

PSE Molekulardynamik Sheet 2: Collision of two bodies

Exercise at 10th November 2010

Task 1 „Unit Tests“

Basis for the further development of the simulator will be that it is possible to test the functionality of components before they are completely integrated with the existing code.

- Inform yourself about CppUnit. Download CppUnit (<http://apps.sourceforge.net/mediawiki/cppunit/>).
- Build the CppUnit-library according to the instructions (file INSTALL).
- Write a simple UnitTest for the particle container you created in sheet 1, as described in the CppUnit CookBook. Also implement a runner. The unit tests should be executed when your programme is called with the option “-test”.
- Extend the code so that it is possible to specify the name of a single test case which is then being executed.
- In the following parts of the PSE always add new tests for the components you implement!

Task 2 „Logging“

For debugging it can be very useful to make use of a logging framework. We will use Log4CXX, a c++-port of the java logging framework log4j.

- Make yourself familiar with Log4CXX (<http://logging.apache.org/log4cxx/>). Download the code of the library in the version 0.10.0 and build it with the autotools. *Remarks:*
 - Additionally, you need the libraries apr1-dev and apr-util1-dev installed on your system.

– If you build log4cxx with a newer Compiler (*gcc geq 4*), you need to add the following header includes to the files: `src/main/cpp/inputstreamreader.cpp` and `src/main/cpp/socketoutputstream.cpp`:
`#include <cstring>`
`src/examples/cpp/console.cpp #include <cstdio> und #include <cstring>.`

- Think about a reasonable structure for the loggers and use log-instructions instead of `std::cout` in your code

For the configuration use a file in the property format.

Task 3 „Collision of two bodies“

- Implement a particle generator with which we can initialize the simulation. The generator should create a cuboid, where the molecules are arranged in a 3d rectangular grid.

The cuboid is being described by the following parameters:

- The coordinate of the lower left front-side corner.
- Number of particles per dimension: $N_1 \times N_2 \times N_3$.
- Distance h of the particles (mesh width of the grid)
- Initial velocity of the particles (3 Components).
- The mean-value of the velocity of the Brownian Motion. For now it is sufficient if you hard-code it in the code.

The movement of the molecules should be superposed by Brownian Motion. Use the code from the website to add the thermal friction!

Specify the parameters via the command line, or read them from a file. It has to be possible to add several cuboids! Moreover, it should be still possible to use a file for input.

- The interaction between two molecules i and j can be described with the help of the Lennard-Jones potential:

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

.

The resulting force can be calculated as

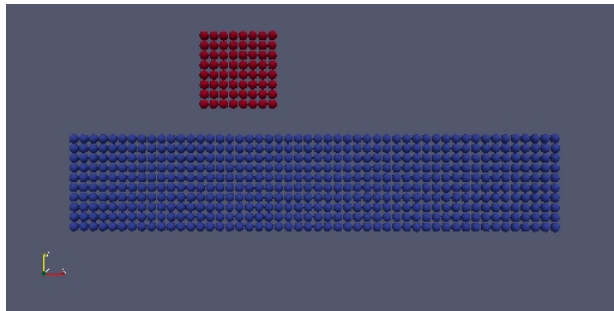
$$F_{ij} = -\nabla U(r_{ij}) = \frac{24 \cdot \epsilon}{r_{ij}} \cdot \left(\left(\frac{\sigma}{r_{ij}} \right)^6 - 2 \cdot \left(\frac{\sigma}{r_{ij}} \right)^{12} \right) \cdot \frac{\vec{r}_{ij}}{r_{ij}}$$

where $\frac{\vec{r}_{ij}}{r_{ij}}$ is the normalized distance vector and $r_{ij} = x_j - x_i$.

Implement a new method for force calculation, which computes the Lennard-Jones force between two molecules! For the moment it's ok if you hard-code the Lennard-Jones parameters ϵ und σ .

- If not already done, change the traversal of the particle pairs in such a way that the method for calculating the force is only called once for every pair and that the force for each pair is not evaluated twice, making use of Newton's third law.
- Now perform the simulation of the collision of two bodies with the parameters listed below.

$$\begin{aligned}x_1 &= \{0, 0, 0\} & x_2 &= \{15, 15, 0\} \\v_1 &= \{0, 0, 0\} & v_2 &= \{0, -10, 0\} \\N_1 &= \{40, 8, 1\} & N_2 &= \{8, 8, 1\} \\h &= 2^{1/6} \cdot \sigma \approx 1.1225 \\ \epsilon &= 5 & \sigma &= 1 \\ \delta t &= 0.0002 & t_{end} &= 5\end{aligned}$$



Good luck!

Deliver by 23rd November 2010, 12 pm per mail to eckhardw@in.tum.de and auckenth@in.tum.de! http://www5.in.tum.de/wiki/index.php/PSE_Molekulardynamik_WS10