Pysic

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Pysic is a calculator incorporating various empirical pair and many-body potentials in an object-based Python environment and user interface while implementing an efficient numeric core written in Fortran. The immediate aim of the Pysic project is to implement advanced variable charge potentials.

Pysic is designed to interface with the ASE simulation environment.

The code was initially developed as part of the Mordred project, and further supported as part of the PAMS project.

Pysic is an open source code with emphasis on making the program simple to learn and control as well as the source code readable, extendable and conforming to good programming standards. The source code is freely available at the github repository.

Pysic is in development. Simulations can be run with it, but many parts of the program are not yet fully tested and so bugs must be expected. Similarly, also this documentation is being constantly updated.

CHAPTER

ONE

PHYSICAL BACKGROUND

1.1 Physics of Pysic

In this section we briefly describe the physical motivation and main ideas behind Pysic. The details of actual algorithms, functions, and implementations included in Pysic are discussed later in sections *Running Pysic* and *Structure and syntax of Pysic*.

1.2 Applications and goals

Phenomena such as Si covalent bonding and charge redistribution at defects and interfaces make semiconductors a very challenging group of materials to describe computationally. Usually quantum mechanical methods such as density functional theory are used, but these approaches are limited by their high computational cost. More sophisticated empirical potentials are being developed for these materials, however, combining fairly accurate precision with a reasonable cost. Notably, the ReaxFF [1] and COMB [2] [3] variable charge potentials have been recently introduced and shown to reproduce the structural properties of for instance Si, SiO_2 and HfO_2. Still these methods are efficient enough to allow the simulation of semiconductor systems at size and time scales relevant for actual device performance (hundreds of thousands of atoms).

1.3 Atomistic interactions

To accurately model condensed matter systems, one often needs to know how the electrons behave, as electrons determine the chemical properies of atoms. Even if the primary interest is the atomic structure, not the electronic one, it may be necessary to include electrons in the simulations in order to calculate the atomistic interactions. The electronic structure must be treated on a quantum mechanical level making these kinds of calculations quite heavy, and so one would often wish to bypass the electronic level of detail and only work with the atomistic structure and a classical description. If we assume that the atomic and electronic degrees of freedom are separate (this is the Born-Oppenheimer approximation, and it is often justified), then in principle the electronic ground state $|\psi\rangle$ is determined by the atomic coordinates $\{\mathbf{R}_i\}$ and nuclear charges $\{Q_i\}$ through the Schrödinger equation

$$H(\{\mathbf{R}_i\},\{Q_i\})|\psi\rangle = E|\psi\rangle \tag{1.1}$$

$$\Rightarrow |\psi\rangle = \psi(\{\mathbf{R}_i\},\{Q_i\}), \tag{1.2}$$

[1] A. van Duin, S. Dasgupta, F. Lorant, and W. Goddard, J Phys Chem A 105, 9396 (2001).
[2] T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, and S. R. Phillpot, Phys Rev B 81, 125328 (2010).
[3] T.-R. Shan, D. Bryce, J. Hawkins, A. Asthagiri, S. Phillpot, and S. Sinnott, Phys Rev B 82, 235302 (2010).

where $H = H(\{\mathbf{R}_i\}, \{Q_i\})$ is the Hamiltonian. As the total energy of the system, E, is determined by the electronic state, it too is a function of the atomic configuration

$$E = \langle\psi|H|\psi\rangle = E(\{\mathbf{R}_i\}, \{Q_i\}).$$

So, in principle, the energy of the system and the atomic forces $F_\alpha = -\nabla_{\mathbf{R}_\alpha} E$ can be determined from the atomic configuration. Construction of the energy function $E(\{\mathbf{R}_i\}, \{Q_i\})$ is very challenging though. It is a very complicated function of the coordinates of *all* the atoms in the system, and in practice one needs to further assume that the system can be split in local substructures for which the energy function can be parameterized, and that the total energy is obtained as a sum of the local contributions. For n-body local interactions, this could be written

$$E \approx \sum_{(i_1, i_2, \ldots, i_n)} E_{\mathrm{local}}(\mathbf{R}_{i_1}, \ldots, \mathbf{R}_{i_n}, Q_{i_1}, \ldots, Q_{i_n}), \tag{1.3}$$

where $(i_1, i_2, \ldots, i_n)$ are all the sets of n atoms in the system.

1.4 Dynamic charges

In practice, calculations get exponentially more complex when the number of bodies included in the local n-body energy $E_{\mathrm{local}}(\mathbf{R}_{i_1}, \ldots, \mathbf{R}_{i_n}, Q_{i_1}, \ldots, Q_{i_n})$ in (1.3) increases. Therefore usually only few particles close to each other are included in the local energy function, and all configurations with distant atoms are given a zero energy. This approach does not work, however, if the system exhibits long-ranged collective electronic reconstruction such as local charging or polarization, for instance, due to the presence of defects or interfaces. Changes in charge distribution can drastically alter the local energy function E_{local}. Increasing the number of bodies n in the local interaction function does not solve this problem in general, since the charge redistribution may be a system wide phenomenon that no local function can properly capture.

One way to treat the redistribution of charge is to make the local energy also a function of the total atomic charge $q_i = Q_i - \eta_i e$, where η_i is the (possibly fractional) number of electrons associated with the atom

$$E_{\mathrm{local}} = E_{\mathrm{local}}(\mathbf{R}_{i_1}, \ldots, \mathbf{R}_{i_n}, Q_{i_1}, \ldots, Q_{i_n}, q_{i_1}, \ldots, q_{i_n}).$$

Although electrons do not specifically belong to any atom making η_i ambiguous, this approach allows the inclusion of long ranged charge distribution in the model with reasonable computational cost.

In addition, having the local charge as a parameter of the energy function allows for the optimization of the energy with respect to the local charges, allowing one to search for an equilibrium charge distribution. This is analogous to finding equilibrium structures by optimizing the energy with respect to the atomic coordinates $\mathbf{R}_i$.

1.5 Hybrid QM/MM calculations in Pysic

Pysic provides a framework for creating and running hybrid QM/MM simulations. Within this framework it is possible to calculate the potential energy and forces in an atomistic configuration which has multiple subsystems and interactions between them. Any external calculator with an ASE interface can be assigned to a subsystem or the classical potentials provided by Pysic can be used. The QM/MM implementation in Pysic uses the mechanical embedding scheme with hydrogen link atoms. It is possible to enable any Pysic-supported interaction potentials between the subsystems, with special functions provided for the easy use of Coulomb and COMB interactions.

1.6 Pysic approach

The immediate aim in the development of Pysic is to implement atomistic potentials with variable local atomic charges and apply them in the study of semiconductor interfaces, e.g., silicon-hafnia. In the long term, Pysic will include a full library of different atomistic potentials.

Pysic implements a very general framework for calculating energies and forces due to arbitrary local atomistic pair or many body potentials. It is straightforward to implement new types of interactions in the code, and mixing different potentials during the simulations is simple. Furthermore, one can easily evaluate the contribution of different interactions on the total energy and forces by switching on and off specific interactions. So called bond order, or Tersoff, potentials [4] are also supported, and the user is free to scale any potential with a bond-dependent factor. In addition, in a system with local charges, long ranged Coulomb interactions need to be evaluated. Such $1/r$-potentials are calculated with the standard Ewald summation algorithm. Implementation of other algorithms such as Particle mesh Ewald [5] or Wolf summation [6] is also planned.

In addition, it is planned that various advanced analysis tools are included with the Pysic package. These would include tools for tasks such as potential parametrization or structural analysis using techniques like evolutionary algorithms, machine learning, or Bayesian mehods.

[4] J. Tersoff, Phys Rev B 37, 6991 (1988).
[5] T. Darden, D. York, and L. Pedersen, Journal of Chemical Physics 98, 10089 (1993).
[6] D. Wolf, P. Keblinski, S. Phillpot, and J. Eggebrecht, Journal of Chemical Physics 110, 8254 (1999).

CHAPTER

TWO

GETTING PYSIC

2.1 Getting Pysic

Pysic is currently in development and not yet properly tested. Nonetheless, the source code is available through github if you wish to try it out. The code is provided with no warranty or support.

2.1.1 Contents of the Pysic repository

When you download Pysic, you should receive a package containing three directories *doc*, *fortran*, and *pysic*. The directory *doc* contains the reStructuredText (`.rst`) source files used for generating the documentation (with Sphinx). For readability, check the online version. The directories *fortran* and *pysic* contain the Fortran and Python source code, respectively. In addition to these folders, there should be a `readme.txt` file containing installation instructions and a `Makefile` for compiling with `make`.

2.2 Compiling Pysic

This section gives brief instructions on how to compile Pysic.

2.2.1 Requirements

To run Pysic, you will need Python 2.x and the numpy and scipy modules. For dynamic simulation, the ASE package is required. Some plotting tools also require the matplotlib package, but Pysic will work without it.

To compile the Fortran core, one needs a Fortran 90 compiler and f2py (the latter is part of numpy.) For compiling an MPI compatible version, an MPI-Fortran compiler is needed.

2.2.2 Quick compilation

To compile Pysic, go to the directory where you have the `Makefile` and folders *fortran* and *pysic*, and enter the command `make <target>` on command line, where `<target>` is for instance `serial` or `parallel`. A list of available targets are shown with the command `make help`.

The default compilers listed in the `Makefile` are `gfortran` and `mpif90`. You may need to edit the names of the compilers to match those available on your system.

By default, `make` creates the pysic Python module as a folder named *pysic* (or *pysic_debug* etc., depending on the type of compilation) in the folder *build*. To run Pysic, copy the folder *pysic* to wherever you wish to run your simulations and import it in Python with `import pysic`.

2.2.3 Compilation under the hood

The Python part of Pysic does not have to be compiled separately, but the Fortran core must be. In order to link the Fortran and Python sides together, you need to compile the code with the f2py tool, which is part of the numpy package.

The Fortran part is compiled with the commands:

```
f2py -m pysic_fortran -h pysic_fortran.pyf PyInterface.F90
f2py -c --fcompiler=gfortran --f90exec=mpif90 --f90flags="-D MPI" \
pysic_fortran.pyf Mersenne.F90 MPI.F90 Quaternions.F90 Utility.F90 \
Geometry.F90 Potentials.F90 Core.F90 PyInterface.F90
```

The first run creates the interface file `pysic_fortran.pyf` from the Fortran source file `PyInterface.F90`. The second run compiles the rest of the code in a native Fortran mode and creates the Python accessible binary file `pysic_fortran.so`. From this file, the subroutines of `PyInterface.F90` are callable as Python functions.

Above, the `gfortran` and `mpif90` compilers are used, but change the names to whichever compilers you wish to call. The flag `--f90flags="-D MPI"` invokes the preprocessor which picks the MPI part of the source code. To compile a serial version, leave this flag out.

The created `pysic_fortran.so` appears in Python as a module `pysic_fortran.pysic_interface`. The package structure of pysic expects to find it at `pysic.pysic_fortran.pysic_interface`, i.e., the `.so` file should be in the folder *pysic* (the root folder of the Python package). The `Makefile` should take care of putting it in the right place, but if you decide to compile the Fortran part manually, keep in mind that the file needs to be moved there.

For further information on compiling with f2py, consult the f2py manual.

2.3 External resources

Below is a list of tools one may find useful or even necessary when using Pysic:

- Python: The Python language
- Python documentation: The official documentation for Python
- Python tutorial: The official tutorials for Python
- F2py: Fortran to Python interface generator
- F2py manual: The (old) official F2py manual
- github: Version control and repository storing Pysic
- ASE: Atomistic Simulation Environment (ASE)
- ASE tutorials: The official ASE tutorials
- NumPy: Numerical Python
- SciPy: Scientific Python
- Matplotlib: Matplotlib Python plotting library
- iPython: iPython enhanced Python interpreter

CHAPTER

THREE

PERFORMING SIMULATIONS WITH PYSIC

3.1 Running Pysic

Once you have Python and Pysic working, it's time to learn how to use them. Next we will go through the basic concepts and ideas behind running simulations with Pysic. A collection of examples will demonstrate how to set up simulations in practice.

3.2 Why Python?

Python is a programming language with a simple human readable syntax yet powerful features and an extensive library. Python is an interpreted language meaning it does not need to be compiled. One can simply feed the source code to an interpreter which reads and interprets it during run. The Python interpreter can also perform calculations, read and write files, render graphics, etc. making Python a powerful tool for scripting. Python is also an object based language enabling sophisticated *Thinking in objects* programming.

In computational physics codes, the most common method of performing the calculations is to have the program read input files to extract the necessary parameters, perform the simulation based on the given input, and print output based on the results. The generated data is then analysed using separate tools. In some cases, more common in commercial programs, the user can control the program through a graphical user interface.

In Pysic, another approach is chosen. Pysic is not a "black box" simulator that turns input data to output data. Instead, Pysic is a *Python module*. In essence, it is a library of tools one can use within Python to perform complicated calculations. Instead of writing an input file - often a complicated and error prone collection of numbers - the user needs to build the simulation in Python. Pysic can then be used in evaluating the energies, forces and other physical quantities of the given system. Python syntax is in general simple and simplicity and user friendliness has also been a key goal in the design of Pysic syntax.

Since Python is a programming language, having Pysic be a part of the language makes it straightforward to write scripts that generate the physical system to be studied and also extract the needed information from the simulations. Instead of generating enormous amounts of data which would then have to be fed to some other analysis program, one can precisely control what kind of data should be produced in the simulations and even analyse the results simultaneously as the simulation is run. Even controlling the simulation based on the produced data is not only possible but easy.

The downside of Pysic being a Python module instead of an independent program is that one has to know the basics of how to run Python. Python documentation is the best resource for getting started, but some simple first step instructions and *Examples* are also given in this document.

3.3 The Atomic Simulation Environment

The Atomistic Simulation Environment (ASE [1]) is a simulation tool developed originally at CAMd, DTU (Technical University of Denmark). The package defines a full atomistic simulation environment for Python, including utilities such as a graphical user interface. Like Pysic, ASE is a collection of Python modules. These modules allow the user to construct atomistic systems, run molecular dynamics or geometry optimization, do calculations and analysis, etc.

ASE is easily extendable, and in fact, the common way to use ASE is join it with an external calculator which produces the needed physical quantities based on the structures defined by ASE. Pysic is such an extension. In the terms used in ASE, Pysic is a calculator. The main role of calculators in ASE is to calculate forces and energies, and this is also what Pysic does. In addition, Pysic incorporates variable charge potentials with dynamic charge equilibration routines. Since ASE does not contain such routines, they are also handled by Pysic, making it more than just an extension of ASE. ASE does contain efficient dynamics and optimization routines including constrained algorithms and nudged elastic band as well as a choice of thermostats, and so Pysic does not implement any such functionality.

The central object in ASE, also used by Pysic, is the Atoms class. This class defines the complete system geometry including atomic species, coordinates, momenta, supercell, and boundary conditions. Pysic interprets instances of this class as the simulation geometry.

3.4 Thinking in objects

If you are already familiar with Python or languages such as Java or C++, you probably know what object oriented programming is. If you are more of a Fortran77 type, maybe not. Since Pysic relies heavily on the object paradigm, a few words should be said about it.

Let's say we want to simulate a bunch of atoms. To do this, we need to know where they are (coordinates), what element they are, what are their charges, momenta, etc. One way to store the information would be to assign indices to the atoms and create arrays containing the data. One for coordinates, another for momenta, third for charges etc. However, this type of bookkeeping approach gets more and more complicated the more strucuted data one needs to store. E.g., if we have a neighbor list as an array of atomic indices and wish to find the coordinates of a neighbor of a given atom, we first need to find the correct entry in the list of neighbors to find the index of the neighbor, and then find the entry corresponding to this index in the list of coordinates. In code, it could look like this:

```
neighbor_atom_index = neighbor_lists[atom_index, neighbor_index]
neighbor_atom_coordinates = coordinates[neighbor_atom_index, 1:3]
```

For complicated data hierarchies one may need to do this kind of index juggling for several rounds, which leads to code that is difficult to read and very susceptible to bugs. Furthermore, if one would want to edit the lists of atoms by, say, removing an atom from the system, all the arrays containing data related to atoms would have to be checked in case they contain the to be deleted particle and updated accordingly.

In the object oriented approach, one defines a data structure (called a *class* in Python) capable of storing various types of information in a single instance. So one can define an 'atom' datatype which contains the coordinates (as real numbers), momenta, etc. in one neat package. One can also define a 'neighbor list' datatype which contains a list of 'atom' datatypes. And the 'atom' datatype can contain a 'neighbor list' (although, this is not exactly how ASE handles neighbor lists). Now, the problem of finding the coordinates of a neighbor is solved in a more intuitive way by asking the atom who the neigbor is and the neighbor its coordinates. This might look something like this:

```
neighbor_atom_coordinates = atom.get_neighbor(neighbor_index).get_coordinates()
```

The above example also demonstrates *methods* - object specific functions allowing one to essentially give orders to objects. Objects and methods make it easy to write code that is simple to read and understand, since we humans

[1] ASE: Comput. Sci. Eng., Vol. 4, 56-66, 2002; https://wiki.fysik.dtu.dk/ase/

intuitively see the world as objects, not as arrays of data. Another great benefit of the object based model is that when an object is modified, the changes automatically propagate everywhere where that object is referred.

The classes and their methods defined in Pysic are documented in detail in *Structure and syntax of Pysic*, and their basic use is shown in the collection of provided *Examples*. The central class in Pysic is `Pysic`, which is an energy and force calculator for ASE. The interactions according to which the energies are calculated are constructed through the class `Potential`. Utilizing these classes is necessary to run meaningful calculations, though also other classes are defined for special purposes.

3.5 Examples

Next, we go through some basic examples on how to use Pysic, starting from launching Python, finishing with relatively advanced scripting techniques.

3.5.1 First steps with Python

Once you have installed Python - chances are it is already preinstalled in your system - you can launch the Python interpreter with the command `python` on the command line:

```
> python
Python 2.7.2 (#1, Feb 28 2010, 00:02:06)
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

This will start up Python in interactive mode and you can start writing commands. For instance:

```
>>> a = 1+1
>>> a
2
>>> b = 'hello'
>>> c = b + ' world!'
>>> c
'hello world!'
```

Another way to run Python is by feeding a source file to the interpreter. Say you have the file `first_step.py` containing:

```
left_first = False
if left_first:
   print "Left, right, left!"
else:
   print "Right, left, right!"
```

This can be run with either:

```
> python first_step.py
Right, left, right!
```

or simply:

```
> ./first_step.py
Right, left, right!
```

assuming you have execution permissions for the script. You can also pass command line arguments to a Python script when launching one.

That's it, basically! In the following examples it is shown how Pysic is set up within Python and how simulations can be run. However, as Python is a powerful language, you will certainly get the most out of Pysic by learning some of the basic features of Python. Taking a look at the official Python tutorial is a good place to start.

3.5.2 Importing Pysic to Python

Modules are accessed in Python by importing them with the `import` command. To get access to Pysic, simply write:

```
>>> import pysic
```

Then, you can access all the functionality in the module `pysic`:

```
>>> pysic_calculator = pysic.Pysic()
>>> pysic.get_names_of_parameters('LJ')
['epsilon', 'sigma']
```

The Fortran interface module is imported with `pysic` as `pysic.pf.pysic_interface`, but it is strongly recommended you do not touch the Fortran core directly.

Altogether, when the module `pysic` is imported, it imports the following non-standard modules:

```
>>> import pysic.pysic_fortran as pf
>>> import numpy as np
>>> import ase.calculators.neighborlist as nbl
```

and defines the functions and classes as documented in the syntax description of `pysic`. In addition, the `start_potentials()` and `start_bond_order_factors()` routines of the Fortran core are automatically invoked in order to initialize the descriptors in the core (see *potentials (Potentials.f90)*). In an MPI environment, the MPI initialization routines `start_mpi()` are also called from the Fortran core. Finally, the random number generator is initialized in the Fortran core by `start_rng()`.

3.5.3 Minimal example of running Pysic

Here is an example of setting up a Pysic calculator for ASE:

```
>>> from ase import Atoms
>>> import pysic
>>> system = Atoms('He2', [[0.0, 0.0, 0.0], [0.0, 0.0, 3.0]])
>>> calc = pysic.Pysic()
>>> system.set_calculator(calc)
>>> physics = pysic.Potential('LJ', cutoff = 10.0)
>>> physics.set_symbols(['He', 'He'])
>>> physics.set_parameter_value('epsilon', 0.1)
>>> physics.set_parameter_value('sigma', 2.5)
>>> calc.add_potential(physics)
```

The example above creates a system of two helium atoms interacting via a Lennard-Jones potential

$$V(r) = \varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$
$$\varepsilon = 0.1$$
$$\sigma = 2.5$$

In the code above, `system` is an ASE Atoms object containing the structure of the system to be calculated - two He atoms in this case. The object `calc` is an instance of `Pysic`, the ASE calculator class defined by Pysic. The

interactions governing the system are defined by the `physics` object, which is an instance of the `Potential` class of Pysic.

Now, the potential energy of the system and the forces acting on the atoms can be calculated with:

```
>>> system.get_potential_energy()
-0.022274132189576905
>>> system.get_forces()
array([[ 0.        ,  0.        ,  0.02211693],
       [ 0.        ,  0.        , -0.02211693]])
```

These commands are addressed to the `system` object, but under the hood `system` asks `calc`, i.e., Pysic, to do the actual calculations. In order to evaluate the requested quantities, Pysic needs the parameters contained in `physics`.

A more compact way to create the calculator would be:

```
>>> physics = pysic.Potential('LJ',
...                           cutoff = 10.0,
...                           symbols = ['He','He'],
...                           parameters = [0.1, 2.5])
>>> calc = pysic.Pysic(system, physics)
```

Setting up more complicated interactions works similarly, as is shown in later examples.

3.5.4 Running molecular dynamics

This example shows how to set up a dynamic simulation with ASE (also see the ASE MD tutorial).

First set up a MgO crystal:

```
from ase.lattice.compounds import Rocksalt

# Set up a crystal
size = 4
lattice_constant = 4.212
system = Rocksalt(size=(size,size,size), symbol=("Mg", "O"),
                  latticeconstant=lattice_constant, pbc=True)
# Set charges for the atoms
for i in range(len(system)):
    if system[i].get_symbol() == "Mg":
        system[i].set_charge(2)
    elif system[i].get_symbol() == "O":
        system[i].set_charge(-2)
```

Create a Pysic calculator. We set up pairwise interactions with the *Buckingham potential* and a Coulomb interaction:

```
import pysic

# Set up a calculator
calc = pysic.Pysic()

# Mg-O pair potential
pot_mgo = pysic.Potential('Buckingham', symbols=['Mg','O'], cutoff=8.0, cutoff_margin=1.0)
pot_mgo.set_parameter_value('A', 1284.38)
pot_mgo.set_parameter_value('C', 0.0)
pot_mgo.set_parameter_value('sigma', 0.2997)
calc.add_potential(pot_mgo)

# O-O pair potential
```

```
pot_oo = pysic.Potential('Buckingham', symbols=['O','O'], cutoff=10.0, cutoff_margin=1.0)
pot_oo.set_parameter_value('A', 9574.96)
pot_oo.set_parameter_value('C', 288474.00)
pot_oo.set_parameter_value('sigma', 0.2192)
calc.add_potential(pot_oo)

# Coulomb interaction
ewald = pysic.CoulombSummation()
ewald.set_parameter_value('epsilon',0.00552635) # epsilon_0 in e**2/(eV A)
ewald.set_parameter_value('k_cutoff',0.7)      # one should always test the Ewald parameters for conve
ewald.set_parameter_value('real_cutoff',10.0) # and optimal speed - long cutoffs can substantially i
ewald.set_parameter_value('sigma',1.4)         # needed cpu time while short cutoffs give incorrect re
calc.set_coulomb_summation(ewald)

system.set_calculator(calc)
```

Now, let us set up the dynamic simulation.

We initialize the velocity distribution:

```
from ase.md.velocitydistribution import MaxwellBoltzmannDistribution
from ase import units

# Set the momenta corresponding to T=300K
MaxwellBoltzmannDistribution(system, 300*units.kB)
```

And define the dynamics as a `VelocityVerlet` object:

```
from ase.md.verlet import VelocityVerlet

# We want to run MD with constant energy using the VelocityVerlet algorithm.
dyn = VelocityVerlet(system, 5*units.fs)  # 5 fs time step.
```

In order to record the ASE trajectory and print information during simulation, we also define observers and attach them to the dynamics. In a similar fashion we can collect whatever information we need:

```
# Function to print the potential, kinetic and total energy.
def print_energy(a=system):
    epot = a.get_potential_energy() / len(a)
    ekin = a.get_kinetic_energy() / len(a)
    print ("Energy per atom: Epot = %.3feV  Ekin = %.3feV (T=%3.0fK)  Etot = %.3feV" %
           (epot, ekin, ekin/(1.5*units.kB), epot+ekin))
dyn.attach(print_energy, interval=100) # print after every 100 steps

# Save a trajectory
from ase.io.trajectory import PickleTrajectory

traj = PickleTrajectory("example.traj", "w", system) # write a trajectory to the file 'example.traj'
dyn.attach(traj.write, interval=10) # save every 10 step
```

Finally, we run the dynamics:

```
dyn.run(1000) # run for 1000 steps
traj.close()  # close the trajectory recording
```

3.5.5 A hybrid calculation

The following python script demonstrates the Python interface for creating a simple hybrid QM/MM simulation with Pysic. The potentials and calculator parameters used in this example are not physically justified and serve only to illustrate the usage:

```
#! /usr/bin/env python
from ase.structure import molecule
from pysic import *
from gpaw import GPAW

# Create the atomic system as an ASE Atoms object
ethane = molecule('C2H6', cell=(6, 6, 6))
ethane.center()

# Create the hybrid calculator
hybrid_calc = HybridCalculator()

# Setup the primary system
gpaw_calc = GPAW(h=0.25, txt=None)
PS = SubSystem("primary", indices=(0, 2, 3, 4), calculator=gpaw_calc)
hybrid_calc.add_subsystem(PS)

# Setup the secondary system
1pysic_calc = Pysic()
pysic_calc.add_potential(Potential('LJ', symbols=[['H', 'C']], parameters=[0.05, 2.5], cutoff=5))
SS = SubSystem("secondary", indices="remaining", calculator=pysic_calc)
hybrid_calc.add_subsystem(SS)

# Setup the interaction between the subsystems
interaction = Interaction("primary", "secondary")
interaction.set_potentials(Potential('LJ', symbols=[['C', 'C']], parameters=[0.05, 3], cutoff=5))
interaction.add_hydrogen_links((0, 1), CHL=0.5)
hybrid_calc.add_interaction(interaction)

# Do some calculations
ethane.set_calculator(hybrid_calc)
ethane.get_potential_energy()
ethane.get_forces()

# Output results
hybrid_calc.print_energy_summary()
hybrid_calc.print_force_summary()
hybrid_calc.print_time_summary()
```

The code is now split into sections that are further elaborated:

- First we define the entire structure that we want to analyze. It is a regular ASE Atoms object:

  ```
  ethane = molecule('C2H6', cell=(6, 6, 6))
  ethane.center()
  ```

- A HybridCalculator object is then created. It is the core class in Pysic's hybrid calculations. The end-user may treat is like any other ASE compatible calculator:

```
hybrid_calc = HybridCalculator()
```

- A SubSystem object is created for each desired subsystem. A subsystem is defined by giving it a unique name, the indices of the atoms in the subsystem and the calculator which is to be used for it. The newly created SubSystem object is then passed to the HybridCalculator:

```
# Setup the primary system
gpaw_calc = GPAW(h=0.25, txt=None)
PS = SubSystem("primary", indices=(0, 2, 3, 4), calculator=gpaw_calc)
hybrid_calc.add_subsystem(PS)

# Setup the secondary system
pysic_calc = Pysic()
pysic_calc.add_potential(Potential('LJ', symbols=[['H', 'C']], parameters=[0.05, 2.5], cutoff=5)
SS = SubSystem("secondary", indices="remaining", calculator=pysic_calc)
hybrid_calc.add_subsystem(SS)
```

- Interaction potentials and hydrogen link atoms between any two subsystems are set up by creating an Interaction object. The names of the interacting subsystems are given in the constructor, the first being the primary system, and the latter being the secondary system. Potentials and link atoms are created through simple function calls. Finally the Interaction object is passed to the HybridCalculator:

```
interaction = Interaction("primary", "secondary")
interaction.set_potentials(Potential('LJ', symbols=[['C', 'C']], parameters=[0.05, 3], cutoff=5)
interaction.add_hydrogen_links((0, 1), CHL=0.5)
hybrid_calc.add_interaction(interaction)
```

- When the subsystems and interactions are successfully configured, the HybridCalculator can be used like any regular ASE calculator to calculate the potential energy and forces in the system:

```
ethane.set_calculator(hybrid_calc)
ethane.get_potential_energy()
ethane.get_forces()
```

- The HybridCalculator provides useful tools for inspecting the energies, calculation times and forces related to the different subsystems and interactions:

```
hybrid_calc.print_energy_summary()
hybrid_calc.print_force_summary()
hybrid_calc.print_time_summary()
```

3.6 Screencasts

We have also prepared screencasts demonstrating the use of Pysic.

3.6.1 Pysic basics

This is a demonstration of a very simple simulation setup while running Pysic in an interactive Python session.

YouTube link

3.6.2 Pysic in a script

This is a demonstration of running Pysic with a script, including an MPI parallel run.

YouTube link (high definition)

CHAPTER

FOUR

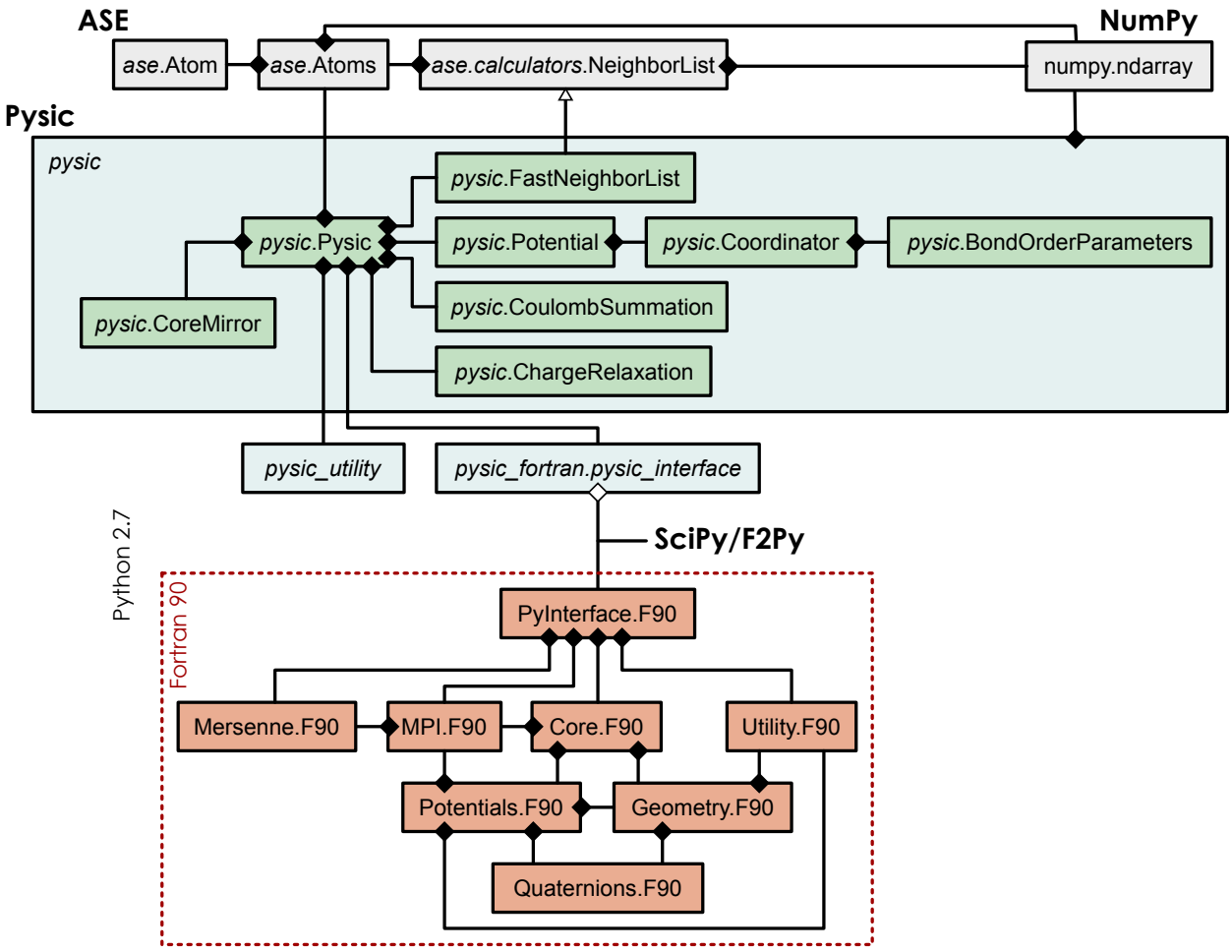
STRUCTURE AND SYNTAX IN PYSIC

4.1 Structure and syntax of Pysic

Pysic can be used with basic functionality with just a few commands. To give access to all the functionality in Pysic, the full API of Pysic is documented in the following section. All the classes and methods including their arguments are explained in detail. Also the types of potentials and bond order factors available are documented, including their mathematical descriptions and the keywords needed for access.

In addition to the Python documentation, also the variables, types, and routines in the Fortran core are listed with comments and explanations. Besides the interface module *pysic_interface (PyInterface.f90)*, this part of the code is not accessible through Python. Thus, you need not know what the core contains. However, if you plan to modify the core, studying also the Fortran documentation is useful.

The graph below show the main dependancies between the Python and Fortran classes and modules. (This is not a full UML diagram, just a schematic presentation.)



4.2 Pysic module

Pysic is an object based calculator for atomistic many-body interactions. It is controlled via several classes such as `Pysic`, which defines a calculator for the ASE simulation environment [1], and `Potential`, which defines potentials to be used by for calculating atomic interactions.

4.2.1 Classes of the pysic module

Pysic class

This class provides an interface both to the ASE environment and the Fortran core of Pysic through the `pysic_fortran` module. In ASE terms, Pysic is a calculator, i.e., an object that calculates forces and energies of given atomistic structures provided as an ASE Atoms object.

Pysic is not a fixed potential calculator, where the interactions are determined solely based on the elements present in the system. Instead, Pysic allows and requires the user to specify the interactions governing the system. This is done by providing the calculator with one or several `Potential` objects.

[1] ASE: Comput. Sci. Eng., Vol. 4, 56-66, 2002; https://wiki.fysik.dtu.dk/ase/

Calculators in ASE

Calculators in ASE are a class representing the physics of the atomistic system. Or put in another way, a calculator is the mathematical machine containing the algorithms and routines for calculating, for instance, the total potential energy of the atomistic system represented as an ASE atoms object (hence the name). As ASE itself contains only some very simple calculators, in practice the calculators are often just Python interfaces to other atomistic simulators. Pysic too is such a calculator.

Pysic implements classical potentials, where the interactions between atomic pairs, triplets etc. are represented via simple mathematical functions or a *Tabulated potential*. These can be combined freely using the *Potential class* and its modifiers and extensions such as the *Coordinator*, *Bond order parameter*, *Product potential*, *Compound Potential*, and *Coulomb summation* classes.

Wrapping calculators

Although Pysic can be used as a calculator on its own, it is also possible to use it as a wrapper for other ASE calculators. By doing so, one may combine different simulators and even different descriptions in one calculator, and all the wrapped calculators will be executed when the Pysic calculator needs to calculate energies or forces. This is done simply by adding the external ASE calculators to Pysic using the `add_calculator()` method.

As a simple example, one can use Pysic to add simple components like springs in an ab initio calculation. This example uses the Gpaw code.:

```
import pysic
from ase import Atoms
from gpaw import GPAW

# create the system
system = Atoms( ... )

# create the pysic calculator
calc = pysic.Pysic()

# create a classical spring potential between atoms '0' and '1'
spr = pysic.Potential('spring', indices=[0,1], parameters=[10.0, 3.0], cutoff=10.0, cutoff_margin=1.0
calc.add_potential(spr)

# create an ab initio calculator
dft = GPAW(h=0.18, nbands=1, xc='PBE', txt='wrapped.out')

# wrap the calculators
calc.add_calculator(dft)

# calculate the energy
system.set_calculator(calc)
print system.get_potential_energy()
```

It is also possible to wrap several instances of Pysic together, but usually there should be no need to do this. It is more efficient to just add all the potentials in one Pysic instance. However, as an example, here is how it works:

```
import pysic
import ase

# create some test system
system = ase.Atoms('COH',[[0.0,0.0,0.0], [2.0,0.0,0.0], [2.0,2.0,2.0]])

# create two calculators
```

```
calc1 = pysic.Pysic()
calc2 = pysic.Pysic()

# potential 1
pot1 = pysic.Potential('LJ',symbols=['C','O'],parameters=[1,1],cutoff=10.0)
# potential 2
pot2 = pysic.Potential('LJ',symbols=['O','H'],parameters=[1,1],cutoff=10.0)

# add potentials to respective calculators
calc1.add_potential(pot1)
calc2.add_potential(pot2)
system.set_calculator(calc1)

# write energies and forces for the calculators both separately and combined
print "Only potential 1"
print system.get_potential_energy()
print system.get_forces()
print "\n"

print "Only potential 2"
print calc2.get_potential_energy(system)
print calc2.get_forces(system)
print "\n"

print "Both potentials by calculator wrapping"
calc1.add_calculator(calc2)
print system.get_potential_energy()
print system.get_forces()
print "\n"

calc1.remove_calculator(calc2)
calc1.add_potential(pot2)
print "Both potentials in one calculator"
print system.get_potential_energy()
print system.get_forces()
print "\n"
```

This will output:

```
Only potential 1
-0.015380859375
[[ 0.04541016  0.          0.        ]
 [-0.04541016  0.          0.        ]
 [ 0.          0.          0.        ]]


Only potential 2
-0.00194931030273
[[ 0.          0.          0.        ]
 [ 0.          0.00291824  0.00291824]
 [ 0.         -0.00291824 -0.00291824]]


Both potentials by calculator wrapping
-0.0173301696777
[[ 0.04541016  0.          0.        ]
 [-0.04541016  0.00291824  0.00291824]
 [ 0.         -0.00291824 -0.00291824]]
```

```
Both potentials in one calculator
-0.0173301696777
[[ 0.04541016  0.          0.        ]
 [-0.04541016  0.00291824  0.00291824]
 [ 0.         -0.00291824 -0.00291824]]
```

Notice how in the third printout the calculators *calc1* and *calc2* are wrapped together, and the result is their sum. In the fourth case, *calc2* is discarded and instead *pot2* is added directly to *calc1*. The result is the same, but the latter option is better performance wise, since wrapping the calculators requires both to be separately managed during calculation.

List of methods

Below is a list of methods in `Pysic`, grouped according to the type of functionality.

Structure handling

- `create_neighbor_lists()` (meant for internal use)
- `get_atoms()`
- `get_neighbor_lists()`
- `neighbor_lists_expanded()` (meant for internal use)
- `set_atoms()`

Potential handling

- `add_potential()`
- `get_individual_cutoffs()`
- `get_potentials()`
- `remove_potential()`
- `set_potentials()`

Coulomb handling

- `get_coulomb_summation()`
- `set_coulomb_summation()`

Charge relaxation handling

- `get_charge_relaxation()`
- `set_charge_relaxation()`

Calculator handling

- `add_calculator()`
- `get_calculators()`
- `remove_calculator()`

Calculations

- calculate_electronegativities() (meant for internal use)
- calculate_energy() (meant for internal use)
- calculate_forces() (meant for internal use)
- calculate_stress() (meant for internal use)
- calculation_required() (meant for internal use)
- get_electronegativities()
- get_electronegativity_differences()
- get_forces()
- get_numerical_bond_order_gradient() (for testing)
- get_numerical_energy_gradient() (for testing)
- get_numerical_electronegativity() (for testing)
- get_potential_energy()
- get_stress()

Core

- core
- core_initialization_is_forced()
- force_core_initialization()
- initialize_fortran_core()
- set_core()
- update_core_charges() (meant for internal use)
- update_core_coordinates() (meant for internal use)
- update_core_coulomb() (meant for internal use)
- update_core_neighbor_lists() (meant for internal use)
- update_core_potential_lists() (meant for internal use)
- update_core_supercell() (meant for internal use)

Full documentation of the Pysic class

class pysic.calculator.**Pysic**(*atoms=None*, *potentials=None*, *charge_relaxation=None*, *coulomb=None*, *full_initialization=False*)

A calculator class providing the necessary methods for interfacing with ASE.

Pysic is a calculator for evaluating energies and forces for given atomic structures according to the given Potential set. Neither the geometry nor the potentials have to be specified upon creating the calculator, as they can be specified or changed later. They are necessary for actual calculation, of course.

Simulation geometries must be defined as ASE Atoms. This object contains both the atomistic coordinates and supercell parameters.

Potentials must be defined as a list of `Potential` objects. The total potential of the system is then the sum of the individual potentials.

Parameters:

atoms: ASE Atoms object an Atoms object containing the full simulation geometry

potentials: list of `Potential` objects list of potentials for describing interactions

force_initialization: boolean If true, calculations always fully initialize the Fortran core. If false, the Pysic tries to evaluate what needs updating by consulting the `core` instance of `CoreMirror`.

`add_calculator`(*calculator*)
Add a calculator to the list of external calculators.

Parameters:

calculator: an ASE calculator object a new calculator to describe interactions

`add_potential`(*potential*)
Add a potential to the list of potentials.

Also a list of potentials can be given as an argument. In that case, the potentials are added one by one.

If a `CompoundPotential` is given, the addition is done through its `build()` method.

Parameters:

potential: `interactions.local.Potential` object a new potential to describe interactions

`calculate_electronegativities`()
Calculates electronegativities.

Calls the Fortran core to calculate forces for the currently assigned structure.

`calculate_energy`(*skip_charge_relaxation=False*)
Calculates the potential energy.

Calls the Fortran core to calculate the potential energy for the currently assigned structure.

If a link exists to a `ChargeRelaxation`, it is first made to relax the atomic charges before the forces are calculated.

`calculate_forces`(*skip_charge_relaxation=False*)
Calculates forces (and the potential part of the stress tensor).

Calls the Fortran core to calculate forces for the currently assigned structure.

If a link exists to a `ChargeRelaxation`, it is first made to relax the atomic charges before the forces are calculated.

`calculate_stress`(*skip_charge_relaxation=False*)
Calculates the potential part of the stress tensor (and forces).

Calls the Fortran core to calculate the stress tensor for the currently assigned structure.

`calculation_required`(*atoms=None, quantities=['forces', 'energy', 'stress', 'electronegativities']*)
Check if a calculation is required.

When forces or energy are calculated, the calculator saves the result in case it is needed several times. This method tells if a wanted quantity is not yet calculated for the current structure and needs to be calculated explicitly. If a list of several quantities is given, the method returns true if any one of them needs to be calculated.

Parameters:

atoms: ASE Atoms object ignored at the moment

quantities: list of strings list of keywords 'energy', 'forces', 'stress', 'electronegativities'

core = CoreMirror()
An object storing the data passed to the core.

Whenever a `Pysic` calculator alters the Fortran core, it should also modify the `core` object so that it is always a valid representation of the actual core. Then, whenever `Pysic` needs to check if the representation in the core is up to date, it only needs to compare against `core` instead of accessing the Fortran core itself.

core_initialization_is_forced()
Returns true if the core is always fully initialized, false otherwise.

create_neighbor_lists(*cutoffs=None*, *marginal=None*)
Initializes the neighbor lists.

In order to do calculations at reasonable speed, the calculator needs a list of neighbors for each atom. For this purpose, either the list is built in the Fortran core or the ASE NeighborList are used. The ASE lists are very slow, but they will work even for small systems where the cutoff is longer than cell size. The custom list uses `pysic.calculator.FastNeighborList`, but the build succeeds only for cutoffs shorter than cell size. The type of list is determined automatically.

This method initializes these lists according to the given cutoffs.

Parameters:

cutoffs: list of doubles a list containing the cutoff distance for each atom

marginal: double the skin width of the neighbor list

force_core_initialization(*new_mode*)
Set the core initialization mode.

Parameters:

new_mode: logical true if full initialization is required, false if not

get_atoms()
Returns the ASE Atoms object assigned to the calculator.

get_calculators()
Returns the list of other calculators to be used with Pysic.

get_charge_relaxation()
Returns the `ChargeRelaxation` object connected to the calculator.

get_charges(*system=None*)
Update for ASE 3.7

get_coulomb_summation()
Returns the Coulomb summation algorithm of this calculator.

get_electronegativities(*atoms=None*)
Returns the electronegativities of atoms.

get_electronegativity_differences(*atoms=None*)
Returns the electronegativity differences of atoms from the average of the entire system.

get_forces(*atoms=None*, *skip_charge_relaxation=False*)
Returns the forces.

If the atoms parameter is given, it will be used for updating the structure assigned to the calculator prior to calculating the forces. Otherwise the structure already associated with the calculator is used.

The calculator checks if the forces have been calculated already via `calculation_required()`. If the structure has changed, the forces are calculated using `calculate_forces()`

Parameters:

atoms: ASE atoms object the structure for which the forces are determined

get_individual_cutoffs(*scaler=1.0*)
Get a list of maximum cutoffs for all atoms.

For each atom, the interaction with the longest cutoff is found and the associated maximum cutoffs are returned as a list. In case the a list of scaled values are required, the scaler can be adjusted. E.g., scaler = 0.5 will return the cutoffs halved.

Parameters:

scaler: double a number for scaling all values in the generated list

get_neighbor_list()
Returns the neighbor list object.

get_neighbor_lists()
Returns the `FastNeighborList` or ASE NeighborList object assigned to the calculator.

The neighbor lists are generated according to the given ASE Atoms object and the `Potential` objects of the calculator. Note that the lists are created when the core is set or if the method `create_neighbor_lists()` is called.

get_numerical_bond_order_gradient(*coordinator*, *atom_index*, *moved_index*, *shift=0.001*, *atoms=None*)
Numerically calculates the gradient of a bond order factor with respect to moving a single particle.

This is for debugging the bond orders.

get_numerical_electronegativity(*atom_index*, *shift=0.001*, *atoms=None*)
Numerically calculates the derivative of energy with respect to charging a single particle.

This is for debugging the electronegativities.

get_numerical_energy_gradient(*atom_index*, *shift=0.0001*, *atoms=None*)
Numerically calculates the negative gradient of energy with respect to moving a single particle.

This is for debugging the forces.

get_potential_energy(*atoms=None*, *force_consistent=False*, *skip_charge_relaxation=False*)
Returns the potential energy.

If the atoms parameter is given, it will be used for updating the structure assigned to the calculator prior to calculating the energy. Otherwise the structure already associated with the calculator is used.

The calculator checks if the energy has been calculated already via `calculation_required()`. If the structure has changed, the energy is calculated using `calculate_energy()`

Parameters:

atoms: ASE atoms object the structure for which the energy is determined

force_consistent: logical ignored at the moment

get_potentials()
Returns the list of potentials assigned to the calculator.

get_stress(*atoms=None*, *skip_charge_relaxation=False*)
Returns the stress tensor in the format $[\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy}]$

If the atoms parameter is given, it will be used for updating the structure assigned to the calculator prior to calculating the stress. Otherwise the structure already associated with the calculator is used.

The calculator checks if the stress has been calculated already via `calculation_required()`. If the structure has changed, the stress is calculated using `calculate_stress()`

Stress (potential part) and force are evaluated in tandem. Therefore, invoking the evaluation of one automatically leads to the evaluation of the other. Thus, if you have just evaluated the forces, the stress will already be known.

This is because the stress tensor is formally defined as

$$\sigma_{AB} = -\frac{1}{V}\sum_i \left[m_i (v_i)_A (v_i)_B + (r_i)_A (f_i)_B\right],$$

where m, v, r, and f are mass, velocity, position and force of atom i, and A, B denote the cartesian coordinates x, y, z. (The minus sign is there just to be consistent with the NPT routines in ASE.) However, if periodic boundaries are used, the absolute coordinates cannot be used (there would be discontinuities at the boundaries of the simulation cell). Instead, the potential energy terms $(r_i)_A (f_i)_B$ must be evaluated locally for pair, triplet, and many body forces using the relative coordinates of the particles involved in the local interactions. These coordinates are only available during the actual force evaluation when the local interactions are looped over. Thus, calculating the stress requires doing the full force evaluation cycle. On the other hand, calculating the stress is not a great effort compared to the force evaluation, so it is convenient to evaluate the stress always when the forces are evaluated.

Parameters:

atoms: ASE atoms object the structure for which the stress is determined

initialize_fortran_core()
Fully initializes the Fortran core, creating the atoms, supercell, potentials, and neighbor lists.

neighbor_lists_expanded(*cutoffs*)
Check if the cutoffs have been expanded.

If the cutoffs have been made longer than before, the neighbor lists have to be recalculated. This method checks the individual cutoffs of all atoms to check if the cutoffs have changed.

Parameters:

cutoffs: list of doubles new cutoffs

remove_calculator(*calculator*)
Remove a calculator from the list of calculators.

Parameters:

calculator: an ASE calculator object the calculator to be removed

remove_potential(*potential*)
Remove a potential from the list of potentials.

If a `CompoundPotential` is given, the removal is done through its `remove()` method.

Parameters:

potential: `Potential` object the potential to be removed

set_atoms(*atoms=None*)
Assigns the calculator with the given structure.

This method is always called when any method is given the atomic structure as an argument. If the argument is missing or None, nothing is done. Otherwise a copy of the given structure is saved (according to the instructions in ASE API.)

If a structure is already in memory and it is different to the given one (as compared with `__ne__`), it is noted that all quantities are unknown for the new system. If the structure is the same as the one already known, nothing is done. This is because if one wants to access the energy of forces of the same system repeatedly, it is unnecessary to always calculate them from scratch. Therefore the calculator saves the computed values along with a flag stating that the values have been computed.

Parameters:

atoms: ASE atoms object the structure to be calculated

set_charge_relaxation(*charge_relaxation*)
Add a charge relaxation algorithm to the calculator.

If a charge relaxation scheme has been added to the `Pysic` calculator, it will be automatically asked to do the charge relaxation before the calculation of energies or forces via `charge_relaxation()`.

It is also possible to pass the `Pysic` calculator to the `ChargeRelaxation` algorithm without creating the opposite link using `set_calculator()`. In that case, the calculator does not automatically relax the charges, but the user can manually trigger the relaxation with `charge_relaxation()`.

If you wish to remove automatic charge relaxation, just call this method again with None as argument.

Parameters:

charge_relaxation: `ChargeRelaxation` object the charge relaxation algorithm

set_core()
Sets up the Fortran core for calculation.

If the core is not initialized, if the number of atoms has changed, or if full initialization is forced, the core is initialized from scratch. Otherwise, only the atomic coordinates and momenta are updated. Potentials, neighbor lists etc. are also updated if they have been edited.

set_coulomb_summation(*coulomb*)
Set the Coulomb summation algorithm for the calculator.

If a Coulomb summation algorithm is set, the Coulomb interactions between all charged atoms are evaluated automatically during energy and force evaluation. If not, the charges do not directly interact.

Parameters:

coulomb: `interactions.coulomb.CoulombSummation` the Coulomb summation algorithm

set_cutoffs(*cutoffs*)
Copy and save the list of individual cutoff radii.

Parameters:

cutoffs: list of doubles new cutoffs

set_potentials(*potentials*)
Assign a list of potentials to the calculator.

Also a single potential object can be given, instead of a list. Note that this method does not conserve any potentials that were already known by the calculator. To add potentials to the list of known potentials, use `add_potential()`.

Parameters:

potentials: list of `Potential` objects a list of potentials to describe interactinos

update_core_charges()
Updates atomic charges in the core.

update_core_coordinates()
Updates the positions and momenta of atoms in the Fortran core.

The core must be initialized and the number of atoms must match. Upon the update, it is automatically checked if the neighbor lists should be updated as well.

update_core_coulomb()
Updates the Coulomb summation parameters in the Fortran core.

update_core_neighbor_lists()
Updates the neighbor lists in the Fortran core.

If uninitialized, the lists are created first via `create_neighbor_lists()`.

update_core_potential_lists()
Initializes the potential lists.

Since one often runs `Pysic` with a set of potentials, the core pre-analyzes which potentials affect each atom and saves a list of such potentials for every particle. This method asks the core to generate these lists.

update_core_potentials()
Generates potentials for the Fortran core.

update_core_supercell()
Updates the supercell in the Fortran core.

Potential class

This class defines an atomistic potential to be used by `Pysic`. An interaction between two or more particles can be defined and the targets of the interaction can be specified by chemical symbol, tag, or index. The available types of potentials are always inquired from the Fortran core to ensure that any changes made to the core are automatically reflected in the Python interface.

There are a number of utility functions in `pysic` for inquiring the keywords and other data needed for creating the potentials. For example:

- Inquire the names of available potentials: `list_valid_potentials()`
- Inquire the names of parameters for a potential: `names_of_parameters()`
- Ask for a short description of a potential: `description_of_potential()`

Cutoffs

Many potentials decay towards zero in infinity, but in a numeric simulation they are cut at a finite range as specified by a cutoff radius. However, if the potential is not exactly zero at this range, a discontinuity will be introduced. It is possible to avoid this by including a smoothening factor in the potential to force a decay to zero in a finite interval:

$$\tilde{V}(r) = f(r)V(r),$$

where the smoothening factor is (for example)

$$f(r) = \begin{cases} 1, & r < r_{\mathrm{soft}} \\ \frac{1}{2}\left(1 + \cos \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}}\right), & r_{\mathrm{soft}} < r < r_{\mathrm{hard}} \\ 0, & r > r_{\mathrm{hard}} \end{cases}.$$

Pysic allows one to specify both a hard and a soft cutoff for all potentials to include such a smooth cutoff. If no soft cutoff if given or it is zero (or equal to the hard cutoff), no smoothening is applied.

Targets of a Potential

A Potential needs targets to describe interactions. For instance a 2-body potential needs two targets. These targets can be specified as chemical species (through the corresponding chemical symbols), indices, or tags (as defined in ASE Atoms). The most typical use is by symbols.

The targets need to be specified as lists. For example, if one wishes to define a Potential affecting He-He pairs, it can be defined through:

```
>>> pot = Potential(...)
>>> pot.set_symbols(['He','He'])
```

There are also utility functions for generating these lists more conveniently from strings: `pysic.utility.convenience.expand_symbols_string()` and `pysic.utility.convenience.expand_symbols_table()`. For example:

```
>>> from pysic.utility.convenience import expand_symbols_string as sym
>>> from pysic.utility.convenience import expand_symbols_table as tab
>>> print sym('HeHe')
[['He', 'He']]
>>> print tab(sym('Si,SiO'))
[['Si', 'Si'], ['Si', 'O']]
```

List of currently available potentials

Below is a list of potentials currently implemented. Also see the *List of corrently available compound potentials*.

- *Constant potential*
- *Constant force potential*
- *Charge self energy potential*
- *Power decay potential*
- *Shifted power potential*
- *Harmonic potential*
- *Lennard-Jones potential*
- *Buckingham potential*
- *Exponential potential*
- *Charged-pair potential*
- *Absolute charged-pair potential*
- *Charge dependent exponential potential*
- *Tabulated potential*
- *Bond bending potential*
- *Dihedral angle potential*

Constant potential 1-body potential defined as

$$V(\mathbf{r}) = V,$$

i.e., a constant potential.

A constant potential is of course irrelevant in force calculation since the gradient is zero. However, one can add a BondOrderParameters bond order factor with the potential to create essentially a bond order potential.

The constant potential can also be used for assigning an energy offset which depends on the number of atoms of required types.

Keywords:

```
>>> names_of_parameters('constant')
['V']
```

Fortran routines:

- create_potential_characterizer_constant_potential()
- evaluate_energy_constant_potential()

Constant force potential 1-body potential defined as

$$V(\mathbf{r}) = -\mathbf{F} \cdot \mathbf{r},$$

i.e., a constant force $\mathbf{F}$.

Keywords:

```
>>> names_of_parameters('force')
['Fx', 'Fy', 'Fz']
```

Fortran routines:

- create_potential_characterizer_constant_force()
- evaluate_energy_constant_force()
- evaluate_force_constant_force()

Charge self energy potential 1-body potential defined as

$$V(q) = \varepsilon q^n,$$

where ε is an energy scale constant and n an integer exponent. Note that only the integer part of the exponent is taken if a real number is given. This is because you must expect negative values for q and so a non-integer n would be ill-defined.

Keywords:

```
>>> names_of_parameters('charge_self')
['epsilon', 'n']
```

Fortran routines:

- create_potential_characterizer_constant_force()
- evaluate_energy_constant_force()
- evaluate_force_constant_force()

Power decay potential 2-body interaction defined as

$$V(r) = \varepsilon \left(\frac{a}{r}\right)^n$$

where ε is an energy scale constant, a is a lenght scale constant or lattice parameter, and n is an exponent.

There are many potentials defined in Pysic which already incorporate power law terms, and so this potential is often not needed. Still, one can build, for instance, the *Lennard-Jones potential* potential by stacking two power decay potentials. Note that n should be large enough fo the potential to be sensible. Especially if one is creating a Coulomb potential with $n = 1$, one should not define the potential through `Potential` objects, which are directly summed, but with the `CoulombSummation` class instead.

Keywords:

```
>>> names_of_parameters('power')
['epsilon', 'a', 'n']
```

Fortran routines:

- `create_potential_characterizer_power()`
- `evaluate_energy_power()`
- `evaluate_force_power()`

Shifted power potential 2-body interaction defined as

$$V(r) = \varepsilon \left(\frac{r_1 - r}{r_1 - r_2}\right)^n$$

where ε is an energy scale constant, r_1 and r_2 are a lenght scale constants, and n is an exponent.

Keywords:

```
>>> names_of_parameters('shift_power')
['epsilon', 'r1', 'r2', 'n']
```

Fortran routines:

- `create_potential_characterizer_shift()`
- `evaluate_energy_shift()`
- `evaluate_force_shift()`

Harmonic potential 2-body interaction defined as

$$V(r) = \frac{1}{2}k(r - R_0)^2 - \frac{1}{2}k(r_{\mathrm{cut}} - R_0)^2,$$

where k is a spring constant, R_0 is the equilibrium distance, and r_{cut} is the potential cutoff. The latter term is a constant whose purpose is to remove the discontinuity at cutoff.

Keywords:

```
>>> names_of_parameters('spring')
['k', 'R_0']
```

Fortran routines:

- `create_potential_characterizer_spring()`
- `evaluate_energy_spring()`
- `evaluate_force_spring()`

Lennard-Jones potential 2-body interaction defined as

$$V(r) = \varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right],$$

where ε is an energy constant defining the depth of the potential well and σ is the distance where the potential changes from positive to negative in the repulsive region.

Keywords:

```
>>> names_of_parameters('LJ')
['epsilon', 'sigma']
```

Fortran routines:

- create_potential_characterizer_LJ()
- evaluate_energy_LJ()
- evaluate_force_LJ()

Buckingham potential 2-body interaction defined as

$$V(r) = Ae^{-\frac{r}{\sigma}} - C\left(\frac{\sigma}{r}\right)^{6}$$

where σ is a length scale constant, and A and C are the energy scale constants for the exponential and van der Waals parts, respectively.

Keywords:

```
>>> names_of_parameters('Buckingham')
['A', 'C', 'sigma']
```

Fortran routines:

- create_potential_characterizer_buckingham()
- evaluate_energy_buckingham()
- evaluate_force_buckingham()

Exponential potential 2-body interaction defined as

$$V(q) = \varepsilon \exp(-\zeta r)$$

where ε is an energy scale constant and ζ is a length decay constant.

Keywords:

```
>>> names_of_parameters('exponential')
['epsilon', 'zeta']
```

Fortran routines:

- create_potential_characterizer_exp()
- evaluate_energy_exp()
- evaluate_force_exp()

Charged-pair potential 2-body interaction defined as

$$V(q_1, q_2) = \varepsilon q_1^{n_1} q_2^{n_2}$$

where ε is an energy scale constant, and n_i are integer exponents.

This potential is similar to the *Charge self energy potential*, but it affects two atoms. It is mainly meant to be used together with distance dependent potentials in a `ProductPotential` to add charge dependence to other potentials. For instance:

```
pot1 = pysic.Potential('power')
pot2 = pysic.Potential('charge_pair')
prod = pysic.ProductPotential([pot1,pot2])
```

Defines the potential

$$V(q_1, q_2, r) = \varepsilon q_1^{n_1} q_2^{n_2} \left(\frac{a}{r}\right)^n$$

Keywords:

```
>>> names_of_parameters('charge_pair')
['epsilon', 'n1', 'n2']
```

Fortran routines:

- `create_potential_characterizer_charge_pair()`
- `evaluate_energy_charge_pair()`
- `evaluate_electronegativity_charge_pair()`

Absolute charged-pair potential 2-body interaction defined as

$$V(q_1, q_2) = \sqrt{B_1(q_1) B_2(q_2)}$$
$$B_i(q_i) = a_i + b_i |q_i - Q_i|^{n_i}$$

where a_i is an energy shift, b_i is a scale constant, Q_i is a charge shift, and n_i are real exponents.

This potential is similar to the *Charged-pair potential*, but it affects the absolute values of charges. This allows one to use real valued exponents instead of just integers. Note though, that the product $B_1(q_1)B_2(q_2)$ must be positive for all relevant values of q_i.

Keywords:

```
>>> names_of_parameters('charge_abs')
['a1', 'b1', 'Q1', 'n1',
 'a2', 'b2', 'Q2', 'n2']
```

Fortran routines:

- `create_potential_characterizer_charge_pair_abs()`
- `evaluate_energy_charge_pair_abs()`
- `evaluate_electronegativity_charge_pair_abs()`

Charge dependent exponential potential 2-body interaction defined as

$$
\begin{aligned}
V(q) &= \varepsilon_{ij} \exp\left(\frac{\xi_i D_i(q_i) + \xi_j D_j(q_j)}{2}\right) \\
D_i(q) &= R_{i,\max} + |\beta_i (Q_{i,\max} - q)|^{\eta_i} \\
\beta_i &= \frac{(R_{i,\min} - R_{i,\max})^{\frac{1}{\eta_i}}}{Q_{i,\max} - Q_{i,\min}} \\
\eta_i &= \frac{\ln \frac{R_{i,\max}}{R_{i,\max} - R_{i,\min}}}{\ln \frac{Q_{i,\max}}{Q_{i,\max} - Q_{i,\min}}},
\end{aligned}
$$

where ε is an energy scale constant, ξ_i are charge decay constants, and $R_{i,\min\,/\,\max}$ and $Q_{i,\min\,/\,\max}$ are the changes in valence radii and charge, respectively, of the ions for the minimum and maximum charge. $D_i(q)$ is the effective atomic radius for the charge q.

Keywords:

```
>>> names_of_parameters('charge_exp')
['epsilon',
 'Rmax1', 'Rmin1', 'Qmax1', 'Qmin1',
 'Rmax2', 'Rmin2', 'Qmax2', 'Qmin2',
 'xi1', 'xi2']
```

Fortran routines:

- `create_potential_characterizer_charge_exp()`
- `evaluate_energy_charge_exp()`
- `evaluate_electronegativity_charge_exp()`

Tabulated potential 2-body interaction of the type $V(r)$ defined with a tabulated list of values.

The values of the potential are read from text files of the format:

```
V(0)      V'(0)*R
V(dr)     V'(dr)*R
V(2*dr)   V'(2*dr)*R
...       ...
V(R)      V'(R)*R
```

where `V` and `V'` are the numberic values of the potential and its derivative ($V(r)$ and $V'(r)$), respectively, for the given values of atomic separation r. The grid is assumed to be uniform and starting from 0, so that the values of r are $0, \mathrm{d}r, 2\mathrm{d}r, \ldots, R$, where R is the range of the tabulation and $\mathrm{d}r = R/(n-1)$ where n is the number of value pairs (lines) in the table. Note that the first and last derivatives are forced to be zero regardless of what is given in the table ($V'(0) = V'(R) = 0$).

For each interval $[r_i, r_{i+1}]$ the value of the potential is calculated using third degree spline (cspline) interpolation

$$
\begin{aligned}
r \in & [r_i, r_{i+1}]: \\
t(r) = & \frac{r - r_i}{r_{i+1} - r_i} \\
V(r) = & V(r_i)h_{00}(t) + V'(r_i)(r_{i+1} - r_i)h_{10}(t) + \\
& V(r_{i+1})h_{01}(t) + V'(r_{i+1})(r_{i+1} - r_i)h_{11}(t) \\
h_{00}(t) = & 2t^3 - 3t^2 + 1 \\
h_{10}(t) = & t^3 - 2t^2 + t \\
h_{01}(t) = & -2t^3 + 3t^2 \\
h_{11}(t) = & t^3 - t^2
\end{aligned}
$$

The range of the tabulation R is given as a parameter when creating the potential. The tabulated values should be given in a text file with the name `table_xxxx.txt`, where `xxxx` is an identification integer with leading zeros (e.g., `table_0001.txt`). The id is also given as a parameter when defining the potential.

The tabulation range R is not the same as a cutoff. It merely defines the value of r for the last given value in the table. If the cutoff is longer than that, then $V(r) = V(R)$ for all $r > R$. If the cutoff is shorter than the range, then as for all potentials, $V(r) = 0$ for all $r > r_{\mathrm{cut}}$. A smooth cutoff (see *Cutoffs*) can also be applied on top of the tabulation. The reason for this formalism is that once you have tabulated your potential, you may change the cutoff and smoothening marginal without having to retabulate the potential.

You can also scale the potential in r-axis just by changing the range R, which is the reason why the table needs to include the derivatives multiplied by R: Say you tabulate a potential for a given R, obtaining values $V(r), V'(r)R$. If you scale the r-axis of the potential by a factor ρ, $R^* = \rho R$, you obtain a new potential $U(r)$. This new potential is a scaling of the original potential $U(r) = V(r/\rho), U'(r) = V'(r/\rho)/\rho$. The tabulated r values are scaled so that the ith value becomes $r_i^* = \rho r_i$, and so the expected tabulated values are for the potential $U(r_i^*) = V(r_i^*/\rho) = V(r_i)$ and for the derivative $U'(r_i^*)R^* = V'(r_i^*/\rho)R^*/\rho = V'(r_i)R$. That is, the tabulated values are invariant under the scaling of R.

Finally, another parameter is available for scaling the energy scale $V(r) \to \varepsilon V(r)$.

The file containing the tabulated values is directly read in by the Fortran core, and it is not allowed to contain anything besides two equally long columns of real numbers separated by white spaces.

Keywords:

```
>>> names_of_parameters('tabulated')
['id', 'range', 'scale']
```

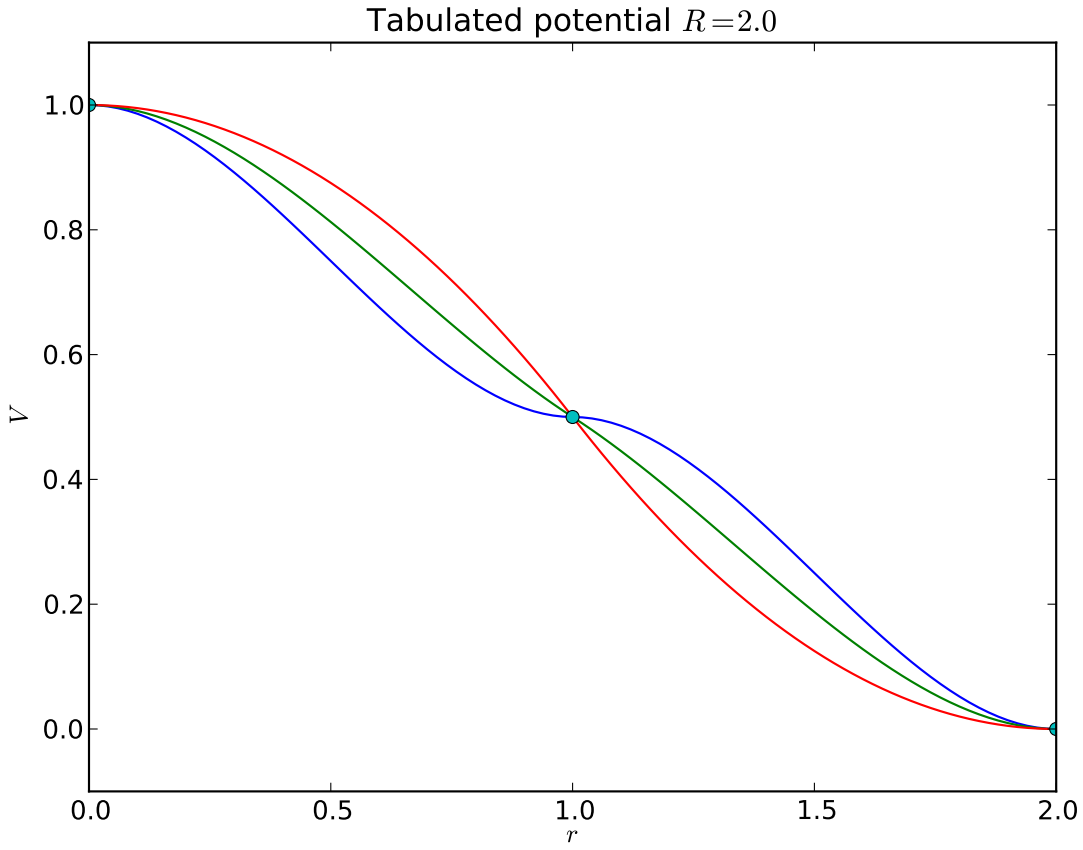
The example plot below shows the resulting potentials for table:

```
1.0  0.0
0.5  0.0
0.0  0.0
```

as well as similar tables with the second number on the second row replaced by -1.0 or -2.0 with range $R = 2.0$ (i.e., the midpoint gets derivative values of 0.0, -0.5, or -1.0).

Fortran routines:

- `create_potential_characterizer_table()`
- `evaluate_energy_table()`
- `evaluate_force_table()`


Tabulated potential $R=2.0$
1.0
0.8
0.6
0.4
0.2
0.0
V
0.0
0.5
1.0
1.5
2.0
r

Bond bending potential 3-body interaction defined as

$$V(\theta) = \varepsilon(\cos^n\theta - \cos^n\theta_0)^m,$$

where ε is an energy scale constant, n and m are integer exponents, θ is an angle defined by three points in space (atomic positions) and θ_0 is the equilibrium angle. As a apecial case, the cosine harmonic potential is obtined with $\varepsilon = k/2, n = 1, m = 2$.

Keywords:

```
>>> names_of_parameters('bond_bend')
['epsilon', 'theta_0', 'n', 'm']
```

Three bodies form a triangle and so there are three possible angles the potential could bend. To remove this ambiguousness, the angle is defined so that as the potential is given a list of targets, the middle target is considered to be at the tip of the angle.

Example:

```
>>> pot = Potential('bond_bend')
>>> pot.set_symbols(['H', 'O', 'H'])
```

This creates a potential for H-O-H angles, but not for H-H-O angles.

Also remember that the bond bending potential does not include any actual bonding potential between particles - it only generates an angular force component. It must be coupled with other potentials to build a full bonding potential.

Fortran routines:

- `create_potential_characterizer_bond_bending()`
- `evaluate_energy_bond_bending()`
- `evaluate_force_bond_bending()`

Dihedral angle potential 4-body interaction defined as

$$V(r) = \frac{k}{2}(\cos\theta - \cos\theta_0)^2$$

where k is a spring constant and θ is the dihedral angle, with θ_0 denoting the equilibrium angle. (So, this is the cosine harmonic variant of the dihedral angle potential.)

For an atom chain 1-2-3-4 the dihedral angle is the angle between the bonds 1-2 and 3-4 when projected on the plane perpendicular to the bond 2-3. In other words, it is the torsion angle of the bond chain. If we write $\mathbf{r}_{ij} = \mathbf{R}_j - \mathbf{R}_i$, where $\mathbf{R}_i$ is the coordinate vector of the atom i, the angle is given by

$$\begin{aligned}\cos\theta &= \frac{\mathbf{p}\cdot\mathbf{p}'}{|\mathbf{p}||\mathbf{p}'|}\\ \mathbf{p} &= -\mathbf{r}_{12} + \frac{\mathbf{r}_{12}\cdot\mathbf{r}_{23}}{|\mathbf{r}_{23}|^2}\mathbf{r}_{23}\\ \mathbf{p}' &= \mathbf{r}_{34} - \frac{\mathbf{r}_{34}\cdot\mathbf{r}_{23}}{|\mathbf{r}_{23}|^2}\mathbf{r}_{23}\end{aligned}$$

Keywords:

```
>>> names_of_parameters('dihedral')
['k', 'theta_0']
```

Fortran routines:

- `create_potential_characterizer_dihedral()`

- evaluate_energy_dihedral()
- evaluate_force_dihedral()

List of methods

Below is a list of methods in Potential, grouped according to the type of functionality.

Interaction handling

- get_cutoff()
- get_cutoff_margin()
- get_number_of_parameters()
- get_parameter_names()
- get_parameter_value()
- get_parameter_values()
- get_potential_type()
- get_soft_cutoff()
- set_cutoff()
- set_cutoff_margin()
- set_parameter_value()
- set_parameter_values()
- set_soft_cutoff()

Coordinator handling

- get_coordinator()
- set_coordinator()

Target handling

- accepts_target_list()
- add_indices()
- add_symbols()
- add_tags()
- get_different_indices()
- get_different_symbols()
- get_different_tags()
- get_indices()
- get_number_of_targets()
- get_symbols()
- get_tags()

- set_indices()
- set_symbols()
- set_tags()

Description

- describe()
- is_multiplier() (meant for internal use)
- get_potentials() (meant for internal use)

Full documentation of the Potential class

class pysic.interactions.local.**Potential**(*potential_type*, *symbols=None*, *tags=None*, *indices=None*, *parameters=None*, *cutoff=0.0*, *cutoff_margin=0.0*, *coordinator=None*)

Class for representing a potential.

Several types of potentials can be defined by specifying the type of the potential as a keyword. The potentials contain a host of parameters and information on what types of particles they act on. To view a list of available potentials, use the method `list_valid_potentials()`.

A potential may be a pair or many-body potential: here, the bodies a potential acts on are called targets. Thus specifying the number of targets of a potential also determines if the potential is a many-body potential.

A potential may be defined for atom types or specifically for certain atoms. These are specified by the symbols, tags, and indices. Each of these should be either 'None' or a list of lists of n values where n is the number of targets. For example, if:

```
indices = [[0, 1], [1, 2], [2, 3]]
```

the potential will be applied between atoms 0 and 1, 1 and 2, and 2 and 3.

Parameters:

symbols: list of string the chemical symbols (elements) on which the potential acts

tags: integer atoms with specific tags on which the potential acts

indices: list of integers atoms with specific indices on which the potential acts

potential_type: string a keyword specifying the type of the potential

parameters: list of doubles a list of parameters for characterizing the potential; their meaning depends on the type of potential

cutoff: double the maximum atomic separation at which the potential is applied

cutoff_margin: double the margin in which the potential is smoothly truncated to zero

coordinator: Coordinator object the coordinator defining a bond order factor for scaling the potential

accepts_target_list(*targets*)

Tests whether a list is suitable as a list of targets, i.e., symbols, tags, or indices and returns True or False accordingly.

A list of targets should be of the format:

```
targets = [[a, b], [c, d]]
```

where the length of the sublists must equal the number of targets.

It is not tested that the values contained in the list are valid.

Parameters:

targets: list of strings or integers a list whose format is checked

add_indices(*indices*)
Adds the given indices to the list of indices.

Parameters:

indices: list of integers list of additional indices on which the potential acts

add_symbols(*symbols*)
Adds the given symbols to the list of symbols.

Parameters:

symbols: list of strings list of additional symbols on which the potential acts

add_tags(*tags*)
Adds the given tags to the list of tags.

Parameters:

tags: list of integers list of additional tags on which the potential acts

describe()
Prints a short description of the potential using the method `describe_potential()`.

get_coordinator()
Returns the Coordinator.

get_cutoff()
Returns the cutoff.

get_cutoff_margin()
Returns the margin for a smooth cutoff.

get_different_indices()
Returns a list containing each index the potential affects once.

get_different_symbols()
Returns a list containing each symbol the potential affects once.

get_different_tags()
Returns a list containing each tag the potential affects once.

get_indices()
Return a list of indices on which the potential acts on.

get_number_of_parameters()
Return the number of parameters the potential expects.

get_number_of_targets()
Returns the number of targets.

get_parameter_names()
Returns a list of the names of the parameters of the potential.

get_parameter_value(*param_name*)
Returns the value of the given parameter.

Parameters:

param_name: string name of the parameter

get_parameter_values()
Returns a list containing the current parameter values of the potential.

get_potential_type()
Returns the keyword specifying the type of the potential.

get_potentials()
Returns a list containing the potential itself.

This is a method ensuring cross compatibility with the `ProductPotential` class.

get_soft_cutoff()
Returns the lower limit for a smooth cutoff.

get_symbols()
Return a list of the chemical symbols (elements) on which the potential acts on.

get_tags()
Return the tags on which the potential acts on.

is_multiplier()
Returns a list containing False.

This is a method ensuring cross compatibility with the `ProductPotential` class.

set_coordinator(*coordinator*)
Sets a new Coordinator.

Parameters:

coordinator: a `Coordinator` object the Coordinator

set_cutoff(*cutoff*)
Sets the cutoff to a given value.

This method affects the hard cutoff. For a detailed explanation on how to define a soft cutoff, see `set_cutoff_margin()`.

Parameters:

cutoff: double new cutoff for the potential

set_cutoff_margin(*margin*)
Sets the margin for smooth cutoff to a given value.

Many potentials decay towards zero in infinity, but in a numeric simulation they are cut at a finite range as specified by the cutoff radius. If the potential is not exactly zero at this range, a discontinuity will be introduced. It is possible to avoid this by including a smoothening factor in the potential to force a decay to zero in a finite interval.

This method defines the decay interval $r_{\mathrm{hard}} - r_{\mathrm{soft}}$. Note that if the soft cutoff value is made smaller than 0 or larger than the hard cutoff value an `InvalidPotentialError` is raised.

Parameters:

margin: double The new cutoff margin

set_indices(*indices*)
Sets the list of indices to equal the given list.

Parameters:

indices: list of integers list of integers on which the potential acts

set_parameter_value(*parameter_name*, *value*)
Sets a given parameter to the desired value.

Parameters:

parameter_name: string name of the parameter

value: double the new value of the parameter

set_parameter_values(*values*)
Sets the numeric values of all parameters.

Parameters:

values: list of doubles list of values to be assigned to parameters

set_parameters(*values*)
Sets the numeric values of all parameters.

Equivalent to `set_parameter_values()`.

Parameters:

values: list of doubles list of values to be assigned to parameters

set_soft_cutoff(*cutoff*)
Sets the soft cutoff to a given value.

For a detailed explanation on the meaning of a soft cutoff, see `set_cutoff_margin()`. Note that actually the cutoff margin is recorded, so changing the hard cutoff (see `set_cutoff()`) will also affect the soft cutoff.

Parameters:

cutoff: double The new soft cutoff

set_symbols(*symbols*)
Sets the list of symbols to equal the given list.

Parameters:

symbols: list of strings list of element symbols on which the potential acts

set_tags(*tags*)
Sets the list of tags to equal the given list.

Parameters:

tags: list of integers list of tags on which the potential acts

ProductPotential class

This class defines an interaction as a product of `Potential`s.

Adding and multiplying potentials

The ordinary `Potential` defines a local interaction for n bodies $(i, j, \ldots)$, so that the total potential energy is

$$V = \sum_{(i,j,\ldots)} v_{i,j,\ldots}.$$

Defining several such potentials (p) for the same set of atoms simply adds them together

$$V = \sum_{(i,j,\ldots)} \sum_{p} v^{p}_{i,j,\ldots}.$$

In code, this could be done for instance this way:

```
pot1 = pysic.Potential(...)
pot2 = pysic.Potential(...)
calc = pysic.Pysic()
calc.set_potentials( [pot1, pot2] )
```

However, you may also wish to *multiply* the potentials to obtain

$$V = \sum_{(i,j,\ldots)} \prod_{p} v^{p}_{i,j,\ldots}.$$

This can be done by wrapping the potentials to be multiplied in a `ProductPotential`:

```
pot1 = pysic.Potential(...)
pot2 = pysic.Potential(...)
prod = pysic.ProductPotential( [pot1, pot2] )
calc = pysic.Pysic()
calc.set_potentials( prod )
```

An immediate benefit of this functionality is the possibility to construct complicated potentials from simple building blocks without having to hardcode all the different variants.

As an example:

```
pot1 = pysic.Potential('power', parameters=[1,1])
pot2 = pysic.Potential('charge_pair', parameters=[1,1,1])
prod = pysic.ProductPotential([pot1,pot2])
```

defines the potentials

$$\begin{aligned} v^{1}_{ij} &= q_i q_j \\ v^{2}_{ij} &= \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \\ V = \sum_{ij} v^{1}_{ij} v^{2}_{ij} &= \sum_{ij} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \end{aligned}$$

Parameterization

The `ProductPotential` class has mostly a similar interface as the elemental `Potential` class. However, the object does not store parameters itself. It merely wraps a group of potentials and these potentials are used for storing the parameters. More precisely, the *first* `Potential` object in the list contained by the `ProductPotential` defines all the general parameters of the potential. We call this the *leading potential* in the following discussion:

```
# Here, pot1 is the leading potential
prod = pysic.ProductPotential( [pot1, pot2, pot3] )
```

Since the product potential is defined as

$$V = \sum_{(i,j,\ldots)} \prod_{p} v^{p}_{i,j,\ldots},$$

the potentials $v^p_{i,j,\ldots}$ being multiplied need to be defined for the same group of atoms - both the number of atoms and their types must match. Also the cutoffs should be equal, since if one $v^p = 0$, the whole product is. Because of this, the targets and cutoffs defined by the *leading* potential are used for the entire product.

In fact, since the cutoff and targets of the potentials forming the product besides the leading one are ignored, they need not be defined at all. Also possible `Coordinator` objects defining bond order factors need to be attached to the leading potential in order to have an effect.

As an example, the following code:

```
pot1 = pysic.Potential(..., symbols=[['H','O']])
pot2 = pysic.Potential(..., symbols=[['H','H']])
prod1 = pysic.ProductPotential( [pot1, pot2] )
prod2 = pysic.ProductPotential( [pot2, pot1] )
```

defines two products, `prod1` and `prod2`, which are both a product of the potentials `pot1` and `pot2`. However, the former, `prod1`, targets H-O pairs (`pot1` is the leading potential) while the latter, `prod2`, affects H-H pairs (`pot2` is the leading potential).

Furthermore, the `ProductPotential` defines methods for handling the general parameters similarly to the `Potential` class, and these methods directly affect the leading potential. That is, methods of the type:

```
prod = pysic.ProductPotential( [pot1, pot2] )
# method call on prod
prod.set_cutoff(8.0)
# is equivalent to a method call on the leading potential in prod
prod.get_potentials()[0].set_cutoff(8.0)
```

are equivalent.

To avoid changing the original potentials, the objects are copied when passed to the product. However, this also means that you are unable to modify the product by changing the component potentials after having wrapped them:

```
prod = pysic.ProductPotential( [pot1, pot2] )
# method call on prod
prod.set_cutoff(8.0)
# is not the same as a method call on the original pot1
pot1.set_cutoff(8.0)
```

For instance:

```
calc = pysic.Pysic()
pot1 = pysic.Potential(..., symbols=[['H','O']])   # Define a potential for H-O
calc.add_potential( pot1 )                          # Add pot1 to the calculator
pot2 = pysic.Potential(...)                         # Define another potential
prod = pysic.ProductPotential( [pot1, pot2] )       # Multiply pot1 and pot2 to make prod
prod.set_symbols( [['H','H']] )                     # Set prod to target H-H
calc.add_potential( prod )                          # Add the prod to the calculator
```

creates two potentials, `pot1` and `prod` affecting H-O and H-H pairs. Although `prod` is constructed from `pot1` and `pot2`, is actually contains only copies of these potentials. If `prod` contained the original potential objects `prod.set_symbols( [['H','H']] )` would affect `pot1`, the leading potential, and change `symbols` in `pot1` as well having both potentials end up targeting H-H pairs. This kind of behaviour could lead to unintentional changes in the properties of other potentials

On the other hand, this example:

```
calc = pysic.Pysic()
pot1 = pysic.Potential(..., symbols=[['H','O']])   # Define a potential for H-O
calc.add_potential( pot1 )                          # Add pot1 to the calculator
pot2 = pysic.Potential(...)                         # Define another potential
```

```
prod = pysic.ProductPotential( [pot1, pot2] )       # Multiply pot1 and pot2 to make prod
pot1.set_symbols( [['H','H']] )                     # Set pot1 to target H-H
calc.add_potential( prod )                          # Add the prod to the calculator
```

Leads to `pot1` and `prod` affecting H-H and H-O pairs, respectively. This is because `pot1.set_symbols( [['H','H']] )` only changes the original potential, not the copy stored in `prod`.

The physical parameters of the potential components are naturally defined separately for each potential. Therefore the `ProductPotential` has no methods for accessing these parameters of its constituents. Instead, one has to directly access the `Potential` objects themselves:

```
pot1 = pysic.Potential(...)                              # Define a potential
pot2 = pysic.Potential(...)                              # Define another potential
prod = pysic.ProductPotential( [pot1, pot2] )            # Multiply pot1 and pot2 to make prod
prod.get_potentials()[1].set_parameter_value('a', 1.0) # set parameter a to 1.0
pot2.set_parameter_value('a' 2.0)                        # set parameter a to 2.0
```

Above, the second potential in `prod` gets the parameter value `a = 1.0`. The last command changes the parameter value in `pot2`, but the change does not propagate to the copy stored in `prod`.

List of methods

Below is a list of methods in `ProductPotential`, grouped according to the type of functionality.

Interaction handling

- `get_cutoff()`
- `get_cutoff_margin()`
- `get_soft_cutoff()`
- `set_cutoff()`
- `set_cutoff_margin()`
- `set_soft_cutoff()`

Coordinator handling

- `get_coordinator()`
- `set_coordinator()`

Target handling

- `accepts_target_list()`
- `add_indices()`
- `add_symbols()`
- `add_tags()`
- `get_different_indices()`
- `get_different_symbols()`
- `get_different_tags()`

- get_indices()
- get_number_of_targets()
- get_symbols()
- get_tags()
- set_indices()
- set_symbols()
- set_tags()

Description

- is_multiplier() (meant for internal use)
- get_potentials() (meant for internal use)

Full documentation of the ProductPotential class

class pysic.interactions.local.**ProductPotential**(*potentials*)
Class representing an interaction obtained by multiplying several Potential objects.

Parameters:

potentials: a list of Potential objects the potentials

accepts_target_list(*targets*)
Tests whether a list is suitable as a list of targets, i.e., symbols, tags, or indices and returns True or False accordingly.

A list of targets should be of the format:

```
targets = [[a, b], [c, d]]
```

where the length of the sublists must equal the number of targets.

It is not tested that the values contained in the list are valid.

Parameters:

targets: list of strings or integers a list whose format is checked

add_indices(*indices*)
Adds the given indices to the list of indices.

Parameters:

indices: list of integers list of additional indices on which the potential acts

add_potential(*potential*)
Adds a potential in the product.

If another ProductPotential is given as an argument, the individual potentials in the product are added one by one to this product.

Also a list of potentials can be given. Then all the listed potentials are added to the product.

Parameters:

potential: a Potential object the potential to be added

add_symbols(*symbols*)
Adds the given symbols to the list of symbols.

Parameters:

symbols: list of strings list of additional symbols on which the potential acts

add_tags(*tags*)
Adds the given tags to the list of tags.

Parameters:

tags: list of integers list of additional tags on which the potential acts

get_coordinator()
Returns the Coordinator.

get_cutoff()
Returns the cutoff.

get_cutoff_margin()
Returns the margin for a smooth cutoff.

get_different_indices()
Returns a list containing each index the potential affects once.

get_different_symbols()
Returns a list containing each symbol the potential affects once.

get_different_tags()
Returns a list containing each tag the potential affects once.

get_indices()
Return a list of indices on which the potential acts on.

get_number_of_targets()
Returns the number of targets.

get_potentials()
Returns the potentials stored in the ProductPotential.

get_soft_cutoff()
Returns the lower limit for a smooth cutoff.

get_symbols()
Return a list of the chemical symbols (elements) on which the potential acts on.

get_tags()
Return the tags on which the potential acts on.

is_multiplier()
Returns a list of logical values specifying if the potentials are multipliers for a product.

The leading potential is considered not to be a multiplier, while the rest are multipliers. Therefore the returned list is [False, True, ..., True], withlength equal to the length of potentials in the product.

set_coordinator(*coordinator*)
Sets a new Coordinator.

Parameters:

coordinator: a Coordinator object the Coordinator

set_cutoff(*cutoff*)
Sets the cutoff to a given value.

This method affects the hard cutoff. For a detailed explanation on how to define a soft cutoff, see `set_cutoff_margin()`.

Parameters:

cutoff: double new cutoff for the potential

set_cutoff_margin (*cutoff_margin*)
Sets the margin for smooth cutoff to a given value.

Many potentials decay towards zero in infinity, but in a numeric simulation they are cut at a finite range as specified by the cutoff radius. If the potential is not exactly zero at this range, a discontinuity will be introduced. It is possible to avoid this by including a smoothening factor in the potential to force a decay to zero in a finite interval.

This method defines the decay interval $r_{\mathrm{hard}} - r_{\mathrm{soft}}$. Note that if the soft cutoff value is made smaller than 0 or larger than the hard cutoff value an `InvalidPotentialError` is raised.

Parameters:

margin: double The new cutoff margin

set_indices (*indices*)
Sets the list of indices to equal the given list.

Parameters:

indices: list of integers list of integers on which the potential acts

set_potentials (*potentials*)
Sets the list of potentials for the product.

Parameters:

potentials: a list of `Potential` objects the potentials

set_soft_cutoff (*cutoff*)
Sets the soft cutoff to a given value.

For a detailed explanation on the meaning of a soft cutoff, see `set_cutoff_margin()`. Note that actually the cutoff margin is recorded, so changing the hard cutoff (see `set_cutoff()`) will also affect the soft cutoff.

Parameters:

cutoff: double The new soft cutoff

set_symbols (*symbols*)
Sets the list of symbols to equal the given list.

Parameters:

symbols: list of strings list of element symbols on which the potential acts

set_tags (*tags*)
Sets the list of tags to equal the given list.

Parameters:

tags: list of integers list of tags on which the potential acts

CoulombSummation class

If a periodic system contains charges interacting via the $\frac{1}{r}$ Coulomb potential, direct summation of the interactions

$$E = \sum_{(i,j)} \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}}, \tag{4.1}$$

where the sum is over pairs of charges q_i, q_j (charges of the entire system, not just the simulation cell) and the distance between the charges is $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$, does not work in general because the sum (4.1) converges very slowly (it actually converges only conditionally). Therefore truncating the sum may lead to severe errors. More advanced techniques must be used in order to accurately evaluate such sums.

This class represents the algorithms used for evaluating the $1/r$ sums. It wraps the summation parameters and activates the summation of Coulomb interactions. If an instance of `CoulombSummation` is given to the `Pysic` calculator, Coulomb interactions between all charged atoms are automatically included in the calculations, regardless of possible `Potential` potentials the calculator may also contain. Otherwise the charges do not directly interact. This is due to two reasons: First, the direct Coulomb interaction is usually always required and it is convenient that it is easily enabled. Second, the specific potentials described by `Potential` are evaluated by direct summation and so the Coulomb summation is separate also on algorithm level in the core.

Charge scaling

Sometimes, you may want to scale the effective charges before calculating the Coulomb sum. Especially, you may want to exclude some atoms from the long range summation. This can be done by giving the `CoulombSummation` a list of scaling values, one per atom. The actual charges of the atoms are then multiplied by the given scaling values before the Coulomb potential is calculated. If a scaling value is 0, the corresponding atom is always treated as if it had no charge. Note though, that scaling with unequal scaling constants may lead to the cell being effectively charged.

Using the Python map function is a convenient way to generate such atom-by-atom lists. For instance, if you want to generate a list by element:

```
>>> atoms = ase.Atoms('H2O')
>>> def charge_by_elem(elem):
...     if elem == 'H':
...         return 0.1
...     elif elem == 'O':
...         return -0.2
...     else:
...         return 0.0
...
>>> system.set_initial_charges(map(charge_by_elem, system.get_chemical_symbols()))
>>> charges
[0.1, 0.1, -0.2]
```

Automatic parameters

As the summation algorithms are parameter dependent, one should always check numeric convergence before real simulations. As a first guess, the utility function `pysic.interactions.coulomb.estimate_ewald_parameters()` can be used for estimating the parameters of the Ewald method.

List of currently available summation algorithms

Below is a list of summation algorithms currently implemented.

Ewald summation The standard technique for overcoming the problem of summing long ranged periodic potentials is the so called Ewald summation method. The idea is to split the long ranged and singular Coulomb potential to a short ranged singular and long ranged smooth parts, and calculate the long ranged part in reciprocal space via Fourier transformations. This is possible (for a smooth potential) since the system is periodic and the same supercell repeats infinitely in all directions. In practice the calculation can be done by adding (and subtracting) Gaussian charge densities over the point charges to screen the potential in real space. That is, the original charge density $\rho(\mathbf{r}) = \sum_i q_i \delta(\mathbf{r} - \mathbf{r}_i)$ is split by

$$\begin{aligned}
\rho(\mathbf{r}) &= \rho_s(\mathbf{r}) + \rho_l(\mathbf{r}) && (4.2)\\
\rho_s(\mathbf{r}) &= \sum_i \left[q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i G_\sigma(\mathbf{r} - \mathbf{r}_i)\right] && (4.3)\\
\rho_l(\mathbf{r}) &= \sum_i q_i G_\sigma(\mathbf{r} - \mathbf{r}_i) && (4.4)\\
G_\sigma(\mathbf{r}) &= \frac{1}{(2\pi\sigma^2)^{3/2}} \exp\left(-\frac{|\mathbf{r}|^2}{2\sigma^2}\right) && (4.5)
\end{aligned}$$

Here ρ_l generates a long range interaction since at large distances the Gaussian densities G_σ appear the same as point charges ($\lim_{\sigma/r\to 0} G_\sigma(\mathbf{r}) = \delta(\mathbf{r})$). Since the charge density is smooth, so will be the potential it creates. The density ρ_s exhibits short ranged interactions for the same reason: At distances longer than the width of the Gaussians the point charges are screened by the Gaussians which exactly cancel them ($\lim_{\sigma/r\to 0} \delta(\mathbf{r}) - G_\sigma(\mathbf{r}) = 0$).

The short ranged interactions are directly calculated in real space

$$\begin{aligned}
E_s &= \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_s(\mathbf{r})\rho_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r \mathrm{d}^3 r' && (4.6)\\
&= \frac{1}{4\pi\varepsilon_0} \sum_{(i,j)} \frac{q_i q_j}{r_{ij}} \mathrm{erfc}\left(\frac{r_{ij}}{\sigma\sqrt{2}}\right) - \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_i^N q_i^2. && (4.7)
\end{aligned}$$

The complementary error function $\mathrm{erfc}(r) = 1 - \mathrm{erf}(r) = 1 - \frac{2}{\sqrt{\pi}} \int_0^r e^{-t^2/2} \mathrm{d}t$ makes the sum converge rapidly as $\frac{r_{ij}}{\sigma} \to \infty$. The latter sum is the self energy of each point charge in the potential of the particular Gaussian that screens the charge, and the sum runs over all charges in the supercell spanning the periodic system. (The self energy is cancelled by the long range part of the energy.)

The long ranged interaction

$$E_l = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_l(\mathbf{r})\rho_l(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r \mathrm{d}^3 r'$$

can be calculated in reciprocal space by Fourier transformation. The result is

$$\begin{aligned}
E_l &= \frac{1}{2V\varepsilon_0} \sum_{\mathbf{k}\neq 0} \frac{e^{-\sigma^2 k^2/2}}{k^2} |S(\mathbf{k})|^2 && (4.8)\\
S(\mathbf{k}) &= \sum_i^N q_i e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} && (4.9)
\end{aligned}$$

The sum in E_l runs over the reciprocal lattice $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$ where $\mathbf{b}_i$ are the vectors spanning the reciprocal cell ($[\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3] = ([\mathbf{v}_1\mathbf{v}_2\mathbf{v}_3]^{-1})^T$ where $\mathbf{v}_i$ are the real space cell vectors). Likewise the sum in the structure factor $S(\mathbf{k})$ runs over all charges in the supercell.

The total energy is then the sum of the short and long range energies

$$E = E_s + E_l.$$

If the system carries a net charge, the total Coulomb potential of the infinite periodic system is infinite. Excess charge can be neutralized by imposing a uniform background charge of opposite sign, which results in the correction term

$$E_c = -\frac{\sigma^2}{4V\varepsilon_0}\left|\sum_i q_i\right|^2.$$

This correction is applied automatically.

Forces are obtained as the gradient of the total energy. For atom α, the force is

$$\mathbf{F}_\alpha = -\nabla_\alpha E = -\nabla_\alpha E_s - \nabla_\alpha E_l.$$

(There is no contribution from E_c.) The short ranged interactions are easily calculated in real space

$$-\nabla_\alpha E_s = \frac{q_\alpha}{4\pi\varepsilon_0}\sum_j q_j\left[\mathrm{erfc}\left(\frac{r_{\alpha j}}{\sigma\sqrt{2}}\right)\frac{1}{r_{\alpha j}^2} + \frac{1}{\sigma}\sqrt{\frac{2}{\pi}}\exp\left(-\frac{r_{\alpha j}^2}{2\sigma^2}\right)\frac{1}{r_{\alpha j}}\right]\hat{r}_{\alpha j},$$

where $\hat{r}_{\alpha j} = \mathbf{r}_{\alpha j}/r_{\alpha j}$ is the unit vector pointing from atom α to j. The long range forces are obtained by differentiating the structure factor

$$-\nabla_\alpha E_l = -\frac{1}{2V\varepsilon_0}\sum_{\mathbf{k}\neq 0}\frac{e^{-\sigma^2k^2/2}}{k^2}2\mathrm{Re}[S^*(\mathbf{k})\nabla_\alpha S(\mathbf{k})] \quad (4.10)$$

$$\nabla_\alpha S(\mathbf{k}) = q_\alpha\mathbf{k}(-\sin\mathbf{k}\cdot\mathbf{r}_\alpha + i\cos\mathbf{k}\cdot\mathbf{r}_\alpha). \quad (4.11)$$

List of methods

Below is a list of methods in `CoulombSummation`, grouped according to the type of functionality.

Initialization

- `initialize_parameters()` (meant for internal use)
- `get_summation()`
- `set_summation()`
- `summation_modes`
- `summation_parameter_descriptions`
- `summation_parameters`

Parameter handling

- `get_parameters()`
- `set_parameter_value()`
- `set_parameter_values()`
- `set_parameters()`

Miscellaneous

- get_realspace_cutoff()
- get_scaling_factors()
- set_scaling_factors()

Full documentation of the CoulombSummation class

class pysic.interactions.coulomb.**CoulombSummation**(*method='ewald'*, *parameters=None*, *scaler=None*)

Class for representing a collection of parameters for evaluating Coulomb potentials.

Summing $1/r$ potentials in periodic systems requires more advanced techniques than just direct summation of pair interactions. The starndard method for evaluating these kinds of potentials is through Ewald summation, where the long range part of the potential is evaluated in reciprocal space.

Instances of this class are used for wrapping the parameters controlling the summations. Passing such an instance to the Pysic calculator activates the evaluation of Coulomb interactions.

Currently, only Ewald summation is available as a calculation method.

Parameters:

method: string keyword specifying the method of summation

parameters: list of doubles numeric values of summation parameters

scaler: list of doubles numeric values for scaling the atomic charges in summation

get_parameters()
Returns a list containing the numeric values of the parameters.

get_realspace_cutoff()
Returns the real space cutoff.

get_scaling_factors()
Returns the list of scaling parameters for atomic charges.

get_summation()
Returns the mode of summation.

initialize_parameters()
Creates a dictionary of parameters and initializes all values to 0.0.

set_parameter_value(*parameter_name*, *value*)
Sets a given parameter to the desired value.

Parameters:

parameter_name: string name of the parameter

value: double the new value of the parameter

set_parameter_values(*parameters*)
Sets the numeric values for all parameters.

Parameters:

parameters: list of doubles list of values to be assigned to parameters

set_parameters(*parameters*)
Sets the numeric values for all parameters.

Equivalent to `set_parameter_values()`

Parameters:

parameters: list of doubles list of values to be assigned to parameters

set_scaling_factors(*scaler*)
Set the list of scaling parameters for atomic charges.

Parameters:

scaler: list of doubles the list of scaling factors

set_summation(*method*)
Sets the summation method.

The method also creates a dictionary of parameters initialized to 0.0 by invoking `initialize_parameters()`.

Parameters:

method: string a keyword specifying the mode of summation

summation_modes = ['ewald']
Names of the summation methods. These are keywords used for setting up the summation algorithms.

summation_parameter_descriptions = {'ewald': ['real space cutoff radius', 'reciprocal space cutoff radius', 'ewa
Short descriptions of the parameters of the summation algorithm.

summation_parameters = {'ewald': ['real_cutoff', 'k_cutoff', 'sigma', 'epsilon']}
Names of the parameters of the summation algorithm.

pysic.interactions.coulomb.**estimate_ewald_parameters**(*real_cutoff=10.0*, *accuracy='normal'*)
Returns a tuple containing a good initial guess for Ewald parameters in the order *real_cutoff, k_cutoff, sigma, epsilon*.

The returned values are (real_cutoff, k_cutoff, sigma, epsilon). Epsilon is always 0.00552635 ε_0 in units of $\frac{e^2}{eVA}$ Real cutoff can be given by the user and should be short enough to make the real space summation efficient (note that this affects neighborlisting and thus also other real space summations). Sigma and k_cutoff are determined by simple scaling rules where $\sigma \sim r_{\mathrm{cut}}$ and $k_{\mathrm{cut}} \sim \sigma^{-1}$. The scaling constants are determined by the accuracy setting.

Note that the given parameters are not analysed in any way - they are only a first guess. You should always test the parameters for accuracy and speed before production simulations.

Parameters:

real_cutoff: double the real space cutoff to be used - it should be shorter than the size of the simulation box

accuracy: string either 'low', 'normal', 'high', 'real' or 'reciprocal'

Coordinator class

Coordinator is short for 'Coordination Calculator'.

This class provides a utility for calculating and storing bond order factors needed for bond order or Tersoff-like potentials. Here, bond order refers roughly to the number of neighbors of an atom, however, the bond order factors may depend also on the atomic distances, angles and other local geometric factors.

To use a `Coordinator`, one must pass it first to a `Potential` object, which is further given to a `Pysic` calculator. Then, one can use the calculator to calculate forces or just the bond order factors. When a `Coordinator` is added to a `Potential`, the potential is multiplied by the bond order factors as defined by the Coordinator.

Bond order potentials

A bond order factor can be added to any `Potential` object. This means that the potential is multiplied by the bond order factor. The factors are always defined by atom, but for a two and many body potentials the average is applied. To put in other words, if we have, say, a three-body potential

$$V = \sum_{(i,j,k)} v_{ijk},$$

where the sum goes over all atom triplets (i,j,k), adding a bond order factor 'b' will modify this to

$$V = \sum_{(i,j,k)} \frac{1}{3}(b_i + b_j + b_k)v_{ijk}.$$

The corresponding modified force (acting on atom alpha) would be

$$F_\alpha = -\nabla_\alpha V = -\sum_{(i,j,k)} \frac{1}{3}(\nabla_\alpha b_i + \nabla_\alpha b_j + \nabla_\alpha b_k)v_{ijk} + \sum_{(i,j,k)} \frac{1}{3}(b_i + b_j + b_k)f_{\alpha,ijk}.$$

where

$$f_{\alpha,ijk} = -\nabla_\alpha v_{ijk}$$

is the gradient of the unmodified potential.

Note that since the bond factor of an atom usually depends on its whole neighborhood, moving a neighbor of an atom may change the bond factors. In other words, the gradients

$$\nabla_\alpha b_i + \nabla_\alpha b_j + \nabla_\alpha b_k$$

can be non-zero for values of alpha other than i, j, k. Thus adding a bond factor to a potential effectively increases the number of bodies in the interaction.

Parameter wrapping

Bond order factors are defined by atomic elements (chemical symbols). Unlike potentials, however, they may incorporate different parameters and cutoffs for different elements and in addition, they may contain parameters separately for single elements, pairs of elements, element triplets etc. Due to this, a bond order factor can contain plenty of parameters.

To ease the handling of all the parameters, a wrapper class `BondOrderParameters` is defined. A single instance of this class defines the type of bond order factor and contains the cutoffs and parameters for one set of elements. The `Coordinator` object then collects these parameters in one bundle.

The bond order types and all associated parameters are explained in the documentation of `BondOrderParameters`.

Bond order mixing

In general, bond order factors are of the form

$$b_i = s_i(\sum_{(i,j,\ldots)} c_{ij\ldots})$$

where $c_{ij\ldots}$ are local environment contributors and s_i is a per-atom scaling function. For example, if one would define a factor

$$b_i = 1 + \sum_{(i,j)} f(r_{ij}),$$

then

$$c_{ij} = f(r_{ij})$$
$$s_i(x) = 1 + x.$$

When bond order factors are evaluated, the sums $\sum_{(i,j,\ldots)} b_{ij\ldots}$ are always calculated first and only then the scaling s_i is applied atom-by-atom.

When a `Coordinator` contains several `BondOrderParameters`:

```
>>> crd = pysic.Coordinator( [ bond1, bond2, bond3 ] )
```

they are all added together in the bond order sums $\sum_{(i,j,\ldots)} b_{ij\ldots}$. Mixing different types of bond order factors is possible but not recommenended as the results may be unexpected.

The scaling is always carried out at most only once per atom. This is done as follows. The list of bond order parameters is searched for a parameter set which requires scaling and which contains 1-body parameters for the correct element. (That is, the first atomic symbol of the list of targets of the parameter must equal the element of the atom for which the scaling is done.) Once such parameters are found, they are used for scaling and the rest of the parameters are ignored. In practice this means that the first applicable set of parameters in the list of `BondOrderParameters` in the `Coordinator` is used.

Because of this behaviour, the default scaling can be overridden as shown in the following example.

Let's say we wish to create a potential to bias the coordination number of Cu-O bonds of Cu atoms, n, according to

$$V(n) = \varepsilon \frac{\Delta N}{1 + \exp(\gamma \Delta N)}$$
$$\Delta N = C(n - N).$$

In general, this type of a potential tries to push n towards N, a given parameter.

We can define this in pysic by overriding the scaling of the coordination bond order factor.:

```
>>> bond_sum = pysic.BondOrderParameters( 'neighbors', cutoff = 4.0,
...                                       cutoff_margin = 1.0,
...                                       symbols = [['Cu','O']] )
>>> bond_scale = pysic.BondOrderParameters( 'c_scale', symbols = ['Cu'],
...                                         parameters=[epsilon,
...                                         N,
...                                         C,
...                                         gamma] )
>>> crd = pysic.Coordinator( [bond_scale, bond_sum] )
>>> pot = pysic.Potential( 'constant', symbols = ['Cu'],
...                        parameters = [1.0], coordinator = crd )
```

In the final step, the `Coordinator` is attached to a `Potential` with a constant value of 1.0. Since the result is a product between the bond order factor and the potential, the resulting potential is just the bond order factor.

List of methods

Below is a list of methods in `Coordinator`, grouped according to the type of functionality.

Parameter handling

- `add_bond_order_parameters()`
- `set_bond_order_parameters()`
- `get_bond_order_parameters()`

Coordination and bond order

- calculate_bond_order_factors()
- get_bond_order_factors()
- get_bond_order_gradients()
- get_bond_order_gradients_of_factor()

Miscellaneous

- get_group_index() (meant for internal use)
- set_group_index() (meant for internal use)

Full documentation of the Coordinator class

class pysic.interactions.bondorder.**Coordinator**(*bond_order_parameters=None*)
Class for representing a calculator for atomic coordination numbers and bond order factors.

Pysic can utilise 'Tersoff-like' potentials which are locally scaled according to bond order factors, related to the number of neighbors of each atom. The coordination calculator keeps track of updating the bond order factors and holds the parameters for calculating the values.

When calculating forces also the derivatives of the coordination numbers are needed. Coordination numbers may be used repeatedly when calculating energies and forces even within one evaluation of the forces and therefore they are stored by the calculator. Derivatives are not stored since storing them could potentially require an N x N matrix, where N is the number of particles.

The calculation of coordination is an operation on the geometry, not the complete physical system including the interactions, and so one can define coordination calculators as standalone objects as well. They always operate on the geometry currently allocated in the core.

Parameters:

bond_order_parameters: list of BondOrderParameters objects Parameters for calculating bond order factors.

add_bond_order_parameters(*params*)
Adds the given parameters to this Coordinator.

Parameters:

params: BondOrderParameters new bond order parameters

calculate_bond_order_factors()
Recalculates the bond order factors for all atoms and stores them.

Similarly to coordination numbers (calculate_coordination()), this method only calculates the factors and stores them but does not return them.

get_bond_order_factors()
Returns an array containing the bond order factors of all atoms.

This method does not calculate the bond order factors but returns the precalculated array.

get_bond_order_gradients(*atom_index*)
Returns an array containing the gradients of bond order factors of all atoms with respect to moving one atom.

Parameters:

atom_index: integer the index of the atom the position of which is being differentiated with

get_bond_order_gradients_of_factor(*atom_index*)
Returns an array containing the gradients of the bond order factor of one atom with respect to moving any atom.

Parameters:

atom_index: integer the index of the atom the position of which is being differentiated with

get_bond_order_parameters()
Returns the bond order parameters of this Coordinator.

get_group_index()
Returns the group index of the Coordinator.

set_bond_order_parameters(*params*)
Assigns new bond order parameters to this Coordinator.

Parameters:

params: BondOrderParameters new bond order parameters

set_group_index(*index*)
Sets an index for the coordinator object.

In the fortran core, bond order parameters are calculated by bond order parameters. Since a coordinator contains many, they are grouped to a coordinator via a grouping index when the core is initialized. This method is meant to be used for telling the Coordinator of this index. That allows the bond orders can be calculated by calling the Coordinator itself, since the index tells which bond parameters in the core are needed.

Parameters:

index: integer an index for grouping bond order parameters in the core

BondOrderParameters class

This class defines a set of parameters for a bond order factor, to be used in conjunction with the `Coordinator` class.

Similarly to the potentials, the available types of bond order factors are always inquired from the Fortran core to ensure that any changes made to the core are automatically reflected in the Python interface.

The same utility functions in `pysic` for inquiring keywords and other data needed for creating the potentials also work for fetching information on bond order factors, if applicable. The functions check automatically if the inquired name matches a potential or a bond order factor and gather the correct type of information based on this.

For example:

- Inquire the names of available bond order factors: `list_valid_bond_order_factors()`
- Inquire the names of parameters for a bond order factors: `names_of_parameters()`

Bond order cutoffs

Atomic coordination is an example of a simple bond order factor. It is calculated by checking all atom pairs and counting which ones are “close” to each others. Close naturally means closer than some predefined cutoff distance. However, in order to make the coordination a continuous and differentiable function, a continuous cutoff has to be

applied. This is done similarly to the smooth cutoffs used in `Potential` by defining a proximity function which is 1 for small separations and 0 for large distances.

$$f(r) = \begin{cases} 1, & r < r_{\mathrm{soft}} \\ \frac{1}{2}\left(1 + \cos \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}}\right), & r_{\mathrm{soft}} < r < r_{\mathrm{hard}} \\ 0, & r > r_{\mathrm{hard}} \end{cases}.$$

Since bond order factors such as atomic coordination need not decay as a function of distance, one must always define a margin for continuous cutoff in bond order factors.

Atomic and pairwise factors

Two types of factors can be defined: atomic or pairwise (per bond) factors. Let us first give formal definitions for these types and then discuss the differences in their use and behavior.

Atomic factors Atomic factors are of the form

$$b_i = s_i(\sum_{j,\ldots} c_{ij\ldots}),$$

where the local factors $c_{ij\ldots}$ may have 2, 3, or more indices depending on how many bodies affect the factor. When this kind of a factor is applied on an n-body potential, $v_{ij\ldots}$, an n-body factor is created as the average of the atomic factors

$$b_{ij\ldots} = \frac{1}{n}(b_i + b_j + \ldots).$$

The resulting potential is then

$$U = \sum_{i,j,\ldots} b_{ij\ldots} v_{ij\ldots},$$

where the summation goes over all n-chains.

Pairwise factors Pairwise factors, on the other hand are only defined for pair potentials v_{ij}. These factors scale the interaction by

$$U = \sum_{i,j} b_{ij} v_{ij},$$

where the summation goes over all pairs (i, j). Note that this form requires b_{ij} to be symmetric with respect to i and j. It would also be possible to define the factor through

$$U = \frac{1}{2} \sum_{i \neq j} \tilde{b}_{ij} v_{ij},$$

where the sum goes over all indices — and thus over all pairs twice. Using the notation above, this is equivalent to

$$U = \sum_{i,j} \frac{1}{2}(\tilde{b}_{ij} + \tilde{b}_{ji}) v_{ij}.$$

Clearly, $b_{ij} = \frac{1}{2}(\tilde{b}_{ij} + \tilde{b}_{ji})$. The factor $\tilde{b}_{ij}$ defined in this manner need not be symmetric, since the summation automatically leads to the symmetric form. Because of this, to avoid the need to force symmetry on b_{ij}, Pysic calculates

the pairwise factors using $b_{ij} = \frac{1}{2}(\tilde{b}_{ij} + \tilde{b}_{ji})$. Therefore it is only necessary to implement the non-symmetric factors $\tilde{b}_{ij}$.

It is important to note that any scaling functions are applied on the factors $\tilde{b}_{ij}$, not on b_{ij}. The difference can be seen with a simple example. Let our factor be $\tilde{b}_{ij} = \sqrt{\sum_k c_{ijk}}$. Then, $b_{ij} = \frac{1}{2}(\sqrt{\sum_k c_{ijk}} + \sqrt{\sum_k c_{jik}}) \neq \sqrt{\frac{1}{2}(\sum_k c_{ijk} + c_{jik})}$. Also note that *Bond order mixing* is not possible between atomic and pairwise factors.

Only use a pairwise factor with a pair potential! If a pairwise factor is applied on an n-body potential where $n \neq 2$, it will automatically be zero. However, applying such a factor will result in the potential being multiplied by the factor, and so the potential becomes zero also.

Pairwise and atomic factors can be used on one and the same pair potential, in which case they are simply added together:

$$b_{ij} = \frac{1}{2}(b_i + b_j + \tilde{b}_{ij} + \tilde{b}_{ji}).$$

The usefulness of this is probably limited — this behavior is adopted to avoid conflicts.

Defining parameters

A `BondOrderParameters` instance defines the type of the bond order factor, the cutoffs, and parameters for one set of elements. The parameters are formally split to scaling function parameters and local summation parameters, where for a factor of type

$$b_i = s_i(\sum_j c_{ij})$$

s_i is the scaling function and $\sum_j c_{ij}$ is the local sum (similarly for many-body factors).

This division is mostly cosmetic, though, and the parameters could just as well be defined as a single list.

Bond order factors are applied and parameterized by atomic element types (chemical symbols). An n-body factor must always have one or several sets of n symbols to designate the atoms it affects. So, 2- and 3-body factors could accept for instance the following lists of symbols, respectively:

```
>>> two_body_targets = [['H', 'H'], ['H', 'O'], ['O', 'O']]
>>> three_body_targets = [['Si', 'O', 'H']]
```

Atomic factors As an example, the *Power decay bond order factor*

$$b_i = \sum_{j \neq i} f(r_{ij}) \left(\frac{a}{r_{ij}}\right)^n$$

is a two-body factor and therefore requires two elements as its target. It includes no scaling and two local summation factors.

Such a bond order factor could be created with the following command:

```
>>> bonds = pysic.BondOrderParameters('power_bond', cutoff=3.2, cutoff_margin=0.4,
...                                   symbols=[['Si', 'Si']],
...                                   parameters=[[],[a, n]])
```

or alternatively in pieces by a series of commands:

```
>>> bonds = pysic.BondOrderParameters('power_bond')
>>> bonds.set_cutoff(3.2)
>>> bonds.set_cutoff_margin(0.4)
>>> bonds.set_symbols([['Si', 'Si']])
>>> bonds.set_parameter_value('a', a)
>>> bonds.set_parameter_value('n', n)
```

To be used in calculations, this is then passed on to a `Coordinator`, `Potential`, and `Pysic` with:

```
>>> crd = pysic.Coordinator( bonds )
>>> pot = pysic.Potential( ... , coordinator=crd )
>>> cal = pysic.Pysic( potentials=pot )
```

The above factor will only consider Si-Si pairs in the local summation $b_i = \sum_j c_{ij}$, i.e., the atoms i and j must both be silicons. If also, say Si-O pairs should be taken into account, the list needs to be expanded:

```
>>> bonds.add_symbols([['Si','O']])
>>> bonds.get_symbols()
[['Si', 'Si'], ['Si', 'O']]
```

This will apply the factor on Si atoms so that the summation $b_i = \sum_j c_{ij}$ goes over Si-Si and Si-O pairs, i.e., atom i is Si but atom j may be either Si or O.

If you want to define a bond factor also for oxygens, this can be done separately with for instance:

```
>>> bonds2 = pysic.BondOrderParameters('power_bond', cutoff=3.2, cutoff_margin=0.4,
...                                    symbols=[['O', 'O'], ['O', 'Si']],
...                                    parameters=[[],[a, n]])
>>> crd2 = pysic.Coordinator( bonds2 )
>>> pot2 = pysic.Potential( ... , coordinator=crd2 )
>>> cal.add_potential( pot2 )
```

Here one needs to be careful. If you apply a bond order factor on a potential, say a Si-O pair potential, the factor is applied on both Si and O atoms. However, if no parameters are applied for O, the factor for it is zero. That is, in the case of a Si-O pair (Si is i and O is j) the bond factor $b_{ij} = \frac{1}{2}(b_i + b_j) = \frac{1}{2}b_i$, which may be not the intended result.

If you want to have different local parameters for the different pairs O-O and O-Si, you must define two `BondOrderParameters` objects and wrap them in a `Coordinator`:

```
>>> bonds_oo  = pysic.BondOrderParameters('power_bond', cutoff=3.2, cutoff_margin=0.4,
...                                       symbols=[['O', 'O']],
...                                       parameters=[[],[a_oo, n_oo]])
>>> bonds_osi = pysic.BondOrderParameters('power_bond', cutoff=3.2, cutoff_margin=0.4,
...                                       symbols=[['O', 'Si']],
...                                       parameters=[[],[a_osi, n_osi]])
>>> crd3 = pysic.Coordinator( [bonds_oo, bonds_osi] )
>>> pot3 = pysic.Potential( ... , coordinator=crd3 )
>>> cal.set_potentials( [pot, pot3] )
```

That is, local summation is done using all the given parameters summed together. If you apply a scaling factor on a bond order factor, however, it is applied only once. The scaling is determined by the first `BondOrderParameters` object in the `Coordinator` which defines a scaling function and whose first target is the atom for which the factor is being calculated. This can be used for *Bond order mixing*.

As a rule of thumb, remember that one `Potential` can contain only one `Coordinator`, but a `Coordinator` can contain many `BondOrderParameters`. So if your bond order factor requires several sets of parameters due to the different element pairs, it is safest to define each set of parameters using its own `BondOrderParameters` object and wrap the parameters involved in one local summation in a `Coordinator`.

Pairwise factors As an example, the *Tersoff bond order factor*

$$\tilde{b}_{ij} = \left[1 + \left(\beta \sum_{k \neq i,j} \xi_{ijk} g_{ijk}\right)^{\eta}\right]^{-\frac{1}{2\eta}}$$

$$\xi_{ijk} = f(r_{ik}) \exp\left[a^{\mu}(r_{ij} - r_{ik})^{\mu}\right]$$

$$g_{ijk} = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2}$$

is a three-body factor (it includes terms depending on atom triplets (i, j, k)) and therefore requires a set of three elements as its target. It incorporates two scaling and five local sum parameters. Such a bond order factor could be created with the following command:

```
>>> bonds = pysic.BondOrderParameters('tersoff', cutoff=3.2, cutoff_margin=0.4,
...                                   symbols=[['Si', 'Si', 'Si']],
...                                   parameters=[[beta, eta],
...                                               [a, c, d, h, mu]])
```

or alternatively in pieces by a series of commands:

```
>>> bonds = pysic.BondOrderParameters('tersoff')
>>> bonds.set_cutoff(3.2)
>>> bonds.set_cutoff_margin(0.4)
>>> bonds.set_symbols([['Si', 'Si', 'Si']])
>>> bonds.set_parameter_value('beta', beta)
>>> bonds.set_parameter_value('eta', eta)
>>> bonds.set_parameter_value('a', a)
>>> bonds.set_parameter_value('c', c)
>>> bonds.set_parameter_value('d', d)
>>> bonds.set_parameter_value('h', h)
>>> bonds.set_parameter_value('mu', mu)
```

The above example creates a bond order factor which is applied to all Si triplets (symbols=[['Si','Si','Si']]). The command also assigns scaling parameters β, η, and μ, and local summation parameters a, c, d, and h. If there are other elements in the system besides silicon, they will be completely ignored: The bond order factors are calculated as if the other elements do not exist. If one wishes to include, say, Si-O bonds in the bond order factor calculation, the list of symbols needs to be expanded by:

```
>>> bonds.add_symbols([['Si', 'Si', 'O'],
...                    ['Si', 'O', 'Si'],
...                    ['O', 'Si', 'Si'],
...                    ['Si', 'O', 'O'],
...                    ['O', 'Si', 'O']])
>>> bonds.get_symbols()
[['Si', 'Si', 'Si'], ['Si', 'Si', 'O'], ['Si', 'O', 'Si'], ['O', 'Si', 'Si'], ['Si', 'O', 'O'], ['O',
```

The format of the symbol list is as follows. In each triplet, the first two symbols determine the bond on which the factor is calculated (atoms i and j). (For atomic factors, the first symbol determines the element on which the factor is applied.) The third symbol defines the other atoms in the triplets which are taken in to account (atom k). That is, in the example above, Si-(Si-O) bond parameters are included with:

```
>>> ['Si', 'O', 'Si']
```

O-(Si-O) with:

```
>>> ['Si', 'O', 'O']
```

Si-(O-Si) with:

```
>>> ['O', 'Si', 'Si']
```

and O-(O-Si) with:

```
>>> ['O', 'Si', 'O']
```

The definition is complicated like this to enable the tuning of parameters of all the various bond combinations separately.

Instead of giving a list of symbols to a single `BondOrderParameters`, one can define many instances with different symbols and different parameters, and feed a list of these to a `Coordinator` object.:

```
>>> bond_sioo = pysic.BondOrderParameters('tersoff', cutoff=3.2, cutoff_margin=0.4,
...                                       symbols=[['Si', 'O', 'O']],
...                                       parameters=[[beta_si, eta_si],
...                                                   [a_sio, c_sio, d_sio, h_sio, mu_si]])
>>> bond_sisio = pysic.BondOrderParameters('tersoff', cutoff=3.5, cutoff_margin=0.5,
...                                       symbols=[['Si', 'Si', 'O']],
...                                       parameters=[[beta_si, eta_si],
...                                                   [a_sisi, c_sisi, d_sisi, h_sisi, mu_si]])
>>> bond_list = [bond_sioo,bond_sisio]
>>> crd = pysic.Coordinator( bond_list )
```

The above example would assign the parameter values

$$\begin{aligned}
\beta_{\mathrm{Si}} &= \texttt{beta_si} \\
\eta_{\mathrm{Si}} &= \texttt{eta_si} \\
\mu_{\mathrm{Si}} &= \texttt{mu_si} \\
a_{\mathrm{Si-O}} &= \texttt{a_sio} \\
c_{\mathrm{Si-O}} &= \texttt{c_sio} \\
d_{\mathrm{Si-O}} &= \texttt{d_sio} \\
h_{\mathrm{Si-O}} &= \texttt{h_sio} \\
a_{\mathrm{Si-Si}} &= \texttt{a_sisi} \\
c_{\mathrm{Si-Si}} &= \texttt{c_sisi} \\
d_{\mathrm{Si-Si}} &= \texttt{d_sisi} \\
h_{\mathrm{Si-Si}} &= \texttt{h_sisi}
\end{aligned}$$

This gives the user the possibility to precisely control the parameters, including cutoffs, for different elements.

Note that the beta, eta, and mu parameters are the same for both `BondOrderParameters` objects defined in the above example. They could be different in principle, but when the factors are calculated, the scaling parameters are taken from the first object in the list of bonds (*bond_list*) for which the first element is of the correct type. Because of this, the scaling parameters in *bond_sisio* are in fact ignored. This feature can be exploited for *Bond order mixing*.

For three different elements, say C, O, and H, the possible triplets are:

```
>>> [ ['H', 'H', 'H'],  # H-H bond in an H-H-H triplet
...   ['H', 'H', 'C'],  # H-H bond in an H-H-C triplet
...   ['H', 'H', 'O'],  # H-H bond in an H-H-O triplet
...   ['H', 'O', 'H'],  # H-O bond in an H-H-O triplet
...   ['H', 'O', 'C'],  # H-O bond in an O-H-C triplet
...   ['H', 'O', 'O'],  # H-O bond in an O-H-O triplet
...   ['H', 'C', 'H'],  # etc.
```

```
...     ['H', 'C', 'C'],
...     ['H', 'C', 'O'],
...     ['O', 'H', 'H'],
...     ['O', 'H', 'C'],
...     ['O', 'H', 'O'],
...     ['O', 'O', 'H'],
...     ['O', 'O', 'C'],
...     ['O', 'O', 'O'],
...     ['O', 'C', 'H'],
...     ['O', 'C', 'C'],
...     ['O', 'C', 'O'],
...     ['C', 'H', 'H'],
...     ['C', 'H', 'C'],
...     ['C', 'H', 'O'],
...     ['C', 'O', 'H'],
...     ['C', 'O', 'C'],
...     ['C', 'O', 'O'],
...     ['C', 'C', 'H'],
...     ['C', 'C', 'C'],
...     ['C', 'C', 'O'] ]
```

In principle, one can attach a different set of parameters to each of these. Often though the parameters are mostly the same, and writing these kinds of lists for all possible combinations is cumbersome. To help in generating the tables, the utility method `expand_symbols_table()` can be used. For instance, the full list of triplets above can be created with:

```
>>> pysic.utility.convenience.expand_symbols_table([['C', 'O', 'H'],
...                                                 ['C', 'O', 'H'],
...                                                 ['C', 'O', 'H']])
```

List of currently available bond order factors

Below is a list of bond order factors currently implemented.

- *Coordination scaling function*
- *Square root scaling function*
- *Tabulated scaling function*
- *Coordination bond order factor*
- *Power decay bond order factor*
- *Tabulated bond order factor*
- *Tersoff bond order factor*

Coordination scaling function 1-body bond order factor defined as

$$b_i(\Sigma_i) = \begin{cases} \varepsilon_i \frac{\Delta\Sigma_i}{1+\exp(\gamma_i \Delta\Sigma_i)}, & \Delta\Sigma_i > \min_\Sigma \\ 0, & \Delta\Sigma_i < \min_\Sigma \end{cases}$$
$$\Delta\Sigma_i = C_i(\Sigma_i - N_i).$$

where Σ_i is the bond order sum.

In other words, this factor only overrides the scaling function of another bond order factor when mixed. Especially, it is zero if not paired with other bond order factors.

Keywords:

```
>>> names_of_parameters('c_scale')
[['epsilon', 'N', 'C', 'gamma', 'min'], []]
```

Square root scaling function 1-body bond order factor defined as

$$b_i(\Sigma_i) = \varepsilon_i \sqrt{\Sigma_i}$$

where Σ_i is the bond order sum and ε is a scaling constant.

Keywords:

```
>>> names_of_parameters('sqrt_scale')
[['epsilon'], []]
```

Tabulated scaling function 1-body bond order factor of the type

$$b_i(\Sigma_i) = s_i(\Sigma_i),$$

where $s_i(\Sigma)$ is a tabulated function. The tabulation works similarly to the *Tabulated potential*.

Keywords:

```
>>> names_of_parameters('table_scale')
[[id, range, scale], []]
```

Coordination bond order factor 2-body bond order factor defined as

$$b_i = \sum_{j \neq i} f(r_{ij}).$$

The coordination of an atom is simply the sum of the proximity functions. This is a parameterless (besides cutoffs) 2-body bond order factor.

Keywords:

```
>>> names_of_parameters('neighbors')
[[], []]
```

Power decay bond order factor 2-body bond order factor defined as

$$b_i = \sum_{j \neq i} f(r_{ij}) \left(\frac{a_{ij}}{r_{ij}} \right)^{n_{ij}}.$$

This is a density-like bond factor, where the contributions of atomic pairs decay with interatomic distance according to a power law. In form, it is similar to the *Power decay potential* potential.

Keywords:

```
>>> names_of_parameters('power_bond')
[[], [a, n]]
```

Tabulated bond order factor 2-body bond order factor of the type

$$b_i = \sum_{j \neq i} f(r_{ij}) t(r_{ij}),$$

where $t(r)$ is a tabulated function. The tabulation works similarly to the *Tabulated potential*.

Similarly, to tabulate bond scaling, use the *Tabulated scaling function*.

Keywords:

```
>>> names_of_parameters('table_bond')
[[], [id, range, scale]]
```

Tersoff bond order factor Pairwise 3-body bond order factor defined as

$$\tilde{b}_{ij} = \left[1 + \left(\beta_{ij} \sum_{k \neq i,j} \xi_{ijk} g_{ijk} \right)^{\eta_{ij}} \right]^{-\frac{1}{2\eta_{ij}}}$$

$$\xi_{ijk} = f(r_{ik}) \exp \left[a_{ijk}^{\mu_{ijk}} (r_{ij} - r_{ik})^{\mu_{ijk}} \right]$$

$$g_{ijk} = 1 + \frac{c_{ijk}^2}{d_{ijk}^2} - \frac{c_{ijk}^2}{d_{ijk}^2 + (h_{ijk} - \cos\theta_{ijk})^2}$$

where r and theta are distances and angles between the atoms. This rather complicated bond factor takes also into account the directionality of bonds in its angle dependency.

Keywords:

```
>>> names_of_parameters('tersoff')
[['beta', 'eta'], ['a', 'c', 'd', 'h', 'mu']]
```

List of methods

Below is a list of methods in `BondOrderParameters`, grouped according to the type of functionality.

Parameter handling

- `accepts_parameters()`
- `get_bond_order_type()`
- `get_cutoff()`
- `get_cutoff_margin()`
- `get_number_of_parameters()`
- `get_parameter_names()`
- `get_parameter_value()`
- `get_parameter_values()`
- `get_parameters_as_list()`

- get_soft_cutoff()
- set_cutoff()
- set_cutoff_margin()
- set_parameter_value()
- set_parameter_values()
- set_parameters()
- set_soft_cutoff()

Target handling

- accepts_target_list()
- add_symbols()
- get_different_symbols()
- get_number_of_targets()
- get_symbols()
- set_symbols()

Full documentation of the BondOrderParameters class

class pysic.interactions.bondorder.**BondOrderParameters**(*bond_order_type*, *cutoff=0.0*, *cutoff_margin=0.0*, *parameters=None*, *symbols=None*)

Class for representing a collection of parameters for bond order calculations.

Calculating bond order factors using Tersoff-like methods defined in Coordinator requires several parameters per element and element pair. To facilitate the handling of all these parameters, they are wrapped in a BondOrderParameters object.

The object can be created empty and filled later with the parameters. Alternatively, a list of parameters can be given upon initialization in which case it is passed to the set_parameters() method.

Parameters:

bond_order_type: string a keyword specifying the type of the bond order factor

soft_cut: double The soft cutoff for calculating partial coordination. Any atom closer than this is considered a full neighbor.

hard_cut: double The hard cutoff for calculating partial coordination. Any atom closer than this is considered (at least) a partial neighbor and will give a fractional contribution to the total coordination. Any atom farther than this will not contribute to the neighbor count.

parameters: list of doubles a list of parameters to be contained in the parameter object

symbols: list of strings a list of elements on which the factor is applied

accepts_parameters(*params*)

Test if the given parameters array has the correct dimensions.

A bond order parameter can contain separate parameters for single, pair etc. elements and each class can have a different number of parameters. This method checks if the given list has the correct dimensions.

Parameters:

params: list of doubles list of parameters

accepts_target_list(*targets*)
Tests whether a list is suitable as a list of targets, i.e., element symbols and returns True or False accordingly.

A list of targets should be of the format:

```
targets = [[a, b], [c, d]]
```

where the length of the sublists must equal the number of targets.

It is not tested that the values contained in the list are valid.

Parameters:

targets: list of strings or integers a list whose format is checked

add_symbols(*symbols*)
Adds the given symbols to the list of symbols.

Parameters:

symbols: list of strings list of additional symbols on which the bond order factor acts

get_bond_order_type()
Returns the keyword specifying the type of the bond order factor.

get_cutoff()
Returns the cutoff.

get_cutoff_margin()
Returns the margin for a smooth cutoff.

get_different_symbols()
Returns a list containing each symbol the potential affects once.

get_level()
Returns the level of the factor, i.e., is it a per-atom or par-pair factor.

get_number_of_parameters()
Returns the number of parameters the bond order parameter object contains.

get_number_of_targets()
Returns the (maximum) number of targets the bond order factor affects.

get_parameter_names()
Returns a list of the names of the parameters of the potential.

get_parameter_value(*param_name*)
Returns the value of the given parameter.

Parameters:

param_name: string name of the parameter

get_parameter_values()
Returns a list containing the current parameter values of the potential.

get_parameters_as_list()
Returns the parameters of the bond order factor as a single list.

The generated list first contains the single element parameters, then pair parameters, etc.

get_soft_cutoff()
Returns the lower limit for a smooth cutoff.

get_symbols()
Returns the symbols the bond parameters affect.

includes_scaling()
Returns True iff there are scaling paramters.

set_cutoff(*cutoff*)
Sets the cutoff to a given value.

This method affects the hard cutoff.

Parameters:

cutoff: double new cutoff for the bond order factor

set_cutoff_margin(*margin*)
Sets the margin for smooth cutoff to a given value.

This method defines the decay interval $r_{\mathrm{hard}} - r_{\mathrm{soft}}$. Note that if the soft cutoff value is made smaller than 0 or larger than the hard cutoff value an `InvalidParametersError` is raised.

Parameters:

margin: double The new cutoff margin

set_parameter_value(*parameter_name*, *value*)
Sets a given parameter to the desired value.

Parameters:

parameter_name: string name of the parameter

value: double the new value of the parameter

set_parameter_values(*values*)
Sets the numeric values of all parameters.

Parameters:

params: list of doubles list of values to be assigned to parameters

set_parameters(*params*)
Sets the numeric values of all parameters.

Equivalent to `set_parameter_values()`.

Parameters:

params: list of doubles list of values to be assigned to parameters

set_soft_cutoff(*cutoff*)
Sets the soft cutoff to a given value.

Note that actually the cutoff margin is recorded, so changing the hard cutoff (see `set_cutoff()`) will also affect the soft cutoff.

Parameters:

cutoff: double The new soft cutoff

set_symbols(*symbols*)
Sets the list of symbols to equal the given list.

Parameters:

symbols: list of strings list of element symbols on which the bond order factor acts

CompoundPotential class

This class defines an interaction as a collection of `Potential`s, `ProductPotential`s, `Coordinator`s, and `BondOrderParameters`. It is a wrapper to ease the handling of complicated potentials.

Using CompoundPotential

The `CompoundPotential` class does not define a potential itself, but it defines an abstract superclass which can be used for defining particular potentials as subclasses. One such subclass is the Sutton-Chen potential, which will be used as an example here.

Sutton-Chen potential combines a simple power-law potential with a similar density-like term

$$U = \varepsilon \left[\sum_{i,j} \left(\frac{a}{r_{ij}} \right)^n - c \sum_i \sqrt{\rho_i} \right]$$

$$\rho_i = \sum_j \left(\frac{a}{r_{ij}} \right)^m$$

where r_{ij} is the interatomic distance, and ε, a, c, m, n are parameters.

In Pysic, this can be defined by a structure like this:

```
>>> power_pot = pysic.Potential('power', ...)
>>> rho = pysic.BondOrderParameters('power_bond', ...)
>>> root = pysic.BondOrderParameters('sqrt_scale', ...)
>>> sqrt_rho = pysic.Coordinator([root, rho])
>>> rho_pot = pysic.Potential('constant', coordinator=sqrt_rho)
>>> calc = pysic.Pysic()
>>> calc.set_potentials([power_pot, rho_pot])
```

but this is already somewhat cumbersome and requires *Bond order mixing*. It would be much nicer to wrap the definitions in a container:

```
>>> sutton_chen_pot = SuttonChenPotential(...)
>>> calc = pysic.Pysic()
>>> calc.set_potentials(sutton_chen_pot)
```

This is the purpose of `CompoundPotential` and its subclasses.

The central classes such as `pysic.interactions.local.Potential` are imported automatically with the `pysic` module, which is why you can refer to them with `pysic.Potential`. Compound potentials are not, so you need to manually import them, for instance like this:

```
>>> from pysic.interactions.suttonchen import SuttonChenPotential
>>> sutton_chen_pot = SuttonChenPotential(...)
```

Defining new wrappers

`CompoundPotential` inherits the interface of `Potential` and it is used in a similar fashion. A subclass of `CompoundPotential` then also inherits the interface, and so it is easy to create new potentials this way without having to care about the interface. Defining a subclass in Python is done like this:

```
>>> class SuttonChenPotential(CompoundPotential):
...     def __init__(self, ...):
...         super(SuttonChenPotential, self).__init__(...)
...
```

The brackets in the class definition, `(CompoundPotential)`, tell that the class derives from another class and inherits its functionality. In the constructor, `__init__`, the superclass constructor is called with `super(SuttonChenPotential, self).__init__(...)`, but it is also possible to extend the constructor with additional commands.

Compound potentials store their components in a list called `self.pieces`, and this is done in the method `define_elements()`. The components are passed to the calculator via the `build()` method. This is automatically called when a compound potential is given to the `pysic.calculator.Pysic.add_potential()` method, so that the interface is similar to that of simple potentials. For the Sutton-Chen example, the definitions could look something like this:

```
...     def define_elements(self):
...         power_pot = pysic.Potential('power', ...)
...         rho = pysic.BondOrderParameters('power_bond', ...)
...         root = pysic.BondOrderParameters('sqrt_scale', ...)
...         sqrt_rho = pysic.Coordinator([root, rho])
...         rho_pot = pysic.Potential('constant', coordinator=sqrt_rho)
...         self.pieces = [power_pot, rho_pot]
...
```

In principle, this is the only method that a new potential has to override, since the rest is done automatically. Of course, it is possible to override other methods as well or write new ones. The potentials can be made very general, accepting free parameters and target lists, but it is also possible to hard code the parameters. The latter tends to be easier since handling arbitrary lists of parameters can be a code-intensive task.

List of corrently available compound potentials

The potentials provided with Pysic are all found in `pysic.interactions.x` where `x` is the name of the submodule containing the potential.

SuttonChenPotential class This class constructs the Sutton-Chen potential [2] as a subclass of `CompoundPotential`.

This potential contains 2-body and many-body terms defined as

$$U = \varepsilon \left[\sum_{i,j} \left(\frac{a}{r_{ij}} \right)^n - c \sum_i \sqrt{\rho_i} \right]$$

$$\rho_i = \sum_j \left(\frac{a}{r_{ij}} \right)^m$$

where r_{ij} is the interatomic distance, and ε, a, c, m, n are parameters.

Load the potential with:

```
>>> from pysic.interactions.suttonchen import SuttonChenPotential
>>> pot = SuttonChenPotential(symbols=...,
...                           tags=...,
...                           indices=...,
...                           parameters=...,
...                           cutoff=...,
...                           cutoff_margin=...)
```

The same cutoff is used for both the 2-body and many-body terms.

[2] Sutton, A. P., and Chen, J., 1990, Philos. Mag. Lett., 61, 139.

If the potential is given several target pairs, e.g., `symbols = [['A', 'B'], ['A', 'C']]`, all possible combinations are targeted by default. For the above list, the 2-body interaction would be evaluated for A-B and A-C pairs (not B-C), and the many-body interaction would be evaluated for elements A with A-B and A-C pairs, for element B with B-A terms, and for element C with C-A terms. If the many-body term should be only evaluated for certain elements, the method `set_density_symbols()` can be used for specifying the specific target symbols. For instance:

```
>>> pot.set_symbols( [['A', 'B'], ['A', 'C']] )
>>> pot.set_density_symbols( ['A'] )
```

will have the 2-body terms evaluated for A-B and A-C pairs while the many-body term is only evaluated for neighborhoods of element A, taking into account the pairs A-B and A-C.

Full documentation of the SuttonChenPotential class

class `pysic.interactions.suttonchen.`**`SuttonChenPotential`**(*symbols=None*, *tags=None*, *indices=None*, *parameters=None*, *cutoff=0.0*, *cutoff_margin=0.0*)

Class representing the Sutton-Chen potential as a `CompoundPotential` object.

Parameters:

symbols: list of string the chemical symbols (elements) on which the potential acts

tags: integer atoms with specific tags on which the potential acts

indices: list of integers atoms with specific indices on which the potential acts

parameters: list of doubles a list of parameters for characterizing the potential; their meaning depends on the type of potential

cutoff: double the maximum atomic separation at which the potential is applied

cutoff_margin: double the margin in which the potential is smoothly truncated to zero

`define_elements`()

`describe`()

`set_density_symbols`(*symbols*)

CombPotential class This class constructs the Comb potential for silicon and silica [3] as a subclass of `CompoundPotential`.

Load the potential with:

```
>>> from pysic.interactions.comb import CombPotential
>>> import pysic
>>> calc = pysic.Pysic()
>>> pot = CombPotential()
>>> pot.set_calculator(calc, True)
```

The potential is only defined for Si and SiO and parameters have been hard coded, so symbols need not be set. The potential also automatically includes screened `CoulombSummation`, which is why the calculator should be given to it explicitly with `set_calculator()`.

Comb is a fairly complicated potential with many components such as local attractive and repulsive terms, bond angle terms and electrostatics. The class allows the user to switch terms on and off in order to analyze their contribution.

[3] T.-R. Shan, D. Bryce, J. Hawkins, A. Asthagiri, S. Phillpot, and S. Sinnott, Phys Rev B 82, 235302 (2010).

Full documentation of the CombPotential class

class pysic.interactions.comb.**CombPotential**(*excludes=['direct_coulomb', 'long_coulomb']*)

Class representing a COMB potential.

Use:

```
import pysic
import pysic.interactions.comb as comb_sio

calc = pysic.Pysic()
pot = comb_sio.CombPotential()
pot.set_calculator(calc, True)
```

Since the potential may also define CoulombSummation (which it by default does), you should always pass the calculator to the potential in addition to passing the potential to the calculator.

The potential can be modified through the exclusion list. This defines which chuncks of the potential are incorporated at any time. For instance:

```
pot.exclude('si_self')
calc.set_potentials(pot)
```

will remove the self energy contribution from Si atoms. If you modify the potential, you need to confirm the changes by passing the potential to the calculator. This is because the potential is built in the calculator as it is passed. Therefore any changes made after that to the potential will not propagate to the calculator.

check_exclude(*ex*)
Returns True, if `ex` is a valid keyword of the list of components for this potential.

define_elements()
Creates the components of the potential.

exclude(*ex*)
Excludes the given component from the potential.

exclude_all()
Excludes everything.

get_parameter_value(*param_name*)

include(*ex*)
Includes the given component in the potential.

include_all()
Includes all components in the potential, except long range Coulomb interaction.

is_excluded(*ex*)
Returns `True` if the given component is excluded from the potential.

is_included(*ex*)
Returns `True` if the given component is included in the potential.

list_excludes()
Lists the excluded components.

list_possible_excludes()
Lists the keywords of the list of components of the potential.

set_calculator(*calc*, *reciprocal=False*)
Attaches the calculator to the potential. This is needed so that a CoulombSummation can be set. If the argument `reciprocal=True` is given, also the command `calc.set_potentials(self)` is run.

set_ewald(*calc*, *cheat*)
Switches on Ewald summation in `calc`. If `cheat == True`, a short ranged screened interaction is used. For internal use.

set_parameter_value(*param_name*, *value*)

toggle_exclude(*ex*)
Changes the state of the given component from included to excluded, or from excluded to included.

List of methods

Below is a list of methods in `CompoundPotential`, grouped according to the type of functionality. Note that most methods are inherited from the `Potential` class.

Interaction handling

- `build()`
- `pysic.interactions.local.Potential.get_cutoff()`
- `pysic.interactions.local.Potential.get_cutoff_margin()`
- `get_elements()`
- `get_number_of_parameters()`
- `pysic.interactions.local.Potential.get_parameter_names()`
- `pysic.interactions.local.Potential.get_parameter_value()`
- `pysic.interactions.local.Potential.get_parameter_values()`
- `set_potential_type()` (meant for internal use)
- `pysic.interactions.local.Potential.get_soft_cutoff()`
- `remove()`
- `pysic.interactions.local.Potential.set_cutoff()`
- `pysic.interactions.local.Potential.set_cutoff_margin()`
- `pysic.interactions.local.Potential.set_parameter_value()`
- `pysic.interactions.local.Potential.set_parameter_values()`
- `pysic.interactions.local.Potential.set_soft_cutoff()`

Coordinator handling

- `get_coordinator()`
- `set_coordinator()`

Target handling

- `accepts_target_list()`
- `add_indices()`
- `add_symbols()`
- `add_tags()`

- get_different_indices()
- get_different_symbols()
- get_different_tags()
- get_indices()
- get_number_of_targets()
- get_symbols()
- get_tags()
- set_indices()
- set_symbols()
- set_tags()

Description

- describe()
- is_multiplier() (meant for internal use)
- get_potentials() (meant for internal use)

Full documentation of the CompoundPotential class

class pysic.interactions.compound.**CompoundPotential**(*n_targets*, *n_params*, *symbols=None*, *tags=None*, *indices=None*, *parameters=None*, *cutoff=0.0*, *cutoff_margin=0.0*)

Class representing an interaction constructed of several Potential and ProductPotential objects.

This class implements the framework for wrapping complicated potentials as Python objects. The class itself implements an empty potential. To utilize the compound potential for real calculations, subclasses should be used for defining the actual contents of the potential.

Parameters:

n_targets: integer number of targets the potential acts on

n_params: integer number of parameters needed for describing the potential

symbols: list of string the chemical symbols (elements) on which the potential acts

tags: integer atoms with specific tags on which the potential acts

indices: list of integers atoms with specific indices on which the potential acts

parameters: list of doubles a list of parameters for characterizing the potential; their meaning depends on the type of potential

cutoff: double the maximum atomic separation at which the potential is applied

cutoff_margin: double the margin in which the potential is smoothly truncated to zero

build(*calculator*)

Constructs the potential for the calculator as a collection of elemental potentials.

The method adds all the elemental potentials it consists of one by one through the pysic.calculator.Pysic.add_potential() method.

Parameters:

calculator: `Pysic` object the Pysic calculator to which the potential is added

`define_elements`()
Fills the compound potential with the elemental potentials it is made of.

This method just stores an empty list. Any subclass to be used as a compound potential should re-implement this method.

`describe`()
Prints a description of the potential on-screen.

`get_elements`()
Returns the elemental potentials this compund potential consists of.

`get_number_of_parameters`()
Returns the number of parameters the potential accepts.

`remove`(*calculator*)
Removes the elemental potentials this compound contains from the calculator.

The method removes all the elemental potentials it consists of one by one through the `pysic.calculator.Pysic.remove_potential()` method. If a match is not found in the set of potentials in the calculator, a message will be printed but the removal process continues.

Parameters:

calculator: `Pysic` object the Pysic calculator from which the potential is removed

`set_potential_type`(*type*)
Sets the name of the potential.

This can be used by subclasses to set the name of the potential. Since normal potentials are distinguished by their names (keywords) compound potentials should also have a name for consistency.

Parameters:

type: string The name of the potential

ChargeRelaxation class

This class controls equilibration of atomic charges in the system.

It is possible for the user to define the charges of atoms in ASE. If a system exhibits charge transfer, polarization, charged defects etc., one may not know the charges beforehand or the charges may change dynamically during simulation. To handle such systems, it is possible to let the charges in the system develop dynamically.

Since charge dynamics are usually much faster than dynamics of the ions, it is usually reasonable to allow the charges to equilibrate between ionic steps. This does not conserve energy exactly, however, since the charge equilibration drives the system charge distribution towards a lower energy. The energy change in charge redistribution is lost unless it is fed back to the system.

Connecting the structure, calculator and relaxation algorithm

Special care must be taken when setting up links between the atomic structure (ASE Atoms), the calculator (`Pysic`), and the charge relaxation algorithm (`ChargeRelaxation`). While some of the objects must know the others, in some cases the behavior of the simulator changes depending on whether or not they have access to the other objects.

The atoms and the calculator are linked as required in the ASE calculator interface: One can link the two by either the `set_atoms()` method of `Pysic`, or the set_calculator method of ASE Atoms. In either case, the atomic structure

is given a link to the calculator, and a **copy** of the structure is stored in the calculator. This must be done in order to do any calculations on the system.

Also the relaxation algorithm has to know the `Pysic` calculator, since the relaxation is done according to the `Potential` interactions stored in the calculator. The algorithm can be made to know the calculator via the `set_calculator()` method of `ChargeRelaxation`. By default, this does not make the calculator know the relaxation algorithm, however. Only if the optional argument `reciprocal=True` is given the backwards link is also made. `Pysic` can be made to know the relaxation algorithm also by calling the method `set_charge_relaxation()`. Unlike the opposite case, by making the link from the calculator, the backwards link from the relaxation algorithm is always made automatically. In fact, even though linking an algorithm to a calculator does not automatically link the calculator to the algorithm, if a different calculator was linked to the algorithm, the link is automatically removed.

This slightly complicated behavior is summarized as follows: The algorithm should always have a link to a calculator, but a calculator need not have a link to an algorithm. If a calculator does link to an algorithm, the algorithm must link back to the same calculator. Clearly one does not always want to perform charge relaxation on the system and so it makes sense that the calculator need not have a link to a charge relaxation algorithm. If such a link does exist, then the relaxation is *automatically* invoked prior to each energy and force evaluation. This is necessary in simulations such as molecular dynamics (MD). A charge relaxation can be linked to a calculator in order to do charge equilibration, but if one does not wish to trigger the charge relaxation automatically, then it is enough to just not let the calculator know the relaxation algorithm.

The atomic structure cannot be given a link to the relaxation algorithm since the charge relaxation is not part of the ASE API and so the atoms object does not know how to interact with it. In essence, from the point of view of the structure, the charge relaxation is fully contained in the calculator.

The charge relaxation algorithm always acts on the structure contained in the calculator. The atomic charges of this structure are automatically updated during the relaxation. Since the calculator only stores a copy of the original structure, the original is not updated. This may be desired if, for instance, one wishes to revert back to the original charges. However, during strucural dynamics simulations such as MD, it is necessary that the relaxed charges are saved between structural steps. This is a problem, since structural dynamics are handled by ASE, and ASE invokes the calculation of forces with the original ASE Atoms object. Therefore, if the relaxed charges are not saved, charge relaxation is always started from the original charges, which may be very inefficient. In order to have also the original structure updated automatically, the charge relaxation can be made to know the original structure with `set_atoms()`. Note that the structure given to the algorithm is not used in the actual relaxation; the algorithm always works on the structure in the calculator, which may be different. The given structure is merely updated according to the calculation results.

Piping ChargeRelaxation algorithms

Sometimes the most efficient way to optimize a system is to combine several algorithms or several parameterizations of a single algorithm in a sequence. First, one can run a robust but less efficient algorithm to find a rough solution and follow with a more efficient method to pinpoint the optimum at high precision. For a plain relaxation, this can be done manually. However, if the optimization needs to happen automatically, e.g., between molecular dynamics steps, one needs to combine several ChargeRelaxation objects together. This can be done through the method `add_relaxation_pipe()`.

Adding a piped ChargeRelaxation object simply calls the `charge_relaxation()` methods of both objects one after another when relaxation is invoked. Several objects can be piped by recursive piping. For instance, the following:

```
rel1 = ChargeRelaxation(...)
rel2 = ChargeRelaxation(...)
rel3 = ChargeRelaxation(...)

rel1.add_relaxation_pipe(rel2)
rel2.add_relaxation_pipe(rel3)
```

creates a pipe `rel1-rel2-rel3`, where `rel1` is executed first and `rel3` last. Creating looped pipes where the same relaxation appears twice is not allowed.

By default, when a pipe is created, the calculator and structure objects of the first relaxation are copied also to all the piped ChargeRelaxation objects (including recursively defined ones).

Observers

Similarly to ASE molecular dynamics, also the ChargeRelaxation allows one to attach callback functions to the dynamics. That is, one can have a specific functions be automatically invoked at given intervals. This can be used for instance for printing statistics or saving data during the optimization run. For instance, the following example saves and plots the charge of the atom with index 0:

```
system = Atoms(...)
calc = Pysic(...)
rel = ChargeRelaxation(calculator = calc, system = system)

charge0 = []
def save_charge():
    charge0.append(calc.get_atoms().get_charges()[0])

rel.add_observer(save_charge)
rel.charge_relaxation()

import matplotlib.pyplot as plt
plt.plot(np.array(range(len(charge0))), thecharges)
plt.show()
```

List of currently available relaxation methods

Below is a list of the charge relaxation methods currently implemented.

Damped dynamics Assigning an inertia, M_q, on the atomic charges, q_i, we can describe the system with the Lagrangian

$$L = \sum_i \frac{1}{2} m_i \dot{\mathbf{r}}_i^2 + \sum_i \frac{1}{2} M_q \dot{q}_i^2 - U(\{q\}, \{\mathbf{r}\}) - \nu \sum_i q_i,$$

where $m_i, \mathbf{r}_i$ are the mass and position of atom i, respectively. The last term is a Lagrange multiplier corresponding to the constraint of fixed total charge, i.e., $\sum_i q_i = Q_{\mathrm{tot}}$ being constant. The total potential energy U is a function of all charges and positions.

The equations of motion for this system are

$$m_i \ddot{\mathbf{r}}_i = -\nabla_i U \tag{4.12}$$

$$M_q \ddot{q}_i = -\frac{\partial U}{\partial q_i} - \nu. \tag{4.13}$$

In the charge equation, the Lagrange multiplier can be shown to equal the average electronegativity of the system, $\nu = \bar{\chi}$, and the derivative is the effective electronegativity of atom i, $-\frac{\partial U}{\partial q_i} = \chi_i$. Thus, the effective force driving the change in atomic charges is the electronegativity difference from the avarage

$$M_q \ddot{q}_i = -\frac{\partial U}{\partial q_i} - \nu = \chi_i - \bar{\chi} = \Delta\chi_i.$$

In the damped dynamic equilibration, the charges are developed dynamically according to the equation of motion with an added damping (friction) term $-\eta\dot{q}_i$

$$M_q\ddot{q}_i = \Delta\chi_i - \eta\dot{q}_i. \tag{4.14}$$

This leads to the charges being driven towards a state where the driving force vanishes $\Delta\chi_i = 0$, i.e., the electronegativities are equal.

During simulation such as molecular dynamics or geometry optimization, charge equilibration is done by running the damped charge dynamics (4.14) before each force or energy evaluation.

Keywords:

```
>>> names_of_parameters('dynamic')
['n_steps', 'timestep', 'inertia', 'friction', 'tolerance']
```

Potentiostat Similarly to *Damped dynamics*, a potentiostat drives the atomic charges q_i with the dynamics

$$m_i\ddot{\mathbf{r}}_i = -\nabla_i U \tag{4.15}$$

$$M_q\ddot{q}_i = -\frac{\partial U}{\partial q_i} - \Phi. \tag{4.16}$$

Charge equilibration tries to optimize the charge distribution (with fixed total charge) so that the total energy is minimized. The potentiostat, however, connects the system to an electrode (a charge resevoir) at constant potential Φ. This means that the total charge of the system is allowed to change so that the electronegativity of each atom equals the external potential $\chi_i = -\frac{\partial U}{\partial q_i} = \Phi$.

Keywords:

```
>>> names_of_parameters('potentiostat')
['n_steps', 'timestep', 'inertia', 'potential']
```

Optimization This charge optimization method uses the Scipy fmin_slsqp function for constrained optimization using Sequential Least Squares Programming (SLSQP).

Instead of dynamic simulation, the algorithm searches for energy minimum $U(\mathbf{q})$ with the constraint of constant charge $\sum_i q_i = Q$.

As the external function does not support callback functions, observers cannot be attached to this algorithm.

Keywords:

```
>>> names_of_parameters('optimize')
['n_steps', 'tolerance']
```

List of methods

Below is a list of methods in `ChargeRelaxation`, grouped according to the type of functionality.

Initialization

- `initialize_parameters()`
- `get_relaxation()`
- `set_relaxation()`
- `relaxation_modes`

- relaxation_parameter_descriptions
- relaxation_parameters

Atoms handling

- get_atoms()
- set_atoms()

Calculator handling

- get_calculator()
- set_calculator()

Parameter handling

- get_parameters()
- set_parameter_value()
- set_parameter_values()
- set_parameters()

Pipe handling

- clear_relaxation_pipe()
- get_relaxation_pipe()
- set_relaxation_pipe()

Observer handling

- add_observer()
- call_observers()
- clear_observers()

Charge relaxation

- charge_relaxation()

Full documentation of the ChargeRelaxation class

class pysic.charges.relaxation.**ChargeRelaxation**(*relaxation='dynamic'*, *calculator=None*, *parameters=None*, *atoms=None*)

A class for handling charge dynamics and relaxation.

Pysic does not implement molecular dynamics or geometric optimization since they are handled by ASE. Conceptually, the structural dynamics of the system are properties of the atomic geometry and so it makes sense that they are handled by ASE, which defines the atomic structure in the first place, in the ASE Atoms class.

On the other hand, charge dynamics are related to the electronic structure of the system. Since ASE is meant to use methods such as density functional theory (DFT) in the calculators is employs, all electronic properties

are left at the responsibilty of the calculator. This makes sense since in DFT the electron density is needed for calculations of forces and energies.

Pysic is not a DFT calculator and there is no electron density but the atomic charges can be made to develop dynamically. The ChargeRelaxation class handles these dynamics.

Parameters:

relaxation: string a keyword specifying the mode of charge relaxation

calculator: `Pysic` object a Pysic calculator

parameters: list of doubles numeric values for parameters

atoms: ASE Atoms object The system whose charges are to be relaxed. Note! The relaxation is always done using the atoms copy in `Pysic`, but if the original structure needs to be updated as well, the relaxation algorithm must have access to it.

`add_observer` (*function*, *interval=1*, **args*, ***kwargs*)
Attach a callback function.

Call the given function with the given arguments at constant intervals, after a given number of relaxation steps.

Parameters:

function: Python function the function to be called

interval: integer the number of steps between callback

args: string arguments for the callback function

kwargs: string keyword arguments for the callback function

`call_observers` (*step*)
Calls all the attached callback functions.

Parameters:

step: integer the number of dynamics steps taken during the relaxation

`charge_relaxation`()
Performs the charge relaxation.

The relaxation is always performed on the system associated with the `Pysic` calculator joint with this `ChargeRelaxation`. The calculated equilibrium charges are returned as a numeric array.

If an ASE Atoms structure is known by the `ChargeRelaxation` (given through `set_atoms()`), the charges of the structure are updated according to the calculation result. If the structure is not known, the charges are updated in the structure stored in the `Pysic` calculator, but not in any other object. Since `Pysic` only stores a copy of the structure it is given, the original ASE Atoms object will not be updated.

`clear_observers`()
Removes all observers.

`clear_relaxation_pipe`()
Equivalent to set_relaxation_pipe(None).

`get_atoms`()
Returns the atoms object known by the algorithm.

This is the ASE Atoms which will be automatically updated when charge relaxation is invoked.

`get_calculator`()
Returns the `Pysic` calculator assigned to this `ChargeRelaxation`.

get_parameters()
Returns a list containing the numeric values of the parameters.

get_relaxation()
Returns the keyword specifying the mode of relaxation.

get_relaxation_pipe(*recursive=True*)
Return the piped ChargeRelaxation objects.

By default, a list is given containing all the ChargeRelaxation objects in the pipeline (or an empty list).

If called with the argument False, only the ChargeRelaxation next-in-line will be returned (or None).

Parameters:

recursive: boolean If True, will return a list containing all the piped objects. Otherwise, only the next-in-line is returned.

initialize_parameters()
Creates a dictionary of parameters and initializes all values to 0.0.

relaxation_modes = ['dynamic', 'potentiostat', 'optimize']
Names of the charge relaxation algorithms available.

These are keywords needed when creating the ChargeRelaxation objects as type specifiers.

relaxation_parameter_descriptions = {'dynamic': ['number of time steps of charge dynamics between molecul
Short descriptions of the relaxation parameters.

relaxation_parameters = {'dynamic': ['n_steps', 'timestep', 'inertia', 'friction', 'tolerance'], 'optimize': ['n_steps',
Names of the parameters of the charge relaxation algorithms.

set_atoms(*atoms*, *pass_to_calculator=False*)
Lets the relaxation algorithm know the atomic structure to be updated.

The relaxation algorithm always works with the structure stored in the Pysic calculator it knows. If pass_to_calculator = True, this method also updates the structure known by the calculator. However, this is not the main purpose of letting the ChargeRelaxation know the structure - it is not even necessary that the structure known by the relaxation algorithm is the same as that known by the calculator.

The structure given to the algorithm is the structure whose charges it automatically updates after relaxing the charges in charge_relaxation(). In other words, if no structure is given, the relaxation will update the charges in the strucure known by Pysic, but this is always just a copy and so the original structure is left untouched.

Parameters:

atoms: ASE Atoms object The system whose charges are to be relaxed. Note! The relaxation is always done using the atoms copy in Pysic, but if the original structure needs to be updated as well, the relaxation algorithm must have access to it.

pass_to_calculator: logical if True, the atoms are also set for the calculator via set_atoms()

set_calculator(*calculator*, *reciprocal=False*)
Assigns a Pysic calculator.

The calculator is necessary for calculation of electronegativities. It is also possible to automatically assign the charge relaxation method to the calculator by setting reciprocal = True.

Note though that it does make a difference whether the calculator knows the charge relaxation or not: If the Pysic has a connection to the ChargeRelaxation, every time force or energy calculations are requested the charges are first relaxed by automatically invoking charge_relaxation(). If there is no link, it is up to the user to start the relaxation.

Parameters:

calculator: `Pysic` object a Pysic calculator

reciprocal: logical if True, also the `ChargeRelaxation` is passed to the `Pysic` through `set_charge_relaxation()`.

`set_parameter_value`(*parameter_name*, *value*)
Sets a given parameter to the desired value.

Parameters:

parameter_name: string name of the parameter

value: double the new value of the parameter

`set_parameter_values`(*parameters*)
Sets the numeric values for all parameters.

Use get_parameters() to see the correct order of values.

Parameters:

parameters: list of doubles list of values to be assigned to parameters

`set_parameters`(*parameters*)
Sets the numeric values for all parameters.

Equivalent to `set_parameter_values()`

Parameters:

parameters: list of doubles list of values to be assigned to parameters

`set_relaxation`(*relaxation*)
Sets the relaxation method.

The method also creates a dictionary of parameters initialized to 0.0 by invoking `initialize_parameters()`.

Parameters:

relaxation: string a keyword specifying the mode of charge relaxation

`set_relaxation_pipe`(*relaxation*, *pass_info=True*)
Add another `ChargeRelaxation` to take place immediately after this relaxation.

Sometimes it is most efficient to start the relaxation with a robust but possibly slow algorithm and switch to a more advanced one once closer to equilibrium. On the other hand, when relaxation is needed between MD steps, this is not possible manually. Therefore, one can link several ChargeRelaxation objects together to automatically invoke a sequential relaxation procedure.

You should only give one ChargeRelaxation for piping. If you want to pipe more than two relaxation sequences together, you should always link the additional relaxation to the currently final ChargeRelaxation object to create a nested pipeline:

```
rel1 = ChargeRelaxation()
rel2 = ChargeRelaxation()
rel3 = ChargeRelaxation()

rel1.set_relaxation_pipe(rel2)
rel2.set_relaxation_pipe(rel3)

rel1.charge_relaxation() # will do rel1 -> rel2 -> rel3
```

Parameters:

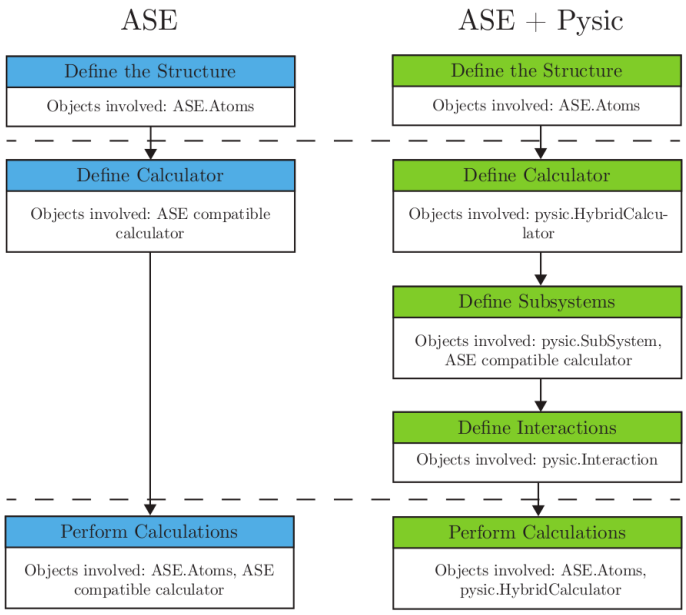
relaxation: `ChargeRelaxation` object the relaxation to be piped after this one

pass_info: boolean If True, the calculator and atoms of this calculator will be automatically copied over to the piped calculator.

HybridCalculator class

The HybridCalculator provides a regular ASE calculator interface, but internally combines results from multiple different calculators and interactions between them. Currently you can use it for potential energy and force calculations (stress calculations not yet implemented). Like with any ASE calculator, you can also run molecular dynamics and local geometry optimizations with it, but global energy optimization schemes that require a stress implementation will naturally not work due to missing stress implementation.

The following figure demonstrates the simplified workflow comparison of a regular ASE calculation vs. Pysic's hybrid QM/MM calculation.



HybridCalculator is meant to be used in conjunction with the classes `SubSystem` and `Interaction`. See also the *run example*.

Mechanical Embedding

The electrostatic interaction between subsystems is treated with the mechanical embedding scheme. The Coulomb interaction is thus calculated in the MM level by assigning point charges for the atoms in the primary and secondary system. The charges in the secondary system are static and can be obtained from experimental data or theoretical calculations. Rather than also parametrizing the charges in the primary system, in Pysic they can be dynamically calculated by using the electron density provided by the DFT calculator. The positive charge of the nuclei can be accurately modeled as an atom-centered point charge. The effect of the negative electron charge density is approximated also as a single atom-centered point charge. The value of this point charge is calculated by integrating the electron charge density inside a certain volume. Primarily Pysic uses the Bader partitioning scheme to determine these volumes, but a spherical partitioning scheme is also available.

Hydrogen links in Pysic

The covalent bonds between subsystems are treated with the link atom approach, i.e. hydrogen atoms are used to cap the bonds in the primary QM system. The hydrogen link atoms are placed on the line connecting the two atoms that form the bond. The exact position of the link atoms in this line can be controlled with the CHL parameter, given when defining the links in `add_hydrogen_links()`. The link atoms automatically keep their correct position when running dynamics or geometry optimization.

List of methods

The following methods form the basis for creating and performing hybrid simulations with HybridCalculator:

- `add_subsystem()`
- `add_interaction()`
- `get_potential_energy()`
- `get_forces()`
- `print_energy_summary()`
- `print_force_summary()`
- `print_time_summary()`
- `print_interaction_charge_summary()`
- `view_subsystems()`

Full documentation of the HybridCalculator class

class `pysic.hybridcalculator.`**`HybridCalculator`**(*atoms=None*)

Used to create and perform hybrid calculations.

This class is a fully compatible ASE calculator that provides the possibility of dividing the Atoms object into subsystems with different ASE calculators attached to them.

You can also define hydrogen link atoms in the interfaces of these subsystems or define any Pysic Potentials through which the subsystems interact with each other.

Attributes:

total_timer: :class:'~pysic.utility.timer.Timer' Keeps track of the total time spent in the calculations.

subsystem_energies: dictionary Name to energy.

subsystems: dictionary Name to SubSystemInternal.

subsystem_interactions: dictionary Pair of names to InteractionInternal.

subsystem_info: dictionary Name to SubSystem.

interaction_info: dictionary Pair of names to Interaction.

forces: numpy array

-

stress: None

-

potential_energy: float

-

system_initialized: bool Indicates whether the SubSystemInternals and InteractionInternals have been constructed.

self.atoms: ASE Atoms The full system.

add_interaction(*interaction*)
Used to add a interaction between two subsystems.

Parameters:

interaction: Interaction The Interaction object containing the information.

add_subsystem(*subsystem*)
Used to define subsystems

You can define a subsystem with a oneliner, or then call setters on the SubSystemInfo object returned by this function.

Parameters: subsystem: SubSystem object

calculate_forces()
Calculates the forces in the current structure.

This force includes the forces internal to the subsystems and the forces that bind the subsystems together.

calculate_potential_energy()
Calculates the potential energy in the current structure.

calculate_subsystem_interaction_charges(*name*)
Returns the calculated interaction charges for the given subsystem.

Before the charges can be calulated, one energy calculation has to be made so that the electron density is available

calculation_required(*atoms, quantities=['forces', 'energy', 'stress']*)
Check if a calculation is required for any of the the given properties.

Check if the quantities in the quantities list have already been calculated for the atomic configuration atoms. The quantities can be one or more of: 'energy', 'forces', 'stress'. This method is used to check if a quantity is available without further calculations. For this reason, calculators should react to unknown/unsupported quantities by returning True, indicating that the quantity is not available.

Two sets of atoms are considered identical if they have the same positions, atomic numbers, unit cell and periodic boundary conditions.

Parameters:

atoms: ASE Atoms This structure is compared to the currently stored.

quantities: list of strings list of keywords 'energy', 'forces', 'stress'

Returns: bool: True if the quantities need to be calculated, false otherwise.

check_subsystem_indices(*atom_indices*, *name*)
Check that the atomic indices of the subsystem are present.

check_subsystem_overlap(*atom_indices*, *name*)
Check that the subsystem doesn't overlap with another one.

full_system_set()
Checks whether the full system has been defined.

generate_subsystem_indices(*name*)
Generates the indices for the given subsystem.

get_atoms()
Return a copy of the full system.

get_colors()
Returns a color set for AtomEyeViewer with different colours for the different subsystems.

When the subsystems have been defined with add_subsystem() and the atoms have been set, this function will return a list of colors for each atom. The different subsystems have different colours for easy identification. You can provide this list of colors to an AtomEyeViewer object for visualization.

get_forces(*atoms=None*)
Returns the forces acting on the atoms.

If the atoms parameter is given, it will be used for updating the structure assigned to the calculator prior to calculating the forces. Otherwise the structure already associated with the calculator is used.

The calculator checks if the forces have been calculated already via `calculation_required()`. If the structure has changed, the forces are calculated using `calculate_forces()`

Parameters:

atoms: ASE Atoms object The structure to calculate the forces on.

get_potential_energy(*atoms=None*, *force_consistent=False*)
Returns the potential energy of the hybrid system.

get_stress(*atoms=None*, *skip_charge_relaxation=False*)
This function has not been implemented.

get_subsystem(*name*)
Returns a copy of the ASE Atoms object for a certain subsystem.

The returned subsystem can be used for e.g. visualization or debugging.

get_subsystem_indices(*name*)
Return the indices of the atoms in the subsystem in the full system.

You can ask the indices even if the subsystems have not been initialized, but the indices of different subsystems may overlap in this case. If the subsystems have been initialized this function will only return indices if they are valid.

get_subsystem_pseudo_density(*name*)
Returns the electron pseudo density for the given subsystem.

get_unsubsystemized_atoms()
Return a list of indices for the atoms not already in a subsystem.

identical_atoms(*atoms*)
Compares the given atoms to the stored atoms object. The Atoms are identical if the positions, atomic numbers, periodic boundary conditions and cell are the same.

initialize_interaction(*info*)
Initializes a InteractionInternal from the given Interaction.

Parameters: info: Interaction

initialize_subsystem(*info*)
Initializes a SubsystemInternal from the given Subsystem.

Parameters: info: SubSystem

initialize_system()
Initializes the subsystems and interactions.

Called once during the lifetime of the calculator. Typically when calling set_atoms for the first time, or when calculating any quantity for the first time. If the atoms in the simulation need to be updated, update_system() is used.

print_energy_summary()
Print a detailed summary of the different energies in the system. This includes the energies in the subsystems, interaction energies and possible energy corrections.

print_force_summary()
Print a detailed summary of forces in the system.

print_interaction_charge_summary()
Print a summary of the atomic charges that are used in the electrostatic interaction between subsystems.

print_time_summary()
Print a detailed summary of the time usage.

set_atoms(*atoms*)
Set the full system for hybrid calculations.

Use `add_subsystem()` for setting up the subsystems.

Parameters:

atoms: ASE Atoms The full system.

subsystem_defined(*name*)
Checks that there is a subsystem with the given name.

update_system(*atoms*)
Update the subsystem atoms.

view_subsystems()
Views the subsystems with ASE:s built in viewer.

Subsystem class

The SubSystem class works as an interface for defining subsystems in hybrid simulations. Through it you can define the atoms that belong to the subsystem and the calculator that is used for it. SubSystem objects also provides special options for QM subsystems: you can setup dynamical charge calculation with `enable_charge_calculation()` and cell optimization with `enable_cell_optimization()`.

You can define the atoms in the subsystem as a list of indices, with a tag or with a special string: "remaining", which means all the atoms that are not yet assigned to a subsystem.

Full documentation of the Subsystem class

class pysic.subsystem.**SubSystem**(*name*, *indices=None*, *tag=None*, *calculator=None*)
Used to create and store information about a subsystem.

The end user can create and manipulate these objects when defining subsystems. The subsystems are added to the calculation by calling `add_subsystem()` which adds a SubSystem-object to the calculation.

When the HybridCalculator sees fit, the subsystems are materialized by converting the stored SubSystems into SubSystemInternals.

Attributes:

name: string The unique name for this subsystem.

calculator: ASE Calculator The calculator used.

cell_size_optimization_enabled: bool

-

cell_padding: float The padding used when optimizing the cell size.

charge_calculation_enabled: bool

-

charge_source: string Indicates the electron density that is used in charge calculation. Can be "pseudo" or "all-electron".

division: string Indicates the division algorithm used in charge caluclation. Can be "Bader" or "van Der Waals".

gridrefinement: int The factor by which the calculation grid is densified in charge calculation.

indices: list of ints

-

tag: int

-

enable_cell_optimization(*padding*)
Enable cell size optimization.

A subsystem might spatially reside in only a small portion of the entire system. DFT calculators will then waste time doing calculations in empty space, where almost none of electron density reaches.

This optimization minimizes the cell size, so that the atoms in the subsystem fit the cell with the given padding. If the padding is too small, the DFT-calculator might not work properly!

The optimization is off by default. It cannot be turned on in systems with periodic boundary conditions. The new optimized cell is always ortorhombic, regardless of the shape of the original, unoptimized cell.

Parameters:

padding: float The minimum distance between the subsystem atoms and the cell walls.

enable_charge_calculation(*division='Bader'*, *source='all-electron'*, *gridrefinement=4*)
Enable the dynamic calculation of atom-centered charges with the specified algorithm and from the specified electron density. These charges are only used for the interaction between other subsystems.

Parameters:

division: string Indicates the division algorithm that is used. Available options are:

- "Bader": Bader algorithm
- "van Der Waals": Spheres with van Der Waals radius

source: string Indicates what type of electron density is used. Available options are:

- "pseudo": Use the pseudo electron density provided by all ASE DFT calculators
- "all-electron": Use the all-electron density provided by at least GPAW

gridrefinement: int Indicates the subdivision that is used for the all-electron density. Can be other than unity only for Bader algorithm with all-electron density.

is_valid(*indices*, *tag*)
Checks that the given atom specifiers are correctly given. Does not yet check that they exist or don't overlap with other subssystems.

set_atoms(*indices=None*, *tag=None*)
Set the atoms that belong to this subsystem. Give only one of the specifiers: indices or tag.

Parameters:

indices: list of integers or string A list of atom indices or a special string "remaining", which assigns all the yet unassigned atoms to this subsystem.

tag: int The atoms with this tag belong to this subsystem.

set_calculator(*calculator*)
Set the calculator for the subsystem.

Parameters: calculator: ASE compatible calculator

SubSystemInternal class This class is meant for internal use only.

Full documentation of the SubSystemInternal class

class pysic.subsystem.**SubSystemInternal**(*atoms*, *info*, *index_map*, *reverse_index_map*, *n_atoms*)
A materialization of a SubSystem object.

This class is materialised from a SubSystem, and should not be accessible to the end user.

Attributes:

name: string The unique name for this subsystem.

calculator: ASE Calculator The calculator used.

cell_size_optimization_enabled: bool

-

cell_padding: float

-

charge_calculation_enabled: bool

-

charge_source: string

-

division: string

-

gridrefinement: int

-

n_atoms: int Number of atoms in the full system.

atoms_for_interaction: ASE Atoms The copy of subsystems atoms used in interaction calculations.

atoms_for_subsystem: ASE Atoms The copy of subsystems atoms used in calculating subsystem energies etc.

index_map: dictionary of int to int The keys are the atom indices in the full system, values are indices in the subssystem.

reverse_index_map: dicitonary of int to int The keys are the atom indices in the subsystem, values are the keys in the full system.

potential_energy: float

-

forces: numpy array

-

density_grid: numpy array Stored if spherical division is used in charge calculation.

pseudo_density: numpy array

-

link_atom_indices: list

-

timer: :class:'~pysic.utility.timer.Timer' Used to keep track of time usage.

get_forces()
Returns a 3D numpy array that contains forces for this subsystem.

The returned array contains a row for each atom in the full system, but there is only an entry for the atoms in this subsystem. This makes it easier to calculate the total forces later on.

get_potential_energy()
Returns the potential energy contained in this subsystem.

get_pseudo_density()
Returns the electron pseudo density if available.

optimize_cell()
Tries to optimize the cell of the subsystem so only the atoms in this subsystem fit in it with the defined padding to the edges. The new cell is always ortorhombic.

update_charges()
Updates the charges in the system. Depending on the value of self.division, calls either update_charges_bader(), or update_charges_van_der_waals()

update_charges_bader()
Updates the charges in the atoms used for interaction with the Bader algorithm.

This function uses an external Bader charge calculator from http://theory.cm.utexas.edu/henkelman/code/bader/. This tool is provided also in pysic/tools. Before using this function the bader executable directory has to be added to PATH.

update_charges_van_der_waals()
Updates the atomic charges by using the electron density within a sphere of van Der Waals radius.

The charge for each atom in the system is integrated from the electron density inside the van Der Waals radius of the atom in hand. The link atoms will affect the distribution of the electron density.

update_density_grid()
Precalculates a grid of 3D points for the charge calculation with van Der Waals radius.

Interaction class

The Interaction class works as an interface for defining interactions and link atoms between subsystems in hybrid calulations. With the methods `add_potential()`, `set_potentials()`, `enable_coulomb_potential()` and `enable_comb_potential()` you can define the Pysic Potentials that are present between the subsystems. With `add_hydrogen_links()` you can setup the hydrogen link atoms.

Full documentation of the Interaction class

class `pysic.interaction.`**`Interaction`**(*primary*, *secondary*)

Used to store information about a interaction between subsystems.

The end user can create and manipulate these objects when defining interactions between subsystems. The interactions between subsystems are added to the calculation by calling `add_interaction()` which adds a Interaction object to the calculation.

When the HybridCalculator sees fit, the subsystem bindings are materialized by converting the stored Interactions to InteractionInternals.

Attributes:

primary: string Name of the primary subsystem.

secondary: string Name of the secondary subsystem.

links: list of tuples Contains a list of different link types. Each list item is a tuple with two items: the first is a list of link pairs, the second one is the CHL parameter for these links.

electrostatic_parameters: dictionary Contains all the parameters used for creating a Coulomb potential.

coulomb_potential_enabled: bool

-

comb_potential_enabled: bool

-

link_atom_correction_enabled: bool

-

potentials: list of `Potential`

-

`add_hydrogen_links`(*pairs*, *CHL*)

Defines hydrogen links in the system.

Parameters:

pairs: tuple or list of tuples A set of tuples containing two indices, the first index in the tuple should point to the subsystem in which the hydrogen link atom is actually added to (=primary system).

CHL: float Indicates the position of the hydrogen atom on the line defined by the atom pairs. Values should be between 0-1. 0 means that the link atom overlaps with the atom in the primary system, 1 means that the link atom overlaps with the atom in the secondary system. The scale is linear.

`add_potential`(*potential*)

Used to add a Pysic potential between the subsystems.

Parameters: potential: `Potential`

enable_comb_potential()
Enable the COMB potential between the subsystems. Valid for Si-Si and Si-O interactions.

enable_coulomb_potential(*epsilon=0.00552635*, *real_cutoff=None*, *k_cutoff=None*, *sigma=None*)
Enables the electrical Coulomb interaction between the subsystems.

Parameters:

epsilon: float The vacumm permittivity. Has a default value from the literature, in Atomic units.

r_cutoff: float Real space cutoff radius. Provide if system has periodic boundary conditions.

k_cutoff: float Reciprocal space cutoff radius. Provide if system has periodic boundary conditions.

sigma: float Ewald summation split parameter. Provide if system has periodic boundary conditions.

set_link_atom_correction(*value*)
Sets whether the link interaction correction energy is calculated or not.

By default the correction is enabled, but you have to provide a secondary calculator that can calculate the interaction energies between the link atoms themselves and between link atoms and the primary system.

The link atom correction is defined as: .. math:

```
E^  ext{link} &= - E^       ext{int}_       ext{MM} ext{(PS, HL)} - E^      ext{tot}_
```

set_potentials(*potentials*)
Used to set a list of additional Pysic potentials between the subsystems.

Parameters: potentials: list of or single `Potential`

InteractionInternal class This class is meant for internal use only.

Full documentation of the InteractionInternal class

class pysic.interaction.**InteractionInternal**(*full_system*, *primary_subsystem*, *secondary_subsystem*, *info*)
The internal version of the Interaction-class.

This class is meant only for internal use, and should not be accessed by the end-user.

Attributes:

info: :class:'~Pysic.interaction.Interaction' Contains all the info about the interaction given by the user.

full_system: ASE Atoms

-

primary_subsystem: SubSystem

-

secondary_subsystem: SubSystem

-

uncorrected_interaction_energy: float The interaction energy without the link atom correction.

uncorrected_interaction_forces: numpy array The interaction forces without the link atom correction.

link_atom_correction_energy: float

-

link_atom_correction_forces: numpy array

-

interaction_energy: float The total interaction energy = uncorrected_interaction_energy + link_atom_correction_energy

interaction_forces: numpy array The total interaction forces = uncorrected_interaction_forces + link_atom_correction_forces

has_interaction_potentials: bool True if any potentials are defined.

calculator: :class:'~pysic.calculator.Pysic' The pysic calculator used for non-pbc systems.

pbc_calculator: :class:'~pysic.calculator.Pysic' The pysic calculator used for pbc systems.

timer: :class:'~pysic.utility.timer.Timer' Used for tracking time usage.

has_pbc: bool

-

link_atoms: ASE Atoms Contains all the hydrogen link atoms. Needed when calculating link atom correction.

n_primary: int Number of atoms in primary subsystem.

n_secondary: int Number of atoms in secondary subsystem.

n_full: int Number of atoms in full system.

n_links: int Number of link atoms.

calculate_link_atom_correction_energy()
Calculates the link atom interaction energy defined as

$$E^{\text{link}} = -E^{\text{tot}}_{\text{MM}}(\text{HL}) - E^{\text{int}}_{\text{MM}}(\text{PS, HL})$$

calculate_link_atom_correction_forces()
Calculates the link atom correction forces defined as

$$F^{\text{link}} = -\nabla(-E^{\text{tot}}_{\text{MM}}(\text{HL}) - E^{\text{int}}_{\text{MM}}(\text{PS, HL}))$$

calculate_uncorrected_interaction_energy()
Calculates the interaction energy of a non-pbc system without the link atom correction.

calculate_uncorrected_interaction_energy_pbc()
Calculates the interaction energy of a pbc system without the link atom correction.

calculate_uncorrected_interaction_forces()
Calculates the interaction forces of a non-pbc system without the link atom correction.

calculate_uncorrected_interaction_forces_pbc()
Calculates the interaction forces of a pbc system without the link atom correction.

get_interaction_energy()
Returns the total interaction energy which consists of the uncorrected energies and possible the link atom correction.

Returns: float: the interaction energy

get_interaction_forces()
Return a numpy array of total 3D forces for each atom in the whole system.

The forces consists of the uncorrected forces and possibly the link atom correction forces. The row index refers to the atom index in the original structure.

Returns: numpy array: the forces for each atom in the full system

setup_comb_potential()
Setups a COMB-potential between the subsystems.

setup_coulomb_potential()
Setups a Coulomb potential between the subsystems.

Ewald calculation is automatically used for pbc-systems. Non-pbc systems use the ProductPotential to reproduce the Coulomb potential.

setup_hydrogen_links(*links*)
Setup the hydrogen link atoms to the primary system.

Parameters:

link_parameters: list of tuples Contains the link atom parameters from the Interaction-object. Each tuple in the list is a link atom specification for a covalent bond of different type. The first item in the tuple is a list of tuples containing atom index pairs. The second item in the tuple is the CHL parameter for these links.

setup_potentials()
Setups the additional Pysic potentials given in the Interaction-object.

update_hydrogen_link_positions()
Used to update the position of the hydrogen link atoms specified in this interaction

It is assumed that the position of the host atoms have already been updated.

update_subsystem_charges()
Updates the charges in the subsystems involved in the interaction (if charge update is enabled in them).

FastNeighborList class

This class extends the ASE NeighborList class to provide a more efficient neighbor finding tool. The neighbor finding routine searches the neighborhoods of all atoms and for each atom records which other atoms are closer than a given cutoff distance.

The benefit of neighbor lists

Atomistic pair and many-body potentials typically depend on the local atomic structure and especially the relative coordinates of the atoms. However, finding the separation vector and distance between coordinates in periodic 3D space is computationally fairly costly operation and the number of atom-atom pairs in the system grows as $\mathcal{O}(n^2)$. Therefore the evaluation of local potentials can be made efficient by storing lists of nearby atoms for all particles to narrow down the scope of search for interacting neighbors.

Typically one chooses a cutoff distance r_{cut} beyond which the atoms do not see each other. Then, the neighbor lists should always contain all the atoms within this cutoff radius $r_{ij} \leq r_{\mathrm{cut}}$. In dynamic simulations where the atoms move, the typical scheme is to list atoms within a slightly longer radius, $r_{\mathrm{cut}} + r_{\mathrm{skin}}$ because then the lists need not be updated until an atom has moved by more than r_{skin}.

The skin width is a static variable of `FastNeighborList`, which you can directly change with:

```
new_skin_width = 1.0
pysic.calculator.FastNeighborList.neighbor_marginal = new_skin_width
```

The currently set default value is automatically used when `Pysic` needs to build the neighbor list.

Faster neighbor search

There is a built in neighbor searching tool in ASE, ASE NeighborList. It is, however, a pure Python implementation using a brute-force $\mathcal{O}(n^2)$ algorithm making it slow - even prohibitively slow - for large systems especially when periodic boundary conditions are used.

To overcome this performance bottleneck, Pysic implements the `FastNeighborList` class. This class inherits other properties from the built-in ASE class except for the `build()` method, which is replaced by a faster algorithm. The fast neighbor search is implemented in Fortran and parallelized with MPI. The algorithm is based on a spatial divisioning, i.e.

- the simulation volume is divided in subvolumes
- for each atom the subvolume where it is contained is found
- for each atom, the neighbors are searched for only in the adjacent subvolumes

For a fixed cutoff, the neighborhood searched for each atom is constant and thus this is an $\mathcal{O}(n)$ algorithm. [4] The method is also faster the shorter the cutoffs are. For short cutoffs (~ 5 Å), a 10000 atom periodic system is expected to be handled 100 or even 1000 fold faster with `FastNeighborList` than with the ASE method.

Limitations in the implementation

Since the fast algorithm is implemented in Fortran, it operates on the structure allocated in the Fortran core. Therefore, even though the `build()` method takes an ASE Atoms object as an argument, it does not analyze the given structure. It does check against `CoreMirror` to see if the given structure matches the one in the core and raises an error if not, but accessing the core has to still be done through `Pysic`. When `Pysic` is run normally, this is automatically taken care of. As the implementation is MPI parallelized, it is also necessary that the MPI environment has been set up - especially the distribution of load (i.e. atoms) between processors must be done before the lists can be built.

Another more profound limitation in the current implementation of the algorithm is the fact that it limits the neighbor finding to neighboring subvolumes. Since the subvolumes are not allowed to be larger than the actual simulation volume, the cutoffs cannot be longer than the shortest perpendicular separation between facets of the subvolume. For rectangular cells, this is just the minimum of the lengths of the vectors spanning the cell, $\mathbf{v}_{i,j,k}$. For inclined cell shapes, the perpendicular distance between cell facets, d, is

$$d_i = \frac{|\mathbf{v}_i \cdot \mathbf{n_i}|}{|\mathbf{n}_i|} \tag{4.17}$$

$$\mathbf{n}_i = \mathbf{v}_j \times \mathbf{v}_k \tag{4.18}$$

where $\mathbf{n}_i$ are the normal vectors of the plane spanned by the vectors $\mathbf{v}_{j,k}$. If one wishes to find neighbors in a radius containing the simulation volume several times, the original ASE NeighborList should be used instead. `Pysic` does this choice automatically when building the neighbor lists. One should usually avoid such long cutoffs in the first place, but if your system is very small that may not be possible.

Accessing neighbor lists

Although the neighbor lists are automatically used by the calculator, it is also possible to use the list for manually analysing local atomic neighborhoods. This can be done with the methods

- `get_neighbors()`
- `get_neighbor_separations()`

[4] For very large systems the number of subdivisions is limited to conserve memory so the $\mathcal{O}(n)$ scaling is eventually lost. Say we divide the volume in a hundred subvolumes along each axis; we end up with a million subvolumes which is a lot!

- get_neighbor_distances()

which list, for a specified atom, the indices and periodic boundary offsets of neighbors (cf. get_neighbors of the ASE neighbor list), separation vectors, and separation distances, respectively. The arrays can also be requested pre-sorted according to the atom-atom distance by providing the keyword `sort=True`.

Since the lists are created in the Fortran core according to specified interaction cutoffs, it is unfortunately not possible to inquire the neighbors within arbitrary radii without touching the potentials. Normally the lists contain the atoms which interact. In order to just analyse structures, a dummy calculator needs to be created:

```
system = ase.Atoms(...)

# create a dummy calculator
dummy = pysic.Pysic()
# Find neighbors at distance 3.0 + 0.5 (0.5 is the default marginal).
# Note that the list finds all neighbors within the maximum interaction
# radius of the particular atom.
pot = pysic.Potential('LJ', cutoff=3.0, symbols=...)
dummy.add_potential(pot)
system.set_calculator(dummy)
# It is important to manually initialize the core since no actual calculations are carried out.
dummy.set_core()

# get the list and access its contents
nbl = dummy.get_neighbor_list()
neighbors, offsets = nbl.get_neighbors(0, system, True)
separations = nbl.get_neighbor_separations(0, system, True)
distances = nbl.get_neighbor_distances(0, system, True)
```

Methods inherited from ASE NeighborList

- update

List of methods

- build()
- get_neighbors()
- get_neighbor_separations()
- get_neighbor_distances()

Full documentation of the FastNeighborList class

class pysic.calculator.**FastNeighborList**(*cutoffs*, *skin=None*)

ASE has a neighbor list class built in, ASE NeighborList, but its implementation is currently inefficient, and building of the list is an $O(n^2)$ operation. This neighbor list class overrides the build() method with an $O(n)$ time routine. The fast routine is based on a spatial partitioning algorithm.

The way cutoffs are handled is also somewhat different to the original ASE list. In ASE, the distances for two atoms are compared against the sum of the individual cutoffs + neighbor list skin. This list, however, searches for the neighbors of each atom at a distance of the cutoff of the given atom only, plus skin.

build(*atoms*)

Builds the neighbor list.

The routine requires that the given atomic structure matches the one in the core. This is because the method invokes the Fortran core to do the neighbor search. The method overrides the similar method in the original ASE neighborlist class, which directly operates on the given structure, so this method also takes the atomic structure as an argument. However, in order to keep the core modification routines in the `Pysic` class, this method does not change the core structure. It does raise an error if the structures do not match, though.

The neighbor search is done via the `generate_neighbor_lists()` routine. The routine builds the neighbor list in the core, after which the list is fed back to the `FastNeighborList` object by looping over all atoms and saving the lists of neighbors and offsets.

Parameters:

atoms: ASE Atoms object the structure for which the neighbors are searched

get_neighbor_distances (*index*, *atoms*, *sort=False*)
Returns a list of atom-atom distances between the given atom and its neighbors.

Parameters:

index: integer the index of the central atom

atoms: ASE Atoms the atoms object containing the absolute coordinates

sort: boolean if True, the list will be sorted according to distance

get_neighbor_separations (*index*, *atoms*, *sort=False*)
Returns an array of atom-atom separation vectors between the given atom and its neighbors.

Parameters:

index: integer the index of the central atom

atoms: ASE Atoms the atoms object containing the absolute coordinates

sort: boolean if True, the list will be sorted according to distance

get_neighbors (*index*, *atoms=None*, *sort=False*)
Returns arrays containing the indices and offsets of the neighbors of the given atom.

Overrides the method in ASE NeighborList.

Parameters:

index: integer the index of the central atom

atoms: ASE Atoms the atoms object containing the absolute coordinates - needed only if sorting is necessary

sort: boolean if True, the list will be sorted according to distance

neighbor_marginal = 0.5
Default skin width for the neighbor list

CoreMirror class

CoreMirror is a Python representation of the Fortran core. When running pysic, it is intended that a single instance of CoreMirror exists, created automatically when importing `pysic` as the `core` object in `Pysic`.

Whenever changes are made in the Fortran core, they should also be reflected in the CoreMirror. This way one has always easy access to the state of the Fortran core without having to directly access the core and parse the data.

Normally, the user should not touch the CoreMirror directly. It is automatically handled through `Pysic`.

List of Methods

- atoms_ready() (meant for internal use)
- cell_ready() (meant for internal use)
- charges_ready() (meant for internal use)
- coulomb_summation_ready() (meant for internal use)
- get_atoms() (meant for internal use)
- neighbor_lists_ready() (meant for internal use)
- potentials_ready() (meant for internal use)
- set_atomic_momenta() (meant for internal use)
- set_atomic_positions() (meant for internal use)
- set_atoms() (meant for internal use)
- set_cell() (meant for internal use)
- set_charges() (meant for internal use)
- set_coulomb() (meant for internal use)
- set_neighbor_lists() (meant for internal use)
- set_potentials() (meant for internal use)
- view_fortran() (for testing)

Full documentation of the CoreMirror class

class pysic.core.**CoreMirror**

A class representing the status of the core.

Whenever data is being passed over to the core for calculation, it should also be saved in the CoreMirror. This makes the CoreMirror reflect the current status of the core. Then, when something needs to be calculated, the Pysic calculator can simply check that it contains the same system as the CoreMirror to ensure that the core operates on the correct data.

All data given to CoreMirror is saved as deep copies, i.e., not as the objects themselves but objects with exactly the same contents. This way if the original objects are modified, the ones in CoreMirror are not. This is the proper way to work, since the Fortran core obviously does not change without pushing the changes in the Python side to the core first.

Since exactly one CoreMirror should exist during the simulation, deletion of the instance (which should happen at program termination automatically) will automatically trigger release of memory in the Fortran core as well as termination of the MPI framework.

atoms_ready(*atoms*)

Checks if the positions and momenta of the given atoms match those in the core.

True is returned if the structures match, False otherwise.

Parameters:

atoms: ASE Atoms object The atoms to be compared.

cell_ready (*atoms*)
Checks if the given supercell matches that in the core.

True is returned if the structures match, False otherwise.

Parameters:

atoms: ASE Atoms object The cell to be compared.

charges_ready (*atoms*)
Checks if the charges of the given atoms match those in the core.

True is returned if the charges match, False otherwise.

Parameters:

atoms: ASE Atoms object The atoms to be compared.

coulomb_summation_ready (*coulomb*)
Checks if the given Coulomb summation matches that in the core.

True is returned if the summation algorithms match, False otherwise.

Parameters: CoulombSummation the summation algorithm to be compared

get_atoms ()
Returns the ASE Atoms structure stored in the CoreMirror.

neighbor_lists_ready (*lists*)
Checks if the given neighbor lists match those in the core.

True is returned if the structures match, False otherwise.

Parameters:

atoms: ASE NeighborList object The neighbor lists to be compared.

potentials_ready (*pots*)
Checks if the given potentials match those in the core.

True is returned if the potentials match, False otherwise.

Parameters:

atoms: list of Potential objects The potentials to be compared.

set_atomic_momenta (*atoms*)
Copies and stores the momenta of atoms in the ASE Atoms instance.

Parameters:

atoms: ASE Atoms object atomic structure containing the momenta to be saved.

set_atomic_positions (*atoms*)
Copies and stores the positions of atoms in the ASE Atoms instance.

Parameters:

atoms: ASE Atoms object atomic structure containing the positions to be saved.

set_atoms (*atoms*)
Copies and stores the entire ASE Atoms instance.

Parameters:

atoms: ASE Atoms object atomic structure to be saved

set_cell (*atoms*)
Copies and stores the supercell in the ASE Atoms instance.

Parameters:

atoms: ASE Atoms object atomic structure containing the supercell to be saved.

set_charges (*charges*)
Copies and stores the charges of atoms in the ASE Atoms instance.

Parameters:

atoms: ASE Atoms object atomic structure containing the positions to be saved.

set_coulomb (*coulomb*)
Copies and stores the Coulomb summation algorithm.

Parameters:

coulomb: CoulombSummation Coulomb summation algorithm to be saved

set_neighbor_lists (*lists*)
Copies and stores the neighbor lists.

Parameters:

atoms: ASE NeighborList object Neighbor lists to be saved.

set_potentials (*potentials*)
Copies and stores Potential potentials.

The Potential instances are copied as a whole, so any possible Coordinator and BondOrderParameters objects are also stored.

Parameters:

atoms: list of Potential objects Potentials to be saved.

view_fortran ()
Print some information on the data allocated in the Fortran core.

This is mainly a debugging utility for directly seeing the status of the core. It can be accessed through:

```
>>> pysic.Pysic.core.view_fortran()
```

The result is a bunch of data dumped to stdout. The function does not return anything.

4.2.2 List of methods

Below is a list of methods in pysic.

Potential and bond order factor inquiry

- list_potentials()
- list_valid_potentials()
- is_potential()
- is_valid_potential()
- list_bond_order_factors()
- list_valid_bond_order_factors()

- is_bond_order_factor()
- is_valid_bond_order_factor()
- number_of_targets()
- number_of_parameters()
- names_of_parameters()
- index_of_parameter()
- descriptions_of_parameters()
- description_of_potential()

Charge relaxation inquiry

- is_valid_charge_relaxation()
- is_charge_relaxation()

Message Parsing Interface

- finish_mpi()
- get_number_of_cpus()
- get_cpu_id()

4.2.3 Functions of the pysic module

The module defines a group of functions to directly access the Fortran core for information on available potentials.

pysic.**list_potentials**()
Same as list_valid_potentials()

pysic.**list_valid_potentials**()
A list of names of potentials currently known by the core.

The method retrieves from the core a list of the names of different potentials currently implemented. Since the fortran core is directly accessed, any updates made in the core source code should get noticed automatically.

pysic.**is_potential**(*potential_name*)
Same as is_valid_potential()

Parameters:

potential_name: string the name of the potential

pysic.**is_charge_relaxation**(*relaxation_name*)
Same as is_valid_charge_relaxation()

Parameters:

relaxation_name: string the name of the relaxation mode

pysic.**is_valid_charge_relaxation**(*relaxation_name*)
Tells if the given string is the name of a charge relaxation mode.

Parameters:

relaxation_name: string the name of the relaxation mode

pysic.**is_valid_potential**(*potential_name*)
Tells if the given string is the name of a potential.

Parameters:

potential_name: string the name of the potential

pysic.**list_bond_order_factors**()
Same as `list_valid_bond_order_factors()`

pysic.**list_valid_bond_order_factors**()
A list of names of bond order factors currently known by the core.

The method retrieves from the core a list of the names of different bond factors currently implemented. Since the fortran core is directly accessed, any updates made in the core source code should get noticed automatically.

pysic.**is_bond_order_factor**(*bond_order_name*)
Same as `is_valid_bond_order_factor()`

Parameters:

bond_order_name: string the name of the bond order factor

pysic.**is_valid_bond_order_factor**(*bond_order_name*)
Tells if the given string is the name of a bond order factor.

Parameters:

bond_order_name: string the name of the bond order factor

pysic.**number_of_targets**(*potential_name*)
Tells how many targets a potential or bond order factor acts on, i.e., is it pair or many-body.

Parameters:

potential_name: string the name of the potential or bond order factor

pysic.**number_of_parameters**(*potential_name*, *as_list=False*)
Tells how many parameters a potential, bond order factor, charge relaxation mode or coulomb summation mode incorporates.

A potential has a simple list of parameters and thus the function returns by default a single number. A bond order factor can incorporate parameters for different number of targets (some for single elements, others for pairs, etc.), and so a list of numbers is returned, representing the number of single, pair etc. parameters. If the parameter 'as_list' is given and is True, the result is a list containing one number also for a potential.

Parameters:

potential_name: string the name of the potential or bond order factor

as_list: logical should the result always be a list

pysic.**names_of_parameters**(*potential_name*)
Lists the names of the parameters of a potential, bond order factor, charge relaxation mode or coulomb summation mode.

For a potential, a simple list of names is returned. For a bond order factor, the parameters are categorised according to the number of targets they apply to (single element, pair, etc.). So, for a bond order factor, a list of lists is returned, where the first list contains the single element parameters, the second list the pair parameters etc.

Parameters:

potential_name: string the name of the potential or bond order factor

pysic.**index_of_parameter**(*potential_name*, *parameter_name*)
Tells the index of a parameter of a potential or bond order factor in the list of parameters the potential uses.

For a potential, the index of the specified parameter is given. For a bond order factor, a list of two integers is given. These give the number of targets (single element, pair etc.) the parameter is associated with and the list index.

Note especially that an index is returned, and these start counting from 0. So for a bond order factor, a parameter for pairs (2 targets) will return 1 as the index for number of targets.

Parameters:

potential_name: string the name of the potential or bond order factor

parameter_name: string the name of the parameter

pysic.**descriptions_of_parameters**(*potential_name*)
Returns a list of strings containing physical names of the parameters of a potential, bond order factor, or charge relaxation mode, e.g., 'spring constant' or 'decay length'.

For a potential, a simple list of descriptions is returned. For a bond order factor, the parameters are categorised according to the number of targets they apply to (single element, pair, etc.). So, for a bond order factor, a list of lists is returned, where the first list contains the single element parameters, the second list the pair parameters etc.

Parameters:

potential_name: string the name of the potential or bond order factor

pysic.**description_of_potential**(*potential_name*, *parameter_values=None*, *cutoff=None*, *elements=None*, *tags=None*, *indices=None*)
Prints a brief description of a potential.

If optional arguments are provided, they are incorporated in the description. That is, by default the method describes the general features of a potential, but it can also be used for describing a particular potential with set parameters.

Parameters:

potential_name: string the name of the potential

pysic.**finish_mpi**()
Terminates the MPI framework.

If the Fortran core is compiled in MPI mode, pysic will automatically initialize MPI upon being imported. This method terminates the MPI.

pysic.**get_number_of_cpus**()
Gets the number of cpus from the Fortran MPI.

pysic.**get_cpu_id**()
Gets the cpu ID from the Fortran MPI.

4.3 Pysic Utility modules

Modules for providing utility tools and parameters.

4.3.1 Plot

The plot utility defines a group of tools for exploring and plotting energy and force landscapes. It uses the matplotlib library.

pysic.utility.plot.**plot_abs_force_on_line**(*index, system, direction=None, length=None, steps=100, start=None, end=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the absolute value of the force on a particle as a function of the position.

The method probes the system by moving a single particle on a line and recording the force. A plot is drawn. Also a tuple containing arrays of the distance traveled and the recorded forces is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

direction: double 3-vector the direction where the atom is moved

length: double the distance moved

steps: integer number of points (taken uniformly on the movement path) for measuring the force

start: double 3-vector (array or list) starting point for the trajectory - if not specified, the position of the particle in 'system' is used

end: double 3-vector (array or list) end point for the trajectory - alternative for direction and length (will override them)

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_abs_force_on_plane**(*index, system, directions, lengths, steps=100, start=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the absolute value of force on a particle as a function of the position.

The method probes the system by moving a single particle on a plane and recording the force. A contour plot is drawn. Also a tuple containing arrays of the distances traveled on the plane and the recorded forces is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

directions: double 2x3-matrix The directions where the atom is moved - i.e., the vectors defining the plane. If the second vector is not perpendicular to the first, the normal component is automatically used instead.

lengths: double 2-vector the distances moved in the given directions

steps: integer number of points (taken uniformly on the movement plane) for measuring the force

start: double 3-vector (array or list) starting point for the trajectory, i.e., a corner for the plane to be probed - if not specified, the position of the particle in 'system' is used

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_energy_on_line**(*index, system, direction=None, length=None, steps=100, start=None, end=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the energy of the system as a function of the position of a single particle.

The method probes the system by moving a single particle on a line and recording the energy. A plot is drawn. Also a tuple containing arrays of the distance traveled and the recorded energies is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

direction: double 3-vector the direction where the atom is moved

length: double the distance moved

steps: integer number of points (taken uniformly on the movement path) for measuring the energy

start: double 3-vector (array or list) starting point for the trajectory - if not specified, the position of the particle in 'system' is used

end: double 3-vector (array or list) end point for the trajectory - alternative for direction and length (will override them)

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_energy_on_plane**(*index, system, directions, lengths, steps=100, start=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the energy of the system as a function of the position of a particle.

The method probes the system by moving a single particle on a plane and recording the energy. A contour plot is drawn. Also a tuple containing arrays of the distances traveled on the plane and the recorded energies is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

directions: double 2x3-matrix The directions where the atom is moved - i.e., the vectors defining the plane. If the second vector is not perpendicular to the first, the normal component is automatically used instead.

lengths: double 2-vector the distances moved in the given directions

steps: integer number of points (taken uniformly on the movement plane) for measuring the energy

start: double 3-vector (array or list) starting point for the trajectory, i.e., a corner for the plane to be probed - if not specified, the position of the particle in 'system' is used

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_force_component_on_plane**(*index, system, directions, lengths, component, steps=100, start=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the projected component of force on a particle as a function of the position.

The method probes the system by moving a single particle on a plane and recording the force. The component of the force projected on a given vector is recorded. A contour plot is drawn. Also a tuple containing arrays of the distances traveled on the plane and the recorded forces is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

directions: double 2x3-matrix The directions where the atom is moved - i.e., the vectors defining the plane. If the second vector is not perpendicular to the first, the normal component is automatically used instead.

lengths: double 2-vector the distances moved in the given directions

component: double 3-vector the direction on which the force is projected - e.g., if component is [1,0,0], the x-component is recorded

steps: integer number of points (taken uniformly on the movement plane) for measuring the force

start: double 3-vector (array or list) starting point for the trajectory, i.e., a corner for the plane to be probed - if not specified, the position of the particle in 'system' is used

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_tangent_force_on_line**(*index, system, direction=None, length=None, steps=100, start=None, end=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the tangential force on a particle as a function of the position.

The method probes the system by moving a single particle on a line and recording the force tangent. A plot is drawn. Also a tuple containing arrays of the distance traveled and the recorded forces is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

direction: double 3-vector the direction where the atom is moved

length: double the distance moved

steps: integer number of points (taken uniformly on the movement path) for measuring the energy

start: double 3-vector (array or list) starting point for the trajectory - if not specified, the position of the particle in 'system' is used

end: double 3-vector (array or list) end point for the trajectory - alternative for direction and length (will override them)

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

pysic.utility.plot.**plot_tangent_force_on_plane**(*index, system, directions, lengths, steps=100, start=None, lims=[-10000000000.0, 10000000000.0]*)

Plots the absolute value of the tangent component of force on a particle as a function of the position.

The method probes the system by moving a single particle on a plane and recording the force. The force is projected on the same plane, and the absolute value of the projection is calculated. A contour plot is drawn. Also a tuple containing arrays of the distances traveled on the plane and the recorded forces is returned.

After the operation is complete, the initial structure is restored.

Parameters:

index: integer index of the particle to be moved

system: ASE Atoms object the structure to be explored

directions: double 2x3-matrix The directions where the atom is moved - i.e., the vectors defining the plane. If the second vector is not perpendicular to the first, the normal component is automatically used instead.

lengths: double 2-vector the distances moved in the given directions

steps: integer number of points (taken uniformly on the movement plane) for measuring the force

start: double 3-vector (array or list) starting point for the trajectory, i.e., a corner for the plane to be probed - if not specified, the position of the particle in 'system' is used

lims: double 2-vector (array or list) lower and upper truncation limits - if a recorded value is smaller than the lower limit or larger than the upper, it is replaced by the corresponding truncation value

4.3.2 Outliers

This module contains tools for statistical analysis of atomic structures. It can be used for calculating the bond length and angle distributions in a given structure according to bond rules given by the user. Log-likelihood distributions are generated based on these distributions, which can be further grouped or used to create false color representations of the structure.

This is an example of how to create the distributions:

```
import pysic
from pysic.utility.outliers import *
from ase.io import read

def do_everything(inputfile, outputfile, radii, periodic_directions, cell_lengths):
    """Stitch everything together.
    """

    system = read(inputfile)
    system.set_pbc(periodic_directions)
    system.set_cell(cell_lengths)
    structure = Structure(system)

    structure.add_bond(['Si','Si'], radii['Si']*2*0.6)
    structure.add_bond(['Si','O'], (radii['Si']+radii['O'])*0.6)
    structure.add_bond(['O','O'], radii['O']*2*0.6)
    structure.add_bond(['Si','H'], (radii['Si']+radii['H'])*0.6)
    structure.add_bond(['H','O'], (radii['H']+radii['O'])*0.6)
    structure.create_neighbor_lists()
    angles = structure.get_all_angles()
    distances = structure.get_all_distances()
    max_n = np.shape(system)[0]

    for a in angles:
        print "a", a.center_index, a.type1, a.type2, a.type3, a.value
```

```
    for d in distances:
        print "d", d.primary_index, d.type1, d.type2, d.value

    angle_distribs, dist_distribs = get_distributions(angles, distances, radii)
    a_logls, d_logls = get_log_likelihoods(angles, distances, angle_distribs,
                                           dist_distribs, max_n)
    write_to_file(outputfile, cell_lengths, system.get_chemical_symbols(),
                    system.get_positions(), a_logls, d_logls)


inputfile           = 'sio2.xyz'
outputfile          = 'sio2_analysis.txt'
periodic_directions = [True, True, True]
cell_lengths = [14.835, 14.835, 14.835]

radii = {'O' : 1.52,
         'Si': 2.10}


# All set? Run.
do_everything(inputfile, outputfile, radii, periodic_directions, cell_lengths)
```

The atomic system is first read from an xyz file using ASE read method. It is then translated to a Structure class, which the outliers tools use, and bonding rules are created based on element types. Once bonding has been defined, bond lengths, bond angles, and their distributions are calculated with the outliers tools. The results are printed in a file in this example, but it would of course be possible to access them directly in the script for further analysis.

Structure class

class pysic.utility.outliers.**Structure**(*atoms*)

add_bond(*elements*, *cutoff*)
Adds a bond between atoms of the given elements, up to the cutoff separation.

create_neighbor_lists()
Creates neighbor lists for the structure.

get_all_angles()
Returns a list of all 3-atom angles as Angle objects.

get_all_distances()
Returns a list of all 2-atom distances as Distance objects.

get_bond_length(*elements*)
Returns the stored bond length for the given pair of elements.

get_distances(*index*)
Returns the distances between a given atom and its neighbors. (Sorted.)

get_neighbors(*index*)
Returns the indices of neighboring atoms for the given atom. (Sorted according to distance.)

get_separations(*index*)
Returns the separation vectors from a given atom to its neighbors. (Sorted according to distance.)

Distance class

class pysic.utility.outliers.**Distance**(*primary_index*, *type1*, *type2*, *distance*)

Angle class

class pysic.utility.outliers.**Angle**(*center_index*, *type1*, *type2*, *type3*, *angle*)

Outliers module

Detection of irregular atomic neighborhoods by bond distance and angle analysis.

pysic.utility.outliers.**angle**(*A*, *O*, *B*)
Return the angle between vectors OA and OB

Parameters O, A, B: coordinates in 3d-space

pysic.utility.outliers.**get_distributions**(*angles*, *distances*, *radii*)
Return observed log-distributions of angles and distances

Distributions are obtained for all combinations of observed atom types. They are histogram-based, using the breakpoints specified by parameters 'angle.grid' and 'dist.grid'. The distributions are represented by vectors giving the log-probability of each "bin". These are not normalized by the "bin" widths. This is not a problem as these would cancel out later.

pysic.utility.outliers.**get_log_likelihoods**(*angles*, *distances*, *angle_distribs*, *dist_distribs*, *n_atoms*)
Calculate log-likelihoods of each atom

All observed angles and distances are considered independent. Parameters 'angles' and .distances' supplie the observations, 'angle_distribs' and 'dist_distribs" the histogram-based distributions and 'angle.grid' & 'dist.grid' the breakpoints of these histograms. Parameter 'n_atoms' gives the number of atoms in the original data.

pysic.utility.outliers.**vec_angle**(*A*, *B*)
Return the angle between vectors A and B

Parameters A, B: coordinates in 3d-space

pysic.utility.outliers.**write_to_file**(*filename*, *boxsize*, *atoms*, *coordinates*, *a_logls*, *d_logls*)
Write original data + results into a file

Creates/overwrites an xyz-like file with two additional columns. These additional columns will contain the log-likelihood contributions from (1) angles and (2) distances.

4.3.3 MPI

The mpi utility defines a group of tools for parallel computations. Defines MPI safe routines for printing, file access etc.

pysic.utility.mpi.**append_file**(*lines*, *filename*)
Appends the given lines to a text file so that only the master cpu writes.

Parameters:

lines: list of strings lines to be written

filename: string the name of the file

pysic.utility.mpi.**cd**(*dir*)
Changes to the given directory on all cpus.

Parameters:

dir: string the name of the directory

pysic.utility.mpi.**cpu_id**()
Gets the cpu ID from the Fortran MPI.

Equivalent to `get_cpu_id()`.

pysic.utility.mpi.**finish_mpi**()
Terminates the MPI framework.

If the Fortran core is compiled in MPI mode, `pysic` will automatically initialize MPI upon being imported. This method terminates the MPI.

pysic.utility.mpi.**get_cpu_id**()
Gets the cpu ID from the Fortran MPI.

pysic.utility.mpi.**get_number_of_cpus**()
Gets the number of cpus from the Fortran MPI.

pysic.utility.mpi.**is_master**()
Returns `True` for the cpu with ID 0.

pysic.utility.mpi.**mkdir**(*dir*)
Creates a new directory only with the master cpu.

Parameters:

dir: string the name of the directory

pysic.utility.mpi.**mpi_barrier**()
Calls MPI barrier from the Fortran core MPI framework.

This is equivalent to `sync_mpi()`

pysic.utility.mpi.**mprint**(*string*)
Prints the string to stdout only from the master cpu.

Parameters:

string: string the string to be written

pysic.utility.mpi.**sync_mpi**()
Calls MPI barrier from the Fortran core MPI framework.

pysic.utility.mpi.**write_file**(*lines*, *filename*)
Writes the given lines to a text file so that only the master cpu writes.

Parameters:

lines: list of strings lines to be written

filename: string the name of the file

4.3.4 Archive

The archive utility defines a group of functions for archiving and retrieving simulation data in the hdf5 format. This requires hdf5 and the h5py Python library.

class pysic.utility.archive.**Archive**(*filename*)

A class representing a data archive in the hdf5 format.

The archive is built on h5py. See its documentation to access further functionality.

Parameters:

filename: string path to the file storing the data

access_dataset(*name*)

add_dataset_metadata(*attribute*, *metadata*)

add_group_metadata(*attribute*, *metadata*)

create_dataset(*name*, *data*, ***kwds*)

create_subgroup(*name*)

data()

delete_current_dataset()

delete_dataset(*name*)

delete_group()

delete_subgroup(*name*)

get_contents()

get_dataset()

get_dataset_metadata()

get_dataset_name()

get_group()

get_group_metadata()

get_group_name()

get_system(*name*)

Restore a stored system.

The function returns a tuple with the data:

```
system, energy, forces, stress, electronegativities
```

Parameters:

name: string name of the group storing the system

group()

list()

move(*source*, *destination*)

move_to_group(*name*)

move_to_parent_group()

move_to_root_group()

remove_dataset_metadata(*attribute*)

remove_group_metadata(*attribute*)

state()

store_system(*name*, *atoms*, *calculate=True*)
Stores the information of an atomic system.

The routine creates a group with the given name and stores the atomic information there as named datasets:

```
'atomic numbers'
'positions'
'charges'
'magnetic moments'
'tags'
'cell'
'pbc'
'momenta'
'potential energy'
'forces'
'stress'
'electronegativites'
```

The data requiring calculation is stored only if a calculator is attached to the atoms, electronegativities only if the calculator is `Pysic`.

Parameters:

name: string the name of the group for storing the data

atoms: Atoms object the structure to be stored

calculate: boolean if True, the data requiring calculations will not be stored

4.3.5 Convenience

The convenience utility defines functions to ease the handling of complicated data structures.

pysic.utility.convenience.**expand_symbols_string**(*symbol_string*)
Expands a string of chemical symbols to list.

The function parses a string of chemical symbols and turns it to a list such as those expected by `Potential`.

Examples:

```
>>> print expand_symbols_string("HH")
[['H', 'H']]
>>> print expand_symbols_string("SiSi,SiO,SiH")
[['Si', 'Si'], ['Si', 'O'], ['Si', 'H']]
```

Parameters:

symbol_string: string the string to be expanded

pysic.utility.convenience.**expand_symbols_table**(*symbol_list*, *type=None*)
Creates a table of symbols object.

The syntax for defining the targets is precise but somewhat cumbersome due to the large number of permutations one gets when the number of bodies increases. Oftentimes one does not need such fine control over all the parameters since many of them have the same numerical values. Therefore it is convenient to be able to define the targets in a more compact way.

This method generates the detailed target tables from compact syntax. By default, the method takes a list of list and multiplies each list with the others (note the call for a static method):

```
>>> pysic.utility.convenience.expand_symbols_table([  'Si',
...                                                  ['O', 'C'],
...                                                  ['H', 'O'] ])
[['Si', 'O', 'H'],
 ['Si', 'C', 'H'],
 ['Si', 'O', 'O'],
 ['Si', 'C', 'O']]
```

Other custom types of formatting can be defined with the type parameter.

For type 'triplet', the target list is created for triplets A-B-C from an input list of the form:

```
['A', 'B', 'C']
```

Remember that in the symbol table accepted by the BondOrderParameters, one needs to define the B-A and B-C bonds separately and so B appears as the first symbol in the output and the other two appear as second and third (both cases):

```
[['B', 'A', 'C'],
 ['B', 'C', 'A']]
```

However, for an A-B-A triplet, the A-B bond should only be defined once to prevent double counting. Like the default function, also here several triplets can be defined at once:

```
>>> pysic.BondOrderParameters.expand_symbols_table([ ['H', 'O'],
...                                                   'Si',
...                                                  ['O', 'C'] ],
...                                                type='triplet')
[['Si', 'H', 'O'],
 ['Si', 'O', 'H'],
 ['Si', 'H', 'C'],
 ['Si', 'C', 'H'],
 ['Si', 'O', 'O'],
 ['Si', 'O', 'C'],
 ['Si', 'C', 'O']]
```

Parameters:

symbol_list: list of strings list to be expanded to a table type: string specifies a custom way of generating the table

4.3.6 Geometry

The geometry utility defines tools for geometric operations.

class `pysic.utility.geometry.`**`Cell`**(*vector1*, *vector2*, *vector3*, *pbc*)

Cell describing the simulation volume of a subvolume.

This class can be used by the user for coordinate manipulation. Note however, that ASE does not use on this class, as it is part of Pysic. The class is merely a tool for examining the geometry.

Parameters:

vector1: list of doubles 3-vector specifying the first vector spanning the cell $\mathbf{v}_1$

vector2: list of doubles 3-vector specifying the second vector spanning the cell $\mathbf{v}_2$

vector3: list of doubles 3-vector specifying the third vector spanning the cell $\mathbf{v}_3$

pbc: list of logicals three logic switches for specifying periodic boundaries - True denotes periodicity

get_absolute_coordinates (*fractional*)
For the given fractional coordinates, returns the absolute coordinates.

The absolute coordinates are the cell vectors multiplied by the fractional coordinates.

Parameters:

fractional: numpy double 3-vector the fractional coordinates

get_distance (*atom1*, *atom2*, *offsets=None*)
Calculates the distance between two atoms.

Offsets are multipliers for the cell vectors to be added to the plain separation vector r1-r2 between the atoms.

Parameters:

atom1: ASE Atoms object first atom

atom2: ASE Atoms object second atom

offsets: Numpy integer 3-vector the periodic boundary offsets

get_relative_coordinates (*coordinates*)
Returns the coordinates of the given atom in fractional coordinates.

The absolute position of the atom is given by multiplying the cell vectors by the fractional coordinates.

Parameters:

coordinates: numpy double 3-vector the absolute coordinates

get_separation (*atom1*, *atom2*, *offsets=None*)
Returns the separation vector between two atoms, r1-r2.

Offsets are multipliers for the cell vectors to be added to the plain separation vector r1-r2 between the atoms.

Parameters:

atom1: ASE Atoms object first atom

atom2: ASE Atoms object second atom

offsets: Numpy integer 3-vector the periodic boundary offsets

get_wrapped_coordinates (*coordinates*)
Wraps the coordinates of the given atom inside the simulation cell.

This method return the equivalent position (with respect to the periodic boundaries) of the atom inside the cell.

For instance, if the cell is spanned by vectors of length 10.0 in directions of x, y, and z, an the coordinates [-1.0, 12.0, 3.0] wrap to [9.0, 2.0, 3.0].

Parameters:

coordinates: numpy double 3-vector the absolute coordinates

4.3.7 Error

The error utility defines a group of intrinsic errors to describe situations where one tries to use or set up the calculator with errorneous or insufficient information.

The module also defines the `Warning` class and related routines for displaying warnings for the user upon suspicious but non-critical behavior.

exception pysic.utility.error.**InvalidCoordinatorError**(*message=''*, *coordinator=None*)
An error raised when an invalid coordination calculator is about to be created or used.

Parameters:

message: string information describing why the error occurred

coordinator: Coordinator the errorneous coordinator

exception pysic.utility.error.**InvalidParametersError**(*message=''*, *params=None*)
An error raised when an invalid set of parameters is about to be created.

Parameters:

message: string information describing why the error occurred

params: BondOrderParameters the errorneous parameters

exception pysic.utility.error.**InvalidPotentialError**(*message=''*, *potential=None*)
An error raised when an invalid potential is about to be created or used.

Parameters:

message: string information describing why the error occurred

potential: Potential the errorneous potential

exception pysic.utility.error.**InvalidRelaxationError**(*message=''*, *relaxation=None*)
An error raised when an invalid charge relaxation is about to be created.

Parameters:

message: string information describing why the error occurred

params: ChargeRelaxation the errorneous parameters

exception pysic.utility.error.**InvalidSummationError**(*message=''*, *summer=None*)
An error raised when an invalid coulomb summation is about to be created.

Parameters:

message: string information describing why the error occurred

params: CoulombSummation the errorneous summation

exception pysic.utility.error.**LockedCoreError**(*message=''*)
An error raised when a Pysic tries to access the core which is locked by another calculator.

Parameters:

message: string information describing why the error occurred

exception pysic.utility.error.**MissingAtomsError**(*message=''*)
An error raised when the core is being updated with per atom information before updating the atoms.

Parameters:

message: string information describing why the error occurred

exception pysic.utility.error.**MissingNeighborsError**(*message=''*)
An error raised when a calculation is initiated without initializing the neighbor lists.

In principle Pysic should always take care of handling the neighbors automatically. This error is an indication that there is loophole in the built-in preparations.

Parameters:

message: string information describing why the error occurred

class pysic.utility.error.**Warning**(*message*, *level*)
A warning raised due to a potentially dangerous action.

The warning is not an exception, so it doesn't by default interrupt execution. It will, however, display a message or perform an action depending on the warning settings.

The warning levels are:

1: a condition that leads to unwanted behaviour (e.g., creating redundant potential in core) 2: a condition that is likely unwanted, but possibly a hack 3: a condition that is likely unwanted, but is a featured hack (e.g., bond order mixing) 4: a condition that is harmless but may lead to errors later (e.g., defining a potential without targets - often you'll specify the targets later) 5: a condition that may call for attention (notes to user)

Parameters:

message: string information describing the cause for the warning

level: int severity of the warning (1-5, 1 being most severe)

display()
Displays the message related to this warning, but only if the level of the warning is smaller (more severe) than the global warning_level.

exception pysic.utility.error.**WarningInterruptException**(*message*)
An error raised automatically for any warning when strict warnings are in use (warning_level = 6).

pysic.utility.error.**error**(*message*)
Raises an error and displays the reason. Independent of the warning level.

Parameters:

message: string information describing the cause for the warning

pysic.utility.error.**set_warning_level**(*level*)
Set the warning level.

Parameters:

level: int The level of warnings displayed. Should be an integer between 0 (no warnings) and 6 (warnings are treated as errors).

pysic.utility.error.**style_message**(*header*, *message*, *width=80*, *x_pad=2*, *y_pad=1*)
Styles a message to be printed into console.

The message can be a list of string, where each list item corresponds to a row. If a single string is provided, it is converted to a list. Rows are cut into pieces so that they will fit into the defined width.

pysic.utility.error.**warn**(*message*, *level*)
Raise and display a warning.

Parameters:

message: string information describing the cause for the warning

level: int severity of the warning (1-5, 1 being most severe)

4.3.8 Debug

The debug utility defines debugging tools.

4.3.9 F2py

The f2py utility defines tools for the Python-Fortran interfacing.

pysic.utility.f2py.**char2int**(*char_in*)
Codes a single character to an integer.

pysic.utility.f2py.**int2char**(*int_in*)
Decodes an integer to a single character.

pysic.utility.f2py.**ints2str**(*ints_in*)
Decodes a list of integers to a string.

pysic.utility.f2py.**str2ints**(*string_in*, *target_length=0*)
Codes a string to a list of integers.

Turns a string to a list of integers for f2py interfacing. If required, the length of the list can be specified and trailing spaces will be added to the end.

4.4 Pysic Fortran module

Pysic Fortran (pysic.pysic_fortran) is the Python interface of the Fortran core generated using f2py from PyInterface.F90. This is the only Fortran source file of Pysic that should be wrapped with f2py: the rest of the core needs to be directly compiled with a Fortran compiler to .mod Fortran modules.

The module is naturally accessible from within Python, but usually there should be no need to directly invoke its functions as pysic defines a more refined interface to the Fortran core, mainly through the class Pysic. It is assumed that the arguments passed to the functions have proper data types and array dimensions, and that they are called in such an order that the necessary memory allocations have been done within Fortran before data structures are accessed. Methods in Pysic do this automatically and are thus much safer to use than directly calling the functions in this module. The Fortran routines are documented here mostly for development purposes.

4.4.1 Modules of the Fortran core of Pysic

pysic_interface (PyInterface.f90)

Pysic_interface is an interface module between the Python and Fortran sides of pysic. When pysic is compiled, only this file is interfaced to Python via f2py while the rest of the Fortran source files are directly compiled to .mod Fortran modules. The main reason for this is that F90 derived types are used extensively in the core and these are not yet (2011) supported by f2py (although the support for derived types is planned in third generation f2py). Because of this, most data is passed from pysic to *pysic_interface (PyInterface.f90)* as NumPy arrays, and conversions from objects is needed on both sides. This is cumbersome and adds overhead, but it is not an efficiency issue since most of the information is only passed from Python to Fortran once and saved. Even during a molecular dynamics simulation only the forces, coordinates and momenta of atoms need to be communicated through the interface, which is naturally and efficiently handled using just numeric arrays anyway.

Another limitation in current f2py is handling of string arrays. To overcome this, string arrays are converted to integer arrays and back using simple mapping functions in pysic_utility and *utility (Utility.f90)*.

Due to the current limitations of f2py, no derived types can appear in the module. This severly limits what the module can do, and therefore the module has been by design made to be very light in terms of functionality: No data is stored in the module and almost all routines simply redirect the call to a submodule, most often *pysic_core (Core.f90)*. In the descriptions of the routines in this documentation, links are provided to the submodule routines that the call is directed to, if the routine is just a redirect of the call.

Full documentation of subroutines in pysic_interface

add_bond_order_factor (*n_targets*, *n_params*, *n_split*, *bond_name*, *parameters*, *param_split*, *cutoff*, *smooth_cut*, *elements*, *orig_elements*, *group_index*, *success*)

Creates a bond order factor in the core. The memory must have been allocated first using allocate_potentials.

Calls `core_add_bond_order_factor()`

Parameters:

n_targets: integer *intent(in) scalar* number of targets (interacting bodies)

n_params: integer *intent(in) scalar* number of parameters

n_split: integer *intent(in) scalar* number of subsets in the list of parameters, should equal n_targets

bond_name: character(len=*) *intent(in) scalar* bond order factor names

parameters: double precision *intent(in) size(n_params)* numeric parameters

param_split: integer *intent(in) size(n_split)* the numbers of parameters for 1-body, 2-body etc.

cutoff: double precision *intent(in) scalar* interaction hard cutoff

smooth_cut: double precision *intent(in) scalar* interaction soft cutoff

elements: integer *intent(in) size(2, n_targets)* atomic symbols specifying the elements the interaction acts on

orig_elements: integer *intent(in) size(2, n_targets)* original atomic symbols specifying the elements the interaction acts on

group_index: integer *intent(in) scalar* index denoting the potential to which the factor is connected

success: logical intent(out) *scalar* logical tag specifying if creation of the factor succeeded

add_potential (*n_targets*, *n_params*, *pot_name*, *parameters*, *cutoff*, *smooth_cut*, *elements*, *tags*, *indices*, *orig_elements*, *orig_tags*, *orig_indices*, *pot_index*, *is_multiplier*, *success*)

Creates a potential in the core. The memory must have been allocated first using allocate_potentials.

Calls `core_add_potential()`

Parameters:

n_targets: integer *intent(in) scalar* number of targets (interacting bodies)

n_params: integer *intent(in) scalar* number of parameters

pot_name: character(len=*) *intent(in) scalar* potential names

parameters: double precision *intent(in) size(n_params)* numeric parameters

cutoff: double precision *intent(in) scalar* interaction hard cutoff

smooth_cut: double precision *intent(in) scalar* interaction soft cutoff

elements: integer *intent(in) size(2, n_targets)* atomic symbols specifying the elements the interaction acts on

tags: integer *intent(in) size(n_targets)* tags specifying the atoms the interaction acts on

indices: integer *intent(in) size(n_targets)* indices specifying the atoms the interaction acts on

orig_elements: integer *intent(in) size(2, n_targets)* original atomic symbols specifying the elements the interaction acts on

orig_tags: integer *intent(in) size(n_targets)* original tags specifying the atoms the interaction acts on

orig_indices: integer *intent(in) size(n_targets)* original indices specifying the atoms the interaction acts on

pot_index: integer *intent(in) scalar* index of the potential

is_multiplier: logical *intent(in) scalar* logical tag defining if the potential is a multiplier for a product potential

success: logical intent(out) *scalar* logical tag specifying if creation of the potential succeeded

allocate_bond_order_factors (*n_bonds*)

Allocates memory for storing bond order parameters for describing the atomic interactions. Similar to the allocate_potentials routine.

Calls `core_allocate_bond_order_factors()`

Parameters:

n_bonds: integer *intent(in) scalar* number of bond order factors

allocate_bond_order_storage (*n_atoms*, *n_groups*, *n_factors*)

Allocates memory for storing bond order factors for describing the atomic interactions. The difference to allocate_bond_order_factors is that this method allocates space for arrays used in storing actual calculated bond order factors. The other routine allocates space for storing the parameters used in the calculations.

Calls `core_allocate_bond_order_storage()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

n_groups: integer *intent(in) scalar* number of bond order groups

n_factors: integer *intent(in) scalar* number of bond order parameters

allocate_potentials (*n_pots*)

Allocates memory for storing potentials for describing the atomic interactions. It is more convenient to loop through the potentials and format them in a suitable way in python than in fortran. Therefore the core is first called through this routine in order to allocate memory for the potentials. Then, each potential is created individually.

Calls `core_allocate_potentials()`

Parameters:

n_pots: integer *intent(in) scalar* number of potentials

calculate_bond_order_factors (*n_atoms*, *group_index*, *bond_orders*)

Returns bond order factors of the given group for all atoms. The group index is an identifier for the bond order parameters which are used for calculating one and the same factors. In practice, the Coordinators in pysic are indexed and this indexing is copied in the core. Thus the group index specifies the coordinator / potential.

Calls `core_get_bond_order_factors()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

group_index: integer *intent(in) scalar* index for the bond order factor group

bond_orders: double precision intent(out) *size(n_atoms)* the calculated bond order factors

calculate_bond_order_gradients (*n_atoms*, *group_index*, *atom_index*, *gradients*)
Returns bond order factors gradients of the given group. The gradients of all factors are given with respect to moving the given atom. The group index is an identifier for the bond order parameters which are used for calculating one and the same factors. In practice, the Coordinators in pysic are indexed and this indexing is copied in the core. Thus the group index specifies the coordinator / potential.

Calls core_get_bond_order_sums()

and core_calculate_bond_order_gradients()

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

atom_index: integer *intent(in) scalar* index of the atom with respect to which the factors are differentiated

gradients: double precision intent(out) *size(3, n_atoms)* the calculated bond order gradients

calculate_bond_order_gradients_of_factor (*n_atoms*, *group_index*, *atom_index*, *gradients*)
Returns bond order factors gradients of the given group. The gradients of the given factors is given with respect to moving all atoms. The group index is an identifier for the bond order parameters which are used for calculating one and the same factors. In practice, the Coordinators in pysic are indexed and this indexing is copied in the core. Thus the group index specifies the coordinator / potential.

Calls core_get_bond_order_sums()

and core_calculate_bond_order_gradients_of_factor()

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

atom_index: integer *intent(in) scalar* index of the atom whose factor is differentiated

gradients: double precision intent(out) *size(3, n_atoms)* the calculated bond order gradients

calculate_electronegativities (*n_atoms*, *enegs*)
Returns electronegativities of the particles

Calls core_calculate_electronegativities()

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

enegs: double precision intent(out) *size(n_atoms)* array of electronegativities on all atoms

calculate_energy (*energy*)
Returns the total potential energy of the system

Calls core_calculate_energy()

Parameters:

energy: double precision intent(out) ***scalar*** total potential energy

calculate_forces(*n_atoms*, *forces*, *stress*)
Returns forces acting on the particles and the stress tensor

Calls core_calculate_forces()

Parameters:

n_atoms: integer ***intent(in) scalar*** number of atoms

forces: double precision intent(out) ***size(3, n_atoms)*** array of forces on all atoms

stress: double precision intent(out) ***size(6)*** array containing the components of the stress tensor (in order xx, yy, zz, yz, xz, xy)

clear_potential_multipliers()
Clears the temporary stored array of multiplier potentials

create_atoms(*n_atoms*, *masses*, *charges*, *positions*, *momenta*, *tags*, *elements*)
Creates atomic particles. Atoms are handled as custom fortran types atom in the core. Currently f2py does not support direct creation of types from Python, so instead all the necessary data is passed from Python as arrays and reassembled as types in Fortran. This is not much of an added overhead - the memory allocation itself already makes this a routine one does not wish to call repeatedly. Instead, one should call the routines for updating atoms whenever the actual atoms do not change (e.g., between MD timesteps).

Calls core_generate_atoms()

Parameters:

n_atoms: integer ***intent(in) scalar*** number of atoms

masses: double precision ***intent(in) size(n_atoms)*** masses of atoms

charges: double precision ***intent(in) size(n_atoms)*** electric charges of atoms

positions: double precision ***intent(in) size(3, n_atoms)*** coordinates of atoms

momenta: double precision ***intent(in) size(3, n_atoms)*** momenta of atoms

tags: integer ***intent(in) size(n_atoms)*** numeric tags for the atoms

elements: integer ***intent(in) size(2, n_atoms)*** atomic symbols of the atoms

create_bond_order_factor_list()
Similarly to the potential lists, also list containing all the bond order factors that may affect an atom are stored in a list.

Calls core_assign_bond_order_factor_indices()

create_cell(*vectors*, *inverse*, *periodicity*)
Creates a supercell for containing the calculation geometry Also the inverse cell matrix must be given, although it is not checked that the given inverse actually is the true inverse.

Calls core_create_cell()

Parameters:

vectors: double precision ***intent(in) size(3, 3)*** A 3x3 matrix containing the vectors spanning the supercell. The first index runs over xyz and the second index runs over the three vectors.

inverse: double precision ***intent(in) size(3, 3)*** A 3x3 matrix containing the inverse matrix of the one given in vectors, i.e. $M^{-1} * M = I$ for the two matrices. Since the latter represents a cell of non-zero volume, this inverse must exist. It is not tested that the given matrix actually is the inverse, the user must make sure it is.

periodicity: logical *intent(in) size(3)* A 3-element vector containing logical tags specifying if the system is periodic in the directions of the three vectors spanning the supercell.

create_neighbor_list(*n_nbs*, *atom_index*, *neighbors*, *offsets*)
Creates neighbor lists for a single atom telling it which other atoms are in its immediate neighborhood. The neighbor list must be precalculated, this method only stores them in the core. The list must contain an array storing the indices of the neighboring atoms as well as the supercell offsets. The offsets are integer triplets showing how many times must the supercell vectors be added to the position of the neighbor to find the neighboring image in a periodic system. Note that if the system is small, one atom can in principle appear several times in the neighbor list.

Calls core_create_neighbor_list()

Parameters:

n_nbs: integer *intent(in) scalar* number of neighbors

atom_index: integer *intent(in) scalar* index of the atom for which the neighbor list is created

neighbors: integer *intent(in) size(n_nbs)* An array containing the indices of the neighboring atoms

offsets: integer *intent(in) size(3, n_nbs)* An array containing vectors specifying the offsets of the neighbors in periodic systems.

create_potential_list()
Creates a list of indices for all atoms showing which potentials act on them. The user may define many potentials to sum up the potential energy of the system. However, if some potentials only act on certain atoms, they will be redundant for the other atoms. The potential lists are lists given to each atom containing the potentials which can act on the atom.

Calls core_assign_potential_indices()

description_of_bond_order_factor(*bond_name*, *description*)
Returns a description of the given bond order factor

Calls get_description_of_bond_order_factor()

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

description: character(len=500) intent(out) *scalar* description of the bond order actor

description_of_potential(*pot_name*, *description*)
Returns a description of the given potential

Calls get_description_of_potential()

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

description: character(len=500) intent(out) *scalar* description of the potential

descriptions_of_parameters_of_bond_order_factor(*bond_name*, *n_targets*, *param_notes*)
Lists descriptions for parameters the given bond order factor. Output is an array of integers. This is because f2py doesn't currently support string arrays. So, the characters are translated to integers and back in fortran and python. This adds a bit of overhead, but the routine is only invoked on user command so it doesn't matter.

Calls get_descriptions_of_parameters_of_bond_order_factor()

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

n_targets: integer *intent(in) scalar* number of targets

param_notes: integer intent(out) *size(100, 12)* descriptions of the parameters

descriptions_of_parameters_of_potential (*pot_name*, *param_notes*)
Lists descriptions for parameters the given potential. Output is an array of integers. This is because f2py doesn't currently support string arrays. So, the characters are translated to integers and back in fortran and python. This adds a bit of overhead, but the routine is only invoked on user command so it doesn't matter.

Calls `get_descriptions_of_parameters_of_potential()`

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

param_notes: integer intent(out) *size(100, 12)* descriptions of the parameters

distribute_mpi (*n_atoms*)
Distributes atoms among the processors. In the MPI scheme, atoms are distributed among the cpus for force and energy calculations. This routine initializes the arrays that tell each cpu which atoms it has to calculate interactions for. It can be called before the atoms are created in the core but one has to make sure the number of atoms specified in the last call matches the number of atoms in the core when a calculation is invoked.

Calls `mpi_distribute()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

examine_atoms()
Prints some information about the atoms allocated in the core. This is mainly for debugging, as the python side should always dictate what is in the core.

Calls `list_atoms()`

examine_bond_order_factors()
Prints some information about the bond order factors allocated in the core. This is mainly for debugging, as the python side should always dictate what is in the core.

Calls `list_bonds()`

examine_cell()
Prints some information about the supercell allocated in the core. This is mainly for debugging, as the python side should always dictate what is in the core.

Calls `list_cell()`

examine_potentials()
Prints some information about the potential allocated in the core. This is mainly for debugging, as the python side should always dictate what is in the core.

Calls `list_interactions()`

finish_mpi()
Finishes MPI for parallel calculations.

Calls `mpi_finish()`

generate_neighbor_lists (*n_atoms*, *cutoffs*)
calculates and allocates neighbor lists

Parameters:

n_atoms: integer *intent(in) scalar*

cutoffs: double precision *intent(in) size(n_atoms)*

get_cell_vectors (*vectors*)
Returns the vectors defining the simulation supercell.

Calls `core_get_cell_vectors()`

Parameters:

vectors: double precision intent(out) ***size(3, 3)*** A 3x3 matrix containing the vectors spanning the supercell. The first index runs over xyz and the second index runs over the three vectors.

get_cpu_id (*id*)
Returns the MPI cpu id number, which is an integer between 0 and $n_{\mathrm{cpus}} - 1$, where n_{cpus} is the total number of cpus.

Parameters:

id: integer intent(out) ***scalar*** cpu id number in MPI - 0 in serial mode

get_ewald_energy (*real_cut*, *k_cut*, *reciprocal_cut*, *sigma*, *epsilon*, *energy*)
Debugging routine for Ewald

Parameters:

real_cut: double precision *intent(in) scalar*

k_cut: double precision *intent(in) scalar*

reciprocal_cut: integer *intent(in) size(3)*

sigma: double precision *intent(in) scalar*

epsilon: double precision *intent(in) scalar*

energy: double precision **intent(out)** *scalar*

get_mpi_list_of_atoms (*n_atoms*, *cpu_atoms*)
Returns a logical array containing true for every atom that is allocated to this cpu, and false for all other atoms.

Parameters:

n_atoms: integer ***intent(in) scalar*** number of atoms

cpu_atoms: logical intent(out) ***size(n_atoms)*** array of logical values showing which atoms are marked to be handled by this cpu

get_neighbor_list_of_atom (*atom_index*, *n_neighbors*, *neighbors*, *offsets*)
Returns the list of neighbors for an atom

Parameters:

atom_index: integer *intent(in) scalar*

n_neighbors: integer *intent(in) scalar*

neighbors: integer **intent(out)** *size(n_neighbors)*

offsets: integer **intent(out)** *size(3, n_neighbors)*

get_number_of_atoms (*n_atoms*)
Counts the number of atoms in the current core

Calls `core_get_number_of_atoms()`

Parameters:

n_atoms: integer intent(out) ***scalar*** number of atoms

get_number_of_cpus (*ncpu*)
Returns the MPI cpu count

Parameters:

ncpu: integer intent(out) ***scalar*** the total number of cpus available

get_number_of_neighbors_of_atom (*atom_index*, *n_neighbors*)
Returns the number of neighbors for an atom

Parameters:

atom_index: integer *intent(in) scalar*

n_neighbors: integer **intent(out)** *scalar*

is_bond_order_factor (*string*, *is_ok*)
Tells whether a given keyword defines a bond order factor or not

Calls `is_valid_bond_order_factor()`

Parameters:

string: character(len=*) ***intent(in) scalar*** name of a bond order factor

is_ok: logical intent(out) ***scalar*** true if string is a name of a bond order factor

is_potential (*string*, *is_ok*)
Tells whether a given keyword defines a potential or not

Calls `is_valid_potential()`

Parameters:

string: character(len=*) ***intent(in) scalar*** name of a potential

is_ok: logical intent(out) ***scalar*** true if string is a name of a potential

level_of_bond_order_factor (*bond_name*, *n_target*)
Tells the level of a bond order factor has, i.e., is it per-atom or per-pair

Calls `get_level_of_bond_order_factor()`

Parameters:

bond_name: character(len=*) ***intent(in) scalar*** name of the bond order factor

n_target: integer intent(out) ***scalar*** number of targets

list_valid_bond_order_factors (*n_bonds*, *bond_factors*)
Lists all the keywords which define a bond order factor

Calls `list_bond_order_factors()`

Parameters:

n_bonds: integer ***intent(in) scalar*** number of bond order factor types

bond_factors: integer intent(out) ***size(11, n_bonds)*** names of the bond order factor types

list_valid_potentials (*n_pots*, *potentials*)
Lists all the keywords which define a potential

Calls `list_potentials()`

Parameters:

n_pots: integer *intent(in) scalar* number of potential types

potentials: integer intent(out) *size(11, n_pots)* names of the potential types

names_of_parameters_of_bond_order_factor (*bond_name*, *n_targets*, *param_names*)
Lists the names of parameters the given bond order factor knows. Output is an array of integers. This is because f2py doesn't currently support string arrays. So, the characters are translated to integers and back in fortran and python. This adds a bit of overhead, but the routine is only invoked on user command so it doesn't matter.

Calls `get_names_of_parameters_of_bond_order_factor()`

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

n_targets: integer *intent(in) scalar* number of targets

param_names: integer intent(out) *size(10, 12)* names of the parameters

names_of_parameters_of_potential (*pot_name*, *param_names*)
Lists the names of parameters the given potential knows. Output is an array of integers. This is because f2py doesn't currently support string arrays. So, the characters are translated to integers and back in fortran and python. This adds a bit of overhead, but the routine is only invoked on user command so it doesn't matter.

Calls `get_names_of_parameters_of_potential()`

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

param_names: integer intent(out) *size(10, 12)* names of the parameters

number_of_bond_order_factors (*n_bonds*)
Tells the number of differently named bond order factors the core knows

Calls `get_number_of_bond_order_factors()`

Parameters:

n_bonds: integer intent(out) *scalar* number of bond order factors

number_of_parameters_of_bond_order_factor (*bond_name*, *n_targets*, *n_params*)
Tells how many numeric parameters a bond order factor incorporates

Calls `get_number_of_parameters_of_bond_order_factor()`

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

n_targets: integer *intent(in) scalar* number of targets

n_params: integer intent(out) *scalar* number of parameters

number_of_parameters_of_potential (*pot_name*, *n_params*)
Tells how many numeric parameters a potential incorporates

Calls `get_number_of_parameters_of_potential()`

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

n_params: integer intent(out) ***scalar*** number of parameters

number_of_potentials(*n_pots*)
Tells the number of differently named potentials the core knows

Calls `get_number_of_potentials()`

Parameters:

n_pots: integer intent(out) ***scalar*** number of potentials

number_of_targets_of_bond_order_factor(*bond_name*, *n_target*)
Tells how many targets a bond order factor has, i.e., is it many-body

Calls `get_number_of_targets_of_bond_order_factor()`

Parameters:

bond_name: character(len=*) ***intent(in) scalar*** name of the bond order factor

n_target: integer intent(out) ***scalar*** number of targets

number_of_targets_of_potential(*pot_name*, *n_target*)
Tells how many targets a potential has, i.e., is it a many-body potential

Calls `get_number_of_targets_of_potential()`

Parameters:

pot_name: character(len=*) ***intent(in) scalar*** name of the potential

n_target: integer intent(out) ***scalar*** number of targets

release()
Deallocates all the arrays in the core

Calls `core_release_all_memory()`

set_ewald_parameters(*n_atoms*, *real_cut*, *k_radius*, *reciprocal_cut*, *sigma*, *epsilon*, *scaler*)
Sets the parameters for Ewald summation in the core.

Parameters:

n_atoms: integer *intent(in) scalar*

real_cut: double precision ***intent(in) scalar*** the real-space cutoff

k_radius: double precision ***intent(in) scalar*** the k-space cutoff

reciprocal_cut: integer ***intent(in) size(3)*** the k-space cutoffs (in numbers of cells)

sigma: double precision ***intent(in) scalar*** the split parameter

epsilon: double precision ***intent(in) scalar*** electric constant

scaler: double precision ***intent(in) size(n_atoms)*** scaling factors for the individual charges

start_bond_order_factors()
Initializes the bond order factors. A routine is called to generate descriptors for potentials. These descriptors are needed by the python interface in order to directly inquire the core on the types of factors available.

Calls `initialize_bond_order_factor_characterizers()`

start_mpi()
Initializes MPI for parallel calculations.

Calls `mpi_initialize()`

start_potentials()
Initializes the potentials. A routine is called to generate descriptors for potentials. These descriptors are needed by the python interface in order to directly inquire the core on the types of potentials available.

Calls initialize_potential_characterizers()

start_rng(*seed*)
Initialize Mersenne Twister random number generator.

A seed number has to be given. In case we run in MPI mode, the master cpu will broadcast its seed to all other cpus to ensure that the random number sequences match in all the cpus.

Parameters:

seed: integer *intent(in) scalar* a seed for the random number generator

sync_mpi()
Syncs MPI. This just calls mpi_barrier, so it makes all cpus wait until everyone is at this particular point in execution.

Calls mpi_sync()

update_atom_charges(*n_atoms*, *charges*)
Updates the charges of existing atoms. This method does not allocate memory and so the atoms must already exist in the core.

Calls core_update_atom_charges()

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

charges: double precision *intent(in) size(n_atoms)* new charges for the atoms

update_atom_coordinates(*n_atoms*, *positions*, *momenta*)
Updates the positions and velocities of existing atoms. This method does not allocate memory and so the atoms must already exist in the core.

Calls core_update_atom_coordinates()

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

positions: double precision *intent(in) size(3, n_atoms)* new coordinates for the atoms

momenta: double precision *intent(in) size(3, n_atoms)* new momenta for the atoms

pysic_core (Core.f90)

Core, true to its name, is the heart of the Fortran core of Pysic. It contains the data structures defining the simulation geometry and interactions and defines the central routines for calculating the total energy of and the forces acting on the system.

Many of the routines in *pysic_interface (PyInterface.f90)* which f2py interfaces to Python are simply calling routines here.

Full documentation of global variables in pysic_core

atoms
type(atom) *pointer size(:)*

an array of atom objects representing the system

atoms_created
logical *scalar*

initial value = .false.

logical tag indicating if atom storing arrays have been created

bo_factors
double precision *pointer size(:)*

bo_gradients
double precision *pointer size(:, :, :)*

bo_scaling
logical *pointer size(:)*

bo_sums
double precision *pointer size(:)*

bo_temp
double precision *pointer size(:)*

bond_factors
type(bond_order_parameters) *pointer size(:)*

an array of bond_order_parameters objects representing bond order factors modifying the potentials

bond_factors_allocated
logical *scalar*

initial value = .false.

logical tag indicating if bond order parameter storing arrays have been allocated

bond_storage_allocated
logical *scalar*

initial value = .false.

logical tag indicating if bond order factor storing arrays have been allocated

cell
type(supercell) *scalar*

a supercell object representing the simulation cell

electronegativity_evaluation_index
integer *scalar parameter*

initial value = 3

energy_evaluation_index
integer *scalar parameter*

initial value = 1

evaluate_ewald
logical *scalar*

initial value = .false.

switch for enabling Ewald summation of coulomb interactions

ewald_allocated
logical *scalar*

initial value = .false.

ewald_cutoff
double precision *scalar*

ewald_epsilon
double precision *scalar*

ewald_k_cutoffs
integer *size(3)*

ewald_k_radius
double precision *scalar*

ewald_scaler
double precision *pointer size(:)*

ewald_sigma
double precision *scalar*

force_evaluation_index
integer *scalar parameter*

initial value = 2

group_index_save_slot
integer *pointer size(:)*

interactions
type(potential) *pointer size(:)*

an array of `potential` objects representing the interactions

multipliers
type(potential) *allocatable size(:)*

a temporary array for storing multiplying potentials before associating them with a master potential

n_bond_factors
integer *scalar*

initial value = 0

n_interactions
integer *scalar*

initial value = 0

number of potentials

n_multi
integer *scalar*

initial value = 0

number of temporary product potentials

n_nbs
integer *pointer size(:)*

n_saved_bond_order_factors
integer *scalar*

initial value = 0

number of saved bond order factors

number_of_atoms
integer *scalar*

potentials_allocated
logical *scalar*

initial value = .false.

logical tag indicating if potential storing arrays have been allocated

saved_bond_order_factors
double precision *pointer size(:, :)*

Array for storing calculated bond order factors. Indexing: (atom index, group_index_save_slot(group index))

saved_bond_order_gradients
double precision *pointer size(:, :, :, :)*

Array for storing calculated bond order gradients. Indexing: (xyz, atom index, group_index_save_slot(group index), target index)

saved_bond_order_sums
double precision *pointer size(:, :)*

Array for storing calculated bond order sums. Indexing: (atom index, group_index_save_slot(group index))

saved_bond_order_virials
double precision *pointer size(:, :, :)*

Array for storing calculated bond order virials. Indexing: (xyz, group_index_save_slot(group index), target index)

temp_enegs
double precision *pointer size(:)*

temp_forces
double precision *pointer size(:, :)*

temp_gradient
double precision *pointer size(:, :, :)*

total_n_nbs
integer *pointer size(:)*

use_saved_bond_order_factors
logical *scalar*

initial value = .false.

Logical tag which enables / disables bond order saving. If true, bond order calculation routines try to find the precalculated factors in the saved bond order arrays instead of calculating.

use_saved_bond_order_gradients
integer *pointer size(:, :)*

Array storing the atom index of the bond gradient stored for indices (group index, target index). Since gradients are needed for all factors (N) with respect to moving all atoms (N), storing them all would require an N x N matrix. Therefore only some are stored. This array is used for searching the stroage to see if the needed gradient is there or needs to be calculated.

Full documentation of subroutines in pysic_core

core_add_bond_order_factor(*n_targets*, *n_params*, *n_split*, *bond_name*, *parameters*, *param_split*, *cutoff*, *smooth_cut*, *elements*, *orig_elements*, *group_index*, *success*)

Creates one additional bond_order_factor in the core. The routine assumes that adequate memory has been allocated already using core_allocate_bond_order_factors.

When the bond order parameters in the Python interface are imported to the Fortran core, the target specifiers (elements) are permutated to create all equivalent bond order parameters. That is, if we have parameters for Si-O, both Si-O and O-Si parameters are created. This is because the energy and force calculation loops only deal with atom pairs A-B once (so only A-B or B-A is considered, not both) and if, say, the loop only finds an O-Si pair, it is important to apply the Si-O parameters also on that pair. In some cases, such as with the tersoff factor affecting triplets (A-B-C), the contribution is not symmetric for all the atoms. Therefore it is necessary to also store the original targets of the potential as specified in the Python interface. These are to be given in the 'orig_elements' lists.

called from PyInterface: `add_bond_order_factor()`

Parameters:

n_targets: integer ***intent(in) scalar*** number of targets (interacting bodies)

n_params: integer ***intent(in) scalar*** number of parameters

n_split: integer ***intent(in) scalar*** number of subsets in the list of parameters, should equal n_targets

bond_name: character(len=*) ***intent(in) scalar*** bond order factor names

parameters: double precision ***intent(in) size(n_params)*** numeric parameters

param_split: integer ***intent(in) size(n_split)*** the numbers of parameters for 1-body, 2-body etc.

cutoff: double precision ***intent(in) scalar*** interaction hard cutoff

smooth_cut: double precision ***intent(in) scalar*** interaction soft cutoff

elements: character(len=label_length) ***intent(in) size(n_targets)*** atomic symbols specifying the elements the interaction acts on

orig_elements: character(len=label_length) ***intent(in) size(n_targets)*** original atomic symbols specifying the elements the interaction acts on

group_index: integer ***intent(in) scalar*** index denoting the potential to which the factor is connected

success: logical intent(out) ***scalar*** logical tag specifying if creation of the factor succeeded

core_add_bond_order_forces(*group_index*, *atom_index*, *prefactor*, *forces*, *stress*)

Parameters:

group_index: integer *intent(in) scalar*

atom_index: integer *intent(in) scalar*

prefactor: double precision *intent(in) scalar*

forces: double precision **intent(inout)** *size(:, :)*

stress: double precision **intent(inout)** *size(6)*

core_add_pair_bond_order_forces(*index1*, *index2*, *prefactor*, *separation*, *direction*, *distance*, *group_index*, *pair_bo_sums*, *pair_bo_factors*, *forces*, *stress*)

Evaluates the local force affecting two atoms from bond order factors.

Parameters:

index1: integer *intent(in) scalar* index of the atom 1

index2: integer *intent(in) scalar* index of the atom 2

prefactor: double precision *intent(in) scalar*

separation: double precision *intent(in) size(3)*

direction: double precision *intent(in) size(3)*

distance: double precision *intent(in) scalar*

group_index: integer *intent(in) scalar*

pair_bo_sums: double precision *intent(in) size(2)*

pair_bo_factors: double precision *intent(in) size(2)*

forces: double precision intent(inout) *size(:, :)* calculated forces

stress: double precision intent(inout) *size(6)* calculated stress

core_add_potential(*n_targets*, *n_params*, *pot_name*, *parameters*, *cutoff*, *smooth_cut*, *elements*, *tags*, *indices*, *orig_elements*, *orig_tags*, *orig_indices*, *pot_index*, *is_multiplier*, *success*)

Creates one additional potential in the core. The routine assumes that adequate memory has been allocated already using core_allocate_potentials.

When the potentials in the Python interface are imported to the Fortran core, the target specifiers (elements, tags, indices) are permutated to create all equivalent potentials. That is, if we have a potential for Si-O, both Si-O and O-Si potentials are created. This is because the energy and force calculation loops only deal with atom pairs A-B once (so only A-B or B-A is considered, not both) and if, say, the loop only finds an O-Si pair, it is important to apply the Si-O interaction also on that pair. In some cases, such as with the bond-bending potential affecting triplets (A-B-C), the interaction is not symmetric for all the atoms. Therefore it is necessary to also store the original targets of the potential as specified in the Python interface. These are to be given in the 'orig_*' lists.

If product potentials are created, all but the first one of the potentials are created with `is_multiplier == .true.`. This leads to the potentials being stored in the global temporary array `multipliers`. The last potential of a group should be created with `is_multiplier = .false.` and the stored multipliers are attached to it. The list of multipliers is not cleared automatically, since usually one creates copies of the same potential with permutated targets and all of these need the same multipiers. Instead the multipliers are cleared with a call of `clear_potential_multipliers()`.

called from PyInterface: `add_potential()`

Parameters:

n_targets: integer *intent(in) scalar* number of targets (interacting bodies)

n_params: integer *intent(in) scalar* number of parameters

pot_name: character(len=*) *intent(in) scalar* potential names

parameters: double precision *intent(in) size(n_params)* numeric parameters

cutoff: double precision *intent(in) scalar* interaction hard cutoff

smooth_cut: double precision *intent(in) scalar* interaction soft cutoff

elements: character(len=label_length) *intent(in) size(n_targets)* atomic symbols specifying the elements the interaction acts on

tags: integer *intent(in) size(n_targets)* tags specifying the atoms the interaction acts on

indices: integer *intent(in) size(n_targets)* indices specifying the atoms the interaction acts on

orig_elements: character(len=label_length) *intent(in) size(n_targets)* original atomic symbols specifying the elements the interaction acts on

orig_tags: integer *intent(in) size(n_targets)* original tags specifying the atoms the interaction acts on

orig_indices: integer *intent(in) size(n_targets)* original indices specifying the atoms the interaction acts on

pot_index: integer *intent(in) scalar* index of the potential

is_multiplier: logical *intent(in) scalar* logical tag specifying if this potential should be treated as a multiplier

success: logical intent(out) *scalar* logical tag specifying if creation of the potential succeeded

core_allocate_bond_order_factors (*n_bond_factors*)
Allocates pointers for storing bond order factors.

called from PyInterface: `allocate_bond_order_factors()`

Parameters:

n_bond_factors: integer *intent(in) scalar*

core_allocate_bond_order_storage (*n_atoms*, *n_groups*, *n_factors*)
Allocates arrays for storing precalculated values of bond order factors and gradients.

called from PyInterface: `allocate_bond_order_factors()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

n_groups: integer *intent(in) scalar* number of bond order groups

n_factors: integer *intent(in) scalar* number of bond order parameters

core_allocate_potentials (*n_pots*)
Allocates pointers for storing potentials.

called from PyInterface: `allocate_potentials()`

Parameters:

n_pots: integer *intent(in) scalar* number of potentials

core_assign_bond_order_factor_indices ()
This routine finds for each atom the potentials for which the atom is an accepted target at the first position. First position here means that for instance in an A-B-C triplet. A is in first position. Being an accepted target means that the atom has the correct element.

called from PyInterface: `create_bond_order_factor_list()`

core_assign_potential_indices()
This routine finds for each atom the potentials for which the atom is an accepted target at the first position. First position here means that for instance in an A-B-C triplet. A is in first position. Being an accepted target means that the atom has the correct element, index or tag (one that the potential targets).

called from PyInterface: `create_potential_list()`

core_build_neighbor_lists(*cutoffs*)
Builds the neighbor lists in the core. The simulation cell must be partitioned with `core_create_space_partitioning()` before this routine can be called.

Parameters:

cutoffs: double precision *intent(in) size(:)* list of cutoffs, atom by atom

core_calculate_bond_order_factors(*group_index*, *total_bond_orders*)
Calculates the bond order sums of all atoms for the given group.

For a factor such as

$$b_i = f(\sum_j c_{ij})$$

The routine calculates

$$\sum_j c_{ij}.$$

The full bond order factor is then obtained by applying the scaling function f. This is done with `core_post_process_bond_order_factors()`.

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

total_bond_orders: double precision intent(inout) *size(:)* the calculated bond order sums

core_calculate_bond_order_gradients(*group_index*, *atom_index*, *raw_sums*, *total_gradient*, *total_virial*, *for_factor*)
Returns the gradients of bond order factors.

For a factor such as

$$b_i = f(\sum_j c_{ij})$$

The routine calculates

$$\nabla_\alpha b_i = f'(\sum_j c_{ij}) \nabla_\alpha \sum_j c_{ij}.$$

By default, the gradients of all factors i are calculated with respect to moving the given atom α. If for_factor is .true., the gradients of the bond factor of the given atom are calculated with respect to moving all atoms.

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

atom_index: integer *intent(in) scalar* index of the atom with respect to which the factors are differentiated (α), or the atoms whose factor is differentiated (i) if for_factor is .true.

raw_sums: double precision *intent(in) size(:)* precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

total_gradient: double precision intent(inout) *size(:, :)* the calculated bond order gradients $\nabla_\alpha b_i$

total_virial: double precision intent(inout) *size(6)* the components of the virial due to the bond order gradients

for_factor: logical *intent(in) scalar optional* a switch for requesting the gradients for a given i instead of a given α

core_calculate_bond_order_gradients_of_factor(*group_index*, *atom_index*, *raw_sums*, *total_gradient*, *total_virial*)

Returns the gradients of one bond order factor with respect to moving all atoms.

This calls `core_calculate_bond_order_gradients()` with for_factor = .true.

For a factor such as

$$b_i = f(\sum_j c_{ij})$$

The routine calculates

$$\nabla_\alpha b_i = f'(\sum_j c_{ij}) \nabla_\alpha \sum_j c_{ij}.$$

The gradients of the bond factor of the given atom i are calculated with respect to moving all atoms α.

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

atom_index: integer *intent(in) scalar* index of the atom whose factor is differentiated (i)

raw_sums: double precision *intent(in) size(:)* precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

total_gradient: double precision intent(inout) *size(:, :)* the calculated bond order gradients $\nabla_\alpha b_i$

total_virial: double precision intent(inout) *size(6)* the components of the virial due to the bond order gradient

core_calculate_electronegativities(*total_enegs*)

Calculates electronegativity forces acting on all atomic charges of the system.

The routine calculates the electronegativities

$$\chi_\alpha = -\frac{\partial V}{\partial q_\alpha}$$

for all atoms α. This is done according to the the structure and potentials allocated in the core, so the routine does not accept arguments. Instead, the core modifying routines such as `core_generate_atoms()` must be called first to set up the calculation.

called from PyInterface: `calculate_electronegativities()`

Parameters:

total_enegs: double precision intent(inout) *size(:)* an array containing the calculated charge forces for all atoms

core_calculate_energy (*total_energy*)
Calculates the total potential energy of the system.

This is done according to the the structure and potentials allocated in the core, so the routine does not accept arguments. Instead, the core modifying routines such as `core_generate_atoms()` must be called first to set up the calculation.

called from PyInterface: `calculate_energy()`

Parameters:

total_energy: double precision intent(out) ***scalar*** calculated total potential energy

core_calculate_forces (*total_forces*, *total_stress*)
Calculates forces acting on all atoms of the system.

The routine calculates the potential gradient

$$\mathbf{F}_\alpha = -\nabla_\alpha V$$

for all atoms α. This is done according to the the structure and potentials allocated in the core, so the routine does not accept arguments. Instead, the core modifying routines such as `core_generate_atoms()` must be called first to set up the calculation.

called from PyInterface: `calculate_forces()`

Parameters:

total_forces: double precision intent(inout) ***size(:, :)*** an array containing the calculated forces for all atoms

total_stress: double precision intent(inout) ***size(6)*** as array containing the calculated stress tensor

core_calculate_pair_bond_order_factor (*atom_pair*, *separation*, *distance*, *direction*, *group_index*, *bond_order_sum*)
Calculates the bond order sum for a given pair of atoms for the given group.

For a factor such as

$$b_i j = f(\sum_k c_{ijk})$$

The routine calculates

$$\sum_k c_{ijk}.$$

The full bond order factor is then obtained by applying the scaling function f. This is done with `core_post_process_bond_order_factors()`.

Parameters:

atom_pair: integer *intent(in) size(2)*

separation: double precision *intent(in) size(3)*

distance: double precision *intent(in) scalar*

direction: double precision *intent(in) size(3)*

group_index: integer ***intent(in) scalar*** an index denoting the potential to which the factor is connected

bond_order_sum: double precision intent(out) ***size(2)*** the calculated bond order sums

core_calculate_pair_bond_order_gradients(*atom_pair*, *separation*, *distance*, *direction*, *group_index*, *raw_sums*, *total_gradient*, *total_virial*)

Returns the gradients of a pair bond order factor.

For a factor such as

$$b_{ij} = f(\sum_k c_{ijk})$$

The routine calculates

$$\nabla_\alpha b_{ij} = f'(\sum_k c_{ijk}) \nabla_\alpha \sum_k c_{ijk}.$$

By default, the gradients the factor ij is calculated with respect to moving all atoms α.

Parameters:

atom_pair: integer *intent(in) size(2)*

separation: double precision *intent(in) size(3)*

distance: double precision *intent(in) scalar*

direction: double precision *intent(in) size(3)*

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

raw_sums: double precision *intent(in) size(2)* precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

total_gradient: double precision intent(inout) *size(:, :, :)* the calculated bond order gradients $\nabla_\alpha b_i$

total_virial: double precision intent(inout) *size(6, 2)* the components of the virial due to the bond order gradient

core_clear_atoms()
Deallocates the array of atoms in the core, if allocated.

core_clear_bond_order_factors()
Deallocates pointers for bond order factors (the parameters)

core_clear_bond_order_storage()
Deallocates pointers for bond order factors (the precalculated factor values).

core_clear_ewald_arrays()

core_clear_potential_multipliers()

core_clear_potentials()
Deallocates pointers for potentials

core_create_cell(*vectors*, *inverse*, *periodicity*)
Creates a supercell for containing the calculation geometry.

called from PyInterface: `create_cell()`

Parameters:

vectors: double precision *intent(in) size(3, 3)* A 3x3 matrix containing the vectors spanning the supercell. The first index runs over xyz and the second index runs over the three vectors.

inverse: double precision *intent(in) size(3, 3)* A 3x3 matrix containing the inverse matrix of the one given in vectors, i.e. $A * B = I$ for the two matrices. Since the latter represents a cell of non-zero volume, this inverse must exist. It is not tested that the given matrix actually is the inverse, the user must make sure it is.

periodicity: logical *intent(in) size(3)* A 3-element vector containing logical tags specifying if the system is periodic in the directions of the three vectors spanning the supercell.

core_create_neighbor_list (*n_nbors*, *atom_index*, *neighbors*, *offsets*)

Assigns a precalculated neighbor list to a single atom of the given index. The neighbor list must be precalculated, this method only stores them in the core. The list must contain an array storing the indices of the neighboring atoms as well as the supercell offsets. The offsets are integer triplets showing how many times must the supercell vectors be added to the position of the neighbor to find the neighboring image in a periodic system. For example, let the supercell be:

```
[[1.0, 0, 0], [0, 1.0, 0], [0, 0, 1.0]],
```

i.e., a unit cube, with periodic boundaries. Now, if we have particles with coordinates:

```
a = [1.5, 0.5, 0.5]
b = [0.4, 1.6, 3.3]
```

the closest separation vector $\mathbf{r}_b - \mathbf{r}_a$ between the particles is:

```
[-.1, .1, -.2]
```

obtained if we add the vector of periodicity:

```
[1.0, -1.0, -3.0]
```

to the coordinates of particle b. The offset vector (for particle b, when listing neighbors of a) is then:

```
[1, -1, -3]
```

Note that if the system is small, one atom can in principle appear several times in the neighbor list with different offsets.

called from PyInterface: `create_neighbor_list()`

Parameters:

n_nbors: integer *intent(in) scalar*

atom_index: integer *intent(in) scalar* index of the atom for which the neighbor list is created

neighbors: integer *intent(in) size(n_nbors)* An array containing the indices of the neighboring atoms

offsets: integer *intent(in) size(3, n_nbors)* An array containing vectors specifying the offsets of the neighbors in periodic systems.

core_create_space_partitioning (*max_cutoff*)

Partitions the simulation volume in subvolumes for fast neighbor searching

Parameters:

max_cutoff: double precision *intent(in) scalar* the maximum cutoff radius for neighbor search

core_debug_dump (*forces*)

Write atomic coordinates and other info in a file. This is only for debugging.

Parameters:

forces: double precision *intent(in) size(:, :)*

core_empty_bond_order_gradient_storage(*index*)
Clears bond order factor gradients (the precalculated gradient values) but does not deallocate the arrays. If an index is given, then only that column is emptied.

Parameters:

index: integer *intent(in) scalar optional* the column to be emptied

core_empty_bond_order_storage()
Clears bond order factors (the precalculated factor values) but does not deallocate the arrays.

core_evaluate_local_doublet(*n_atoms*, *atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *calculation_type*, *energy*, *forces*, *enegs*, *stress*, *many_bodies_found*)
Evaluates the interactions affecting two atoms.

Parameters:

n_atoms: integer *intent(in) scalar* total number of atoms in the system

atom_doublet: type(atom) *intent(in) size(2)* the atoms that are targeted

index1: integer *intent(in) scalar* index of the atom 1

index2: integer *intent(in) scalar* index of the atom 2

test_index1: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer *intent() pointer size(:)* the interactions targeting the given atoms

separations: double precision *intent(in) size(3, 1)* distance vector from 1 to 2, as an array

directions: double precision *intent(in) size(3, 1)* unit vector from 1 to 2, as an array

distances: double precision *intent(in) size(1)* distance from 1 to 2, as an array

calculation_type: integer *intent(in) scalar* the type of information requested

energy: double precision intent(inout) *scalar* calculated energy

forces: double precision intent(inout) *size(3, n_atoms)* calculated forces

enegs: double precision intent(inout) *size(n_atoms)* calculated electronegativities

stress: double precision intent(inout) *size(6)* calculated stress

many_bodies_found: logical intent(out) *scalar* returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_doublet_electronegativities(*n_atoms*, *atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *enegs*, *many_bodies_found*)
Evaluates the local electronegativity affecting two atoms.

Parameters:

n_atoms: integer *intent(in) scalar*

atom_doublet: type(atom) *intent(in) size(2)* the atoms that are targeted

index1: integer *intent(in) scalar* index of the atom 1

index2: integer *intent(in) scalar* index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

enegs: double precision intent(inout) ***size(n_atoms)*** calculated electronegativities

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_doublet_electronegativities_B(*atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *enegs*, *many_bodies_found*, *manybody_indices*, *n_manybody*)

Evaluates the local electronegativity affecting two atoms. (Rearranged internally.)

Parameters:

atom_doublet: type(atom) ***intent(in) size(2)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

enegs: double precision intent(inout) ***size(:)*** calculated electronegativities

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

manybody_indices: integer *intent() pointer size(:)*

n_manybody: integer **intent(out)** *scalar*

core_evaluate_local_doublet_energy(*n_atoms*, *atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *energy*, *many_bodies_found*)

Evaluates the local potential affecting two atoms.

Parameters:

n_atoms: integer *intent(in) scalar*

atom_doublet: type(atom) ***intent(in) size(2)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

energy: double precision intent(inout) ***scalar*** calculated energy

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_doublet_energy_B(*atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *energy*, *many_bodies_found*, *manybody_indices*, *n_manybody*)

Evaluates the local potential affecting two atoms. (Rearranged internally compared to 'A'.)

Parameters:

atom_doublet: type(atom) ***intent(in) size(2)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

energy: double precision intent(inout) ***scalar*** calculated energy

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

manybody_indices: integer *intent() pointer size(:)*

n_manybody: integer **intent(out)** *scalar*

core_evaluate_local_doublet_forces(*n_atoms*, *atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *forces*, *stress*, *many_bodies_found*)

Evaluates the local force affecting two atoms.

Parameters:

n_atoms: integer ***intent(in) scalar*** total number of atoms in the system

atom_doublet: type(atom) ***intent(in) size(2)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

forces: double precision intent(inout) ***size(3, n_atoms)*** calculated forces

stress: double precision intent(inout) ***size(6)*** calculated stress

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_doublet_forces_B(*atom_doublet*, *index1*, *index2*, *test_index1*, *interaction_indices*, *separations*, *directions*, *distances*, *forces*, *stress*, *many_bodies_found*, *manybody_indices*, *n_manybody*)

Evaluates the local force affecting two atoms. (Rearranged internally.)

Parameters:

atom_doublet: type(atom) ***intent(in) size(2)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

test_index1: integer ***intent(in) scalar*** if 1, test if the interaction targets atom1; similarly for 2

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 1)*** distance vector from 1 to 2, as an array

directions: double precision ***intent(in) size(3, 1)*** unit vector from 1 to 2, as an array

distances: double precision ***intent(in) size(1)*** distance from 1 to 2, as an array

forces: double precision intent(inout) ***size(:, :)*** calculated forces

stress: double precision intent(inout) ***size(6)*** calculated stress

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

manybody_indices: integer *intent() pointer size(:)*

n_manybody: integer **intent(out)** *scalar*

core_evaluate_local_quadruplet(*n_atoms*, *atom_quadruplet*, *index1*, *index2*, *index3*, *index4*, *test_index1*, *test_index2*, *test_index3*, *interaction_indices*, *separations*, *directions*, *distances*, *calculation_type*, *energy*, *forces*, *enegs*, *stress*, *many_bodies_found*)

Evaluates the interactions affecting four atoms.

Parameters:

n_atoms: integer ***intent(in) scalar*** total number of atoms in the system

atom_quadruplet: type(atom) ***intent(in) size(4)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

index3: integer ***intent(in) scalar*** index of the atom 3

index4: integer ***intent(in) scalar*** index of the atom 4

test_index1: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index2: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index3: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

interaction_indices: integer *intent() pointer size(:)* the interactions targeting the given atoms

separations: double precision *intent(in) size(3, 3)* distance vector from 1 to 2, 2 to 3 and 3 to 4 as an array

directions: double precision *intent(in) size(3, 3)* unit vector from 1 to 2, 2 to 3 and 3 to 4 as an array

distances: double precision *intent(in) size(3)* distance from 1 to 2, 2 to 3 and 3 to 4 as an array

calculation_type: integer *intent(in) scalar* the type of information requested

energy: double precision intent(out) *scalar* calculated energy

forces: double precision intent(out) *size(3, n_atoms)* calculated forces

enegs: double precision intent(out) *size(n_atoms)* calculated electronegativities

stress: double precision intent(out) *size(6)* calculated stress

many_bodies_found: logical intent(out) *scalar* returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_quadruplet_B(*atom_quadruplet*, *index1*, *index2*, *index3*, *index4*, *test_index1*, *test_index2*, *test_index3*, *separations*, *directions*, *distances*, *calculation_type*, *energy*, *forces*, *enegs*, *stress*, *many_bodies_found*, *many-body_indices*, *n_manybody*)

Evaluates the interactions affecting four atoms. (Rearranged internally.)

Parameters:

atom_quadruplet: type(atom) *intent(in) size(4)* the atoms that are targeted

index1: integer *intent(in) scalar* index of the atom 1

index2: integer *intent(in) scalar* index of the atom 2

index3: integer *intent(in) scalar* index of the atom 3

index4: integer *intent(in) scalar* index of the atom 4

test_index1: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index2: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index3: integer *intent(in) scalar* if 1, test if the ineraction targets atom1; similarly for 2, 3

separations: double precision *intent(in) size(3, 3)* distance vector from 1 to 2, 2 to 3 and 3 to 4 as an array

directions: double precision *intent(in) size(3, 3)* unit vector from 1 to 2, 2 to 3 and 3 to 4 as an array

distances: double precision *intent(in) size(3)* distance from 1 to 2, 2 to 3 and 3 to 4 as an array

calculation_type: integer *intent(in) scalar* the type of information requested

energy: double precision intent(inout) *scalar* calculated energy

forces: double precision intent(inout) *size(:, :)* calculated forces

enegs: double precision intent(inout) *size(:)* calculated electronegativities

stress: double precision intent(inout) ***size(6)*** calculated stress

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

manybody_indices: integer *intent() pointer size(:)*

n_manybody: integer *intent(in) scalar*

core_evaluate_local_singlet(*index1*, *atom_singlet*, *interaction_indices*, *calculation_type*, *energy*, *forces*, *stress*, *enegs*)

Evaluates the local potential affecting a single atom

Parameters:

index1: integer ***intent(in) scalar*** index of the atom

atom_singlet: type(atom) ***intent(in) scalar*** the atom that is targeted

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atom

calculation_type: integer ***intent(in) scalar*** specifies if we are evaluating the energy, forces, or electronegativities

energy: double precision intent(inout) ***scalar*** calculated energy

forces: double precision intent(inout) ***size(:, :)*** calculated forces

stress: double precision intent(inout) ***size(6)*** calculated stress

enegs: double precision intent(inout) ***size(:)*** calculated electronegativities

core_evaluate_local_triplet(*n_atoms*, *atom_triplet*, *index1*, *index2*, *index3*, *test_index1*, *test_index2*, *interaction_indices*, *separations*, *directions*, *distances*, *calculation_type*, *energy*, *forces*, *enegs*, *stress*, *many_bodies_found*)

Evaluates the interactions affecting three atoms.

Parameters:

n_atoms: integer ***intent(in) scalar*** total number of atoms in the system

atom_triplet: type(atom) ***intent(in) size(3)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

index3: integer ***intent(in) scalar*** index of the atom 3

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index2: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2, 3

interaction_indices: integer ***intent() pointer size(:)*** the interactions targeting the given atoms

separations: double precision ***intent(in) size(3, 2)*** distance vector from 1 to 2 and 2 to 3 as an array

directions: double precision ***intent(in) size(3, 2)*** unit vector from 1 to 2 and 2 to 3 as an array

distances: double precision ***intent(in) size(2)*** distance from 1 to 2 and 2 to 3 as an array

calculation_type: integer ***intent(in) scalar*** the type of information requested

energy: double precision intent(out) ***scalar*** calculated energy

forces: double precision intent(out) ***size(3, n_atoms)*** calculated forces

enegs: double precision intent(out) ***size(n_atoms)*** calculated electronegativities

stress: double precision intent(out) ***size(6)*** calculated stress

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

core_evaluate_local_triplet_B(*atom_triplet*, *index1*, *index2*, *index3*, *test_index1*, *test_index2*, *separations*, *directions*, *distances*, *calculation_type*, *energy*, *forces*, *enegs*, *stress*, *many_bodies_found*, *manybody_indices*, *n_manybody*)

Evaluates the interactions affecting three atoms. (Rearranged internally.)

Parameters:

atom_triplet: type(atom) ***intent(in) size(3)*** the atoms that are targeted

index1: integer ***intent(in) scalar*** index of the atom 1

index2: integer ***intent(in) scalar*** index of the atom 2

index3: integer ***intent(in) scalar*** index of the atom 3

test_index1: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2, 3

test_index2: integer ***intent(in) scalar*** if 1, test if the ineraction targets atom1; similarly for 2, 3

separations: double precision ***intent(in) size(3, 2)*** distance vector from 1 to 2 and 2 to 3 as an array

directions: double precision ***intent(in) size(3, 2)*** unit vector from 1 to 2 and 2 to 3 as an array

distances: double precision ***intent(in) size(2)*** distance from 1 to 2 and 2 to 3 as an array

calculation_type: integer ***intent(in) scalar*** the type of information requested

energy: double precision intent(inout) ***scalar*** calculated energy

forces: double precision intent(inout) ***size(:, :)*** calculated forces

enegs: double precision intent(inout) ***size(:)*** calculated electronegativities

stress: double precision intent(inout) ***size(6)*** calculated stress

many_bodies_found: logical intent(out) ***scalar*** returns true if the loop finds an interaction with 3 or more targets

manybody_indices: integer *intent() pointer size(:)*

n_manybody: integer *intent(in) scalar*

core_fill_bond_order_storage()

Fills the storage for bond order factors and bond order sums. This is meant to be called in the beginning of force and energy evaluation. The routine calculates all bond order factors (in parallel, if run in MPI) and stores them. Then during the energy or force calculation, it is sufficient to just look up the needed values in the arrays. The routine does not calculate and store bond factor gradients.

core_generate_atoms(*n_atoms*, *masses*, *charges*, *positions*, *momenta*, *tags*, *elements*)

Creates the atomic particles by invoking a subroutine in the geometry module.

called from PyInterface: `create_atoms()`

Parameters:

n_atoms: integer ***intent(in) scalar*** number of atoms

masses: double precision ***intent(in) size(n_atoms)*** masses of atoms

charges: double precision *intent(in) size(n_atoms)* electric charges of atoms

positions: double precision *intent(in) size(3, n_atoms)* coordinates of atoms

momenta: double precision *intent(in) size(3, n_atoms)* momenta of atoms

tags: integer *intent(in) size(n_atoms)* numeric tags for the atoms

elements: character(len=label_length) *intent(in) size(n_atoms)* atomic symbols of the atoms

core_get_bond_order_factor_of_atom(*group_index*, *atom_index*, *bond_order_factor*)
Returns the bond order factors of the given atom for the given group.

Parameters:

group_index: integer *intent(in) scalar* index for the bond order factor group

atom_index: integer *intent(in) scalar* index of the atom whose bond order factor is returned

bond_order_factor: double precision intent(inout) *scalar* the calculated bond order factor

core_get_bond_order_factors(*group_index*, *bond_order_factors*)
Returns the bond order factors of all atoms for the given group. The routines tries to find the values in the stored precalculated values first if use_saved_bond_order_factors is true, and saves the calculated values if it does not find them.

Parameters:

group_index: integer *intent(in) scalar* index for the bond order factor group

bond_order_factors: double precision intent(inout) *size(:)* the calculated bond order factors

core_get_bond_order_gradients(*group_index*, *atom_index*, *slot_index*, *bond_order_gradients*, *bond_order_virial*)
Returns the gradients of the bond order factor of the given atom with respect to moving all atoms, for the given group. The routine tries to find the values in the stored precalculated values first if use_saved_bond_order_factors is true, and saves the calculated values if it does not find them.

The slot index is the index of the atom in the interaction being evaluated (so for a triplet A-B-C, A would have slot 1, B slot 2, and C slot 3). This is only used for storing the values.

Parameters:

group_index: integer *intent(in) scalar* index for the bond order factor group

atom_index: integer *intent(in) scalar* index of the atom whose bond order factor is differentiated

slot_index: integer *intent(in) scalar* index denoting the position of the atom in an interacting group (such as A-B-C triplet)

bond_order_gradients: double precision intent(inout) *size(:, :)* the calculated gradients of the bond order factor

bond_order_virial: double precision intent(inout) *size(6)* the components of the virial due to the bond order factors

core_get_bond_order_sums(*group_index*, *bond_order_sums*)
Returns the bond order sums of all atoms for the given group. By 'bond order sum', we mean the summation of local terms without per atom scaling. E.g., for $b_i = 1 + \sum c_{ij}$, $\sum c_{ij}$ is the sum. The routines tries to find the values in the stored precalculated values first if use_saved_bond_order_factors is true, and saves the calculated values if it does not find them.

Parameters:

group_index: integer *intent(in) scalar* index for the bond order factor group

bond_order_sums: double precision intent(inout) *size(:)* the calculated bond order sums

core_get_cell_vectors (*vectors*)
Returns the vectors defining the supercell stored in the core.

called from PyInterface: `get_cell_vectors()`

Parameters:

vectors: double precision intent(out) ***size(3, 3)*** A 3x3 matrix containing the vectors spanning the supercell. The first index runs over xyz and the second index runs over the three vectors.

core_get_ewald_energy (*real_cut*, *k_cut*, *reciprocal_cut*, *sigma*, *epsilon*, *energy*)
Debug routine for Ewald

Parameters:

real_cut: double precision *intent(in) scalar*

k_cut: double precision *intent(in) scalar*

reciprocal_cut: integer *intent(in) size(3)*

sigma: double precision *intent(in) scalar*

epsilon: double precision *intent(in) scalar*

energy: double precision **intent(out)** *scalar*

core_get_neighbor_list_of_atom (*atom_index*, *n_neighbors*, *neighbors*, *offsets*)
Returns the list of neighbros for an atom

Parameters:

atom_index: integer ***intent(in) scalar*** the index of the atom whose neighbors are returned

n_neighbors: integer ***intent(in) scalar*** the number of neighbors

neighbors: integer intent(out) ***size(n_neighbors)*** the indices of the neighboring atoms

offsets: integer intent(out) ***size(3, n_neighbors)*** the offsets for periodic boundaries

core_get_number_of_atoms (*n_atoms*)
Returns the number of atoms in the array allocated in the core.

called from PyInterface: `get_number_of_atoms()`

Parameters:

n_atoms: integer intent(out) ***scalar*** number of atoms

core_get_number_of_neighbors (*atom_index*, *n_neighbors*)
Returns the number of neighbors for an atom

Parameters:

atom_index: integer ***intent(in) scalar*** the index of the atoms

n_neighbors: integer intent(out) ***scalar*** the number of neighbors

core_loop_over_local_interactions (*calculation_type*, *total_energy*, *total_forces*, *total_enegs*, *total_stress*)
Loops over atoms, atomic pairs, atomic triplets, and atomic quadruplets and calculates the contributions from local potentials to energy, forces, or electronegativities. This routine is called from the routines

- `core_calculate_energy()`
- `core_calculate_forces()`
- `core_calculate_electronegaivities()`

Parameters:

calculation_type: integer *intent(in) scalar* index to specify if the loop calculates energies, forces, or e-negativities

total_energy: double precision intent(inout) *scalar* calculated energy

total_forces: double precision intent(inout) *size(:, :)* calculated forces

total_enegs: double precision intent(inout) *size(:)* calculated electronegativities

total_stress: double precision intent(inout) *size(6)* calculated stress

core_post_process_bond_order_factors (*group_index*, *raw_sums*, *total_bond_orders*)

Bond-order post processing, i.e., application of per-atom scaling functions.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_i = f(\sum_j c_{ij}) = 1 + \sum_j c_{ij},$$

the $\sum_j c_{ij}$ would have been calculated already (with `core_calculate_bond_order_factors()`) and the operation $f(x) = 1 + x$ remains to be carried out. The post processing is done per atom regardless of if the bond factor is of a pair or many body type.

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

raw_sums: double precision *intent(in) size(:)* precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

total_bond_orders: double precision intent(inout) *size(:)* the calculated bond order factors b_i

core_post_process_bond_order_gradients (*group_index*, *raw_sums*, *raw_gradients*, *total_bond_gradients*, *mpi_split*)

Bond-order post processing, i.e., application of per-atom scaling functions. This routine does the scaling for all bond factors with the given bond order sums and gradients of these sums.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_i = f(\sum_j c_{ij}) = 1 + \sum_j c_{ij},$$

the $\sum_j c_{ij}$ would have been calculated already and the operation $f(x) = 1 + x$ remains to be carried out. The post processing is done per atom regardless of if the bond factor is of a pair or many body type.

For gradients, one needs to evaluate

$$\nabla_\alpha b_i = f'(\sum_j c_{ij}) \nabla_\alpha \sum_j c_{ij}$$

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

raw_sums: double precision *intent(in) size(:)* precalculated bond order sums, $\sum_j c_{ij}$, in the above example

raw_gradients: double precision *intent(in) size(:, :)* precalculated gradients of bond order sums, $\nabla_\alpha \sum_j c_{ij}$, in the above example

total_bond_gradients: double precision intent(inout) *size(:, :)* the calculated bond order gradients $\nabla_\alpha b_i$

mpi_split: logical *intent(in) scalar optional* A switch for enabling MPI parallelization. By default the routine is sequential since the calculation may be called from within an already parallelized routine.

core_post_process_bond_order_gradients_of_factor(*group_index*, *atom_index*, *raw_sum*, *raw_gradients*, *total_bond_gradients*, *raw_virial*, *total_virial*, *mpi_split*)

Bond-order post processing, i.e., application of per-atom scaling functions. This routine does the scaling for the bond order factor of the given atom with respect to moving all atoms with the given bond order sum for the factor and the gradients of the sum with respect to moving all atoms.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_i = f(\sum_j c_{ij}) = 1 + \sum_j c_{ij},$$

the $\sum_j c_{ij}$ would have been calculated already and the operation $f(x) = 1 + x$ remains to be carried out. The post processing is done per atom regardless of if the bond factor is of a pair or many body type.

For gradients, one needs to evaluate

$$\nabla_\alpha b_i = f'(\sum_j c_{ij}) \nabla_\alpha \sum_j c_{ij}$$

Parameters:

group_index: integer *intent(in) scalar* an index denoting the potential to which the factor is connected

atom_index: integer *intent(in) scalar* the index of the atom whose factor is differentiated (i)

raw_sum: double precision *intent(in) scalar* precalculated bond order sum for the given atom, $\sum_j c_{ij}$, in the above example

raw_gradients: double precision *intent(in) size(:, :)* precalculated gradients of bond order sums, $\nabla_\alpha \sum_j c_{ij}$, in the above example

total_bond_gradients: double precision intent(inout) *size(:, :)* the calculated bond order gradients $\nabla_\alpha b_i$

raw_virial: double precision *intent(in) size(6)* the precalculated virial due to the bond order gradient

total_virial: double precision intent(inout) *size(6)* the scaled virial due to the bond order gradient

mpi_split: logical *intent(in) scalar optional* A switch for enabling MPI parallelization. By default the routine is sequential since the calculation may be called from within an already parallelized routine.

core_post_process_pair_bond_order_factor(*atom1*, *group_index*, *raw_sum*, *total_bond_order*)

Bond-order post processing, i.e., application of per-pair scaling functions.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_{ij} = f(\sum_k c_{ijk}) = 1 + \sum_k c_{ijk},$$

the $\sum_k c_{ijk}$ would have been calculated already (with `core_calculate_pair_bond_order_factor()`) and the operation $f(x) = 1 + x$ remains to be carried out.

Parameters:

atom1: type(atom) ***intent(in) scalar*** the central atom of the pair bond order factor

group_index: integer ***intent(in) scalar*** an index denoting the potential to which the factor is connected

raw_sum: double precision ***intent(in) scalar*** precalculated bond order sum, $\sum_k c_{ijk}$, in the above example.

total_bond_order: double precision intent(out) ***scalar*** the calculated bond order factor b_{ij}

core_post_process_pair_bond_order_gradients(*group_index*, *atom1*, *raw_sum*, *raw_gradients*, *total_bond_gradients*, *raw_virial*, *total_virial*, *mpi_split*)

Bond-order post processing, i.e., application of per-pair scaling functions. This routine does the scaling for the bond order factor of the given pair with respect to moving all atoms with the given bond order sum for the factor and the gradients of the sum with respect to moving all atoms.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_{ij} = f(\sum_k c_{ijk}) = 1 + \sum_k c_{ijk},$$

the $\sum_k c_{ijk}$ would have been calculated already and the operation $f(x) = 1 + x$ remains to be carried out. The post processing is done per pair.

For gradients, one needs to evaluate

$$\nabla_\alpha b_{ij} = f'(\sum_k c_{ijk}) \nabla_\alpha \sum_k c_{ijk}$$

Parameters:

group_index: integer ***intent(in) scalar*** an index denoting the potential to which the factor is connected

atom1: type(atom) ***intent(in) scalar*** the central atom of the pair bond order factor

raw_sum: double precision ***intent(in) scalar*** precalculated bond order sum for the given atom, $\sum_j c_{ij}$, in the above example

raw_gradients: double precision ***intent(in) size(:, :)*** precalculated gradients of bond order sums, $\nabla_\alpha \sum_j c_{ij}$, in the above example

total_bond_gradients: double precision intent(out) ***size(:, :)*** the calculated bond order gradients $\nabla_\alpha b_i$

raw_virial: double precision ***intent(in) size(6)*** the precalculated virial due to the bond order gradient

total_virial: double precision intent(out) ***size(6)*** the scaled virial due to the bond order gradient

mpi_split: logical *intent(in) scalar optional* A switch for enabling MPI parallelization. By default the routine is sequential since the calculation may be called from within an already parallelized routine.

core_release_all_memory()
Release all allocated pointer arrays in the core.

core_set_ewald_parameters(*real_cut*, *k_radius*, *reciprocal_cut*, *sigma*, *epsilon*, *scaler*)
Sets the parameters for Ewald summation in the core.

Parameters:

real_cut: double precision *intent(in) scalar* the real-space cutoff

k_radius: double precision *intent(in) scalar* the k-space cutoff (in inverse length)

reciprocal_cut: integer *intent(in) size(3)* the k-space cutoffs (in numbers of k-space cells)

sigma: double precision *intent(in) scalar* the split parameter

epsilon: double precision *intent(in) scalar* electric constant

scaler: double precision *intent(in) size(:)* scaling factors for the individual charges

core_update_atom_charges(*n_atoms*, *charges*)
Updates the charges of atomic particles.

called from PyInterface: `update_atom_charges()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

charges: double precision *intent(in) size(n_atoms)* new charges for the atoms

core_update_atom_coordinates(*n_atoms*, *positions*, *momenta*)
Updates the positions and momenta of atomic particles.

called from PyInterface: `update_atom_coordinates()`

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

positions: double precision *intent(in) size(3, n_atoms)* new coordinates for the atoms

momenta: double precision *intent(in) size(3, n_atoms)* new momenta for the atoms

expand_neighbor_storage(*nbors_and_offsets*, *length*, *new_length*, *n_atoms*)
Expands the allocated memory for storing neighbor lists

Parameters:

nbors_and_offsets: integer *intent() pointer size(:, :, :)*

length: integer *intent(in) scalar*

new_length: integer *intent(in) scalar*

n_atoms: integer *intent(in) scalar*

list_atoms()
Prints some information on the atoms stored in the core in stdout.

list_bonds()
Prints some information on the bond order factors stored in the core in stdout.

list_cell()
Prints some information on the supercell stored in the core in stdout.

list_interactions()
Prints some information on the potentials stored in the core in stdout.

potentials (Potentials.f90)

Potentials contains the low-level routines for handling interactions. The module defines custom types for both describing the types of potentials and bond order factors (potential_descriptor, bond_order_descriptor) as well as for storing the parameters of actual interactions in use for the Fortran calculations (potential, bond_order_parameters). Tools for creating the custom datatypes (create_potential(), create_bond_order_factor()) are provided.

The types of potentials and bond order factors are defined using the types potential_descriptor and bond_order_descriptor. These should be created at start-up and remain untouched during simulation. They are used by the Fortran core for checking the types of parameters a potential needs, for instance, but they are also accessible from the Python interface. Especially, upon creation of Potential and BondOrderParameters instances, one needs to specify the type as a keyword. This keyword is then compared to the list of characterizers in the core to determine the type of the interaction.

The basic routines for calculating the actual forces and energies are also defined in this module (evaluate_energy(), evaluate_forces(), evaluate_bond_order_factor(), evaluate_bond_order_gradient()). However, these routines do not calculate the total potential energy of the system, V, or the total forces acting on the particles, $\mathbf{F} = -\nabla_\alpha V$. Instead, the routines evaluate the contributions from individual atoms, atom pairs, atom triplets, etc. For instance, let the total energy of the system be

$$V = \sum_p \left(\sum_i v_i^p + \sum_{(i,j)} v_{ij}^p + \sum_{(i,j,k)} v_{ijk}^p \right),$$

where p sums over the different potentials acting on the system and i, (i,j) and (i,j,k) sum over all atoms, pairs and triplet, respectively. Then the energy terms v are obtained from evaluate_energy(). In pseudo-code,

$$v_S^p = \texttt{evaluate\_energy}(S, p),$$

where S is a set of atoms. The summation over potentials and atoms is done in *pysic_core (Core.f90)* in calculate_energy(). Similarly for forces, the summation is carried out in calculate_forces().

The reason for separating the calculation of individual interaction terms to *potentials (Potentials.f90)* and the overall summation to *pysic_core (Core.f90)* is that only the core knows the current structure and interactions of the system. It is the task of this module to tell the core how all the potentials behave given any local structure, but the overall system information is kept in the core. So during energy evaluation, *pysic_core (Core.f90)* finds all local structures that possibly contribute with an interaction and asks *potentials (Potentials.f90)* to calculate this contribution.

Bond order factors are potential modifiers, not direct interactions themselves. In general, the factors are scalar functions defined per atom, for instance,

$$b_i^p = s_i^p \left(\sum_{(i,j)} c_{ij}^p + \sum_{(i,j,k)} c_{ijk}^p \right)$$

for a three-body factor, where c^p are local contributions (usually representing chemical bonds) and s_i^p is a per atom scaling function. The bond factors multiply the potentials p leading to the total energy

$$V = \sum_p \left(\sum_i b_i^p v_i^p + \sum_{(i,j)} \frac{1}{2}(b_i^p + b_j^p) v_{ij}^p + \sum_{(i,j,k)} \frac{1}{3}(b_i^p + b_j^p + b_k^p) v_{ijk}^p \right).$$

The corresponding total force on atom α is then

$$\mathbf{F}_\alpha = -\nabla_\alpha V = -\sum_p \left(\sum_i ((\nabla_\alpha b_i^p) v_i^p + b_i^p (\nabla_\alpha v_i^p)) + \dots \right).$$

The contributions $\mathbf{f}_\alpha^p = -\nabla_\alpha v^p$, c^p, and $\nabla_\alpha c^p$ are calculated in `evaluate_forces()`, `evaluate_bond_order_factor()`, and `evaluate_bond_order_gradient()`. Application of the scaling functions s_i and s_i' on the sums $\sum_{(i,j)} c_{ij}^p + \sum_{(i,j,k)} c_{ijk}^p$ is done in the routines `post_process_bond_order_factor()` and `post_process_bond_order_gradient()` to produce the actual bond order factors b_i^p and gradients $\nabla_\alpha b_i^p$. These sums, similarly to the energy and force summations, are evaluated with `core_calculate_bond_order_factors()` in *pysic_core (Core.f90)*.

Note when adding potentials or bond order factors in the source code:

The parameters defined in Potentials.f90 are used for determining the maximum sizes of arrays, numbers of potentials and bond factors, and the internally used indices for them. When adding new potentials of bond factors, make sure to update the relevant numbers. Especially the number of potentials (`n_potential_types`) or number of bond order factors (`n_bond_order_types`) must be increased when more types are defined.

Also note that in *pysic_interface (PyInterface.f90)*, some of these parameters are used for determining array sizes. However, the actual parameters are not used because f2py does not read the values from here. Therefore if you change a parameter here, search for its name in *pysic_interface (PyInterface.f90)* to see if the name appears in a comment. That is an indicator that a numeric value must be updated accordingly.

Full documentation of global variables in potentials

bond_descriptors_created
logical *scalar*

initial value = .false.

logical tag used for managing pointer allocations for bond order factor descriptors

bond_order_descriptors
type(bond_order_descriptor) *pointer size(:)*

an array for storing descriptors for the different *types* of bond order factors

c_scale_index
integer *scalar parameter*

initial value = 3

internal index for the coordination scaling function

coordination_index
integer *scalar parameter*

initial value = 1

descriptors_created
logical *scalar*

initial value = .false.

logical tag used for managing pointer allocations for potential descriptors

ewald_arrays_allocated
logical *scalar*

initial value = .false.

ewald_forces
double precision *pointer size(:, :, :)*

ewald_sum_forces
double precision *pointer size(:, :, :)*

ewald_tmp_enegs
double precision *pointer size(:)*

mono_const_index
integer *scalar parameter*

initial value = 3

internal index for the constant force potential

mono_none_index
integer *scalar parameter*

initial value = 6

internal index for the constant potential

mono_qself_index
integer *scalar parameter*

initial value = 11

n_bond_order_types
integer *scalar parameter*

initial value = 8

number of different types of bond order factors known

n_max_params
integer *scalar parameter*

initial value = 12

n_potential_types
integer *scalar parameter*

initial value = 16

number of different types of potentials known

no_name
character(len=label_length) *scalar parameter*

initial value = "xx"

The label for unlabeled atoms. In other words, there are routines that expect atomic symbols as arguments, but if there are no symbols to pass, this should be given to mark an empty entry.

pair_buck_index
integer *scalar parameter*

initial value = 7

internal index for the Buckingham potential

pair_exp_index
integer *scalar parameter*

initial value = 5

pair_lj_index
integer *scalar parameter*

initial value = 1

internal index for the Lennard-Jones potential

pair_power_index
integer *scalar parameter*

initial value = 9

internal index for the power law potential

pair_qabs_index
integer *scalar parameter*

initial value = 14

pair_qexp_index
integer *scalar parameter*

initial value = 13

pair_qpair_index
integer *scalar parameter*

initial value = 12

pair_shift_index
integer *scalar parameter*

initial value = 15

pair_spring_index
integer *scalar parameter*

initial value = 2

internal index for the spring potential

pair_step_index
integer *scalar parameter*

initial value = 16

pair_table_index
integer *scalar parameter*

initial value = 10

internal index for the tabulated potential

param_name_length
integer *scalar parameter*

initial value = 10

param_note_length
integer *scalar parameter*

initial value = 100

maximum length allowed for the descriptions of parameters

pot_name_length
integer *scalar parameter*

initial value = 11

maximum length allowed for the names of potentials

pot_note_length
integer *scalar parameter*

initial value = 500

maximum lenght allowed for the description of the potential

potential_descriptors
type(potential_descriptor) *pointer size(:)*

an array for storing descriptors for the different *types* of potentials

power_index
integer *scalar parameter*

initial value = 5

internal index for the power law bond order factor

quad_dihedral_index
integer *scalar parameter*

initial value = 8

internal index for the dihedral angle potential

s_factor
double precision *pointer size(:, :, :, :)*

s_factor_allocated
logical *scalar*

initial value = .false.

sqrt_scale_index
integer *scalar parameter*

initial value = 6

internal index for the square root scaling function

stored_factor_cutoffs
integer *size(3)*

table_bond_index
integer *scalar parameter*

initial value = 7

internal index for the tabulated bond order factor

table_prefix
character(len=6) *scalar parameter*

initial value = "**table_**"

prefix for filenames for storing tables

table_scale_index
integer *scalar parameter*

initial value = 8

internal index for the tabulated scaling function

table_suffix
character(len=4) *scalar parameter*

initial value = ".txt"

tersoff_index
integer *scalar parameter*

initial value = 2

internal index for the Tersoff bond order factor

tmp_factor
double precision *pointer size(:, :, :, :)*

tri_bend_index
integer *scalar parameter*

initial value = 4

internal index for the bond bending potential

triplet_index
integer *scalar parameter*

initial value = 4

internal index for the triplet bond order factor

Full documentation of custom types in potentials

bond_order_descriptor
Description of a type of a bond order factor. The type contains the name and description of the bond order factor and the parameters it contains. The descriptors contain the information that the inquiry methods in the python interface fetch.

Contained data:

parameter_notes: character(len=param_note_length) ***pointer size(:, :)*** Descriptions of the parameters. The descriptions should be very short indicators such as 'spring constant' or 'energy coefficient'. For more detailed explanations, the proper documentation should be used.

n_parameters: integer ***pointer size(:)*** number of parameters for each number of bodies (1-body parameters, 2-body parameters etc.)

n_level: integer ***scalar*** 1 for atomic bond order factors, 2 for pairwise factors

name: character(len=pot_name_length) ***scalar*** The name of the bond order factor: this is a keyword according to which the factor may be recognized.

description: character(len=pot_note_length) ***scalar*** A description of the bond order factor. This should contain the mathematical formulation as well as a short verbal explanation.

includes_post_processing: logical ***scalar*** a logical tag specifying if there is a scaling function s_i attached to the factor.

type_index: integer ***scalar*** The internal index of the bond order factor. This can also be used for recognizing the factor and must therefore match the name. For instance, if name = 'neighbors', type_index = `coordination_index`.

n_targets: integer ***scalar*** number of targets, i.e., interacting bodies

parameter_names: character(len=param_name_length) ***pointer size(:, :)*** The names of the parameters of the bond order factor: these are keywords according to which the parameters may be recognized.

`bond_order_parameters`

Defines a particular bond order factor. The factor should correspond to the description of some built-in type and hold actual numeric values for parameters. In addition a real bond order factor must have information on the particles it acts on and the range it operates in. These are created based on the `BondOrderParameters` objects in the Python interface when calculations are invoked.

Contained data:

cutoff: double precision ***scalar*** The hard cutoff for the bond order factor. If the atoms are farther away from each other than this, they do not contribute to the total bond order factor does not affect them.

n_level: integer ***scalar*** 1 for atomic bond order factors, 2 for pairwise

soft_cutoff: double precision ***scalar*** The soft cutoff for the bond order factor. If this is smaller than the hard cutoff, the bond contribution is scaled to zero continuously when the interatomic distances grow from the soft to the hard cutoff.

parameters: double precision ***pointer size(:, :)*** numerical values for parameters

group_index: integer ***scalar*** The internal index of the *potential* the bond order factor is modifying.

includes_post_processing: logical ***scalar*** a logical switch specifying if there is a scaling function s_i attached to the factor

type_index: integer ***scalar*** The internal index of the bond order factor *type*. This is used for recognizing the factor. Note that the bond order parameters instance does not have a name. If the name is needed, it can be obtained from the `bond_order_descriptor` of the correct index.

n_params: integer ***pointer size(:)*** array containing the numbers of parameters for different number of targets (1-body parameters, 2-body parameters, etc.)

table: double precision ***pointer size(:, :)*** array for storing tabulated values

original_elements: character(len=2) ***pointer size(:)*** The list of elements (atomic symbols) of the original `BondOrderParameters` in the Python interface from which this factor was created. Whereas the apply_elements lists are used for finding all pairs and triplets of atoms which could contribute to the bond order factor, the original_elements lists specify the roles of atoms in the factor.

derived_parameters: double precision ***pointer size(:, :)*** numerical values for parameters calculated based on the parameters specified by the user

apply_elements: character(len=2) ***pointer size(:)*** A list of elements (atomic symbols) the factor affects. E.g., for Si-O bonds, it would be ('Si','O'). Note that unlike in the Python interface, a single `bond_order_parameters` only has one set of targets, and for multiple target options several `bond_order_parameters` instances are created.

`potential`

Defines a particular potential. The potential should correspond to the description of some built-in

type and hold actual numeric values for parameters. In addition, a real potential must have information on the particles it acts on and the range it operates in. These are to be created based on the `Potential` objects in the Python interface when calculations are invoked.

Contained data:

pot_index: integer ***scalar*** The internal index of the *actual potential*. This is needed when bond order factors are included so that the factors may be joint with the correct potentials.

smoothened: logical ***scalar*** logical switch specifying if a smooth cutoff is applied to the potential

n_product: integer ***scalar*** number of multipliers for a product potential

filter_elements: logical ***scalar*** a logical switch specifying whether the potential targets atoms based on the atomic symbols

parameters: double precision ***pointer size(:)*** numerical values for parameters

cutoff: double precision ***scalar*** The hard cutoff for the potential. If the atoms are farther away from each other than this, the potential does not affect them.

soft_cutoff: double precision ***scalar*** The soft cutoff for the potential. If this is smaller than the hard cutoff, the potential is scaled to zero continuously when the interatomic distances grow from the soft to the hard cutoff.

apply_tags: integer ***pointer size(:)*** A list of atom tags the potential affects. Note that unlike in the Python interface, a single `potential` only has one set of targets, and for multiple target options several `potential` instances are created.

original_indices: integer ***pointer size(:)*** The list of atom indices of the original `Potential` in the Python interface from which this potential was created. Whereas the apply_* lists are used for finding all pairs and triplets of atoms for which the potential could act on, the original_* lists specify the roles of atoms in the interaction.

apply_indices: integer ***pointer size(:)*** A list of atom indices the potential affects. Note that unlike in the Python interface, a single `potential` only has one set of targets, and for multiple target options several `potential` instances are created.

filter_indices: logical ***scalar*** a logical switch specifying whether the potential targets atoms based on the atom indices

type_index: integer ***scalar*** The internal index of the potential *type*. This is used for recognizing the potential. Note that the potential instance does not have a name. If the name is needed, it can be obtained from the `potential_descriptor` of the correct index.

original_tags: integer ***pointer size(:)*** The list of atom tags of the original `Potential` in the Python interface from which this potential was created. Whereas the apply_* lists are used for finding all pairs and triplets of atoms for which the potential could act on, the original_* lists specify the roles of atoms in the interaction.

table: double precision ***pointer size(:, :)*** array for storing tabulated values

original_elements: character(len=2) ***pointer size(:)*** The list of elements (atomic symbols) of the original `Potential` in the Python interface from which this potential was created. Whereas the apply_* lists are used for finding all pairs and triplets of atoms for which the potential could act on, the original_* lists specify the roles of atoms in the interaction.

multipliers: type(potential) ***pointer size(:)*** additional potentials with the same targets and cutoff, for potential multiplication

derived_parameters: double precision ***pointer size(:)*** numerical values for parameters calculated based on the parameters specified by the user

apply_elements: character(len=2) ***pointer size(:)*** A list of elements (atomic symbols) the potential affects. E.g., for a Si-O potential, it would be ('Si','O'). Note that unlike in the Python interface, a single `potential` only has one set of targets, and for multiple target options several `potential` instances are created.

filter_tags: logical ***scalar*** a logical switch specifying whether the potential targets atoms based on the atom tags

`potential_descriptor`

Description of a type of a potential. The type contains the name and description of the potential and the parameters it contains. The descriptors contain the information that the inquiry methods in the python interface fetch.

Contained data:

parameter_notes: character(len=param_note_length) ***pointer size(:)*** Descriptions of the parameters. The descriptions should be very short indicators such as 'spring constant' or 'energy coefficient'. For more detailed explanations, the proper documentation should be used.

n_parameters: integer ***scalar*** number of parameters

description: character(len=pot_note_length) ***scalar*** A description of the potential. This should contain the mathematical formulation as well as a short verbal explanation.

type_index: integer ***scalar*** The internal index of the potential. This can also be used for recognizing the potential and must therefore match the name. For instance, if name = 'LJ', type_index = `pair_lj_index`.

n_targets: integer ***scalar*** number of targets, i.e., interacting bodies

parameter_names: character(len=param_name_length) ***pointer size(:)*** The names of the parameters of the potential: these are keywords according to which the parameters may be recognized.

name: character(len=pot_name_length) ***scalar*** The name of the potential: this is a keyword according to which the potentials may be recognized.

Full documentation of subroutines in potentials

`allocate_ewald_arrays`(*n_atoms*)

Parameters:

n_atoms: integer *intent(in) scalar*

`bond_order_factor_affects_atom`(*factor*, *atom_in*, *affects*, *position*)

Tests whether the given bond order factor affects the specific atom.

For bond order factors, the atoms are specified as valid targets by the atomic symbol only.

If position is not given, then the routine returns true if the atom can appear in the bond order factor in any role. If position is given, then true is returned only if the atom is valid for that particular position.

For instance, we may want to calculate the coordination of Cu-O bonds for Cu but not for O.

Parameters:

factor: type(bond_order_parameters) ***intent(in) scalar*** the `bond_order_parameters`

atom_in: type(atom) ***intent(in) scalar*** the `atom`

affects: logical intent(out) ***scalar*** true if the bond order factor is affected by the atom

position: integer *intent(in) scalar optional* specifies the particular role of the atom in the bond order factor

bond_order_factor_is_in_group (*factor*, *group_index*, *in_group*)
Tests whether the given bond order factor is a member of a specific group, i.e., if it affects the potential specifiesd by the group index.

Parameters:

factor: type(bond_order_parameters) *intent(in) scalar* the bond_order_parameters

group_index: integer *intent(in) scalar* the index for the potential

in_group: logical intent(out) *scalar* true if the factor is a member of the group

calculate_derived_parameters_bond_bending (*n_params*, *parameters*, *new_potential*)
Bond bending derived parameters

Parameters:

n_params: integer *intent(in) scalar*

parameters: double precision *intent(in) size(n_params)*

new_potential: type(potential) intent(inout) *scalar* the potential object for which the parameters are calculated

calculate_derived_parameters_charge_exp (*n_params*, *parameters*, *new_potential*)
Charge exponential derived parameters

Parameters:

n_params: integer *intent(in) scalar*

parameters: double precision *intent(in) size(n_params)*

new_potential: type(potential) intent(inout) *scalar* the potential object for which the parameters are calculated

calculate_derived_parameters_dihedral (*n_params*, *parameters*, *new_potential*)
Dihedral angle derived parameters

Parameters:

n_params: integer *intent(in) scalar*

parameters: double precision *intent(in) size(n_params)*

new_potential: type(potential) intent(inout) *scalar* the potential object for which the parameters are calculated

calculate_ewald_electronegativities (*atoms*, *cell*, *real_cutoff*, *k_radius*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *scaler*, *include_dipole_correction*, *total_enegs*, *include_realspace*)
Calculates the electronegativities due to long ranged $\frac{1}{r}$ potentials. These electronegativities are the derivatives of the energies U given by calculate_ewald_energy()

$$\chi_\alpha = -\frac{\partial U}{\partial q_\alpha}$$

Parameters:

atoms: type(atom) *intent(in) size(:)* list of atoms

cell: type(supercell) *intent(in) scalar* the supercell containing the system

real_cutoff: double precision *intent(in) scalar* Cutoff radius of real-space interactions. Note that the neighbor lists stored in the atoms are used for neighbor finding so the cutoff cannot exceed the cutoff for the neighbor lists. (Or, it can, but the neighbors not in the lists will not be found.)

k_radius: double precision *intent(in) scalar* Cutoff radius of k-space summation in inverse length. This is an absolute cutoff so that any k-point at a greater distance will be ignored. THis makes the k-cutoff spherical instead of summing over a rectangular box. (It also speeds up the summation.)

reciprocal_cutoff: integer *intent(in) size(3)* The number of cells to be included in the reciprocal sum in the directions of the reciprocal cell vectors. For example, if `reciprocal_cutoff = [3,4,5]`, the reciprocal sum will be truncated as $\sum_{\mathbf{k}\neq 0} = \sum_{k_1=-3}^{3}\sum_{k_2=-4}^{4}\sum_{k_3=-5,(k_1,k_2,k_3)\neq(0,0,0)}^{5}$.

gaussian_width: double precision *intent(in) scalar* The σ parameter, i.e., the distribution width of the screening Gaussians. This should not influence the actual value of the energy, but it does influence the convergence of the summation. If σ is large, the real space sum E_s converges slowly and a large real space cutoff is needed. If it is small, the reciprocal term E_l converges slowly and the sum over the reciprocal lattice has to be evaluated over several cell lengths.

electric_constant: double precision *intent(in) scalar* The electic constant, i.e., vacuum permittivity ε_0. In atomic units, it is $\varepsilon_0 = 0.00552635\frac{e^2}{\mathrm{eV}}$, but if one wishes to scale the results to some other unit system (such as reduced units with $\varepsilon_0 = 1$), that is possible as well.

scaler: double precision *intent(in) size(:)* a list of numerical values to scale the individual charges of the atoms

include_dipole_correction: logical *intent(in) scalar* if true, a dipole correction term is included

total_enegs: double precision intent(inout) *size(:)* the calculated electronegativities

include_realspace: logical *intent(in) scalar optional* By default, also the real space summation is carried out, but giving the .false. flag here will prevent the calculation. This is used in the normal evaluation loop where the real space sum is calculated during the evaluation of other pairwise interactions.

`calculate_ewald_energy` (*atoms*, *cell*, *real_cutoff*, *k_radius*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *scaler*, *include_dipole_correction*, *total_energy*, *include_realspace*)

Calculates the energy of $\frac{1}{r}$ potentials through Ewald summation.

If a periodic system contains charges interacting via the $\frac{1}{r}$ Coulomb potential, direct summation of the interactions

$$E = \sum_{(i,j)} \frac{1}{4\pi\epsilon_0}\frac{q_i q_j}{r_{ij}}, \tag{4.19}$$

where the sum is over pairs of charges q_i, q_j (charges of the entire system, not just the simulation cell) and the distance between the charges is $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$, does not work in general because the sum (4.19) converges very slowly. [5] Therefore truncating the sum may lead to severe errors.

The standard technique for overcoming this problem is the so called Ewald summation method. The idea is to split the long ranged and singular Coulomb potential to a short ranged singular and long ranged smooth parts, and calculate the long ranged part in reciprocal space via Fourier transformations. This is possible since the system is periodic and the same supercell repeats infinitely in all

[5] In fact, the sum converges only conditionally meaning the result depends on the order of summation. Physically this is not a problem, because one never has infinite lattices.

directions. In practice the calculation can be done by adding (and subtracting) Gaussian charge densities over the point charges to screen the potential in real space. That is, the original charge density $\rho(\mathbf{r}) = \sum_i q_i \delta(\mathbf{r} - \mathbf{r}_i)$ is split by

$$\rho(\mathbf{r}) = \rho_s(\mathbf{r}) + \rho_l(\mathbf{r}) \tag{4.20}$$

$$\rho_s(\mathbf{r}) = \sum_i \left[q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i G_\sigma(\mathbf{r} - \mathbf{r}_i) \right] \tag{4.21}$$

$$\rho_l(\mathbf{r}) = \sum_i q_i G_\sigma(\mathbf{r} - \mathbf{r}_i) \tag{4.22}$$

$$G_\sigma(\mathbf{r}) = \frac{1}{(2\pi\sigma^2)^{3/2}} \exp\left(-\frac{|\mathbf{r}|^2}{2\sigma^2} \right) \tag{4.23}$$

Here ρ_l generates a long range interaction since at large distances the Gaussian densities G_σ appear the same as point charges ($\lim_{\sigma/r \to 0} G_\sigma(\mathbf{r}) = \delta(\mathbf{r})$). Since the charge density is smooth, so will be the potential it creates. The density ρ_s exhibits short ranged interactions for the same reason: At distances longer than the width of the Gaussians the point charges are screened by the Gaussians which exactly cancel them ($\lim_{\sigma/r \to 0} \delta(\mathbf{r}) - G_\sigma(\mathbf{r}) = 0$).

The short ranged interactions are directly calculated in real space

$$E_s = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_s(\mathbf{r}) \rho_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r \mathrm{d}^3 r' \tag{4.24}$$

$$= \frac{1}{4\pi\varepsilon_0} \sum_{(i,j)} \frac{q_i q_j}{r_{ij}} \mathrm{erfc}\left(\frac{r_{ij}}{\sigma\sqrt{2}} \right). \tag{4.25}$$

The complementary error function $\mathrm{erfc}(r) = 1 - \mathrm{erf}(r) = 1 - \frac{2}{\sqrt{\pi}} \int_0^r e^{-t^2/2} \mathrm{d}t$ makes the sum converge rapidly as $\frac{r_{ij}}{\sigma} \to \infty$.

The long ranged interaction can be calculated in reciprocal space by Fourier transformation. The result is

$$E_l = \frac{1}{2V\varepsilon_0} \sum_{\mathbf{k} \neq 0} \frac{e^{-\sigma^2 k^2/2}}{k^2} |S(\mathbf{k})|^2 - \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_i^N q_i^2 \tag{4.26}$$

$$S(\mathbf{k}) = \sum_i^N q_i e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} \tag{4.27}$$

The first sum in E_l runs over the reciprocal lattice $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$ where $\mathbf{b}_i$ are the vectors spanning the reciprocal cell ($[\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3] = ([\mathbf{v}_1\mathbf{v}_2\mathbf{v}_3]^{-1})^T$ where $\mathbf{v}_i$ are the real space cell vectors). The latter sum is the self energy of each point charge in the potential of the particular Gaussian that screens the charge, and the sum runs over all charges in the supercell spanning the periodic system. (The self energy must be removed because it is present in the first sum even though when evaluating the potential at the position of a charge due to the other charges, no screening Gaussian function should be placed over the charge itself.) Likewise the sum in the structure factor $S(\mathbf{k})$ runs over all charges in the supercell.

The total energy is then the sum of the short and long range energies

$$E = E_s + E_l.$$

Parameters:

atoms: type(atom) ***intent(in) size(:)*** list of atoms

cell: type(supercell) ***intent(in) scalar*** the supercell containing the system

real_cutoff: double precision *intent(in) scalar* Cutoff radius of real-space interactions. Note that the neighbor lists stored in the atoms are used for neighbor finding so the cutoff cannot exceed the cutoff for the neighbor lists. (Or, it can, but the neighbors not in the lists will not be found.)

k_radius: double precision *intent(in) scalar* absolute k-space cutoff

reciprocal_cutoff: integer *intent(in) size(3)* The number of cells to be included in the reciprocal sum in the directions of the reciprocal cell vectors. For example, if `reciprocal_cutoff = [3,4,5]`, the reciprocal sum will be truncated as $\sum_{\mathbf{k}\neq 0} = \sum_{k_1=-3}^{3}\sum_{k_2=-4}^{4}\sum_{k_3=-5,(k_1,k_2,k_3)\neq(0,0,0)}^{5}$.

gaussian_width: double precision *intent(in) scalar* The σ parameter, i.e., the distribution width of the screening Gaussians. This should not influence the actual value of the energy, but it does influence the convergence of the summation. If σ is large, the real space sum E_s converges slowly and a large real space cutoff is needed. If it is small, the reciprocal term E_l converges slowly and the sum over the reciprocal lattice has to be evaluated over several cell lengths.

electric_constant: double precision *intent(in) scalar* The electic constant, i.e., vacuum permittivity ε_0. In atomic units, it is $\varepsilon_0 = 0.00552635\frac{e^2}{\mathrm{eV}}$, but if one wishes to scale the results to some other unit system (such as reduced units with $\varepsilon_0 = 1$), that is possible as well.

scaler: double precision *intent(in) size(:)* a list of numerical values to scale the individual charges of the atoms

include_dipole_correction: logical *intent(in) scalar* if true, a dipole correction term is included in the energy

total_energy: double precision intent(out) *scalar* the calculated energy

include_realspace: logical *intent(in) scalar optional* By default, also the real space summation is carried out, but giving the .false. flag here will prevent the calculation. This is used in the normal evaluation loop where the real space sum is calculated during the evaluation of other pairwise interactions.

`calculate_ewald_forces`(*atoms*, *cell*, *real_cutoff*, *k_radius*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *scaler*, *include_dipole_correction*, *total_forces*, *total_stress*, *include_realspace*)

Calculates the forces due to long ranged $\frac{1}{r}$ potentials. These forces are the gradients of the energies U given by `calculate_ewald_energy()`

$$\mathbf{F}_\alpha = -\nabla_\alpha U$$

Parameters:

atoms: type(atom) *intent(in) size(:)* list of atoms

cell: type(supercell) *intent(in) scalar* the supercell containing the system

real_cutoff: double precision *intent(in) scalar* Cutoff radius of real-space interactions. Note that the neighbor lists stored in the atoms are used for neighbor finding so the cutoff cannot exceed the cutoff for the neighbor lists. (Or, it can, but the neighbors not in the lists will not be found.)

k_radius: double precision *intent(in) scalar* Cutoff radius of k-space summation in inverse length. This is an absolute cutoff so that any k-point at a greater distance will be ignored. THis makes the k-cutoff spherical instead of summing over a rectangular box. (It also speeds up the summation.)

reciprocal_cutoff: integer *intent(in) size(3)* The number of cells to be included in the reciprocal sum in the directions of the reciprocal cell vectors. For example, if `reciprocal_cutoff = [3,4,5]`, the reciprocal sum will be truncated as $\sum_{\mathbf{k}\neq 0} = \sum_{k_1=-3}^{3}\sum_{k_2=-4}^{4}\sum_{k_3=-5,(k_1,k_2,k_3)\neq(0,0,0)}^{5}$.

gaussian_width: double precision *intent(in) scalar* The σ parameter, i.e., the distribution width of the screening Gaussians. This should not influence the actual value of the energy, but it does influence the convergence of the summation. If σ is large, the real space sum E_s converges slowly and a large real space cutoff is needed. If it is small, the reciprocal term E_l converges slowly and the sum over the reciprocal lattice has to be evaluated over several cell lengths.

electric_constant: double precision *intent(in) scalar* The electic constant, i.e., vacuum permittivity ε_0. In atomic units, it is $\varepsilon_0 = 0.00552635 \frac{e^2}{\mathrm{eV}}$, but if one wishes to scale the results to some other unit system (such as reduced units with $\varepsilon_0 = 1$), that is possible as well.

scaler: double precision *intent(in) size(:)* a list of numerical values to scale the individual charges of the atoms

include_dipole_correction: logical *intent(in) scalar* if true, a dipole correction term is included in the energy

total_forces: double precision intent(inout) *size(:, :)* the calculated forces

total_stress: double precision intent(inout) *size(6)* the calculated stress

include_realspace: logical *intent(in) scalar optional* By default, also the real space summation is carried out, but giving the .false. flag here will prevent the calculation. This is used in the normal evaluation loop where the real space sum is calculated during the evaluation of other pairwise interactions.

check_s_factor_array_allocation (*n_atoms*, *reciprocal_cutoff*)
Parameters:

n_atoms: integer *intent(in) scalar*

reciprocal_cutoff: integer *intent(in) size(3)*

clear_bond_order_factor_characterizers ()
Deallocates all memory associated with bond order factor characterizes.

clear_potential_characterizers ()
Deallocates all memory associated with potential characterizes.

create_bond_order_factor (*n_targets*, *n_params*, *n_split*, *bond_name*, *parameters*, *param_split*, *cutoff*, *soft_cutoff*, *elements*, *orig_elements*, *group_index*, *new_bond*, *success*)
Returns a bond_order_parameters.

The routine takes as arguments all the necessary parameters and returns a bond order parameters type wrapping them in one package.

Parameters:

n_targets: integer *intent(in) scalar* number of targets, i.e., interacting bodies

n_params: integer *intent(in) scalar* array containing the numbers of parameters for different number of targets (1-body parameters, 2-body parameters, etc.)

n_split: integer *intent(in) scalar* number of groupings in the list of parameters, per number of bodies - should equal n_targets

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor - a keyword that must match a name of one of the bond_order_descriptors

parameters: double precision *intent(in) size(n_params)* numerical values for parameters as a one-dimensional array

param_split: integer *intent(in) size(n_split)* Array containing the numbers of 1-body, 2-body, etc. parameters. The parameters are given as a list, but a bond order factor may have parameters

separately for different numbers of targets. This list specifies the number of parameters for each.

cutoff: double precision *intent(in) scalar* The hard cutoff for the bond order factor. If the atoms are farther away from each other than this, they do not contribute to the total bond order factor does not affect them.

soft_cutoff: double precision *intent(in) scalar* The soft cutoff for the bond order factor. If this is smaller than the hard cutoff, the bond contribution is scaled to zero continuously when the interatomic distances grow from the soft to the hard cutoff.

elements: character(len=2) *intent(in) size(n_targets)* a list of elements (atomic symbols) the factor affects

orig_elements: character(len=2) *intent(in) size(n_targets)* the list of elements (atomic symbols) of the original `BondOrderParameters` in the Python interface from which this factor was created

group_index: integer *intent(in) scalar* The internal index of the *potential* the bond order factor is modifying.

new_bond: type(bond_order_parameters) intent(out) *scalar* the created `bond_order_parameters`

success: logical intent(out) *scalar* logical tag specifying if creation of the factor succeeded

`create_bond_order_factor_characterizer_coordination` (*index*)
Coordination characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

`create_bond_order_factor_characterizer_power` (*index*)
Power decay characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

`create_bond_order_factor_characterizer_scaler_1` (*index*)
Scaler characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

`create_bond_order_factor_characterizer_scaler_sqrt` (*index*)
Square root scaler characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

`create_bond_order_factor_characterizer_scaler_table` (*index*)
Square root scaler characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

`create_bond_order_factor_characterizer_table` (*index*)
Tabulated characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

create_bond_order_factor_characterizer_tersoff (*index*)
Tersoff characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

create_bond_order_factor_characterizer_triplet (*index*)
Triplet characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the bond order factor

create_potential (*n_targets*, *n_params*, *pot_name*, *parameters*, *cutoff*, *soft_cutoff*, *elements*, *tags*, *indices*, *orig_elements*, *orig_tags*, *orig_indices*, *pot_index*, *n_multi*, *multipliers*, *new_potential*, *success*)
Returns a potential.

The routine takes as arguments all the necessary parameters and returns a potential type wrapping them in one package.

Parameters:

n_targets: integer *intent(in) scalar* number of targets, i.e., interacting bodies

n_params: integer *intent(in) scalar* number of parameters

pot_name: character(len=*) *intent(in) scalar* name of the potential - a keyword that must match a name of one of the potential_descriptors

parameters: double precision *intent(in) size(n_params)* array of numerical values for the parameters

cutoff: double precision *intent(in) scalar* the hard cutoff for the potential

soft_cutoff: double precision *intent(in) scalar* the soft cutoff for the potential

elements: character(len=2) *intent(in) size(n_targets)* the elements (atomic symbols) the potential acts on

tags: integer *intent(in) size(n_targets)* the atom tags the potential acts on

indices: integer *intent(in) size(n_targets)* the atom indices the potential acts on

orig_elements: character(len=2) *intent(in) size(n_targets)* The elements (atomic symbols) in the Potential used for generating the potential. This is needed to specify the roles of the atoms in the interaction.

orig_tags: integer *intent(in) size(n_targets)* The atom tags in the Potential used for generating the potential. This is needed to specify the roles of the atoms in the interaction.

orig_indices: integer *intent(in) size(n_targets)* The atom indices in the Potential used for generating the potential. This is needed to specify the roles of the atoms in the interaction.

pot_index: integer *intent(in) scalar* the internal index of the potential

n_multi: integer *intent(in) scalar* number of multiplying potentials

multipliers: type(potential) *intent(in) size(n_multi)* the multiplying potentials

new_potential: type(potential) intent(out) *scalar* the created potential

success: logical intent(out) *scalar* logical tag specifying if creation of the potential succeeded

create_potential_characterizer_LJ(*index*)
LJ characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_bond_bending(*index*)
bond-bending characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_buckingham(*index*)
Buckingham characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_charge_exp(*index*)
charge exponential characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_charge_pair(*index*)
charge self energy characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_charge_pair_abs(*index*)
charge abs energy characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_charge_self(*index*)
charge self energy characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_constant_force(*index*)
constant F characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_constant_potential(*index*)
constant potential characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_dihedral(*index*)
dihedral angle characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_exp(*index*)
exponential characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_power(*index*)
Power law characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_shift(*index*)
Shift characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_spring(*index*)
spring characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_step(*index*)
Step characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

create_potential_characterizer_table(*index*)
Tabulated characterizer initialization

Parameters:

index: integer *intent(in) scalar* index of the potential

deallocate_ewald_arrays()

evaluate_bond_order_factor(*n_targets*, *separations*, *distances*, *bond_params*, *factor*, *atoms*)
Returns a bond order factor term.

By a bond order factor term, we mean the contribution from specific atoms, c_{ijk}, appearing in the factor

$$b_i = f(\sum_{jk} c_{ijk})$$

This routine evaluates the term c_{ij} or c_{ijk} for the given atoms ij or ijk according to the given parameters.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) ***intent(in) size(n_targets-1)*** a `bond_order_parameters` containing the parameters

factor: double precision intent(out) ***size(n_targets)*** the calculated bond order term c

atoms: type(atom) ***intent(in) size(n_targets)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_bond_order_factor_coordination` (*separations*, *distances*, *bond_params*, *factor*)

Coordination bond order factor

Parameters:

separations: double precision ***intent(in) size(3, 1)*** atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision ***intent(in) size(1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) ***intent(in) size(1)*** a `bond_order_parameters` containing the parameters

factor: double precision intent(out) ***size(2)*** the calculated bond order term c

`evaluate_bond_order_factor_power` (*separations*, *distances*, *bond_params*, *factor*)

Power bond order factor

Parameters:

separations: double precision ***intent(in) size(3, 1)*** atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision ***intent(in) size(1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) ***intent(in) size(1)*** a `bond_order_parameters` containing the parameters

factor: double precision intent(out) ***size(2)*** the calculated bond order term c

`evaluate_bond_order_factor_table` (*separations*, *distances*, *bond_params*, *factor*)

Tabulated bond order factor

Parameters:

separations: double precision ***intent(in) size(3, 1)*** atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision ***intent(in) size(1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) ***intent(in) size(1)*** a `bond_order_parameters` containing the parameters

factor: double precision intent(out) ***size(2)*** the calculated bond order term c

`evaluate_bond_order_factor_triplet` (*separations*, *distances*, *bond_params*, *factor*, *atoms*)

Triplet bond factor

Parameters:

separations: double precision ***intent(in) size(3, 2)*** atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(2)* a `bond_order_parameters` containing the parameters

factor: double precision intent(out) *size(3)* the calculated bond order term c

atoms: type(atom) *intent(in) size(3)* a list of the actual `atom` objects for which the term is calculated

evaluate_bond_order_gradient (*n_targets*, *separations*, *distances*, *bond_params*, *gradient*, *atoms*)

Returns the gradients of bond order terms with respect to moving an atom.

By a bond order factor term, we mean the contribution from specific atoms, c_ijk, appearing in the factor

$$b_i = f(\sum_{jk} c_{ijk})$$

This routine evaluates the gradient term $\nabla_\alpha c_{ij}$ or $\nabla_\alpha c_{ijk}$ for the given atoms ij or ijk according to the given parameters.

The returned array has three dimensions: gradient(coordinates, atom whose factor is differentiated, atom with respect to which we differentiate) So for example, for a three body term atom1-atom2-atom3, gradient(1,2,3) contains the x-coordinate (1), of the factor for atom2 (2), with respect to moving atom3 (3).

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(n_targets-1)* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, n_targets, n_targets)* the calculated bond order term $\nabla_\alpha c$

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

evaluate_bond_order_gradient_coordination (*separations*, *distances*, *bond_params*, *gradient*)

Coordination bond order factor gradient

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(1)* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, 2, 2)* the calculated bond order term c

evaluate_bond_order_gradient_power (*separations*, *distances*, *bond_params*, *gradient*)

Power bond order factor gradient

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(1)* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, 2, 2)* the calculated bond order term c

evaluate_bond_order_gradient_table (*separations*, *distances*, *bond_params*, *gradient*)

Tabulated bond order factor gradient

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(1)* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, 2, 2)* the calculated bond order term c

evaluate_bond_order_gradient_triplet (*separations*, *distances*, *bond_params*, *gradient*, *atoms*)

Coordination bond order factor gradient

Parameters:

separations: double precision *intent(in) size(3, 2)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) size(2)* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, 3, 3)* the calculated bond order term c

atoms: type(atom) *intent(in) size(3)* a list of the actual `atom` objects for which the term is calculated

evaluate_electronegativity (*n_targets*, *n_product*, *separations*, *distances*, *interaction*, *eneg*, *atoms*)

If a potential, say, U_{ijk} depends on the charges of atoms q_i it will not only create a force, but also a difference in chemical potential μ_i for the atomic partial charges. Similarly to `evaluate_forces()`, this function evaluates the chemical 'force' on the atomic charges

$$\chi_{\alpha,ijk} = -\mu_{\alpha,ijk} = -\frac{\partial U_{ijk}}{\partial q_\alpha}$$

This routine can evaluate the contribution from a product potential.

To be consist the forces returned by `evaluate_electronegativity()` must be derivatives of the energies returned by `evaluate_energy()`.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

n_product: integer *intent(in) scalar* the number of potentials for a product potential

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

eneg: double precision intent(out) *size(n_targets)* the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

`evaluate_electronegativity_charge_exp`(*interaction*, *eneg*, *atoms*)
Charge exp electronegativity

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

eneg: double precision intent(out) *size(2)* the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

`evaluate_electronegativity_charge_pair`(*interaction*, *eneg*, *atoms*)
Charge pair energy electronegativity

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

eneg: double precision intent(out) *size(2)* the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

`evaluate_electronegativity_charge_pair_abs`(*interaction*, *eneg*, *atoms*)
Charge pair abs energy electronegativity

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

eneg: double precision intent(out) *size(2)* the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

`evaluate_electronegativity_charge_self`(*interaction*, *eneg*, *atoms*)
Charge self energy electronegativity

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

eneg: double precision intent(out) *size(1)* the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) ***intent(in) size(1)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_electronegativity_component` (*n_targets*, *separations*, *distances*, *interaction*, *eneg*, *atoms*)

If a potential, say, U_{ijk} depends on the charges of atoms q_i it will not only create a force, but also a difference in chemical potential μ_i for the atomic partial charges. Similarly to `evaluate_forces()`, this function evaluates the chemical 'force' on the atomic charges

$$\chi_{\alpha,ijk} = -\mu_{\alpha,ijk} = -\frac{\partial U_{ijk}}{\partial q_\alpha}$$

This routine evaluates an elemental $\chi_{\alpha,ijk}$.

Parameters:

n_targets: integer ***intent(in) scalar*** number of targets

separations: double precision ***intent(in) size(3, n_targets-1)*** atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision ***intent(in) size(n_targets-1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) ***intent(in) scalar*** a `potential` containing the parameters

eneg: double precision intent(out) ***size(n_targets)*** the calculated electronegativity component $\chi_{\alpha,ijk}$

atoms: type(atom) ***intent(in) size(n_targets)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_energy` (*n_targets*, *n_product*, *separations*, *distances*, *interaction*, *energy*, *atoms*)

Evaluates the potential energy due to an interaction between the given atoms. In other words, if the total potential energy is

$$E = \sum_{ijk} v_{ijk}$$

this routine evaluates v_{ijk} for the given atoms i, j, and k.

This routine can evaluate the contribution from a product potential.

To be consist the forces returned by `evaluate_forces()` must be gradients of the energies returned by `evaluate_energy()`.

Parameters:

n_targets: integer ***intent(in) scalar*** number of targets

n_product: integer ***intent(in) scalar*** the number of potentials for a product potential

separations: double precision ***intent(in) size(3, n_targets-1)*** atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision ***intent(in) size(n_targets-1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) ***intent(in) scalar*** a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

atoms: type(atom) ***intent(in) size(n_targets)*** a list of the actual `atom` objects for which the term is calculated

evaluate_energy_LJ (*separations*, *distances*, *interaction*, *energy*)
LJ energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

evaluate_energy_bond_bending (*separations*, *distances*, *interaction*, *energy*, *atoms*)
Bond bending energy

Parameters:

separations: double precision *intent(in) size(3, 2)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

atoms: type(atom) *intent(in) size(3)* a list of the actual `atom` objects for which the term is calculated

evaluate_energy_buckingham (*separations*, *distances*, *interaction*, *energy*)
Buckingham energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

evaluate_energy_charge_exp (*interaction*, *energy*, *atoms*)
Charge exp energy

Parameters:

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

evaluate_energy_charge_pair (*interaction*, *energy*, *atoms*)
Charge pair energy

Parameters:

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

evaluate_energy_charge_pair_abs (*interaction*, *energy*, *atoms*)
Charge pair abs energy

Parameters:

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

atoms: type(atom) *intent(in) size(2)* a list of the actual `atom` objects for which the term is calculated

evaluate_energy_charge_self (*interaction*, *energy*, *atoms*)
Charge self energy

Parameters:

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

atoms: type(atom) *intent(in) size(1)* a list of the actual `atom` objects for which the term is calculated

evaluate_energy_component (*n_targets*, *separations*, *distances*, *interaction*, *energy*, *atoms*)
Evaluates the potential energy due to an interaction between the given atoms. In other words, if the total potential energy is

$$E = \sum_{ijk} v_{ijk}$$

this routine evaluates v_{ijk} for the given atoms i, j, and k.

This routine evaluates an elemental $v_{\alpha,ijk}$.

To be consist the forces returned by `evaluate_forces()` must be gradients of the energies returned by `evaluate_energy()`.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

atoms: type(atom) ***intent(in) size(n_targets)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_energy_constant_force` (*interaction*, *energy*, *atoms*)
constant force energy

Parameters:

interaction: type(potential) ***intent(in) scalar*** a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

atoms: type(atom) ***intent(in) size(1)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_energy_constant_potential` (*interaction*, *energy*)
Constant potential energy

Parameters:

interaction: type(potential) ***intent(in) scalar*** a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

`evaluate_energy_dihedral` (*separations*, *distances*, *interaction*, *energy*, *atoms*)
Dihedral angle energy

Parameters:

separations: double precision ***intent(in) size(3, 3)*** atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision ***intent(in) size(3)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) ***intent(in) scalar*** a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

atoms: type(atom) ***intent(in) size(4)*** a list of the actual `atom` objects for which the term is calculated

`evaluate_energy_exp` (*separations*, *distances*, *interaction*, *energy*)
Exp energy

Parameters:

separations: double precision ***intent(in) size(3, 1)*** atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision ***intent(in) size(1)*** atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) ***intent(in) scalar*** a `bond_order_parameters` containing the parameters

energy: double precision intent(out) ***scalar*** the calculated energy v_{ijk}

`evaluate_energy_power` (*separations*, *distances*, *interaction*, *energy*)
Power energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

`evaluate_energy_shift` (*separations*, *distances*, *interaction*, *energy*)
Shift energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

`evaluate_energy_spring` (*separations*, *distances*, *interaction*, *energy*)
spring energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

`evaluate_energy_step` (*separations*, *distances*, *interaction*, *energy*)
Shift energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

`evaluate_energy_table` (*separations*, *distances*, *interaction*, *energy*)
Tabulated energy

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `bond_order_parameters` containing the parameters

energy: double precision intent(out) *scalar* the calculated energy v_{ijk}

`evaluate_force_LJ` (*separations*, *distances*, *interaction*, *force*)
LJ force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_bond_bending` (*separations*, *distances*, *interaction*, *force*, *atoms*)
Bond bending force

Parameters:

separations: double precision *intent(in) size(3, 2)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 3)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(3)* a list of the actual `atom` objects for which the term is calculated

`evaluate_force_buckingham` (*separations*, *distances*, *interaction*, *force*)
Buckingham force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_component` (*n_targets*, *separations*, *distances*, *interaction*, *force*, *atoms*)
Evaluates the forces due to an interaction between the given atoms. In other words, if the total force on atom α is

$$\mathbf{F}_\alpha = \sum_{ijk} -\nabla_\alpha v_{ijk} = \sum \mathbf{f}_{\alpha,ijk},$$

this routine evaluates $\mathbf{f}_{\alpha,ijk}$ for $\alpha = (i, j, k)$ for the given atoms i, j, and k.

This routine evaluates an elemental $\mathbf{f}_{\alpha,ijk}$.

To be consist the forces returned by `evaluate_forces()` must be gradients of the energies returned by `evaluate_energy()`.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, n_targets)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

evaluate_force_constant_force (*interaction*, *force*)
constant force

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 1)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

evaluate_force_constant_potential (*interaction*, *force*)
constant force

Parameters:

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 1)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

evaluate_force_dihedral (*separations*, *distances*, *interaction*, *force*, *atoms*)
Dihedral angle force

Parameters:

separations: double precision *intent(in) size(3, 3)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(3)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 4)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(4)* a list of the actual `atom` objects for which the term is calculated

evaluate_force_exp (*separations*, *distances*, *interaction*, *force*)
Exp force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_power` (*separations*, *distances*, *interaction*, *force*)
Power force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_shift` (*separations*, *distances*, *interaction*, *force*)
Shift force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_spring` (*separations*, *distances*, *interaction*, *force*)
spring force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

`evaluate_force_step` (*separations*, *distances*, *interaction*, *force*)
Step force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

evaluate_force_table (*separations*, *distances*, *interaction*, *force*)
Tabulated force

Parameters:

separations: double precision *intent(in) size(3, 1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, 2)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

evaluate_forces (*n_targets*, *n_product*, *separations*, *distances*, *interaction*, *force*, *atoms*)
Evaluates the forces due to an interaction between the given atoms. In other words, if the total force on atom α is

$$\mathbf{F}_\alpha = \sum_{ijk} -\nabla_\alpha v_{ijk} = \sum \mathbf{f}_{\alpha,ijk},$$

this routine evaluates $\mathbf{f}_{\alpha,ijk}$ for $\alpha = (i, j, k)$ for the given atoms i, j, and k.

This routine can evaluate the contribution from a product potential.

To be consist the forces returned by `evaluate_forces()` must be gradients of the energies returned by `evaluate_energy()`.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

n_product: integer *intent(in) scalar* the number of potentials for a product potential

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

interaction: type(potential) *intent(in) scalar* a `potential` containing the parameters

force: double precision intent(out) *size(3, n_targets)* the calculated force component $\mathbf{f}_{\alpha,ijk}$

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

evaluate_pair_bond_order_factor (*n_targets*, *separations*, *distances*, *bond_params*, *factor*, *atoms*)
Returns a bond order factor term.

By a bond order factor term, we mean the contribution from specific atoms, c_{ijk}, appearing in the factor

$$b_i j = f(\sum_k c_{ijk})$$

This routine evaluates the term c_{ijk} for the given atoms ijk according to the given parameters.

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) scalar* a `bond_order_parameters` containing the parameters

factor: double precision intent(out) *scalar* the calculated bond order term c

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

evaluate_pair_bond_order_factor_tersoff(*separations*, *distances*, *bond_params*, *factor*, *atoms*)

Parameters:

separations: double precision *intent(in) size(3, 2)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) scalar* a `bond_order_parameters` containing the parameters

factor: double precision intent(out) *scalar* the calculated bond order term c

atoms: type(atom) *intent(in) size(3)* a list of the actual `atom` objects for which the term is calculated

evaluate_pair_bond_order_gradient(*n_targets*, *separations*, *distances*, *bond_params*, *gradient*, *atoms*)

Returns the gradients of bond order terms with respect to moving an atom.

By a bond order factor term, we mean the contribution from specific atoms, c_ijk, appearing in the factor

$$b_i j = f(\sum_k c_{ijk})$$

This routine evaluates the gradient term $\nabla_\alpha c_{ijk}$ for the given atoms ijk according to the given parameters.

The returned array has two dimensions: gradient(coordinates, atom with respect to which we differentiate).

Parameters:

n_targets: integer *intent(in) scalar* number of targets

separations: double precision *intent(in) size(3, n_targets-1)* atom-atom separation vectors r_{12}, r_{23} etc. for the atoms 123...

distances: double precision *intent(in) size(n_targets-1)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) scalar* a `bond_order_parameters` containing the parameters

gradient: double precision intent(out) *size(3, n_targets)* the calculated bond order term $\nabla_\alpha c$

atoms: type(atom) *intent(in) size(n_targets)* a list of the actual `atom` objects for which the term is calculated

evaluate_pair_bond_order_gradient_tersoff (*separations*, *distances*, *bond_params*, *gradient*, *atoms*)

Tersoff bond order factor gradient

Parameters:

separations: double precision *intent(in) size(3, 2)* atom-atom separation vectors $\mathbf{r}_{12}$, $\mathbf{r}_{23}$ etc. for the atoms 123...

distances: double precision *intent(in) size(2)* atom-atom distances r_{12}, r_{23} etc. for the atoms 123..., i.e., the norms of the separation vectors.

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters containing the parameters

gradient: double precision intent(out) *size(3, 3)* the calculated bond order term c

atoms: type(atom) *intent(in) size(3)* a list of the actual atom objects for which the term is calculated

get_bond_descriptor (*bond_name*, *descriptor*)

Returns the bond_order_descriptor of a given name.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

descriptor: type(bond_order_descriptor) intent(out) *scalar* the matching bond_order_descriptor

get_description_of_bond_order_factor (*bond_name*, *description*)

Returns the description of a bond order factor.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

description: character(len=pot_note_length) intent(out) *scalar* description of the bond order factor

get_description_of_potential (*pot_name*, *description*)

Returns the description of a potential.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

description: character(len=pot_note_length) intent(out) *scalar* description of the potential

get_descriptions_of_parameters_of_bond_order_factor (*bond_name*, *n_targets*, *param_notes*)

Returns the descriptions of the parameters of a bond order factor as a list of strings.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

n_targets: integer *intent(in) scalar* 1 for scaling, 2 for local sum parameters

param_notes: character(len=param_note_length) *intent() pointer size(:)* descriptions of the parameters

get_descriptions_of_parameters_of_potential (*pot_name*, *param_notes*)

Returns the descriptions of the parameters of a potential as a list of strings.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

param_notes: character(len=param_note_length) *intent() pointer size(:)* descriptions of the parameters

get_descriptor (*pot_name*, *descriptor*)
Returns the potential_descriptor of a given name.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

descriptor: type(potential_descriptor) intent(out) *scalar* the matching potential_descriptor

get_index_of_bond_order_factor (*bond_name*, *index*)
Returns the index of a bond_order_descriptor in the internal list of bond order factor types bond_order_descriptors.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor - a keyword

index: integer intent(out) *scalar* index of the potential in the internal array

get_index_of_parameter_of_bond_order_factor (*bond_name*, *param_name*, *index*, *n_targets*)
Returns the index of a parameter of a bond order factor in the internal list of parameters. Since bond order factors can have parameters for different number of targets, also the type (scaling vs. local sum) of this parameter is returned.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

param_name: character(len=*) *intent(in) scalar* name of the parameter

index: integer intent(out) *scalar* index of the parameter

n_targets: integer intent(out) *scalar* 1 for scaling, 2 for local sum parameters

get_index_of_parameter_of_potential (*pot_name*, *param_name*, *index*)
Returns the index of a parameter of a potential in the internal list of parameters.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

param_name: character(len=*) *intent(in) scalar* name of the parameter

index: integer intent(out) *scalar* the index of the parameter

get_index_of_potential (*pot_name*, *index*)
Returns the index of a potential_descriptor in the internal list of potential types potential_descriptors.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential - a keyword

index: integer intent(out) *scalar* index of the potential in the internal array

get_level_of_bond_order_factor (*bond_name*, *level*)
Returns the level of a bond order factor (i.e., is the factor per-atom or per-pair).

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

level: integer intent(out) ***scalar*** level of the factor

get_level_of_bond_order_factor_index(*bond_index*, *level*)
Returns the level of a bond order factor (i.e., is the factor per-atom or per-pair).

Parameters:

bond_index: integer ***intent(in) scalar*** name of the bond order factor

level: integer intent(out) ***scalar*** level of the factor

get_names_of_parameters_of_bond_order_factor(*bond_name*, *n_targets*, *param_names*)
Returns the names of parameters of a bond order factor as a list of strings.

Parameters:

bond_name: character(len=*) ***intent(in) scalar*** name of the bond order factor

n_targets: integer ***intent(in) scalar*** 1 for scaling, 2 for local sum parameters

param_names: character(len=param_name_length) ***intent() pointer size(:)*** names of the parameters

get_names_of_parameters_of_potential(*pot_name*, *param_names*)
Returns the names of parameters of a potential as a list of strings.

Parameters:

pot_name: character(len=*) ***intent(in) scalar*** name of the potential

param_names: character(len=param_name_length) ***intent() pointer size(:)*** names of the parameters

get_number_of_bond_order_factors(*n_bond*)
Returns the number of `bond_order_descriptor` known.

Parameters:

n_bond: integer intent(out) ***scalar*** number of bond order factor types

get_number_of_parameters_of_bond_order_factor(*bond_name*, *n_targets*, *n_params*)
Returns the number of parameters of a bond order factor as an integer.

Parameters:

bond_name: character(len=*) ***intent(in) scalar*** name of the bond order factor

n_targets: integer ***intent(in) scalar*** 1 for scaling parameters, 2 for local sum parameters

n_params: integer intent(out) ***scalar*** number of parameters

get_number_of_parameters_of_potential(*pot_name*, *n_params*)
Returns the number of parameters of a potential.

Parameters:

pot_name: character(len=*) ***intent(in) scalar*** name of the potential

n_params: integer intent(out) ***scalar*** number of parameters

get_number_of_potentials(*n_pots*)
Return the number of `potential_descriptor` known.

Parameters:

n_pots: integer intent(out) ***scalar*** number of potential types

get_number_of_targets_of_bond_order_factor (*bond_name*, *n_target*)
Returns the number of targets (i.e., bodies) of a bond order factor.

Parameters:

bond_name: character(len=*) *intent(in) scalar* name of the bond order factor

n_target: integer intent(out) *scalar* number of targets

get_number_of_targets_of_bond_order_factor_index (*bond_index*, *n_target*)
Returns the number of targets (i.e., bodies) of a bond order factor specified by its index.

Parameters:

bond_index: integer *intent(in) scalar* index of the bond order factor

n_target: integer intent(out) *scalar* number of targets

get_number_of_targets_of_potential (*pot_name*, *n_target*)
Returns the number of targets (i.e., bodies) of a potential.

Parameters:

pot_name: character(len=*) *intent(in) scalar* name of the potential

n_target: integer intent(out) *scalar* number of targets

get_number_of_targets_of_potential_index (*pot_index*, *n_target*)
Returns the number of targets (i.e., bodies) of a potential specified by its index.

Parameters:

pot_index: integer *intent(in) scalar* index of the potential

n_target: integer intent(out) *scalar* number of targets

initialize_bond_order_factor_characterizers ()
Creates bond order factor characterizers.

This routine is meant to be run once, as pysic is imported, to create the characterizers for bond order factors. Once created, they are accessible by both the python and fortran sides of pysic as a tool for describing the general structure of bond order factor objects.

initialize_potential_characterizers ()
Creates potential characterizers.

This routine is meant to be run once, as pysic is imported, to create the characterizers for potentials. Once created, they are accessible by both the python and fortran sides of pysic as a tool for describing the general structure of potential objects.

is_valid_bond_order_factor (*string*, *is_valid*)
Returns true if the given keyword is the name of a bond order factor and false otherwise.

Parameters:

string: character(len=*) *intent(in) scalar* name of a bond order factor

is_valid: logical intent(out) *scalar* true if string is a name of a bond order factor

is_valid_potential (*string*, *is_valid*)
Returns true if the given keyword is the name of a potential and false otherwise.

Parameters:

string: character(len=*) *intent(in) scalar* name of a potential

is_valid: logical intent(out) *scalar* true if string is a name of a potential

list_bond_order_factors (*n_bonds*, *bonds*)
Returns the names of bond_order_descriptor objects.

Parameters:

n_bonds: integer *intent(in) scalar* number of bond order factor types

bonds: character(len=pot_name_length) intent(out) *size(n_bonds)* names of the bond order factor types

list_potentials (*n_pots*, *pots*)
Returns the names of potential_descriptor objects.

Parameters:

n_pots: integer *intent(in) scalar* number of potential types

pots: character(len=pot_name_length) intent(out) *size(n_pots)* names of the potential types

post_process_bond_order_factor (*raw_sum*, *bond_params*, *factor_out*)
Bond-order post processing, i.e., application of per-atom scaling functions.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_i = f(\sum_j c_{ij}) = 1 + \sum_j c_{ij},$$

the $\sum_j c_i j$ would have been calculated already and the operation $f(x) = 1+x$ remains to be carried out. The post processing is done per atom regardless of if the bond factor is of a pair or many body type.

This routine applies the scaling function on the given bond order sum accoding to the given parameters.

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) *scalar* the calculated bond order factor b_i

post_process_bond_order_factor_scaler_1 (*raw_sum*, *bond_params*, *factor_out*)
Scaler post process factor

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) *scalar* the calculated bond order factor b_i

post_process_bond_order_factor_scaler_sqrt (*raw_sum*, *bond_params*, *factor_out*)
Square root scaler post process factor

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) *scalar* the calculated bond order factor b_i

post_process_bond_order_factor_scaler_table(*raw_sum*, *bond_params*, *factor_out*)

Tabulated scaler post process factor

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) *scalar* the calculated bond order factor b_i

post_process_bond_order_factor_tersoff(*raw_sum*, *bond_params*, *factor_out*)

Tersoff post process factor

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_k c_{ijk}$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) *scalar* the calculated bond order factor b_{ij}

post_process_bond_order_gradient(*raw_sum*, *raw_gradient*, *bond_params*, *factor_out*)

Bond-order post processing, i.e., application of per-atom scaling functions.

By post processing, we mean any operations done after calculating the sum of pair- and many-body terms. That is, if a factor is, say,

$$b_i = f(\sum_j c_{ij}) = 1 + \sum_j c_{ij},$$

the $\sum_j c_{ij}$ would have been calculated already and the operation $f(x) = 1 + x$ remains to be carried out. The post processing is done per atom regardless of if the bond factor is of a pair or many body type.

For gradients, one needs to evaluate

$$\nabla_\alpha b_i = f'(\sum_j c_{ij}) \nabla_\alpha \sum_j c_{ij}$$

This routine applies the scaling function on the given bond order sum and gradient accoding to the given parameters.

Parameters:

raw_sum: double precision *intent(in) scalar* the precalculated bond order sum, $\sum_j c_i j$ in the above example

raw_gradient: double precision *intent(in) size(3)* the precalculated bond order gradient sum, $\nabla_\alpha \sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a bond_order_parameters specifying the parameters

factor_out: double precision intent(inout) ***size(3)*** the calculated bond order factor $\nabla_\alpha b_i$

post_process_bond_order_gradient_scaler_1(*raw_sum*, *raw_gradient*, *bond_params*, *factor_out*)

Scaler post process gradient

Parameters:

raw_sum: double precision ***intent(in) scalar*** the precalculated bond order sum, $\sum_j c_i j$ in the above example

raw_gradient: double precision ***intent(in) size(3)*** the precalculated bond order gradient sum, $\nabla_\alpha \sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) ***intent(in) scalar*** a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) ***size(3)*** the calculated bond order factor b_i

post_process_bond_order_gradient_scaler_sqrt(*raw_sum*, *raw_gradient*, *bond_params*, *factor_out*)

Square root scaler post process gradient

Parameters:

raw_sum: double precision ***intent(in) scalar*** the precalculated bond order sum, $\sum_j c_i j$ in the above example

raw_gradient: double precision ***intent(in) size(3)*** the precalculated bond order gradient sum, $\nabla_\alpha \sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) ***intent(in) scalar*** a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) ***size(3)*** the calculated bond order factor b_i

post_process_bond_order_gradient_scaler_table(*raw_sum*, *raw_gradient*, *bond_params*, *factor_out*)

Tabulated scaler post process gradient

Parameters:

raw_sum: double precision ***intent(in) scalar*** the precalculated bond order sum, $\sum_j c_i j$ in the above example

raw_gradient: double precision ***intent(in) size(3)*** the precalculated bond order gradient sum, $\nabla_\alpha \sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) ***intent(in) scalar*** a bond_order_parameters specifying the parameters

factor_out: double precision intent(out) ***size(3)*** the calculated bond order factor b_i

post_process_bond_order_gradient_tersoff(*raw_sum*, *raw_gradient*, *bond_params*, *factor_out*)

Tersoff post process gradient

Parameters:

raw_sum: double precision ***intent(in) scalar*** the precalculated bond order sum, $\sum_j c_i j$ in the above example

raw_gradient: double precision ***intent(in) size(3)*** the precalculated bond order gradient sum, $\nabla_\alpha \sum_j c_i j$ in the above example

bond_params: type(bond_order_parameters) *intent(in) scalar* a `bond_order_parameters` specifying the parameters

factor_out: double precision intent(out) *size(3)* the calculated bond order factor b_i

`potential_affects_atom` (*interaction*, *atom_in*, *affects*, *position*)
Tests whether the given potential affects the specific atom.

For potentials, the atoms are specified as valid targets by the atomic symbol, index, or tag.

If position is not given, then the routine returns true if the atom can appear in the potential in any role. If position is given, then true is returned only if the atom is valid for that particular position.

For instance, in a 3-body potential A-B-C, the potential May be specified so that only certain elements are valid for positions A and C while some other elements are valid for B. In a water molecule, for instance, we could have an H-O-H bond bending potential, but no H-H-O potentials.

Parameters:

interaction: type(potential) *intent(in) scalar* the `potential`

atom_in: type(atom) *intent(in) scalar* the `atom`

affects: logical intent(out) *scalar* true if the potential affects the atom

position: integer *intent(in) scalar optional* specifies the particular role of the atom in the interaction

`smoothening_derivative` (*r*, *hard_cut*, *soft_cut*, *factor*)
Derivative of the function for smoothening potential and bond order cutoffs. In principle any "nice" function which goes from 1 to 0 in a finite interval could be used. Here, we choose

$$f(r) = \frac{1}{2}(1 + \cos \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}})$$

for $r \in [r_{\mathrm{soft}}, r_{\mathrm{hard}}]$. The derivative is then

$$f'(r) = \frac{\pi}{2(r_{\mathrm{soft}} - r_{\mathrm{hard}})} \sin \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}}.$$

This routine takes as arguments r, r_{soft}, and r_{hard}, and returns the value of the derivative of the smoothening function.

Parameters:

r: double precision *intent(in) scalar* distance r

hard_cut: double precision *intent(in) scalar* the hard cutoff r_{hard}

soft_cut: double precision *intent(in) scalar* the soft cutoff r_{soft}

factor: double precision intent(out) *scalar* the calculated derivative of the smoothening factor

`smoothening_factor` (*r*, *hard_cut*, *soft_cut*, *factor*)
Function for smoothening potential and bond order cutoffs. In principle any "nice" function which goes from 1 to 0 in a finite interval could be used. Here, we choose

$$f(r) = \frac{1}{2}(1 + \cos \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}})$$

for $r \in [r_{\mathrm{soft}}, r_{\mathrm{hard}}]$.

This routine takes as arguments r, r_{soft}, and r_{hard}, and returns the value of the smoothening function.

Parameters:

r: double precision *intent(in) scalar* distance r

hard_cut: double precision *intent(in) scalar* the hard cutoff r_{hard}

soft_cut: double precision *intent(in) scalar* the soft cutoff r_{soft}

factor: double precision intent(out) *scalar* the calculated smoothening factor

smoothening_gradient (*unit_vector*, *r*, *hard_cut*, *soft_cut*, *gradient*)
Gradient of the function for smoothening potential and bond order cutoffs. In principle any "nice" function which goes from 1 to 0 in a finite interval could be used. Here, we choose

$$f(r) = \frac{1}{2}(1 + \cos \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}})$$

for $r \in [r_{\mathrm{soft}}, r_{\mathrm{hard}}]$. The derivative is then

$$f'(r) = \frac{\pi}{2(r_{\mathrm{soft}} - r_{\mathrm{hard}})} \sin \pi \frac{r - r_{\mathrm{soft}}}{r_{\mathrm{hard}} - r_{\mathrm{soft}}}.$$

and the gradient with respect to r

$$\nabla f(r) = f'(r) \nabla r = f'(r) \hat{r}$$

where $\hat{r}$ is the unit vector in the direction of $\mathbf{r}$.

This routine takes as arguments $\hat{r}$, r, r_{soft}, and r_{hard}, and returns the value of the gradient of the smoothening function.

Parameters:

unit_vector: double precision *intent(in) size(3)* the vector $\hat{r}$

r: double precision *intent(in) scalar* distance r

hard_cut: double precision *intent(in) scalar* the hard cutoff r_{hard}

soft_cut: double precision *intent(in) scalar* the soft cutoff r_{soft}

gradient: double precision intent(out) *size(3)* the calculated derivative of the smoothening factor

geometry (Geometry.f90)

A module for handling the geometric structure of the system.

Full documentation of global variables in geometry

label_length
integer *scalar parameter*

initial value = 2

the number of characters available for denoting chemical symbols

Full documentation of custom types in geometry

atom
Defines an atomic particle.

Contained data:

neighbor_list: type(neighbor_list) ***scalar*** the list of neighbors for the atom

index: integer ***scalar*** index of the atom

n_pots: integer ***scalar*** number of potentials that may affect the atom

max_potential_radius: double precision ***scalar*** the maximum cutoff of any potential listed in potential_indices

tags: integer ***scalar*** integer tag

potential_indices: integer ***pointer size(:)*** the indices of the potentials for which this atom is a valid target at first position (see `potential_affects_atom()`)

potentials_listed: logical ***scalar*** logical tag for checking if the potentials affecting the atom have been listed in potential_indices

bond_indices: integer ***pointer size(:)*** the indices of the bond order factors for which this atom is a valid target at first position (see `bond_order_factor_affects_atom()`)

element: character(len=label_length) ***scalar*** the chemical symbol of the atom

charge: double precision ***scalar*** charge of the atom

subcell_indices: integer ***size(3)*** indices of the subcell containing the atom, used for fast neighbor searching (see `subcell`)

max_bond_radius: double precision ***scalar*** the maximum cutoff of any bond order factor listed in bond_indices

n_bonds: integer ***scalar*** number of bond order factors that may affect the atom

bond_order_factors_listed: logical ***scalar*** logical tag for checking if the bond order factors affecting the atom have been listed in bond_indices

position: double precision ***size(3)*** coordinates of the atom

mass: double precision ***scalar*** mass of th atom

momentum: double precision ***size(3)*** momentum of the atom

`neighbor_list`

Defines a list of neighbors for a single atom. The list contains the indices of the neighboring atoms as well as the periodic boundary condition (PBC) offsets.

The offsets are integer triplets showing how many times must the supercell vectors be added to the position of the neighbor to find the neighboring image in a periodic system. For example, let the supercell be:

```
[[1.0, 0, 0], [0, 1.0, 0], [0, 0, 1.0]],
```

i.e., a unit cube, with periodic boundaries. Now, if we have particles with coordinates:

```
a = [1.5, 0.5, 0.5]
b = [0.4, 1.6, 3.3]
```

the closest separation vector $\mathbf{r}_b - \mathbf{r}_a$ between the particles is:

```
[-.1, .1, -.2]
```

obtained if we add the vector of periodicity:

```
[1.0, -1.0, -3.0]
```

to the coordinates of particle b. The offset vector (for particle b, when listing neighbors of a) is then:

```
[1, -1, -3]
```

Note that if the system is small, one atom can in principle appear several times in the neighbor list with different offsets.

Contained data:

neighbors: integer ***pointer size(:)*** indices of the neighboring atoms

max_length: integer ***scalar*** The allocated length of the neighbor lists. To avoid deallocating and reallocating memory, extra space is reserved for the neighbors in case the number of neighbors increases during simulation (due to atoms moving).

pbc_offsets: integer ***pointer size(:, :)*** offsets for periodic boundaries for each neighbor

n_neighbors: integer ***scalar*** the number of neighbors in the lists

subcell

Subvolume, which is a part of the supercell containing the simulation.

The subcells are used in partitioning of the simulation space in subvolumes. This divisioning of the simulation cell is needed for quickly finding the neighbors of atoms (see also `pysic.FastNeighborList`). The fast neighbor search is based on dividing the system, locating the subcell in which each atom is located, and then searching for neighbors for each atom by only checking the adjacent subcells. For small subvolumes (short cutoffs) this method is much faster than a brute force algorithm that checks all atom pairs. It also scales $\mathcal{O}(n)$.

Contained data:

neighbors: integer ***size(3, -1:1, -1:1, -1:1)*** indices of the 3 x 3 x 3 neighboring subcells (note that the neighboring subcell 0,0,0 is the cell itself)

vector_lengths: double precision ***size(3)*** lengths of the vectors spanning the subcell

offsets: integer ***size(3, -1:1, -1:1, -1:1)*** integer offsets of the neighboring subcells - if a neighboring subcell is beyond a periodic border, the offset records the fact

max_atoms: integer ***scalar*** the maximum number of atoms the cell can contain in the currently allocated memory space

vectors: double precision ***size(3, 3)*** the vectors spanning the subcell

atoms: integer ***pointer size(:)*** indices of the atoms in this subcell

n_atoms: integer ***scalar*** the number of atoms contained by the subcell

indices: integer ***size(3)*** integer coordinates of the subcell in the subcell divisioning of the supercell

include: logical ***size(-1:1, -1:1, -1:1)*** A logical array noting if the neighboring subcells should be included in the neighbor search. Usually all neighbors are included, but in a non-periodic system, there is only a limited number of cells and once the system border is reached, this tag will be set to `.false.` to notify that there is no neighbor to be found.

supercell

Supercell containing the simulation.

The supercell is spanned by three vectors $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ stored as a 3×3 matrix in format

$$\mathbf{M} = \begin{bmatrix} v_{1,x} & v_{1,y} & v_{1,z} \\ v_{2,x} & v_{2,y} & v_{2,z} \\ v_{3,x} & v_{3,y} & v_{3,z} \end{bmatrix}.$$

Also the inverse cell matrix is kept for transformations between the absolute and fractional coordinates.

Contained data:

vector_lengths: double precision *size(3)* the lengths of the cell spanning vectors (stored to avoid calculating the vector norms over and over)

max_subcell_atom_count: integer *scalar* the maximum number of atoms any of the subcells has

n_splits: integer *size(3)* the number of subcells there are in the subdivisioning of the cell, in the directions of the spanning vectors

inverse_cell: double precision *size(3, 3)* the inverse of the cell matrix $\mathbf{M}^{-1}$

subcells: type(subcell) *pointer size(:, :, :)* an array of `subcell` subvolumes which partition the supercell

vectors: double precision *size(3, 3)* vectors spanning the supercell containing the system as a matrix $\mathbf{M}$

volume: double precision *scalar* volume of the cell

periodic: logical *size(3)* logical switch determining if periodic boundary conditions are applied in the directions of the three cell spanning vectors

reciprocal_cell: double precision *size(3, 3)* the reciprocal cell as a matrix, $\mathbf{M}_R = 2\pi(\mathbf{M}^{-1})^T$. That is, if $\mathbf{b}_i$ are the reciprocal lattice vectors and $\mathbf{a}_j$ the real space lattice vectors, then $\mathbf{b}_i\mathbf{a}_j = 2\pi\delta_{ij}$.

Full documentation of subroutines in geometry

absolute_coordinates (*relative*, *cell*, *position*)
Transforms from fractional to absolute coordinates.

Absolute coordinates are the coordinates in the normal xyz base,

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}.$$

Fractional coordiantes are the coordiantes in the base spanned by the vectors defining the supercell, $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$,

$$\mathbf{r} = \tilde{x}\mathbf{v}_1 + \tilde{y}\mathbf{v}_2 + \tilde{z}\mathbf{v}_3.$$

Notably, for positions inside the supercell, the fractional coordinates fall between 0 and 1.

Transformation between the two bases is given by the cell matrix

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \mathbf{M} \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}$$

Parameters:

relative: double precision *intent(in) size(3)* the fractional coordinates

cell: type(supercell) *intent(in) scalar* the supercell

position: double precision intent(out) *size(3)* the absolute coordinates

assign_bond_order_factor_indices (*n_bonds*, *atom_in*, *indices*)
Save the indices of bond order factors affecting an atom.

In bond order factor evaluation, it is important to loop over bond parameters quickly. As the evaluation of factors goes over atoms, atom pairs etc., it is useful to first filter the parameters by the first

atom participating in the factor. Therefore, the atoms can be given a list of bond order parameters for which they are a suitable target as a 'first participant' (in a triplet A-B-C, A is the first participant).

Parameters:

n_bonds: integer *intent(in) scalar* number of bond order factors

atom_in: type(atom) intent(inout) *scalar* the atom for which the bond order factors are assigned

indices: integer *intent(in) size(n_bonds)* the indices of the bond order factors

assign_max_bond_order_factor_cutoff (*atom_in*, *max_cut*)
Parameters:

atom_in: type(atom) **intent(inout)** *scalar*

max_cut: double precision *intent(in) scalar*

assign_max_potential_cutoff (*atom_in*, *max_cut*)
Parameters:

atom_in: type(atom) **intent(inout)** *scalar*

max_cut: double precision *intent(in) scalar*

assign_neighbor_list (*n_nbs*, *nbor_list*, *neighbors*, *offsets*)
Creates a neighbor list for one atom.

The neighbor list will contain an array of the indices of the neighboring atoms as well as periodicity offsets, as explained in `neighbor_list`

The routine takes the neighbor_list object to be created as an argument. If the list is empty, it is initialized. If the list already contains information, the list is emptied and refilled. If the previous list has room to contain the new list (as in, it has enough allocated memory), no memory reallocation is done (since it will be slow if done repeatedly). Only if the new list is too long to fit in the reserved memory, the pointers are deallocated and reallocated.

Parameters:

n_nbs: integer *intent(in) scalar* number of neighbors

nbor_list: type(neighbor_list) intent(inout) *scalar* The list of neighbors to be created.

neighbors: integer *intent(in) size(n_nbs)* array containing the indices of the neighboring atoms

offsets: integer *intent(in) size(3, n_nbs)* periodicity offsets

assign_potential_indices (*n_pots*, *atom_in*, *indices*)
Save the indices of potentials affecting an atom.

In force and energy evaluation, it is important to loop over potentials quickly. As the evaluation of energies goes over atoms, atom pairs etc., it is useful to first filter the potentials by the first atom participating in the interaction. Therefore, the atoms can be given a list of potentials for which they are a suitable target as a 'first participant' (in a triplet A-B-C, A is the first participant).

Parameters:

n_pots: integer *intent(in) scalar* number of potentials

atom_in: type(atom) intent(inout) *scalar* the atom for which the potentials are assigned

indices: integer *intent(in) size(n_pots)* the indices of the potentials

divide_cell (*cell*, *splits*)
Split the cell in subcells according to the given number of divisions.

The argument 'splits' should be a list of three integers determining how many times the cell is split. For instance, if splits = [3,3,5], the cell is divided in 3*3*5 = 45 subcells: 3 cells along the first two cell vectors and 5 along the third.

The Cell itself is not changed, but an array 'subcells' is created, containing the subcells which are Cell instances themselves. These cells will contain additional data arrays 'neighbors' and 'offsets'. These are 3-dimensional arrays with each dimension running from -1 to 1. The neighbors array contains references to the neighboring subcell Cell instances. The offsets contain coordinate offsets with respect to the periodic boundaries. In other words, if a subcell is at the border of the original Cell, it will have neighbors at the other side of the cell due to periodic boundary conditions. But from the point of view of the subcell, the neighboring cell is not on the other side of the master cell, but a periodic image of that cell. Therefore, any coordinates in the the subcell to which the neighbors array refers to must in fact be shifted by a vector of the master cell. The offsets list contains the multipliers for the cell vectors to make these shifts.

Example in 2D for simplicity: `split = [3,4]` creates subcells:

```
(0,3) (1,3) (2,3)
(0,2) (1,2) (2,2)
(0,1) (1,1) (2,1)
(0,0) (1,0) (2,0)
```

subcell (0,3) will have the neighbors:: (2,0) (0,0) (1,0) (2,3) (0,3) (1,3) (2,2) (0,2) (1,2)

and offsets:: [-1,1] [0,1] [0,1] [-1,0] [0,0] [0,0] [-1,0] [0,0] [0,0]

Note that the central 'neighbor' is the cell itself.

If a boundary is not periodic, extra subcells with indices 0 and split+1 are created to pad the simulation cell. These will contain the atoms that are outside the simulation cell.

Parameters:

cell: type(supercell) **intent(inout)** *scalar*

splits: integer *intent(in) size(3)*

expand_subcell_atom_capacity(*atoms_list*, *old_size*, *new_size*)

Parameters:

atoms_list: integer *intent() pointer size(:)*

old_size: integer *intent(in) scalar*

new_size: integer *intent(in) scalar*

find_subcell_for_atom(*cell*, *at*)

Parameters:

cell: type(supercell) **intent(inout)** *scalar*

at: type(atom) **intent(inout)** *scalar*

generate_atoms(*n_atoms*, *masses*, *charges*, *positions*, *momenta*, *tags*, *elements*, *atoms*)

Creates atoms to construct the system to be simulated.

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

masses: double precision *intent(in) size(n_atoms)* array of masses for the atoms

charges: double precision *intent(in) size(n_atoms)* array of charges for the atoms

positions: double precision ***intent(in) size(3, n_atoms)*** array of coordinates for the atoms

momenta: double precision ***intent(in) size(3, n_atoms)*** array of momenta for the atoms

tags: integer ***intent(in) size(n_atoms)*** array of integer tags for the atoms

elements: character(len=label_length) ***intent(in) size(n_atoms)*** array of chemical symbols for the atoms

atoms: type(atom) ***intent() pointer size(:)*** array of the atom objects created

generate_supercell (*vectors*, *inverse*, *periodicity*, *cell*)
Creates the supercell containing the simulation geometry.

The supercell is spanned by three vectors $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ stored as a 3×3 matrix in format

$$\mathbf{M} = \begin{bmatrix} v_{1,x} & v_{1,y} & v_{1,z} \\ v_{2,x} & v_{2,y} & v_{2,z} \\ v_{3,x} & v_{3,y} & v_{3,z} \end{bmatrix}.$$

Also the inverse cell matrix $\mathbf{M}^{-1}$ must be given for transformations between the absolute and fractional coordinates. However, it is not checked that the given matrix and inverse truly fulfill $\mathbf{M}^{-1}\mathbf{M} = \mathbf{I}$ - it is the responsibility of the caller to give the true inverse.

Also the periodicity of the system in the directions of the cell vectors need to be given.

Parameters:

vectors: double precision ***intent(in) size(3, 3)*** the cell spanning matrix $\mathbf{M}$

inverse: double precision ***intent(in) size(3, 3)*** the inverse cell $\mathbf{M}$

periodicity: logical ***intent(in) size(3)*** logical switch, true if the boundaries are periodic

cell: type(supercell) intent(out) ***scalar*** the created cell object

get_optimal_splitting (*cell*, *max_cut*, *splits*)
Parameters:

cell: type(supercell) *intent(in) scalar*

max_cut: double precision *intent(in) scalar*

splits: integer **intent(out)** *size(3)*

relative_coordinates (*position*, *cell*, *relative*)
Transforms from absolute to fractional coordinates.

Absolute coordinates are the coordinates in the normal xyz base,

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}.$$

Fractional coordiantes are the coordiantes in the base spanned by the vectors defining the supercell, $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$,

$$\mathbf{r} = \tilde{x}\mathbf{v}_1 + \tilde{y}\mathbf{v}_2 + \tilde{z}\mathbf{v}_3.$$

Notably, for positions inside the supercell, the fractional coordinates fall between 0 and 1.

Transformation between the two bases is given by the inverse cell matrix

$$\begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix} = \mathbf{M}^{-1} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Parameters:

position: double precision *intent(in) size(3)* the absolute coordinates

cell: type(supercell) *intent(in) scalar* the supercell

relative: double precision intent(out) *size(3)* the fractional coordinates

`separation_vector` (*r1*, *r2*, *offset*, *cell*, *separation*)
Calculates the minimum separation vector between two atoms, $\mathbf{r}_2 - \mathbf{r}_1$, including possible periodicity.

Parameters:

r1: double precision *intent(in) size(3)* coordiantes of atom 1, $\mathbf{r}_1$

r2: double precision *intent(in) size(3)* coordinates of atom 1, $\mathbf{r}_2$

offset: integer *intent(in) size(3)* periodicity offset (see `neighbor_list`)

cell: type(supercell) *intent(in) scalar* supercell spanning the system

separation: double precision intent(out) *size(3)* the calculated separation vector, $\mathbf{r}_2 - \mathbf{r}_1$

`update_atomic_charges` (*n_atoms*, *charges*, *atoms*)
Updates the charges of the given atoms. Other properties are not altered.

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

charges: double precision *intent(in) size(n_atoms)* new charges for the atoms

atoms: type(atom) *intent() pointer size(:)* the atoms to be edited

`update_atomic_positions` (*n_atoms*, *positions*, *momenta*, *atoms*)
Updates the positions and momenta of the given atoms. Other properties are not altered.

This is meant to be used during dynamic simulations or geometry optimization where the atoms are only moved around, not changed in other ways.

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

positions: double precision *intent(in) size(3, n_atoms)* new coordinates for the atoms

momenta: double precision *intent(in) size(3, n_atoms)* new momenta for the atoms

atoms: type(atom) *intent() pointer size(:)* the atoms to be edited

`wrapped_coordinates` (*position*, *cell*, *wrapped*, *offset*)
Wraps a general coordinate inside the supercell if the system is periodic.

In a periodic system, every particle has periodic images at intervals defined by the cell vectors $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. That is, for a particle at $\mathbf{r}$, there are periodic images at

$$\mathbf{R} = \mathbf{r} + a_1\mathbf{v}_1 + a_2\mathbf{v}_2 + a_3\mathbf{v}_3$$

for all $a_1, a_2, a_3 \in \mathbf{Z}$. These are equivalent positions in the sense that if a particle is situated at any of one of them, the set of images is the same. Exactly one of the images is inside the cell - this routine gives the coordinates of that particular image.

If the system is periodic in only some directions, the wrapping is done only along those directions.

Parameters:

position: double precision *intent(in) size(3)* the absolute coordinates

cell: type(supercell) *intent(in) scalar* the supercell

wrapped: double precision intent(out) ***size(3)*** the wrapped absolute coordinates

offset: integer intent(out) ***size(3) optional*** wrapping offset, i.e., the number of times the cell vectors are added to the absolute coordinates in order to obtain the wrapped coordinates

Full documentation of functions in geometry

pick (*index1*, *index2*, *offset*)

A utility function for sorting the atoms.

The function return `true` if `index1 < index2` and `false` otherwise. If `index1 == index2`, the comparison is made through the separation vector. The vector is examined element at a time, and if a positive number is found, `true` is returned, if a negative one, `false`. For values of zero, the next element is examined.

The purpose for this function is to sort the atoms to prevent double counting when summing over pairs. In principle, a sum over pairs (i, j) can be done with $\frac{1}{2}\sum_{i\neq j}$, but this leads to evaluation of all elements twice (both (i, j) and (j, i) are considered separately). It is more efficient to evaluate $\sum_{i<j}$, where only one of (i, j) and (j, i) fullfill the condition.

A special case arises if interactions are so long ranged that an atom can see its own periodic images. Then, one will need to sum terms for atom pairs where both atoms have the same index $\sum_{\text{images}}\sum_{i,j}$ if they are in different periodic copies of the actual simulation cell. In order to still pick only one of the pairs (i, i') and (i', i), we compare the offset vectors. If atom i' is in the neighboring cell of i in the first cell vector direction, it has an offset of $[1, 0, 0]$ and vice versa i has an offset of $[-1, 0, 0]$ from i'. Instead of the index, the sorting $i' < i$ is then done by comparing these offset vectors, element by element.

Parameters:

index1: integer ***intent(in) scalar*** index of first atom

index2: integer ***intent(in) scalar*** index of second atom

offset: integer ***intent(in) size(3)*** pbc offset vector from atom1 to atom2

utility (Utility.f90)

A module containing utility functionas and constants.

The module is a collection of standalone helper tools, not physically relevant functionality.

Full documentation of global variables in utility

pi

double precision *scalar parameter*

initial value = 4.d0 * datan(1.d0)

the constant π calculated as $\pi = 4\arctan 1$

Full documentation of subroutines in utility

int2str (*length*, *ints*, *string_out*)

Transforms an integer array to string through a codec:

```
1 - a
2 - b
...
101 - A
102 - B
...
-1 - 1
-2 - 2
...
```

Unrecognized numbers are treated as white spaces.

The function is used for communicating string arrays between Python and Fortran oer f2py.

Parameters:

length: integer *intent(in) scalar* string length

ints: integer *intent(in) size(length)* the integers

string_out: character(len=length) intent(out) *scalar* the string

pad_string (*str_in*, *str_length*, *str_out*)
Adds spaces after the given string to create a string of a certain length. If the given string is longer than the specified length, it is truncated.

This is used to ensure strings are of a certain length, since character arrays in Fortran may be forced to a certain length.

Parameters:

str_in: character(len=*) *intent(in) scalar* the original string

str_length: integer *intent(in) scalar* the required string length

str_out: character(len=str_length) intent(out) *scalar* the padded string

read_table (*filename*, *table*, *success*)
Reads a 2D real array from a file

Parameters:

filename: character(len=*) *intent(in) scalar* the name of the file to be read

table: double precision *intent() pointer size(:, :)* the read array

success: logical intent(out) *scalar* logical tag showing if the operation was successful

str2int (*length*, *string*, *ints*)
Transforms a string to an integer array through a codec:

```
1 - a
2 - b
...
101 - A
102 - B
...
-1 - 1
-2 - 2
...
```

Unrecognized characters are mapped to 0.

The function is used for communicating string arrays between Python and Fortran oer f2py.

Parameters:

length: integer ***intent(in) scalar*** string length

string: character(len=length) ***intent(in) scalar*** the string

ints: integer intent(out) ***size(length)*** the integers

mpi (MPI.f90)

Module for Message Parsing Interface parallellization utilities.

This module handles the initialization of the MPI environment and assigns the cpus their indices. Parallellization is done by distributing atoms on the processors and the routine for doing this randomly is provided. Also tools for monitoring the loads of all the cpus and redistributing them are also implemented.

Full documentation of global variables in mpi

all_atoms
integer *scalar*

the total number of atoms

all_loads
double precision *allocatable size(:)*

list of the loads of all cpus

atom_buffer
integer *allocatable size(:)*

list used for passing atom indices during load balancing

cpu_id
integer *scalar*

identification number for the cpu, from 0 to $n_{\mathrm{cpus}} - 1$

is_my_atom
logical *allocatable size(:)*

logical array, true for the indices of the atoms that are distributed to this cpu

load_length
integer *scalar*

the number of times loads have been recorded

loadout
integer *scalar*

initial value = 2352

an integer of the output channel for loads

loads_mask
logical *allocatable size(:)*

logical array used in load rebalancing, true for cpus whose loads have not yet been balanced

mpi_atoms_allocated
logical *scalar*

initial value = .false.

logical switch for denoting that the mpi allocatable arrays have been allocated

mpistat
integer *scalar*

mpi return value

mpistatus
integer *size(mpi_status_size)*

array for storing the mpi status return values

my_atoms
integer *scalar*

the number of atoms distributed to this cpu

my_load
double precision *scalar*

storage for the load of this particular cpu

n_cpus
integer *scalar*

number of cpus, n_{cpus}

stopwatch
double precision *scalar*

cpu time storage

track_loads
logical *scalar parameter*

initial value = .false.

logical switch, if true, the loads of cpus are written to a file during run

Full documentation of subroutines in mpi

balance_loads()
Load balancing.

The loads are gathered from all cpus and sorted. Then load (atoms) is passed from the most loaded cpus to the least loaded ones.

close_loadmonitor()
Closes the output for wirting workload data

initialize_load(*reallocate*)
Initializes the load monitoring arrays.

Parameters:

reallocate: logical *intent(in) scalar* Logical switch for reallocating the arrays. If true, the related arrays are allocated. Otherwise only the load counters are set to zero.

mpi_distribute(*n_atoms*)
distributes atoms among processors

Parameters:

n_atoms: integer *intent(in) scalar* number of atoms

mpi_finish()
closes the mpi framework

mpi_initialize()
intializes the mpi framework

mpi_master_bcast_int(*sync_int*)
the master cpu broadcasts an integer value to all other cpus

Parameters:

sync_int: integer intent(inout) *scalar* the broadcast integer

mpi_stack(*list*, *items*, *depth*, *length*, *width*)
stacks the "lists" from all cpus together according to the lengths given in "items" and gathers the complete list to cpu 0. For example:

```
cpu 0          cpu 1          cpu 0
abc....        12.....        abc12..
de.....        3456...   ->   de3456.
fghij..        78.....        fghij78
```

The stacking is done for the second array index: list(1,:,1). The stacking works so that first every cpu 2n+1 sends its data to cpu 2n, then 2*(2n+1) sends data to 2*2n, and so on, until the final cpu 2^m sends its data to cpu 0:

```
cpu
0 1 2 3 4 5 6 7 8 9 10
|-/ |-/ |-/ |-/ |-/ |
|---/   |---/   |---/
|-------/       |
|---------------/
x
```

Parameters:

list: INTEGER *intent() size(:, :, :)* 3d arrays containing lists to be stacked

items: INTEGER *intent() size(:)* the numbers of items to be stacked in each list

depth: INTEGER *intent() scalar* dimensionality of the stacked objects (size of list(:,1,1))

length: INTEGER *intent() scalar* the number of lists (size of list(1,1,:))

width: INTEGER *intent() scalar* max size of lists (size of list(1,:,1))

mpi_sync()
syncs the cpus by calling mpi_barrier

mpi_wall_clock(*clock*)
returns the global time through mpi_wtime

Parameters:

clock: double precision intent(out) *scalar* the measured time

open_loadmonitor()
Opens the output for writing workload data to a file called "mpi_load.out"

record_load(*amount*)
Saves the given load.

Parameters:

amount: double precision *intent(in) scalar* the load to be stored

start_timer()
records the wall clock time to `stopwatch`

timer(*stamp*)
reads the elapsed wall clock time since the previous starting of the timer (saved in `stopwatch`) and then restarts the timer.

Parameters:

stamp: double precision intent(inout) *scalar* the elapsed real time

write_loadmonitor()
Routine for writing force calculation workload analysis data to a file called "mpi_load.out"

quaternions (Quaternions.f90)

A module for basic quarternion operations and 3D spatial rotations using quaternion representation Quaternions are a 4-component analogue to complex numbers

$$\mathbf{q} = w + x\mathbf{i} + y\mathbf{j} + z\mathbf{k} = [w, x, y, z]$$

where the three imaginary components obey $\mathbf{ijk} = \mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1$. This leads to a structure similar to that of complex numbers, except that the quaternion product defined according to the above rules is non-commutative $\mathbf{q}_1\mathbf{q}_2 \neq \mathbf{q}_2\mathbf{q}_1$.

It turns out that unit quaternions $||\mathbf{q}|| = \sqrt{w^2 + x^2 + y^2 + z^2} = 1$ represent the space of 3D rotations so that the rotation by angle α around unit axis $\mathbf{u} = [x, y, z]$ is represented by the quaternion

$$\mathbf{q} = [\cos\frac{\alpha}{2}, x\sin\frac{\alpha}{2}, y\sin\frac{\alpha}{2}, z\sin\frac{\alpha}{2}]$$

and joining rotations is represented as a a quaternion product (rotating first by $\mathbf{q}_1$, then by $\mathbf{q}_2$ yields the combined rotation of $\mathbf{q}_{12} = \mathbf{q}_2\mathbf{q}_1$).

Full documentation of global variables in quaternions

norm_tolerance
double precision *scalar parameter*

initial value = 1.0d-8

the threshold value for the norm for treating vectors as zero vectors

Full documentation of custom types in quaternions

qtrn
The quarternion type. It only contains four real components, but the main advantage for defining it as a custom type is the possibility to write routines and operators for quaternion algebra.

Contained data:

y: double precision *scalar* an "imaginary" component of the quaternion

x: double precision *scalar* an "imaginary" component of the quaternion

z: double precision *scalar* an "imaginary" component of the quaternion

w: double precision *scalar* the "real" component of the quaternion

Full documentation of subroutines in quaternions

norm_quaternion (*qq*)
norms the given quaternion

Parameters:

qq: TYPE(qtrn) *intent() scalar* quaternion to be normed to unity

Full documentation of functions in quaternions

cross (*v*, *u*)
Normal cross product of vectors $\mathbf{v} \times \mathbf{u}$ (Note: for 3-vectors only!)

Parameters:

v: double precision *intent() size(3)* vector

u: double precision *intent() size(3)* vector

dot (*v*, *u*)
Normal dot product of vectors $\mathbf{v} \cdot \mathbf{u}$ (Note: for 3-vectors only!)

Parameters:

v: double precision *intent() size(3)* vector

u: double precision *intent() size(3)* vector

q2angle (*q*)
Returns the angle of rotation described by the UNIT quarternion $\mathbf{q}$. Note that the unity of $\mathbf{q}$ is not checked (as it would be time consuming to calculate the norm all the time if we know the quaternions used have unit length).

Parameters:

q: TYPE(qtrn) *intent() scalar* a quaternion representation of rotation

q2axis (*q*)
Returns the axis of rotation described by the UNIT quarternion $\mathbf{q}$. Note that the unity of $\mathbf{q}$ is not checked (as it would be time consuming to calculate the norm all the time if we know the quaternions used have unit length).

Parameters:

q: TYPE(qtrn) *intent() scalar* a quaternion representation of rotation

q2matrix (*q*)
Returns the rotation matrix described by the UNIT quarternion $\mathbf{q}$. Note that the unity of $\mathbf{q}$ is not checked (as it would be time consuming to calculate the norm all the time if we know the quaternions used have unit length).

Parameters:

q: TYPE(qtrn) *intent() scalar* a quaternion representation of rotation

qconj (*q*)
Returns the quarternion conjugate of $\mathbf{q}$: $\mathbf{q}^* = w + x\mathbf{i} + y\mathbf{j} + z\mathbf{k} \rightarrow w - x\mathbf{i} - y\mathbf{j} - z\mathbf{k}$

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

qdiv (*q*, *r*)
Returns the quarternion $\mathbf{q}$ divided by scalar r component-wise

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

r: double precision ***intent() scalar*** a real scalar

qinv (*q*)
Returns the quarternion inverse of $\mathbf{q}$: $\mathbf{q}^*/||\mathbf{q}||$

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

qminus (*q*, *r*)
Returns the quarternion $\mathbf{q}$ subtracted by scalar r component-wise

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

r: double precision ***intent() scalar*** a real scalar

qnorm (*q*)
Returns the quarternion norm of $\mathbf{q}$: $||\mathbf{q}|| = \sqrt{w^2 + x^2 + y^2 + z^2}$

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

qplus (*q*, *r*)
Returns the quarternion $\mathbf{q}$ added by scalar r component-wise

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

r: double precision ***intent() scalar*** a real scalar

qprod (*q1*, *q2*)
Returns the quarternion product $\mathbf{q}_1\mathbf{q}_2$ Note that the product is non-commutative: $\mathbf{q}_1\mathbf{q}_2 \neq \mathbf{q}_2\mathbf{q}_1$

Parameters:

q1: TYPE(qtrn) ***intent() scalar*** a quaternion

q2: TYPE(qtrn) ***intent() scalar*** a quaternion

qtimes (*r*, *q*)
Returns the quarternion $\mathbf{q}$ multiplied by scalar r component-wise

Parameters:

r: double precision ***intent() scalar*** a real scalar

q: TYPE(qtrn) ***intent() scalar*** a quaternion

qtimesB(*q*, *r*)
Returns the quarternion $\mathbf{q}$ multiplied by scalar r component-wise

Parameters:

q: TYPE(qtrn) ***intent() scalar*** a quaternion

r: double precision ***intent() scalar*** a real scalar

rot2q(*a*, *u*)
Returns the quarternion representing a rotation around axis $\mathbf{u}$ by angle α

Parameters:

a: double precision ***intent() scalar*** angle in radians

u: double precision ***intent() size(3)*** 3D vector, defining an axis of rotation

rotate_a(*vec*, *da*)
Returns the vector rotated according to the vector $\mathbf{d}$. The axis of rotation is given by the direction of $\mathbf{d}$ and the angle by $||\mathbf{d}||$.

Parameters:

vec: double precision ***intent() size(3)*** vector to be rotated

da: double precision ***intent() size(3)*** rotation vector (e.g., angular velocity x time ωt)

rotate_au(*vec*, *a*, *u*)
Returns the vector rotated according to the axis $\mathbf{u}$ and angle α.

Parameters:

vec: double precision ***intent() size(3)*** vector to be rotated

a: double precision ***intent() scalar*** angle of rotation

u: double precision ***intent() size(3)*** axis of rotation

rotate_q(*vec*, *q*)
Returns the 3D vector rotated according to the UNIT quarternion $\mathbf{q}$. Note that the unity of $\mathbf{q}$ is not checked (as it would be time consuming to calculate the norm all the time if we know the quaternions used have unit length).

Parameters:

vec: double precision ***intent() size(3)*** vector to be rotated

q: TYPE(qtrn) ***intent() scalar*** a quaternion representation of rotation

vec2q(*v*)
Returns the quarternion representing a rotation around axis $\mathbf{v}$ by angle $||\mathbf{v}||$. If $\mathbf{v} = 0$, the quaternion $\mathbf{q} = [1000]$ will be returned.

Parameters:

v: double precision ***intent() size(3)*** 3D vector, defining both the angle and axis of rotation

vnorm(*v*)
Norm of a vector, $||\mathbf{v}||$

Parameters:

v: double precision ***intent() size(3)*** vector

mt95 (Mersenne.f90)

The module mt95 contains a random number generator. Currently 'Mersenne twister' is used, but it could in principle be replaced with any generator. This is an external module not written as part of the Pysic project.

The generator is initialized with the routine `genrand_init()` and random real numbers in [0,1] and [0,1) are extracted with `genrand_real1()` and `genrand_real2()`, respectively.

Routines of the mt95 module

genrand_init (*seed*)

genrand_real1 (*random*)

genrand_real2 (*random*)

CHAPTER

FIVE

DEVELOPMENT OF PYSIC

5.1 Version history

This is a list of the main updates in the different versions of Pysic. Descriptions of all incremental changes can be found in the commit log (see also the develop version).

The version number is available in Pysic as the variable:

`pysic.version`

5.1.1 Version 0.6

- Added support for dividing the system to subsystems and allowing the use of different calculators on the subsystems. This allows hybrid QM/MM calculations. See `HybridCalculator`, `SubSystem`, `Interaction`.

5.1.2 Version 0.5

- Added hdf5 archiving module `pysic.utility.archive`.
- Added the Comb potential for Si/SiO

5.1.3 Version 0.4.8

- Fixed compatibility with syntax changes in ASE 3.7.0.
- Added piping of `ChargeRelaxation` objects.
- Added a potentiostat as a `ChargeRelaxation` type.
- Added a constrained optimization as a `ChargeRelaxation` type.
- Added utility functions such as `get_neighbor_distances()`, `expand_symbols_string()`

5.1.4 Version 0.4.7

- Added wrapping of several *Calculators in ASE*

5.1.5 Version 0.4.6

- Code optimization: updates in the memory allocation and computation routines in the Fortran core for better performance.
- Added a warning system (`pysic.utility.error.Warning`)
- Added support for pairwise bond order factors (in addition to per-atom factors), see *Atomic and pairwise factors*.
- Numerous bug fixes, see the github commit log for details.

5.1.6 Version 0.4.5

- Added the `CompoundPotential` class for representing complicated potentials.
- Added the `SuttonChenPotential` class describing the Sutton-Chen potential.
- Added the *Shifted power potential*
- Interface enhancements. E.g., it is possible to pass lists of potentials to methods like `pysic.calculator.Pysic.add_potential()`, or pass `ProductPotential` objects to other `ProductPotential` objects.
- Efficiency fixes. E.g., when bond order factors are created in the core, it is checked that duplicates are not created.

5.1.7 Version 0.4.4

- Added the ability to calculate products of local potentials (see `pysic.interactions.local.ProductPotential`)
- Added the *Charged-pair potential*
- Separated the old charged exponential potential to *Exponential potential* and *Charge dependent exponential potential*
- Changed the *Bond bending potential* to allow more general expressions.
- Added the *Absolute charged-pair potential*

5.1.8 Version 0.4.3

- Major restructuring of the Python source code
- Provided a Makefile for compiling
- Added calculation of the stress tensor with the method `pysic.calculator.Pysic.get_stress()`
- Added the *Tabulated potential*
- Added the *Tabulated scaling function*
- Added the *Tabulated bond order factor*
- Bug fix: Fixed an issue with core initialization where changing the size of the supercell would lead to a conflict in neighbor list updating (the list update was tried before the cell update but failed due to the cell having been changed).
- Bug fix: Fixed an issue with the parallel neighbor list building algorithm which did not properly broadcast the calculated lists to all cpus.

5.1.9 Version 0.4.2

- Restructured the interaction evaluation loops in the Fortran core (*potentials (Potentials.f90)*)
- Added support for 4-body potentials
- Added the *Dihedral angle potential*
- Added the *Buckingham potential*
- Added the *Power decay potential*
- Added the *Power decay bond order factor*
- Added the *Square root scaling function*
- Bug fix: fixed a memory issue in Ewald summation `CoulombSummation`
- Bug fix: fixed an issue with periodic boundaries in `FastNeighborList`
- Bug fix: fixed an issue with special parameter values in Tersoff bond order factor evaluation
- Bug fix: fixed an issue where the cutoff of a bond order factor could overwrite a longer cutoff a potential
- Bug fix: fixed an indexing error in evaluation of 3-body interaction which gave to incorrect forces
- Bug fix: fixed and indexing error in neighbor offsets in `FastNeighborList`

5.1.10 Version 0.4.1

- Implemented an order $\mathcal{O}(n)$ neighbor finding algorithm in Fortran (see `pysic.calculator.FastNeighborList`)

5.1.11 Version 0.4

- Implemented the Ewald summation of $\frac{1}{r}$ potentials (see `pysic.interactions.coulomb.CoulombSummation`)
- The framework allows for the addition of other summation methods later on, but for now only standard Ewald is available

5.1.12 Version 0.3

- Implemented framework for charge relaxation (see `pysic.charges.relaxation.ChargeRelaxation`)
- Implemented the *Damped dynamics* charge relaxation algorithm.
- Implemented the *Charge dependent exponential potential* potential.

5.1.13 Version 0.2

- Implemented bond order factors (see `pysic.interactions.bondorder.Coordinator` and `pysic.interactions.bondorder.BondOrderParameters`) for scaling of potential energy according to local bond structure.
- Implemented a more robust method for tracking the status of the Fortran core (see `pysic.core.CoreMirror`). This makes it less likely that wrong results are produced due to the changes in the user interface not propagating to the core.

5.1.14 Version 0.1

- First publicly available version
- Python interface
  - pysic
  - pysic.calculator.Pysic
  - pysic.interactions.local.Potential
  - pysic_utility
- Framework for handling pair- and three-body potentials
- ASE compatibility
  - pysic.calculator.Pysic.get_forces()
  - pysic.calculator.Pysic.get_potential_energy()

5.2 Development

Please report any bugs you find by mailing to teemu.hynninen utu.fi or contact on Twitter, @thynnine. There is also an issue tracker set up at github, where intended features and bugs are listed.

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