

## PSE Molekulardynamik

### Sheet 5: Applications and Parallelization

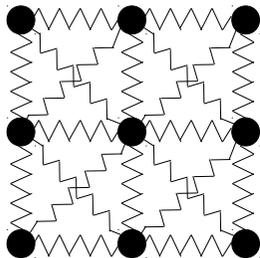
Exercise at 13th January 2012

#### 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 atoms 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 atoms of the membrane "upwards" for the first 15.000 timesteps. Self-penetration is avoided by placing a repulsive Lennard-Jones center at each of the atoms.

- 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

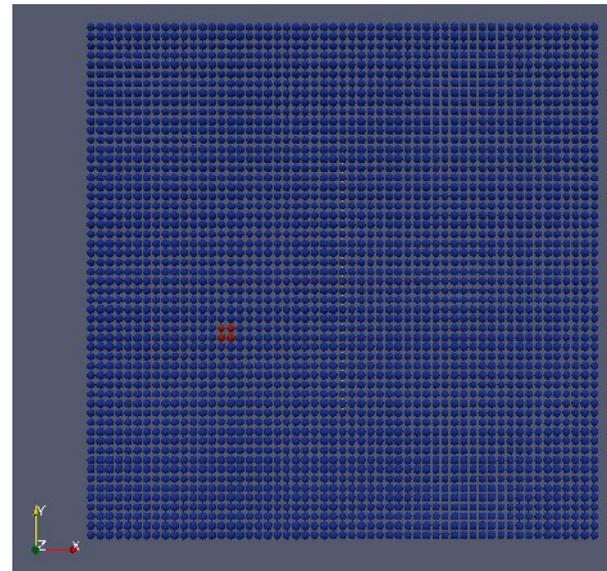
$$F(r_{ij}) = k \cdot (r - r_0)$$

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

Diagonal neighbours interact via

$$F(r_{ij}) = k \cdot (r - \sqrt{2}r_0)$$

- 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: $g_{grav} = -0.001$	$\text{delta}_t = 0.01$	$t_{end} = 500$
Size of domain $L = 148, 148, 148$	$r_{cutoff} = 4.0\sigma$	
$r_0 = 2.2$	$k = 300$	$F_{Z-UP} = 0.8$
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:

$$\begin{array}{lll}
 g_{grav} = -12.44 & \text{delta.t} = 0.0005 & t_{end} = 100 \\
 \text{Size of domain L} = 60, 24, 51 & \text{initial temp. } T_{init} = 40 & n_{thermostat} = 1000 \\
 r_{cutoff} = 2.5\sigma & & 
 \end{array}$$

Liquid 1:

$$\begin{array}{lll}
 m_1 = 40.0 & \epsilon_1 = 2.0 & \sigma_1 = 1.15 \\
 x_1 = \{0.6; 0.6; 0.6\} & v_1 = \{0; 0; 0\} & n_1 = \{48; 9; 42\} \\
 h_1 = 1.2 & & 
 \end{array}$$

Liquid 2:

$$\begin{array}{lll}
 m_2 = 80.0 & \epsilon_2 = 2.0 & \sigma_2 = 1.15 \\
 x_2 = \{0.6; 11.4; 0.6\} & v_2 = \{0; 0; 0\} & n_2 = \{48; 9; 42\} \\
 h_2 = 1.2 & & 
 \end{array}$$

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 4 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.

## Task 4 „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:

$$U(r_{ij}) = 4 \cdot \epsilon \cdot S(r_{ij}) \cdot \left( \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right)$$

with

$$S(r_{ij}) = \begin{cases} 1 & : r \leq r_l \\ 1 - (r - r_l)^2(3r_{cutoff} - r_l - 2r)/(r_{cutoff} - r_l)^3 & : r_l \leq r \leq r_{cutoff} \\ 0 & : r \geq r_{cutoff} \end{cases}$$

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:

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

$$\text{Size of domain L} = \{9.2, 9.2, 9.2\} \quad \text{Simulation time } t_{end} = 150 \quad \text{delta.t} = 0.001$$

$$\begin{array}{lll}
 m_1 = 1.0 & \epsilon_1 = 1.0 & \sigma_1 = 1.0 \\
 x_1 = \{0.575; 0.575; 0.575\} & v_1 = \{0; 0; 0\} & n_1 = \{8; 8; 8\} \\
 h_1 = 1.15 & & 
 \end{array}$$

- 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  $T_{init} = 3.0$ ).

Here, only the parameters which change are given:

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

Simulation time  $t_{end} = 250$      $\text{delta\_t} = 0.001$

- Perform the second experiment (supercooling argon): Use the equilibrated fluid from above as input

Here, only the parameters which change are given:

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

Simulation time  $t_{end} = 100$      $\text{delta\_t} = 0.001$

- 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  $T_{real} = T_{simulation} \cdot 120K$ )?

Good luck!

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