PSE Molekulardynamik

Basics

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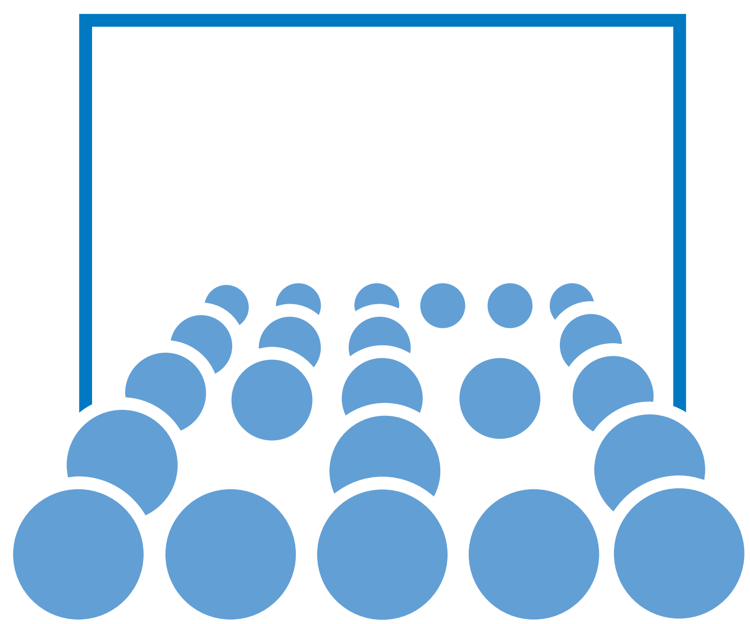
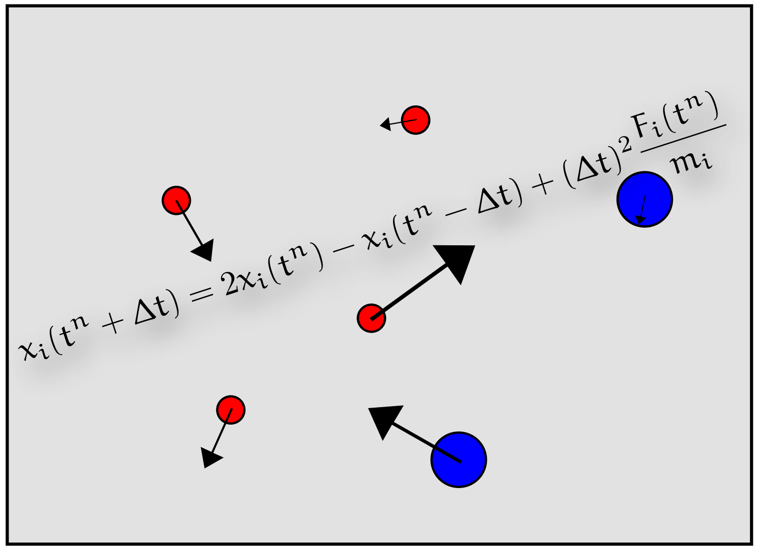
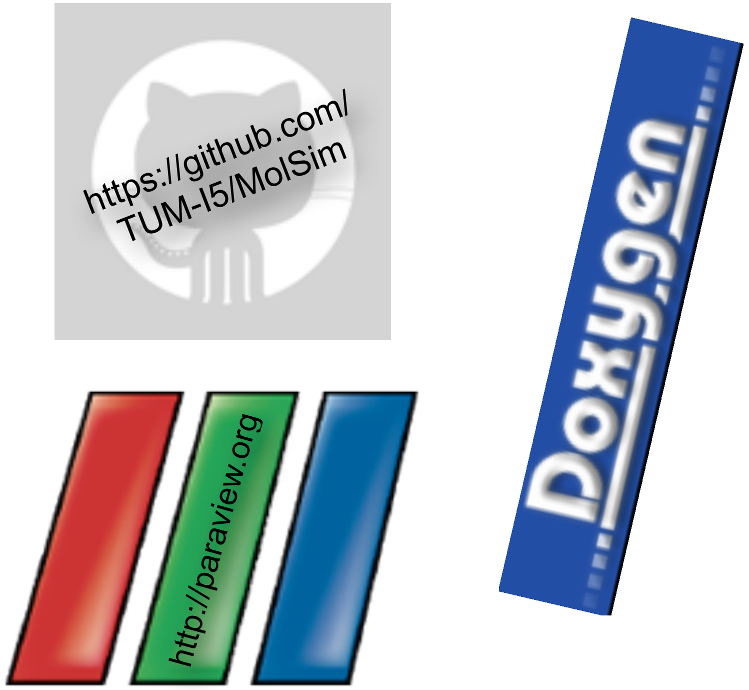
19.10.2012



Outline

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





Schedule (big meetings)

- Attendance is obligatory
- Each group has to prepare a presentation

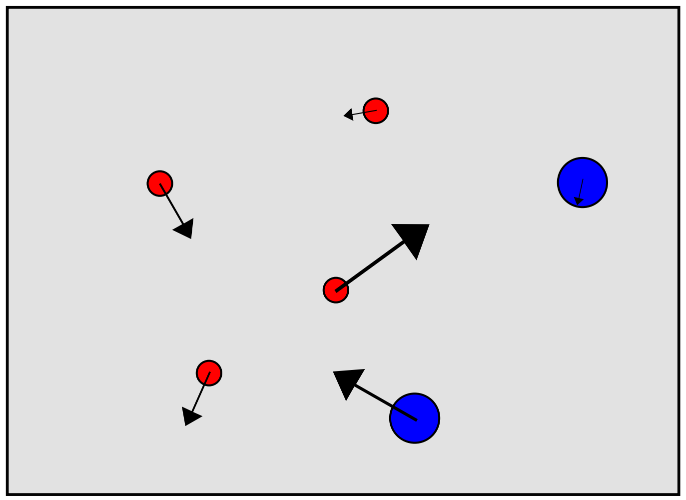
Date	Worksheet
19.10.2012 (today)	
02.11.2012	1
16.11.2012	2
07.12.2012	3
21.12.2012	4
01.02.2012	5

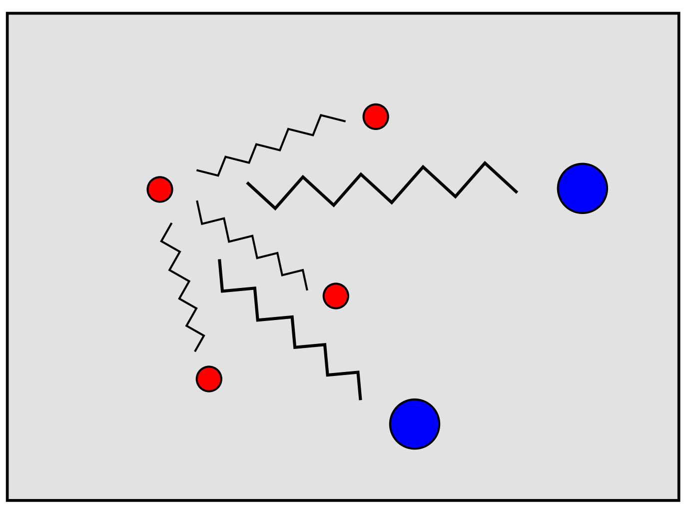
Grading

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

- Grade: Points & presentations

Newton’s laws of motion





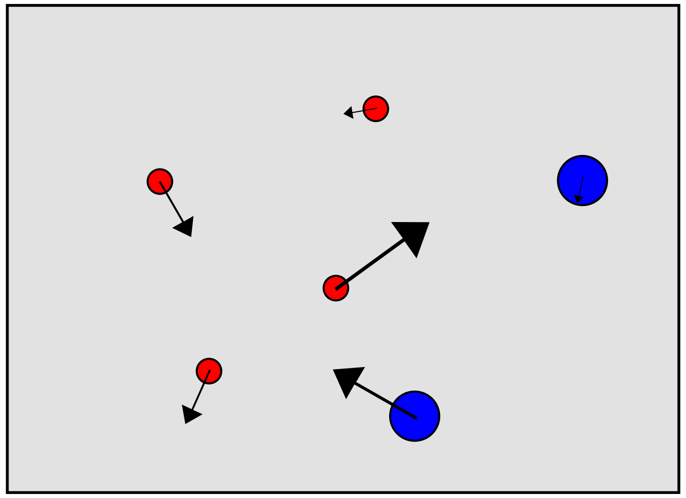
- **First law**: If an object experiences no net force, then its velocity is constant: the object is either at rest (if its velocity is zero), or it moves in a straight line with constant speed (if its velocity is nonzero).

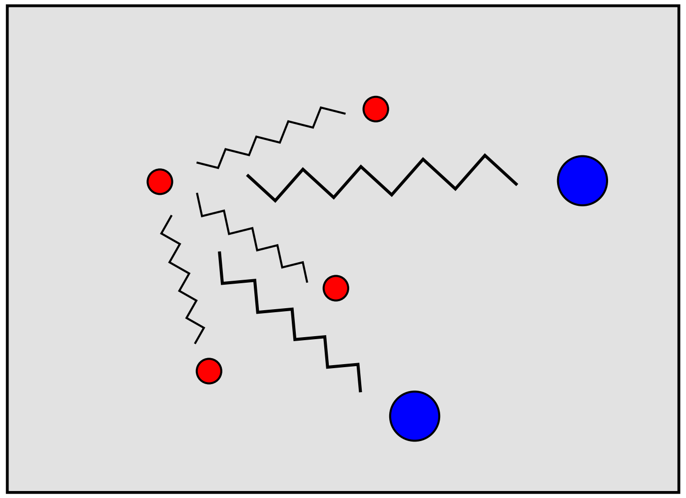
- **Second law**: The acceleration **a** of a body is parallel and directly proportional to the net force **F** acting on the body, is in the direction of the net force, and is inversely proportional to the mass *m* of the body, i.e., $\mathbf{F} = m\mathbf{a}$.

- **Third law**: When a first body exerts a force $\mathbf{F}_1$ on a second body, the second body simultaneously exerts a force $\mathbf{F}_2 = -\mathbf{F}_1$ on the first body. This means that $\mathbf{F}_1$ and $\mathbf{F}_2$ are equal in magnitude and opposite in direction.

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

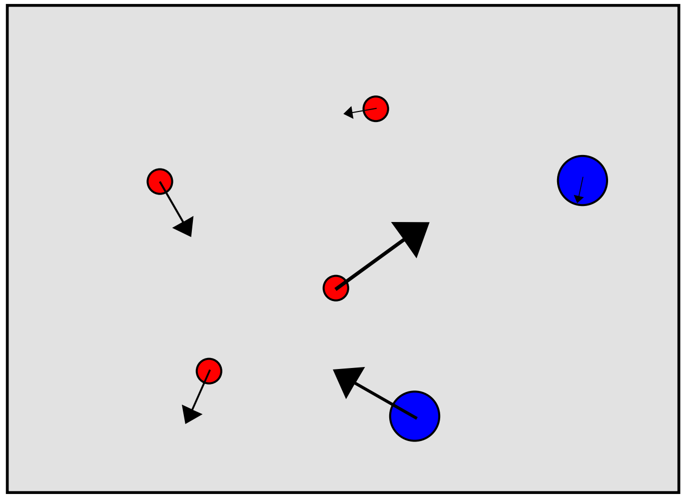
Ordinary Differential Equation

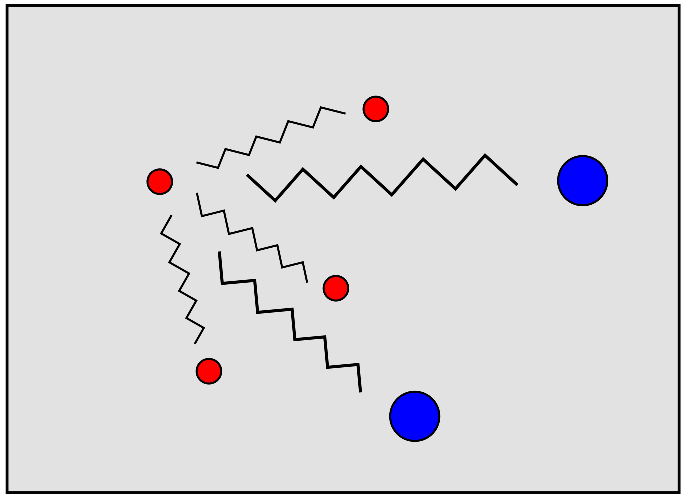




$$\dot{x}_i = v_i$$
$$m_i \dot{v}_i = F_i$$

Ordinary Differential Equation





$$\dot{x}_i = v_i$$
$$m_i \dot{v}_i = F_i$$

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

Time discretization

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

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

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

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$$\Downarrow$$

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

Time discretization

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

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

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

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

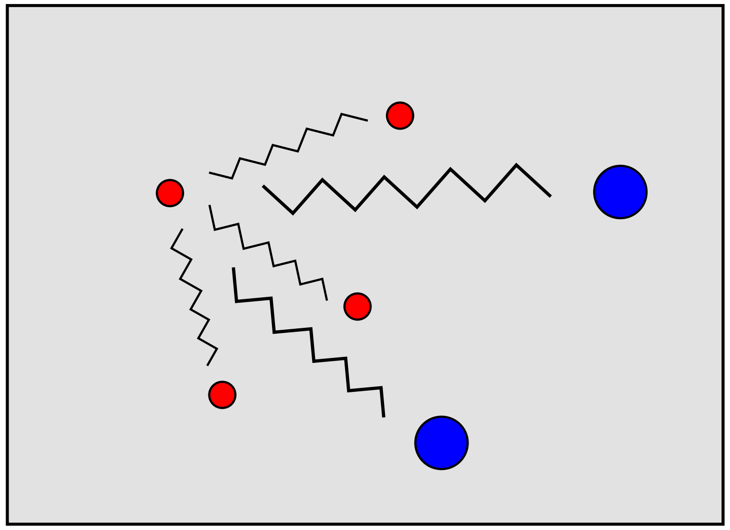
$$x_i(t^{n+1}) = x_i(t^n) + \Delta t \cdot v_i(t^n) + (\Delta t)^2 \frac{F_i(t^n)}{2m_i}$$

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

Simple force calculation

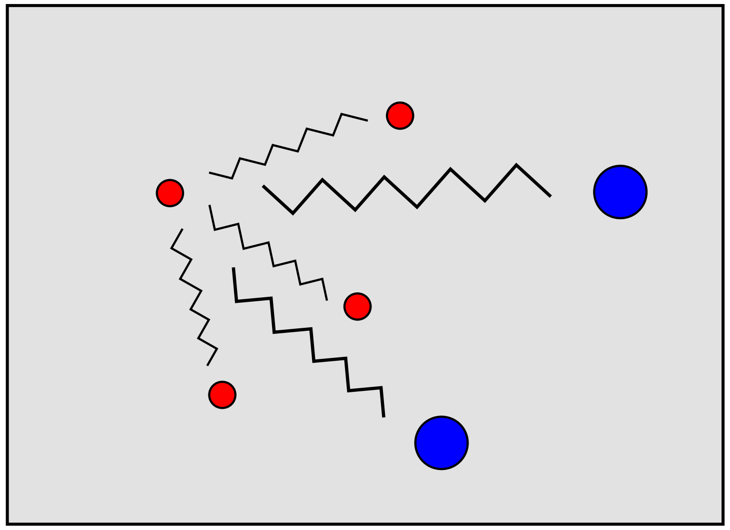
- Used in the first task
- Derived from the gravitational potential:

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



force = -opposing force

Simple force calculation



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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/