PSE Molekulardynamik

Basics

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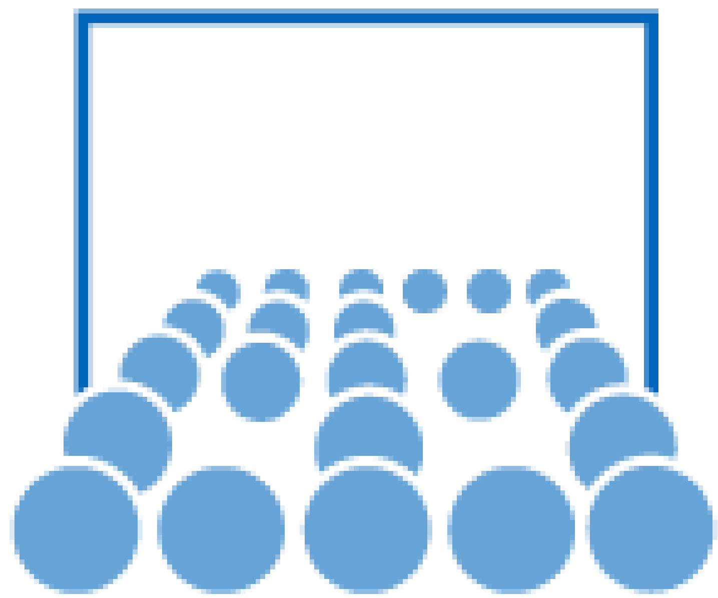
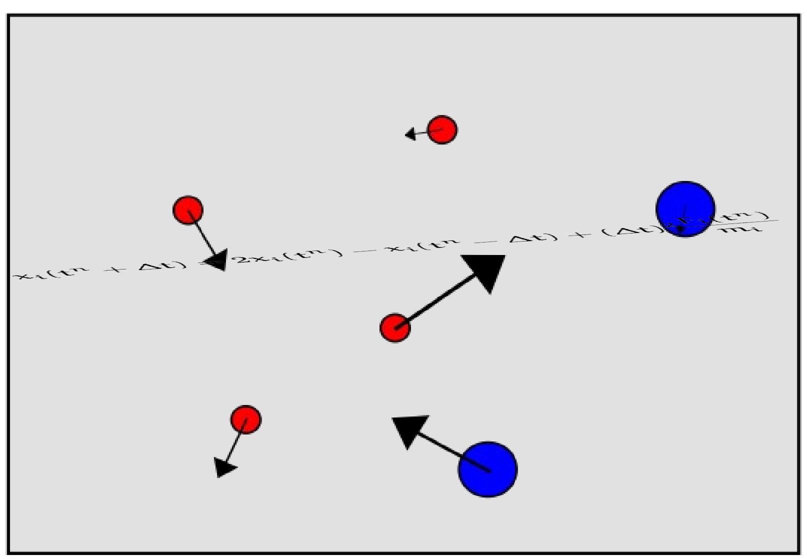
10.10.2014



Outline

- Organization
- Physics and math
- Hands on: Git, ParaView, Doxygen
- First worksheet



https://github.com/TUM-I5/MolSim

http://paraview.org

Schedule (big meetings)

- Presesentation of results (+ questions)
- Theory / algorithms for new exercise sheet
- 12:15 – ~ 14:00

10.10.2014	Intro 1 WS
24.10.2014	Review 1 WS / Intro 2 WS
07.11.2014	Review 2 WS / Intro 3 WS
28.11.2014	Review 3 WS / Intro 4 WS
12.12.2014	Review 4 WS / Intro 5 WS
16.01.2015	Review 5 WS

Grading

- First four worksheets: 10 points
- Last worksheet: 30 points

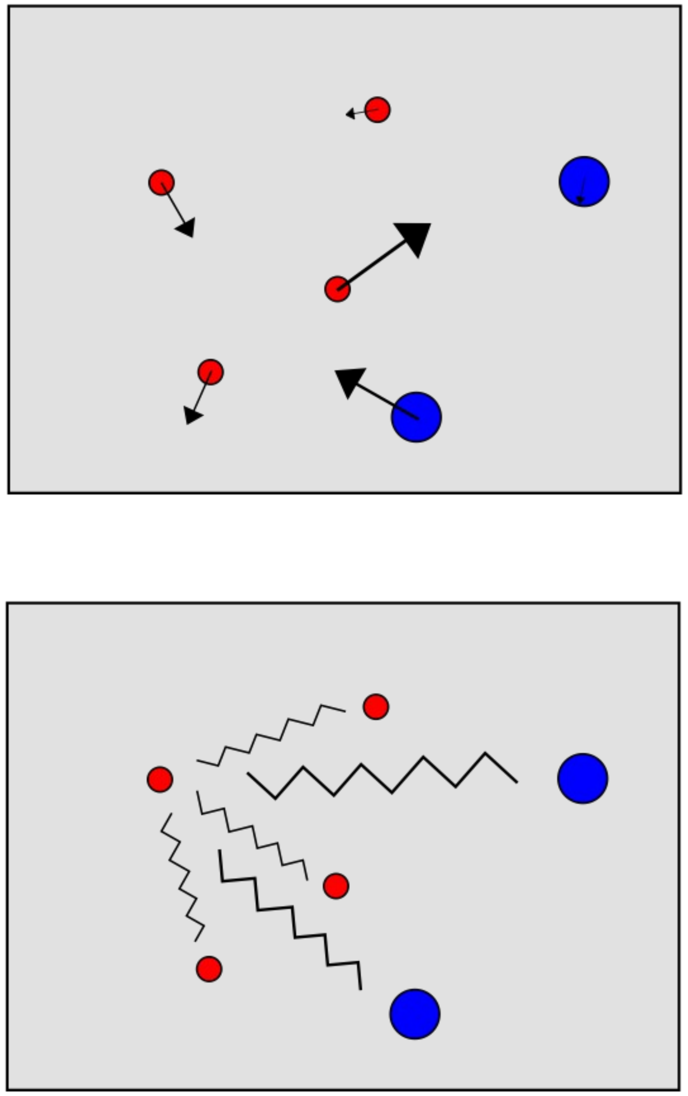
- Grade: Points & presentations

References

- **Molecular Dynamics**
  - Griebel, Knapek, Zumbusch: Numerische Simulation in der Molekulardynamik; Springer 2003
  - Griebel, Knapek, Zumbusch: Numerical Simulation in Molecular Dynamics. Springer, 2007
- **C++ Programming:**
  - Steve Qualline: Practical C++ Programming. O'Reilly, 2003
  - Scott Meyers: Effective C++. Addison-Wesley, 2007
  - Scott Meyers: More Effective C++. Addison-Wesley, 2007
  - www.cppreference.com
  - http://www.cplusplus.com/ (Tutorials/Referenz/Forum)

- **Questions?**
- **Groups?**

Newton’s laws of motion



- First law: If an object experiences no net force, then its velocity is constant: the object is either at rest (if its velocity is zero), or it moves in a straight line with constant speed (if its velocity is nonzero).
- Second law: The acceleration a of a body is parallel and directly proportional to the net force F acting on the body, is in the direction of the net force, and is inversely proportional to the mass m of the body, i.e., $F = ma$.
- Third law: When a first body exerts a force F_1 on a second body, the second body simultaneously exerts a force $F_2 = -F_1$ on the first body. This means that F_1 and F_2 are equal in magnitude and opposite in direction.

http://en.wikipedia.org/wiki/Newton's_laws_of_motion

Time discretization

$$t^n \rightarrow t^{n+1}$$

$$x(t^n + \Delta t) = x(t^n) + \Delta t \frac{\partial}{\partial t} x(t^n) + \frac{(\Delta t)^2}{2!} \frac{\partial^2}{(\partial t)^2} x(t^n) + \frac{(\Delta t)^3}{3!} \frac{\partial^3}{(\partial t)^3} x(t^n) + \mathcal{O}(\Delta t)^4$$

$$x(t^n - \Delta t) = x(t^n) - \Delta t \frac{\partial}{\partial t} x(t^n) + \frac{(\Delta t)^2}{2!} \frac{\partial^2}{(\partial t)^2} x(t^n) - \frac{(\Delta t)^3}{3!} \frac{\partial^3}{(\partial t)^3} x(t^n) + \mathcal{O}(\Delta t)^4$$

$$\Downarrow$$

$$\frac{x(t^n + \Delta t) - 2x(t^n) + x(t^n - \Delta t)}{(\Delta t)^2} = \frac{\partial^2}{(\partial t)^2} x(t^n) + \mathcal{O}(\Delta t)^2$$

Time discretization

$$t^n \rightarrow t^{n+1}$$

$$m_i \ddot{x}_i = F_i$$

$$\frac{x_i(t^n + \Delta t) - 2x_i(t^n) + x_i(t^n - \Delta t)}{(\Delta t)^2} = \frac{\partial^2}{(\partial t)^2} x_i(t^n) + \mathcal{O}(\Delta t)^2$$

$$\Downarrow$$

$$x_i(t^n + \Delta t) = 2x_i(t^n) - x_i(t^n - \Delta t) + (\Delta t)^2 \frac{F_i(t^n)}{m_i}$$

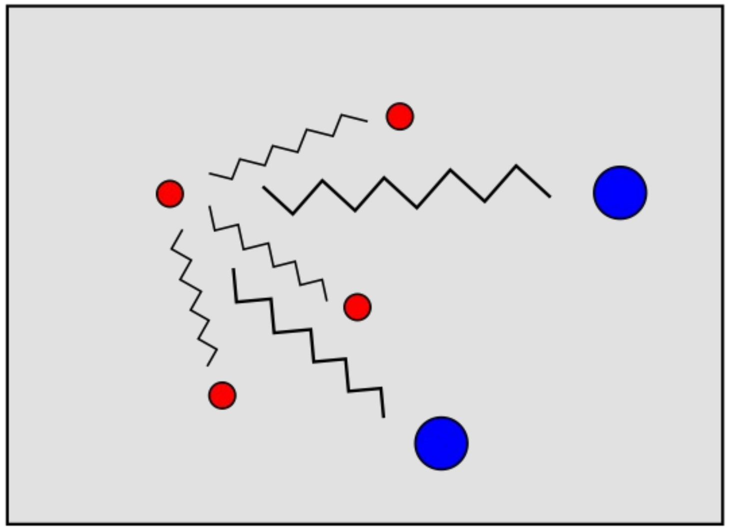
Velocity-Störmer-Verlet-Algorithm

- Used in this course
- Mathematically equivalent (without proof)
- Numerically less rounding errors

$$x_i(t^{n+1}) = x_i(t^n) + \Delta t \cdot v_i(t^n) + (\Delta t)^2 \frac{F_i(t^n)}{2m_i}$$

$$v_i(t^{n+1}) = v_i(t^n) + \Delta t \frac{F_i(t^n)+F_i(t^{n+1})}{2m_i}$$

Simple force calculation



- Used in the first task
- Derived from the gravitational potential:

$$U(x_i, x_j) = -g \frac{m_i m_j}{\|x_i - x_j\|_2}, \quad g := 1$$

force = -opposing force

$$F_i = \sum_{\substack{j=1 \\ j \neq i}}^{\#\text{particles}} F_{ij}, \quad F_{ij} = \frac{m_i m_j}{(\|x_i - x_j\|_2)^3}(x_j - x_i)$$

Hands On: Git and ParaView

- Teaching code: https://github.com/TUM-I5/MolSim
- Git: http://git-scm.com
- ParaView: http://paraview.org, http://www.paraview.org/Wiki/ParaView/Git
- Doxygen: http://www.stack.nl/~dimitri/doxygen/