Institut für Informatik — TU München
Scientific **C**omputing in **C**omputer **S**cience
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WS 2013/14

PSE Molekulardynamik
Sheet 1: First Steps towards a Moleculardynamics Simulation

Exercise on 18th October 2013.

General Information

- Work in groups of 2 or 3 students
- Deliverables:
  - GIT repository containing your source code, compilable with Makefile provided.
  - HTML-Documentation generated with Doxygen.
- Deliver latest by 3 p.m. of the given date per email.

Task 1 „First Steps “

- Download and install Eclipse CDT (http://www.eclipse.org/downloads/)
- Setup GIT (http://git-scm.com/)
- Download the programme frame from GitHub, compile and execute it.
- Download and install VTK/Paraview (http://paraview.org)
- Download and install Doxygen (http://www.doxygen.org). Create a preliminary documentation of the code frame.

Note:

- The directory libxsd/xsd has to be on the include path.
- You have to link against the Xerces XML Parser (flag -lxerces-c)

Task 2 „Completion of the programme frame “

- As we discussed in the lecture, the basic algorithm of the molecular dynamics simulation consists of the following steps:
  - Force calculation.
  - Calculation of the new position according to these forces.
  - Calculation of the new velocities according to these forces.
- Complete the steps of the simulation in the programme frame.
- Create VTK output for visualization with the VTKWriter class.
- Pass the parameters t_end and delta_t via the command line! (You can use the function atof for parsing the string to float)

Note:

- Visualize molecules in paraview with a *glyph*.
- It is possible to export videos (.avi) with “File“ → “save Animation“

Task 3 „Refactoring and Documentation “

The code frame in its current state is not very suitable as base for building up a moleculardynamics simulator. Refactor it, especially with respect to the following issues:

- Encapsulate the molecule list into a class ParticleContainer. It should be possible to iterate over the particles as well as the particle pairs in a simple way. Which design pattern(s) is / are suitable?
- During this course, we will use different methods for I/O and for calculating the force between particles. Think about an easy and extensible way to do that.
- Make yourself familiar with Doxygen. What can you do with a system like Doxygen, what is it useful for?

  Document the interfaces / implementations you created with Doxygen.

Good luck!

Deliver by 30th October 2013, 3 pm per mail to `eckhardw@in.tum.de`!

The programme frame is locatet at
`https://github.com/TUM-I5/MolSim`