

PSE Molekulardynamik Sheet 5: Parallelization

Exercise at 20th December 2013

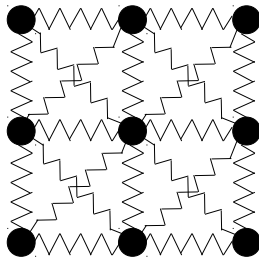
Remark Hand in configurations, animations, performance measurements and analyses of all simulations.

Task 1 “Simulation of a membrane”

Up to now, we assumed molecules to be spherical and of a fixed internal structure. Thinking about e.g. large biomolecules, this clearly isn't true. In this task we want to simulate a membrane, where the molecules have fixed neighbour relationships, but the structure of the whole membrane is nevertheless flexible. Neighbouring particles interact through a harmonic potential.

To demonstrate the dynamical behaviour, the membrane is subject to gravity, and a force pulls a few molecules of the membrane “upwards” for the first 15.000 timesteps. Self-penetration is avoided by placing a repulsive Lennard-Jones center with each of the molecules.

- Extend the molecule class so that the neighbouring molecules can be stored. Adapt the initialisation so that the molecules are arranged on a rectangular grid, and for each molecule it's direct neighbours along the x- and y-axis and it's diagonal neighbours are set:



- Directly neighbouring particles interact via the harmonic potential, i.e. the force is calculated as

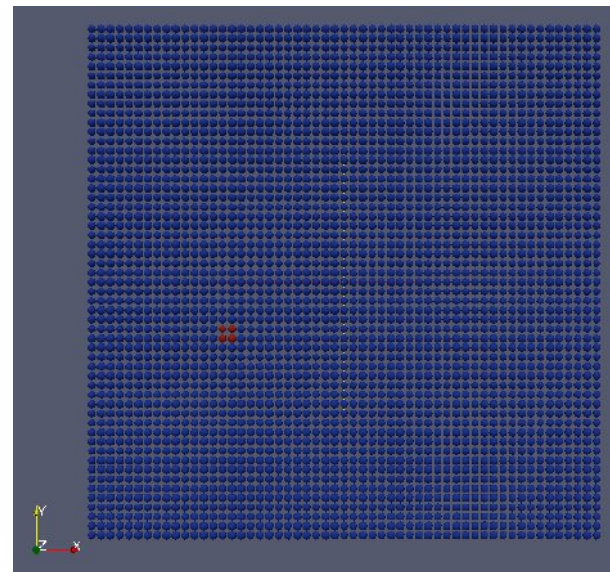
$$F(x_i, x_j) = k \cdot (||x_i - x_j||_2 - r_0),$$

where k is the stiffness constant and r_0 the average bond length of a molecule pair.

Diagonal neighbours interact via

$$F(x_i, x_j) = k \cdot (||x_i - x_j||_2 - \sqrt{2}r_0).$$

- The calculation of the Lennard-Jones potential is truncated at $2^{\frac{1}{6}} \cdot \sigma$, so that only the repulsive part is effective.
- The particles with x/y-indices (17/24), (17/25), (18/24) and (18/25) are pulled by a constant force F_{Z-UP} “upwards” along the z-axis:



That force is only effective until time $t = 150$.

- Perform the simulation with the following parameters:

Gravity along the z-axis: $g_{\text{grav}} = -0.001$ $\text{delta.t} = 0.01$ $t_{\text{end}} = 500$
 Size of domain L = 148, 148, 148 $r_{\text{cutoff}} = 4.0\sigma$

$r_0 = 2.2$ $k = 300$ $F_{Z\text{-UP}} = 0.8$

Membrane:
 $m_1 = 1.0$ $\epsilon_1 = 1.0$ $\sigma_1 = 1.0$
 $x_1 = (15; 15; 1.5)$ $v_1 = (0; 0; 0)$ $n_1 = (50; 50; 1)$
 $h_1 = 2.2$

Use reflecting boundaries in the xy-plane at $z = 0$.

Task 2 "Rayleigh-Taylor instability in 3D"

Extend the "Simulation of the Rayleigh-Taylor instability" from sheet 4 to a 3D-scenario.

- Apply periodic boundaries on the additional 3rd dimension.
- Perform the following experiment:

$g_{\text{grav}} = -12.44$ $\text{delta.t} = 0.0005$ $t_{\text{end}} = 100$
 Size of domain L = 60, 24, 51 initial temp. $T_{\text{init}} = 40$ $n_{\text{thermostat}} = 1000$
 $r_{\text{cutoff}} = 3.0\sigma$

Liquid 1:
 $m_1 = 40.0$ $\epsilon_1 = 2.0$ $\sigma_1 = 1.15$
 $x_1 = \{0.6; 0.6; 0.6\}$ $v_1 = \{0; 0; 0\}$ $n_1 = \{48; 9; 42\}$
 $h_1 = 1.2$

Liquid 2:
 $m_2 = 80.0$ $\epsilon_2 = 2.0$ $\sigma_2 = 1.15$
 $x_2 = \{0.6; 11.4; 0.6\}$ $v_2 = \{0; 0; 0\}$ $n_2 = \{48; 9; 42\}$
 $h_2 = 1.2$

Abort the simulation, if the expected runtime ist too large (> 48h).

Task 3 "Parallelization"

In this task we want to parallelize our application, to reduce the runtime of our simulations to an acceptable length.

Parallelize the most time consuming parts of the algorithm using OpenMP.

- Cut the domain along the longest dimension to get `num_threads` equal sized subdomains. Each thread should now handle such a subdomain. Take care of data dependencies at the border of each subdomain and insert appropriate synchronization points if necessary.

- You application should still work correctly without OpenMP. Use precompiler statements therefore (`#ifdef _OPENMP`). The macro `_OPENMP` is set automatically if the compiler is called using OpenMP.
- Rerun the scenario of task 2 using the parallelized application. Measure the speedup S of your parallel application using up to 16 cores:

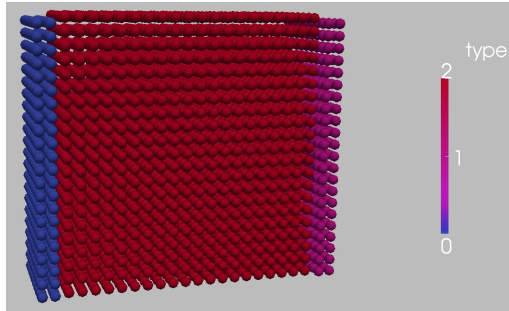
$$S(n) = \frac{T(1)}{T(n)},$$

where T(n) is the runtime for n threads.

- Analyse and optimize your application with PAPI and the Intel®VTune™ Amplifier XE.

Task 4 “Nano-scale Flow Simulation (Optional)”

In this task we want to study the nano-scale flow of liquid “falling” down. Of special interest are the velocity- and density-profile of the flow and its dependence on gravity and material of the wall.



The setup of the experiment consists of three cuboids, as depicted: the outer two cuboids act as walls and are kept fixed, while the molecules of the center cuboid are accelerated by gravity along the y-axis.

- Change the computation of the gravity, so that the weight force is added only to the fluid (use e.g. the type-flag of the molecules).
- Make it possible to fix the particles of the two outer cuboids (use e.g. the type-flag of the molecules to omit the position update).
- Change the thermostat or implement a new one: the velocity scaling has to be applied only to the fluid molecules, and only to the x- and z-component of the velocity-vector. In the computation of the kinetic energy, subtract the mean-velocity of all molecules in y-direction from the y-component of the molecule’s velocity (i.e., the speed of the flow does not contribute to temperature).
- Implement a component to compute the density- and velocity-profile along the x-axis. Subdivide the x-axis in N equal bins. In every time step, compute the bin for each molecule and accumulate the velocity in y-direction.

In fixed intervals of 10.000 iterations, write the statistics computed to a csv file.

- Perform the simulation with the following parameters:

$$\begin{array}{lll}
 g_{\text{grav}} = -0.8 & \text{delta.t} = 0.0005 & t_{\text{end}} = 500 \\
 \text{Size of domain } L = 35, 25, 10 & \text{initial temp. } T_{\text{init}} = 40 & n_{\text{thermostat}} = 10 \\
 r_{\text{cutoff}} = 2.5\sigma & &
 \end{array}$$

Cuboid 1 (left wall):

$$\begin{array}{lll}
 m_1 = 1.0 & \epsilon_1 = 2.0 & \sigma_1 = 1.1 \\
 x_1 = \{1.0; 0.6; 0.6\} & v_1 = \{0; 0; 0\} & n_1 = \{2; 23; 9\} \\
 h_1 = 1.12 & &
 \end{array}$$

Cuboid 2 (right wall):

$$\begin{array}{lll}
 m_2 = 1.0 & \epsilon_2 = 2.0 & \sigma_2 = 1.1 \\
 x_2 = \{27.4; 0.6; 0.6\} & v_2 = \{0; 0; 0\} & n_2 = \{2; 23; 9\} \\
 h_2 = 1.12 & &
 \end{array}$$

Cuboid 3 (fluid):

$$\begin{array}{lll}
 m_3 = 1.0 & \epsilon_3 = 1.0 & \sigma_3 = 1.0 \\
 x_3 = \{3.4; 0.6; 0.6\} & v_3 = \{0; 0; 0\} & n_3 = \{20; 21; 8\} \\
 h_3 = 1.2 & &
 \end{array}$$

Apply outflow boundaries along the x-axis and periodic boundaries along y- and z-axis. For the computation of the profiles in this example, use at least 50 bins along the x-axis.

- Change the gravity factor or mass of the fluid molecules or epsilon of the wall molecules and study the influence on the velocity profile.

Suggestion: Place spheres (fixed or not) in the fluid.

Task 5 “Crystallization of Argon (Optional)”

In this exercise we want to study the cooling process of argon, and especially the influence of how fast it is cooled down. For this experiment we have to adopt the force calculation method, and implement the calculation of thermodynamical statistics.

- Implement the smoothed Lennard-Jones Potential:

$$U(x_i, x_j) = 4 \cdot \epsilon \cdot S(x_i, x_j) \cdot \left(\left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^{12} - \left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^6 \right).$$

with

$$S(x_i, x_j) = \begin{cases} 1 & : \|x_i - x_j\|_2 \leq r_l \\ 1 - (\|x_i - x_j\|_2 - r_l)^2 \frac{3r_{\text{cutoff}} - r_l - 2\|x_i - x_j\|_2}{(r_{\text{cutoff}} - r_l)^3} & : r_l \leq \|x_i - x_j\|_2 \leq r_{\text{cutoff}} \\ 0 & : \|x_i - x_j\|_2 \geq r_{\text{cutoff}} \end{cases}$$

It should be possible to select the force calculation method (LJ, Smoothed LJ, gravitation) via the input file.

- Implement the calculation of thermodynamical statistics:
 - diffusion:

$$Var(t) = \frac{1}{N} \sum_{i=1}^N \|x_i(t) - x_i(t_0)\|^2$$

- Radial Distribution Function (RDF), as explained in the lecture

It is sufficient, if the statistics are calculated e.g. every 1000 time steps. They may be averaged over a few time steps, e.g. 5.

- Create an equilibrated fluid, using the following parameters:

Smoothed LJ with:	$r_{\text{cutoff}} = 2.3\sigma$	$r_l = 1.9$
Initial temperature $T_{\text{init}} = 0.01$	$n_{\text{therm}} = 40$	
target temperature $T_{\text{target}} = 3.0$	$n_{\text{downscaling}} = 40$	$\Delta T = 0.001$

Size of domain $L = (9.2, 9.2, 9.2)$	Simulation time $t_{\text{end}} = 150$	$\text{delta_t} = 0.001$
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$m_1 = 1.0$	$\epsilon_1 = 1.0$	$\sigma_1 = 1.0$
$x_1 = (0.575; 0.575; 0.575)$	$v_1 = (0; 0; 0)$	$n_1 = (8; 8; 8)$
$h_1 = 1.15$		

- Perform the first experiment (cooling argon): Use the equilibrated fluid from above as input (but take care that the thermal motion is not added although the initial temperature is $T_{\text{init}} = 3.0$).

Here, only the parameters which change are given:

Initial temperature $T_{\text{init}} = 3.0$	$n_{\text{therm}} = 50$	
target temperature $T_{\text{target}} = 0.5$	$n_{\text{downscaling}} = 50$	$\Delta T = 7.8 \cdot 10^{-4}$

Simulation time $t_{\text{end}} = 250$	$\text{delta_t} = 0.001$
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- Perform the second experiment (supercooling argon): Use the equilibrated fluid from above as input

Here, only the parameters which change are given:

Initial temperature $T_{\text{init}} = 3.0$	$n_{\text{therm}} = 25$	
target temperature $T_{\text{target}} = 0.02$	$n_{\text{downscaling}} = 25$	$\Delta T = 2.5 \cdot 10^{-3}$

Simulation time $t_{\text{end}} = 100$	$\text{delta_t} = 0.001$
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- Compare the two experiments concerning diffusion, rdf, and graphically, i.e. observe the resulting structure! At which temperature does the phase transition occur (the relation between the simulation temperature and the real temperature is $T_{\text{real}} = T_{\text{simulation}} \cdot 120K$)?

Good luck!

Deliver by 30th January 2014, 3 pm per mail to eckhardw@in.tum.de!