TECHNISCHE
UNIVERSITÄT
WIEN

165.144 Simulation of condensed matter

2025 Ass.Prof. Esther Heid esther.heid@tuwien.ac.at

Topics covered

Properties

- Semester hours: 2.0
- Credits: 3.0
- Type: VU Lecture and Exercise
- Format: Presence

Learning outcomes

After successful completion of the course, students are able to...

- Understand the methodology, approximations, advantages and disadvantages of molecular dynamics
- Use and operate molecular dynamics simulations for soft matter
- Design simple classical and machine-learning based force fields
- Analyze trajectories obtained from molecular dynamics simulations to extract physical/chemical properties

Subject of course

Molecular dynamics methods (force fields, thermostats, and involved approximations). Molecular dynamics simulations of liquids and analysis of their properties (d
force fields obtained from machine learning.

Teaching methods

- Lectures about molecular dynamics
- Practical exercises on a PC

About the course

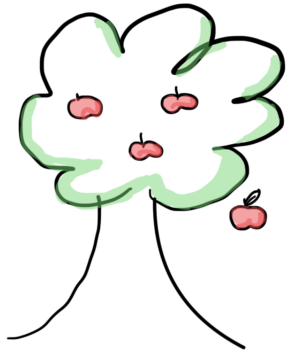
Mode: In-person (but no attendance enforced), recordings

Grading:

- Oral exam at the end of the semester
- Exercise assignments (JupyterHub)
- Voluntary TUWEL quizzes for bonus points

Prerequisites: Theoretical Chemistry (recommended, but not mandatory)

Language: English



Chapter 1: Classical mechanics in the Newtonian formulation

Goal: Study the movements of atoms in a condensed system, here liquids, and relate them to a mascroscopic property.

Theory (Statistical Mechanics)

Averages via phase-space integrals

$$\langle G \rangle = \frac{\int G(r_1 \cdots p_N) e^{-\beta E_{\mathrm{pot}}(r_1 \cdots p_N)} \mathrm{d}r_1 \cdots \mathrm{d}p_N}{\int e^{-\beta E_{\mathrm{pot}}(r_1 \cdots p_N)} \mathrm{d}r_1 \cdots \mathrm{d}p_N}$$

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Simulation (Monte Carlo)

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$$\langle G \rangle = \frac{1}{S} \sum_{s=1}^{S} G(s)$$

where states are chosen with probability $e^{-\beta E_{\mathrm{pot}}(s)}$

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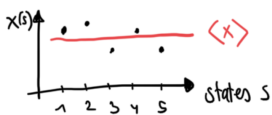

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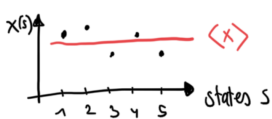

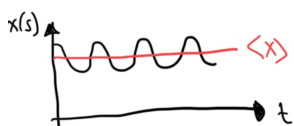

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1. How atoms interact, i.e. given coordinates $\vec{r}$, obtain forces $\vec{f}(\vec{r})$
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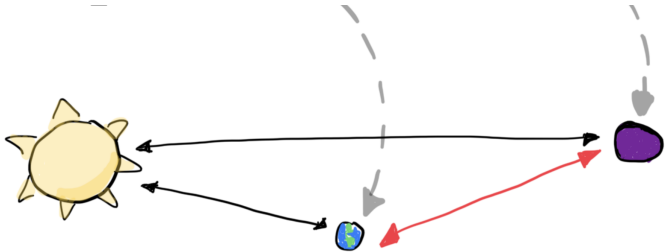

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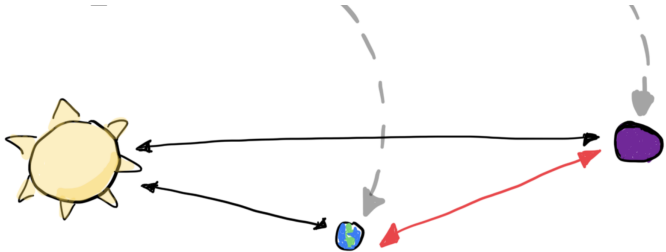
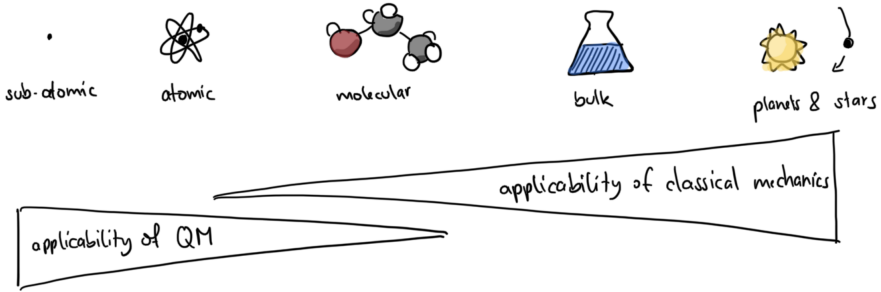


For studying a liquid, we need to follow the motions of thousands of atoms, so it is only possible to solve this problem numerically. For this, we only need Newton's classical mechanics

Classical mechanics: Physical theory describing the motion of macroscopic objects (disregarding quantum mechanics + relativity)



Newtonian mechanics: Earliest and simplest formulation from the 17th century which is directly applicable to the computer simulation of matter

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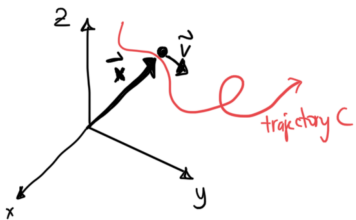
Point particle: Particle is represented using position + mass only, disregarding its structure. Can be a ball, apple, chicken, planet, ...



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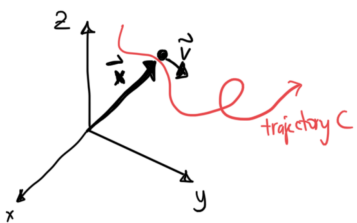

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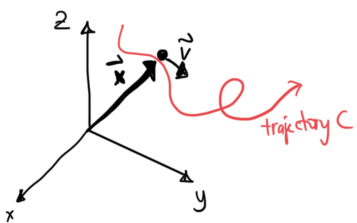

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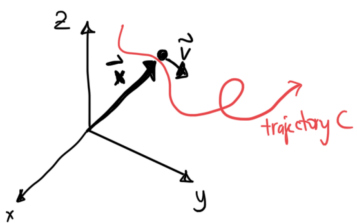

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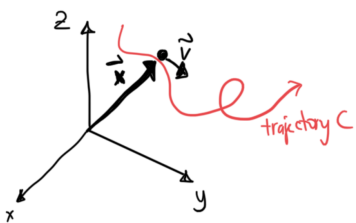

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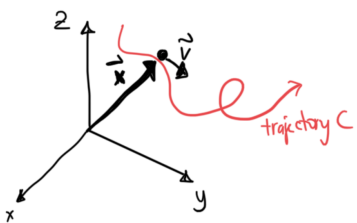

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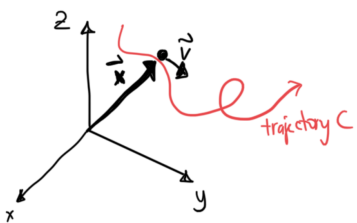

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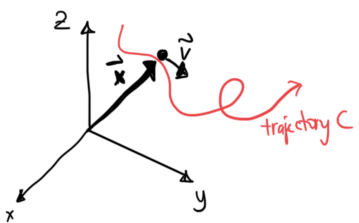

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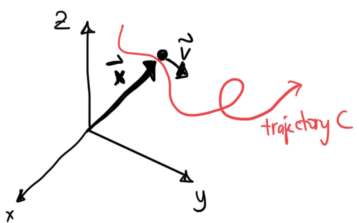

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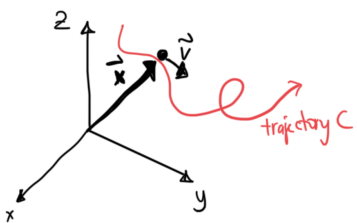

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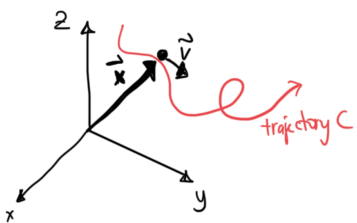

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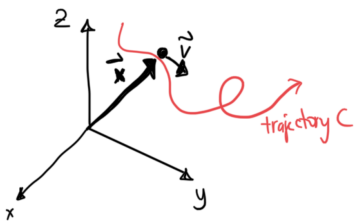

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$$= \frac{m|\mathbf{v}|^2}{2}\Big|_{t_A}^{t_B}$$

1.1 Single point particle

Point particle: Particle is represented using position + mass only, disregarding its structure. Can be a ball, apple, chicken, planet, ...

Position $\mathbf{x}(t)$ ... vector of cartesian coordinates
Velocity $\mathbf{v}(t) = \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}$
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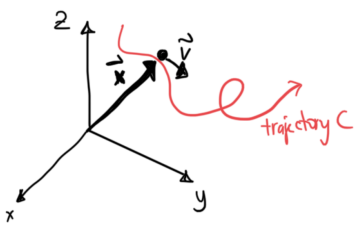
Force $\mathbf{f}(t) = m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = m\mathbf{a}$ = Newton's second law



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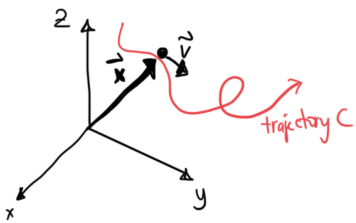

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$$= \frac{m|\mathbf{v}|^2}{2}\Big|_{t_A}^{t_B} = \frac{m}{2}[|\mathbf{v}(t_B)|^2 - |\mathbf{v}(t_A)|^2] = E_k(t_B) - E_k(t_A) \text{ with kinetic energy } E_k = \frac{1}{2}m|\mathbf{v}|^2$$

$\rightarrow$ work does not depend on the path
$\rightarrow$ for a closed curve, i.e. $B = A$: $W_{A\rightarrow B}[C] = \int_C \mathbf{f}\mathrm{d}\mathbf{x} = 0$ ... conservative force field
$\rightarrow$ this is only true for a conservative force field, where $\mathbf{f}$ must be defined over a simply connected region without holes

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Since $W_{A\rightarrow B} = \Delta_{A\rightarrow B} E_k$ and $W_{A\rightarrow B} = -\Delta_{A\rightarrow B} E_{\mathrm{pot}}$, we can derive the conservation of energy
$0 = \Delta_{A\rightarrow B}(E_k + E_{\mathrm{pot}}) = \Delta_{A\rightarrow B} E$ with $E = E_k + E_{\mathrm{pot}}$ ... mechanical energy

Change of energy if we move a particle upwards:
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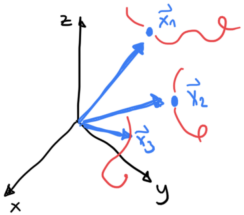
In summary:

- Work is related to the kinetic energy: $W_{A \to B}[C] = E_k(t_B) - E_k(t_A)$
- Work is related to the potential energy if the forces are conservative: $W_{\mathbf{x} \to P} = -W_{P \to \mathbf{x}} = E_{\text{pot}}(\mathbf{x})$
- Mechanical energy is conserved: $0 = \Delta_{A \to B}(E_k + E_{\text{pot}}) = \Delta_{A \to B} E$
- Force is the negative gradient of the potential energy: $\mathbf{f} = -\nabla E_{\text{pot}}$

1.2 System of point particles



For each particle:

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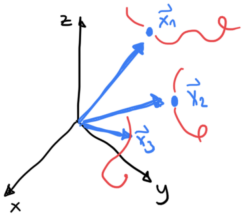

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For all particles:

Instead of several $\mathbf{x_i}$, make one big vector

$\mathbf{x}(t) = (x_1, y_1, z_1, \cdots, x_N, y_N, z_N)$

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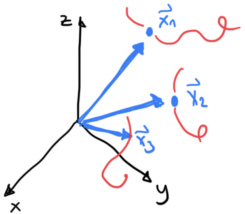

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with $E_k = \frac{1}{2}\sum m_i|\mathbf{v}_i|^2$ ... kinetic energy of all particles

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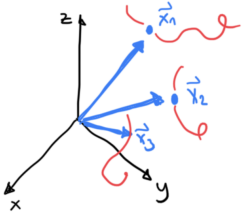

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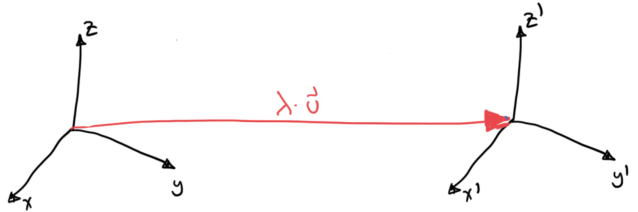
For conservative forcefields:

- $W_{A\to B} = -\Delta_{A\to B} E_{\mathrm{pot}}$
- $\mathbf{f} = -\nabla E_{\mathrm{pot}}$ and $\mathbf{f}_i = -\frac{\partial E_{\mathrm{pot}}}{\partial \mathbf{x}_i}$
- $E = E_k + E_{\mathrm{pot}}$

→ same as for single particle, only in 3N-dimensional space

1.3 Fundamental symmetries of mechanics

Translational symmetry



Mechanics observed from Σ and Σ' must be the same!

Initial conditions: $\vec{x}_0, \vec{v}_0$ trivially consistent, i.e offset in $\vec{x}_0$

Newton's equation of motion, i.e $\vec{F}$:

$\vec{f}$ must transform as a vector for translations

E_{pot} must transform as a scalar, i.e. must be the same for Σ and Σ' since $\vec{f} = -\nabla E_{pot}$

$E_{\mathrm{pot}} = E_{\mathrm{pot}}(x_1, y_1, z_1, \cdots, x_N, y_N, z_N) = E_{\mathrm{pot}}(\{x_i^\alpha\})$

where $i = 1, 2, \cdots, N$ (atomic index) and $\alpha = x, y, z$ (cartesian axis)

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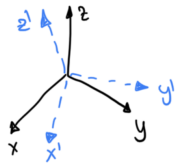
Since $f_i^\alpha = m \frac{\mathrm{d}v_i^\alpha}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} m_i v_i^\alpha = \frac{\mathrm{d}p_i^\alpha}{\mathrm{d}t} \quad \rightarrow \frac{\mathrm{d}}{\mathrm{d}t} \sum_i p_i^\alpha = 0$ and $\frac{\mathrm{d}\mathbf{P}}{\mathrm{d}t} = 0$
$\rightarrow$ conservation of linear momentum

Rotational symmetry



System Σ rotated system Σ'

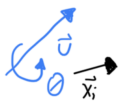
Mechanics observed from Σ and Σ' must be the same

→ $\vec{f}$ must transform as vector with respect to rotation

→ E_{pot} must transform as scalar (= not change)

$$E_{pot}(\vec{x}_1, \vec{x}_2, \dots \vec{x}_N) = E_{pot}\left(t(\vec{x}_1), t(\vec{x}_2) \dots t(\vec{x}_N)\right)$$

Rotation around axis $\vec{v}$, angle θ



using Rodrigues' rotation formula:

$$t(\vec{x}_i) = \underbrace{\vec{x}_i \cos\theta}_{\text{scales vector}} + \underbrace{(\vec{v} \times \vec{x}_i)\sin\theta}_{\text{skews vector toward new position}} + \underbrace{\vec{v} \cdot (\vec{v} \cdot \vec{x}_i)\,(1 - \cos\theta)}_{\text{re-adds the height that was lost in term 1}}$$

$$\frac{\mathrm{d}E_{\mathrm{pot}}}{\mathrm{d}\theta} = \sum_i \frac{\partial E_{\mathrm{pot}}}{\partial \mathbf{x_i}} \frac{\partial \mathbf{x_i}}{\partial \theta} = \sum_i \frac{\partial E_{\mathrm{pot}}}{\partial \mathbf{x}_i} (\mathbf{u} \times \mathbf{x_i}) = -\sum_i \mathbf{f}_i (\mathbf{u} \times \mathbf{x_i}) = -\sum_i \mathbf{u}(\mathbf{x}_i \times \mathbf{f}_i) = -\mathbf{u}[\sum_i m_i (\mathbf{x}_i \times \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t})]$$

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Summary:

- Translational symmetry = Conservation of linear momentum
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Spoiler: In MD, we will sometimes break these symmetries and thus induce energy drifts!