# 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 is developed as part of the Mordred 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 $E_{\mathrm{local}}$. 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 $\eta_i$ 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 $\eta_i$ 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 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.

[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).

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.

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 play with it. However, the code is provided with no warranty or support.

## 2.2 Compiling Pysic

No installers of makefiles are currently provided with Pysic. Once Pysic is in a production capable stage, some kind of an installation tool will be produced.

To run Pysic, you will need Python 2.7 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.

When compiling Pysic, one must wrap the interface module *pysic_interface (PyInterface.f90)* with f2py and compile all other Fortran source directly to `.mod` modules. This can be achieved with:

```
> f2py -m pysic_fortran -h pysic_fortran.pyf PyInterface.F90
> f2py -c pysic_fortran.pyf Mersenne.F90 MPI.F90 Quaternions.F90 \
> Utility.F90 Geometry.F90 Potentials.F90 Core.F90 PyInterface.F90
```

For MPI, use the conditional compiling flag `-D MPI`. This tells the Fortran compiler to include the MPI portions of the code:

```
> 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
```

Above, the `gfortran` and `mpif90` compilers are used, but change the names to whichever compilers you wish to call. 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.

The utility module `pysic_utility` is also imported as `pysic.pu`, but it is also convenient to import it separately:

```
>>> import pysic_utility
>>> pysic_utility.plot_energy_on_plane(0,system,[[1,0,0],[0,1,0]],[10,10])
```

A shorthand can be introduced through the `as` keyword:

```
>>> import pysic_utility as pu
>>> pu.plot_energy_on_plane(0,system,[[1,0,0],[0,1,0]],[10,10])
```

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

```
>>> import pysic_fortran as pf
>>> import pysic_utility as pu
>>> 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
```

## 3.6 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

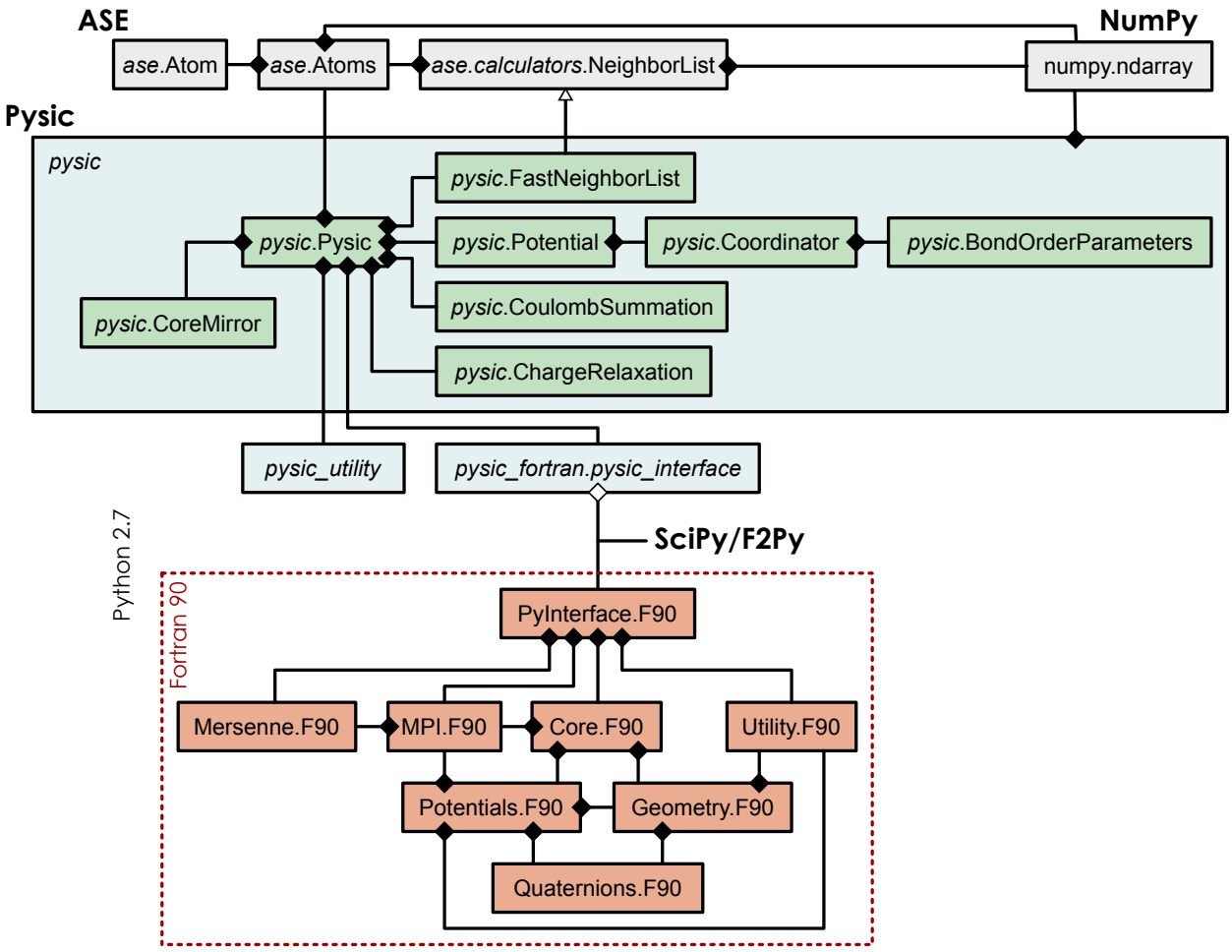
# STRUCTURE AND SYNTAX IN PYSIC

## 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: `Pysic`, which defines a calculator for the ASE simulation environment [1], `Potential`, which defines potentials to be used by `Pysic` for calculating atomic interactions, `Coordinator` which can be used for modifying potentials with bond order factors, and `BondOrderParameters` which are used as a container of parameters for the `Coordinator`.

### 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/

### 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()`
- `set_potentials()`

#### Coulomb handling

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

#### Charge relaxation handling

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

#### 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.**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_potential**(*potential*)

Add a potential to the list of potentials.

Parameters:

**potential: 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**()
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**()
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**()
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=0.5*)
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, the ASE NeighborList are used. 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_charge_relaxation**()
Returns the ChargeRelaxation object connected to the calculator.

**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*)
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_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*)
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*)
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

**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: `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.

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.

#### List of currently available potentials

Below is a list of potentials currently implemented.

- *Constant potential*
- *Constant force potential*
- *Power decay potential*
- *Harmonic potential*
- *Lennard-Jones potential*
- *Buckingham potential*
- *Charge dependent exponential 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()`

**Power decay potential** 2-body interaction defined as

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

where $\varepsilon$ 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()`

**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 $r_{\mathrm{cut}}$ 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 $\varepsilon$ is an energy constant defining the depth of the potential well and $\sigma$ 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 $\sigma$ 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()

**Charge dependent exponential potential** 2-body interaction defined as

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

where $\varepsilon$ is an energy scale constant, $\zeta$ is a length decay constant, $\xi_i$ 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('exponential')
['epsilon', 'zeta',
 'Rmax1', 'Rmin1', 'Qmax1', 'Qmin1',
 'Rmax2', 'Rmin2', 'Qmax2', 'Qmin2',
 'xi1', 'xi2']
```

Fortran routines:

- create_potential_characterizer_charge_exp()
- evaluate_energy_charge_exp()
- evaluate_force_charge_exp()
- evaluate_electronegativity_charge_exp()

**Bond bending potential** 3-body interaction defined as

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

where $k$ is an angular spring constant, $\theta$ is an angle defined by three points in space (atomic positions) and $\theta_0$ is the equilibrium angle. The potential therefore describes an angular spring force related to bending of bonds.

Keywords:

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

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 $\theta$ is the dihedral angle, with $\theta_0$ 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_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()

#### Full documentation of the Potential class

**class** pysic.**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

**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_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_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.

**set_coordinator**(*coordinator*)
Sets a new 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

### 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.

#### 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

$$\rho(\mathbf{r}) = \rho_s(\mathbf{r}) + \rho_l(\mathbf{r}) \tag{4.2}$$

$$\rho_s(\mathbf{r}) = \sum_i \left[q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i G_\sigma(\mathbf{r} - \mathbf{r}_i)\right] \tag{4.3}$$

$$\rho_l(\mathbf{r}) = \sum_i q_i G_\sigma(\mathbf{r} - \mathbf{r}_i) \tag{4.4}$$

$$G_\sigma(\mathbf{r}) = \frac{1}{(2\pi\sigma^2)^{3/2}} \exp\left(-\frac{|\mathbf{r}|^2}{2\sigma^2}\right) \tag{4.5}$$

Here $\rho_l$ generates a long range interaction since at large distances the Gaussian densities $G_\sigma$ 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 $\rho_s$ 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

$$E_s = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_s(\mathbf{r})\rho_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r \mathrm{d}^3 r' \tag{4.6}$$

$$= \frac{1}{4\pi\varepsilon_0} \sum_{(i,j)} \frac{q_i q_j}{r_{ij}} \mathrm{erfc}\left(\frac{r_{ij}}{\sigma\sqrt{2}}\right). \tag{4.7}$$

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

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

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

$$E_l = \frac{1}{2V\varepsilon_0} \sum_{\mathbf{k}\neq 0} \frac{e^{-\sigma^2 k^2/2}}{k^2} |S(\mathbf{k})|^2 - \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_i^N q_i^2 \tag{4.8}$$

$$S(\mathbf{k}) = \sum_i^N q_i e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} \tag{4.9}$$

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

$$E = E_s + E_l.$$

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 $\alpha$, 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 $\alpha$ 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.**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.

### 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.**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: BondOrderCoordinator** 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: BondOrderCoordinator** 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.

### 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 according to the number of atoms they act on. So, an n-body factor can have parameters which are applied for 1-body, 2-body, etc. terms. 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']]
```

As a rule of thumb, if an n-body bond order factor incorporates parameters for m bodies (m <= n), then these parameters are targeted at the first m symbols of the target list. For instance, if a 3-body factor has the targets of the above example (three_body_targets) and it contains 1- and 2-body parameters, then the 1-body parameters are targeted at Si atoms and the 2-body parameters at Si-O bonds.

As an example, the Tersoff bond order factor

$$b_i = \left[ 1 + \left( \beta_i \sum_{j \neq i} \sum_{k \neq i,j} \xi_{ijk} g_{ijk} \right)^{\eta_i} \right]^{-\frac{1}{2\eta_i}}$$

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

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

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 three single body and four two body 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, mu],
...                                               [a, c, d, h],
...                                               [ ]])
```

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('mu', mu)
>>> bonds.set_parameter_value('a', a)
>>> bonds.set_parameter_value('c', c)
>>> bonds.set_parameter_value('d', d)
>>> bonds.set_parameter_value('h', h)
```

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 example creates a bond order factor which is applied to all Si triplets (symbols=[['Si','Si','Si']]). The command also assigns 1-body parameters beta, eta, and mu, and 2-body 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'],
...                    ['Si', 'O', 'O']])
>>> bonds.get_symbols()
[['Si', 'Si', 'Si'], ['Si', 'Si', 'O'], ['Si', 'O', 'Si'], ['Si', 'O', 'O']]
```

The format of the symbol list is as follows. In each triplet, the first symbol determines the element on which the factor is calculated. Since above the first symbol of each triplet is 'Si', the factor will only be applied on Si atoms. The other symbols define the other elements in the triplets which are taken in to account. The second and third symbols are not, however, symmetric. As the bond order factor is defined using 2-body parameters (a_ij etc.), the first two symbols determine the elements of those two atoms (atoms i and j). The third symbol determines the element of the third atom (atom k) of the triplet. I.e., in the example above, Si-O bond parameters are included with:

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

where the first works for triplets O-Si-Si and the second for O-Si-O. However, one should note especially that a triplet A-B-C is only taken in to account if both bonds (A-B) and (B-C) have parameters associated with them. Therefore, ['Si', 'O', 'O'] is enough to fully define O-Si-O bond triplets, but to fully describe Si-Si-O, one also has to define the Si-Si bond with O as the third partner, which is given by:

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

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_siosi = pysic.BondOrderParameters('tersoff', cutoff=3.2, cutoff_margin=0.4,
...                                        symbols=[['Si', 'O', 'Si']],
...                                        parameters=[[beta_si, eta_si, mu_si],
...                                                    [a_sio, c_sio, d_sio, h_sio],
...                                                    [ ]])
>>> bond_sisio = pysic.BondOrderParameters('tersoff', cutoff=3.5, cutoff_margin=0.5,
...                                        symbols=[['Si', 'Si', 'O']],
...                                        parameters=[[beta_si, eta_si, mu_si],
...                                                    [a_sisi, c_sisi, d_sisi, h_sisi],
...                                                    []])
>>> bond_list = [bond_siosi,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 1-body 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 1-body parameters in bond_sisio are in fact ignored. This feature can be exploited for mixing different types of bond order factors, as explained below.

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.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*
- *Coordination bond order factor*
- *Power decay bond order factor*
- *Tersoff bond order factor*

**Coordination scaling function** 1-body bond order factor defined as

$$b_i(\Sigma_i) = \varepsilon_i \frac{\Delta\Sigma_i}{1 + \exp(\gamma_i \Delta\Sigma_i)}$$
$$\Delta\Sigma_i = C_i(\Sigma_i - N_i).$$

where $\Sigma_i$ 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']]
```

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

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

where $\Sigma_i$ is the bond order sum and $\varepsilon$ is a scaling constant.

Keywords:

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

**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

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

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')
[[], [epsilon, a, n]]
```

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

$$b_i = \left[1 + \left(\beta_i \sum_{j \neq i} \sum_{k \neq i,j} \xi_{ijk} g_{ijk}\right)^{\eta_i}\right]^{-\frac{1}{2\eta_i}}$$

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

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

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', 'mu'], ['a', 'c', 'd', 'h'], []]
```

### 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.**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_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.

**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

### 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.

#### 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.

#### 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()

**Charge relaxation**

- charge_relaxation()

#### Full documentation of the ChargeRelaxation class

**class** pysic.**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.

**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.

**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.

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

**relaxation_modes = ['dynamic']**
Names of the charge relaxation algorithms available.

These are keywords needed when creating the ChargeRelaxation objects as type specifiers.

**relaxation_parameter_descriptions = {'dynamic': ['time steps of charge dynamics between molecular dynamic**
Short descriptions of the relaxation parameters.

**relaxation_parameters = {'dynamic': ['n_steps', 'timestep', 'inertia', 'friction', 'tolerance']}**
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.

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

### 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 $r_{\mathrm{cut}}$ 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 $r_{\mathrm{skin}}$.

#### 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. [2] 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

$$d_i = \frac{|\mathbf{v}_i \cdot \mathbf{n_i}|}{|\mathbf{n}_i|} \tag{4.15}$$

$$\mathbf{n}_i = \mathbf{v}_j \times \mathbf{v}_k \tag{4.16}$$

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.

#### Methods inherited from ASE NeighborList

- get_neighbors
- update

#### List of methods

- `build()`

#### Full documentation of the FastNeighborList class

**class** `pysic.`**`FastNeighborList`**(*cutoffs*, *skin=0.5*)

ASE has a neighbor list class built in, 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.

[2] 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!

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

### 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.**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 Errors defined by the pysic module

The module defines a group of intrinsic errors to describe situations where one tries to use or set up the calculator with errorneous or insufficient information.

**exception** pysic.**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.**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.**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.**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.**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

**exception** pysic.**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

### 4.2.4 Functions of the pysic module

The module defines a group of functions to directly access the Fortran core for information on available potentials. The main module of Pysic.

This module defines the user interface in Pysic for setting up potentials and calculators.

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. As the environment won't know when the user is done with his simulation, terminating the MPI is left as a manual operation. If one terminates Python running pysic without finishing the MPI first, the MPI framework in the Fortran core will print an error.

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 module

A module for providing utility tools and parameters. Contains necessary and supporting auxiliary functions for Pysic.

**class** pysic_utility.**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

pysic_utility.**char2int** (*char_in*)
Codes a single character to an integer.

pysic_utility.**expand_symbols_table** (*symbol_list*, *type=None*)
Creates a table of symbols for a BondOrderParameters object.

The syntax for defining the targets of bond order factors 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.BondOrderParameters.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

pysic_utility.**int2char**(*int_in*)
Decodes an integer to a single character.

pysic_utility.**ints2str**(*ints_in*)
Decodes a list of integers to a string.

pysic_utility.**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_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_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_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_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_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_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

pysic_utility.**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_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*)

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

**add_potential** (*n_targets*, *n_params*, *pot_name*, *parameters*, *cutoff*, *smooth_cut*, *elements*, *tags*, *indices*, *orig_elements*, *orig_tags*, *orig_indices*, *pot_index*)

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

**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** (*n_atoms*, *energy*)
Returns the total potential energy of the system

Calls `core_calculate_energy()`

Parameters:

**n_atoms: integer *intent(in) scalar*** number of atoms

**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 $xx, yy, zz, yz, xz, xy$)

**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 $n_{\mathrm{cpus}}$ 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*, *reciprocal_cut*, *sigma*, *epsilon*, *energy*)
Debugging routine for Ewald

Parameters:

real_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*)
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*)
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

**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*, *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

**reciprocal_cut: integer** ***intent(in) size(3)*** the k-space cutoffs

**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

**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_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

**n_bond_factors**
integer *scalar*

*initial value* = 0

**n_interactions**
integer *scalar*

*initial value* = 0

number of potentials

**n_saved_bond_order_factors**
integer *scalar*

*initial value* = 0

number of saved bond order factors

**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)

**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*)
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

**core_add_potential**(*n_targets*, *n_params*, *pot_name*, *parameters*, *cutoff*, *smooth_cut*, *elements*, *tags*, *indices*, *orig_elements*, *orig_tags*, *orig_indices*, *pot_index*)

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.

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

**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** (*n_atoms*, *cutoffs*)
Parameters:

n_atoms: integer *intent(in) scalar*

cutoffs: double precision *intent(in) size(n_atoms)*

**core_calculate_bond_order_factors** (*n_atoms*, *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:

**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

**total_bond_orders: double precision intent(out)** ***size(n_atoms)*** the calculated bond order sums

**core_calculate_bond_order_gradients**(*n_atoms*, *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 $\alpha$. If for_factor is .true., the gradients of the bond factor of the given atom are calculated with respect to moving all atoms.

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 ($\alpha$), or the atoms whose factor is differentiated ($i$) if for_factor is .true.

**raw_sums: double precision** ***intent(in) size(n_atoms)*** precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

**total_gradient: double precision intent(out)** ***size(3, n_atoms)*** the calculated bond order gradients $\nabla_\alpha b_i$

**total_virial**: double precision **intent(out)** *size(6)*

**for_factor: logical** ***intent(in) scalar optional*** a switch for requesting the gradients for a given $i$ instead of a given $\alpha$

**core_calculate_bond_order_gradients_of_factor**(*n_atoms*, *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 $\alpha$.

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 ($i$)

**raw_sums: double precision *intent(in) size(n_atoms)*** precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

**total_gradient: double precision intent(out) *size(3, n_atoms)*** the calculated bond order gradients $\nabla_\alpha b_i$

**total_virial**: double precision **intent(out)** *size(6)*

**core_calculate_electronegativities** (*n_atoms*, *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 $\alpha$. 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:

**n_atoms: integer *intent(in) scalar*** number of atoms

**total_enegs: double precision intent(out) *size(n_atoms)*** an array containing the calculated charge forces for all atoms

**core_calculate_energy** (*n_atoms*, *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:

**n_atoms: integer *intent(in) scalar*** number of atoms

**total_energy: double precision intent(out) *scalar*** calculated total potential energy

**core_calculate_forces** (*n_atoms*, *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 $\alpha$. 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:

**n_atoms: integer *intent(in) scalar*** number of atoms

**total_forces: double precision intent(out)** ***size(3, n_atoms)*** an array containing the calculated forces for all atoms

**total_stress: double precision intent(out)** ***size(6)*** as array containing the calculated stress tensor

**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_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_nbs*, *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_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.

**core_create_space_partitioning**(*max_cutoff*)

Parameters:

max_cutoff: double precision *intent(in) scalar*

**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*)

Parameters:

n_atoms: integer *intent(in) scalar*

atom_doublet: type(atom) *intent(in) size(2)*

index1: integer *intent(in) scalar*

index2: integer *intent(in) scalar*

test_index1: integer *intent(in) scalar*

interaction_indices: integer *intent() pointer size(:)*

separations: double precision *intent(in) size(3, 1)*

directions: double precision *intent(in) size(3, 1)*

distances: double precision *intent(in) size(1)*

calculation_type: integer *intent(in) scalar*

**energy**: double precision **intent(out)** *scalar*

**forces**: double precision **intent(out)** *size(3, n_atoms)*

**enegs**: double precision **intent(out)** *size(n_atoms)*

**stress**: double precision **intent(out)** *size(6)*

**many_bodies_found**: logical **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*)

Parameters:

n_atoms: integer *intent(in) scalar*

atom_quadruplet: type(atom) *intent(in) size(4)*

index1: integer *intent(in) scalar*

index2: integer *intent(in) scalar*

index3: integer *intent(in) scalar*

index4: integer *intent(in) scalar*

test_index1: integer *intent(in) scalar*

test_index2: integer *intent(in) scalar*

test_index3: integer *intent(in) scalar*

interaction_indices: integer *intent() pointer size(:)*

separations: double precision *intent(in) size(3, 3)*

directions: double precision *intent(in) size(3, 3)*

distances: double precision *intent(in) size(3)*

calculation_type: integer *intent(in) scalar*

**energy**: double precision **intent(out)** *scalar*

**forces**: double precision **intent(out)** *size(3, n_atoms)*

**enegs**: double precision **intent(out)** *size(n_atoms)*

**stress**: double precision **intent(out)** *size(6)*

**many_bodies_found**: logical **intent(out)** *scalar*

**core_evaluate_local_singlet** (*n_atoms*, *index1*, *atom_singlet*, *interaction_indices*, *calculation_type*, *energy*, *forces*, *enegs*)

Evaluates the local potential affecting a single atom

Parameters:

**n_atoms: integer *intent(in) scalar*** number of atoms

**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(3, n_atoms)*** calculated forces

**enegs: double precision intent(inout) *size(n_atoms)*** 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*)

Parameters:

n_atoms: integer *intent(in) scalar*

atom_triplet: type(atom) *intent(in) size(3)*

index1: integer *intent(in) scalar*

index2: integer *intent(in) scalar*

index3: integer *intent(in) scalar*

test_index1: integer *intent(in) scalar*

test_index2: integer *intent(in) scalar*

interaction_indices: integer *intent() pointer size(:)*

separations: double precision *intent(in) size(3, 2)*

directions: double precision *intent(in) size(3, 2)*

distances: double precision *intent(in) size(2)*

calculation_type: integer *intent(in) scalar*

**energy**: double precision **intent(out)** *scalar*

**forces**: double precision **intent(out)** *size(3, n_atoms)*

**enegs**: double precision **intent(out)** *size(n_atoms)*

**stress**: double precision **intent(out)** *size(6)*

**many_bodies_found**: logical **intent(out)** *scalar*

**core_fill_bond_order_storage**(*n_atoms*)

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.

Parameters:

**n_atoms: integer *intent(in) scalar*** number of atoms

**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**(*n_atoms*, *group_index*, *atom_index*, *bond_order_factor*)

Returns the bond order factors of the given atom for the given group.

Parameters:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**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(out)** ***scalar*** the calculated bond order factor

**core_get_bond_order_factors**(*n_atoms*, *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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**group_index: integer** ***intent(in) scalar*** index for the bond order factor group

**bond_order_factors: double precision intent(out)** ***size(n_atoms)*** the calculated bond order factors

**core_get_bond_order_gradients**(*n_atoms*, *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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**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(out)** ***size(3, n_atoms)*** the calculated gradients of the bond order factor

**bond_order_virial**: double precision **intent(out)** *size(6)*

**core_get_bond_order_sums**(*n_atoms*, *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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**group_index: integer** ***intent(in) scalar*** index for the bond order factor group

**bond_order_sums: double precision intent(out)** ***size(n_atoms)*** 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*, *reciprocal_cut*, *sigma*, *epsilon*, *energy*)
Debug routine for Ewald

Parameters:

real_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*)
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)*

**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*)
Parameters:

atom_index: integer *intent(in) scalar*

**n_neighbors**: integer **intent(out)** *scalar*

**core_loop_over_local_interactions**(*n_atoms*, *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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**calculation_type: integer *intent(in) scalar*** index to specify if the loop calculates energies, forces, or e-negativities

**total_energy: double precision intent(out) *scalar*** calculated energy

**total_forces: double precision intent(out) *size(3, n_atoms)*** calculated forces

**total_enegs: double precision intent(out) *size(n_atoms)*** calculated electronegativities

**total_stress: double precision intent(out) *size(6)*** calculated stress

**core_post_process_bond_order_factors**(*n_atoms*, *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:

**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

**raw_sums: double precision *intent(in) size(n_atoms)*** precalculated bond order sums, $\sum_j c_{ij}$, in the above example.

**total_bond_orders: double precision intent(out) *size(n_atoms)*** the calculated bond order factors $b_i$

**core_post_process_bond_order_gradients**(*n_atoms*, *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:

**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

**raw_sums: double precision** ***intent(in) size(n_atoms)*** precalculated bond order sums, $\sum_j c_{ij}$, in the above example

**raw_gradients: double precision** ***intent(in) size(3, n_atoms)*** precalculated gradients of bond order sums, $\nabla_\alpha \sum_j c_{ij}$, in the above example

**total_bond_gradients: double precision intent(out)** ***size(3, n_atoms)*** 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**(*n_atoms*, *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:

**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*** 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(3, n_atoms)*** precalculated gradients of bond order sums, $\nabla_\alpha \sum_j c_{ij}$, in the above example

**total_bond_gradients: double precision intent(out)** ***size(3, n_atoms)*** the calculated bond order gradients $\nabla_\alpha b_i$

raw_virial: double precision *intent(in) size(6)*

**total_virial**: double precision **intent(out)** *size(6)*

**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**(*n_atoms*, *real_cut*, *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

**reciprocal_cut: integer *intent(in) size(3)*** the k-space cutoffs

**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

**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*)
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 $\alpha$ 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 potential

**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

**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

**n_bond_order_types**
integer *scalar parameter*

*initial value* = 6

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* = 9

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_spring_index**
integer *scalar parameter*

*initial value* = 2

internal index for the spring 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

**sqrt_scale_index**
integer *scalar parameter*

*initial value* = 6

internal index for the square root scaling potential

**tersoff_index**
integer *scalar parameter*

*initial value* = 2

internal index for the Tersoff bond order factor

**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 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** ***pointer size(:)*** number of parameters for each number of bodies (1-body parameters, 2-body parameters etc.)

**includes_post_processing: logical** ***scalar*** a logical tag specifying if there is a scaling function $s_i$ attached to the factor.

**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.

**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.

**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.

**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.

**includes_post_processing: logical** ***scalar*** a logical switch specifying if there is a scaling function $s_i$ attached to the factor

**group_index: integer** ***scalar*** The internal index of the *potential* the bond order factor is modifying.

**parameters: double precision** ***pointer size(:, :)*** numerical values for parameters

**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.

**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.)

**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

**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.

**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.

**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

**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**(*n_atoms*, *atoms*, *cell*, *real_cutoff*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *filter*, *scaler*, *include_dipole_correction*, *total_enegs*)

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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**atoms: type(atom)** ***intent(in) size(n_atoms)*** 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.)

**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 $\sigma$ 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 $\sigma$ 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 $\varepsilon_0$. 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.

**filter: logical** ***intent(in) size(n_atoms)*** a list of logical values, one per atom, false for the atoms that should be ignored in the calculation

**scaler: double precision** ***intent(in) size(n_atoms)*** 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(out)** ***size(n_atoms)*** the calculated electronegativities

**calculate_ewald_energy**(*n_atoms*, *atoms*, *cell*, *real_cutoff*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *filter*, *scaler*, *include_dipole_correction*, *total_energy*)

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

$$E = \sum_{(i,j)} \frac{1}{4\pi\epsilon_0}\frac{q_i q_j}{r_{ij}}, \tag{4.17}$$

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 (4.17) converges very slowly. [3] 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 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

$$\rho(\mathbf{r}) = \rho_s(\mathbf{r}) + \rho_l(\mathbf{r}) \tag{4.18}$$

$$\rho_s(\mathbf{r}) = \sum_i \left[q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i G_\sigma(\mathbf{r} - \mathbf{r}_i)\right] \tag{4.19}$$

$$\rho_l(\mathbf{r}) = \sum_i q_i G_\sigma(\mathbf{r} - \mathbf{r}_i) \tag{4.20}$$

$$G_\sigma(\mathbf{r}) = \frac{1}{(2\pi\sigma^2)^{3/2}} \exp\left(-\frac{|\mathbf{r}|^2}{2\sigma^2}\right) \tag{4.21}$$

Here $\rho_l$ generates a long range interaction since at large distances the Gaussian densities $G_\sigma$ 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 $\rho_s$ 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

$$E_s = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_s(\mathbf{r})\rho_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r \mathrm{d}^3 r' \tag{4.22}$$

$$= \frac{1}{4\pi\varepsilon_0} \sum_{(i,j)} \frac{q_i q_j}{r_{ij}} \mathrm{erfc}\left(\frac{r_{ij}}{\sigma\sqrt{2}}\right). \tag{4.23}$$

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

$$E_l = \frac{1}{2V\varepsilon_0} \sum_{\mathbf{k}\neq 0} \frac{e^{-\sigma^2 k^2/2}}{k^2} |S(\mathbf{k})|^2 - \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_i^N q_i^2 \tag{4.24}$$

$$S(\mathbf{k}) = \sum_i^N q_i e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} \tag{4.25}$$

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.

[3] 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.

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

$$E = E_s + E_l.$$

Parameters:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**atoms: type(atom)** ***intent(in) size(n_atoms)*** 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.)

**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 $\sigma$ 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 $\sigma$ 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 $\varepsilon_0$. 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.

**filter: logical** ***intent(in) size(n_atoms)*** a list of logical values, one per atom, false for the atoms that should be ignored in the calculation

**scaler: double precision** ***intent(in) size(n_atoms)*** 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

**`calculate_ewald_forces`** (*n_atoms*, *atoms*, *cell*, *real_cutoff*, *reciprocal_cutoff*, *gaussian_width*, *electric_constant*, *filter*, *scaler*, *include_dipole_correction*, *total_forces*, *total_stress*)

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:

**n_atoms: integer** ***intent(in) scalar*** number of atoms

**atoms: type(atom)** ***intent(in) size(n_atoms)*** 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.)

**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 $\sigma$ 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 $\sigma$ 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 $\varepsilon_0$. 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.

**filter: logical *intent(in) size(n_atoms)*** a list of logical values, one per atom, false for the atoms that should be ignored in the calculation

**scaler: double precision *intent(in) size(n_atoms)*** 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(out) *size(3, n_atoms)*** the calculated forces

**total_stress: double precision intent(out) *size(6)*** the calculated stress

**`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*)
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`

**`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_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*, *new_potential*)

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

**new_potential: type(potential) intent(out) *scalar*** the created potential

**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_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_power**(*index*)
Power law 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

**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_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) 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_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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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_tersoff**(*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_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*, *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 $\mu_i$ for the atomic partial charges. Similarly to `evaluate_forces()`, this function evaluates the chemical 'force' on the atomic charges

$$\chi_{\alpha,ijk} = -\mu_{\alpha,ijk} = -\frac{\partial U_{ijk}}{\partial q_\alpha}$$

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

**separations: double precision *intent(in) size(3, n_targets-1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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** (*separations*, *distances*, *interaction*, *eneg*, *atoms*)

Charge exp electronegativity

Parameters:

**separations: double precision *intent(in) size(3, 1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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

**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_energy** (*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.

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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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) optional*** 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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`** (*separations*, *distances*, *interaction*, *energy*, *atoms*)
Charge exp energy

Parameters:

**separations: double precision** ***intent(in) size(3, 1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $v_{ijk}$

**atoms: type(atom)** ***intent(in) size(2)*** 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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_power`** (*separations*, *distances*, *interaction*, *energy*)
Power energy

Parameters:

**separations: double precision** ***intent(in) size(3, 1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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_charge_exp** (*separations*, *distances*, *interaction*, *force*, *atoms*)
charge exp force

Parameters:

**separations: double precision *intent(in) size(3, 1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathbf{f}_{\alpha,ijk}$

**atoms: type(atom) *intent(in) size(2)*** 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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_power** (*separations*, *distances*, *interaction*, *force*)
Power force

Parameters:

**separations: double precision *intent(in) size(3, 1)*** atom-atom separation vectors $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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*, *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 $\alpha$ 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.

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 $\mathrm{r}_{12}$, $\mathrm{r}_{23}$ 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

**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*** number of targets

**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 number of targets 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*** number of targets of the parameter

**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_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*** number of targets

**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 a list of strings, each element showing the number of parameters for that number of bodies.

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

**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*** numner 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_tersoff** (*raw_sum*, *bond_params*, *factor_out*)

Tersoff post process factor

Parameters:

**raw_sum: double precision *intent(in) scalar*** the precalculated bond order sum, $\sum_j c_i j$ 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_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(out) *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_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 $r$, $r_{\mathrm{soft}}$, and $r_{\mathrm{hard}}$, 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 $r_{\mathrm{hard}}$

**soft_cut: double precision *intent(in) scalar*** the soft cutoff $r_{\mathrm{soft}}$

**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 $r$, $r_{\mathrm{soft}}$, and $r_{\mathrm{hard}}$, 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 $r_{\mathrm{hard}}$

**soft_cut: double precision *intent(in) scalar*** the soft cutoff $r_{\mathrm{soft}}$

**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 $\hat{r}$, $r$, $r_{\mathrm{soft}}$, and $r_{\mathrm{hard}}$, 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 $r_{\mathrm{hard}}$

**soft_cut: double precision *intent(in) scalar*** the soft cutoff $r_{\mathrm{soft}}$

**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

**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`)

**mass: double precision *scalar*** mass of th atom

**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

**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 $3 \times 3$ 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_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 $3 \times 3$ 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 $\pi$ 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

**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, $n_{\mathrm{cpus}}$

**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 $\alpha$ 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 $\alpha$

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 $\omega t$)

**rotate_au**(*vec*, *a*, *u*)
Returns the vector rotated according to the axis $\mathbf{u}$ and angle $\alpha$.

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.

### 5.1.1 Version 0.4.3

- Added calculation of the stress tensor with the method `pysic.Pysic.get_stress()`.
- 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.

### 5.1.2 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`

### 5.1.3 Version 0.4.1

- Implemented an order $\mathcal{O}(n)$ neighbor finding algorithm in Fortran (see `pysic.FastNeighborList`)

### 5.1.4 Version 0.4

- Implemented the Ewald summation of $\frac{1}{r}$ potentials (see `pysic.CoulombSummation`)
- The framework allows for the addition of other summation methods later on, but for now only standard Ewald is available

### 5.1.5 Version 0.3

- Implemented framework for charge relaxation (see `pysic.ChargeRelaxation`)
- Implemented the *Damped dynamics* charge relaxation algorithm.
- Implemented the *Charge dependent exponential potential* potential.

### 5.1.6 Version 0.2

- Implemented bond order factors (see `pysic.Coordinator` and `pysic.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.CoreMirror`). This makes it less likely that wrong results are produced due to the changes in the user interface not propagating to the core.

### 5.1.7 Version 0.1

- First publicly available version
- Python interface
  - `pysic`
  - `pysic.Pysic`
  - `pysic.Potential`
  - `pysic_utility`
- Framework for handling pair- and three-body potentials
- ASE compatibility
  - `pysic.Pysic.get_forces()`
  - `pysic.Pysic.get_potential_energy()`

## 5.2 Roadmap

This is a list of the planned major features to be implemented in Pysic.

### 5.2.1 Version 0.5

- Implementation of the COMB potential

### 5.2.2 Version 0.6

- Implementation of the ReaxFF potential

### 5.2.3 Other planned features

- Extensive library of potentials, including tabulated potentials
- Option for other charge relaxation algorithms
- Option for other long range interaction summation algorithms
- Convenience tools for generating parameters for Ewald summation
- Convenience tools for generating chemical symbol lists for Potentials
- Analysis tools for atomic structures
- Analysis tools for potential parameterisation and training

## 5.3 Development

Currently, the main developer and maintainer of the code is Teemu Hynninen (Tampere University of Technology and Aalto University, Helsinki).

Please notify me of any bugs you find by mailing to teemu.hynninen tut.fi or contact me on Twitter, @thynnine. There is also an issue tracker set up at github, where intended features and bugs are listed.

### 5.3.1 Fixed bugs

- Very serious MPI bug in the `build()` method of `pysic.FastNeighborList`: The final lists were not broadcast correctly to all cpus leading to some cpus not having the full neighbor lists. Due to the way interactions are evaluated, this usually allowed the simulations to start normally, but at some point the error would manifest as incorrectly calculated forces. Moreover, the errorneous behavior was not reproducible due to the way the result of the incorrect MPI broadcast depended on the relative speed of the cpus during list building. (4.6.2012, 0.4.3)
- MPI bug in Ewald energy and electronegativity calculation (`pysic.CoulombSummation`): Some energy components were evaluated on all cpus and summed together. (3.6.2012, 0.4.3)
- Core update issue: Changing the size of the supercell lead to conflict in neighbor list update in `pysic.FastNeighborList` since the list update was tried before the cell was updated in the core. This was no problem for the ASE neighbor list, but the new list building method requires that the Fortran core matches the atomic system in Python. (31.5.2012)
- Performance issue in Ewald force calculation (`pysic.CoulombSummation`, `calculate_ewald_forces()`): The force calculation routine saved in memory a huge array of structure factor gradients which were only used once and not calculated in parallel. This was a huge waste of memory and a performance bottleneck. (30.5.2012, 0.4.2)

- Index error in FastNeighborList offsets (`pysic.FastNeighborList`). Also, the offsets passed to Python were in Fortran array order, i.e., transposed. (29.5.2012, 0.4.2)
- Issue with bond order cutoff overwriting longer potential cutoffs: When neighbors are determined, a list of maximum cutoffs (cutoff for each atom) are needed (`pysic.Pysic.get_individual_cutoffs()`). In the determination, the cutoffs of potentials and bond order factors, as well as the Ewald real space cutoff are considered. There was an issue where the bond order factor if present was always used as the maximum even if the other were longer. (24.5.2012, 0.4.2)
- Index error in the 3-body evaluation loop leading to wrong forces. (24.5.2012, 0.4.2)
- Issues with how wrapping was done in the FastNeighborList search (`pysic.FastNeighborList`): The neighbor finding used only wrapped atomic coordinates to locate neighbors. This could lead to atoms crossing a periodic boundary and thus abruptly changing their wrapped position which was not seen by the neighbor offset until the list was refreshed. Changed this so that the list works in terms of absolute coordinate offsets, which do not change discontinuously. This is how the ASE list also works, and the proper way to handle the periodicity in the neighbor list. (18.05.2012, 0.4.2)
- Errorneous values for the Tersoff bond order factor for specific parameter values (`pysic.Potential`, *Tersoff bond order factor*): There were special cases of parameters that allowed for $0^0$ (or `0**0`) and similar ill-defined expressions in the differentiation of the bond order factor, even if the gradient did exist. Added handling for some such cases. Note though that there are still parameter values that must not be used. For instance, if $\eta < 0$, if the sum of local bond terms is zero, one ends up evaluating $\frac{1}{0}$, which is not defined either. (18.05.2012, 0.4.2)

### 5.3.2 Known issues

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