

# Multiscale Simulations of Materials and Structures

## Lecture 2. *Molecular Dynamics II*

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@ Centre des Matériaux  
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- 1 Concept of the temperature
- 2 Maxwell-Boltzmann distribution
- 3 Thermostats
- 4 Mechanical examples
- 5 Applications and limitations
- 6 Other (impressive) examples
- 7 Afterword

# Temperature

- Temperature is one of the central concepts in physics
- Relations between the kinetic energy  $E_{\text{kin}}$  of the system and its temperature  $T$ :

$$E_{\text{kin}} = \frac{1}{2} N_{\text{dof}} k_B T$$

$N_{\text{dof}}$  is the number of degrees of freedom (*need to exclude rigid body motions*),  
 $k_B$  is the Boltzmann constant

$$k_B \approx 1.38065 \cdot 10^{-23} \frac{\text{m}^2 \text{ kg}}{\text{s}^2 \text{ K}}$$

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- Kinetic energy of the system excluding rigid body motions

$$E_{\text{kin}} = \frac{1}{2} \sum_i m_i |\mathbf{v}_i - \mathbf{v}_i^{rb}|^2,$$

where  $\mathbf{v}_i^{rb} = \bar{\mathbf{v}} + \boldsymbol{\omega} \times (\mathbf{r}_i - \mathbf{r}_0)$ ,  $\bar{\mathbf{v}}$  is the velocity of the center of mass  $\mathbf{r}_0$ ,  $\boldsymbol{\omega}$  is the angular velocity, and  $\mathbf{r}_i$  is the point position vector.

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- Attention!

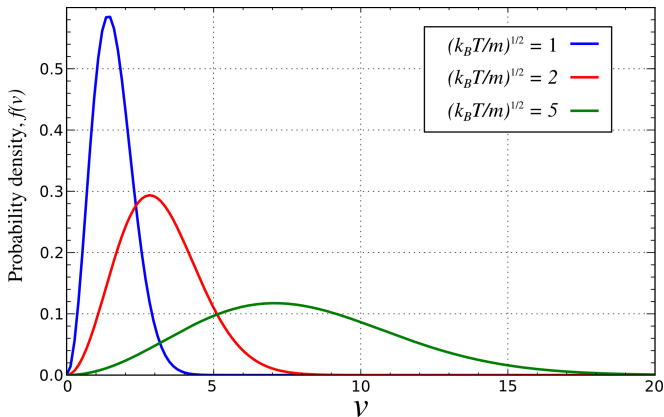
- (1) particles are considered as points (no contribution from angular velocities),
- (2) no contribution from electrons, important carriers of the heat.

# Let's control the temperature: prescribe

## Prescribe a temperature

- In the ideal gas, velocity of particles follows Maxwell-Boltzmann distribution:

$$f(v) = 4\pi \left( \frac{m}{2\pi k_B T} \right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2k_B T}\right), \quad v = |v|$$



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- The mean squared velocity thus satisfies

$$\langle v^2 \rangle = \int_0^\infty v^2 f(v) dv = \frac{3k_B T}{m}$$

- For every degree of freedom:

$$\frac{1}{2} m \langle v_x^2 + v_y^2 + v_z^2 \rangle = \frac{3k_B T}{2} \quad \Leftrightarrow \quad \langle v_d^2 \rangle = \frac{k_B T}{m}$$

- Box-Muller method<sup>[1]</sup>

[1] Box, Muller: A Note on the Generation of Random Normal Deviates, Annals Math. Stat.:29 (1958).

# Let's control the temperature: preserve

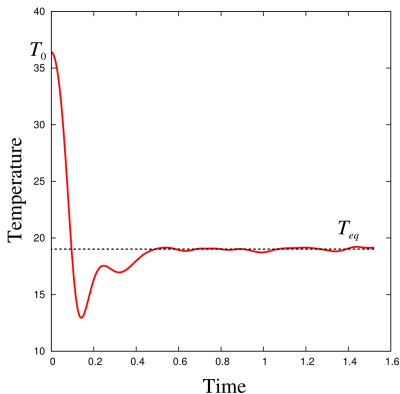
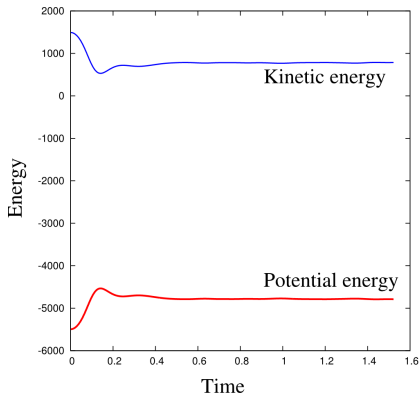
## Preserve the temperature

- Initially inserted energy  $T_0 \dots$

# Let's control the temperature: preserve

## Preserve the temperature

- Initially inserted energy  $T_0$  distributes between the kinetic and potential energy
- Total energy is conserved  $E_{\text{kin}} + E_{\text{pot}}$



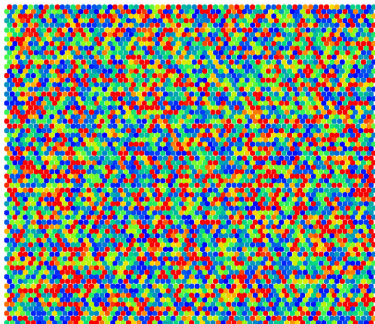


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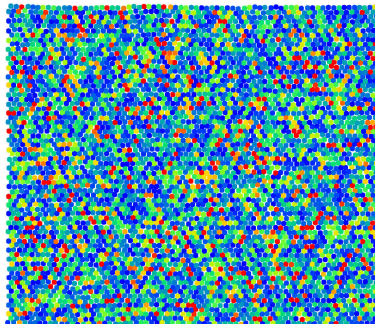
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Initial state,  $T=36$  K



Equilibrium state,  $T=19$  K



Particle velocity

Color represents the velocity of particles

# Let's control the temperature: preserve

## Preserve the temperature

- Initially inserted energy  $T_0$  distributes between the kinetic and potential energy
- Total energy is conserved  $E_{\text{kin}} + E_{\text{pot}}$
- Equipartition theorem: *In thermal equilibrium energy is shared equally among all of its various forms*<sup>[1]</sup>
- Start from a 0K equilibrium perfect crystal  $E_{\text{pot}} = E_{\text{pot}}(0K)$ ,  $E_{\text{kin}} = 0$
- Prescribe initial temperature  $T_0 \rightarrow E_{\text{kin}}(T_0)$ , the total system energy becomes  $E = E_{\text{pot}}(0K) + E_{\text{kin}}(T_0)$  and because of the equal repartition:

$$E = E_{\text{pot}}(0K) + \frac{1}{2} E_{\text{kin}}(T_0) + \frac{1}{2} E_{\text{kin}}(T_0)$$

$$E = E_{\text{pot}}(0K) + \underbrace{E_{\text{kin}}\left(\frac{1}{2}T_0\right)}_{E_{\text{pot}}\left(\frac{1}{2}T_0\right)} + \underbrace{E_{\text{kin}}\left(\frac{1}{2}T_0\right)}_{E_{\text{kin}}\left(\frac{1}{2}T_0\right)} = E_{\text{pot}}(T_{eq}) + E_{\text{kin}}(T_{eq})$$

- In thermal equilibrium  $T_{eq} = \frac{1}{2}T_0$

# Let's control the temperature: preserve

## Preserve the temperature

- **Velocity scaling method** enables us to keep the target temperature  $T^t$ :

$$\beta = \sqrt{T^t/T} = \sqrt{E_{\text{kin}}^t/E_{\text{kin}}} = \sqrt{\langle v^2 \rangle^t / \langle v^2 \rangle}$$

*at every  $m$ -th increment scale velocities:*

$$v(t) = \beta v(t)$$

- A better choice would be to scale temperature more smoothly:

$$\beta = \sqrt{1 + \gamma(T^t/T - 1)}, \quad \gamma \in [0, 1]$$

*for example  $\gamma \sim dt$*

# Let's control the temperature: preserve

## Preserve the temperature

- **Friction/anti-friction term** can be added in dynamical equation:

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i - \xi m_i \dot{\mathbf{r}}_i, \quad \begin{cases} \xi > 0, & \text{if } T > T^t \\ \xi \leq 0, & \text{if } T \leq T^t \end{cases}$$

- Choice of  $\xi$ :

$$\frac{dE_{\text{kin}}}{dt} = - \left( \frac{dE_{\text{pot}}}{dt} + \xi \sum m_i |\mathbf{v}_i|^2 \right) = 0, \quad \Rightarrow \xi = - \frac{dE_{\text{pot}}/dt}{2E_{\text{kin}}}$$

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- **A good strategy:**

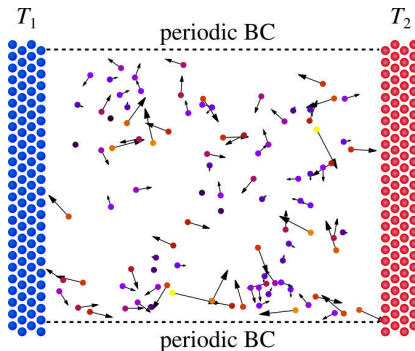
use a thermostat on a part of simulated domain, not too close to the zone of the interest

- See also: Nosé-Hoover thermostat<sup>[1]</sup> and Langevin dynamics.

[1] Hoover. Canonical dynamics: Equilibrium phase-space distributions, Phys. Rev. A 31 (1985)

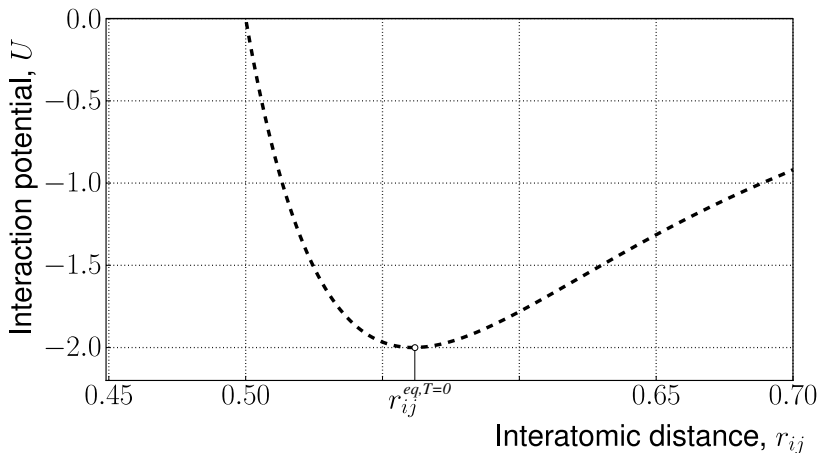
# Let's control the temperature: change

- Prescribe a temperature
- Preserve the temperature
- **Change the temperature during the simulation**
  - Linear scaling of the target temperature during the time  $T^t = T^t(t)$
  - Heating  $\xi > 1$ /cooling  $\xi < 1$  wall  $v_x(t + dt) = -\xi v_x(t)$
  - Rigid walls at prescribed temperature (thermostats)



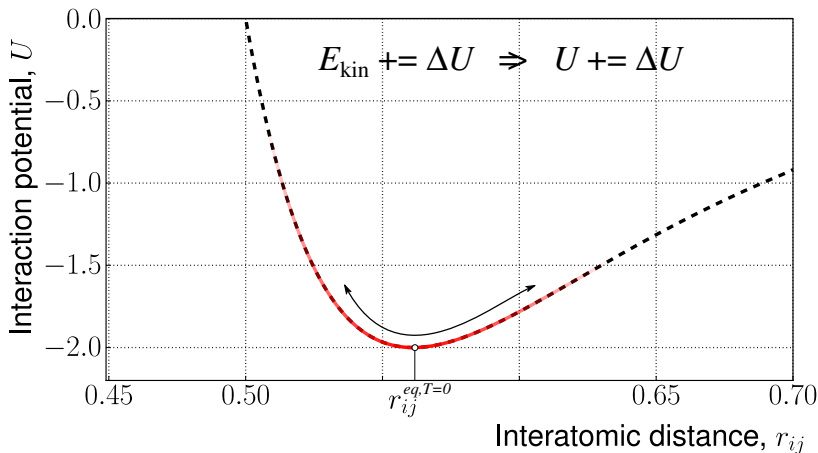
# Thermal expansion 1

Thermal expansion is related to the asymmetry of the potential well.



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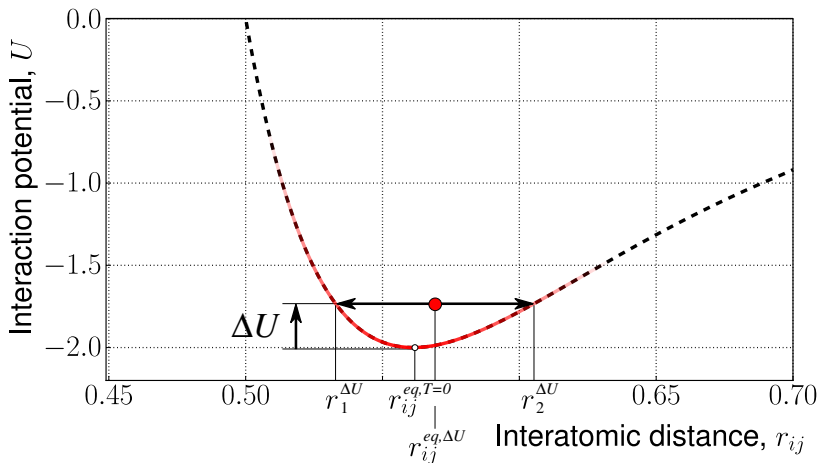
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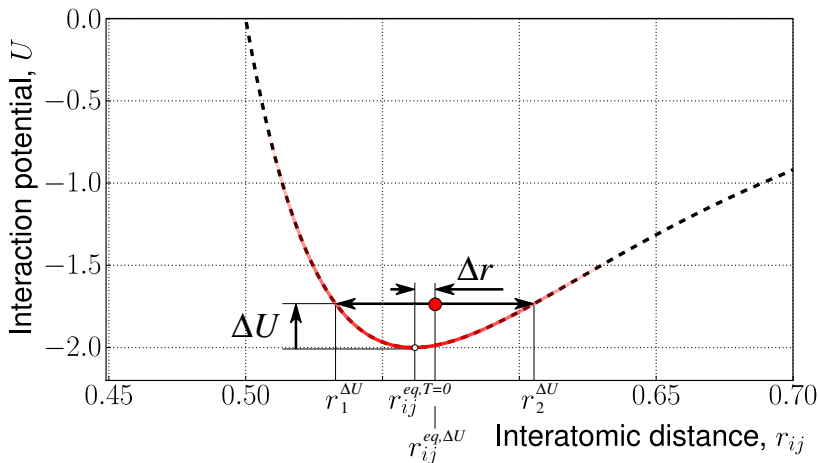
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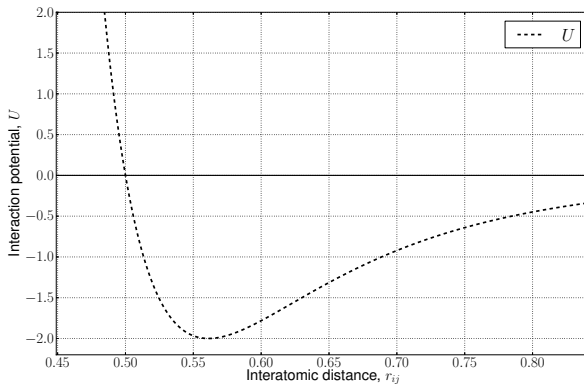


# Thermal expansion 2

- LJ-6-12: Taylor expansion up to the third order:

$$U(r_{ij}^{eq} + \Delta r_{ij})$$

with

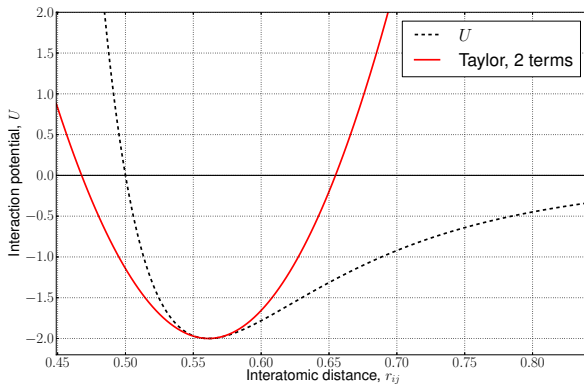


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$$U(r_{ij}^{eq} + \Delta r_{ij}) = U_0(r_{ij}^{eq}) + \frac{1}{2} \frac{\partial^2 U}{\partial r_{ij}^2} \Delta r_{ij}^2 + o(\Delta r_{ij}^2)$$

with  $\partial^2 U / \partial r_{ij}^2 = 288 \varepsilon \sigma^{12} / r_{ij}^{eq14}$ ,

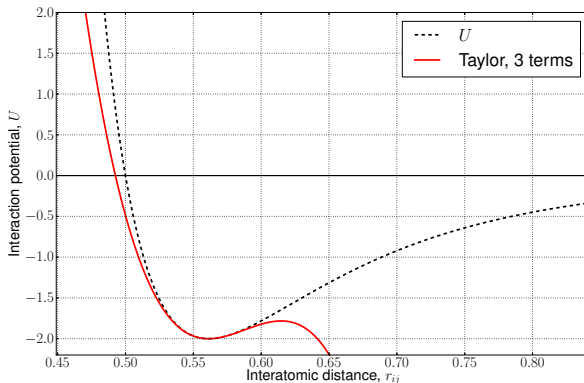


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with  $\partial^2 U / \partial r_{ij}^2 = 288 \varepsilon \sigma^{12} / r_{ij}^{eq14}$ ,  $\partial^3 U / \partial r_{ij}^3 = -6048 \varepsilon \sigma^{12} / r_{ij}^{eq15}$



# Thermal expansion 2

Approximation of the potential in vicinity of the equilibrium:

$$U(r_{ij}^{eq} + \Delta r_{ij}) = U_0 + a\Delta r_{ij}^2 - b\Delta r_{ij}^3, \quad a, b > 0$$

Locations corresponding to  $\Delta U$ :

$$\begin{cases} \Delta U = a\Delta r_1^2 - b\Delta r_1^3 \\ \Delta U = a\Delta r_2^2 - b\Delta r_2^3 \end{cases}$$

Where from

$$a(\Delta r_1^2 - \Delta r_2^2) - b(\Delta r_1^3 - \Delta r_2^3) = 0 \quad \text{or} \quad \boxed{4b\Delta r^2 - 2a\Delta r + b\eta = 0}$$

where  $\Delta r = (\Delta r_1 + \Delta r_2)/2 \geq 0$ ,  $\eta = -\Delta r_1\Delta r_2 \approx \Delta U/a \geq 0$

$$\Delta r = \frac{a - \sqrt{a^2 - 4b^2\eta}}{4b} = \frac{a}{4b} \left(1 - \sqrt{1 - 4b^2\eta/a^2}\right) \approx \frac{a}{4b} \left(1 - \sqrt{1 - 4b^2\Delta U/a^3}\right) \approx \frac{b}{2a} \frac{\Delta U}{a}$$

$$\Delta r \approx \frac{1008r_{ij}^{eq12}}{288\sigma^{12}} \frac{\Delta U}{144\epsilon} r_{ij}^{eq} \Rightarrow \epsilon_{th} = \frac{\Delta r}{r_{ij}^{eq}} \approx 0.097 \frac{\Delta U}{\epsilon} = 0.097 \frac{\Delta E_{kin}}{2\epsilon} = 0.0729 \frac{k_B \Delta T}{\epsilon}$$

# Normalizations

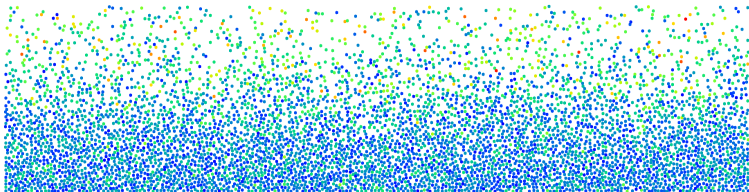
- Energy  $\varepsilon$ :  $E' = E/\varepsilon$
- Distance  $\sigma$ :  $l' = l/\sigma$
- Mass  $M = m_p$ :  $m' = m/M$
- Time  $t_0 = \sqrt{\sigma^2 * m/\varepsilon}$ :  $t' = t/t_0$
- Velocity  $V = \sqrt{\varepsilon/m}$ :  $v' = v/V$
- Force  $F = \varepsilon/\sigma$ :  $f' = f/F$
- Pressure  $P = \varepsilon/\sigma^3$ :  $p' = p/P$
- Temperature  $T_0 = \varepsilon/k_B$ :  $T' = T/T_0$

# Examples



# Example: liquid-gas interface

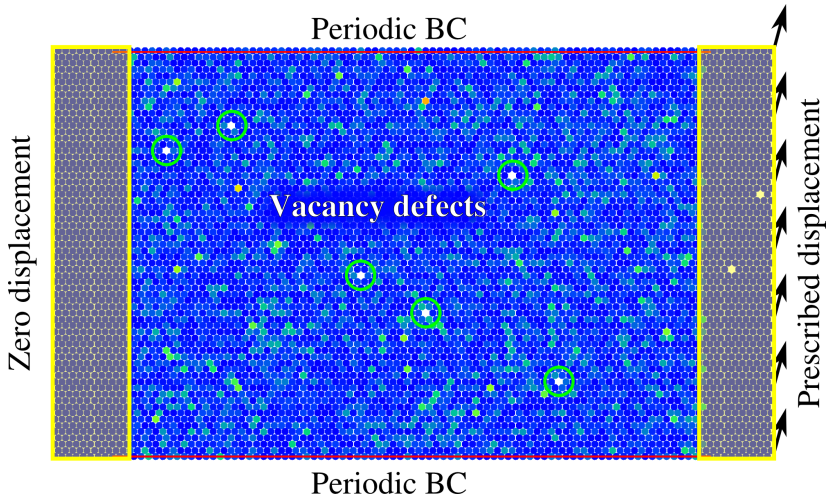
Stabilization phase of a liquid-gas interface under huge gravity.



6000 particles

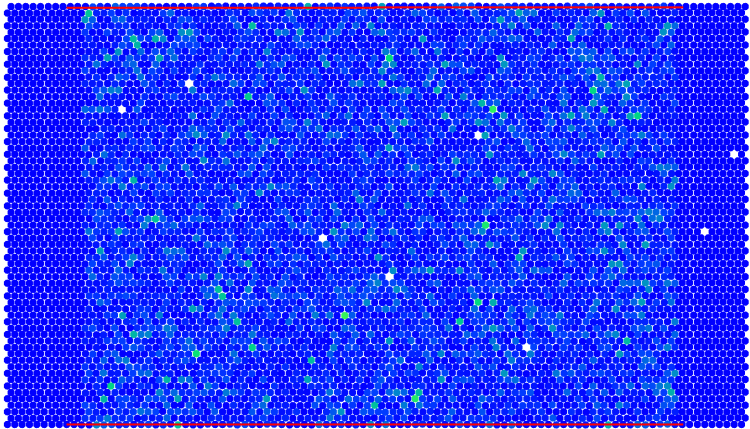
# Example: shear test

Shear test of a crystal with 6 vacancy defects (6 500 atoms)



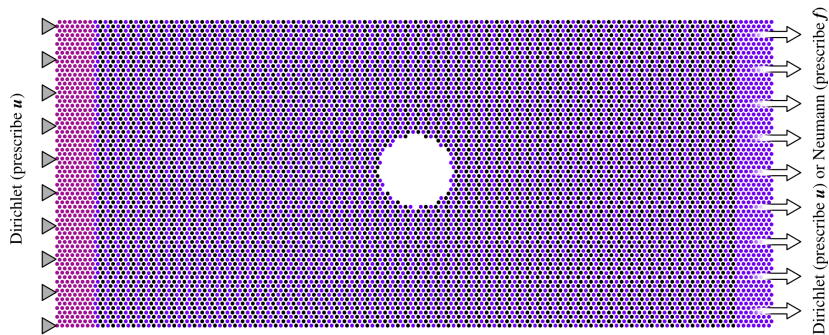
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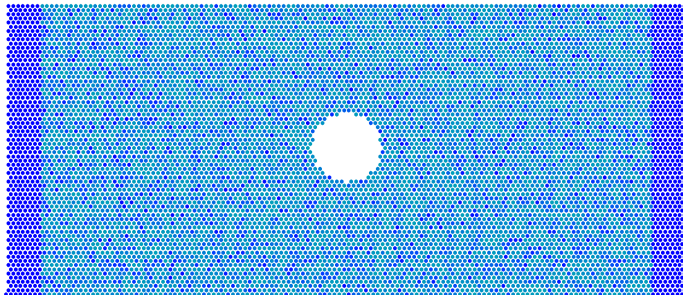
# Example: tensile test

High-velocity tensile test of a bar with a circular defect.



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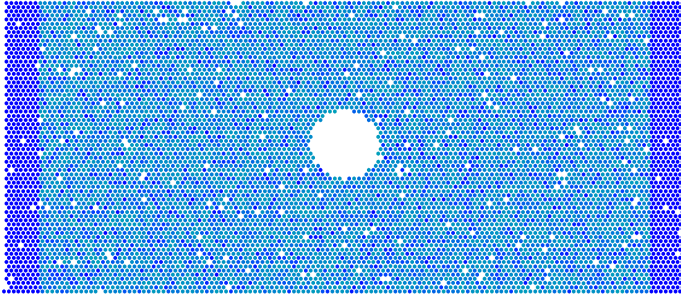
High-velocity tensile test of a bar with a circular defect.



Perfect crystal with a hole, 10 000 particles

# Example: tensile test

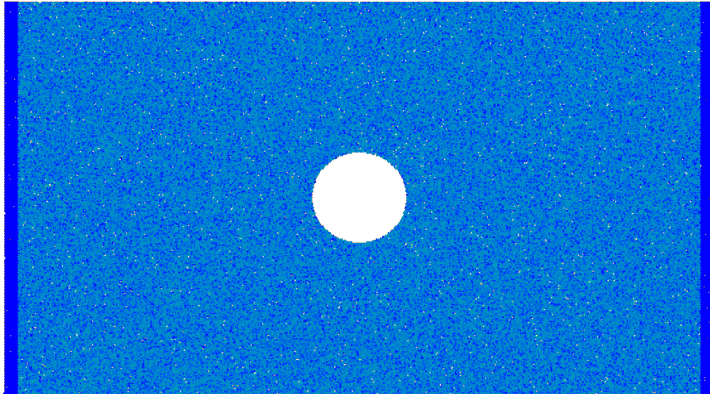
High-velocity tensile test of a bar with a circular defect.



Crystal with 0.5% of vacancy defects and a hole, 10 000 particles

# Example: tensile test

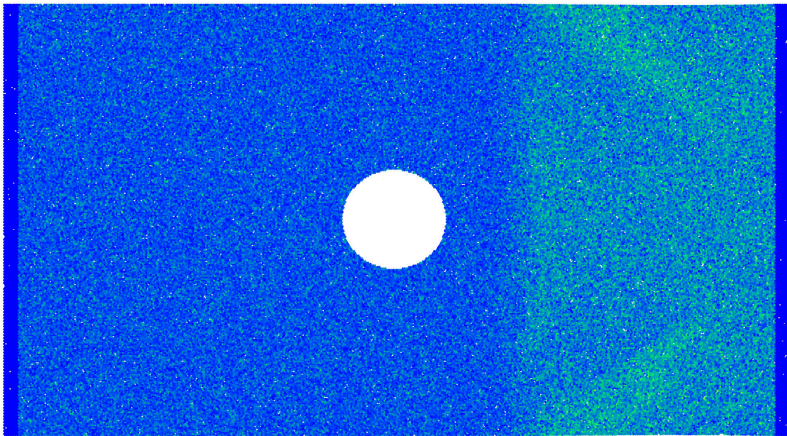
High-velocity tensile test of a bar with a circular defect.



A bigger crystal with 0.5% of vacancy defects and a hole, 130 000 particles

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High-velocity tensile test of a bar with a circular defect.

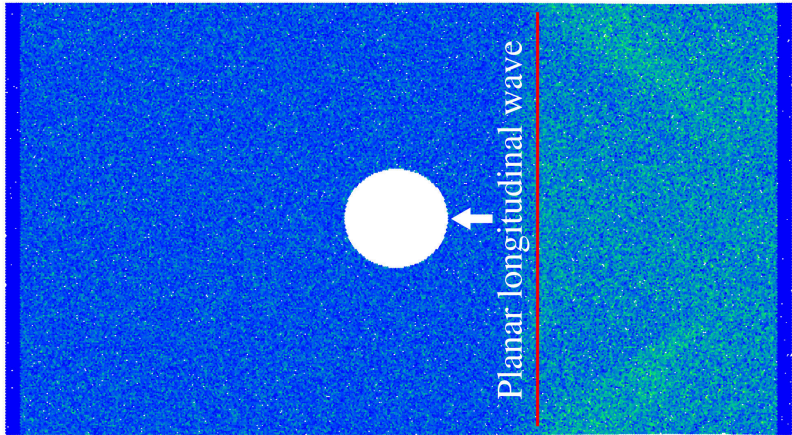


Wave dynamics



# Example: tensile test

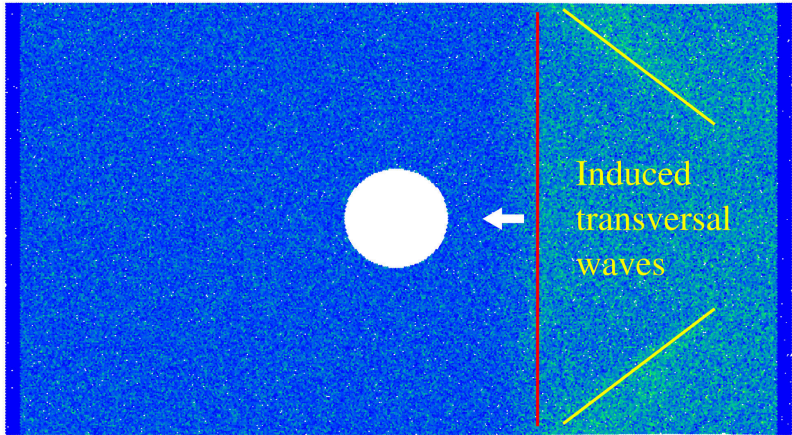
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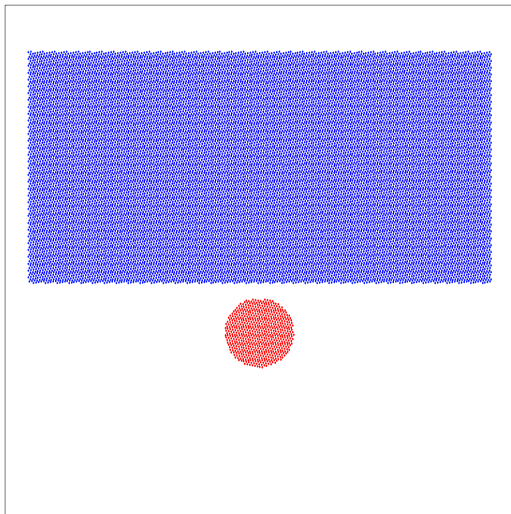
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Wave dynamics

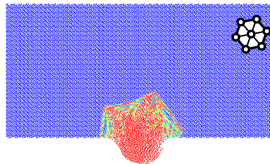
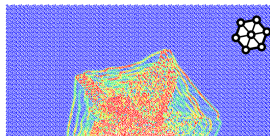
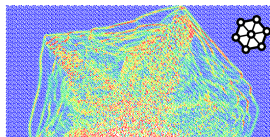
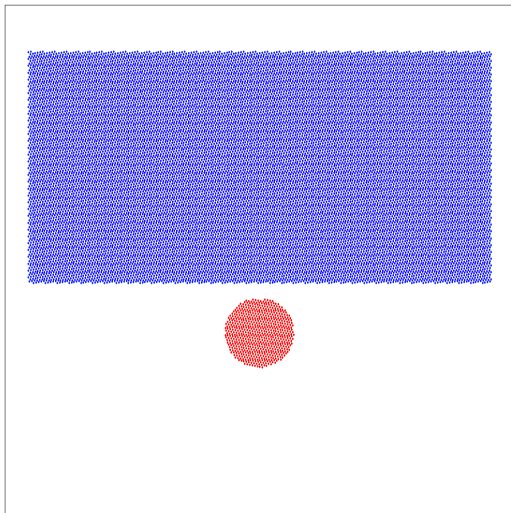
# Example: high-velocity impact

Impact of a perfect crystal by a circular projectile



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Impact of a perfect crystal by a circular projectile: 20 000 particles on 20 000 time steps.



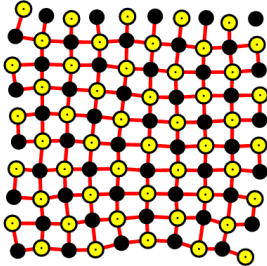
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# Example: martensitic phase transformation

An imitation of martensitic phase transformation with mixed LJ potential<sup>[1]</sup>

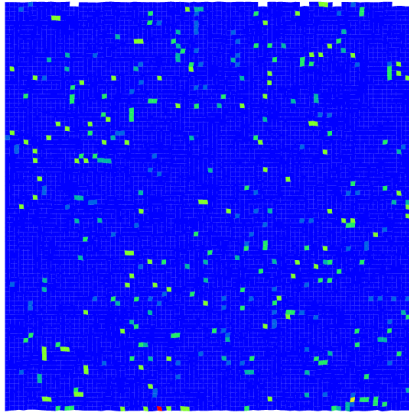


Cooling of a small lattice with high-temperature stable square lattice and low temperature hcp lattice

[1] Kastner O, Eggeler G, Weiss W, Ackland GJ. Molecular dynamics simulation study of microstructure evolution during cyclic martensitic transformations. J Mech Phys Solids 30 (2011)

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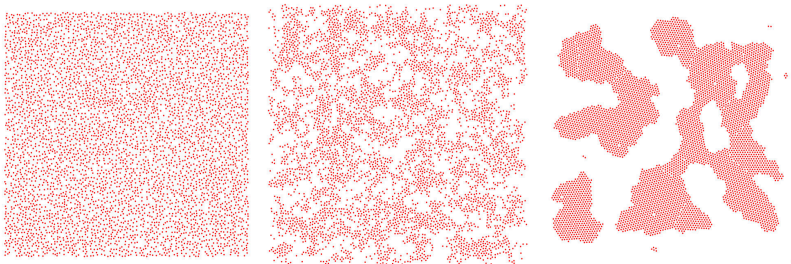
Cooling of a bigger lattice with high-temperature stable square lattice and low temperature hcp lattice  
(atomic cells are colored depending on martensitic variant)

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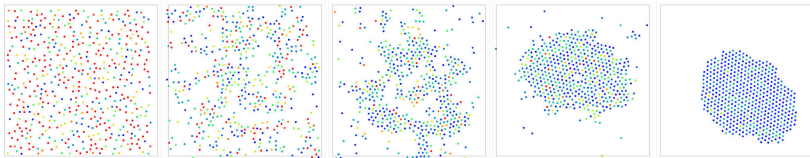
# Example: phase transition in Argon

- Cooling down noble (thus monoatomic) gas Argon in NVT ensemble
- Selecting appropriate parameters  $\sigma = 3.4 \text{ \AA}$ ,  $\varepsilon = 0.0343 \text{ eV}$ ,  $m = 39.95 \text{ u}$



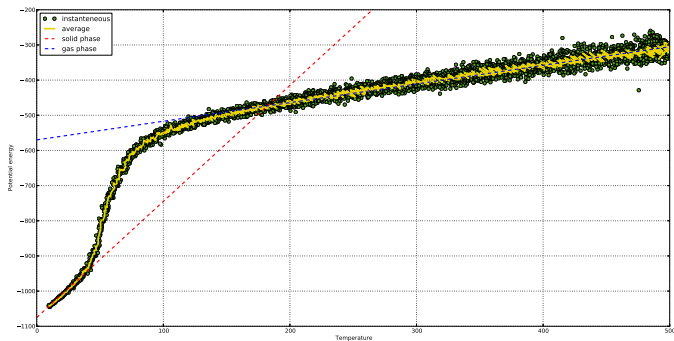
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# Applications of MD

- Popular in materials science, biophysics and biochemistry
- In material science it does not replace continuum models, but complements it with the atomic scale insights
- Naturally couples thermal and mechanical effects (linear and non-linear)

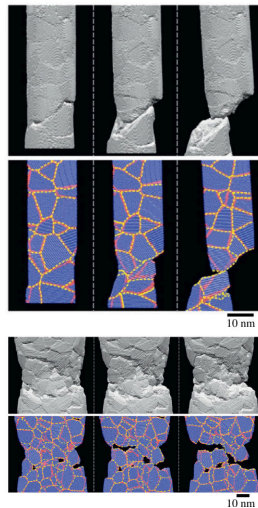
# Applications of MD

- Popular in materials science, biophysics and biochemistry
- In material science it does not replace continuum models, but complements it with the atomic scale insights
- Naturally couples thermal and mechanical effects (linear and non-linear)
- **Applications:**
  - Diffusion and self-diffusion in gas and liquid
  - Instabilities in liquids
  - **Dislocations** (ingredients for upper scale models Dislocation Dynamics)
  - Nanograined materials
  - Atomic-scale heat conduction
  - Phase-transformations
  - Grain boundaries (including GB migration)
  - Collision cascade (impact by a high energy particle (ion, neutron, electron))
  - Thin wetting films
  - Nanolubrication, nanowear
  - NEMS (nano electro mechanical devices)
  - Motion of biological macromolecules (proteins, nuclear acids) and their interaction with other molecules and cell structures

*Nobel prize in Chemistry “for the development of multiscale models for complex chemical systems” was decerned to Michael Levitt*
  - Thin film growth (hard to analyse with conventional experimental methods)

## Several examples:

- Deformation and fracture of nanograined wires



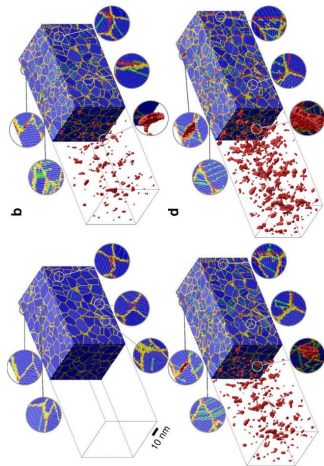
MD simulations vs experiments (size effect)<sup>[1]</sup>

[1] Z. Wu, Y.W. Zhang, M.H. Jhon, D.J. Srolovitz.

Anatomy of nanomaterial deformation: Grain boundary sliding, plasticity and cavitation in nanocrystalline Ni, *Acta Materialia* 61, 2013

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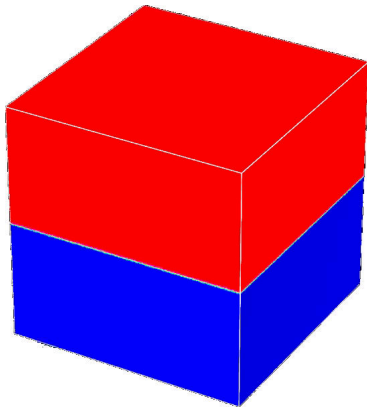


MD simulations of void growth (red zones)<sup>[1]</sup>

[1] Z. Wu, Y.W. Zhang, M.H. Jhon, D.J. Srolovitz.  
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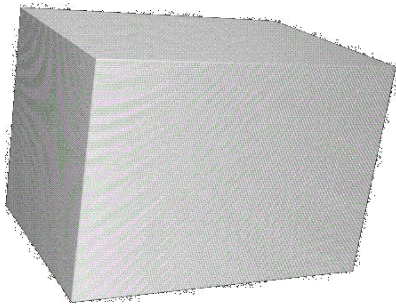
From Kai Kadau home page  
(ex. Los Alamos National Laboratory) <sup>[2]</sup>  
<http://www.thp.uni-duisburg.de>

[2] K. Kadau et al. The importance of fluctuations in fluid mixing. Proc Nat Acad Sci 104 (2007)



## Several examples:

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- Shock-induced structural phase transformation in bcc iron (8 million atoms)



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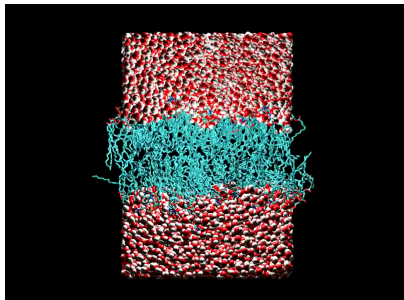
<http://www.thp.uni-duisburg.de>

[3] K. Kadau et al. Shock waves in polycrystalline iron.  
Phys Rev Lett 98 (2007)

# Applications of MD

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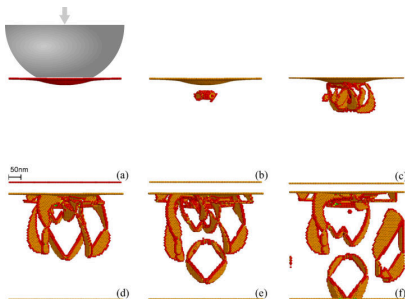


Molecular Dynamics simulation of a lipid bilayer and water<sup>[4]</sup>

[4] M. Stepniewski et al, Effects of the lipid bilayer phase state on the water membrane interface, Phys. Chem. B 114 (2010).

## Several examples:

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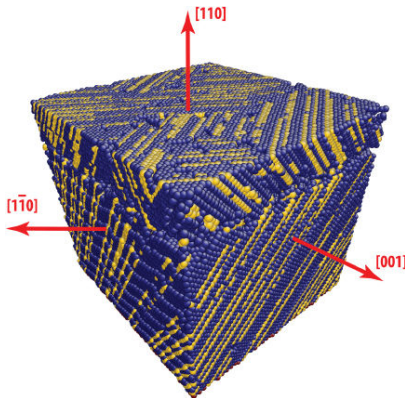


MD simulation of a spherical indentation on (111) FCC cube.

[5] H.J. Chang, M. Fivel, D. Rodney, M. Verdier.  
Multiscale modelling of indentation in FCC metals:  
From atomic to continuum, CR Physique 11 (2010).

## Several examples:

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- Molecular dynamics simulation of the martensitic phase transformation in NiAl alloys



Martensitic structure formed by cooling a simulation block of the  $\text{Ni}_{0.65}\text{Al}_{0.35}$  alloy with a free surface<sup>[5]</sup>

[6] Pun GP, Mishin Y. Molecular dynamics simulation of the martensitic phase transformation in NiAl alloys. J Phys: Condens Mat 22 (2010)

*“The problem of hydrodynamic limits is to obtain rigorous derivations of macroscopic models such as the fundamental partial differential equations (PDEs) of fluid mechanics from a microscopic description of matter, be it molecular dynamics or the kinetic theory of gases.”<sup>[1]</sup>*

[1] F. Golse “The Boltzmann equation and its hydrodynamic limits. Evolutionary equations 2:159-301 (2005).

# Limits of the MD

- It is a long road from an atom to a continuum  
*modeling representative system requires massively parallel computers an adapted software, or even adapted hardware*
- Choice and fit of potential for a particular chemical composition and configuration is non-trivial
- Systems with long-range interactions (e.g., Coulomb) are heavy to simulate  $O(N \log(N))$
- Integration over long time periods require specific numerical methods
- Rare processes are hard to simulate  
*e.g., low temperature diffusion (for example, Cottrell atmosphere), dislocation glide at low stress especially in bcc*  
Either use high temperature and/or high strain rates (see also Kinetic Monte Carlo method)
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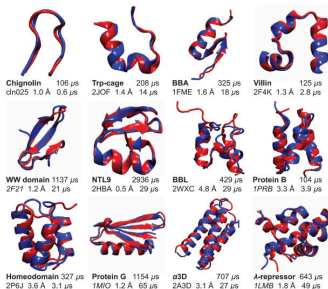
*Apart from the physical simulations, MD is a helpful tool to understand physics of matter in all its states*

## ■ World's **Largest** Molecular Dynamics Simulation<sup>[1]</sup> (2013)

4 125 000 000 000 =  $4.125 \cdot 10^{12}$  atoms on 131 072 cores

## ■ World's **Longest** Molecular Dynamics Simulation<sup>[2]</sup> (2015)

1.112 milliseconds  $\rightarrow 10^{12}$  time steps



Simulation (blue), experimentally determined structure (red)

[1] W. Eckhardt et al. 591 TFLOPS multi-trillion particles simulation on SuperMUC. Supercomputing (2013).

[2] K. Lindorff-Larsen et al. How fast-folding proteins fold. Science 334 (2011)



# Afterword

- It was a very short introduction to the world of molecular dynamic simulations
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- Statistical ensembles (**NVT**, **NPT** & **N $\sigma$ T**)
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- Grid or tree methods for long-range interactions, especially the Fast Multipole Method (**FMM**)
- Kinetic Monte Carlo molecular dynamics which is used to accelerate the time



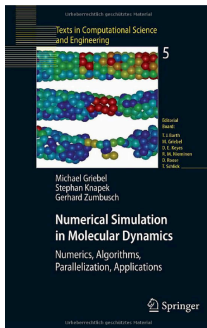
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*I encourage you to consult the literature. . .*

## Recommended reading:



## Sources:

- [1] M. Griebel, S. Knapik, G. Zumbusch. Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications, Springer (2007)
- [2] "Atomistic modelling of metals: introduction and applications" by P.M. Derlet (Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland), Summer school in Bad Herrenalb, Germany, 2009
- [3] D.C. Rapaport. The art of molecular dynamics simulation. Cambridge University Press (2004)

Merci!

Merci de votre attention!