

PSE Molekulardynamik

Sheet 1: First Steps towards a Moleculardynamics Simulation

Exercise on 10th October 2014.

General Information

- Work in groups of 2 or 3 students
- Deliverables:
 - HTML-Documentation generated with Doxygen.
 - Code in a git-repository. Doxygen documentation and unit tests are mandatory.
 - Slides for the presentation during the next meeting; remember to address all questions in the tasks
 - Pictures and animations of all runs.
 - Documentation how to build and use your code, especially if you extend the Makefile.
- Deliver latest by 3 PM 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.

Have fun!

Deliver by 23rd October 2014, 3 PM per mail to uekerman@in.tum.de!

The programme frame is located at
<https://github.com/TUM-I5/MolSim>