Jumos

Main Documentation

Release 0.2

Guillaume Fraux

January 18, 2017

Contents

Jumos is a package for molecular simulations written using the Julia language. It provides a set of customisable blocks for running molecular simulations, and developing novel algorithm for each part of a simulation. Every algorithm (potential computation, long range interactions, pair lists computing, outputs, *etc.*) can easily be customised.

Note: This package is in a very alpha stage, and still in heavy developement. Breaking changes can occurs in the API without any notice at any time.

This documentation is divided in two parts: first come the user manual, starting by some explanation about usal *algorithms in simulations* (page 2) and an *example* (page 4) of how we can use *Jumos* to run a molecular dynamic simulation. The second part is the developer documentation, exposing the internal of *Jumos*, and how we can use them to programm new algorithms.

1 Installation

Jumos uses the 0.4 prerelease version of Julia, and can be installed at julia prompt with the `Pkg.add("Jumos")` command. You also can run the unit tests with the `Pkg.test("Jumos")` command.

2 User manual

2.1 Package overview

This section is a guide to get started with molecular simulations in Jumos. It contains explanations about the how to define and run a basic simulation.

Simulation flow

In every molecular simulation, the main steps are roughly the same. We start by setting the simulated system: positions of the particles, maybe velocities, atomic types, potential to use between the atoms, *etc.* Secondly, we have to choose the simulation type and setup the propagator and the analysis algorithms.

Then we can run the simulation for a given number of steps `nsteps`. During the run, the propagator can be a Newton integrator for Molecular Dynamics, a MonteCarlo propagator for MonteCarlo simulation, a Gradient descent for energy minimization, *etc.* Other algorithms can be added to the simulation, in order to perform live analysis of the simulation or to output data.

All this is summarised in the figure *Simulation flow in Jumos* (page 3).

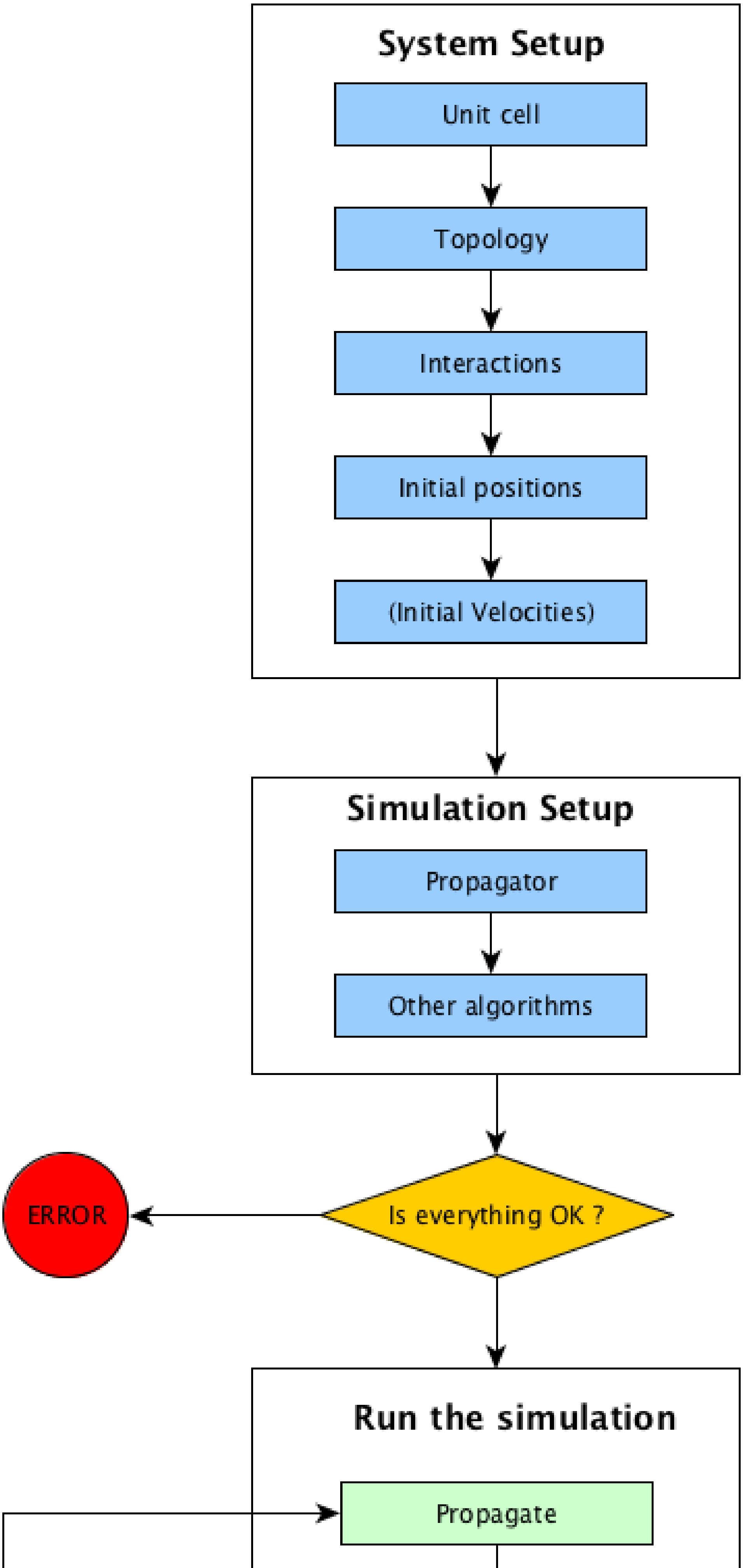
All the steps in the process of running a simulation are described below.

System setup

The system will contain all the physical informations about what we are simulating. In *Jumos*, a system is represented by the *Universe* (page 11) type. It should at least contain data about the *simulation cell* (page 5), the system *topology* (page 8), the initial particles coordinates and the *interactions* (page 9) between the particles.

Simulation setup

During the simulation, the system will be propagated by a *propagator* (page 18): `MolecularDynamics`, `MonteCarlo`, `Minimization` are examples of propagators. Other algorithms can take place here, either algorithms to compute thermodynamic properties or algorithms to modify the behaviour of the simulation.


System Setup
Unit cell
Topology
Interactions
Initial positions
(Initial Velocities)
Simulation Setup
Propagator
Other algorithms
ERROR
Is everything OK ?
Run the simulation
Propagate

Running the simulation

The simulation run is the main part of the simulation, and consist in three main steps:

- Use the propagator to genrerate an update in the particles positions;
- Compute thermodynamical properties of the system;
- Output data to file for later analysis.

Simulation example

In *Jumos*, one run simulations by writting specials Julia scripts. A primer intoduction to the Julia language can be found here, if needed.

Lennard-Jones fluid

Here is a simple simulation script for running a simulation of a Lennard-Jones fluid at $300K$.

```
#!/usr/bin/env julia

# Loading the Jumos module before anything else
using Jumos

# Molecular Dynamics with 1.0fs timestep
sim = Simulation(:MD, 1.0)

# Create a cubic cell with a width of 10A
cell = UnitCell(unit_from(10.0, "A"))
# Read a topology from a file
topology = Topology("lennard-jones.xyz")
# Create an universe from the cell and the topology

universe = Universe(cell, topology)
positions_from_file!(universe, "lennard-jones.xyz")
# Initialize random velocities at 300K
create_velocities!(universe, 300)

# Add Lennard-Jones interactions between He atoms
add_interaction!(
    universe,
    LennardJones(unit_from(0.2, "kJ/mol"), unit_from(2.0, "A")),
    "He", "He"
)

# You can either bind algorithms to variables ...
out_trajectory = TrajectoryOutput("LJ-trajectory.xyz", 1)
push!(sim, out_trajectory)
# ... or create them directly in function call
push!(sim, EnergyOutput("LJ-energy.dat", 10))

propagate!(sim, universe, 5000)

# Simulation scripts are normal Julia scripts !
println("All done")
```

Each simulation script should start by the `using Jumos` directive. This imports the module and the exported names in the current scope.

Then, in this script, we create two main objects: a *simulation* (page 18), and an *universe* (page 11). The topology and the original positions for the universe are read from the same file, as an `.xyz` file contains topological information (mainly the atomics names) and coordinates. The velocities are then initialized from a Boltzmann distribution at 300K.

The only interaction — a *Lennard-Jones* (page 10) interaction — is also added to the universe before the run. The next lines add some outputs to the simulation, namely a *trajectory* (page 17) and an *energy* (page 17) output. Finally, the simulation runs for 5000 steps.

Other example

Some other examples scripts can be found in the example folder in Jumos' source tree. To go there, use the julia prompt:

```
julia> Pkg.dir("Jumos")
"~/.julia/v0.4/Jumos"

julia>; cd $ans/examples
~/.julia/v0.4/Jumos/examples
```

Main types

Jumos is organised around two main types: the `Universe` hold data about the system we are simulating; and the `Simulation` type hold data about the algorithms we should use for the simulation.

Universe

The `Universe` type contains data. It is built around four other basic types:

- The *Topology* (page 8) contains data about the atomic organisation, *i.e.* the particles, bonds, angles and dihedral angles in the system;
- The *UnitCell* (page 5) contains data about the bounding box of the simulation;
- The *Interactions* (page 9) type contains data about the *potentials* (page 9) to use for the atoms in the system;
- The *Frame* (page 8) type contains raw data about the positions and maybe velocities of the particles in the system;

Simulation

The `Simulation` type contains algorithms. The *progagator* (page 18) algorithm is the one responsible for propagating the `Universe` along the simulation. It also contains some analysis algorithms (called *compute* (page 15) in *Jumos*); and some *output* (page 16) algorithms, to save data during the simulation run.

2.2 Universes

UnitCell

A simulation cell (`UnitCell` type) is the virtual container in which all the particles of a simulation move. The UnitCell type is parametrized by the `celltype`. There are three different types of simulation cells:

- Infinite cells (`InfiniteCell`) do not have any boundaries. Any move is allowed inside these cells;
- Orthorombic cells (`OrthorombicCell`) have up to three independent lenghts; all the angles of the cell are set to 90° ($\pi/2$ radians)
- Triclinic cells (`TriclinicCell`) have 6 independent parameters: 3 lenghts and 3 angles.

Creating simulation cell

UnitCell (*A*[, *B*, *C*, *alpha*, *beta*, *gamma*, *celltype*])
Creates an unit cell. If no `celltype` parameter is given, this function tries to guess the cell type using the following behavior: if all the angles are equals to $\pi/2$, then the cell is an `OrthorombicCell`; else, it is a `TriclinicCell`.

If no value is given for `alpha, beta, gamma`, they are set to $\pi/2$. If no value is given for `B, C`, they are set to be equal to `A`. This creates a cubic cell. If no value is given for `A`, a cell with lenghts of 0 Angström and $\pi/2$ angles is constructed.

```
julia> UnitCell() # Without parameters
OrthorombicCell
    Lenghts: 0.0, 0.0, 0.0

julia> UnitCell(10.) # With one lenght
OrthorombicCell
    Lenghts: 10.0, 10.0, 10.0

julia> UnitCell(10., 12, 15) # With three lenghts
OrthorombicCell
    Lenghts: 10.0, 12.0, 15.0

julia> UnitCell(10, 10, 10, pi/2, pi/3, pi/5) # With lenghts and angles
TriclinicCell
    Lenghts: 10.0, 10.0, 10.0
    Angles: 1.5707963267948966, 1.0471975511965976, 0.6283185307179586

julia> UnitCell(InfiniteCell) # With type
InfiniteCell

julia> UnitCell(10., 12, 15, TriclinicCell) # with lenghts and type
TriclinicCell
    Lenghts: 10.0, 12.0, 15.0
    Angles: 1.5707963267948966, 1.5707963267948966, 1.5707963267948966
```

UnitCell (*u::Vector*[, *v::Vector*, *celltype*])
If the size matches, this function expands the vectors and returns the corresponding cell.

```
julia> u = [10, 20, 30]
3-element Array{Int64,1}:
 10
 20
 30

julia> UnitCell(u)
OrthorombicCell
    Lenghts: 10.0, 20.0, 30.0
```

Indexing simulation cell

You can access the cell size and angles either directly, or by integer indexing.

getindex (*b::UnitCell*, *i::Int*)
Calling `b[i]` will return the corresponding length or angle : for `i in [1:3]`, you get the `i`th lenght, and for `i in [4:6]`, you get [avoid get] the angles.

In case of intense use of such indexing, direct field access should be more efficient. The internal fields of a cell are : the three lenghts `a, b, c`, and the three angles `alpha, beta, gamma`.

Boundary conditions and cells

Only fully periodic boundary conditions are implemented for now. This means that if a particle crosses the boundary at some step, it will be wrapped up and will appear at the opposite boundary.

Distances and cells

The distance between two particles depends on the cell type. In all cases, the minimal image convention is used: the distance between two particles is the minimal distance between all the images of theses particles. This is explicited in the *Periodic boundary conditions and distances computations* (page 19) part of this documentation.

Topology

The `Topology` type creates the link between human-readable and computer-readable information about the system. Humans prefer to use string labels for molecules and atoms, whereas a computer will only uses integers.

Atom type

An `Atom` instance is a representation of a type of particle in the system. It is paramerized by an `AtomType`, which can be one of:

- `Element` : an element in the perdiodic classification;
- `DummyAtom` : a dummy atom, for particles without interactions;
- `CorseGrain` : corse-grain particle, for corse-grain simulations;
- `UnknownAtom` : All the other kind of particles.

You can access the following fields for all atoms:

- `label::Symbol` : the atom name;
- `mass` : the atom mass;
- `charge` : the atom charge;
- `properties::Dict{String, Any}` : any other property: dipolar moment, *etc.*;

`Atom`([*label*, *type*])

Creates an atom with the `label` label. If `type` is provided, it is used as the Atom type. Else, a type is guessed according to the following procedure: if the `label` is in the periodic classification, the the atom is an `Element`. Else, it is a `CorseGrain` atom.

```
julia> Atom()
"Atom{UnknownAtom}"

julia> Atom("He")
"Atom{Element} He"

julia> Atom("CH4")
"Atom{CorseGrain} CH4"

julia> Atom("Zn", DummyAtom)
"Atom{DummyAtom} Zn"
```

`mass`(*label::Symbol*)

Try to guess the mass associated with an element, from the periodic table data. If no value could be found, the `0.0` value is returned.

`mass`(*atom::Atom*)

Return the atomic mass if it was set, or call the function `mass(atom.label)`.

Topology

A `Topology` instance stores all the information about the system : atomic types, atomic composition of the system, bonds, angles, dihedral agnles and molecules.

`Topology`([*natoms = 0*])
Create an empty topology with space for `natoms` atoms.

Atoms in the system can be accesed using integer indexing. The following example shows a few operations available on atoms:

```
# topology is a Topology with 10 atoms

atom = topology[3]  # Get a specific atom
println(atom.label) # Get the atom label

atom.mass = 42.9    # Set the atom mass
topology[5] = atom  # Set the 5th atom of the topology
```

Topology functions

`size`(*topology*)
This function returns the number of atoms in the topology.

`atomic_masses`(*topology*)
This function returns a `Vector{Float64}` containing the masses of all the atoms in the system. If no mass was provided, it uses the `ATOMIC_MASSES` dictionnary to guess the values. If no value is found, the mass is set to 0.0. All the values are in *internal units* (page 18).

`add_atom!`(*topology*, *atom*)
Add the `atom` Atom to the end of `topology`.

`remove_atom!`(*topology*, *i*)
Remove the atom at index `i` in `topology`.

`add_liaison!`(*topology*, *i*, *j*)
Add a liaison between the atoms `i` and `j`.

`remove_liaison!`(*topology*, *i*, *j*)
Remove any existing liaison between the atoms `i` and `j`.

`dummy_topology`(*natoms*)
Create a topology with `natoms` of type `DummyAtom`. This function exist mainly for testing purposes.

Periodic table information

The `Universes` module also exports two dictonaries that store information about atoms:

- `ATOMIC_MASSES` is a `Dict{String, Float64}` associating atoms symbols and atomic masses, in *internal units* (page 18) ;
- `VDW_RADIUS` is a `Dict{String, Integer}` associating atoms symbols and Van der Waals radii, in *internal units* (page 18).

Frame

A `Frame` object holds the data which is specific to one step of a simulation. It is defined as:

```
type Frame
    positions::Array3D
    velocities::Array3D
    step::Integer
end
```

i.e. it contains information about the current step, the current positions, and possibly the current velocities. If there is no velocity information, the velocities *Array3D* (page 22) is a 0-sized array.

The `Frame` type have the following constructor:

`Frame`([*natom=0*])
: Creates a frame with space for `natoms` particles.

Interactions

The interaction type contains informations about which *potentials* (page 9) the simulation should use for the atoms in the system. This type is not intended to be manupulated directly, but rather through the *`add_interaction!()`* (page 9) function.

`add_interaction!`(*universe, potential, atoms...[; computation=:auto; kwargs...]*)
: Add an interaction between the `atoms` atomic types, using the `potential` *potential function* (page 10) in the `universe`.

  This function accept many keywords arguments to tweak the *potential computation methode* (page 11) used to effectively compute the potential. The main keyword is `computation` which default to `:auto`. It can be set to other values to choose another computation method than the default one.

```
julia> # Setup an universe with four atoms: two He and one Ar
julia> top = Topology();

julia> add_atom!(top, Atom("He")); add_atom!(top, Atom("He"));

julia> add_atom!(top, Atom("Ar")); add_atom!(top, Atom("Ar"));

julia> universe = Universe(UnitCell(), top);

# Use default values for everything
julia> add_interaction!(universe, LennardJones(0.23, 2.2), "He", "He")

# Set the cutoff to 7.5 A
julia> add_interaction!(universe, LennardJones(0.3, 2.5), "He", "Ar", cutoff=7.5)

# Use table computation with 3000 points, and a maximum distance of 5A
julia> add_interaction!(universe, Harmonic(40, 3.3), "Ar", "Ar", computation=:table, numpoint
```

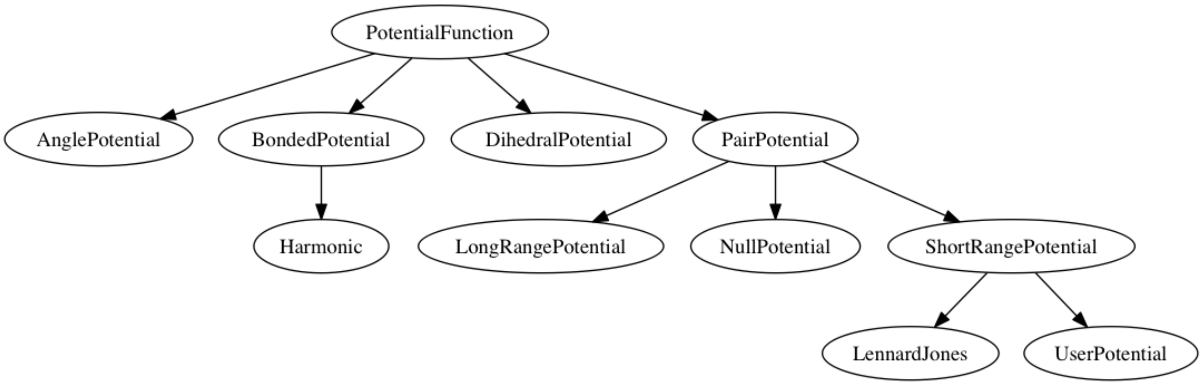
Using non-default computation

By default, the computation algorithm is automatically determined by the potential function type. `ShortRangePotential` are computed with `CutoffComputation`, and all other potentials are computed by `DirectComputation`. If we want to use another computation algorithm, this can be done by providing a `computation` keyword to the `add_interaction!` function. The following values are allowed:

- `:direct` to use a `DirectComputation`;
- `:cutoff` to use a `CutoffComputation`. The cutoff can be specified with the `cutoff` keyword argument;
- `:table`\` to use a `TableComputation`. The table size can be specified with the `numpoints` keyword argument, and the maximum distance with the `rmax` keyword argument.

Potentials

In order to compute the energy or the forces acting on a particle, two informations are needed : a potential energy function, and a computation algorithm. The potential function is a description of the variations of the potential with the particles positions, and a potential computation is a way to compute the values of this potential function. The following image shows the all the potentials functions types currently available in *Jumos*.



We can see these potentials are classified as four main categories: pair potentials, bond potentials, angles potentials (between 3 atoms) and dihedral potentials (between 4 atoms).

The only implemented pair potentials are short-range potentials. Short-range pair potentials go to zero faster than the $1/r^3$ function, and long-range pair potentials go to zero at the same speed or more slowly than $1/r^3$. A typical example of long-range pair potential is the Coulomb potential between charged particles.

Potential functions

Short-range pair potential Short-range pair potential are subtypes of *PairPotential*. They only depends on the distance between the two particles they are acting on. They should have two main properties:

- They should go to zero when the distance goes to infinity;
- They should go to zero faster than the $1/r^3$ function.

Lennard-Jones potential A Lennard-Jones potential is defined by the following expression:

$$V(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

`LennardJones` (*epsilon*, *sigma*)
Creates a Lennard-Jones potential with σ = sigma, and ϵ = epsilon. `sigma` should be in angstroms, and `epsilon` in kJ/mol.

Typical values for Argon are: $\sigma = 3.35\ A, \epsilon = 0.96\ kJ/mol$

Null potential This potential is a potential equal to zero everywhere. It can be used to define "interactions" between non interacting particles.

`NullPotential` ()
Creates a null potential instance.

Bonded potential Bonded potentials acts between two particles, but does no go to zero with an infinite distance. *A contrario*, they goes to infinity as the two particles goes apart of the equilibirum distance.

Harmonic An harmonic potential have the following expression:

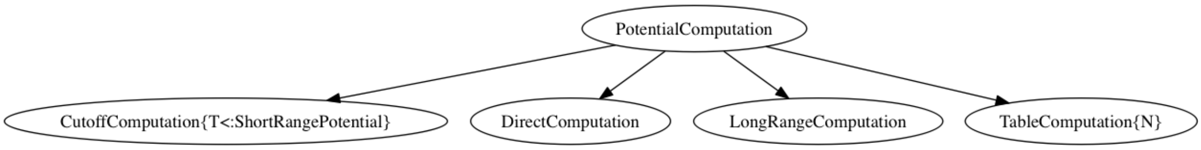
$$V(r) = \frac{1}{2}k(\vec{r} - \vec{r}_0)^2 - D_0$$

D_0 is the depth of the potential well.

`Harmonic` (*k*, *r0*, *depth=0.0*)
Creates an harmonic potential with a spring constant of *k* (in $kJ.mol^{-1}.A^{-2}$), an equilibrium distance r_0 (in angstroms); and a well's depth of D_0 (in kJ/mol).

Potential computation

As stated at the begiging of this section, we need two informations to compute interactions between particles: a potential function, and a potential computation. The potential compuatation algorithms come in four flavors:



- The `DirectComputation` is only a small wrapper on the top of the potential functions, and directly calls the potential function methods for energy and force evaluations.
- The `CutoffComputation` is used for short range potentials. All interactions at a longer distance than the cutoff distance are set to zero. The default cutoff is $12\ A$, and this can be changed by passing a `cutoff` keyword argument to the `add_interaction` function. With this computation, the energy is shifted so that their is a continuity in the energy at the cutoff distance.
- The `TableComputation` use table lookup to extrapolate the potential energy and the forces at a given point. This saves computation time at the cost of accuracy. This algorithm is parametrized by an integer, the size of the undelying array. Increases in this size will result in more accuracy, at the cost of more memory usage. The default size is 2000 points — which corresponds to roughly 15kb. `TableComputation` has also a maximum distance for computations, `rmax`. For any bigger distances, the `TableComputation` will returns a null energy and null forces. So `TableComputation` can only be used if you are sure that the particles will never be at a greater distance than `rmax`.
- The `LongRangeComputation` is not implemented yet.

Which computation for which potential ? Not all computation algorithms are suitable for all potential functions. The usable associations are in the table below.

Function	DirectComputation	CutoffComputation	TableComputation
ShortRangePotential	✓	✓	✓
BondedPotential	✓	✗	✓
AnglePotential	✓	✗	✓
DihedralPotential	✓	✗	✓

`Universe` type

The `Universe` type contains data about a simulation. In order to build an universe, you can use the following functions.

`Universe`(*cell*, *topology*)
Create a new universe with the *simulation cell* (page 5) `cell` and the *Topology* (page 8) `topology`.

`setframe!`(*universe*, *frame*)
Set the *Frame* (page 8) of `universe` to `frame`.

`setcell!`(*universe*, *cell*)
Set the *simulation cell* (page 5) of `universe` to `cell`.

`setcell!`(*universe*[, *celltype*], *paremeters...*)
Set the *simulation cell* (page 5) of `universe` to `UnitCell(parameters..., celltype)`.

`add_atom!`(*u::Universe*, *atom::Atom*)
Add the *Atom* (page 7) `atom` to the `universe` topology.

`add_liaison!`(*u::Universe*, *atom_i::Atom*, *atom_j::Atom*)
Add a liaison between the atoms at indexes `i` and `j` in the `universe` topology.

remove_atom! (*u::Universe*, *index*)
Remove the atom at index `i` in the `universe` topology.

remove_liaison! (*u::Universe*, *atom_i::Atom*, *atom_j::Atom*)
Remove any liaison between the atoms at indexes `i` and `j` in the `universe` topology.

The *add_interaction!()* (page 9) function is already documented in the `Interactions` section of this document.

Loading initial configurations from files

It is often usefull to load initial configurations from files, instead of building it by hand. The *Trajectories* (page 20) module provides functionalities for this.

2.3 Simulations

The simulation module contains types representing algorithms. The main type is the *Simulation* (page 18) type, which is parametrized by a *Propagator* (page 18). This propagator will determine which kind of simulation we are running: *Molecular Dynamics* (page 12); Monte-Carlo; energy minimization; *etc.*

Note: Only molecular dynamic is implemented in *Jumos* for now, but at least Monte-Carlo and energetic optimization should follow.

Molecular Dynamics

The `MolecularDynamics` propagator performs a molecular dynamics simulation, using some specific algorithms. These algorithms are sumarized on the *Algorithms used in MolecularDynamics propagator* (page 13) figure. These algorithms are presented in this documentation section.

The `MolecularDynamics` type have the following constructors:

MolecularDynamics (*timestep*)
Creates a molecular dynamics propagator using a Velocity-Verlet integrator with the specified timestep. Without any *thermostat* (page 13) or *barostat* (page 14), this performs a NVE integration of the system.

MolecularDynamics (*::Integrator*)
Creates a `MolecularDynamics` propagator with the specified *integrator* (page 12).

Time integration

An integrator is an algorithm responsible for updating the positions and the velocities of the current *frame* (page 8) of the *universe* (page 11). It is represented by a subtype of the `Integrator` type. You can set the integrator to use with your simulation using the *set_integrator!()* (page 15) function.

Verlet integrators Verlet integrators are based on Taylor expensions of Newton's second law. They provide a simple way to integrate the movement, and conserve the energy if a sufficently small timestep is used. Assuming the absence of barostat and thermostat, they provide a NVE integration.

type Verlet
The Verlet algorithm is described here for example. The main constructor for this integrator is `Verlet(timestep)`, where `timestep` is the timestep in femtosecond.

type VelocityVerlet
The velocity-Verlet algorithm is descibed extensively in the literature, for example in this webpages. The main constructor for this integrator is `VelocityVerlet(timestep)`, where `timestep` is the integration timestep in femtosecond. This is the default integration algorithm in *Jumos*.

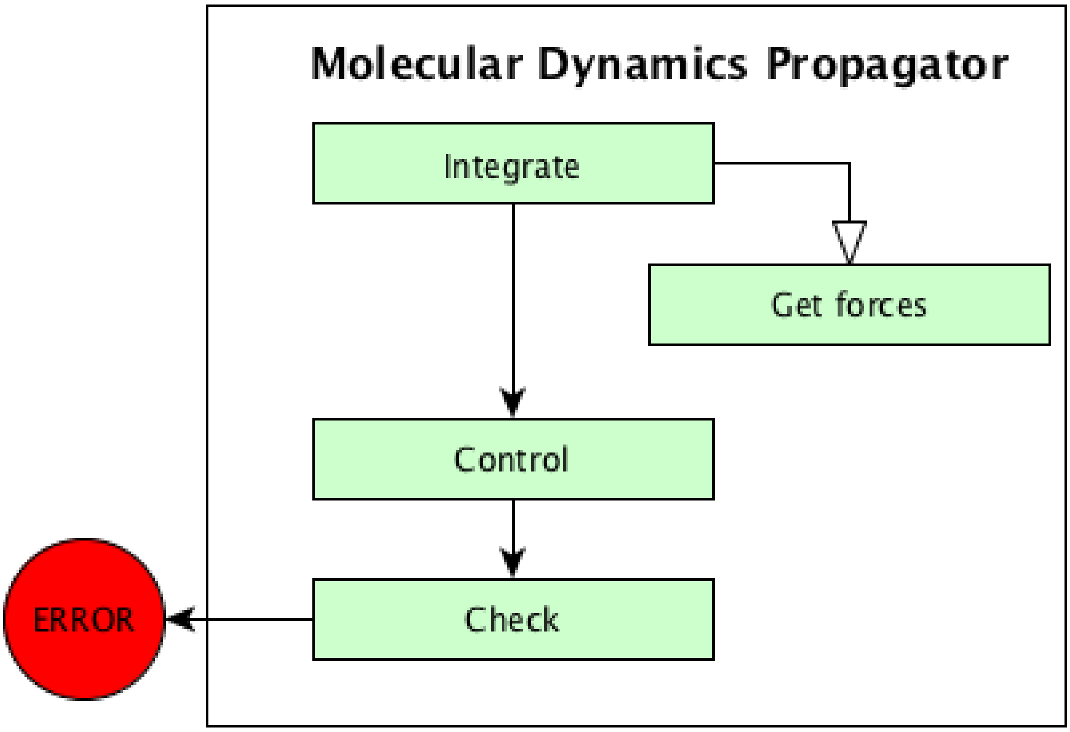


Fig. 2: Algorithms used in MolecularDynamics propagator

Force computation

The `NaiveForces` algorithm computes the forces by iterating over all the pairs of atoms, and calling the appropriate interaction potential. This algorithm is the default in *Jumos*.

Controlling the simulation

While running a simulation, we often want to have control over some simulation parameters: the temperature, the pressure, *etc*. This is the goal of the *control* algorithms, all subtypes of the `Control` type.

Controlling the temperature: Thermostats Various algorithms are available to control the temperature of a simulation and perform NVT simulations. The following thermostating algorithms are currently implemented:

type VelocityRescaleThermostat

The velocity rescale algorithm controls the temperature by rescaling all the velocities when the temperature differs exceedingly from the desired temperature.

The constructor takes two parameters: the desired temperature and a tolerance interval. If the absolute difference between the current temperature and the desired temperature is larger than the tolerance, this algorithm rescales the velocities.

```
sim = Simulation(MolecularDynamics(2.0))

# This sets the temperature to 300K, with a tolerance of 50K
thermostat = VelocityRescaleThermostat(300, 50)
push!(sim, thermostat)
```

type BerendsenThermostat

The berendsen thermostat sets the simulation temperature by exponentially relaxing to a desired temperature. A more complete description of this algorithm can be found in the original article [1].

The constructor takes as parameters the desired temperature, and the coupling parameter, expressed in simulation timestep units. A coupling parameter of 100, will give a coupling time of 150 fs if the simulation timestep is 1.5 fs, and a coupling time of 200 fs if the timestep is 2.0 fs.

`BerendsenThermostat` (*T*[, *coupling = 100*])
Creates a Berendsen thermostat at the temperature `T` with a coupling parameter of `coupling`.

```
sim = Simulation(MolecularDynamic(2.0))

# This sets the temperature to 300K
thermostat = BerendsenThermostat(300)
push!(sim, thermostat)
```

Controlling the pressure: Barostats Barostats provides a way to implement NPT integration. None of them is implemented in *Jumos* for now.

Other controls

type `WrapParticles`
This control wraps the positions of all the particles inside the *unit cell* (page 5).

Checking the simulation consistency

Molecular dynamic is usually a *garbage in, garbage out* set of algorithms. The numeric and physical issues are not caught by the algorithm themselves, and the physical (and chemical) consistency of the simulation should be checked often.

In *Jumos*, this is achieved by the `Check` algorithms, which are presented in this section. Checking algorithms can be added to a simulation by using the `push!` function.

Existing checks

type `GlobalVelocityIsNull`
This algorithm checks if the global velocity (the total moment of inertia) is null for the current simulation. The absolute tolerance is $10^{-5}\ A/fs$.

type `TotalForceIsNull`
This algorithm checks if the sum of the forces is null for the current simulation. The absolute tolerance is $10^{-5}\ uma \cdot A/fs^2$.

type `AllPositionsAreDefined`
This algorithm checks is all the positions and all the velocities are defined numbers, *i.e.* if all the values are not infinity or the `NaN` (not a number) values.

This algorithm is used by default by all the molecular dynamic simulation.

Default algorithms

Default algorithms for molecular dynamic are presented in the following table:

Simulation step	Default algorithms
Integration	*Velocity-Verlet* (page 12)
Forces computation	*Naive computation* (page 13)
Control	None
Check	None

[1] H.J.C. Berendsen, *et al.* J. Chem Phys **81**, 3684 (1984); doi: 10.1063/1.448118

Functions for algorithms selection

The following functions are used to to select specific algorithms for the simulation. They allow to add and change all the algorithms, even in the middle of a simulation run.

set_integrator! (*sim*, *integrator*)
Sets the simulation integrator to `integrator`.

Usage example:

```
sim = Simulation(MolecularDynamic(0.5))

run!(sim, 300)    # Run with a 0.5 fs timestep

set_integrator!(sim, Verlet(1.5))
run!(sim, 3000)  # Run with a 1.5 fs timestep
```

push! (*simulation*, *check*)
Adds a *check* (page 14) or *control* (page 13) algorithm to the simulation list and issues a warning if the algorithm is already present.

Usage example:

```
# Note the parentheses, needed to instanciate the new check.
push!(sim, AllPositionsAreDefined())

push!(sim, RescaleVelocities(300, 10))
```

Computing values of interest

To compute physical values from a simulation, we can use algorithms represented by subtypes of `Compute` and associate these algorithms to a simulation.

Users don't usualy need to use these compute algorithms directly, as the output algorithms (see *Exporting values of interest* (page 16)) set the needed computations by themself.

Computed values can have various usages: they may be used in *outputs* (page 16), or in *controls* (page 13). The data is shared between algorithms using the `Universe.data` field. This field is a dictionnary associating symbols and any kind of value.

This page of documentation presents the implemented computations. Each computation can be associated with a specific *simulation* (page 18) using the `push!` function.

push! (*simulation*, *compute*)
Adds a *compute* (page 15) algorithm to the simulation list. If the algorithm is already present, a warning is issued. Usage example:

```
sim = Simulation(:md, 1.0) # Create a simulation

# Do not forget the parentheses to instanciate the computation
push!(sim, MyCompute())

propagate!(sim, universe, 5000)

# You can access the last computed value in the sim.data dictionnary
universe.data[:my_compute]
```

You can also call directly any instance of `MyCompute`:

```
universe = Universe() # Create an universe
# ...

compute = MyCompute() # Instanciate the compute
value = compute(universe)  # Compute the value
```

The following paragraphs sums up the implemented computations, giving for each algorithm the return value (for direct calling), and the associated keys in `Universe.data`.

Energy related values

type `TemperatureCompute`

Computes the temperature of the universe.

Key: `:temperature`

Return value: The current frame temperature.

type `EnergyCompute`

Computes the potential, kinetic and total energy of the current simulation step.

Keys: `:E_kinetic`, `:E_potential`, `:E_total`

Return value: A tuple containing the kinetic, potential and total energy.

```
energy = EnergyCompute()

# unpacking the tuple
E_kinetic, E_potential, E_total = energy(universe)

# accessing the tuple values
E = energy(sim)

E_kinetic = E[1]
E_potential = E[2]
E_total = E[3]
```

Volume

type `VolumeCompute`

Computes the volume of the current *unit cell* (page 5).

Key: `:volume`

Return value: The current cell volume

Pressure

type `PressureCompute`

TODO

Key:

Return value:

Exporting values of interest

While running a simulation, some basic analysis can be performed and writen to a data file. Further analysis can be differed by writing the trajectory to a file, and running existing tools on these trajectories.

In *Jumos*, outputs are subtypes of the `Output` type, and can be added to a simulation by using the `push!` function.

`push!`(*simulation*, *output*)

Adds an *output* (page 16) algorithm to the simulation list. If the algorithm is already present, a warning is issued. Usage example:

```
    sim = Simulation(:md, 1.0)

    # Direct addition
    push!(sim, TrajectoryOutput("mytraj.xyz"))

    # Binding the output to a variable
    out = TrajectoryOutput("mytraj-2.xyz", 5)
    push!(sim, out)
```

Each output is by default writen to the disk at every simulation step. To speed-up the simulation run and remove useless information, a *write frequency* can be used as the last parameter of each output constructor. If this frequency is set to n, the values will be writen only every n simulaton steps. This frequency can also be changed dynamically:

```
# Frequency is set to 1 by default
traj_out = TrajectoryOutput("mytraj.xyz")

add_output(sim, traj_out)
propagate!(sim, universe, 300) # 300 steps will be writen

# Set frequency to 50
traj_out.frequency = OutputFrequency(50)
propagate!(sim, universe, 500) # 10 steps will be writen
```

Existing outputs

Trajectory output The first thing one might want to save in a simulation run is the trajectory of the system. Such trajectory can be used for visualisation, storage and further analysis. The `TrajectoryOutput` provide a way to write this trajectory to a file.

`TrajectoryOutput` (*filename*[, *frequency = 1*])

This construct a `TrajectoryOutput` which can be used to write a trajectory to a file. The trajectory format is guessed from the `filename` extension. This format must have write capacities, see *the list* (page 22) of supported formats in *Jumos*.

Energy output The energy output write to a file the values of energy and temperature for the current step of the simulation. Values writen are the current step, the kinetic energy, the potential energy, the total energy and the temperature.

`EnergyOutput` (*filename*[, *frequency = 1*])

This construct a `EnergyOutput` which can be used to the energy evolution to a file.

Defining a new output

Adding a new output with custom values, can be done either by using a custom output or by *subtyping* (page 24) the `Output` type to define a new output. The the former wayis to be prefered when adding a *one-shot* output, and the latter when adding an output which will be re-used.

Custom output The `CustomOutput` type provide a way to build specific output. The data to be writen should be *computed* (page 15) before the output by adding the specific algorithms to the current simulation. These computation algorithm set a value in the `MolecularDynamic.data` dictionairy, which can be accessed during the output step. See the *computation algorithms* (page 15) page for a list of keys.

`CustomOutput` (*filename*, *values*[, *frequency = 1; header=""*])

This create a `CustomOutput` to be writen to the file `filename`. The `values` is a vector of symbols, these symbols being the keys of the `Universe.data` dictionary. The `header` string will be writen on the top of the output file, and can contains some metadata.

Usage example:

```
sim = Simulation(:md, 1.0)

# TemperatureCompute register a :temperature key
push!(sim, TemperatureCompute())

temperature_output = CustomOutput("Sim-Temp.dat", [:temperature], header="# step   T/K")
push!(sim, temperature_output)
```

2.4 Propagator

The `Propagator` type is responsible for generating new *frames* (page 8) in the simulated *universe* (page 11). If you want to help adding a new propagator to *Jumos*, please signal yourself in the Gihtub issues list.

`Simulation` type

In *Jumos*, simulations are first-class citizen, *i.e.* objects bound to variables. The following constructors should be used to create a new simulation:

`Simulation` (*propagator::Propagator*)
Create a simulation with the specified `propagator`.

`Simulation` (*propagator::Symbol*, *args...*)
Create a simulation with a *propagator* (page 18) which type is given by the `propagator` symbol. The `args` are passed to the propagator constructor.

If `propagator` takes one of the `:MD`, `:md` and `:moleculardynamics` values, a *MolecularDynamics* (page 12) propagator is created.

The main function to run the simulation is the *`propagate!()`* (page 18) function.

`propagate!` (*simulation*, *universe*, *nsteps*)
Propagate an `universe` for `nsteps` steps, using the `simulation` method. Usage example:

```
julia> sim = Simulation(:MD, 1.0)

julia> universe # This should be an universe, either read from a file or built by hand

julia> propagate!(sim, universe, 4000) # Run the MD simulation for 4000 steps
```

2.5 Utilities

This part of the documentation give some information about basic algebrical types used in *Jumos*.

Internal units

Jumos uses a set of internal units, converting back and forth to these units when needed. Conversion from SI units is always supported. Parenthesis indicate planned conversion that is not implemented yet.

Quantity	Internal unit	Supported conversions
Distances	Ångtröm (A)	(bohr)
Time	Femptosecond (fs)	
Velocities	Ångtröm/Femptosecond (A/fs)	
Mass	Unified atomic mass (u or Da)	g/mol
Temperature	Kelvin (K)	
Energy	Kilo-Joule/Mole (kJ/mol)	(eV), (Ry), $(kcal/mol)$
Force	Kilo-Joule/(Mole-Ångtröm) $kJ/(molA)$	
Pressure	bar	(atm)
Charge	Multiples of $e = 1.602176487\ 10^{-19}C$	

Interaction with others units systems

Jumos uses it's own unit system, and do not track the units in the code. All the interaction with units is based on the SIUnits package. We can convert from and to internal representation using the following functions :

internal (*value::SIQuantity*)

Converts a value with unit to its internal representation.

```
julia> internal(2m)          # Distance
    1.9999999999999996e10

julia> internal(3kg*m/s^2)   # Force
    7.17017208413002e-14
```

with_unit (*value::Number*, *target_unit::SIUnit*)

Converts an internal value to its value in the International System. You shall note that units are not tracked in the code, so you can convert a position to a pressure. And all the results are returned in the main SI unit, without considering any power-of-ten prefix.

This may leads to strange results like:

```
julia> with_unit(45, mJ)
    188280.0 kg m²/s²

julia> with_unit(45, J)
    188280.0 kg m²/s²
```

This behaviour will be corrected in future versions.

Periodic boundary conditions and distances computations

The `PBC` module offers utilities for distance computations using periodic boundary conditions.

Minimal images

These functions take a vector and wrap it inside a *cell* (page 5), by finding the minimal vector fitting inside the cell.

minimal_image (*vect*, *cell::UnitCell*)

Wraps the `vect` vector inside the `cell` unit cell. *vect* can be a `Vector` (*i.e.* a 1D array), or a view from an *Array3D* (page 22). This function returns the wrapped vector.

minimal_image! (*vect*, *cell::UnitCell*)

Wraps `vect` inside of `cell`, and stores the result in `vect`.

minimal_image! (*A::Matrix*, *cell::UnitCell*)

If `A` is a 3xN Array, wraps each one of the columns in the `cell`. The result is stored in `A`. If `A` is not a 3xN array, this throws an error.

Distances

Distances are computed using periodic boundary conditions, by wrapping the $\vec{r}_i - \vec{r}_j$ vector in the cell before computing its norm.

Within one Frame This set of functions computes distances within one frame.

distance (*ref::Frame*, *i::Integer*, *j::Integer*)
Computes the distance between particles `i` and `j` in the frame.

distance_array (*ref::Frame*[, *result*])
Computes all the distances between particles in `frame`. The `result` array can be passed as a pre-allocated storage for the $N \times N$ distances matrix. `result[i, j]` will be the distance between the particle i and the particle j.

distance3d (*ref::Frame*, *i::Integer*, *j::Integer*)
Computes the $\vec{r}_i - \vec{r}_j$ vector and wraps it in the cell. This function returns a 3D vector.

Between two Frames This set of functions computes distances within two frames, either computing the how much a single particle moved between two frames or the distance between the position of a particle i in a reference frame and a particle j in a specific configuration frame.

distance (*ref::Frame*, *conf::Frame*, *i::Integer*, *j::Integer*)
Computes the distance between the position of the particle i in `ref`, and the position of the particle j in `conf`

distance (*ref::Frame*, *conf::Frame*, *i::Integer*)
Computes the distance between the position of the same particle i in `ref` and `conf`.

distance3d (*ref::Frame*, *conf::Frame*, *i::Integer*)
Wraps the `ref[i] - conf[i]` vector in the `ref` unit cell.

distance3d (*ref::Frame*, *conf::Frame*, *i::Integer*, *j::Integer*)
Wraps the `ref[i] - conf[i]` vector in the `ref` unit cell.

Trajectories

When running molecular simulations, the trajectory of the system is commonly saved to the disk in prevision of future analysis or new simulations run. The *Trajectories* module offers facilities to read and write this files.

Reading and writing trajectories

One can read or write *frames* (page 8) from a trajectory. In order to do so, more information is needed : namely an *unit cell* (page 5) and a *topology* (page 8). Both are optional, but allow for better computations. Some file formats already contain this kind of informations so there is no need to provide it.

Trajectories can exist in differents formats: text formats like the XYZ format, or binary formats. In *Jumos*, the format of a trajectory file is automatically determined based on the file extension.

Base types The two basic types for reading and writing trajectories in files are respectively the `Reader` and the `Writer` parametrised types. For each specific format, there is a `FormatWriter` and/or `FormatReader` subtype implementing the basic operations.

Usage The following functions are defined for the interactions with trajectory files.

opentraj (*filename*[, *mode="r"*, *topology=""*, *kwargs...*])
: Opens a trajectory file for reading or writing. The `filename` extension determines the *format* (page 22) of the trajectory.

  The `mode` argument can be `"r"` for reading or `"w"` for writing.

  The `topology` argument can be the path to a *Topology* (page 8) file, if you want to use atomic names with trajectories files in which there is no topological informations.

  All the keyword arguments `kwargs` are passed to the specific constructors.

Reader (*filename*[, *kwargs...*])
: Creates a `Reader` object, by passing the keywords arguments `kwargs` to the specific constructor. This is equivalent to use the *opentraj* function with `"r"` mode.

Writer (*filename*[, *kwargs...*])
: Creates a `Writer` object, by passing the keywords arguments `kwargs` to the specific constructor. This is equivalent to use the *opentraj* function with `"w"` mode.

eachframe (*::Reader [range::Range, start=first_step]*)
: This function creates an [interator] interface to a `Reader`, allowing for constructions like `for frame in eachframe(reader)`.

read_next_frame! (*::Reader*, *frame*)
: Reads the next frame from `Reader`, and stores it into `frame`. Raises an error in case of failure, and returns `true` if there are other frames to read, `false` otherwise.

  This function can be used in constructions such as `while read_next_frame!(traj)`.

read_frame! (*::Reader*, *step*, *frame*)
: Reads a frame at the step `step` from the `Reader`, and stores it into `frame`. Raises an error in the case of failure and returns `true` if there is a frame after the step `step`, `false` otherwise.

write (*::Writer*, *frame*)
: Writes the *Frame* (page 8) `frame` to the file associated with the `Writer`.

close (*trajectory_file*)
: Closes the file associated with a `Reader` or a `Writer`.

Reading frames from a file Here is an example of how you can read frames from a file. In the `Reader` constructor, the `cell` keyword argument will be used to construct an *UnitCell* (page 5).

```
traj_reader = Reader("filename.xyz", cell=[10., 10., 10.])

for frame in eachframe(traj_reader)
    # Do stuff here
end

close(traj_reader)
```

Writing frames in a file Here is an example of how you can write frames to a file. This example converts a trajectory from a file format to another. The `topology` keyword is used to read a *Topology* (page 8) from a file.

```
traj_reader = Reader("filename-in.nc", topology="topology.xyz")
traj_writer = Writer("filename-out.xyz")

for frame in eachframe(traj_reader)
    write(traj_writer, frame)
end

close(traj_writer)
close(traj_reader)
```

Supported formats The following table summarizes the formats supported by *Jumos*, giving the reading and writing capacities of *Jumos*, as well as the presence or absence of the unit cell and the topology information in the files. The last column indicates the accepted keywords.

Format	Extension	Read	Write	Cell	Topology	Keywords
XYZ	`.xyz`	✓	✓	✗	✓	cell
Amber NetCDF	`.nc`	✓	✗	✓	✗	topology

Readind and writing topologies

Topologies can also be represented and stored in files. Some functions allow to read directly these files, but there is usally no need to use them directely.

Supported formats for topology Topology reading supports the formats in the following table.

Format	Reading ?	Writing ?
XYZ	✓	✓
LAMMPS data file	✓	✗

If you want to write a toplogy to a file, the best way for now is to create a frame with this topology, and write this frame to an XYZ file.

Array3D

3-dimensionals vectors are very common in molecular simulations. The `Array3D` type implements arrays of this kind of vectors, provinding all the usual operations between its components.

If `A` is an `Array3D` and `i` an integer, `A[i]` is a 3-dimensional vector implementing `+, -` between vector, `.+, .-, .*, */` between vectors and scalars; `dot` and `cross` products, and the `unit!` function, normalizing its argument.

3 Extending *Jumos*

3.1 Extending *Jumos*

In this section, you will find and how to extend *Jumos* base types to add more fucntionalities to your simulations.

Defining a new potential

User potential

The easier way to define a new potential is to create `UserPotential` instances, providing potential and force functions. To add a potential, for example an harmonic potential, we have to define two functions, a potential function and a force function. These functions should take a `Float64` value (the distance) and return a `Float64` (the value of the potential or the force at this distance).

`UserPotential`(*potential*, *force*)

Creates an UserPotential instance, using the `potential` and `force` functions.

`potential` and `force` should take a `Float64` parameter and return a `Float64` value.

`UserPotential`(*potential*)

Creates an UserPotential instance by automatically computing the force function using a finite difference method, as provided by the Calculus package.

Here is an example of the user potential usage:

```
# potential function
f(x) = 6*(x-3.)^2 - .5
# force function
g(x) = -12.*x + 36.

# Create a potential instance
my_harmonic_potential = UserPotential(f, g)

# One can also create a potential whithout providing a funtion for the force,
# at the cost of a less effective computation.
my_harmonic_2 = UserPotential(f)

force(my_harmonic_2, 3.3) == force(my_harmonic_potential, 3.3)
# false

isapprox(force(my_harmonic_2, 3.3), force(my_harmonic_potential, 3.3))
# true
```

Subtyping PotentialFunction

A more efficient way to use custom potential is to subtype the either `PairPotential`, `BondedPotential`, `AnglePotential` or `DihedralPotential`, according to the new potential from.

For example, we are goning to define a Lennard-Jones potential using an other function:

$$V(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

This is obviously a `ShortRangePotential`, so we are going to subtype this potential function.

To define a new potential, we need to add methods to two functions: *call* and *force*. It is necessary to import these two functions in the current scope before extending them. Potentials should be declared as `immutable`, this allow for optimizations in the code generation.

```
# import the functions to extend
import Base: call
import Jumos: force

immutable LennardJones2 <: PairPotential
    A::Float64
    B::Float64
end

# potential function
function call(pot::LennardJones2, r::Real)
    return pot.A/(r^12) - pot.B/(r^6)
end

# force function
function force(pot::LennardJones2, r::Real)
    return 12 * pot.A/(r^13) - 6 * pot.B/(r^7)
end
```

The above example can the be used like this:

```
# Add a LennardJones2 interaction to an universe
universe = Universe(...)
add_interaction!(universe, LennardJones2(4.5, 5.3), "He", "He")

# Directly compute values
pot = LennardJones2(4.5, 5.3)
```

```
pot(3.3) # value of the potential at r=3.3
force(pot, 8.12) # value of the force at r=8.12
```

Algorithms for all simulations

Computing values

Algorithms to compute properties from a simulation are called `Compute` in *Jumos*. They all act by taking an *Universe* (page 11) as parameter, and then setting a value in the `Universe.data` dictionary.

To add a new compute algorithm (we will call it `MyCompute`), we have to subtype `Jumos.Simulations.BaseCompute` and provide specialised implementation for the `Base.call` function; with the following signature:

`Base.call`(*::Compute*, *::Universe*)
: This function can set a `Universe.data` entry with a `Symbol` key to store the computed value. This value can be anything, but basic types (scalars, arrays, *etc.*) are to be prefered.

Outputing values

An other way to create a custom output is to subtype `Output`. The subtyped type must have at least one field: `frequency::OutputFrequency`, which is responsible for selecting the write frequency of this output. Two functions can be overloaded to set the output behaviour.

`Base.write`(*::Output*, *context::Dict{Symbol, Any}*)
: Write the ouptut. This function will be called every `n` simulation steps according to the `frequency` field.

: The `context` parameter contains all the values set up by the *computation algorithms* (page 15), and a special key `:frame` refering to the current simulation *frame* (page 8).

`Jumos.setup`(*::Output*, *::Simulation*)
: This function is called once, at the begining of a simulation run. It should do some setup job, like adding the needed computations algorithms to the simulation.

As an example, let's build a custom output writing the `x` position of the first atom of the simulation at each step. This position will be taken from the frame, so no specific computation algorithm is needed here. But this position will be writen in bohr, so some conversion from Angstroms will be needed.

```
# File FirstX.jl

using Jumos

import Base.write
import Jumos.setup

type FirstX <: Output
    file::IOStream
    frequency::OutputFrequency
end

# Default values constructor
function FirstX(filename, frequency=1)
    file = open(filename, "w")
    return FirstX(file, OutputFrequency(frequency))
end

function write(out::FirstX, context::Dict)
    frame = context[:frame]
    x = frame.positions[1][1]
    x = x/0.529 # Converting to bohr
    write(out.file, "$x \n")
```

```
end

# Not needed here
# function setup(::FirstX, ::Simulation)
```

This type can be used like this:

```
using Jumos
require("FirstX.jl")

sim = Simulation(:md, 1.0)
# ...

push!(sim, FirstX("The-first-x-file.dat"))
```

Algorithms for molecular dynamics

Writing a new integrator

To create a new integrator, you have to subtype the `Integrator` type, and provide the `call` method, with the following signature: `call(::Integrator, ::MolecularDynamic)`.

The integrator is responsible for calling the `getforces!(::MolecularDynamics, ::Universe)` function when the `MolecularDynamics.forces` field needs to be updated. It should update the two *Array3D* (page 22): `Universe.frame.positions` and `Universe.frame.velocities` with appropriate values.

The `Universe.masses` field is a `Vector{Float64}` containing the particles masses. Any other required information should be stored in the new `Integrator` subtype.

Computing the forces

To create a new force computation algorithm, you have to subtype `ForcesComputer`, and provide the method `call(::ForcesComputer, ::Universe, forces::Array3D)`.

This method should fill the forces array with the forces acting on each particles: `forces[i]` should be the 3D vector of forces acting on the atom `i`. In order to do this, the algorithm can use the `Universe.frame.posistions` and `Universe.frame.velocities` arrays.

Potentials to use for the atoms can be optained throught the following functions:

pairs (*::Interactions*, *i*, *j*)
Get a `Vector{PairPotential}` of interactions betweens atoms `i` and `j`.

bonds (*::Interactions*, *i*, *j*)
Get a `Vector{BondPotential}` of interactions betweens atoms `i` and `j`.

angles (*::Interactions*, *i*, *j*, *k*)
Get a `Vector{AnglePotential}` of interactions betweens atoms `i` and `j` and `k`.

dihedrals (*::Interactions*, *i*, *j*, *k*, *m*)
Get a `Vector{DihedralPotential}` of interactions betweens atoms `i`, `j`, `k` and `m`.

Adding new checks

Adding a new check algorithm is as simple as subtyping `Check` and extending the `call(::Check, ::Universe, ::MolecularDynamic)` method. This method should throw an exception of type `CheckError` if the checked condition is not fullfiled.

type CheckError
Customs exception providing a specific error message for simulation checking.

```
julia> throw(CheckError("This is a message"))
ERROR: Error in simulation :
This is a message
in __text at no file (repeats 3 times)
```

Adding new controls

To add a new type of control to a simulation, the main way is to subtype `Control`, and provide two specialised methods: `call(::Control, ::Universe)` and the optional `setup(::Control, ::Simulation)`. The `call` method should contain the algorithm inplementation, and the `setup` method is called once at each simulation start. It should be used to add add some *computation algorithm* (page 15) to the simulation, as needed.

Index