PSE Molekulardynamik

Thermostats, Lorentz-Berthelot mixing rule, MAC Cluster

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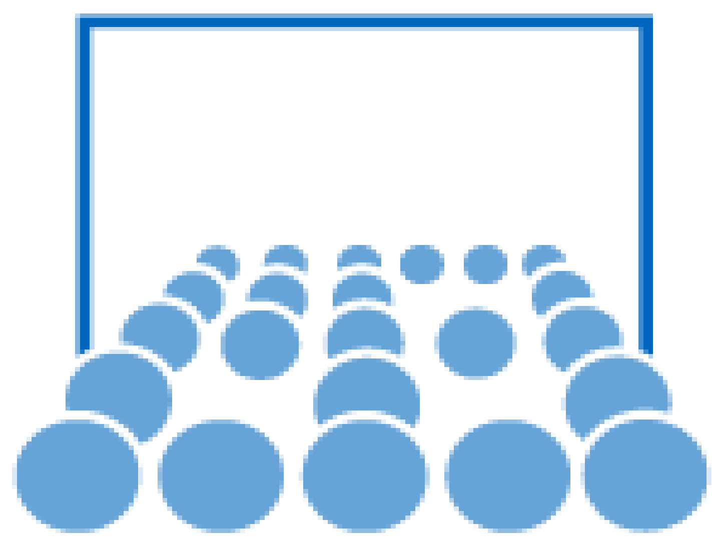


Outline

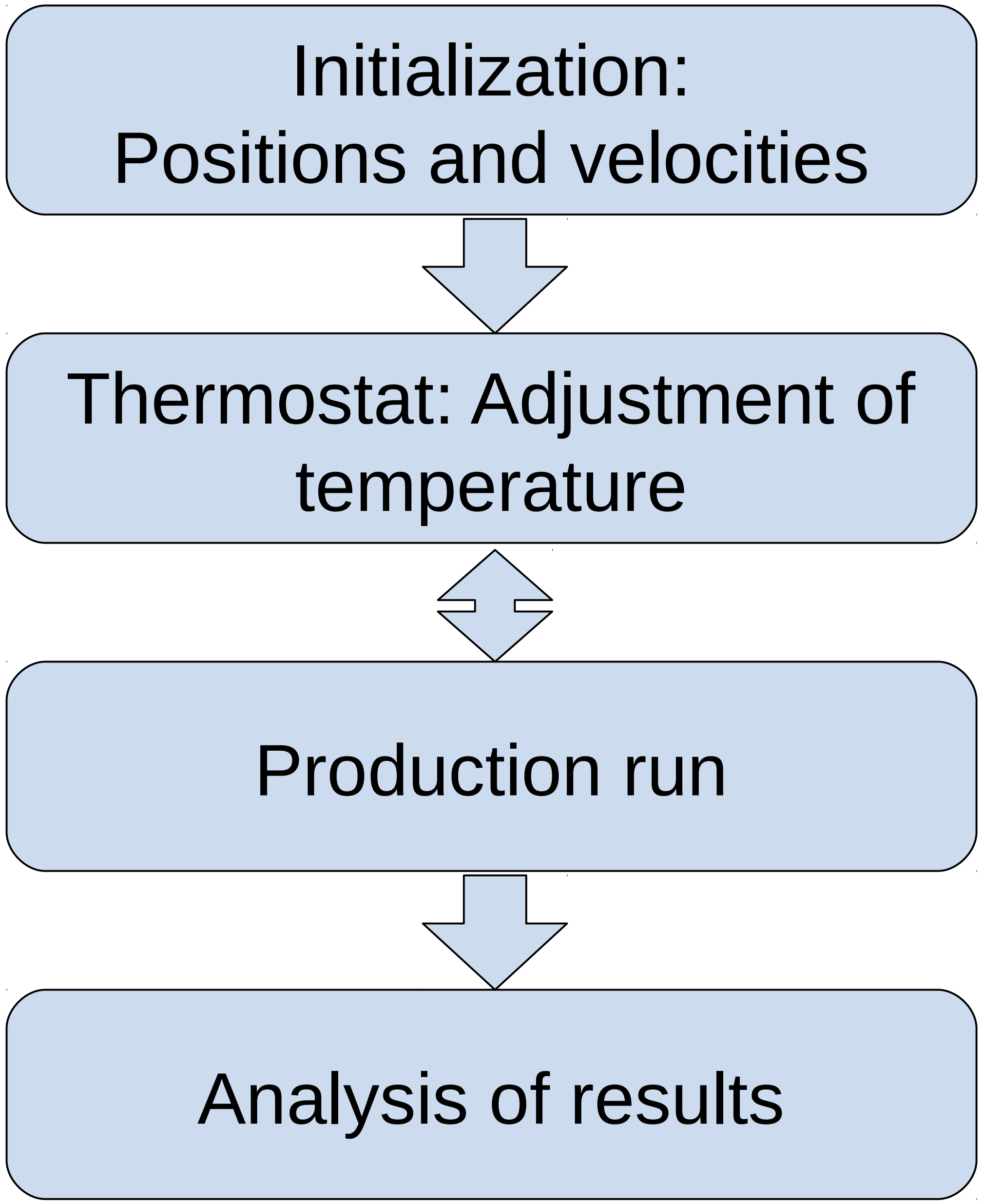
- Schedule
- Presentations: Worksheet 3
- Thermostats
- Lorentz-Berthelot mixing rule
- MAC Cluster
- Preparation: Worksheet 4

Schedule

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

Presentations: Worksheet 3

Thermostats: Simulation overview



Thermostats

- Kinetic energy

$$E_{kin} = \sum_{i=1}^{\#particles} \frac{m_i \langle v_i, v_i \rangle}{2}$$

- Equipartition theorem (thermodynamics): Correlation temperature ↔ kinetic energy

$$E_{kin} = \frac{\#particles \cdot \#dimensions}{2} k_B T$$

- Scale to achieve temperature

$$\beta = \sqrt{\frac{E_{kin}^{D}}{E_{kin}}}, \quad v_i^n := \beta v_i^n$$

Thermostats

- Heating/Cooling smooth process → Smooth energy transfer
- “Adjustment of temperature” over multiple time steps

- Example (worksheet 4):
  - Target temperature: 40
  - Application of thermostat every 1000 time steps

Lorentz-Berthelot mixing rule

- Different materials → Lennard-Jones potential?
- Generalized formulation

$$F_i = \sum_{\substack{j=1 \\ j \neq i}}^{\#\text{particles}} F_{ij}, \quad F_{ij} = \frac{24\epsilon_{ij}}{(\|x_i - x_j\|_2)^2} \left(\left(\frac{\sigma_{ij}}{\|x_i - x_j\|_2} \right)^6 - 2 \left(\frac{\sigma_{ij}}{\|x_i - x_j\|_2} \right)^{12} \right) (x_j - x_i)$$

- Mixing rule

$$\sigma_1 = \sigma_{11}$$
$$\epsilon_1 = \epsilon_{11}$$
$$\sigma_2 = \sigma_{22}$$
$$\epsilon_2 = \epsilon_{22}$$

⇒

$$\sigma_{12} = \sigma_{21} = \frac{\sigma_{11} + \sigma_{22}}{2}$$

$$\epsilon_{12} = \epsilon_{21} = \sqrt{\epsilon_{11}\epsilon_{22}}$$

Preparation: Worksheet 4