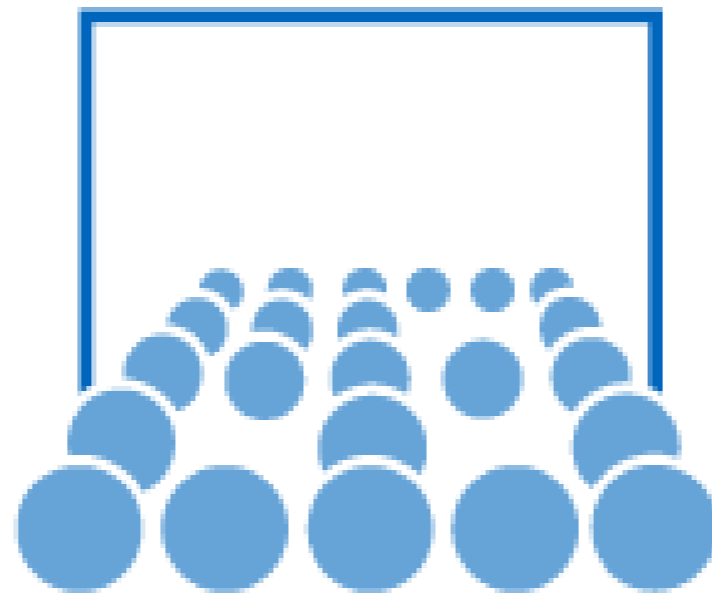


PSE Molekulardynamik

Basics

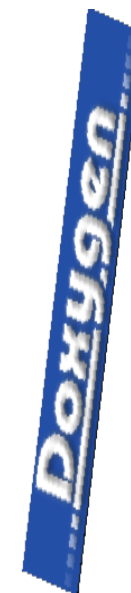
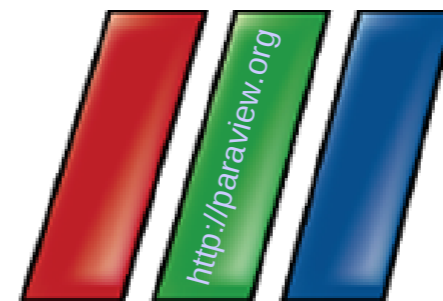
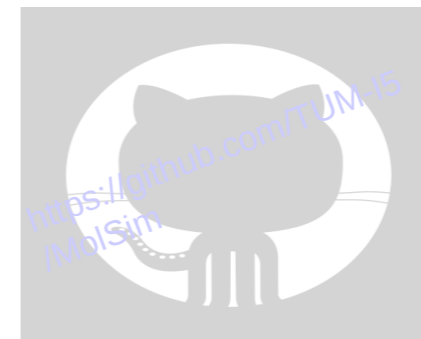
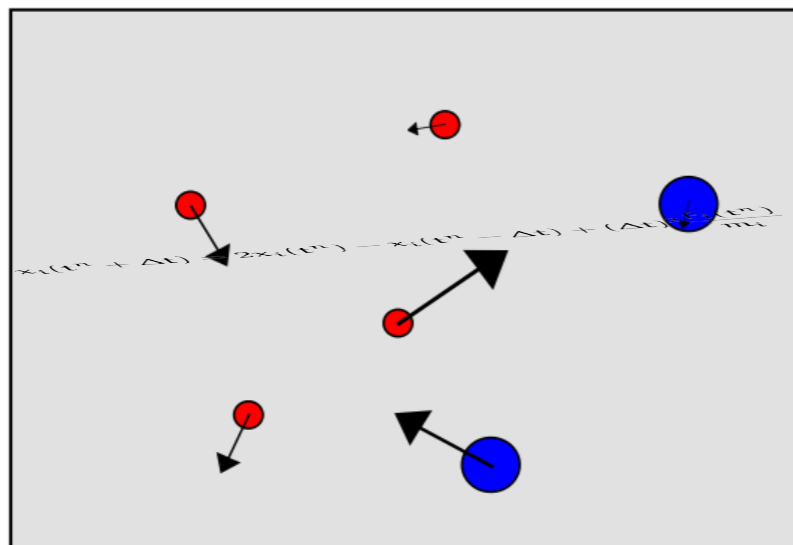
Wolfgang Eckhardt

18.10.2013



Outline

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



Schedule (big meetings)

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

| Date | Worksheet |
|----------------------|-----------|
| 18.10.2013 (today) | |
| 31.10.2013 | 1 |
| 15.11.2013 (Philipp) | 2 |
| 06.12.2013 | 3 |
| 20.12.2013 | 4 |
| 31.01.2014 | 5 |

Grading

- First four worksheets: 10 points
- Last worksheet: 30 points
- Grade: Points & presentations

References

- **Molecular Dynamics**

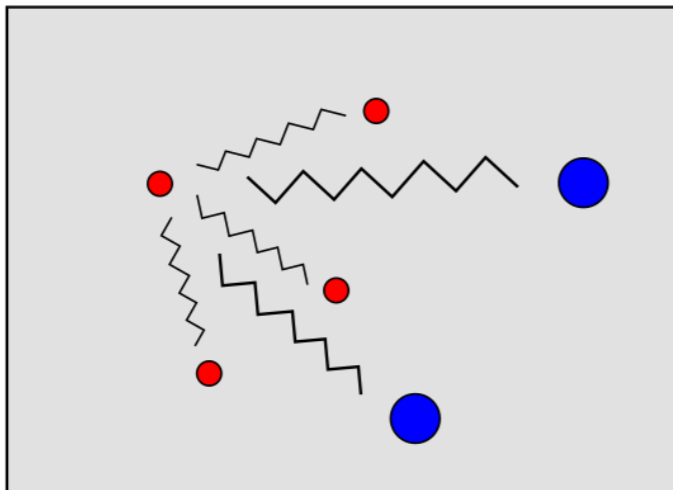
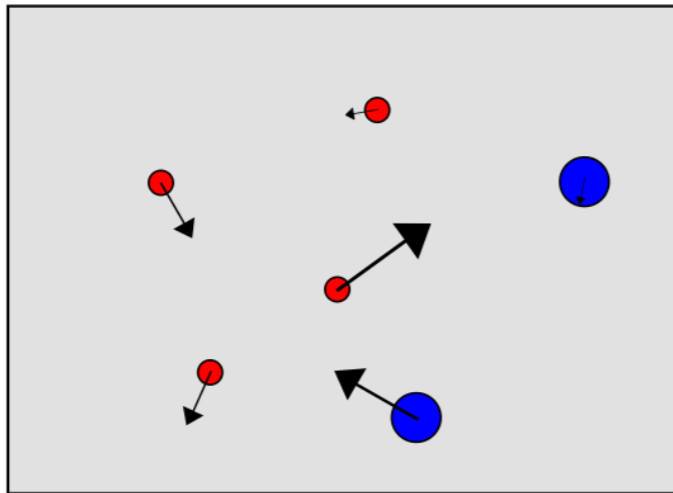
- Griebel, Knapek, Zumbusch: Numerische Simulation in der Molekulardynamik; Springer 2003
- Griebel, Knapek, Zumbusch: Numerical Simulation in Molecular Dynamics. Springer, 2007

- **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.

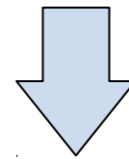
http://en.wikipedia.org/wiki/Newton's_laws_of_motion

Time discretization

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

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

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



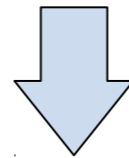
$$\frac{x(t^n + \Delta t) - 2x(t^n) + x(t^n - \Delta t))}{(\Delta t)^2} = \frac{\partial^2}{(\partial t)^2} x(t^n) + \mathcal{O}(\Delta t)^2$$

Time discretization

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

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

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



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

Velocity-Störmer-Verlet-Algorithm

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

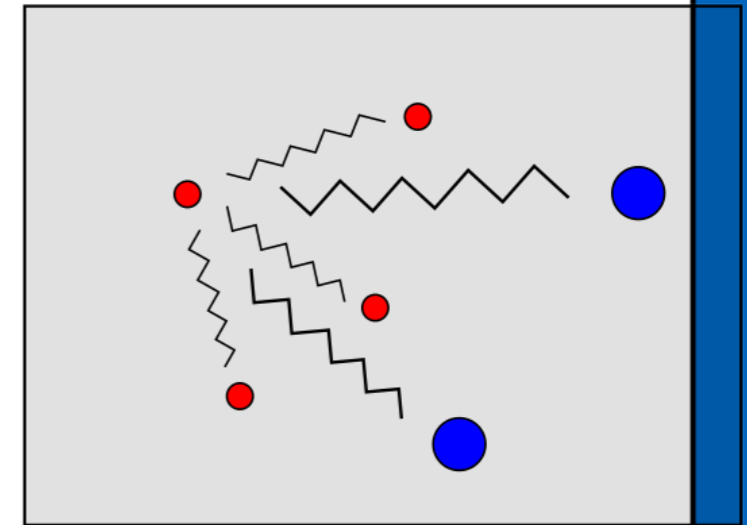
$$x_i(t^{n+1}) = x_i(t^n) + \Delta t \cdot v_i(t^n) + (\Delta t)^2 \frac{F_i(t^n)}{2m_i}$$

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

Simple force calculation

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

$$U(\mathbf{x}_i, \mathbf{x}_j) = -g \frac{m_i m_j}{\|\mathbf{x}_i - \mathbf{x}_j\|_2}, \quad g := 1$$



force = -opposing force

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

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/>

