Overview

This software is a modified version Gromacs 5.0.1 (1, 2) which implements several multi-particle collision (MPC) (3–5) algorithms for efficient simulation of mesoscopic hydrodynamics. An example application called “STRD Martini” (6) is included, which uses stochastic rotation dynamics (SRD) collisions to supplement the Dry Martini (7) forcefield with mesoscopic hydrodynamics. There are five crucial differences between Dry Martini and STRD Martini simulations:

1. Modified topology files are used to define SRD particles and their interactions.
2. Energy exclusion groups are used to prevent nonbonded interactions for all SRD particles. This has the incidental effect of requiring the group neighbor list cutoff scheme.
3. The velocity-verlet integrator must be used in place of the stochastic integrator.
4. A special SRD collision cell thermostat must be used in lieu of a standard Gromacs thermostat. Without a thermostat, the simulation will gradually lose energy over time (at roughly -0.2 K/ns). The new thermostat is designed to conserve the SRD fluid flow field. No thermostat should be applied to the membrane.
5. Barostats should not be used in production simulations. They modify the periodic box, changing the size of SRD collision cells. This size is an important parameter for transport properties of the SRD fluid which should not change during the simulation. The kinetic energy of SRD particles is included in the pressure tensor, causing misleading pressure readings.

Consult the review literature for more comprehensive reviews and detailed descriptions of MPC dynamics (4, 5). The rest of this document will familiarity with MPC on behalf of the reader.

Features

- Three supported MPC collision rules
- Two methods for coupling MPC dynamics to MD force fields
- Output time and space averaged velocity fields from collision cells

Restrictions

- Velocity-Verlet integrator only
- Static load balancing recommended (set -dlb no for mdrun)
- Domain decomposition cells must be larger than MPC collision cells
- Rectangular simulation boxes only, no deformation
- Pressure coupling is compatible, but collision cells will be compressed accordingly
- All colliding particles are assumed to have the same mass as MPC particles

mdp Input Parameters

General input parameters for the collision step:

mpc-type	selected collision rule (off | srd | at | at+a)
mpc-grps	atom groups to include in collision step
mpc-freq	how often to do collisions (# timesteps)
mpc-cellsize	desired collision cell size (nm), actual size will depend on the periodic box size
mpc-seed	seed for collision RNG (-1 for random seed)

The following only apply when the srd collision rule is selected:

srd-angle	collision angle (degrees)
srd-tcouple	enable collision step thermostat (yes | no)
srd-tc-str	thermostat "strength" parameter ϵ
srd-tc-ref-t	thermostat reference temperature T_0 (K)

The following are used for writing out collision cell data:

mpc-out-freq	how often to output cell data (# timesteps)
mpc-out-samp	how often to sample cell data for output averages (# timesteps)
mpc-out-vel	write cell velocities to binary output file (yes | no)
mpc-out-num	write cell occupancies to binary output file (yes | no)

Choosing SRD Parameters

Properties of the SRD fluid are controlled by adjusting these simulation parameters. A set of value should be chosen that produce reasonable dimensionless hydrodynamic numbers and physical fluid properties. A Mathematica 7.0 notebook is provided with interactive plots to visualize how these parameters affect viscosity.

Collision angle: This can be freely adjusted.

Collision frequency: Frequent collisions incur a performance penalty from the increased MPI communication. Infrequent collisions yield large mean free paths, low viscosity, and large Péclet numbers. A value around 200 fs is a good compromise.

Collision cell size: This will set the suggested edge length for collision cells. STRD simulations require an integral number of collision cells along each dimension. Before the simulation begins, a cell grid is chosen that most closely matches the size suggested here.

SRD particle density: This parameter should be chosen such that collision cells contain between 3-30 SRD particles on average.

SRD particle mass: In principle, this can be varied like the other input parameters. However, the STRD implementation assumes all colliding particles have the same mass, so this is fixed at 72 amu – equal to the mass of Dry Martini CG beads.

Running STRD Martini Simulations

Topology files for STRD Martini are included in the "Topology Files" directory. strd_martini.itp is simply dry_martini_v2.1.itp with SRD particles and their interactions added. The "Example System" directory contains all input files required to run an example STRD Martini simulation.

To build your own systems, create and equilibrate a Dry Martini membrane without SRD particles. Then uniformly distribute SRD particles throughout the simulation volume. If you are using forces to couple SRD to your membrane, you may place all the SRD particles at a point far away from the membrane and let them fill the free space through diffusion.

Different Coupling Methods

Pairwise Force Coupling

This method sets repulsive Van der Waals interactions between certain MD atoms and MPC particles. To use this coupling scheme, only set exclusions among MPC particles:

```
energygrp      = Water
energygrp-excl = Water Water
```

And include only MPC particles in the collision group:

```
mpc-grps       = Water
```

The interaction used for STRD Martini is a WCA-like (8) interaction with the phosphate headgroup beads of Dry Martini (PO4). These additional forces may perturb membrane properties and will affect pressure coupling. You may use zero surface-tension coupling, but be aware that the additional normal pressure will cause the membrane to contract laterally in order to balance P_{zz} with $\left(P_{xx} + P_{yy}\right)/2$.

Direct Collision Coupling

This method includes regular MD atoms in the MPC collision step. The atoms are assumed to have the same mass as MPC particles, and are treated exactly like other MPC particles during the collision step. To use this coupling scheme, set exclusions between MPC particles and everything else:

```
energygrp      = Water non-Water
energygrp-excl = Water Water Water non-Water
```

Then include desired atoms in the collision group:

```
mpc-grps       = Water PO4
```

When using this coupling method, STRD Martini is coupled to the phosphate headgroup beads of Dry Martini (PO4). When creating a system, you'll need to create a group using *gmx make_ndx*.

Notation

The following notation will be used throughout the following section:

$\vec{v}_i'$	new velocity for ith particle after collision step
$\vec{v}_i$	absolute velocity of ith particle in cell
$\tilde{v}_i$	relative velocity of ith particle in cell
$\vec{u}_c$	mean cell velocity
$\vec{x}_i$	absolute position of ith particle in cell
$\tilde{x}_i$	relative position of ith particle in cell
$\vec{x}_c$	mean cell position
N_c	number of particles in cell

Since all masses for colliding particles are assumed to be the same, cell averages and relative particle positions/velocities are not weighted:

$$\vec{x}_c = \frac{1}{N_c}\sum_{j=1}^{N_c} \vec{x}_i$$

$$\tilde{x}_i = \vec{x}_i - \vec{x}_c$$

$$\vec{u}_c = \frac{1}{N_c}\sum_{j=1}^{N_c} \vec{v}_i$$

$$\tilde{v}_i = \vec{v}_i - \vec{u}_c$$

Supported Collision Rules

Stochastic Rotation Dynamics (SRD)
mpc-type = srd

$$\vec{v}_i' = \vec{u}_c + R_{\theta,\hat{a}_c}(\tilde{v}_i)$$

This collision rule rotates the relative velocity vectors $\tilde{v}_i$ by a fixed angle θ around random unit axis $\hat{a}_c$. The rotation axis is selected uniformly on the unit sphere with a different axis chosen for each cell. This collision rule conserves energy and momentum. It may be expressed without a rotation matrix as:

$$\vec{v}_i' = \vec{u}_c + \tilde{v}_i^{\parallel} + \tilde{v}_i^{\perp}\cos(\theta) + (\hat{a}_c \times \tilde{v}_i)\sin(\theta)$$

$$\tilde{v}_i^{\parallel} = (\hat{a}_c \cdot \tilde{v}_i)\hat{a}_c$$

$$\tilde{v}_i^{\perp} = \tilde{v}_i - \tilde{v}_i^{\parallel}$$

SRD Cell Thermostat
srd-tcouple = yes
srd-tc-str = 0.10

SRD-compatible thermostats must not disturb the cell velocity vectors $\vec{u}_c$. The thermostat implemented for STRD uses randomly-chosen rescaling factors for each cell that are applied based on a Boltzmann factor using the current kinetic energy of the cell and the target temperature T_0 (9, 10).

Within each cell, a scaling factor S is chosen, with equal probability, to be either $(1+\varepsilon)$ or $(1+\varepsilon)^{-1}$ where ε is an input parameter (srd-tc-str) less than one. A uniform random number is chosen $p \in [0,1]$. If this number is less than the acceptance probability p_A = min(1, A), the relative velocities of SRD particles in the cell are rescaled by S.

$$A = S^{3(N_c-1)} \exp\left(-\frac{(S^2-1)}{2k_B T_0} \sum_{j=1}^{N_c} m_i \tilde{v}_i{}^2 \right)$$

Andersen Thermostat (AT)
mpc-type = at

$$\vec{v}_i' = \vec{u}_c + \vec{w}_i - \frac{1}{N_c}\sum_{j=1}^{N_c} \vec{w}_i = \vec{u}_c + \tilde{v}_i'$$

This collision rule selects new relative velocity vectors at random. The random components of $\vec{w}_i$ are drawn from a gaussian distribution with variance $= \sqrt{k_B T/m_i}$. The sum of these random vectors is subtracted from $\vec{v}_i'$ to keep $\vec{u}_c$ invariant. This collision rule conserves momentum and has an equilibrium temperature, but does not conserve energy.

Andersen Thermostat with Local Angular Momentum Conservation (ATA)
mpc-type = at+a

$$\vec{v}_i' = \vec{u}_c + \tilde{v}_i' - \Delta\vec{\omega}_c \times \tilde{x}_i$$

$$\Delta\vec{\omega}_c = \mathbb{I}_c^{-1}\Delta\vec{L}_c = \mathbb{I}_c^{-1}\sum_{j=1}^{N_c} \tilde{x}_j \times m_j\left(\tilde{v}_j' - \tilde{v}_j\right)$$

This version of the Andersen thermostat collision rule includes an extra term that ensures local angular momentum within each cell is conserved during the collision step. $\mathbb{I}_c$ is the moment of inertia tensor of the cell and m_j is the mass of the jth particle in the cell. Since this collision rule requires additional communication for the MPC particle positions, it will be slower than ordinary Andersen.

Binary Output File Format

Average collision cell vectors and occupancies can be output to a binary data file. The averaging is done both spatially and temporally. Frames are output according to mpc-out-freq, with intervening samples taken according to mpc-out-samp. It is possible to forgo temporal averaging by setting mpc-out-freq equal to the collision frequency, but this often produces very large quantities of data.

Spatial averaging is performed on every sample to account for grid shifting. A gaussian weighting function is used with the distance from the center of each cell to its shifted position and those of its 26 nearest neighbors. The variance is taken to be the MPC grid spacing divided by 3.

Simulations that output cell vectors will run much slower, as global communication is required for each sample to gather cell data to the master node.

A MATLAB script for reading binary cell data files is provided in the "Collision Cell Data" directory. If you'd like to write your own analysis code, the file format is:

File header (0x30 bytes):
(int) magic number to determine endianness (= 2016)
(int) file version (= 1)
(int) size of cell occupancy data (bytes)
(int) size of cell velocity data (bytes)
(int vector) number of collision cells along XYZ
(int) output frame count
(int) collision frequency
(int) sampling frequency
(int) output frequency
(float) time between output frames (ps)

Frame header (0x20 bytes, start of each frame):
(int) frame number (1,2,3…)
(float) frame simulation time (ps)
(float vector) current grid shift (only relevant when dumping every step)
(float vector) time averaged size of collision cells along XYZ

Frame data:
(float x num cells) average occupancy for each cell
(float vector x num cells) average velocity vectors for each cell

Finding Codebase Changes

src/gromacs/srd/ contains new source and build files for STRD. Substantial additions were made to src/gromacs/mdlib/domdec.c to implement the communication protocol. There are dozens of other modifications throughout the Gromacs codebase. These changes are enclosed between comment lines starting with //SRDCODE and //END_SRDCODE.

Wallcycle Accounting Categories

New accounting categories in the output log list time spent in various parts of the STRD code:

MPC – Init	Setting up collision cells
MPC – Cells	Identifying collision cell homes for current node and neighbors
MPC – Comm. pt. 1	Sending particle data to neighbors: $(\vec{v}_i, \vec{x}_i)$
MPC – Collisions	Doing the collision steps (includes thermostatting)
MPC – Comm. pt. 2	Receiving resultant velocities from neighbors: $(\vec{v}_i')$
MPC – Output	Collecting collision cell data and writing it to file
MPC – Comm. Test	Validating communication code (only used with SRD_COMM_TEST)

References

1. Hess, B., C. Kutzner, D. van der Spoel, and E. Lindahl. 2008. GROMACS 4: algorithms for highly efficient, load balanced, and scalable molecular simulations. J. Chem. Theory Comput. 4: 435–447.

2. Abraham, M.J., T. Murtola, R. Schulz, S. Páll, J.C. Smith, B. Hess, and E. Lindah. 2015. Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX. 1–2: 19–25.

3. Malevanets, A., and R. Kapral. 1999. Mesoscopic model for solvent dynamics. J. Chem. Phys. 110: 8605–8613.

4. Padding, J.T., and A.A. Louis. 2006. Hydrodynamic interactions and Brownian forces in colloidal suspensions: Coarse-graining over time and length scales. Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys. 74: 1–29.

5. Gompper, G., T. Ihle, D.M. Kroll, and R.G. Winkler. 2008. Multi-Particle Collision Dynamics -- a Particle-Based Mesoscale Simulation Approach to the Hydrodynamics of Complex Fluids. Adv. Polmer Sci. .

6. Zgorski, A., and E. Lyman. 2016. Toward Hydrodynamics with Solvent Free Lipid Models: STRD Martini. Biophys. J. 111: 2689–2697.

7. Arnarez, C., J.J. Uusitalo, M.F. Masman, H.I. Ingólfsson, D.H. De Jong, M.N. Melo, X. Periole, A.H. De Vries, and S.J. Marrink. 2015. Dry martini, a coarse-grained force field for lipid membrane simulations with implicit solvent. J. Chem. Theory Comput. 11: 260–275.

8. Weeks, J.D., D. Chandler, and H.C. Andersen. 1971. Role of Repulsive Forces in Determining the Equilibrium Structure of Simple Liquids. J. Chem. Phys. 54: 5237–5247.

9. Heyes, D.M. 1983. Molecular dynamics at constant pressure and temperature. Chem. Phys. 82: 285–301.

10. Hecht, M., J. Harting, T. Ihle, and H.J. Herrmann. 2005. Simulation of claylike colloids. Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys. 72: 1–16.