

# RUMD Tutorial

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# 1 Introduction

The CUDA project has enabled scientists to utilise NVIDIA's many-core Graphical Processor Unit (GPU) to solve complex computational problems. Beside being a very fast processor the GPU is relatively cheap, and is thus an ideal computational unit for low-cost high performance supercomputing. Scientific software is currently being developed in a very rapid pace by many different groups world wide, and today there exists optimized software for fluid dynamics and matrix operations just to name a few.

RUMD [ˈrʊm di•] is a high-performance molecular dynamics simulation software package optimized for NVIDIA's graphics cards. RUMD is designed for small to medium size systems of spherical particles and simple molecules. RUMD is developed at The Danish National Research Foundation's centre "Glass and Time" which is located at the Department of Sciences, Roskilde University.

## 1.1 Features

RUMD currently supports:

- van der Waals type pair potentials: Lennard-Jones, Gaussian core, inverse power law, exponential, and more. It is easy to implement new pair potentials.
- Multicomponent simulations
- Bond stretching potentials: Harmonic and FENE
- Bond constraint dynamics
- Angle bending potentials
- Dihedral potentials
- NVE, NVT, NPT (atomic) and NVU ensemble simulations
- Non-equilibrium sheared simulations using Lees-Edwards boundary conditions and the SLLOD equations of motion
- A Python interface including user-defined on-the-fly analysis.
- Tools for setting up configuration files, including molecular systems.
- Post simulation analysis tools

In the near future we plan to implement:

- NPT (molecular) ensemble
- Ewald-based Coulomb interactions (a Coulomb potential using direct pair summation and a shifted-force cut-off is available which gives reasonable performance and accuracy for bulk ionic systems)

## 1.2 User philosophy

We have defined five users of RUMD:

1. A user at level 1 is one who can write or copy a simple python script (for example the one given later in this tutorial) to run a standard molecular dynamics simulation, and use the provided analysis tools to perform standard analysis of the output. This user can make some basic choices, such as the potential, the integrator, and controlling the frequency of output.
2. This user understands the deeper structure of the code—that is the different kinds of classes/objects, the relations between them, and their interfaces—and understands how the python language works, and can therefore write more sophisticated python scripts which access the full power and flexibility of RUMD.
3. A user at level 3 is one with minimal experience in C++ can write her own (pair-)potential functions, to be available as classes derived from `PairPotential`.
4. This user can write their own analysis programs in C++, but does not need to know anything about GPU programming, since analysis is generally carried out on the CPU.
5. RUMD developer. Must have a good knowledge of C++, CUDA programming and knowledge of Subversion.

This tutorial will bring you from level 1 to level 3. Note that level 3 is higher than level 2 in that it requires the user to write some C++ code and re-compile the code, but that involves a relatively limited list of things to do. Level 2, which stays at the python level, but involves access to almost all of the underlying C++ functionality, could take longer to master.

## 1.3 Installation

For Debian-like systems, RUMD can be installed as a package. Use the following repository entries appended to `/etc/apt/sources.list` or in a file in `/etc/apt/sources.d/`

```
deb [trusted=yes] http://carid.ruc.dk/rumd buster main
deb-src [trusted=yes] http://carid.ruc.dk/rumd buster main
```

To install RUMD simply use an equivalent of:

```
apt update
apt install rumd rumd-doc python3-rumd
```

You need to have root privileges, of course.

You can also build the package from the source. To do so, download the source code from the RUMD homepage

```
http://rumd.org/download.html
```

and unpack the file using

```
tar xzvf rumd-X.X.tar.xz
```

where `X.X` is the version number. Enter the source directory

```
cd rumd-X.X
```

and build the package by typing

```
make
```

To test your installation use

```
make test
```

This test will take approximately 5-10 minutes.

Notice, you cannot type `make install` since the default path is different from system to system. We will refer to the installation path as `<RUMD-HOME>`

## 1.4 Setting the path for python

In a proper installation the python modules should be located in a standard place where python will automatically find them. This may not be possible if you do not have root privileges, however. If you have compiled the software yourself, you need to set the environment variable `PYTHONPATH` as follows For C-shell it would go in your `.cshrc` file;

```
setenv PYTHONPATH <RUMD-HOME>/Swig:<RUMD-HOME>/Python:<RUMD-HOME>/Tools
```

For bash you would add the following to your `.profile`;

```
export PYTHONPATH=<RUMD-HOME>/Swig:<RUMD-HOME>/Python:<RUMD-HOME>/Tools
```

## 2 Level 1: How to run your first simulation with RUMD

This tutorial assumes basic GNU/Linux knowledge, a successful installation of RUMD and a little portion of gumption mixed with interest in molecular dynamics. For plotting the results from simulations it is assumed that `xmgrace` is installed, but other plotting programs can be used if you prefer.

The basic work-flow of doing simulations is:

- Specify initial condition, i.e., the initial positions and velocities to be used in the simulation. This also involves the number of particles ( $N$ ) and the (initial) density ( $\rho \equiv N/V$ ).
- Running the actual simulation. This can be done interactively or by a script in python. It includes defining how particles interact with each other (i.e., the potentials used), what integrator to use (and the associated parameters, e.g., time-step and temperature.)
- Post-processing data analysis.

The following sub-sections will take you through these steps.

### 2.1 The initial condition

When conducting simulations it is often convenient to use the end result of one simulation as the initial condition to a new simulation. However, sometimes you need to generate a fresh initial condition. This can be done from a terminal window by executing the commands given below.

First make a directory where you want your first simulation to be performed. Call it e.g. `~/Test/`, and go to that directory:

```
mkdir Test
cd Test
```

Next, run the `rumd_init_conf` program (make sure `RUMD_home/Tools/` is in your path):

```
rumd_init_conf --lattice=fcc --cells=6
```

This command produces a file called `start.xyz.gz` that we will use as the initial configuration. The flag `--lattice=fcc` tells the program to generate a fcc crystal, and the flag `--cells=6` that is should make six unit cells in each direction. The fcc lattice have four particles in the unit cell, and the final configuration will have  $4 \times 6^3 = 864$  particles. We have not specified a density or temperature to the program, and it will use default values of  $\rho = 1.0$  and  $T = 1.0$ , respectively. Note that `rumd_init_conf` have many options for generating configurations. A summary of these can be seen by typing

```
rumd_init_conf --help
```

`rumd_init_conf` also accept “short arguments” and the command to generating the fcc lattice simply done with

```
rumd_init_conf -lfcc -c6
```

## 2.2 Executing your first program using the python interface

In this first example we will simulate a single component Lennard–Jones liquid. We will work with python interactively, so that you can get a feel for what is possible. For production runs you will normally make a script containing the appropriate python commands. Start python by typing

```
python3
```

in a terminal. You will get a python prompt that looks like “>>>”. Type

```
from rumd import *
```

This will import the main RUMD classes into the global namespace<sup>1</sup> (these are actually C++ classes, but we can “talk” to them through python). These are in principle enough to write scripts and thereby run simulations, but to simplify this process, there is an extra python class called `Simulation`: type

```
from rumd.Simulation import Simulation
```

This class combines access to the main data-structures with the main integration loop and various functions for controlling output etc. To start a simulation we first create a `Simulation` object, passing the name of a starting configuration file:

```
sim = Simulation("start.xyz.gz")
```

Here `sim` is an arbitrary name we choose for the object. Next we choose an NVT integrator, giving the time-step, temperature and the relaxation time controlling the thermostat [RUMD versions before 3.4 did not require the latter to be explicitly set and set a default value of 0.2]:

```
itg = IntegratorNVT(timeStep=0.0025, targetTemperature=1.0, thermostatRelaxationTime=0.2)
```

Having an integrator object, we need to connect it to the simulation:

```
sim.SetIntegrator(itg)
```

Next we need to choose the potential. For 12-6 Lennard-Jones we create a potential object, giving it the name `pot`, as follows:

```
pot = Pot_LJ_12_6(cutoff_method=ShiftedPotential)
```

The mandatory argument `cutoff_method` specifies how the cut-off of the pair-potential is to be handled. It must be one of `ShiftedPotential` (the most common method, where the potential is shifted to zero), `ShiftedForce` or `NoShift`. We need to set the parameters, which is done using the method `SetParams`. The arguments to this method depend on which potential class you are working with, but they can be found by typing

```
help(pot.SetParams)
```

which displays a help page generated from the “docstring” of the method (alternatively type `print pot.SetParams.__doc__`). In particular this includes a list of the arguments:

```
SetParams(self, unsigned int i, unsigned int j, float Sigma,
float Epsilon, float Rcut)
```

The first one, `self`, represents the object itself, and is not explicitly given when calling the function. The next two define which particle types we are specifying parameters for—we just have one type of particle so both will be zero; the two after that are the standard Lennard-Jones length and energy parameters, while the last is the cut-off in units of `Sigma`. Press `Q` to exit the help screen. We choose the following:

```
pot.SetParams(0, 0, 1.0, 1.0, 2.5)
```

Note that we can also use python’s “keyword arguments” feature to specify the arguments, which can then be in any order, for example:

<sup>1</sup>Alternatively (recommended by some to avoid possible name clashes in the global namespace) one can type `import rumd`, and then all of the class-names, etc., must be prefixed by `rumd.`, for example `rumd.IntegratorNVE`.

```
pot.SetParams(i=0, j=0, Epsilon=1.0, Rcut= 2.5, Sigma=1.0)
```

The potential also needs to be connected to the simulation:

```
sim.AddPotential(pot)
```

[The old function `SetPotential` is deprecated as of Version 3.5] Now we are ready to run a simulation. To run a simulation with 20000 time steps, we just write

```
sim.Run(20000)
```

Various messages will be printed to the screen while it is running (these can be turned off with `sim.SetVerbose(False)`). If we like, we can get the positions after the 20000 steps by getting them as a numpy array (numpy, or numerical python, is a package that provides efficient array-based numerical methods), and in particular look at the position of particle 0 by typing

```
pos = sim.sample.GetPositions()
print pos[0]
```

However more likely we will run an analysis program on the output files produced by the simulation during the operation of the `Run` function. The available analysis programs are described below in subsection 2.4 in their command-line forms. Some of them (eventually all) can also be called from within python. For now let's write a configuration file for possible use as a starting point for future simulations. Here we go a little deeper into the interface. Objects of type `Simulation` have an attribute called "sample" of type `Sample` (the main C++ class representing the sample we are simulating). We call its `WriteConf` method as follows:

```
sim.WriteConf("end.xyz.gz")
```

Type Ctrl-D to exit python. Next we would like to make scripts. Here is the script that contains the commands we have just worked through (the lines starting with # are comments):

```
from rumd import *
from rumd.Simulation import Simulation

# create simulation object
sim = Simulation("start.xyz.gz")

# create integrator object
itg = IntegratorNVT(timeStep=0.0025, targetTemperature=1.0, thermostatRelaxationTime=0.2)
sim.SetIntegrator(itg)

# create potential object
pot = Pot_LJ_12_6(cutoff_method=ShiftedPotential)
pot.SetParams(0, 0, 1.0, 1.0, 2.5)
sim.AddPotential(pot)

# run the simulation
sim.Run(20000)

# write final configuration
sim.WriteConf("end.xyz.gz")
```

If this script is saved as a file called, for example, `run.py` (it must end in `.py`), then it is run by typing `python3 run.py`. This will exit python when finished. To leave python on after the script has completed, type `python3 -i run.py` (`-i` means run in interactive mode). If it is to be run on a batch queue, the appropriate PBS commands should be included in comments at the top as follows:

```
#!/usr/bin/python3
# pass PYTHONPATH environment variable to the batch process
#PBS -v PYTHONPATH
#PBS (other PBS commands here)
#PBS
#PBS

# this ensures PBS jobs run in the correct directory
import os, sys
if "PBS_O_WORKDIR" in os.environ:
    os.chdir(os.environ["PBS_O_WORKDIR"])
    sys.path.append(".")

from rumd import *
(etc)
```

It should be submitted using `qsub run.py`. Note that the indentation of the two lines following the `if` statement is important!

## 2.3 Setting options with the python interface

Here we present some of the options available for controlling simulations.

### 2.3.1 Choosing the potential and its parameters

Probably the most important thing a user needs to control is the potential. Different potentials are represented by different classes; objects are created just as above, so for example:

```
# generalized LJ potential (here m=18, n=4)
potential = Pot_gLJ_m_n(18,4, cutoff_method=ShiftedPotential)
# inverse power-law (IPL) with exponent n=12
potential = Pot_IPL_12(cutoff_method=ShiftedPotential)
```

To set parameters for the potential, call its `SetParams` method as described above. If a binary system is to be simulated, the parameters should be set separately for each interaction pair as follows

```
potential.SetParams(0, 0, 1.00, 1.00, 1.12246)
potential.SetParams(0, 1, 0.80, 1.50, 1.12246)
potential.SetParams(1, 1, 0.88, 0.50, 1.12246)
```

Note that Newton's third law is assumed to hold, so setting the parameters for  $i=0$  and  $j=1$  automatically sets those for  $i=1$  and  $j=0$  (we could also have called `SetParams` with the latter). An overview of the available potentials is given in the user manual.

### 2.3.2 Choosing the integrator

Perhaps the next most important choice is what kind of integration algorithm to use. Above we did a constant-temperature (NVT) algorithm (the actual algorithm is of the Nosé-Hoover

type). For constant energy (NVE) runs we create the integrator as follows, here passing only the time-step:

```
itg = IntegratorNVE(timeStep=0.0025)
```

(Technical note: this creates an object of the same type as `IntegratorNVT`, but here it defaults to NVE mode—in fact in either case one can switch thermostating on or off using the `SetThermostatOn()` method).

Additional integrators available in RUMD are listed below

Name of Integrator	Description	Arguments
IntegratorNVE	The <i>NVE</i> Leap-frog algorithm.	timeStep
IntegratorNVT	The Nosé-Hoover <i>NVT</i> algorithm.	timeStep, targetTemperature, thermostatRelaxationTime
IntegratorNPTAtomic	<i>NPT</i> algorithm. (JCP 101, N 5, 1994)	timeStep, targetTemperature, thermostatRelaxationTime, targetPressure, barostatRelaxationTime
IntegratorNVU	Algorithm conserving the total potential energy.	dispLength, potentialEnergy
IntegratorMMC	Metropolis <i>NVT</i> Monte Carlo.	dispLength, targetTemperature
IntegratorIHS	Energy minimization via the Leap-frog algorithm.	timeStep
IntegratorSLLOD	Shear an atomic system in the xy-plane using the SLLOD equations.	timeStep, strainRate
IntegratorMolecularSLLOD	Shear a molecular system in the xy-plane using the SLLOD equations.	timeStep, strainRate
IntegratorNPTLangevin	Algorithm which generates the <i>NPT</i> ensemble using Langevin dynamics	timeStep, targetTemperature, friction, targetPressure, barostatFriction, barostatMass

The above integrators are chosen in the usual way with named arguments as given in the table. In the case of `IntegratorNPTAtomic` the user must choose suitable relaxation times for the thermostat and the barostat. An example of reasonable values for the thermostat and barostat relaxation times for the LJ system at  $T = 2.0$  and  $p = 5.0$  are `thermostatRelaxationTime=0.4` and `barostatRelaxationTime=10.0`. For `IntegratorNPTLangevin` the friction may be chosen over a wide range, depending on how strongly individual particles should be coupled to the heat bath. For the box dynamics, note that the ratio of `barostatMass` to `barostatFriction` is a relaxation time which should be reasonable for the system (at least long compared to the time step).

### 2.3.3 Controlling how frequently to write output

To control the output written to files we use the `Simulation` method `SetOutputScheduling`. By default there are two “output managers”: “energies” and “trajectory”. The first is for the files containing potential/kinetic energies and other global quantities, while the second is for trajectories (configuration files containing the particle positions at different times during the run). The write-schedule for either manager can be evenly-spaced in time (“linear”), logarithmic (“logarithmic”), or a kind of combination of the two (“loglin”). Examples of controlling scheduling include

```
sim.SetOutputScheduling( "energies", "linear", interval=50)
sim.SetOutputScheduling( "energies", "none" )
sim.SetOutputScheduling( "trajectory", "logarithmic" )
sim.SetOutputScheduling( "trajectory", "loglin", base=4, maxInterval=64 )
```

The first causes energies to be output equally spaced (linear) in time, once every 50 time steps, while the second turns energy writing off. The third will cause logarithmic saving of configurations (where the interval between saves doubles each time within a “block”, starting with 1. The fourth does logarithmic saving starting with interval 4 until the interval 64 is reached, after which the interval stays fixed at 64 until the end of the block. The details of log-lin are described in a separate document. By default energies are linear, written every 256 steps, and trajectories are logarithmic.

## 2.4 Post processing

The post processing tools are located in the `<RUMD-HOME>/Tools/` directory and each one of them has a help text. To see the help text use the option `-h` or `--help` depending on the tool. The actual output files generated by the program are in a directory called `TrajectoryFiles`. When you start a new simulation in the same directory, this will be moved to `TrajectoryFiles.rumd_bak` as a precaution against accidental overwriting of data. The analysis programs should be run in the original directory where the simulation was run (they know they should look in `TrajectoryFiles` for the data).

`rumd_stats` produces mean values, variances and standard deviations for specific quantities. The `rumd_stats` stdout for the simulation just performed is shown in table 1.

quantity	mean value	variance	standard deviation
ke	1.49802	0.0015541	0.0394221
pe	-5.27922	0.0029679	0.0544784
p	8.64558	0.0529826	0.23018
T	0.999677	0.000692101	0.0263078
Etot	-3.7812	0.00439295	0.0662794
W	7.64591	0.052637	0.229428

Table 1: `rumd_stats` output.

Here ke is the kinetic energy, pe is the potential energy, p is the pressure, T is the kinetic temperature, Ps is the Nose Hoover thermostat, Etot is the total kinetic energy and W is the virial. The program writes the mean and variance in the files `energies_mean.dat` and `energies_var.dat` in one row as the first column of stdout.

The radial distribution function is computed by typing `rumd_rdf -n 1000 -m 1.0` where the first argument is the number of bins in radial distribution function and the second argument, the minimum time between successive configurations to use, is to avoid wasting time doing calculations that are very similar (we assume here that the configurations are uncorrelated after one time unit). Use `rumd_rdf -h` for a full list of arguments. The output is `rdf.dat` and for binary systems the columns are:

$r$   $g_{00}(r)$   $g_{01}(r)$   $g_{10}(r)$   $g_{11}(r)$ . (Single component only has two columns). Plot `rdf.dat` to obtain figure 1.

The static structure factor can be obtained when the radial distribution function is computed. It is done by typing `rumd_sq 2 20 1` where the first argument is the start  $q$  value, the second argument is the final  $q$  value and the third argument is the density. The stdout is the  $q$  value for the maximum of the first peak and it is written in a file called `qmax.dat`. The static structure factor is written in `Sq.dat` and is structured like `rdf.dat`. Plot `Sq.dat` to obtain figure 2.

The mean square displacement and the self part of the incoherent intermediate scattering

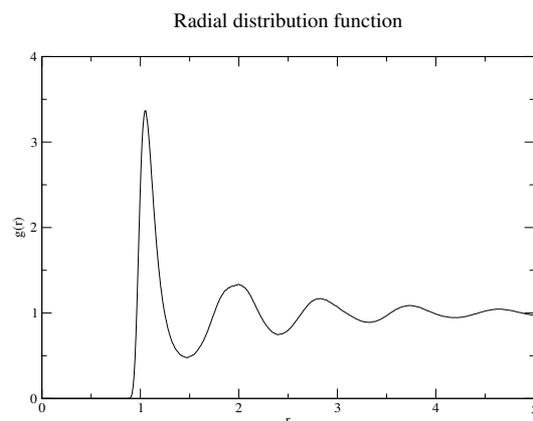


Figure 1: Radial distribution function.

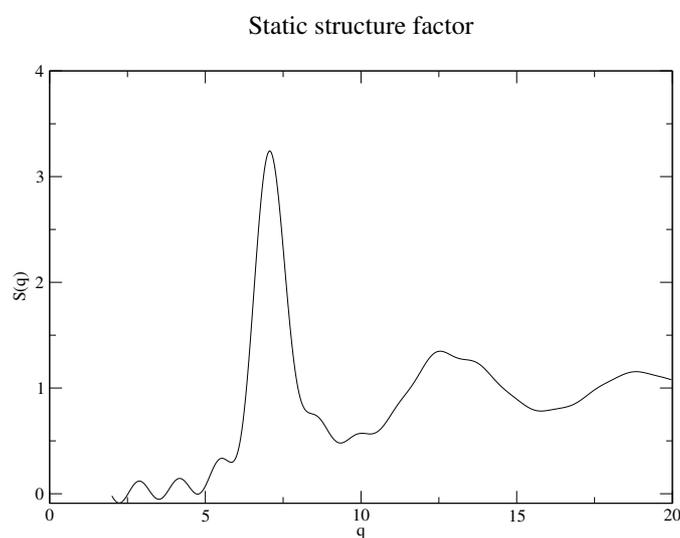


Figure 2: The static structure factor

function  $F_q(t)$  are calculated with the command `rumd_msd`. This generates a `msd.dat` file with time as the first column and the mean square displacement as a function of time as the second column (for binary systems there will be two columns), and a file `Fs.dat` with a similar structure. Before it can be run however, you must create a file called `qvalues.dat` which contains one wavenumber for each type of particle. Typically these correspond to the location of the first peak in the structure factor, so one could copy the file `qmax.dat` created by `rumd_sq`. `rumd_msd` also calculates gaussian parameter `alpha2.dat`. See figure 3 and 4 for mean square displacement and self part of incoherent scattering function. The post processing analysis tools are summarized in table 2. It is evident from table 2 that `rumd_rdf` has to be performed before `rumd_sq` and `rumd_sq` before `rumd_msd`. If you only are interested in the mean square displacement and know which  $q$ -values to use it is not necessary to run `rumd_rdf` and `rumd_sq` first. Then you just have to create a file called `qvalues.dat` with the appropriate  $q$ -values before running `rumd_msd`.

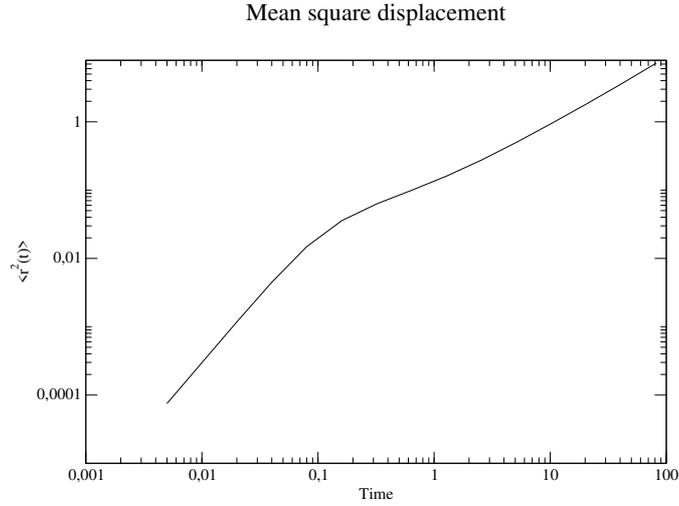
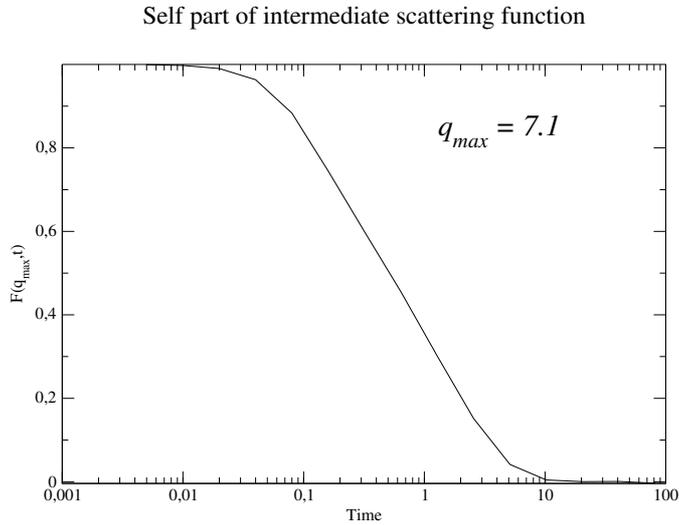


Figure 3: Mean square displacement.

Figure 4: Self part of the intermediate scattering function evaluated at the  $q$  value of the maximum of the first peak in the structure factor.

## 2.5 Simulating molecules

With RUMD you can simulate molecular systems. The intra-molecular force field includes bond, angle and torsion interactions. The total potential energy due to intra-molecular interactions excluding possible pair potentials is given by

$$U(\vec{r}) = \frac{1}{2} \sum_{\text{bonds}} k_s^{(i)} (r_{ij} - l_b^{(i)})^2 + \frac{1}{2} \sum_{\text{angles}} k_\theta^{(i)} [\cos(\theta) - \cos(\theta^{(i)})]^2 + \sum_{\text{dihed}} \sum_{n=0}^5 c_n^{(i)} \cos^n(\phi), \quad (1)$$

Tool	Input	Output	Arguments
rumd_stats	none	std.out: table 1	none
		energies_mean.dat energies_var.dat	
rumd_rdf	none	std.out: Simulation info	1. num. bins
		rdf.dat sdf.dat	2. time diff.
rumd_sq	rdf.dat	std.out: qmax(s)	1. qstart
		Sq.dat qmax.dat	2. qfinal 3. density
rumd_msdl	qvalues.dat	std.out: Simulation info	none
		msd.dat	
		Fs.dat	
		FsSq.dat alpha2.dat	

Table 2: Post processing tools, their input, output and the arguments.

where  $k_s^{(i)}$  is the spring force constant for bond type  $i$ ,  $k_\theta^{(i)}$  the angle force constant for angle force type  $i$ , and  $c_n^{(i)}$  the torsion coefficients for torsional force type  $i$ .  $l_b^{(i)}$  and  $\theta_0^{(i)}$  are the zero force bond length and angle, respectively.

Beside the standard harmonic bond potential RUMD also supports simulation of rigid bonds using constraint method as well as the Finite Extensible Nonlinear Elastic (FENE) potential

$$U(\vec{r}) = -\frac{1}{2}kR_0^2 \sum_{\text{bonds}} \ln \left[ 1 - \left( \frac{r_{ij}}{R_0} \right)^2 \right], \quad (2)$$

where  $k = 30$  and  $R_0 = 1.5$  (in reduced units). At the moment the constraint method is applicable for molecules with few constraints.

### Example

In all one starts by creating (or copying and modifying) a topology file (with extension `.top`). Examples can be found in the subdirectory `Conf/Mol`, in particular one called `mol.top`, which is associated with a configuration file `ExampleMol.xyz.gz`. Copy both of these files to your test directory. They specify a system containing 100 polymeric molecules, each consisting of 10 monomer units. The appropriate lines to include in the python script include one for reading the topology file and one for setting the parameters of the (in this case) single bond-type. Note that this has changed for Version 3.5, so that adding intra-molecular interactions, such as bonds, works similarly to adding ordinary pair interactions.

```
sim = Simulation("ExampleMol.xyz.gz")
# read topology file
sim.ReadMoleculeData("mol.top")

# create integrator object
itg = IntegratorNVE(timeStep=0.0025)
sim.SetIntegrator(itg)
```

```

# create pair potential object
potential = Pot_LJ_12_6(cutoff_method=ShiftedPotential)
potential.SetParams(i=0, j=0, Epsilon=1.0, Sigma=1.0, Rcut=2.5)
sim.AddPotential(potential)

# define harmonic bond and its parameters for bonds of type 0
pot_harm = rumd.BondHarmonic()
pot_harm.SetParams(bond_type=0, bond_length=0.75, stiffness=200.0, exclude=True)
sim.AddPotential(pot_harm)

sim.Run(20000)

```

Specifying `exclude=True` ensure that contributions from the bonds will be removed from the calculation of the pair potential. If you wish to keep the pair force interactions between the bonded particles you can specify this using

```
pot_harm.SetParams(bond_type=0, bond_length=0.75, stiffness=200.0, exclude=False)
```

□

If there are other bond-types which have different lengths or stiffnesses, you just call `SetParams` again; it is not necessary to create another `BondHarmonic` object (this will in fact give an error). In the case you wish to use the FENE potential you simply use

```

pot_fene = rumd.BondFENE()
pot_fene.SetParams(bond_type=0, bond_length=0.75, stiffness=30., exclude=False)
sim.AddPotential(pot_fene)

```

to specify that bond type 0 is a FENE bond type. In the FENE potential, the pair interactions between bonded particles should not be excluded.

As noted above, you can also simulate molecules with rigid bonds. To specify that bond type 0 is a rigid bond you add the bond constraint using an object of type `ConstraintPotential`:

```

pot_cons = rumd.ConstraintPotential()
pot_cons.SetParams(bond_type=0, bond_length=0.75)
sim.AddPotential(pot_cons)

```

Details of the format used for the `.top` files and on tools available for creating them can be found in the user manual.

Table 3: Identifier and column-label for the main quantities that can be written to the energies file.

identifier	column label
potentialEnergy	pe
kineticEnergy	ke
virial	W
totalEnergy	Etot
temperature	T
pressure	p
volume	V
stress_xx	sxx <sup>(a)</sup>

<sup>(a)</sup> Potential part of atomic stress.  
Similarly yy, zz, xy, etc

### 3 Level 2: Fine control

The user at level 2 can use the full `Simulation` interface to control many details of the simulation. Here we present, mostly in the form of python code-snippets, some of the more advanced aspects of the interface, though without trying to present a complete documentation. The next step is to look on the RUMD web-page ([rumd.org](http://rumd.org)) under “example scripts” for ideas about how to get the most out of RUMD.

#### 3.1 Controlling how the simulation run is divided into blocks

The simulation output is divided into blocks of size `blockSize`. By default the block-size is chosen when `Run` is called, so that there will be of order 100-200 blocks in the given number of time-steps. Sometimes it is useful to explicitly specify the block-size (this will sometimes be necessary when using log-lin because there are some constraints on the block-size in relation to the log-lin parameters). The following will set the `blockSize` (we denote by `sim` the `Simulation` object):

```
sim.SetBlockSize(1024)
```

#### 3.2 Controlling what gets written to energies and trajectory files

To change what gets written we call the `SetOutputMetaData` method, which functions similar to `SetOutputScheduling` in that it takes a string with the name of the output manager, and one or more keyword arguments specifying either that a parameter should be included or not, or what the overall precision should be.

```
sim.SetOutputMetaData("energies",totalEnergy=False,stress_xy=True, precision=7)
```

which turns off writing the total energy, turns on writing the xy component of the stress tensor, and sets the precision to seven decimal places. Table 3 shows the most important available quantities. To each of these are associated two strings: an “identifier” for use in scripts, to refer to a given quantity when turning it “on” or “off”; and a “column-label”, which appears in the comment-line of the energies file to identify which column corresponds to which quantity.

For simulations in which more than one potential is present, the contributions from different terms to the total potential energy can be included in the energies file. Each potential class has an ID string. For example for `Pot_LJ_12_6` it is “potLJ”. If desired the ID string can be changed (for example to the simpler “LJ”) via

```
pot.SetID_String("LJ")
```

In the case of contributions to potential energy this ID-string functions as both the identifier in scripts, and the column-label in the energies-file. So for example, after changing the ID-string to “LJ” as above, to cause it to be written we would write

```
sim.SetOutputMetaData("energies", LJ=True)
```

There is a mechanism for additional quantities to be defined and included in the energies file, via classes of type `ExternalCalculator`. This is described in the user manual.

### 3.3 Changing the sample volume within the script

It can be useful to take a configuration corresponding to one density and rescale the box and particle coordinates such that it has a different density. This is accomplished by the following lines (which also show how to get the current volume and number of particles).

```
nParticles = sim.GetNumberOfParticles()
vol = sim.GetVolume()
currentDensity = nParticles/vol
sim.ScaleSystem( pow(newDensity/currentDensity, -1./3) )
```

where `newDensity` is understood to be the desired density.

### 3.4 Options for Run: Restarting a simulation, suppressing output, continuing output

Under default conditions a “restart file” will be written, once per output-block. If a simulation is interrupted (due to hardware problems for example), it can be restarted from the last completed block (here 12) by

```
sim.Run(20000, restartBlock=12)
```

where the original number of time-steps should be specified, and the last completed block can be found by looking at the file “LastComplete\_restart.txt” in `TrajectoryFiles`. It is possible to suppress writing of restart files (so restarts will not be possible), and all other output, by calling

```
sim.Run(20000, suppressAllOutput=True)
```

This might be done for example, during an initial period of equilibration, although if this is planned to take a long time, it may be advisable to allow restart files to be written, in case of possible interruptions.

To avoid re-initializing the output, so that repeated calls to `Run` will append to the existing energies and trajectory files, do

```
sim.Run(20000, initializeOutput=False)
```

This will give an error if `Run` was not called previously in the normal way (`initializeOutput=True`, which is its default value).

### 3.5 Getting optimum performance via the autotuner

RUMD involves several internal parameters whose values do not affect the results of the simulation within round-off error, but they can have a noticeable effect on performance. The easiest way to identify the optimal values is to use the autotuner, which is a python script that takes a simulation object which is ready to run (the potential(s) and integrator have been set), and determines the best values for the internal parameters. The following snippet shows how this is done.

```
from rumd.Autotune import Autotune
at = Autotune()
[create sim with associated potential(s) and integrator]
at.Tune(sim)
sim.Run()
```

The time taken to do the tuning is of order a minute for small systems (longer if constraints are involved). The autotuner writes a file, `autotune.dat` in the directory. If the simulation is re-run in the same directory with the same user parameters and on the same type of graphics card, then the autotuner will simply use the previously determined internal parameters.

## 4 Level 3: How to implement your own pair potential in RUMD

This tutorial will describe how to implement a new pair potential and test it. Let us say we want to implement a Gaussian core potential:

$$v(r) = \epsilon \exp \left[ - \left( \frac{r}{\sigma} \right)^2 \right] \quad (3)$$

When implementing a new pair potential there are a number of things to do:

1. Implement the potential and force into the RUMD source code
2. Include the new potential in the Python interface
3. Compile
4. Test the potential
5. Use it

The `PairPotential.h` in the directory `<RUMD-HOME>/include /rumd` contains all the pair potentials, implemented as classes in C++.

We start with a review of the general 12-6 Lennard-Jones potential - it is the first pair potential in the file (search for `Pot_IPL_12_6`). Note that this is not the one most typically used in simulations; that would be one of its derived classes `Pot_LJ_12_6`. The difference is only in how the parameters are specified: for the `Pot_IPL_12_6` potential, rather than `Epsilon` and `Sigma`, we specify the coefficients of the IPL terms, `A12` and `A6`. We will make a copy of it and change it to the Gaussian core potential.

The implementation is split into two major parts: The first part is the function `SetParams(...)` which is called by the user via the python interface. The last part is the function `ComputeInteraction` where the actual computation (on the GPU) is taking place.

`SetParams(...)` is called via the python interface once for each type of interaction, with `i` and `j` denoting the types of the two particles involved in the particular interaction. The user specifies the coefficients `A12` and `A6` and the cut-off `Rcut` (in other potentials the parameters might include a characteristic length `σ` and characteristic energy `ε` and possibly more parameters). The parameters of the potential are communicated by storing them in `h_params[i][j][ ]`. NOTE: the correctness of the program relies on `h_params[i][j][0]` containing the cut-off in absolute units. In other words, interactions between particles of type `i` and `j` are only computed if the distance between the two particles is less than `h_params[i][j][0]`. The rest of the stored parameters are chosen to facilitate fast computation.

The actual computation of the potential and the associated force is done on the GPU by the function `ComputeInteraction(...)`. When this is called `dist2` contains the square of the distance between the two particles in question, and `param` contains the appropriate parameters as set up by `SetParams(...)`. From this information, the function calculates `s` (i.e. the force, see below in equation (5)) and the potential. In the Lennard-Jones potential it is convenient to define two inverse lengths `invDist2` and `invDist6` to minimize the number of calculations. With these lengths it is easy to calculate `s` and the potential energy. `(*my_f).w +=` is the contribution to the potential energy.

We will now proceed to implement a Gaussian core potential. First step is to write up the equations we will implement. We will here implement the Gaussian core potential (repeated

below)

$$v(r) = \epsilon \exp \left[ - \left( \frac{r}{\sigma} \right)^2 \right] \quad (4)$$

We have to provide the function  $s$  which is used by RUMD to calculate the force:

$$s(r) \equiv -\frac{1}{r} \frac{dU(r)}{dr} = \frac{2\epsilon}{\sigma^2} \exp \left[ - \left( \frac{r}{\sigma} \right)^2 \right] \quad (5)$$

Now copy the entire Lennard-Jones potential and paste it somewhere in the file `PairPotential.h`. Replace `Pot_IPL_12_6` with `Pot_Gaussian` (four places). Choose a default identity string, e.g. `SetID_String("potGauss");`.

We will change the arguments in the `SetParams(...)` to match those of the other LJ potential `Pot_LJ_12_6` which uses  $\epsilon$  and  $\sigma$  instead of  $A_{12}$  and  $A_6$ , since the Gaussian potential also has a characteristic length  $\sigma$  and a characteristic energy  $\epsilon$ . But we need to make corresponding changes to the `h_params[i][j][ ]`'s. For the Gaussian potential they become:

- `h_params[i][j][0] = Rcut * Sigma;`
- `h_params[i][j][1] = 1.f / ( Sigma * Sigma );`
- `h_params[i][j][2] = Epsilon;`

Note that here the user parameter `Rcut` is to be interpreted as a scaled cutoff, in units of the corresponding  $\sigma$ . Now we can write the part taking place on the GPU. Since we do not need any inverse distances delete the lines computing `invDist2` and `invDist6`. We define instead a float called `Dist2`:

```
float Dist2 = dist2 * param[1];
```

which is  $(r/\sigma)^2$ . To avoid computing the exponential more than once, we define:

```
float exponential = exp(-Dist2);
```

With these definitions,  $s$  is simply implemented as:

```
float s = 2.f * param[1] * param[2] * exponential;
```

The next line is the potential:

```
(*my_f).w += param[2] * exponential;
```

This finishes the actual implementation, and we now proceed with a number of more technical changes ensuring that RUMD knows your new pair potential exists.

- In the file `Potentials.i` in the directory `<RUMD-HOME>/Swig` copy the entry (see below) relating to `Pot_IPL_12_6`, replace `Pot_IPL_12_6` with your potential name, change the arguments to `SetParams` in accordance with how it was defined in `PairPotential.h`, and replace the docstring with a similar brief description of your potential. To be 100% clear about what needs to be copied, here is the entry for `Pot_IPL_12_6`:

```
// docstring for Pot_IPL_12_6
%feature("autodoc", "Standard 12-6 Lennard-Jones (cut and shifted potential)
v(r) = ( A12/r^12 + A6/r^6 ) - v_cut
s(r) = 12 A12/r^14 + 6 A6/r^8 = -r^-1*dv/dr (F_ij = s * r_ij)") Pot_IPL_12_6;
```

```

class Pot_IPL_12_6 : public PairPotential
{
public:
    Pot_IPL_12_6( CutoffMethod cutoff_method );
    void SetParams(unsigned int i, unsigned int j, float A12, float A6, float Rcut);
};

```

- In the directory <RUMD-HOME> do  
make

If everything compiled without errors the new pair potential will now be available from the python interface, and you need to test it. Run a simulation as described in the Level 1 tutorial, but choose the new potential.

Check that the simulation ran with the correct potential by plotting it by adding `potential.WritePotentials(sim.sample.GetSimulationBox())` to your script. This command produces a file "potentials\_PotID.dat" where the potential  $v(r)$  is followed by the radial force  $f(r)$  in each column for all possible particle pairs.

Make sure that the cut-off is done correctly by the program by zooming in on that distance. An example is shown in figure 5. Next, run a NVE simulation and test that the total energy is

### Gaussian core potential

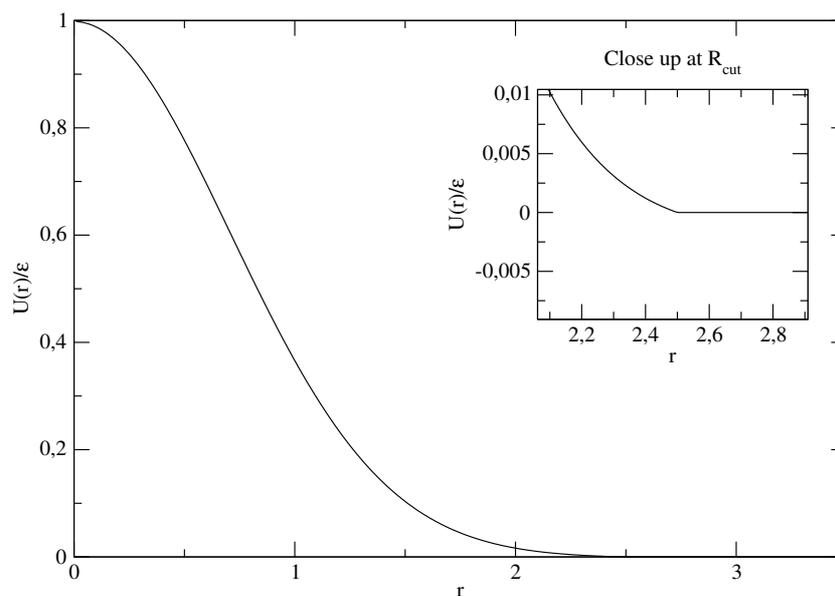


Figure 5: The Gaussian core potential.

conserved (i.e., have fluctuations that are much smaller than for the potential and kinetic energy).

Have fun with RUMD!