Multiscale Simulations of Materials and Structures

Lecture 2.
Molecular Dynamics II

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Outline

Temperature

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

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

N_{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

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

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

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- Attention!

(1) particles are considered as points (no contribution from angular velocities),

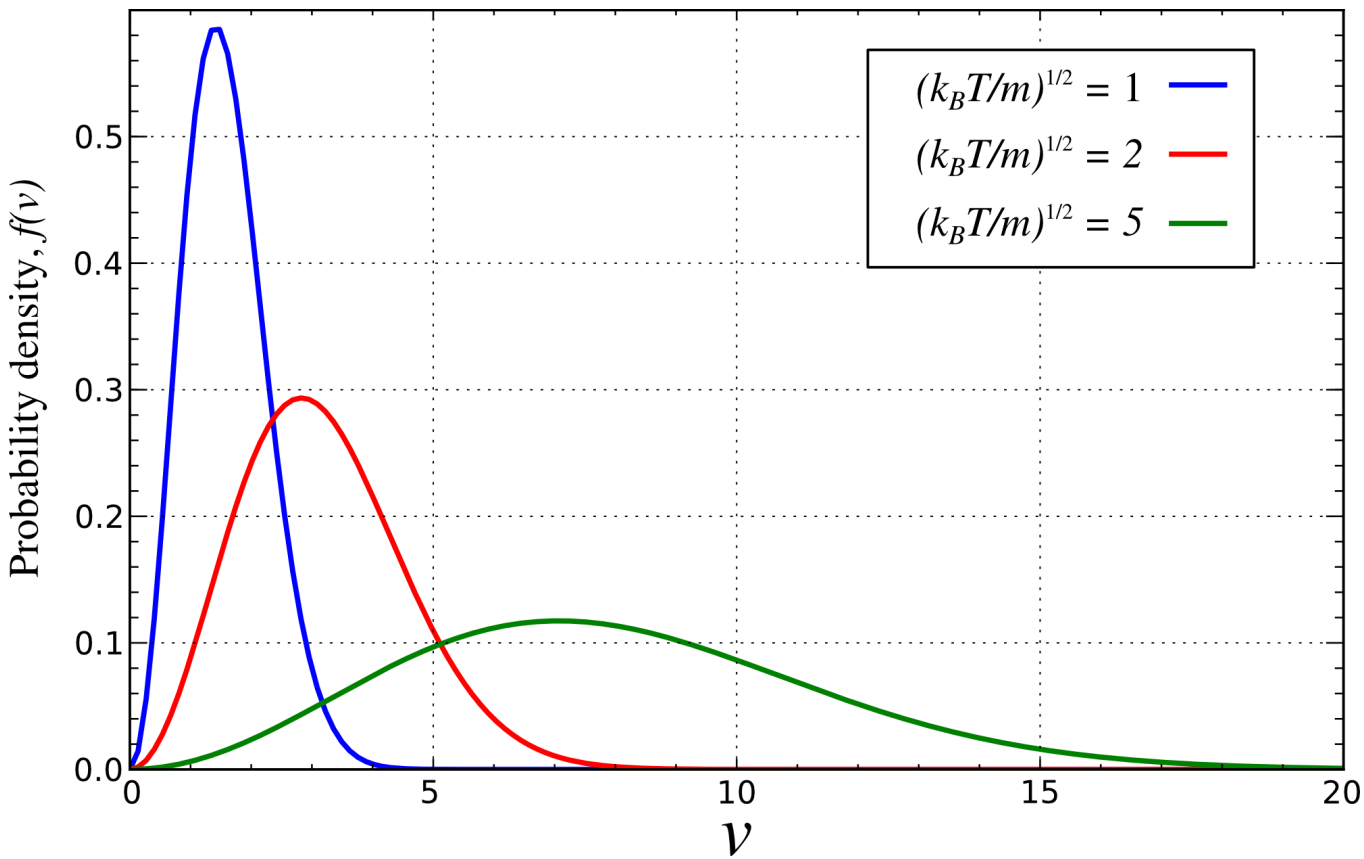
(2) no contribution from electrons, important carriers of the heat.

Let's control the temperature: prescribe

Prescribe a temperature

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

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



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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:

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

- Box-Muller method[1]

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

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Preserve the temperature

- Initially inserted energy T_0 ...

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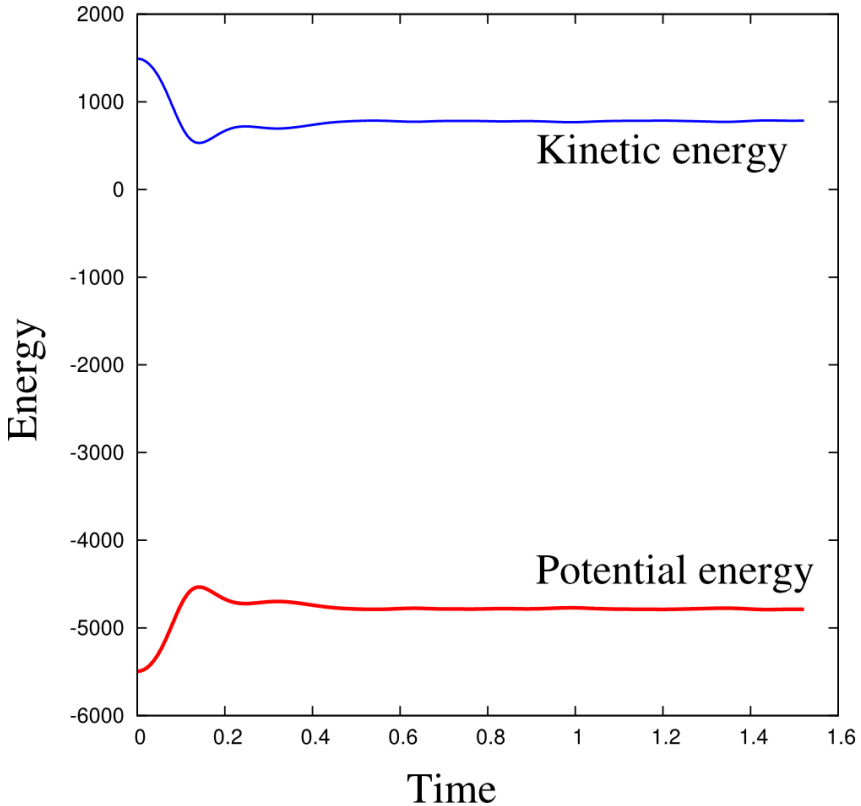
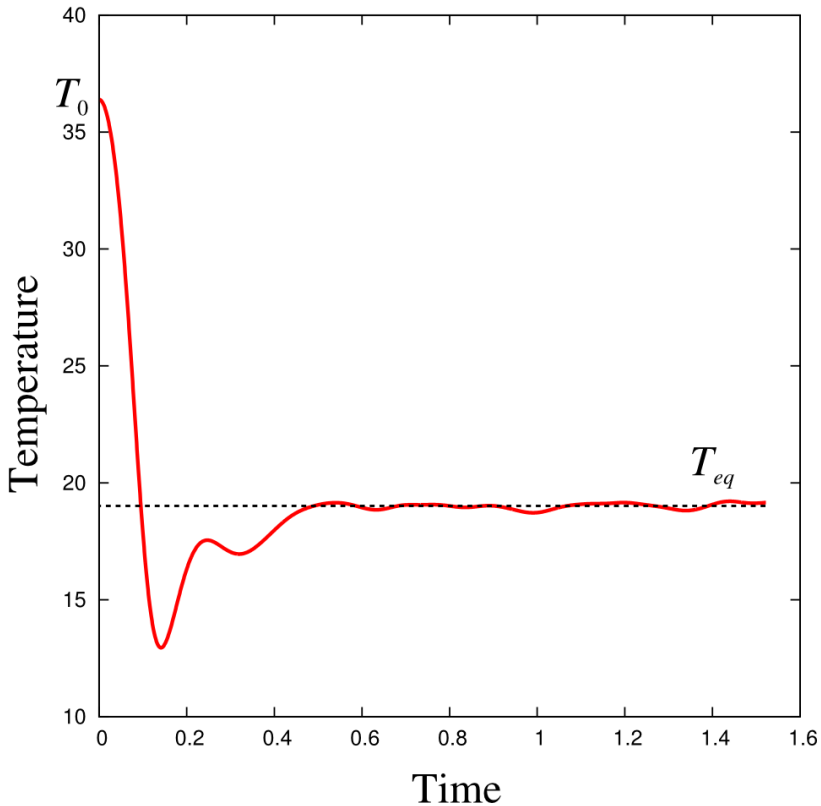
- Total energy is conserved $E_{\text{kin}} + E_{\text{pot}}$





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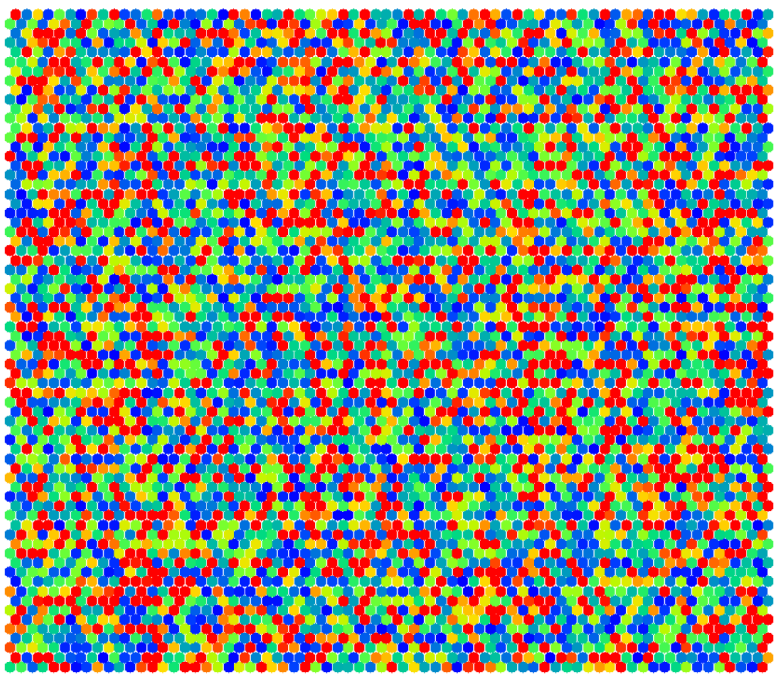
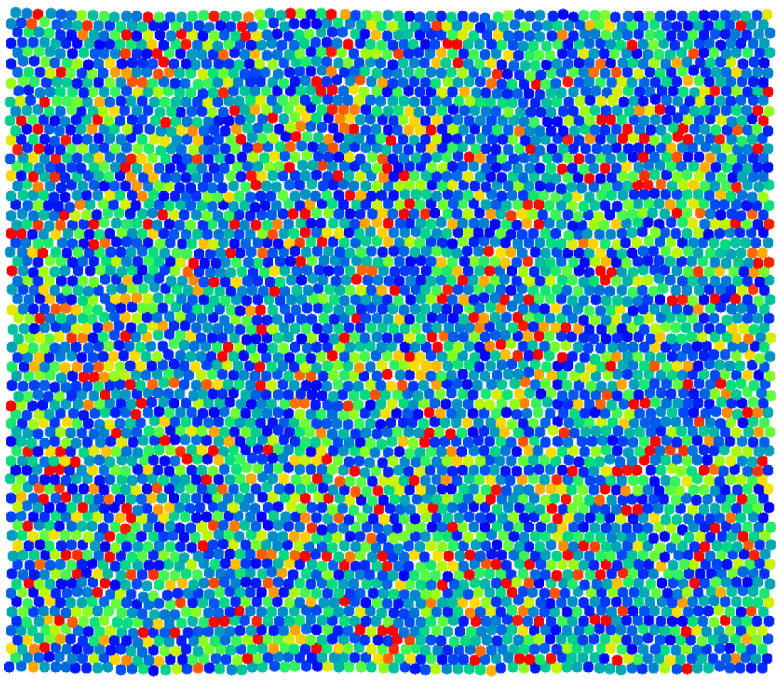
Initial state, T=36 K



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*[1]
- 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:

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

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

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

Let's control the temperature: preserve

Preserve the temperature

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

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

at every m-th increment scale velocities:

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

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

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

for example $\gamma \sim dt$

Let's control the temperature: preserve

Preserve the temperature

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

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

- Choice of ξ:

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

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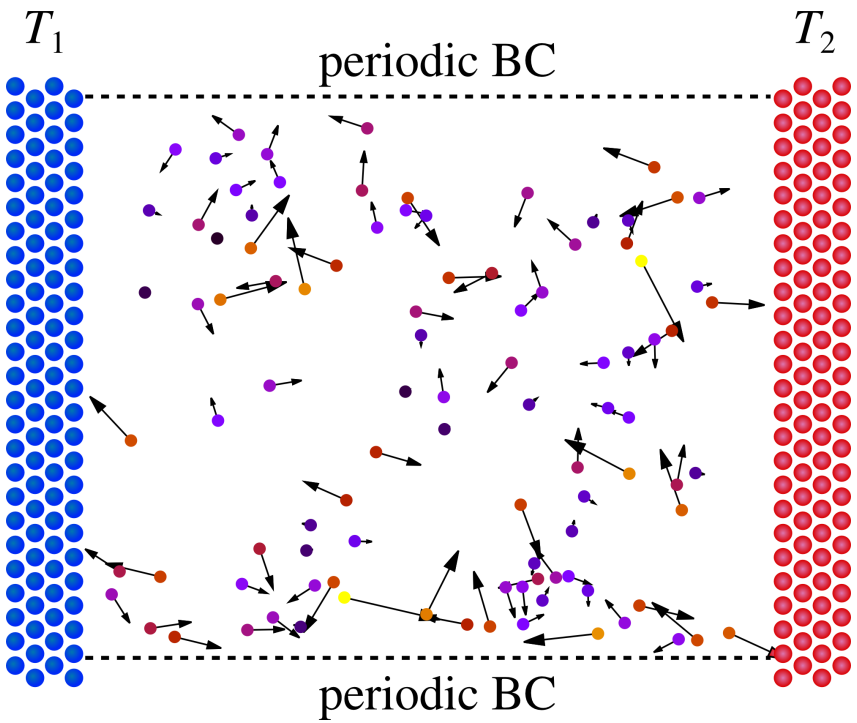
- **A good strategy**:
  use a thermostat on a part of simulated domain, not too close to the zone of the interest
- See also: Nosé-Hoover thermostat[1] and Langevin dynamics.

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

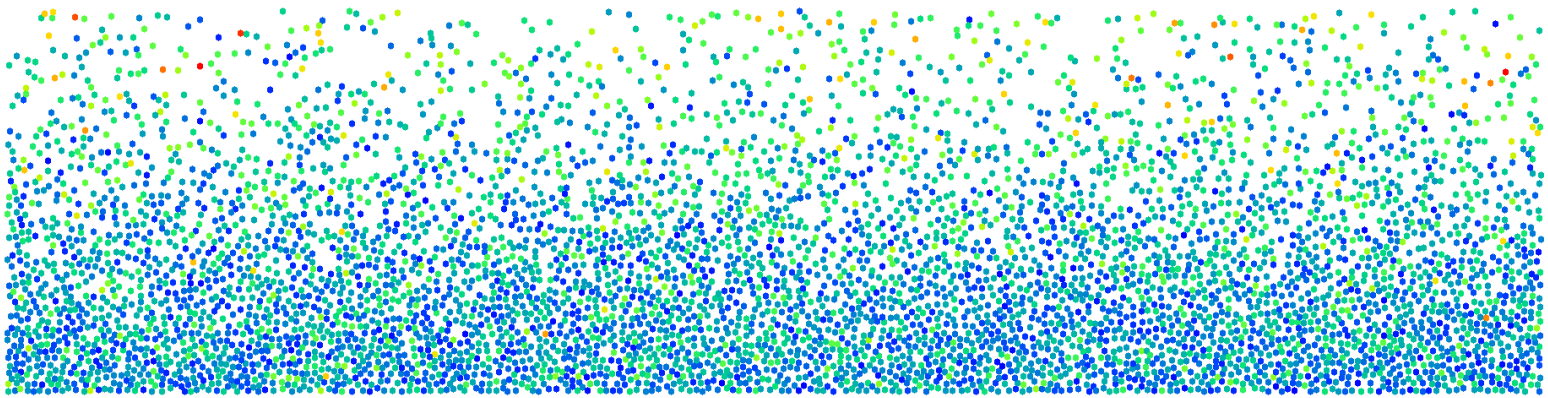
Let's control the temperature: change

- 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 $\quad v_x(t + dt) = -\xi v_x(t)$
  - Rigid walls at prescribed temperature (thermostats)



Example: liquid-gas interface

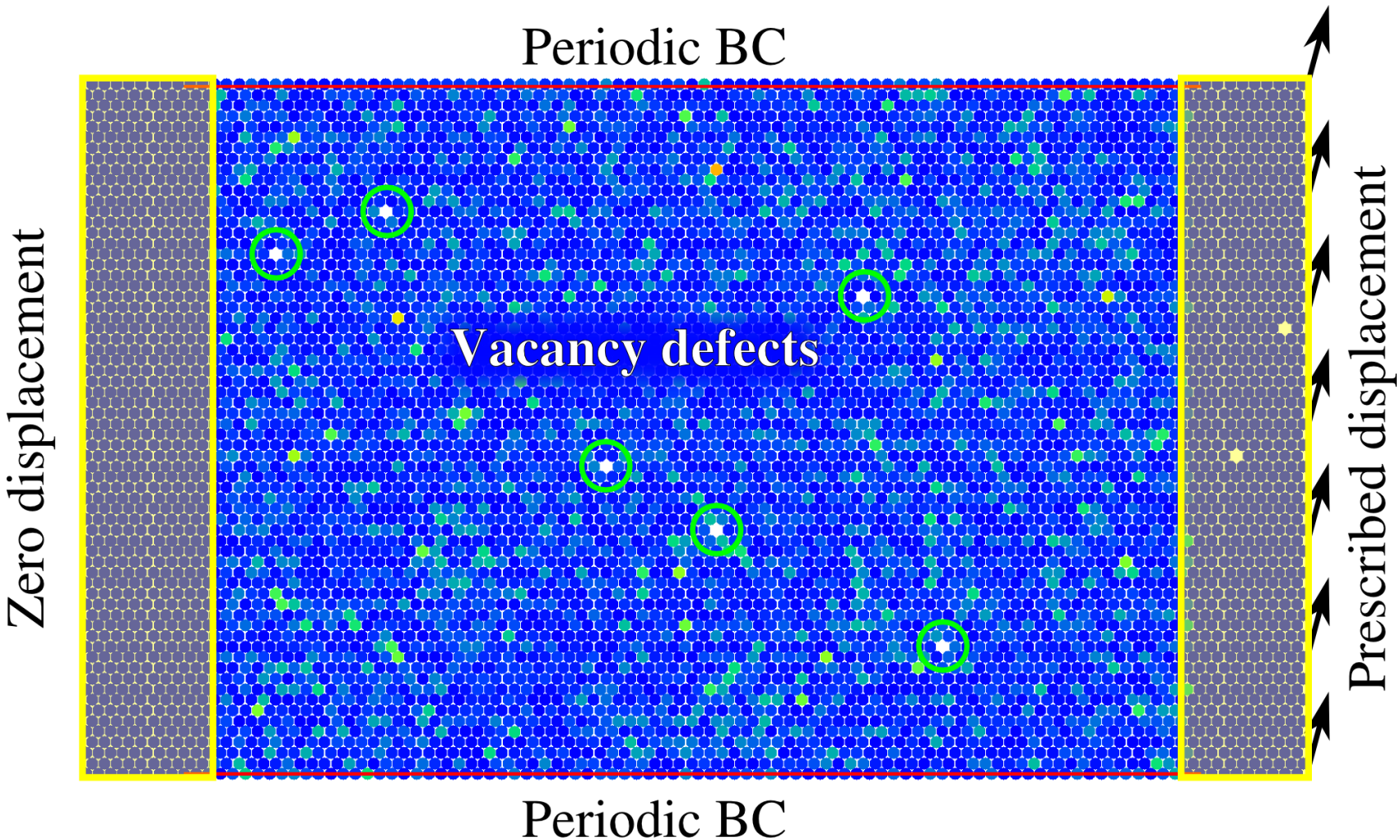
Stabilization phase of a liquid-gas interface under huge gravity.



6000 particles

Example: shear test

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



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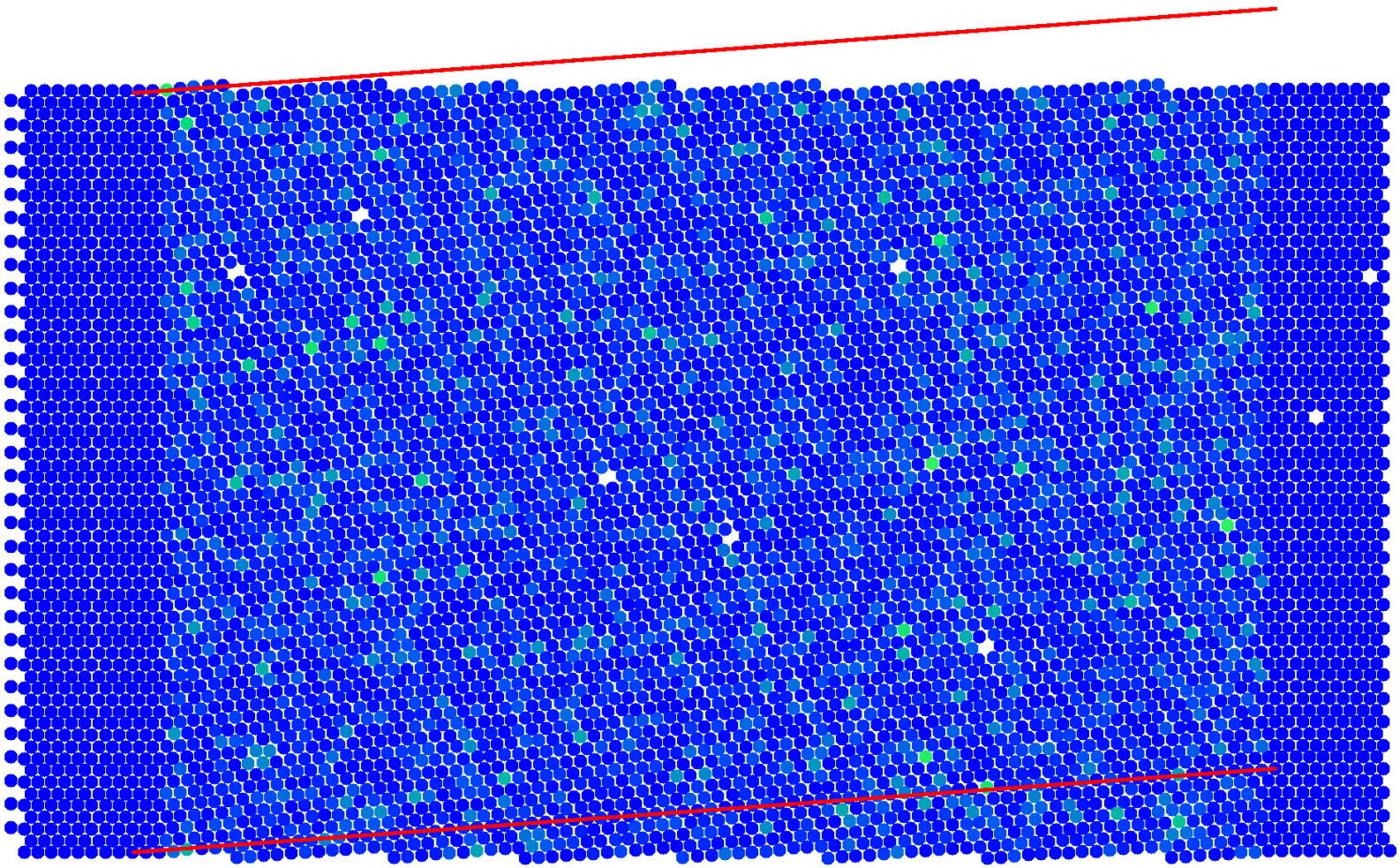
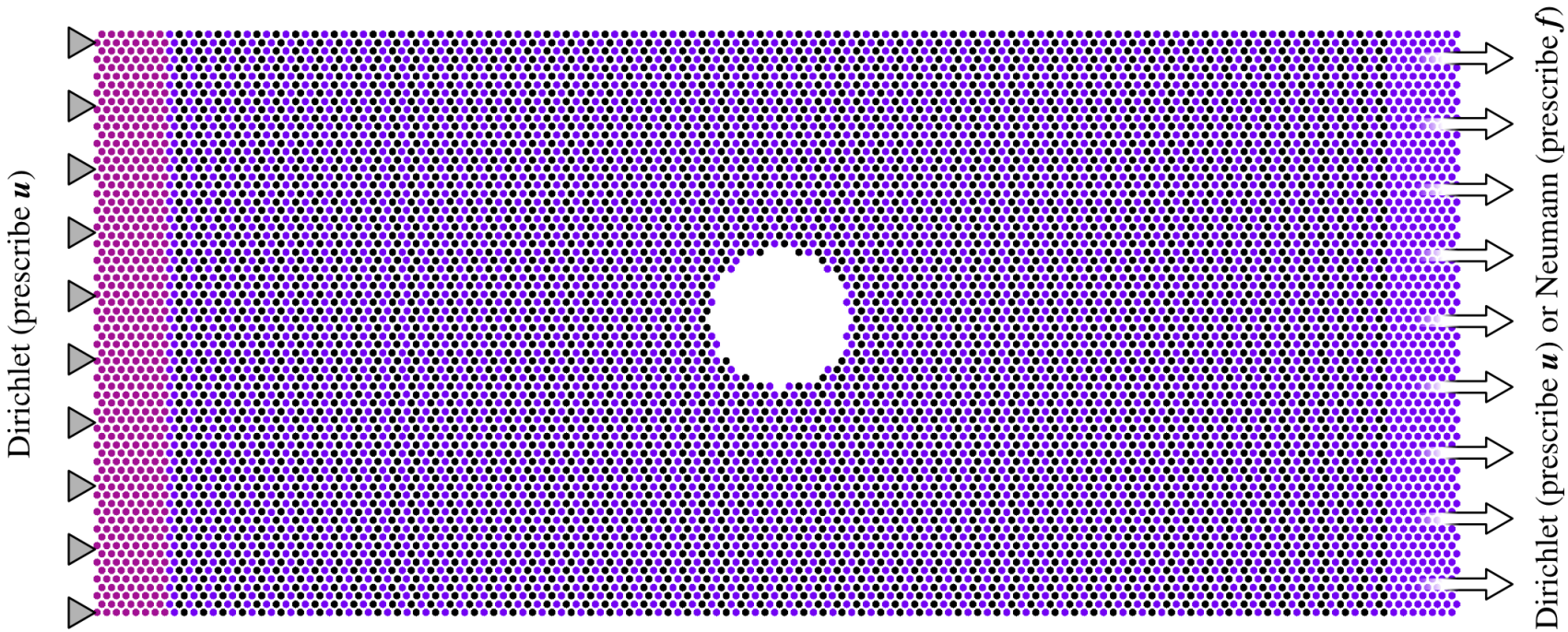


Example: tensile test

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



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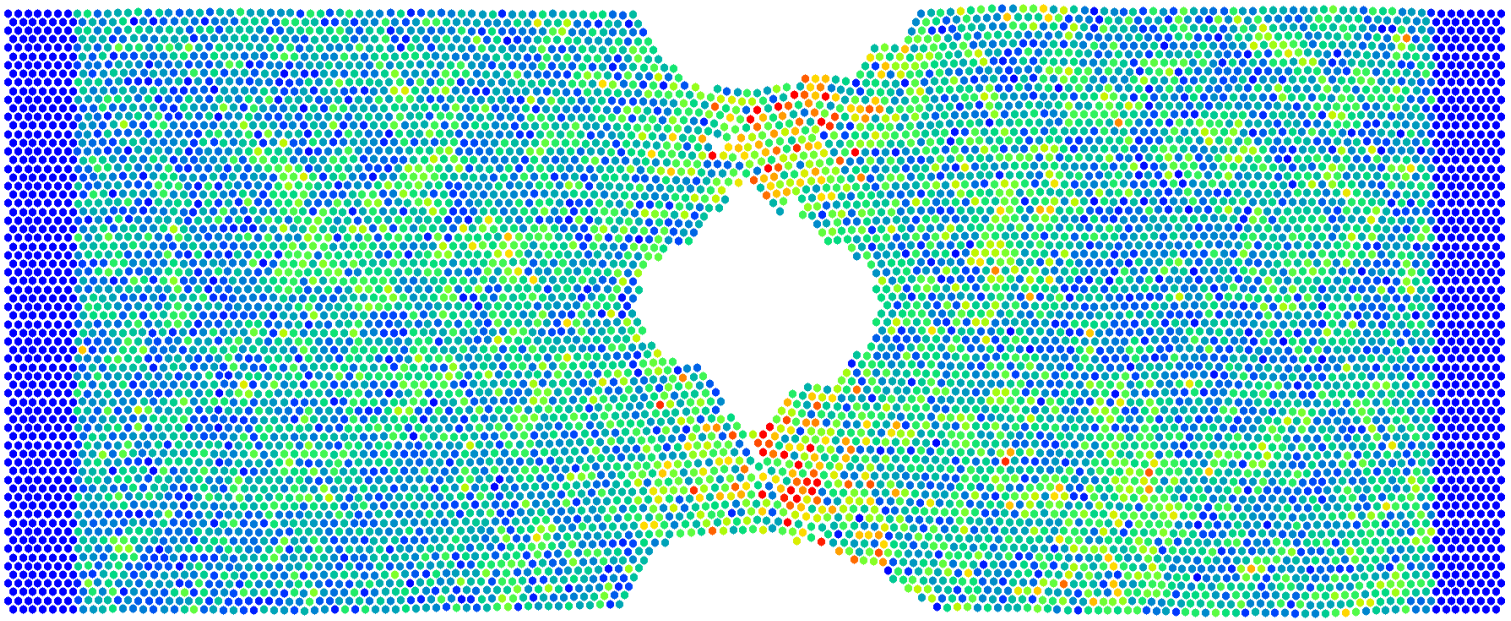

Perfect crystal with a hole, 10 000 particles

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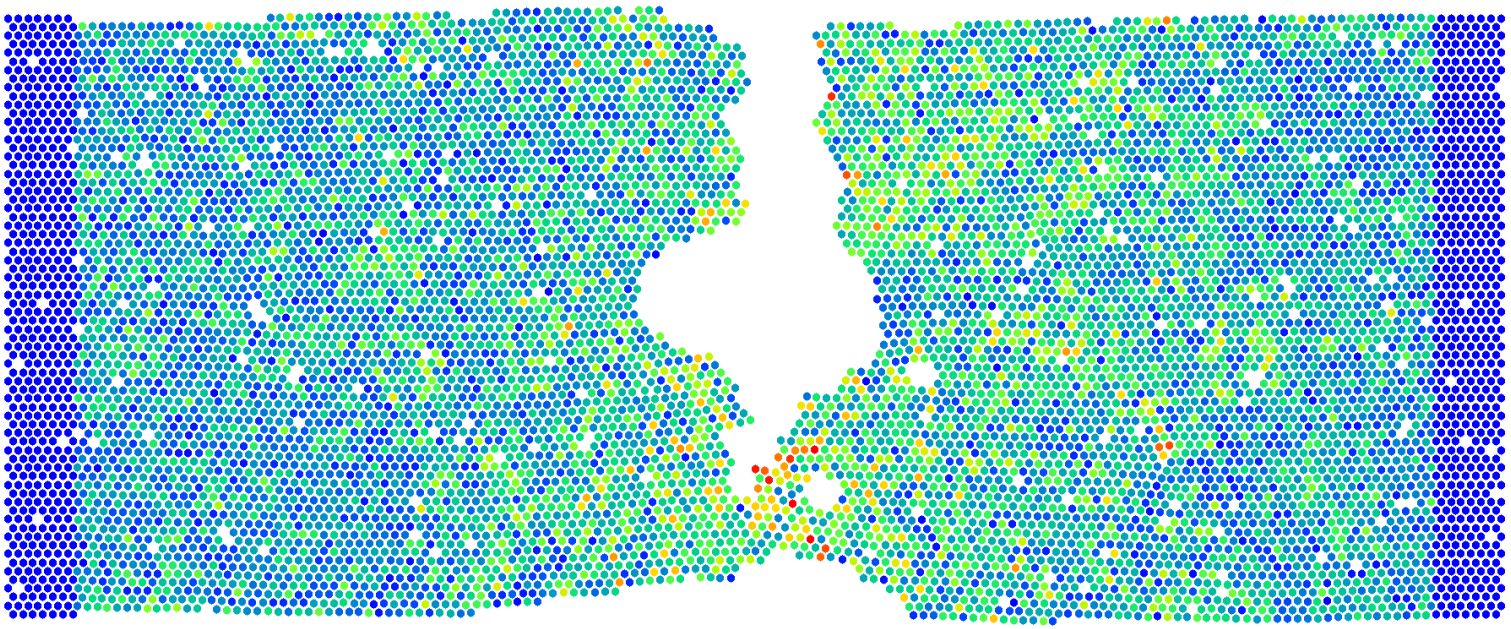
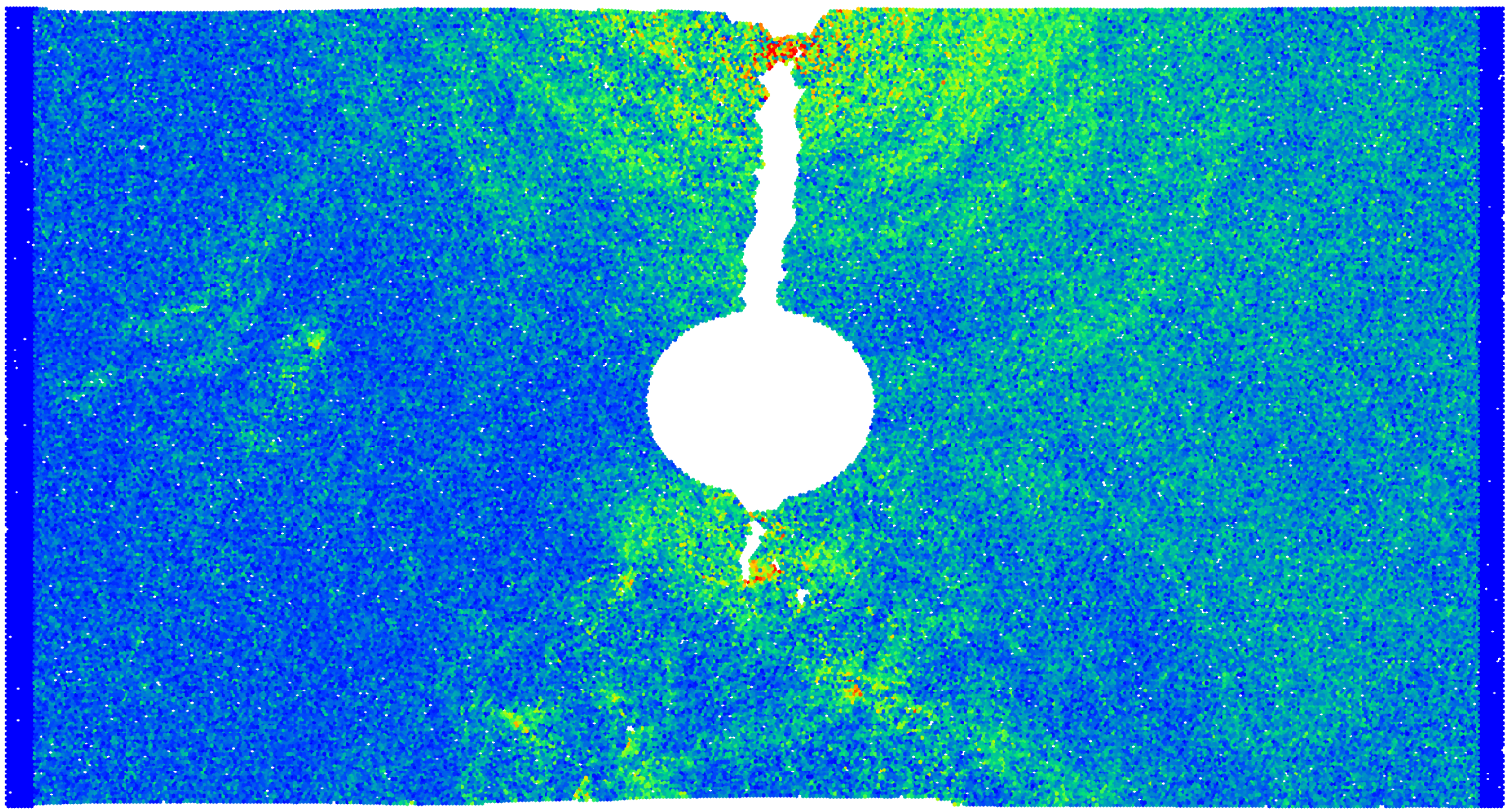


Crystal with 0.5% of vacancy defects and a hole, 10 000 particles

Example: tensile test

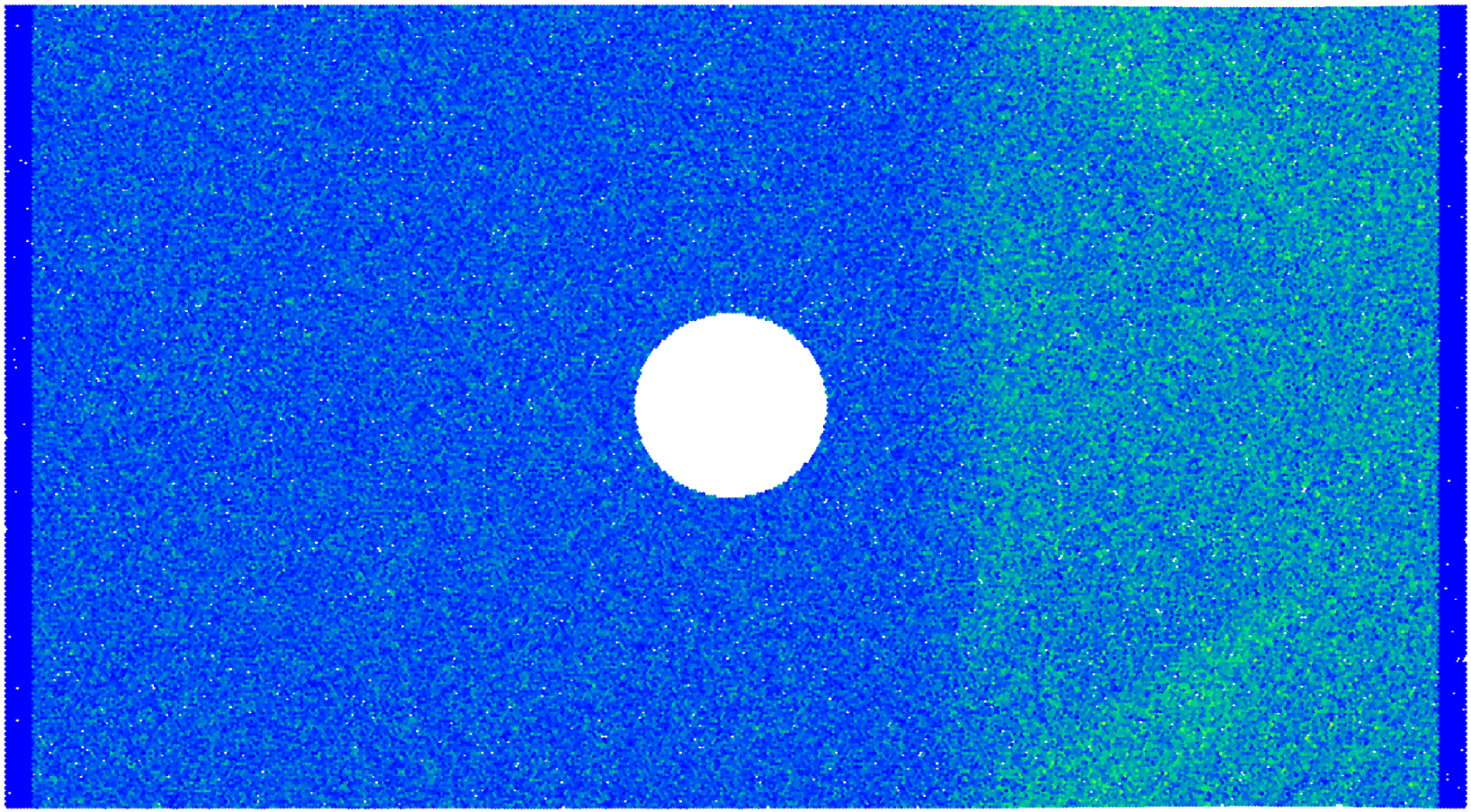
High-velocity tensile test of a bar with a circular defect.



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

Example: tensile test

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



Wave dynamics

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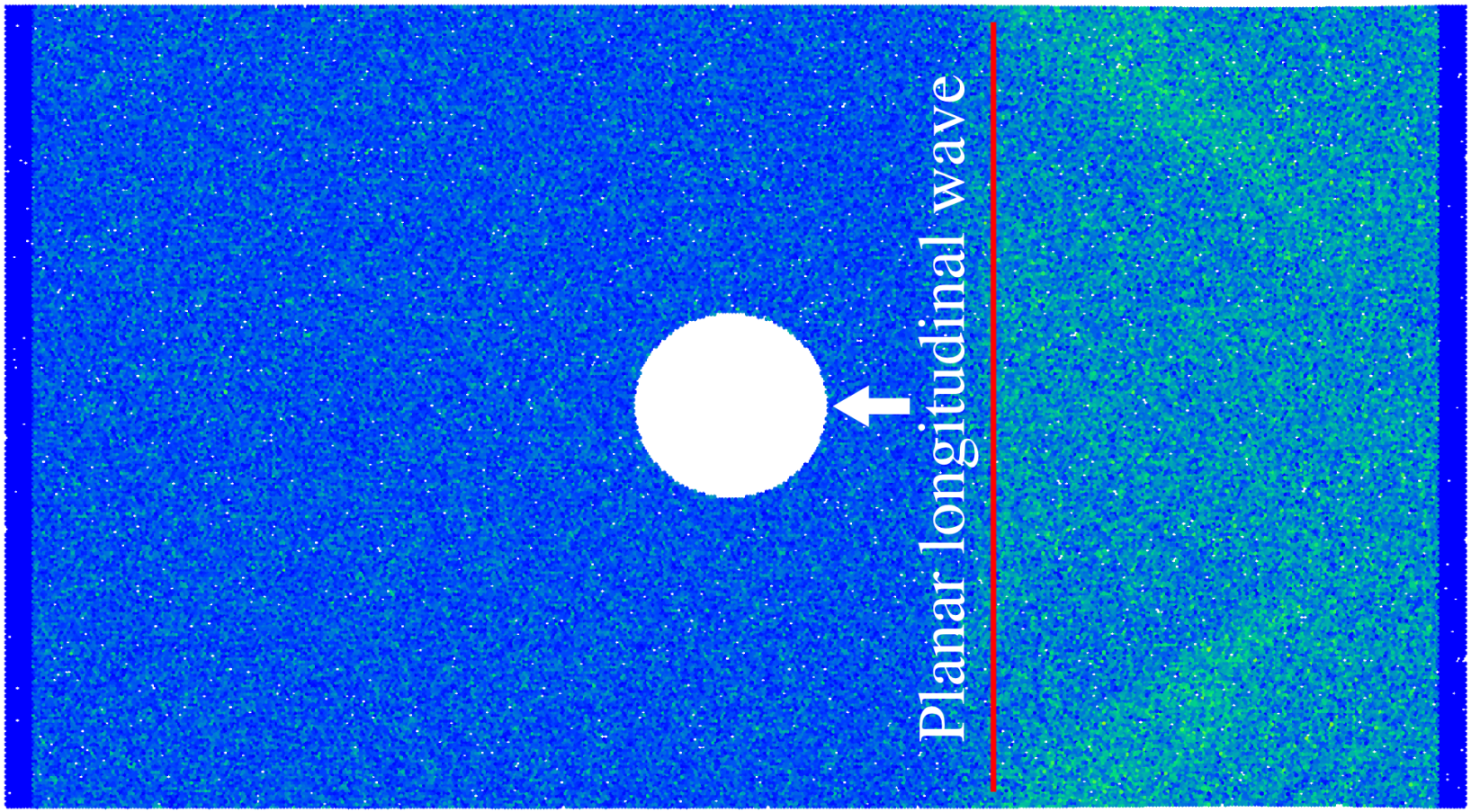

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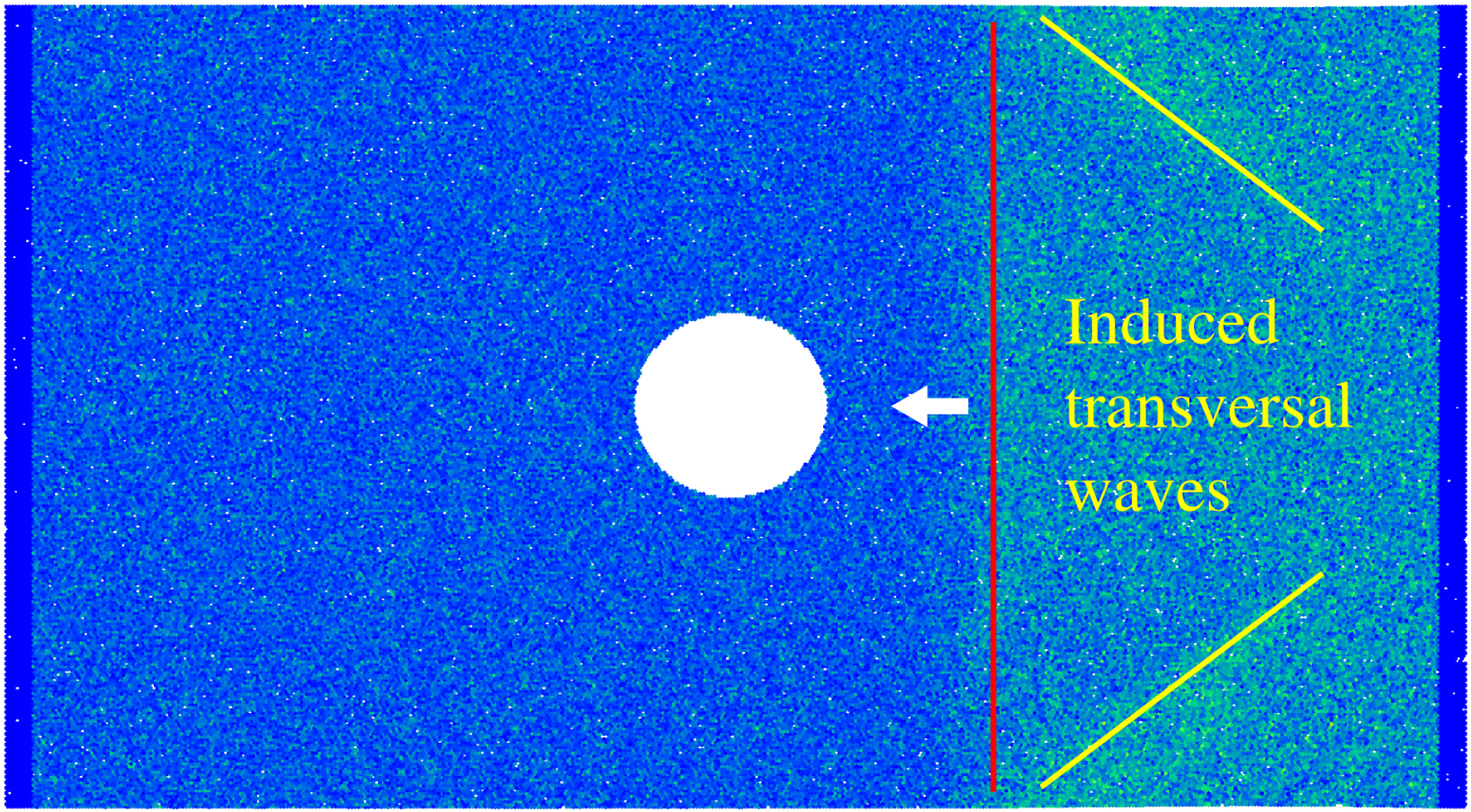
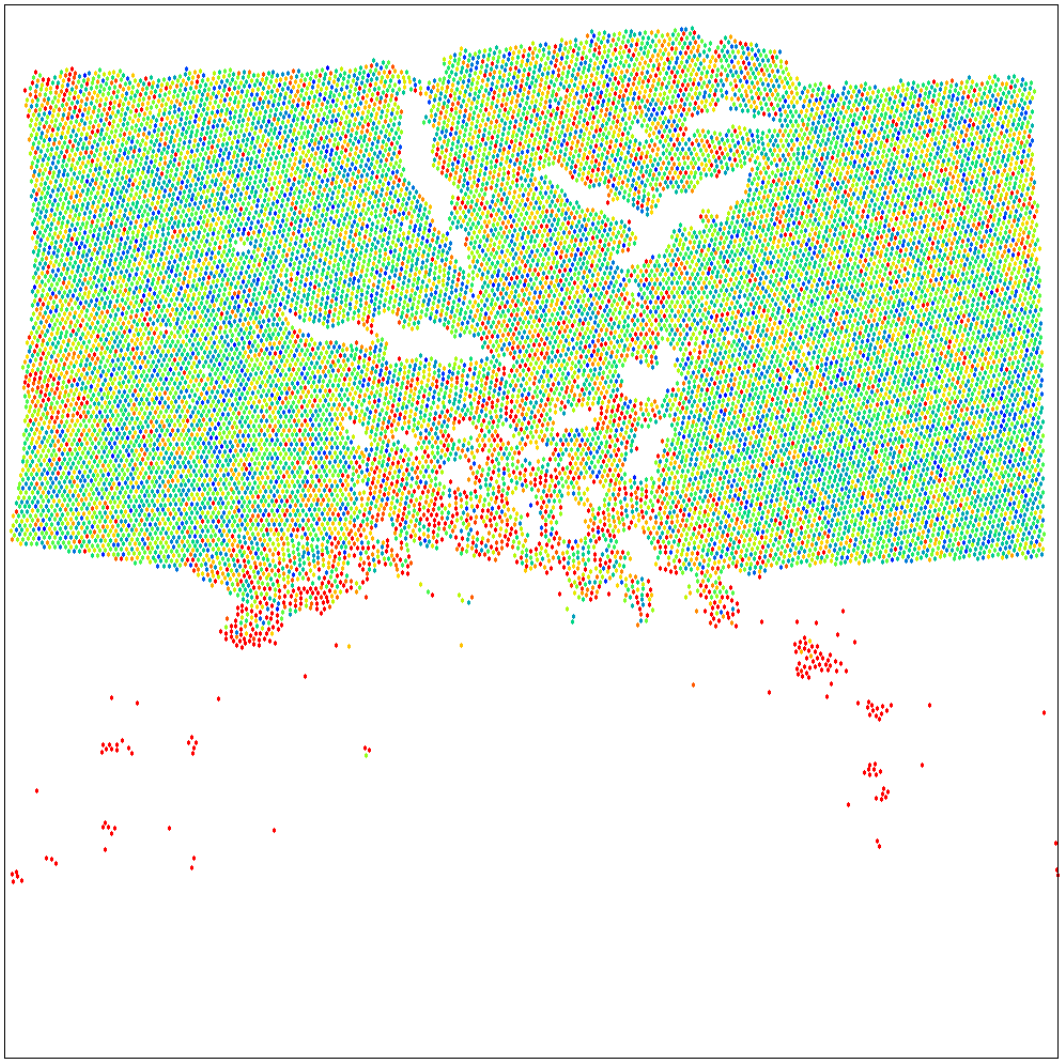


Wave dynamics

Example: high-velocity impact

Impact of a perfect crystal by a circular projectile



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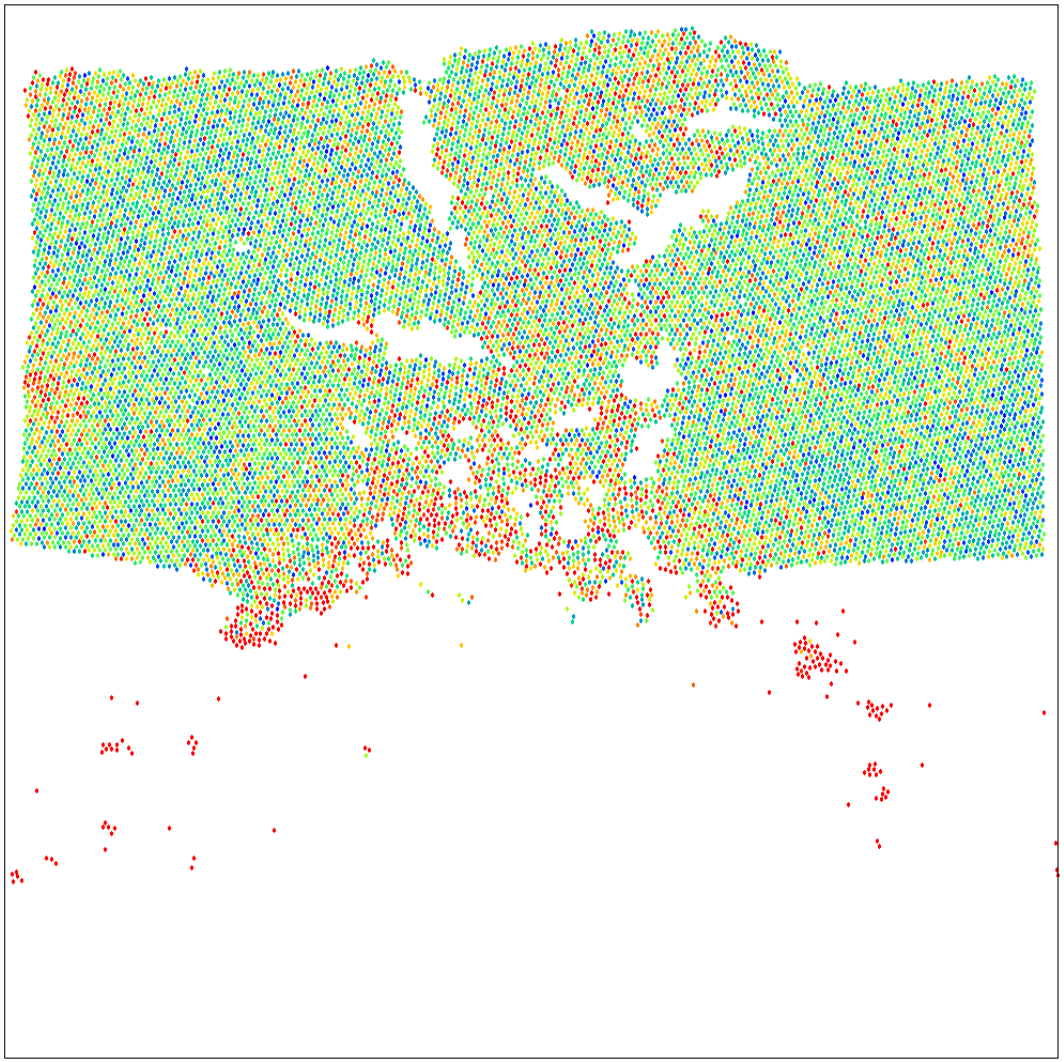

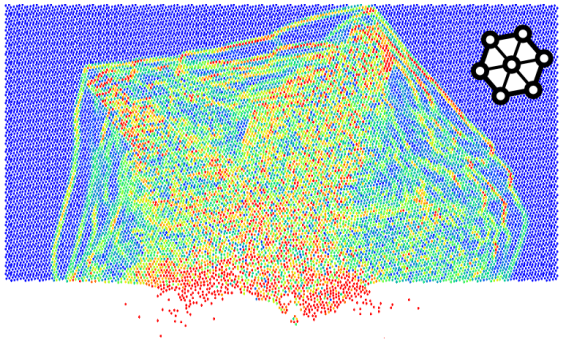

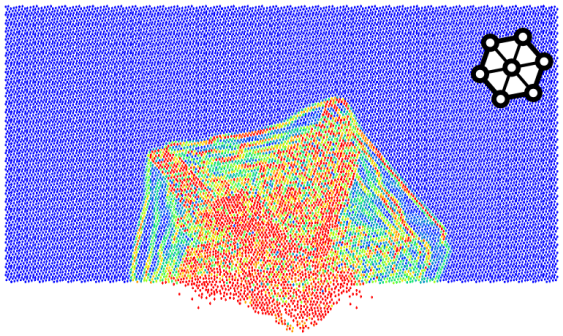

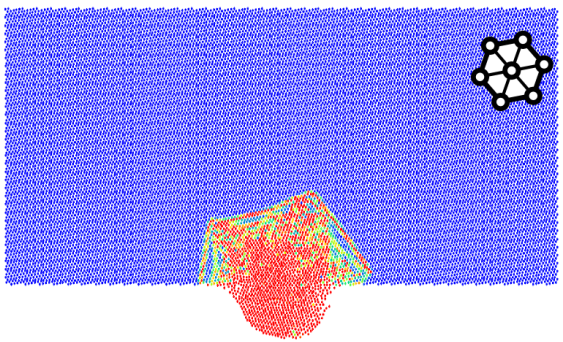

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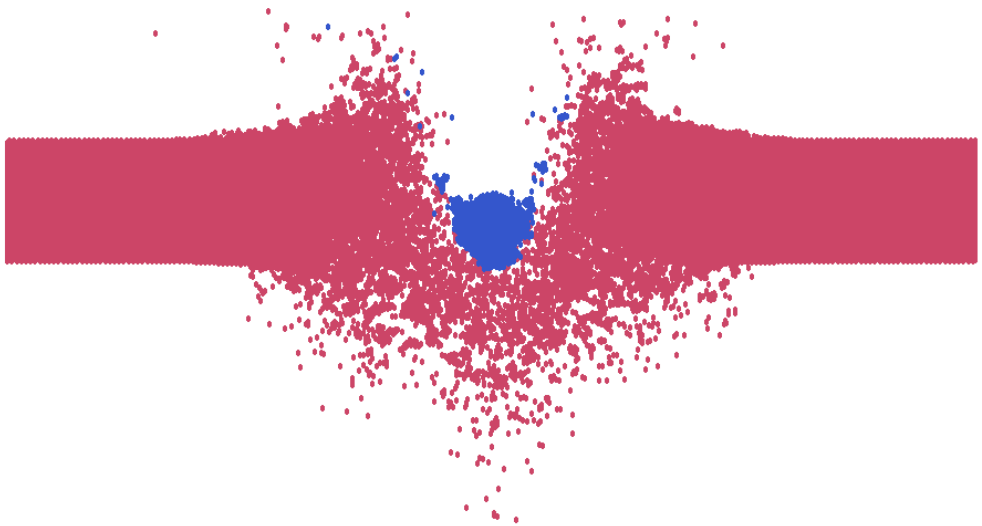
Impact of a perfect crystal by a circular projectile: 20 000 particles on 20 000 time steps.



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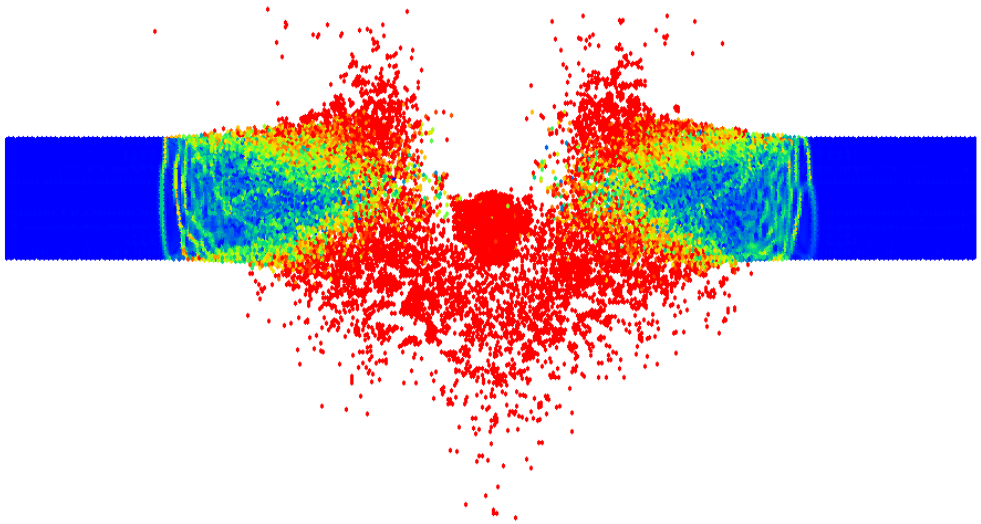
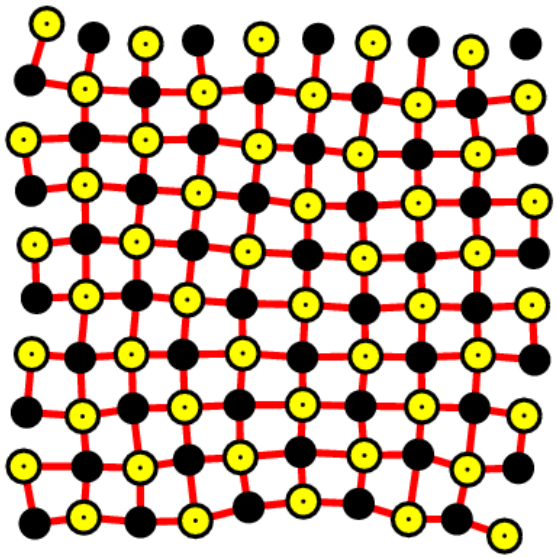


Example: martensitic phase transformation

An imitation of martensitic phase transformation with mixed LJ potential[1]



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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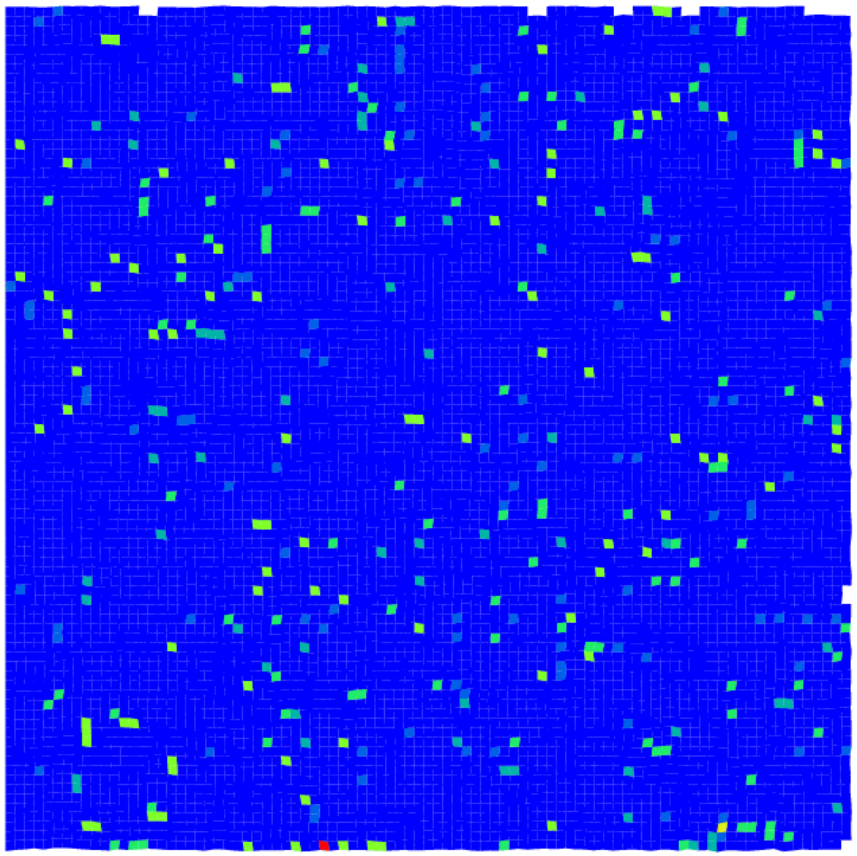

Cooling of a bigger lattice with high-temperature stable square lattice and low temperature hcp lattice (atomic cells are colored depending on martensitic variant)

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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)

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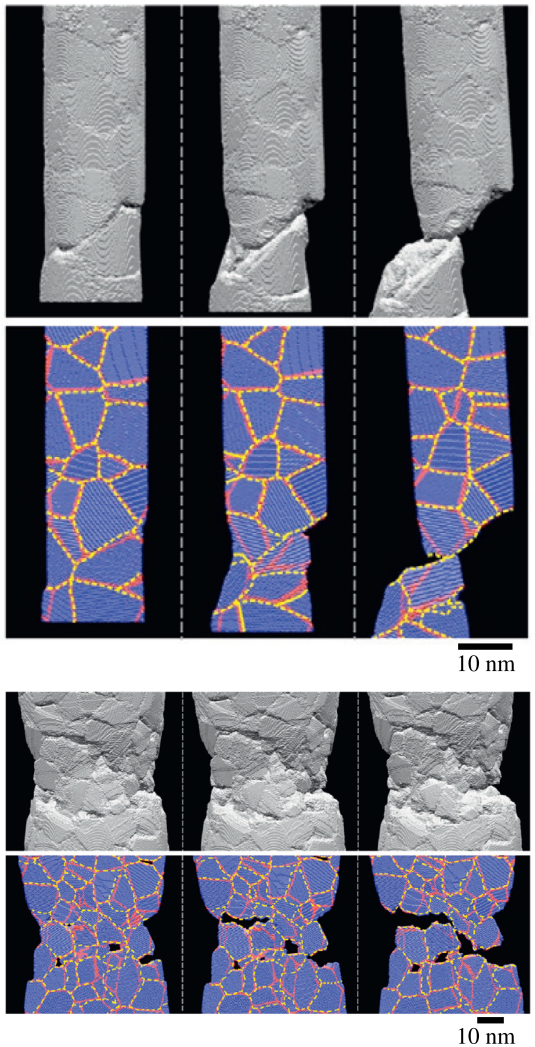
- In material science it does not replace continuum models, but complements it with the atomic scale insights
- Naturally couples thermal and mechanical effects (linear and non-linear)
- **Applications:**
  - Diffusion and self-diffusion in gas and liquid
  - Instabilities in liquids
  - **Dislocations** (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 bilogical 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)

Applications of MD

Several examples:

- Deformation and fracture of nanograined wires



MD simulations vs experiments (size effect)[1]

[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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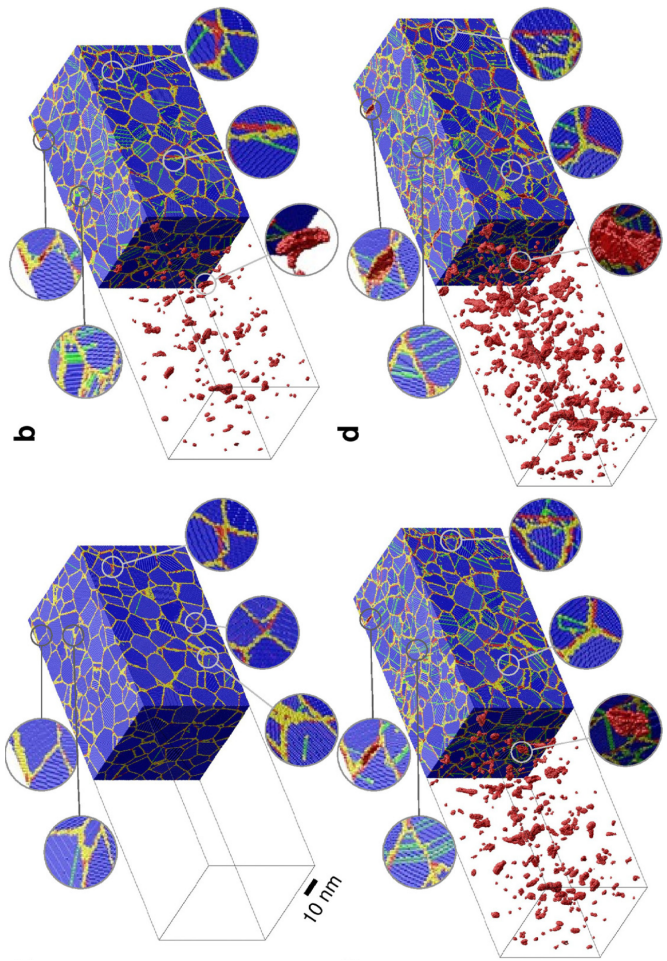

MD simulations of void growth (red zones)[1]

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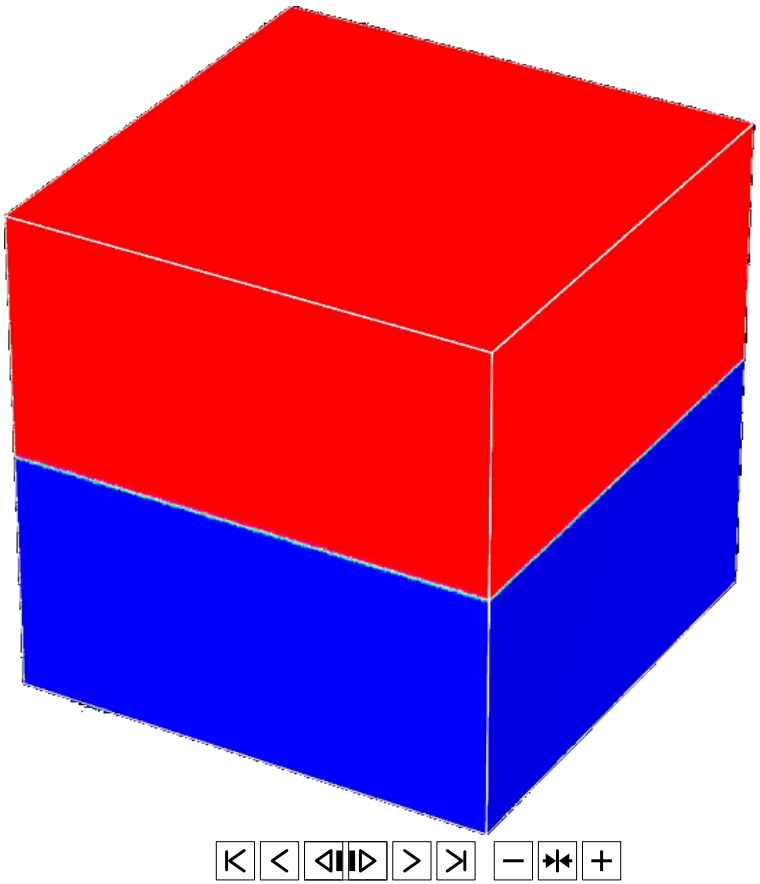
- Rayleigh-Taylor instability (7 billion particles)



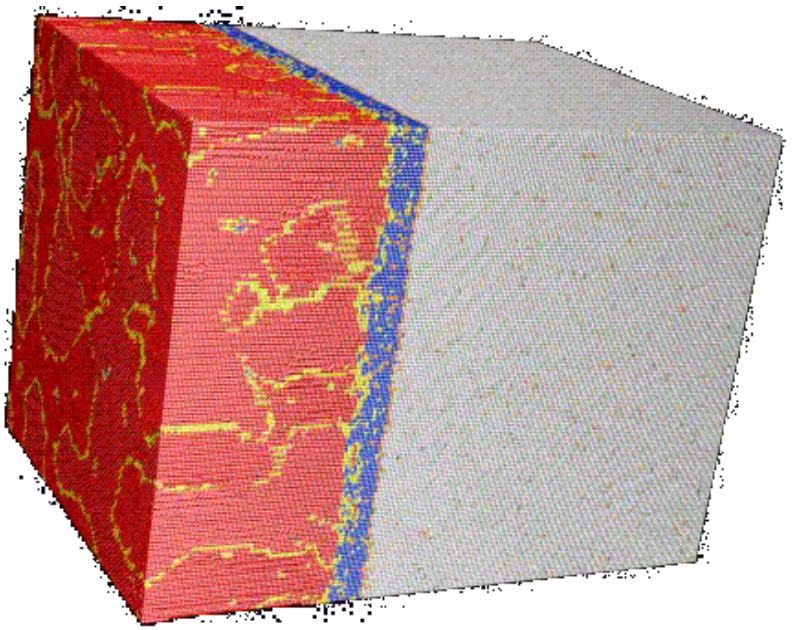
From Kai Kadau home page
(ex. Los Alamos National Laboratory)[2]
`http://www.thp.uni-duisburg.de`

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

Applications of MD

Several examples:

- Deformation and fracture of nanograined wires
- Rayleigh-Taylor instability (7 billion particles)
- Shock-induced structural phase transformation in bcc iron (8 million atoms)



From Kai Kadau home page[3]
`http://www.thp.uni-duisburg.de`

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

Applications of MD

Several examples:

- Deformation and fracture of nanograined wires
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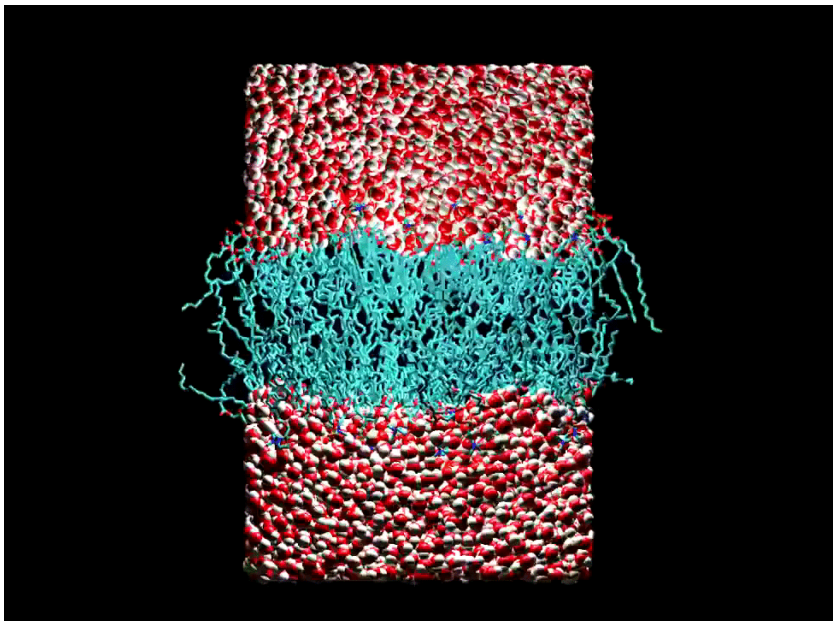

Molecular Dynamics simulation of a lipid bilayer and water[4]

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

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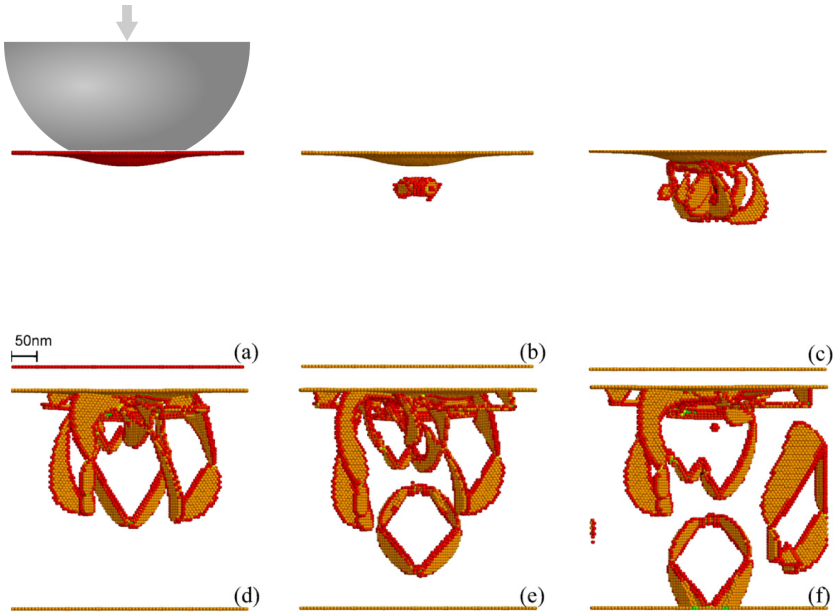

MD simulation of a spherical indentation on (111) FCC cube.

[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).

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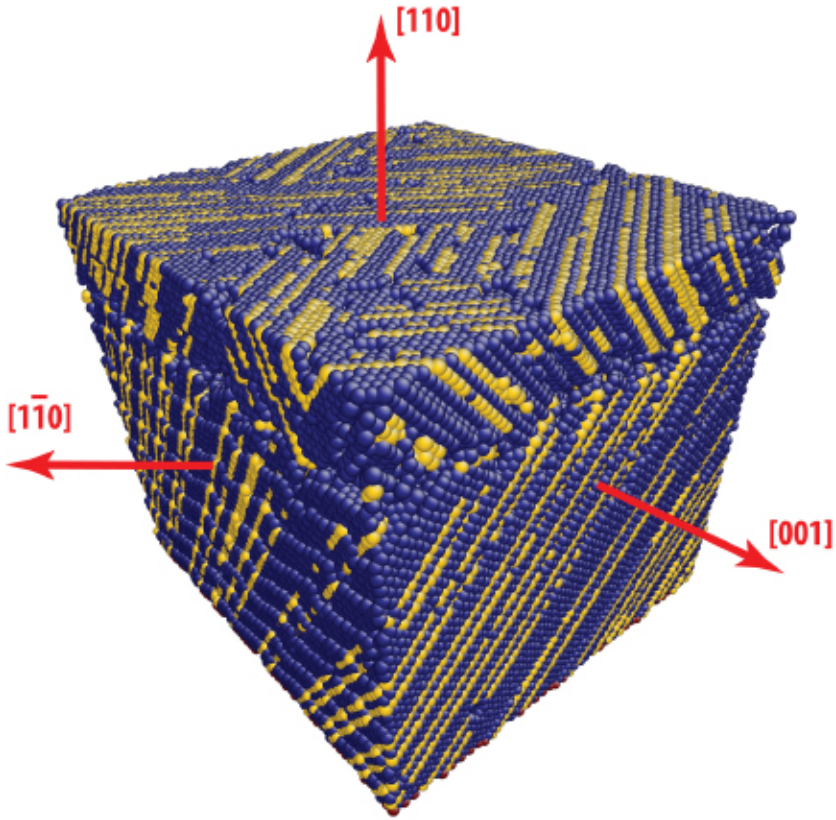

Martensitic structure formed by cooling a simulation block of the $Ni_{0.65}Al_{0.35}$ alloy with a free surface[5]

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

Fundamental problem

"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."[1]

[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 $\mathcal{O}(N \log(N))$
- Integration over long time periods require specific numerical methods
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Apart from the physical simulations, MD is a helpful tool to understand physics of matter in all its states

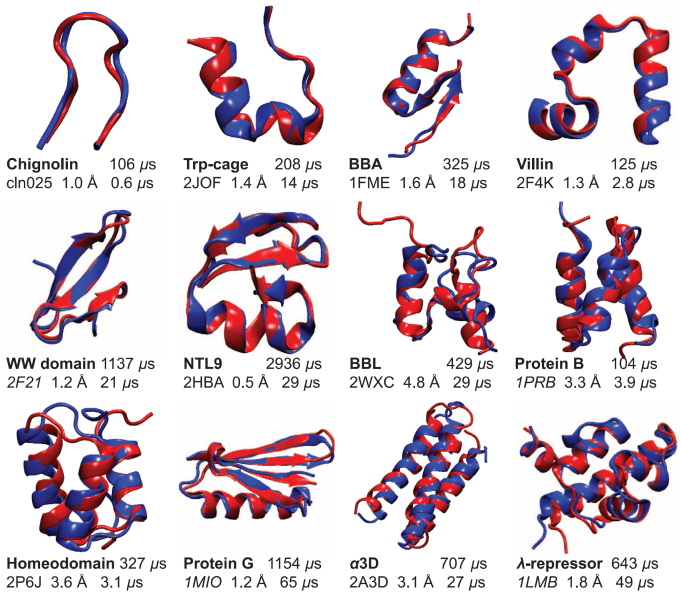
Records in MD simulations

- **World's Largest Molecular Dynamics Simulation**[1] (2013)

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

- **World's Longest Molecular Dynamics Simulation**[2] (2015)

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



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

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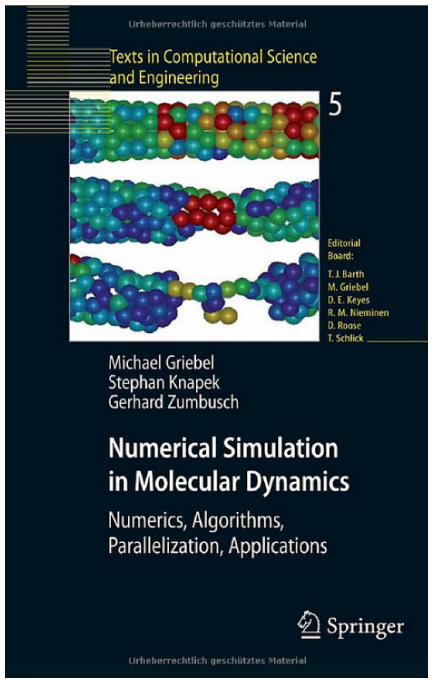
I encourage you to consult the literature. . .

Sources & Reading

Recommended reading:



Sources:

[1] M. Griebel, S. Knapek, 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!