Multiscale Simulations of Materials and Structures

Lecture 1.
Molecular Dynamics I

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Outline

Matter constituents

Standard Model

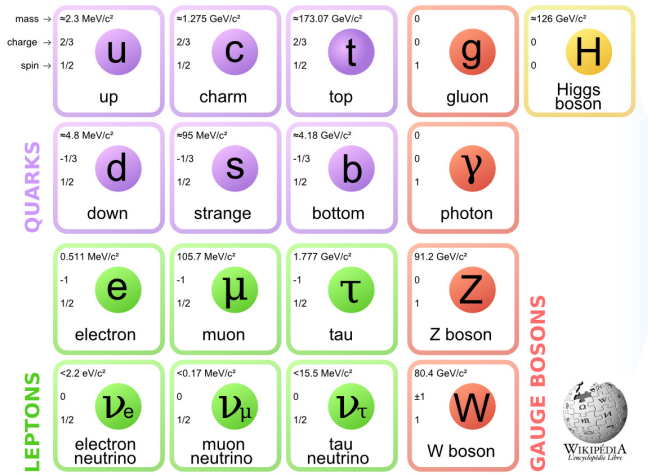
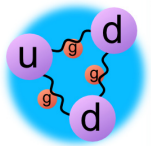


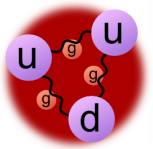
Table from WikipediA

QCD

Neutron



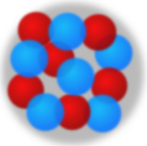
Proton



Quarks are tied by gluons
(strong interaction)

Nuclear physics

Nucleus

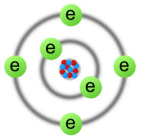


Z protons
(atomic number)
N neutrons
(neutron number)

Nucleons are tied by mesons
(quark+antiquark)
nuclear forces

Chemistry (QED)

Atom



Atoms are tied by photons
(electromegnetic forces)

$A \sim 10^{-16}$ m $R \sim Z^{1/3}$ $5\ 10^{-15}$ m 10^{-10} m Size

Chemical bonds

Nature of bonds :

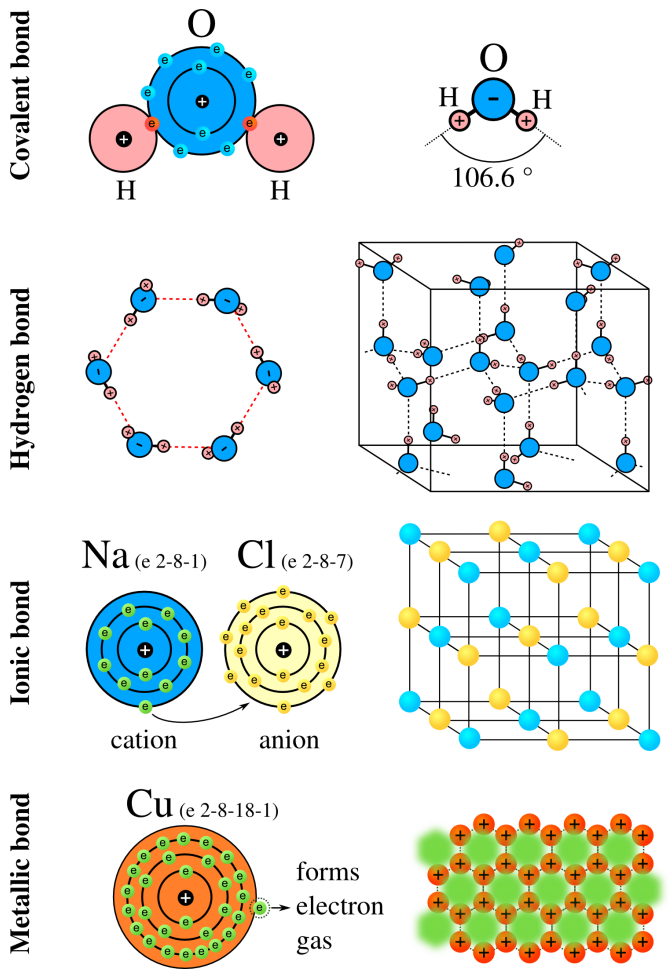
- Electrostatic force
- Electrons sharing mechanism

Strength of bonds :

- Strong (ionic, covalent)
- Weak (hydrogen, van der Waals)

Examples :

- Covalent (H_2O, H_2)
- Hydrogen (H_2O, DNA)
- Ionic (NaCl, NaF)
- Metallic (all metals)
- Van der Waals (dipole-dipole e.g. HCl-HCl, induced dipoles)



Linus Pauling "The Nature of the Chemical Bond"
http://scarc.library.oregonstate.edu/coll/pauling/bond/index.html

Assemblies

Lattices

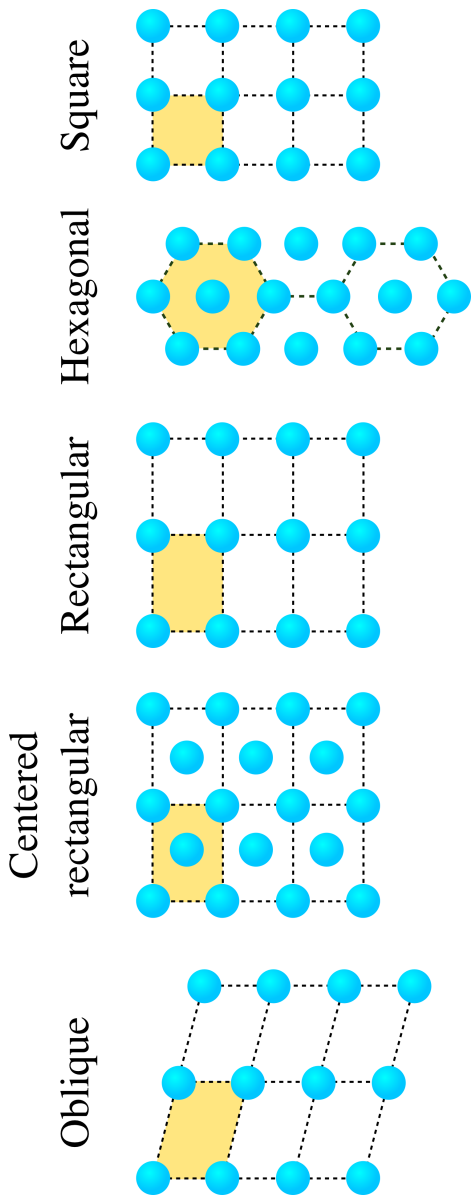
- In 2D : 5 Bravais lattices
- In 3D : 14 Bravais lattices

Molecules

- Diatomic gas (N_2, O_2)
- Ethanol (C_2H_50H)
- Macromolecules (rubber, DNA, polyethene, protein)

Amorphous

- Silica SiO_2
- Metallic glass



Complexity

- Non-relativistic Schrödinger equation for a single particle in an electric field

$$i\hbar\frac{\partial\Psi(\boldsymbol{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\boldsymbol{r},t)\right]\Psi(\boldsymbol{r},t),$$

  where Ψ is the wave function, V is particle's potential energy, μ is its reduced mass

- For n particles

$$i\hbar\frac{\partial\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t)}{\partial t} = \left[-\frac{\hbar^2}{2}\left(\frac{\nabla_1^2}{\mu_1}+\cdots+\frac{\nabla_n^2}{\mu_n}\right) + V(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t)\right]\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t),$$

- Time independent form :

$$E\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t) = \left[-\frac{\hbar^2}{2}\left(\frac{\nabla_1^2}{\mu_1}+\cdots+\frac{\nabla_n^2}{\mu_n}\right) + V(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t)\right]\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t),$$

- Modern chemistry can solve Schrödinger equation with up to 40-50 electrons (only !).

Density Functional Theory

- The DFT is the most successfull approach to compute the electronic structure of matter

  (Nicely presented in http://www.uam.es/personal_pdi/ciencias/jcuevas/Talks/JC-Cuevas-DFT.pdf)

- Applicable from nuclei to solids and fluids :
  molecular structures, vibrational frequencies, energies of atomization, ionization energies, electromagnetic properties, reaction paths, etc.

- Many-particle Schrödinger equation is reduced to minimization of an energy functional with respect to the non-universal functional V (system-dependent part of the total system energy)

- Nobel prize in Chemistry was attributed to Walter Kohn and John Pople for their developments in computational methods in quantum chemistry

  W Kohn, LJ Sham. Self-consistent equations including exchange and correlation effects, Phys Rev, 1965 (37 540 citations)

  RG Parr, W Yang. Density-functional theory of atoms and molecules. Oxford university press, 1989 (16 830 citations)

- Software : e.g. *QuantumEspresso* (www.quantum-espresso.org)

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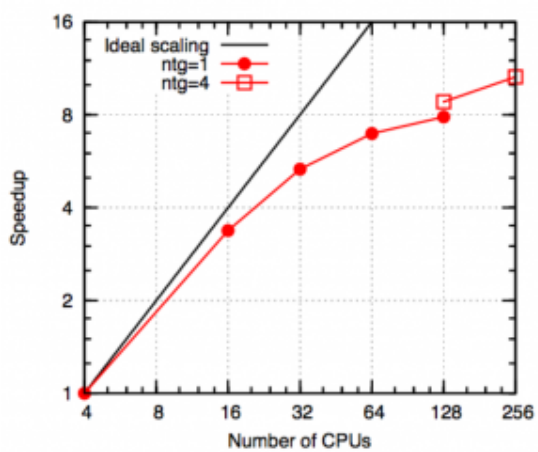
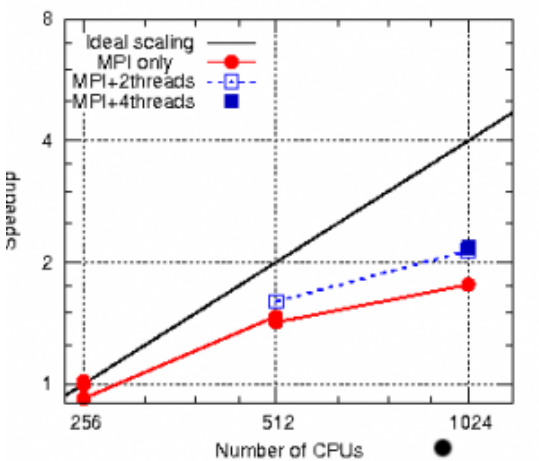


128 Water molecules (1024 electrons) in a cubic box 13.35 Å side, MPI only.



Fragment of an Aβ-peptide in water containing 838 atoms and 2312 electrons in a 22.1×22.9×19.9 $Å^3$ cell : MPI+OpenMP

Simulating bonds

Straightforward in classical mechanics (Coulomb), non-trivial in quantum one (Schrödinger, DFT)

- **Ionic bonds**

Non-trivial (Schrödinger, DFT)

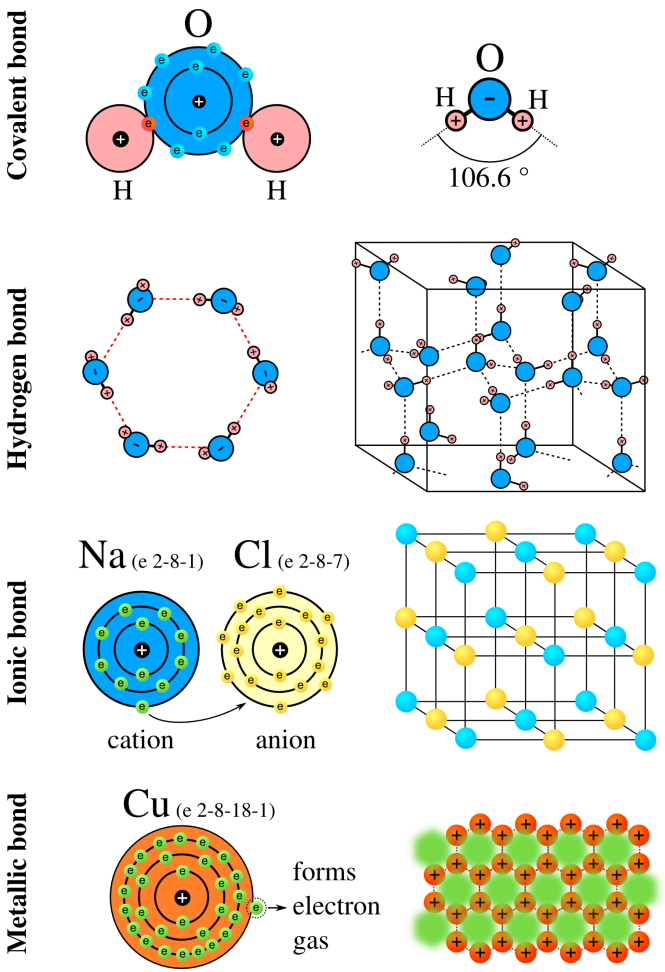
- **Covalent bonds**

If electronic structure of the molecule is well resolved (DFT) then feasible :

- **Hydrogen bonds**
- **Dipole-dipole**
- **Induced dipoles**

If electronic structure of the **lattice** *is well resolved (DFT) then feasible :*

- **Metallic bonds**



From Schrödinger equation to MD I

- Split wave function (nuclei $\boldsymbol{R}_i$, electrons $\boldsymbol{r}_j$)

$$\Psi(\boldsymbol{r}_i, \boldsymbol{R}_j, t) = \phi(\boldsymbol{r}_i, t)\chi(\boldsymbol{R}_j, t)$$

- Wave function for nuclei are generated to expectation values
- Restriction to the ground state ($\phi = \phi_0$ is retained, i.e. $\Delta E(\phi_0, \phi_1)$ is big)
- Simplified mixed quantum-mechanical and classical problem :

$$\begin{cases} M_k \ddot{\boldsymbol{R}}_k(t) = \boldsymbol{F}_{R_k} = -\nabla_{R_k} V_e(\boldsymbol{R}(t)) \\ i\hbar \frac{\partial \phi_0(\boldsymbol{r},t)}{\partial t} = \hat{\mathcal{H}}(\boldsymbol{R}(t), \boldsymbol{r})\phi_0(\boldsymbol{r}, t) \end{cases}$$

- Taylor expansion for V_e :

$$V_e(\boldsymbol{R}) \approx V_{\text{approx}}(\boldsymbol{R}) = \sum_i V_1(\boldsymbol{R}_i) + \sum_{ij} V_2(\boldsymbol{R}_i, \boldsymbol{R}_j) + \sum_{ijk} V_3(\boldsymbol{R}_i, \boldsymbol{R}_j, \boldsymbol{R}_k) + \ldots,$$

where potentials V_n contain electronic degrees of freedom.

[1] Griebel M, Knapek S, Zumbusch G. "Numerical simulation in molecular dynamics". Springer (2007).

[2] Marx D, Hutter J. "Ab initio molecular dynamics : Theory and implementation" in *Modern methods and algorithms of quantum chemistry* (2000)

From Schrödinger equation to MD II

- Global potential energy hyper-surface

$$V_{\text{approx}}(\boldsymbol{R}) = \sum_i V_1(\boldsymbol{R}_i) + \sum_{ij} V_2(\boldsymbol{R}_i, \boldsymbol{R}_j) + \sum_{ijk} V_3(\boldsymbol{R}_i, \boldsymbol{R}_j, \boldsymbol{R}_k) + \dots$$

- Newton's equation of motion in classical Molecular Dynamics

$$M_k \ddot{\boldsymbol{R}}_k(t) = -\nabla_{R_k} V_{\text{approx}}(\boldsymbol{R}(t))$$

- Potential $V_{\text{approx}}(\boldsymbol{R})$ is often approximated as a 1D pair potential

$$V_{\text{approx}}(\boldsymbol{R}) \approx \sum_{ij} V_2(r_{ij}), \quad r_{ij} = |\boldsymbol{R}_i - \boldsymbol{R}_j|$$

- Justification and error estimation are problematic
- Quantum effects and thus chemical reactions are excluded by construction

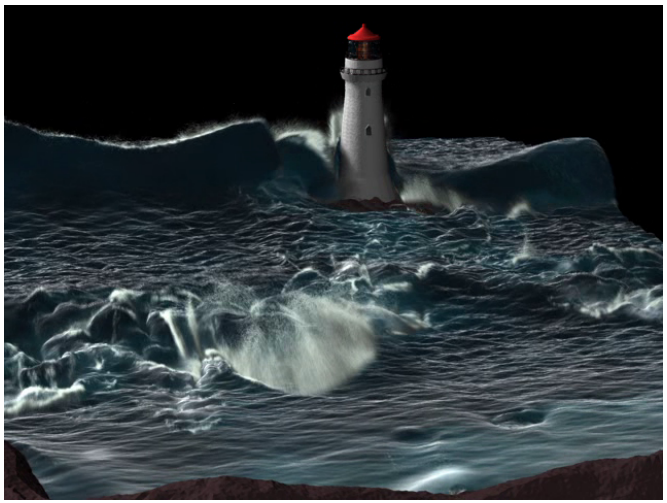
MD from the family of Particle Methods

Particle methods

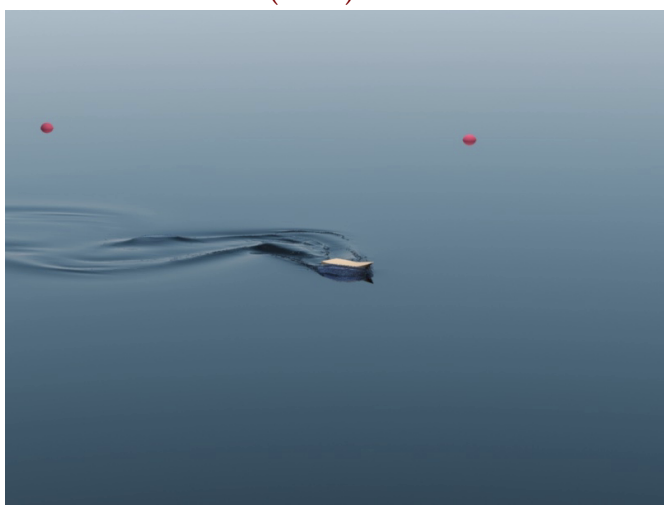
- **SPH**
  Smooth-particle hydrodynamics (fluids, solids)
- **DEM**
  Discrete element method (granular matter)
- **LBM**
  Lattice Boltzmann Method (fluids)
- Multi-body gravity methods (space scale systems)

Common algorithms

- Search and detection
- Data structure
- Parallelization



Coupled SPH and particle level-set
Losasso, Talton, Kwatra, Fedkiw. IEEE TVCG (2008).



Coupling grid+particle
Zheng, Zhu, Kim, Fedkiw, J. Comp. Phys. (2015)

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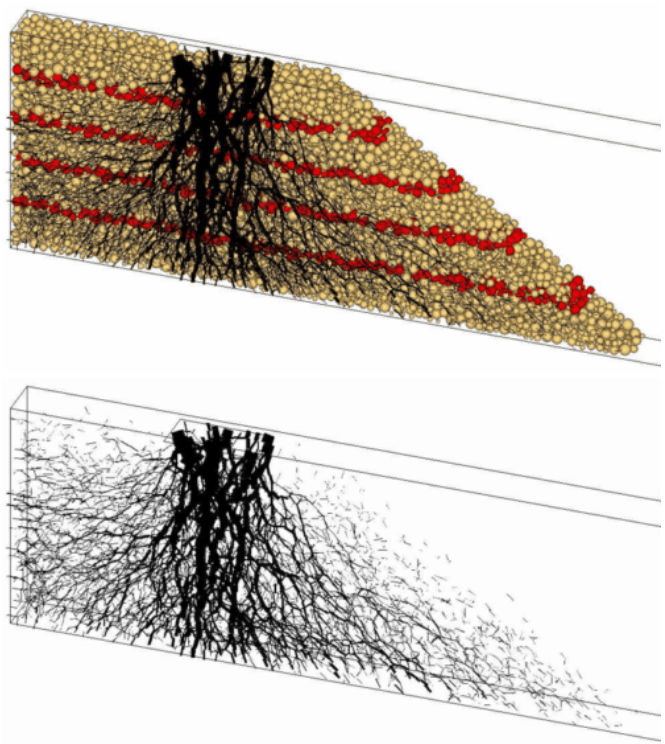

DEM simulation
Fabio Gabrieli (University of Padova)
`geotechlab.wordpress.com`

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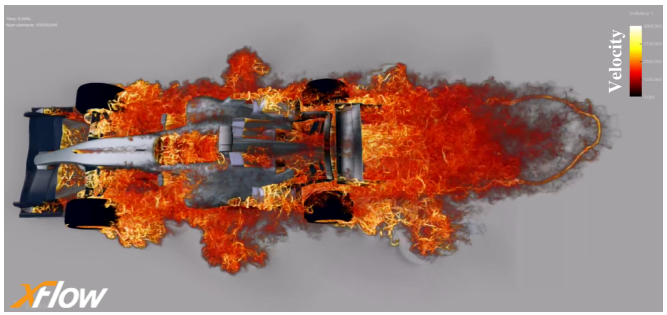
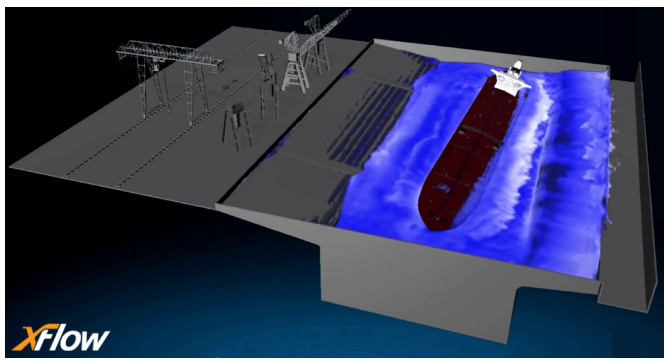


Formula 1 simulation



Ship launch simulation

BLM simulations
`www.xflowcfd.com`

Examples of simple pair potentials

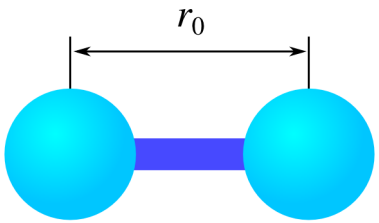
- **Short-range potentials (possible cut-off, fast)**
  - Lennard-Jones potential $U(r_{ij}) = \alpha\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^n - \left(\frac{\sigma}{r_{ij}}\right)^m\right], \quad m < n$
  - Morse potential $U(r_{ij}) = \alpha\left[1 - \exp(-\beta(r_{ij} - r_0)\right]^2$
  - Van der Waals potential $U(r_{ij}) = -\alpha\varepsilon\left(\frac{\sigma}{r_{ij}}\right)^6$
- **Long-range potentials (cut-off prohibited, slow)**
  - Gravitational potential $U(r_{ij}) = -G\frac{m_1 m_2}{r_{ij}}$
  - Electrostatic (Coulomb) potential : $U(r_{ij}) = -\frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r_{ij}}$
  - Elastic (harmonic) potential : $U(r_{ij}) = \frac{k}{2}(r_{ij} - r_0)^2$
- **Regularization**

$$\frac{1}{r_{ij}} \sim \frac{1}{\sqrt{r_{ij}^2 + \varepsilon^2}}$$

Examples of simple molecular models

- Covalent bonds approximated by harmonic potential

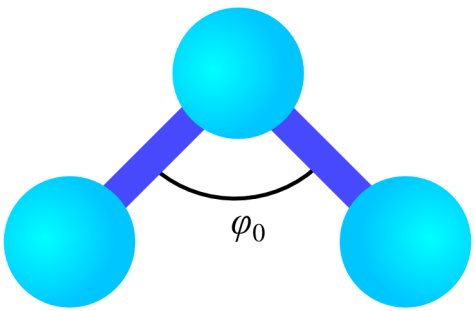
$$V_l(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{k_l}{2}(|\boldsymbol{r}_1 - \boldsymbol{r}_2| - r_0)^2$$



- In-plane angular potential

$$V_a(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \frac{k_a}{2}(1 - \cos(\phi - \phi_0))^2$$

$$V_a(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) \approx \frac{k_a}{2}(\phi - \phi_0)^2$$

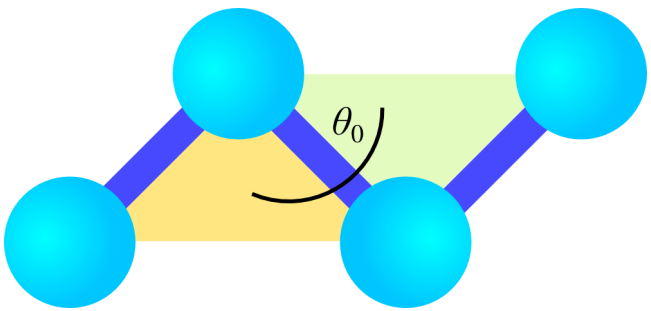


- Torsional potential

$$V_t(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}_4) \approx \frac{k_t}{2}(\theta - \theta_0)^2$$

- Intra-molecular potential

$$V_m(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots, \boldsymbol{r}_n) = \frac{1}{2}\left(\sum_{i=1}^{n-1} V_l(r^i) + \sum_{i=1}^{n-2} V_a(\phi^i) + \sum_{i=1}^{n-3} V_t(\theta^i)\right)$$



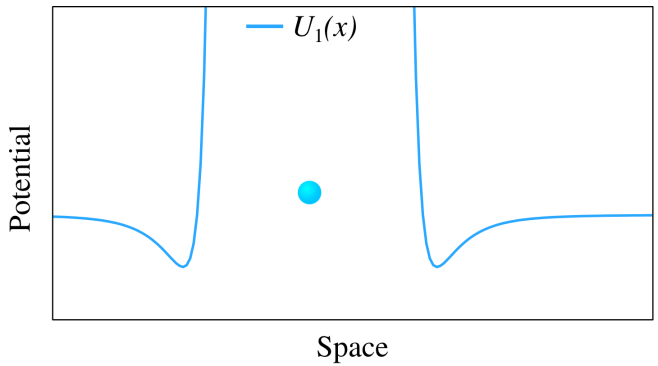
- **Total potential is complemented by an interaction potential with other molecules**

$$V(\boldsymbol{r}) = \sum_{\text{molecules}} V_m(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n) + V_i(\boldsymbol{r})$$

Many-body Hamiltonian system

General algorithm

- Potential :
  $U(r_{ij})$
- System pair potential :
  $V(\boldsymbol{r}) = \sum_{\forall i,j:\, i<j} U(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$
- Compute force $\boldsymbol{f}_0$ on particle $\boldsymbol{r}_0$:
  $\boldsymbol{F}_0 = -\nabla_{r_0} V(\boldsymbol{r}) = -\sum_{j\neq 0} \nabla_{r_0} U(|\boldsymbol{r}_0 - \boldsymbol{r}_j|)$
- 2^{nd} Newton's law :
  $\ddot{\boldsymbol{r}}_0 = \frac{1}{m_0}\boldsymbol{F}_0$
- Integrate in time :
  $\boldsymbol{r}_0(t) \rightarrow \boldsymbol{r}_0(t + \Delta t)$



Properties :

- Energy conservation
  $E = \underbrace{\frac{1}{2}\sum_i m_i \dot{\boldsymbol{r}}_i^2}_{Kinetic} + \underbrace{V(\boldsymbol{r})}_{Potential}$

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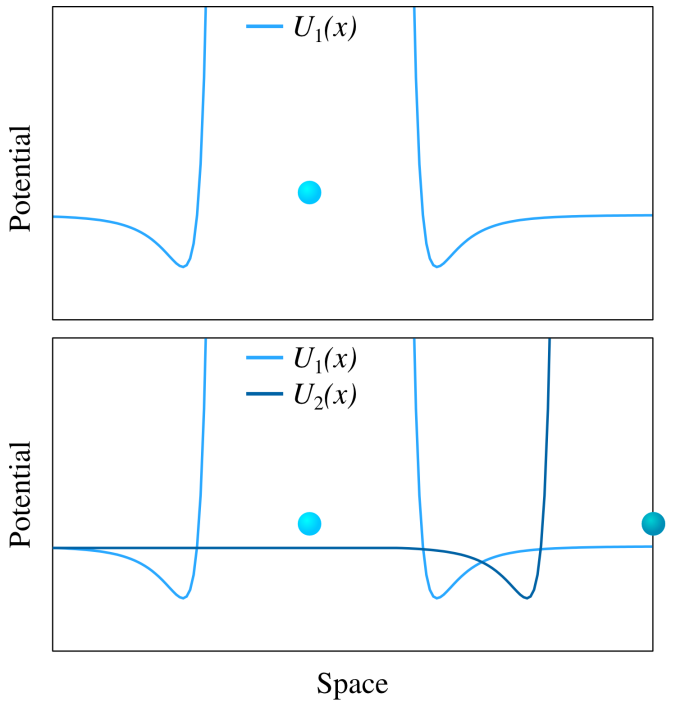

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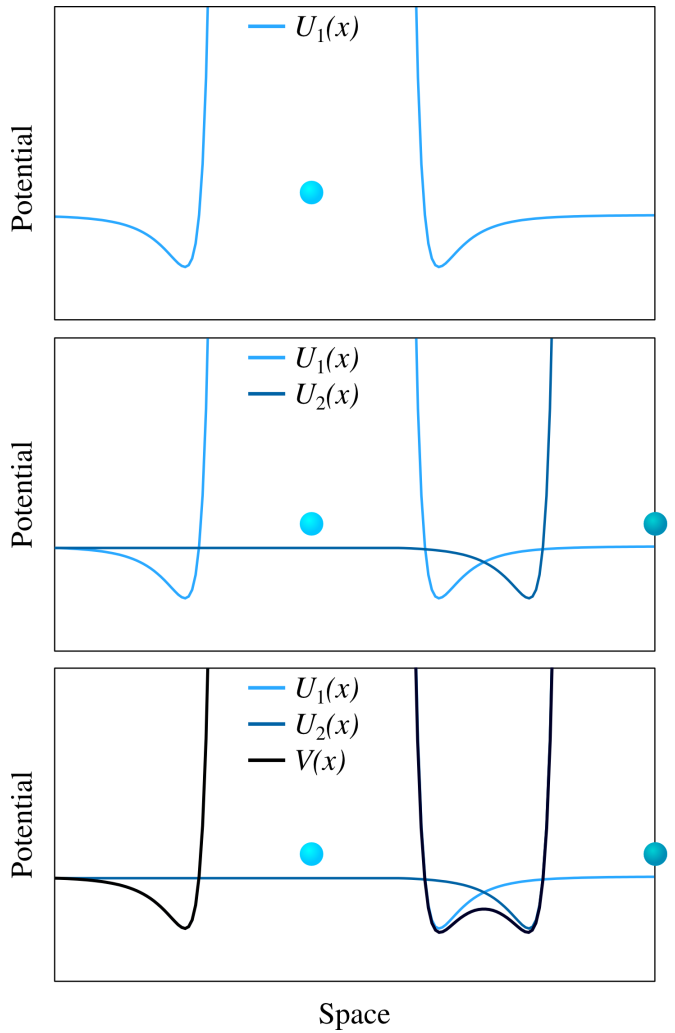

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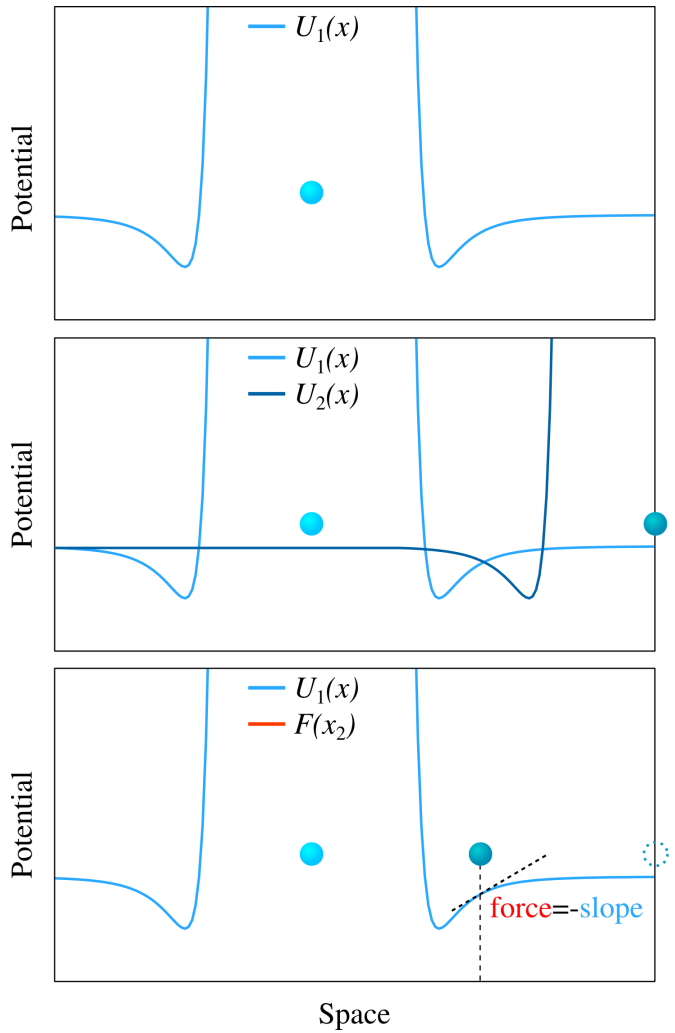

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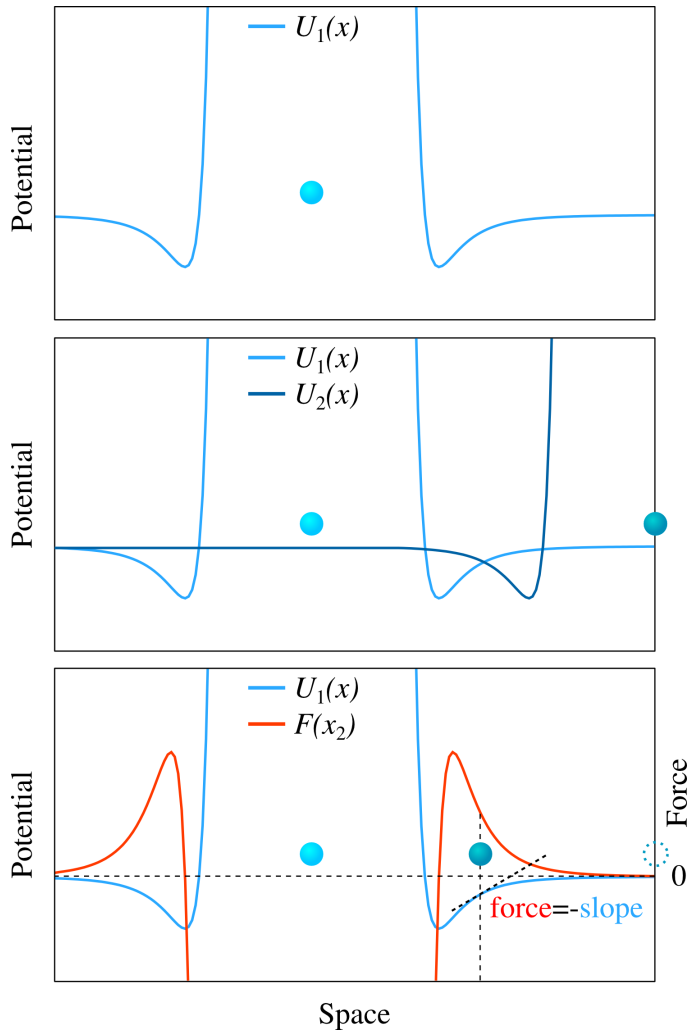

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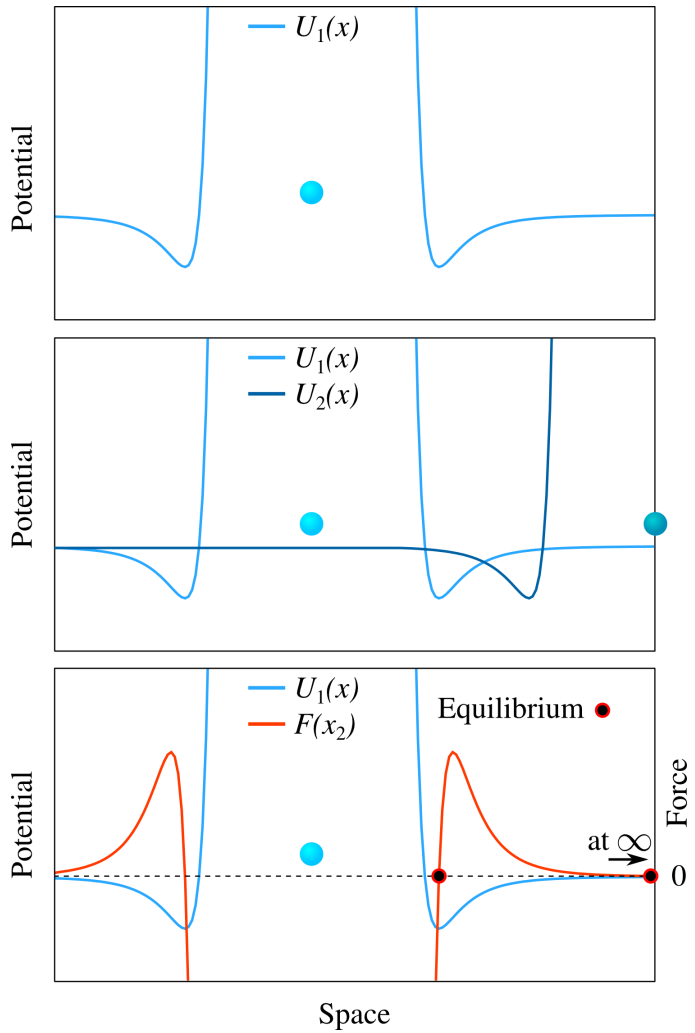

Example : Lennard-Jones potential

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- Lennard-Jones 6-12 (LJ 6-12) :

$$U(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

- Force :

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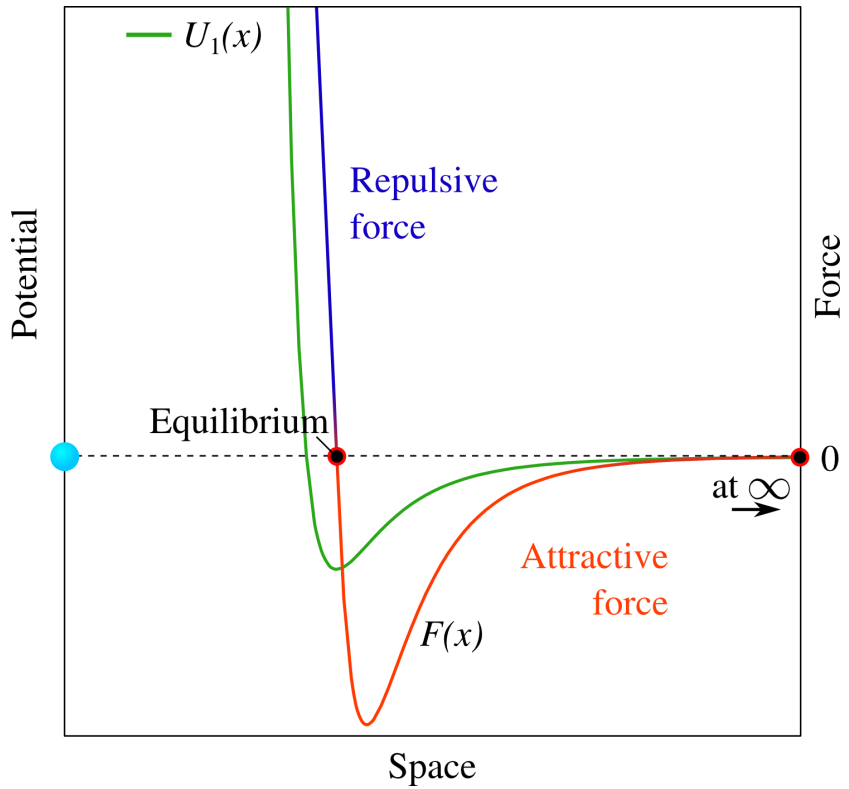

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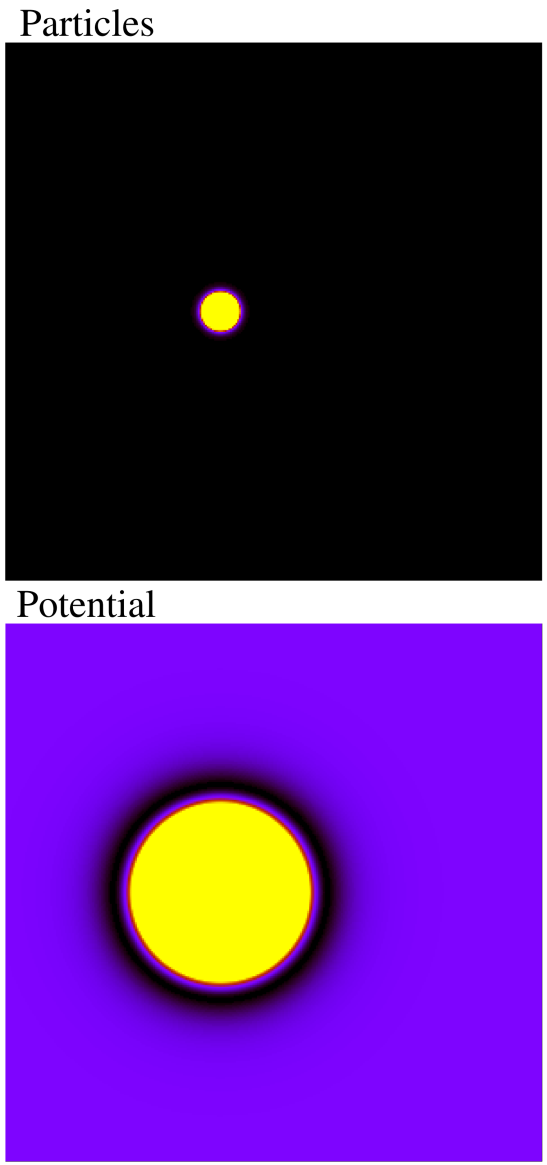

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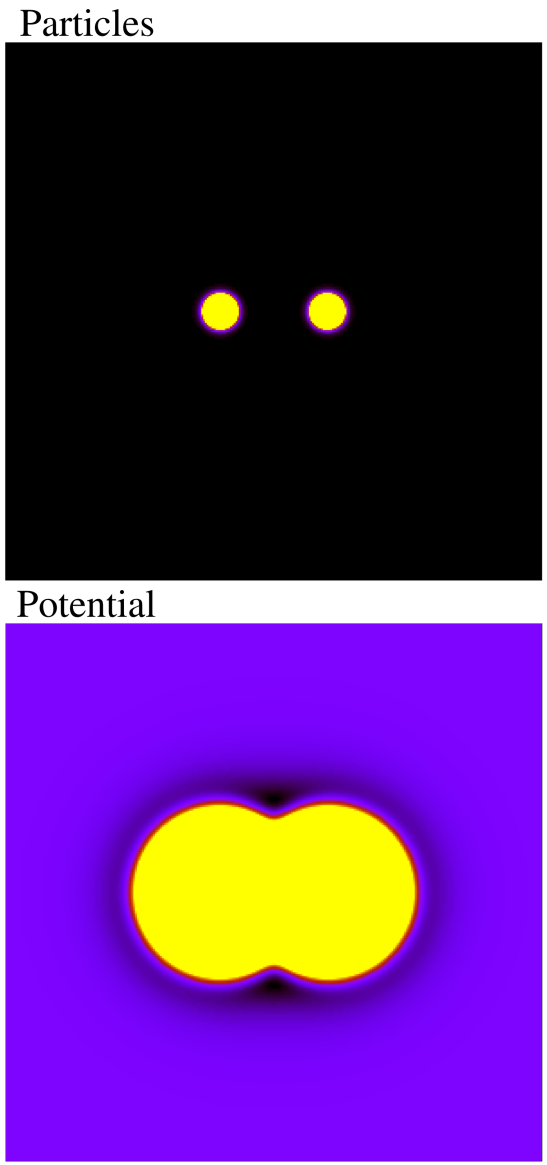

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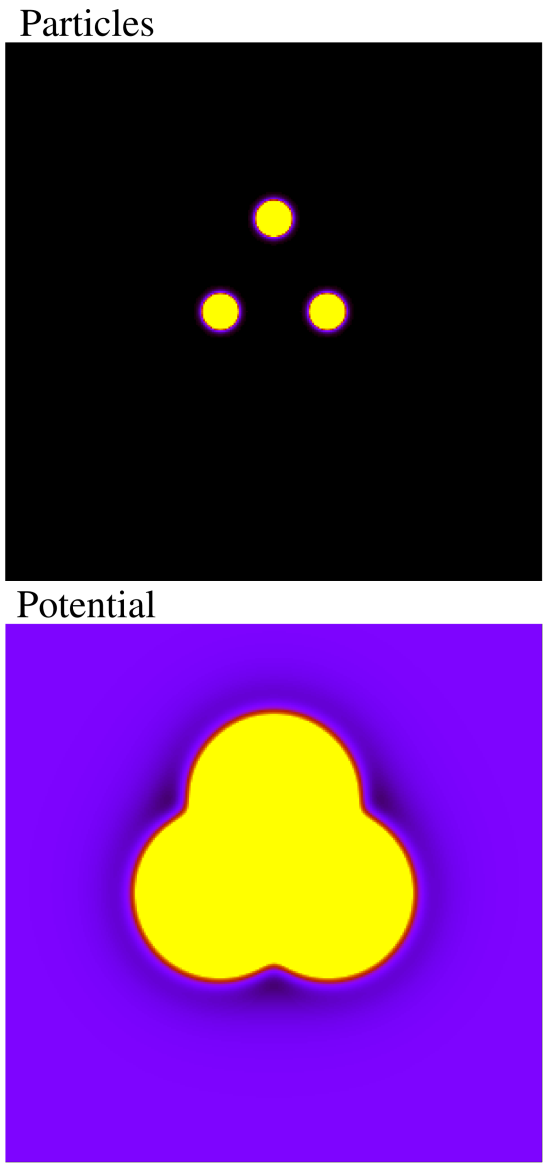

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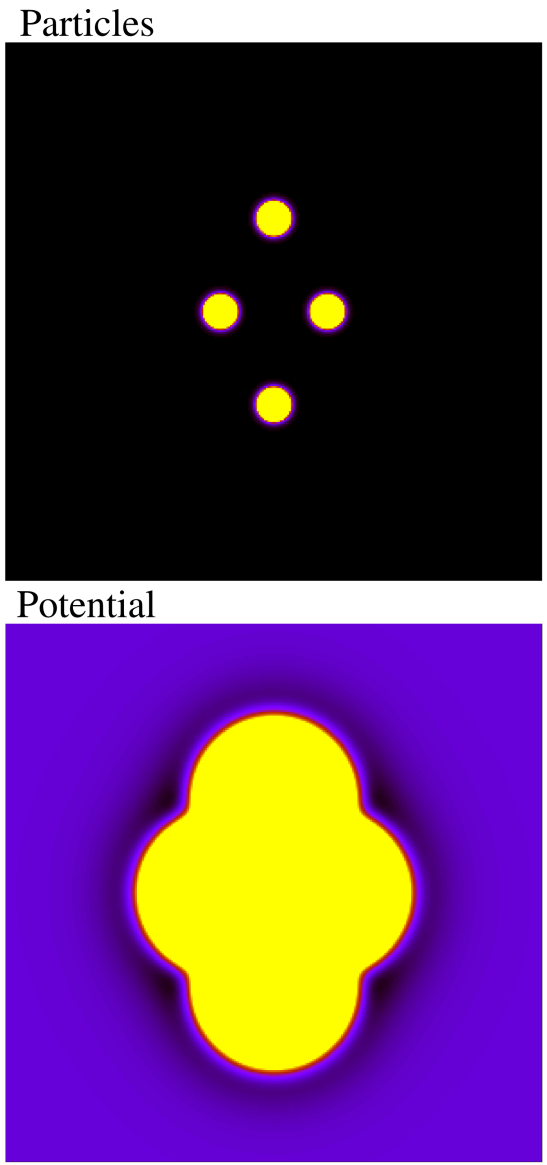

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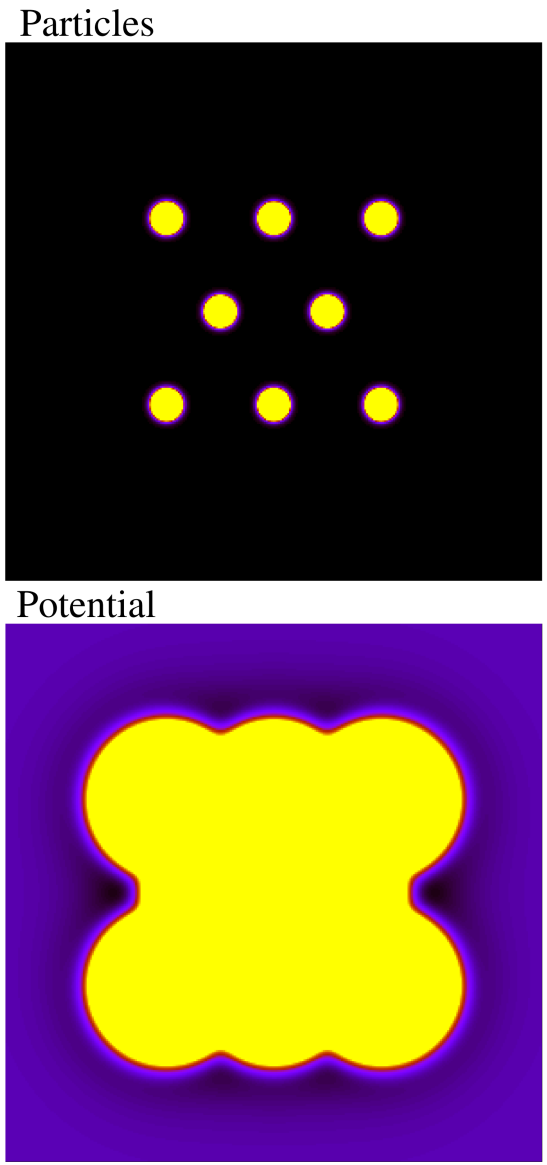

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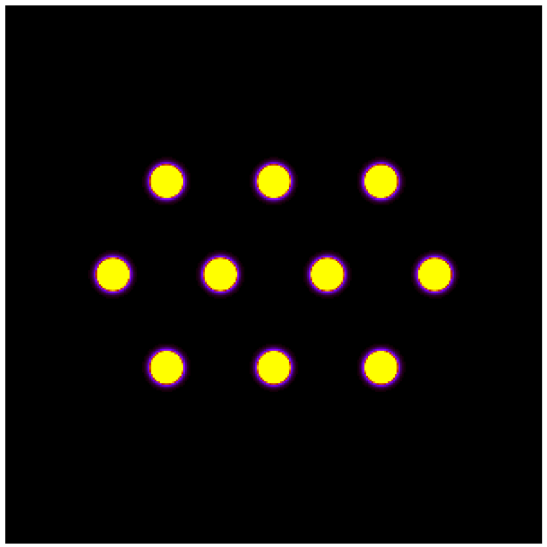
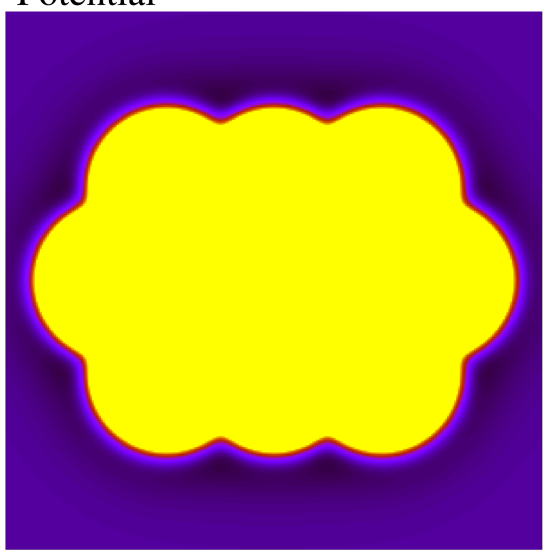
Particles



Potential



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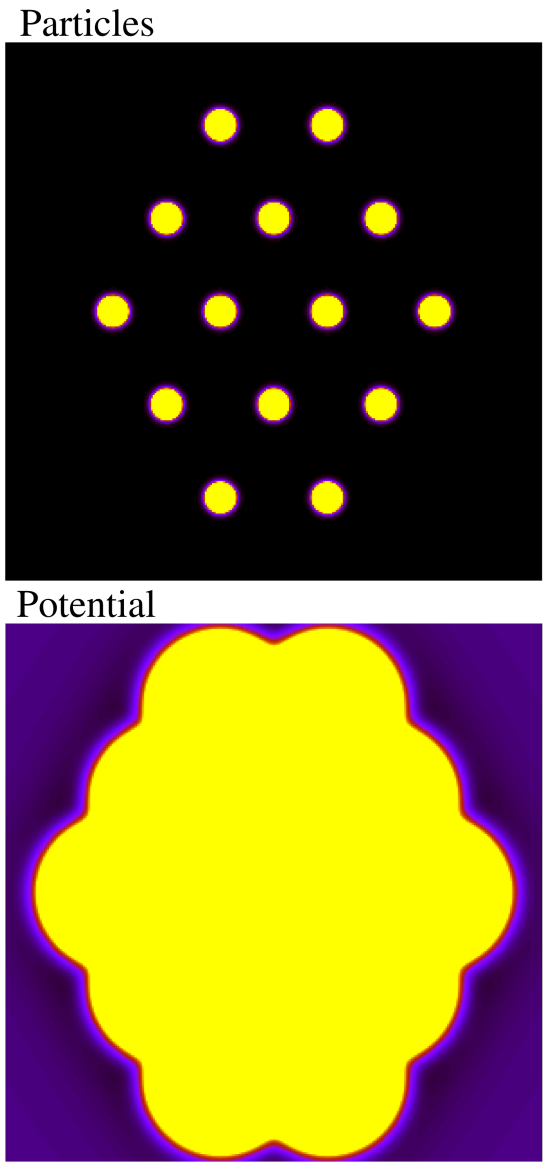


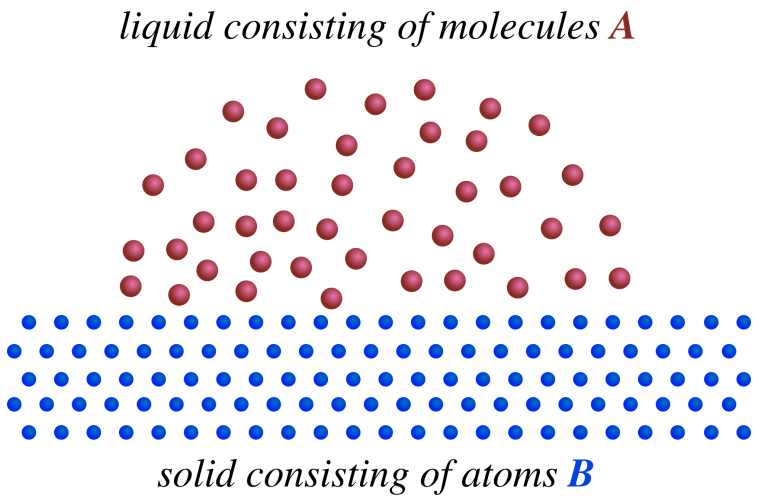
Mixing rule

- Consider a system containing 2 different atoms (molecules) : A, B
- We know ε_{AA}, σ_{AA} and ε_{BB}, σ_{BB}
- To compute energy and forces between atoms A and B we need σ_{AB} and ε_{AB}
- The classical mixing rule by Lorentz-Berthelot[1] :

$$\sigma_{AB} = \frac{1}{2}(\sigma_{AA} + \sigma_{BB})$$

$$\varepsilon_{AB} = \sqrt{\varepsilon_{AA}\varepsilon_{BB}}$$

- From algorithmic point of view one needs to check atom types
- For a liquid drop on surface, values of σ_{AB} and ε_{AB} can be obtained from the macroscopic value of the contact angle



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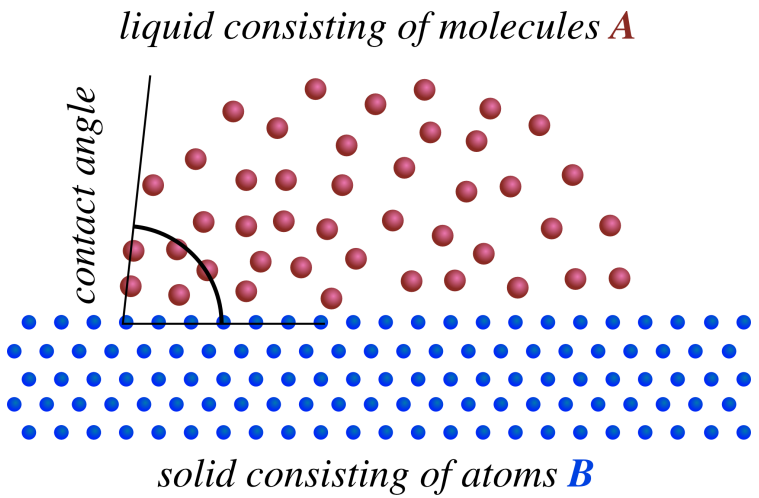


Parameters of interactions:

σ_{BB}, ε_{BB} ●↔●

σ_{AA}, ε_{AA} ●↔●

σ_{AB}, ε_{AB} ●↔●

Short-range potentials and a cutoff

- Short-range potential

$$V \sim \frac{1}{r_{ij}^{\alpha}}, \quad \alpha > \dim$$

- System pair potential :

$$V(\boldsymbol{r}) = \sum_{\forall i,j:\, i<j} U(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$$

- Complexity of the force evaluation : $O(N^2)$
- First simplification, for two particles :

$$\boldsymbol{F}_{ij} = -\boldsymbol{F}_{ji}$$

- Critical simplification : **cutoff radius** r_{cut} :

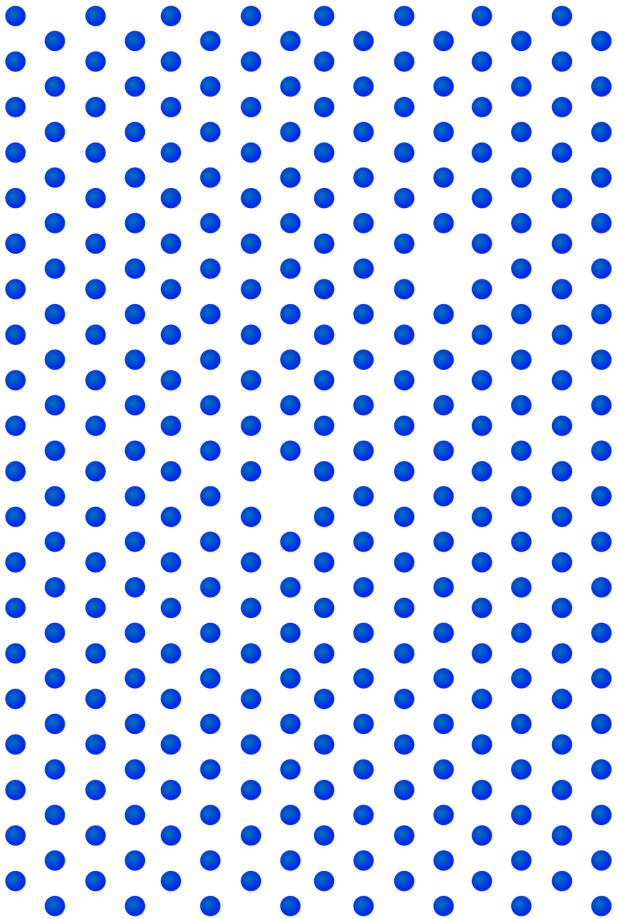
$$U(r_{ij}) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], & \text{if } r_{ij} \le r_{\text{cut}} \\ 0, & \text{if } r_{ij} > r_{\text{cut}} \end{cases}$$

- Cutoff value : $r_{\text{cut}} > 2.5\sigma$
- Attention : truncated potential is discontinuous, additional errors are introduced.

Algorithm : linked-cell method

- Create a spatial grid $d \geq r_{\text{cut}}$
- Every cell contains a list of particles and a list of neighbouring cells
- Forces are evaluated in the cell and with respect to the neighbouring cells
- 3^{rd} Newton's law is used

  Instead of checking 8 neighbouring cells, we check only 4.



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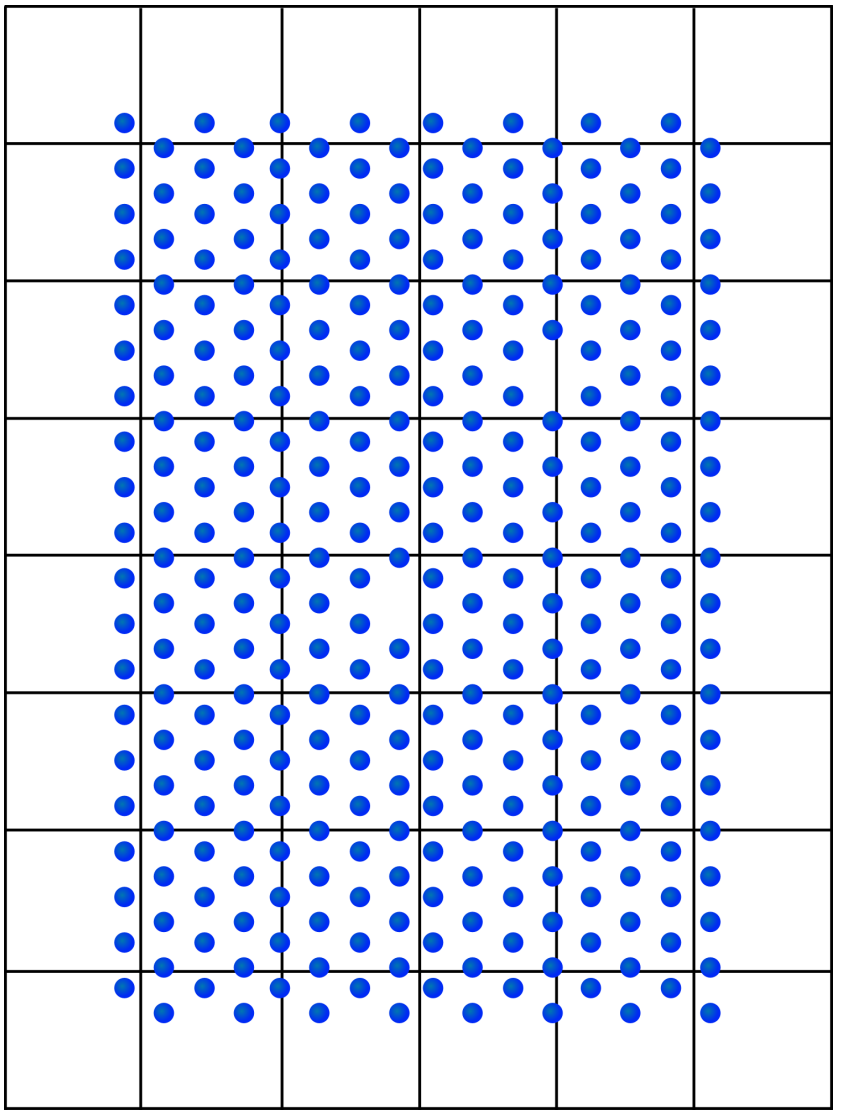

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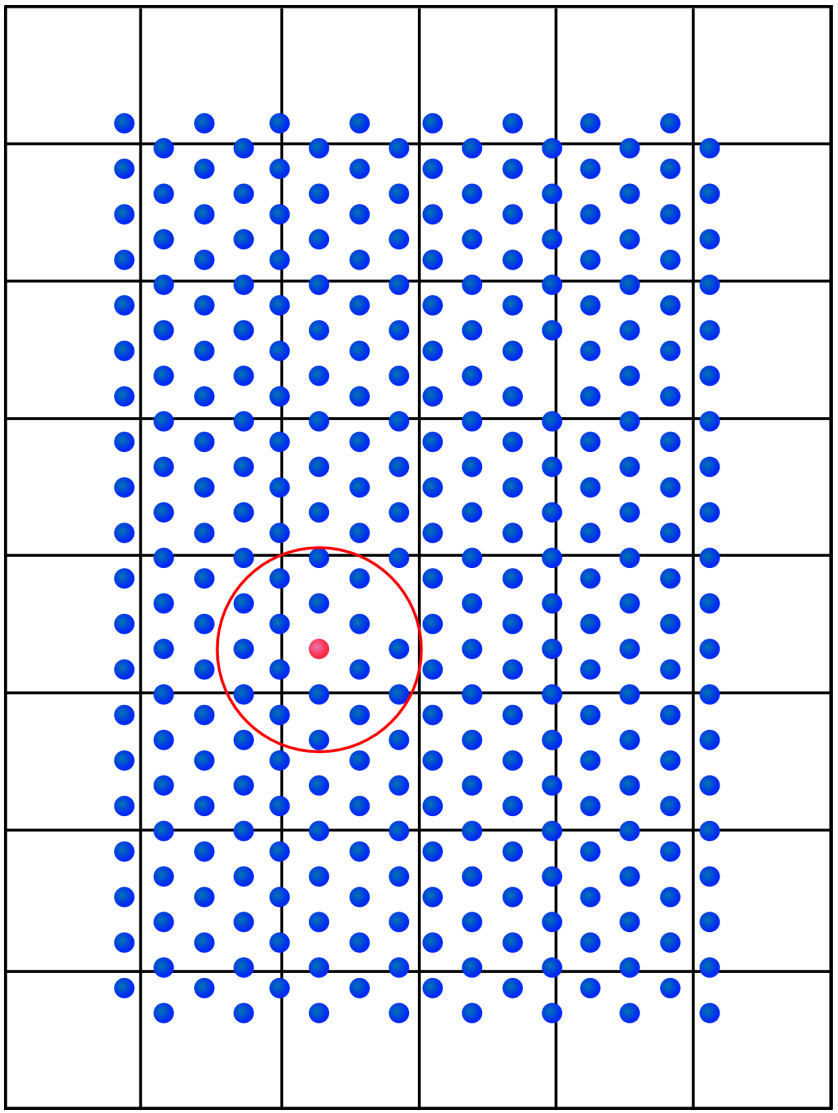

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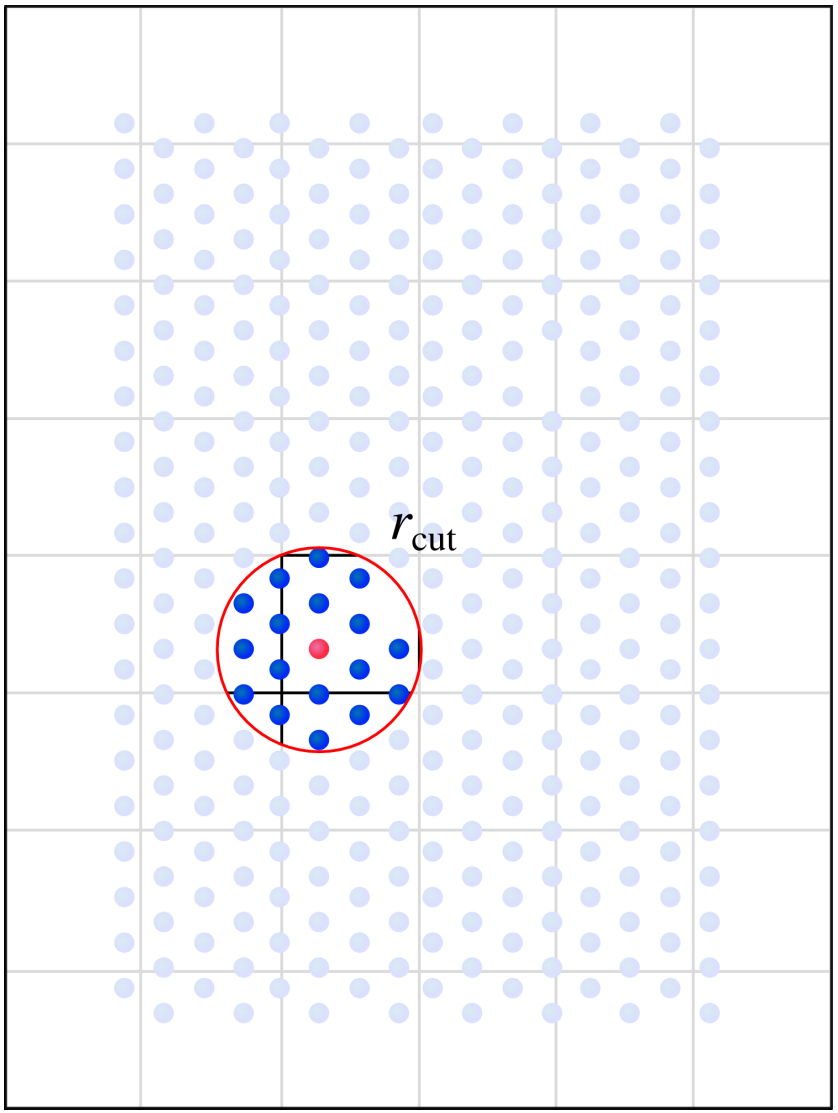

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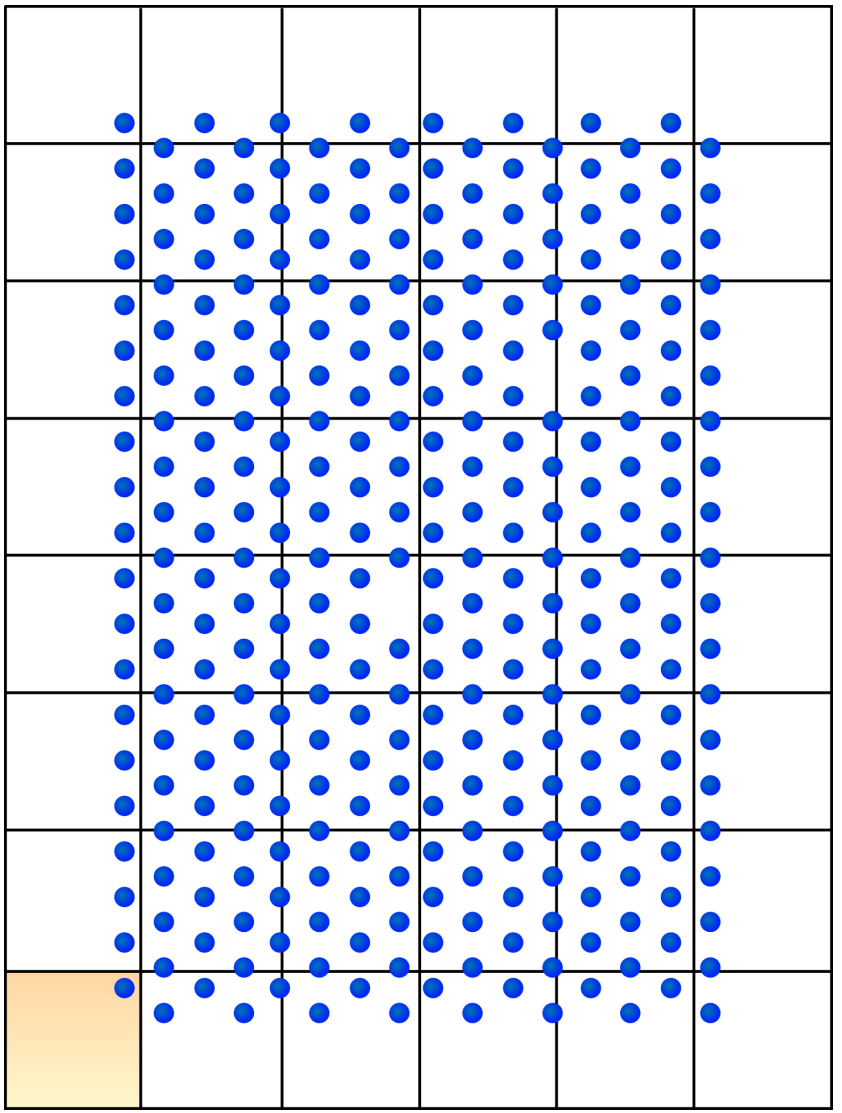

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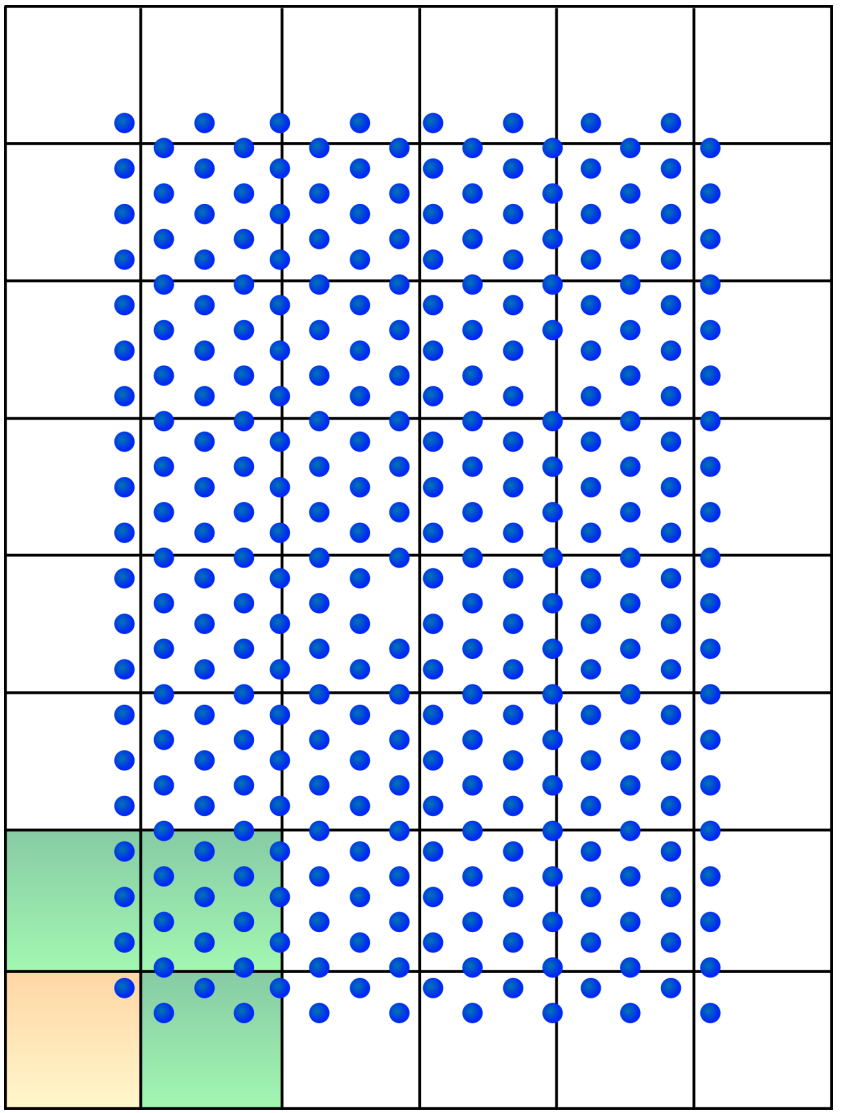

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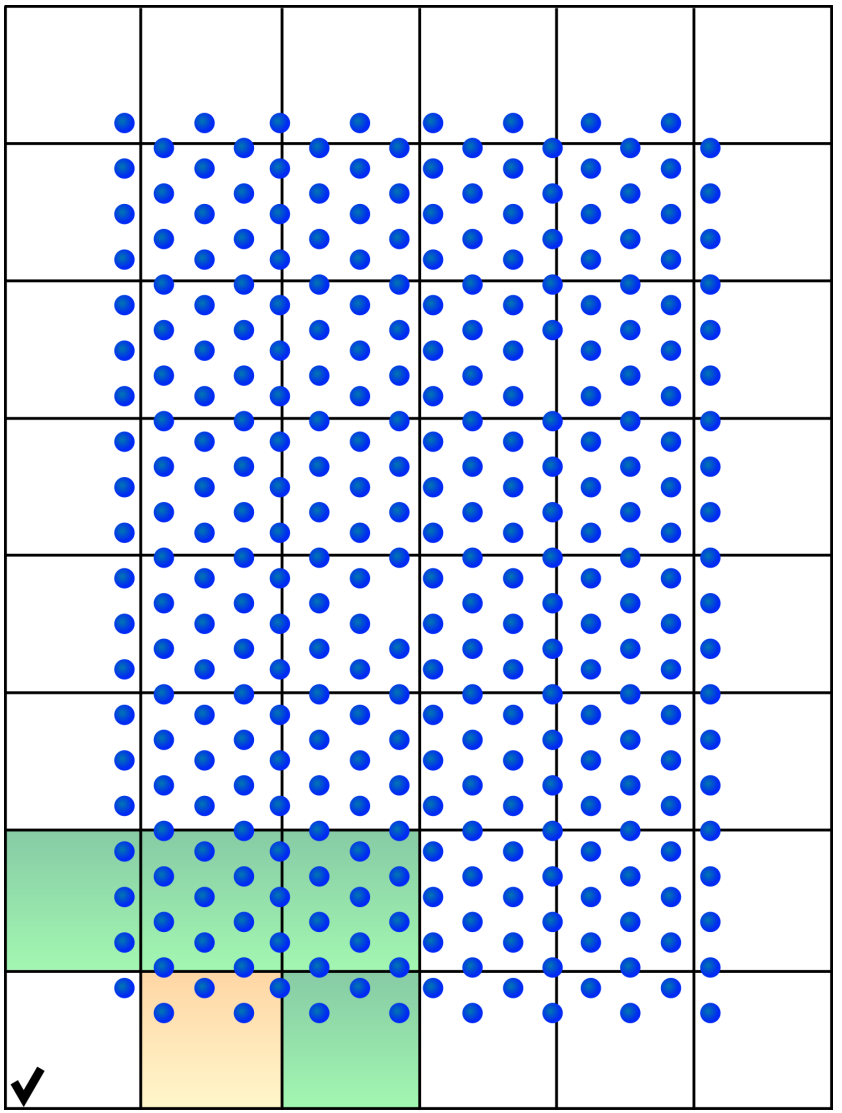

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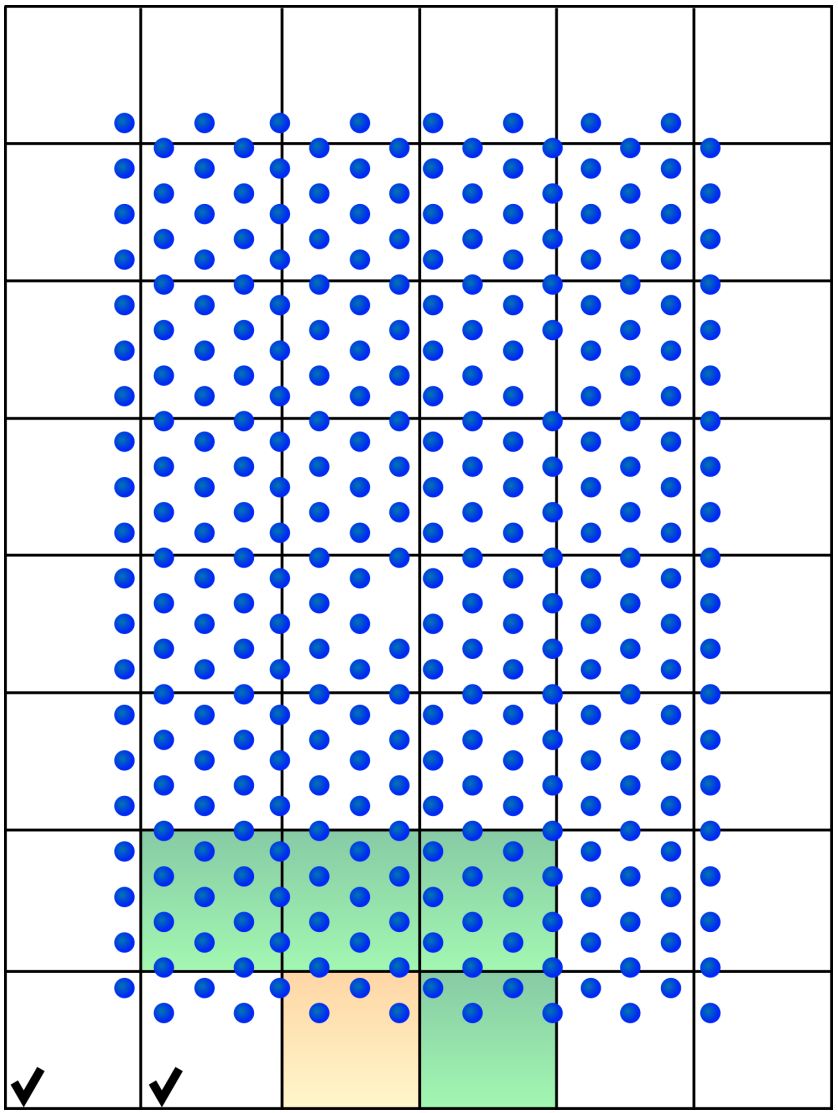

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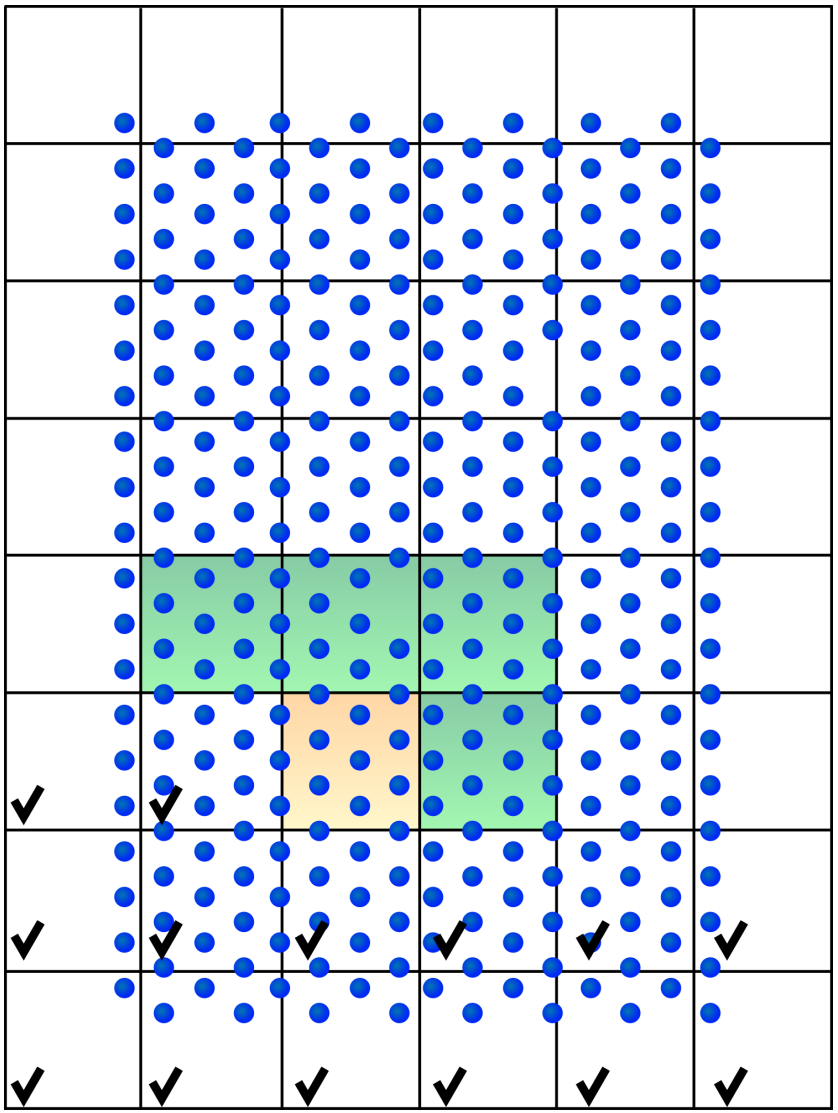

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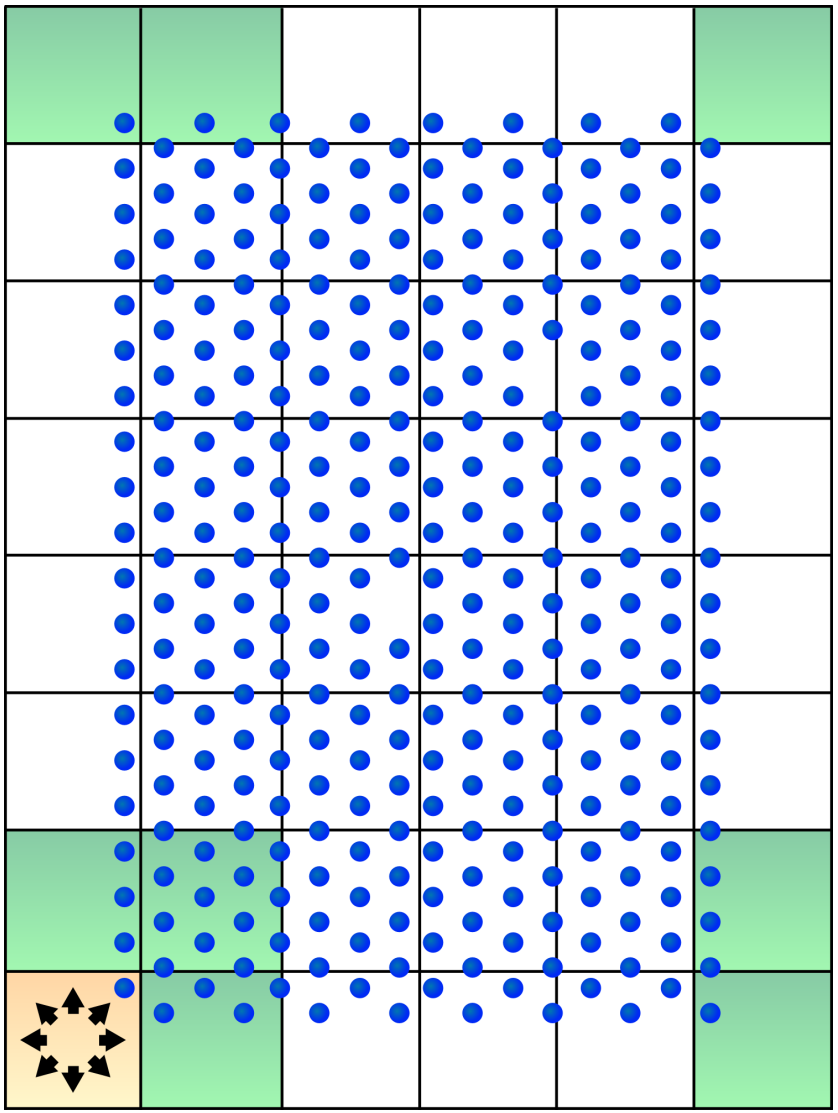


Time integration : explicit Euler

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

- Straight forward approach (**explicit Euler**)

  Compute : $f_i(x(t))$

$$m\ddot{x}_i = f_i$$

$$m\frac{\dot{x}_i(t+\Delta t)-\dot{x}_i(t)}{\Delta t} = f_i$$

  Compute :

$$\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{m_i} f_i}$$

$$\dot{x}_i(t+\Delta t) = \frac{x_i(t+\Delta t)-x_i(t)}{\Delta t}$$

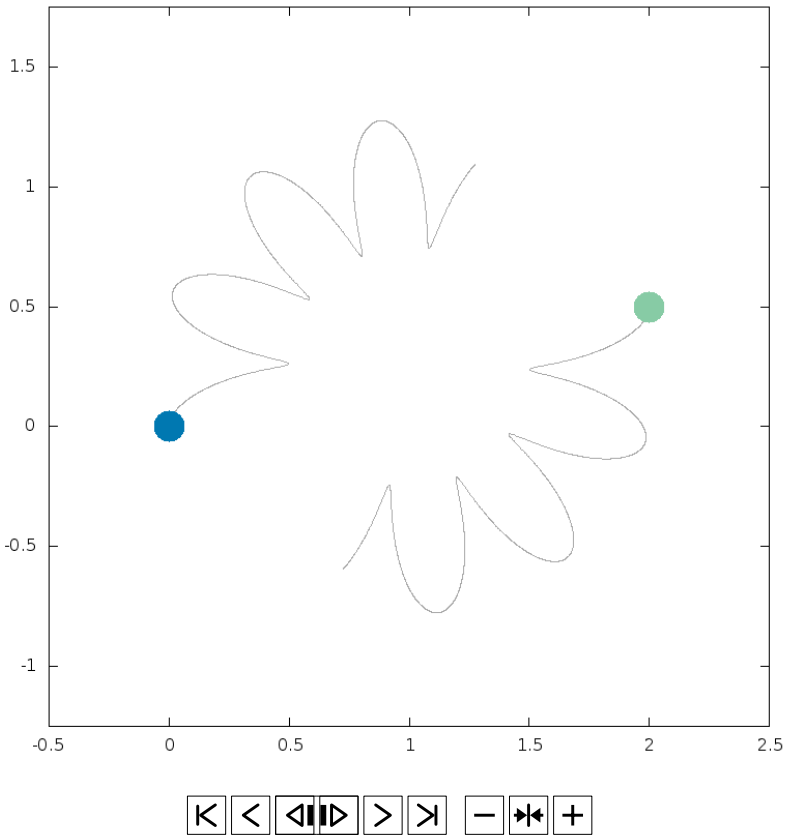
  Compute :

$$\boxed{x_i(t+\Delta t) = x_i(t) + \dot{x}_i(t)\Delta t}$$

- Let's see how fast it diverges

Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.00001$



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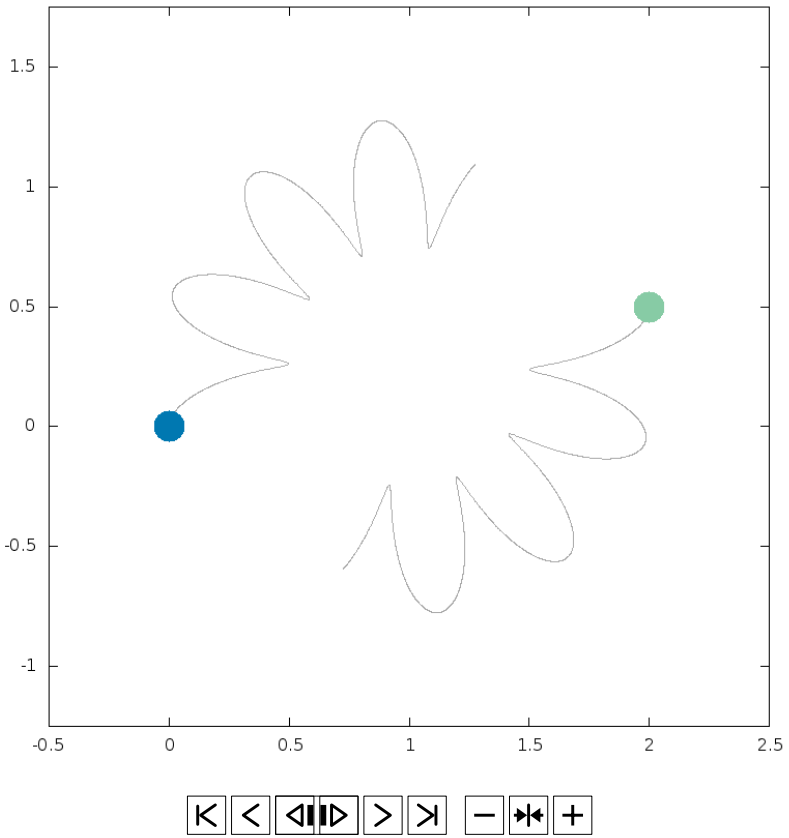

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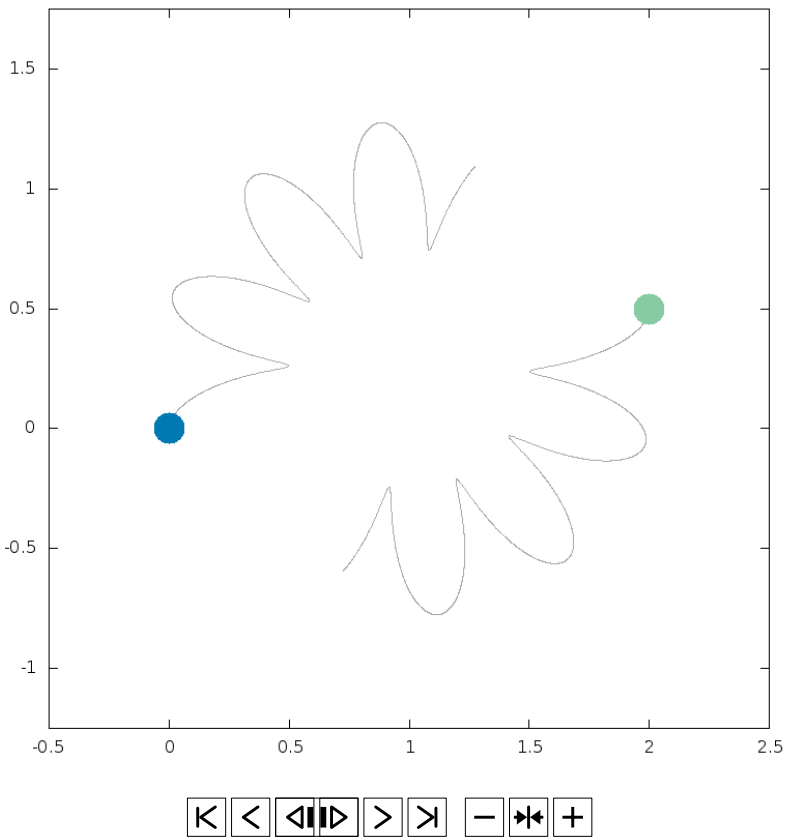


Time integration : semi-implicit Euler

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

- **A better approach**
  (**semi-implicit Euler**)

  Compute : $f_i(x(t))$

$$m\ddot{x}_i = f_i$$

$$m\frac{\dot{x}_i(t+\Delta t)-\dot{x}_i(t)}{\Delta t} = f_i$$

  Compute :

$$\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{m_i} f_i}$$

$$\dot{x}_i(t+\Delta t) = \frac{x_i(t+\Delta t)-x_i(t)}{\Delta t}$$

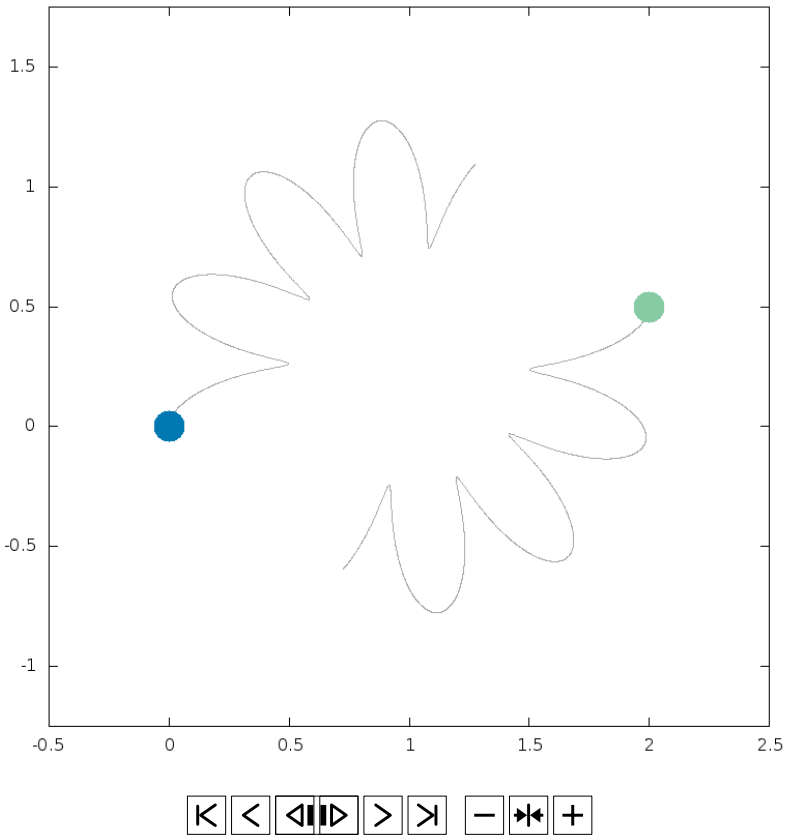
  Compute :

$$\boxed{x_i(t+\Delta t) = x_i(t) + \dot{x}_i(t+\Delta t)\Delta t}$$

- Symplectic integrator !
  In average it preserves the energy.

Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.01$



Time integration : semi-implicit Euler

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.02$

- **A better approach**

  (**semi-implicit Euler**)

  Compute : $f_i(x(t))$

$$m\ddot{x}_i = f_i$$

$$m\frac{\dot{x}_i(t+\Delta t)-\dot{x}_i(t)}{\Delta t} = f_i$$

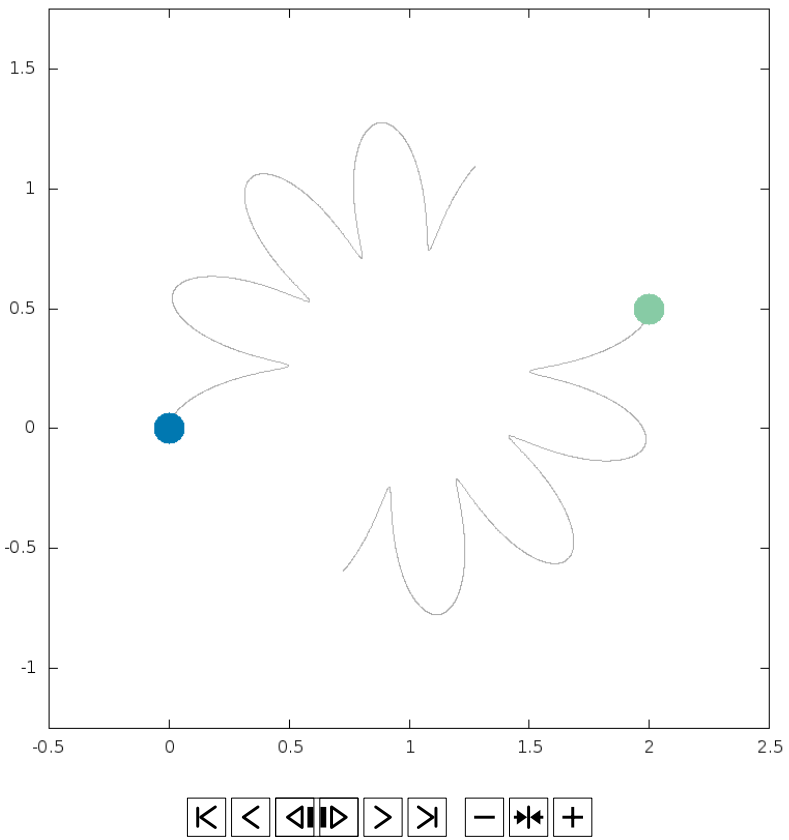
  Compute :

$$\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{m_i} f_i}$$

$$\dot{x}_i(t+\Delta t) = \frac{x_i(t+\Delta t)-x_i(t)}{\Delta t}$$

  Compute :

$$\boxed{x_i(t+\Delta t) = x_i(t) + \dot{x}_i(t+\Delta t)\Delta t}$$



- Symplectic integrator !
  In average it preserves the energy.

Time integration : semi-implicit Euler

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

- **A better approach**
  (**semi-implicit Euler**)

  Compute : $f_i(x(t))$

$$m\ddot{x}_i = f_i$$

$$m\frac{\dot{x}_i(t+\Delta t)-\dot{x}_i(t)}{\Delta t} = f_i$$

  Compute :

$$\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{m_i} f_i}$$

$$\dot{x}_i(t+\Delta t) = \frac{x_i(t+\Delta t)-x_i(t)}{\Delta t}$$

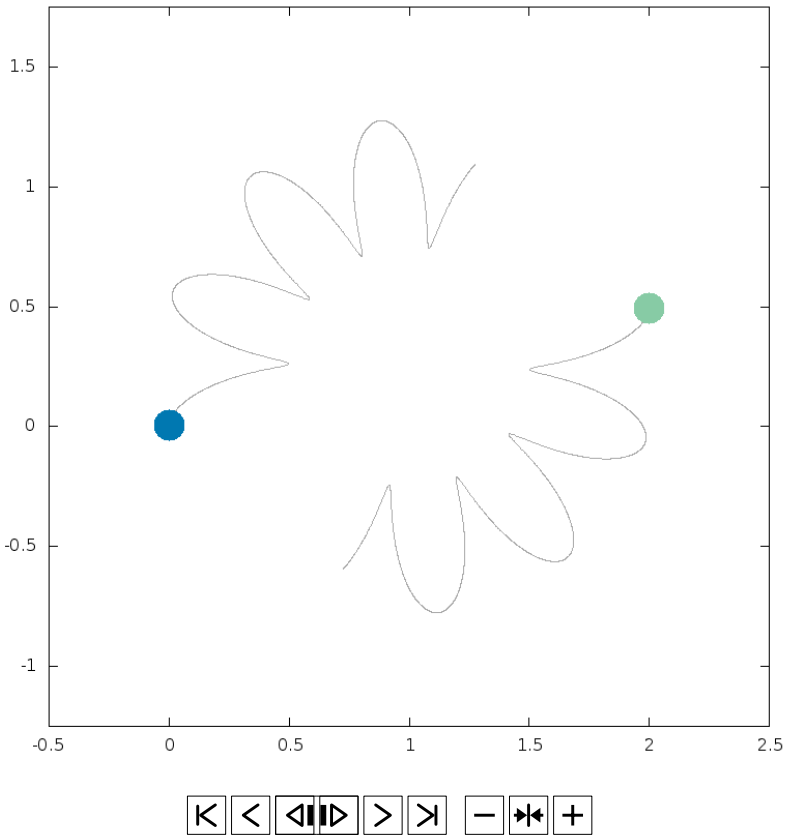
  Compute :

$$\boxed{x_i(t+\Delta t) = x_i(t) + \dot{x}_i(t+\Delta t)\Delta t}$$

- Symplectic integrator !
  In average it preserves the energy.

Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.05$



Time integration : semi-implicit Euler

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

- **A better approach**
  (**semi-implicit Euler**)

  Compute : $f_i(x(t))$

$$m\ddot{x}_i = f_i$$

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$$\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{m_i} f_i}$$

$$\dot{x}_i(t+\Delta t) = \frac{x_i(t+\Delta t)-x_i(t)}{\Delta t}$$

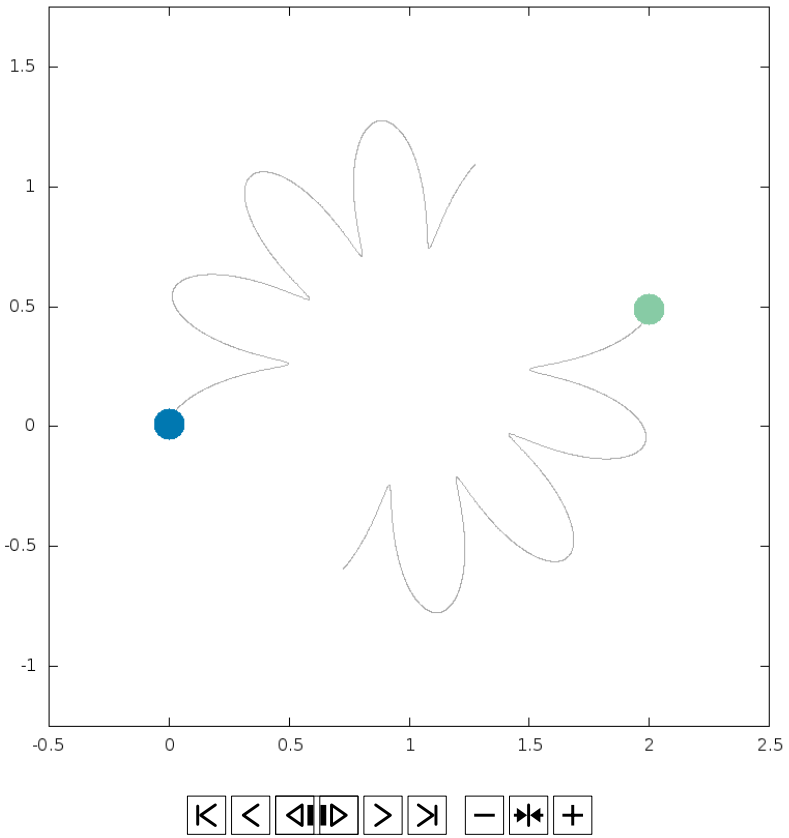
  Compute :

$$\boxed{x_i(t+\Delta t) = x_i(t) + \dot{x}_i(t+\Delta t)\Delta t}$$

- Symplectic integrator !
  In average it preserves the energy.

Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.10$



Time integration : Verlet method

- Initial value problem

$$\begin{cases} M\ddot{X}(t) = F(X) \\ X(0) = X_0, \quad \dot{X}(0) = \dot{X}_0 \end{cases}$$

- Velocity-Verlet method[1]

Compute : $\boxed{x_i(t+\Delta t) = x_i(t) + \left[\dot{x}_i(t) + \frac{\Delta t}{2m_i} f_i(t)\right]\Delta t}$

Store $f_i(t)$

Compute : $f_i(t+\Delta t) = f_i(x(t+\Delta t))$

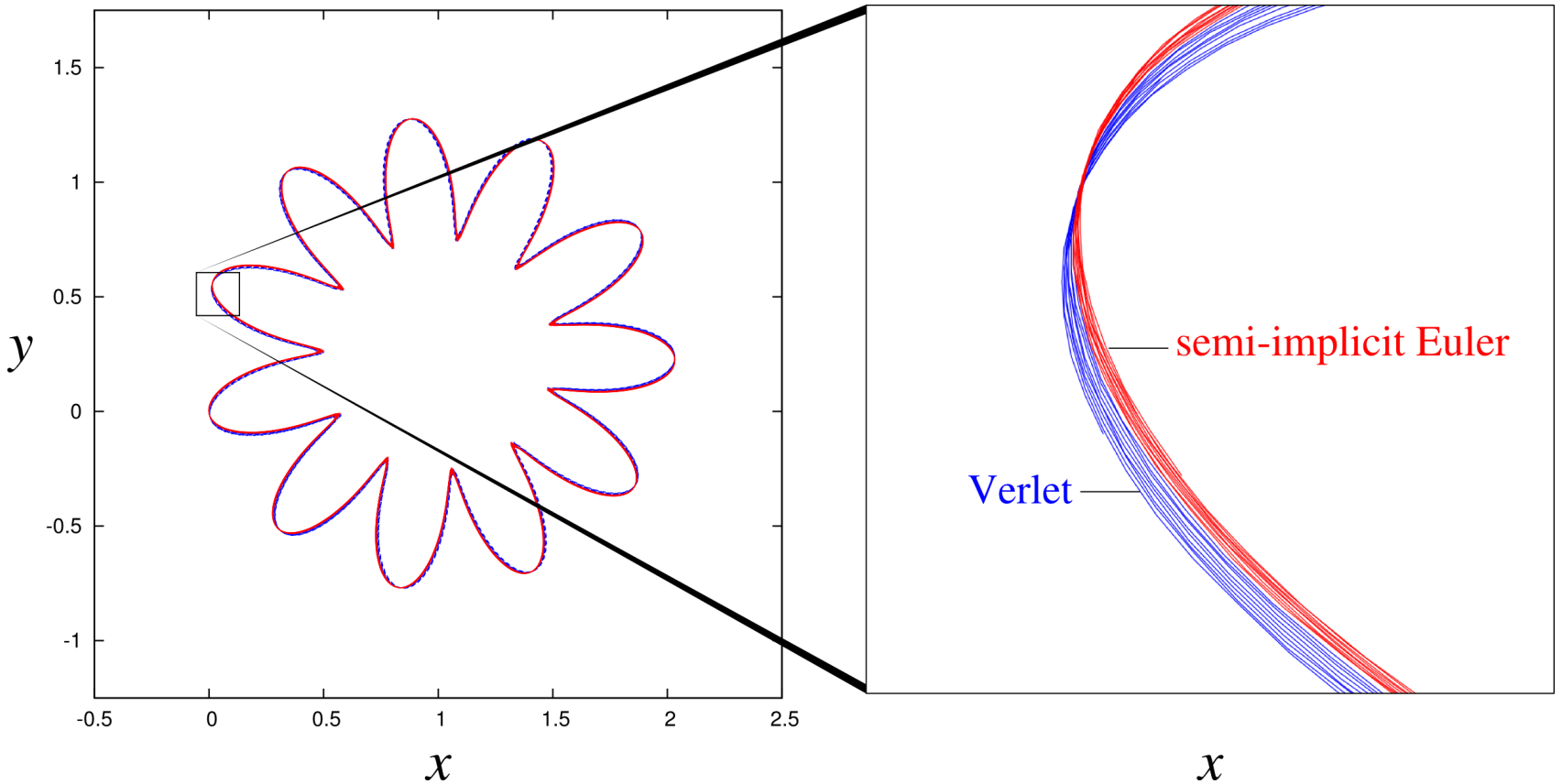
Compute : $\boxed{\dot{x}_i(t+\Delta t) = \dot{x}_i(t) + \frac{\Delta t}{2m_i}\left[f_i(t) + f_i(t+\Delta t)\right]}$

- Requires additional storage for $f_i(t)$.
- Symplectic integrator !
  In average it preserves the energy.

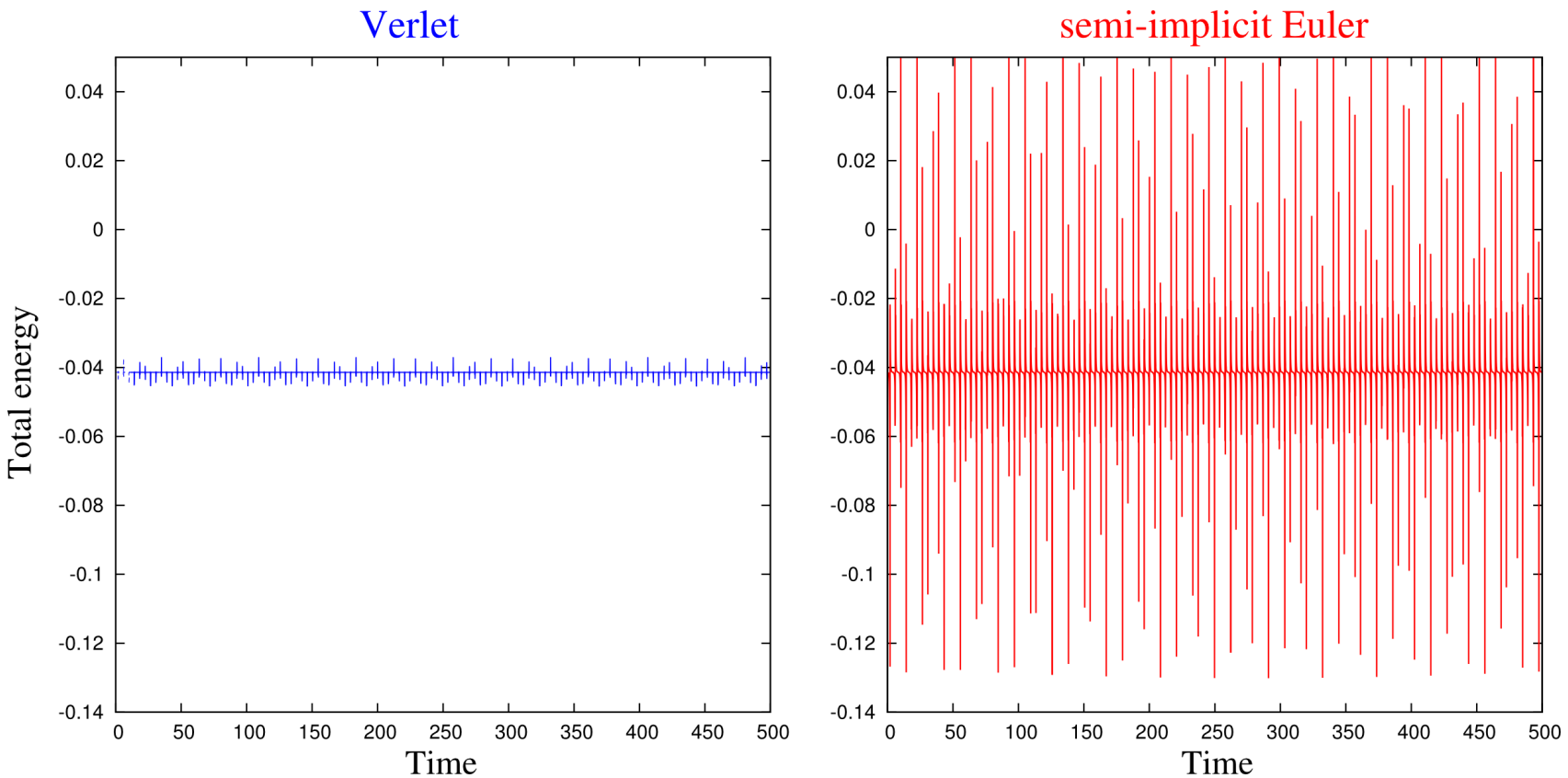
---

[1] Verlet L. "Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules". Phys Rev (1967)

Comparison Verlet vs Euler



Comparison Verlet vs Euler



- *Explicit Euler* method is of no use
- Both *Velocity-Verlet* method and *semi-implicit Euler* methods are simplectic, i.e. in average they preserve the system energy
- *Velocity-Verlet* has better energy preserving properties

General algorithm

- **Initialize :**
  1. distribute particles $x_i(0)$ for $i \in [0, N]$
  2. assign initial velocity field $\dot{x}_i(0)$
  3. assign boundary conditions
  4. evaluate forces on particles $f_i(x(0))$
- **Integrate in time (velocity Verlet method) :**
  1. $t \to t + \Delta t$
  2. update boundary conditions
  3. compute new positions

     $$x_i(t + \Delta t) = x_i(t) + \left[\dot{x}_i(t) + \frac{\Delta t}{2m_i} f_i(t)\right] \Delta t$$
  4. store forces $f_i(t)$
  5. evaluate new forces (using, e.g., linked-cell method) $f_i(x(t + \Delta t))$
  6. compute new velocities

     $$\dot{x}_i(t + \Delta t) = \dot{x}_i(t) + \frac{\Delta t}{2m_i} \left[f_i(t) + f_i(t + \Delta t)\right]$$
  7. if needed store data and compute energies.

General algorithm

- **Initialize :**
  1. **distribute particles** $x_i(0)$ **for** $i \in [0, N]$
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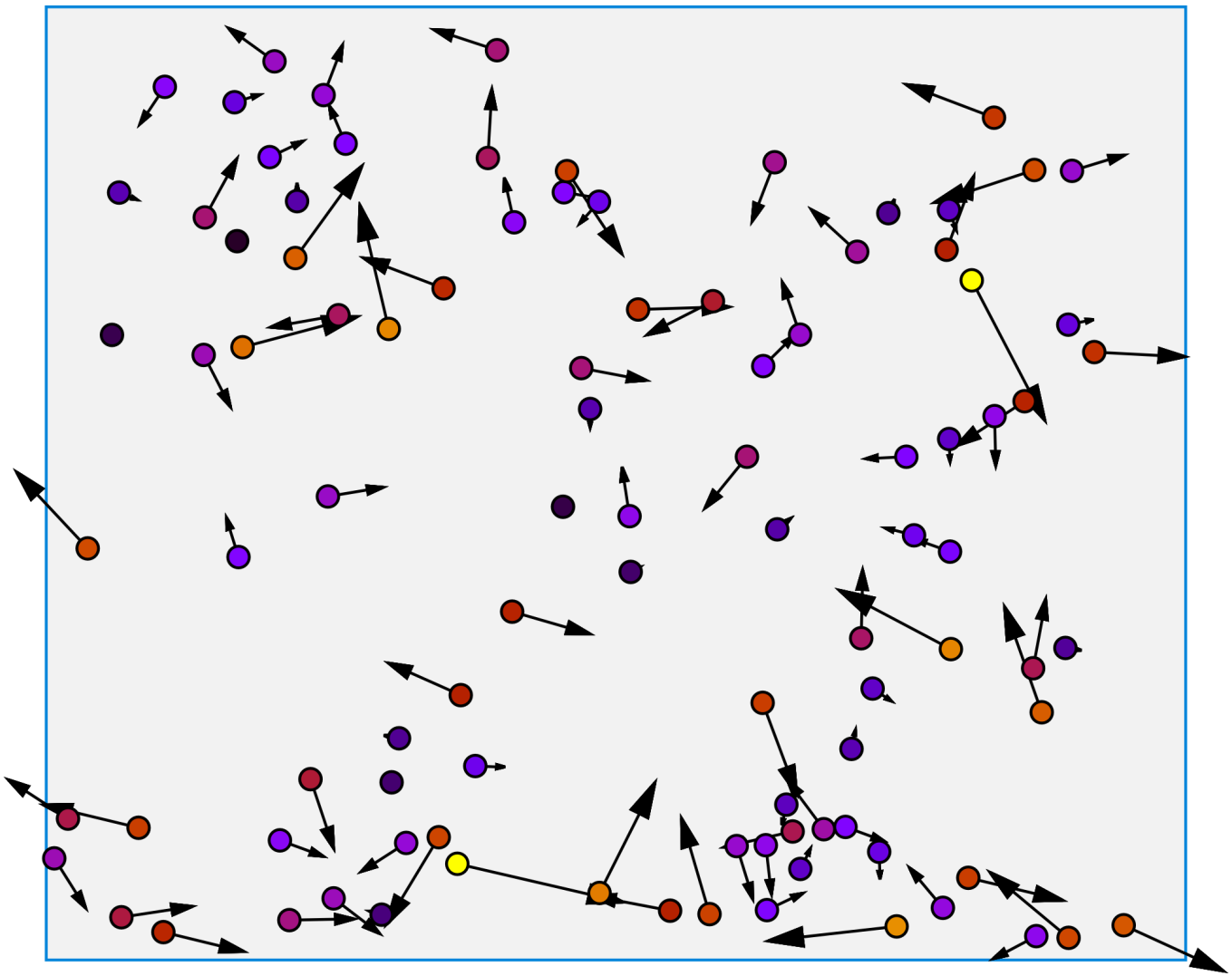
  7. if needed store data and compute energies.

Boundary conditions I

Animation `pbc.gif`

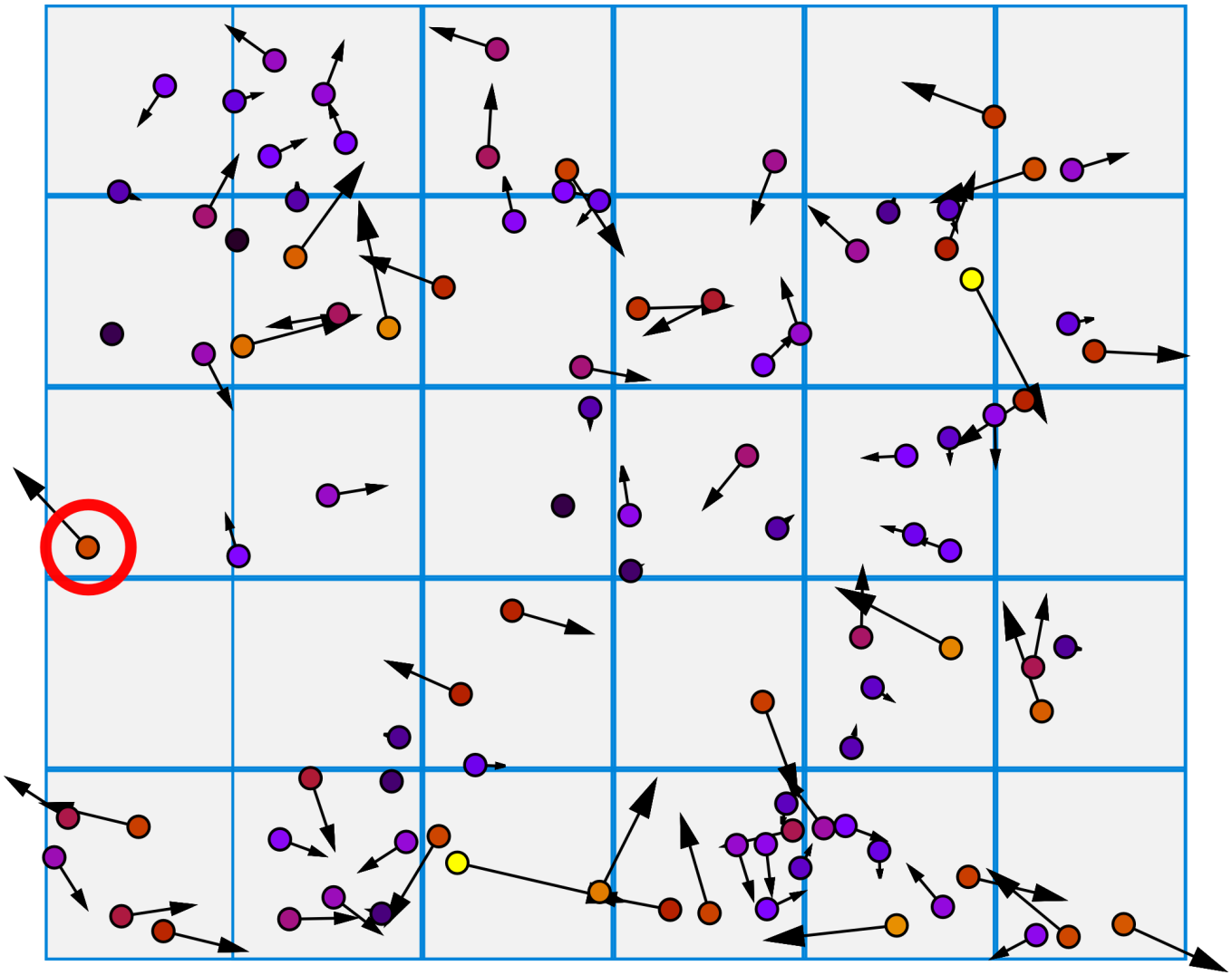
Boundary conditions I

- Periodic boundary conditions



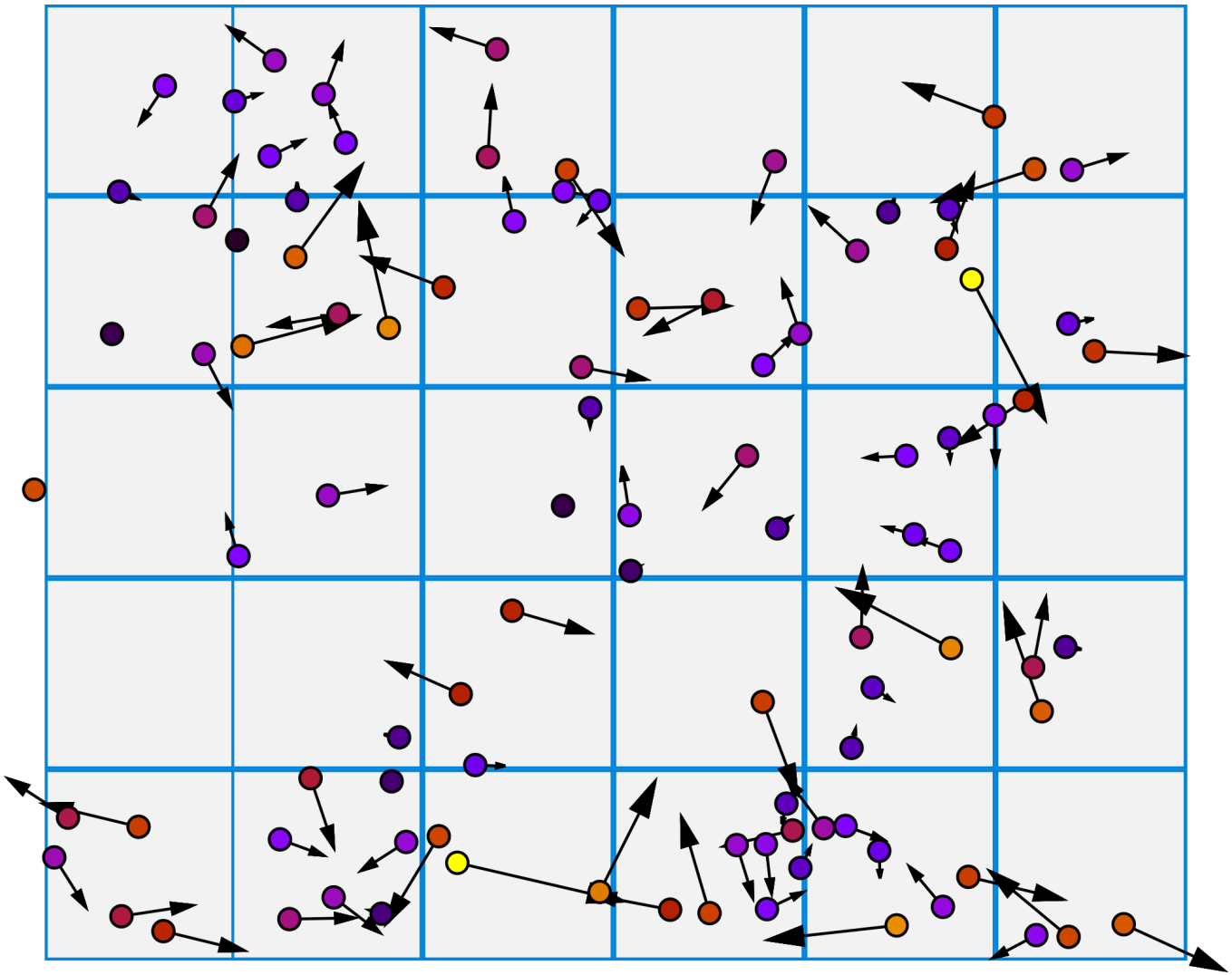
Boundary conditions I

- Periodic boundary conditions



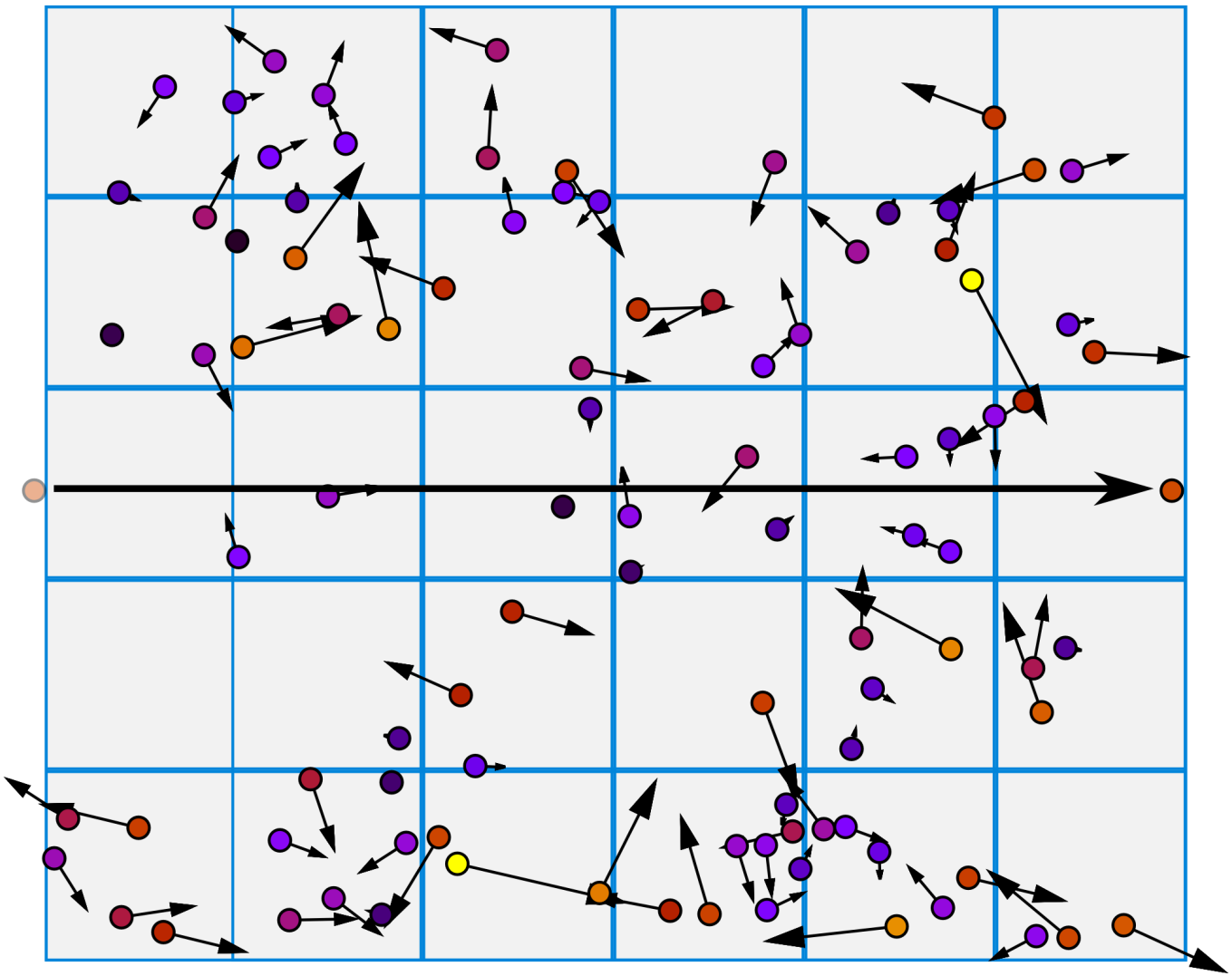
Boundary conditions I

- Periodic boundary conditions



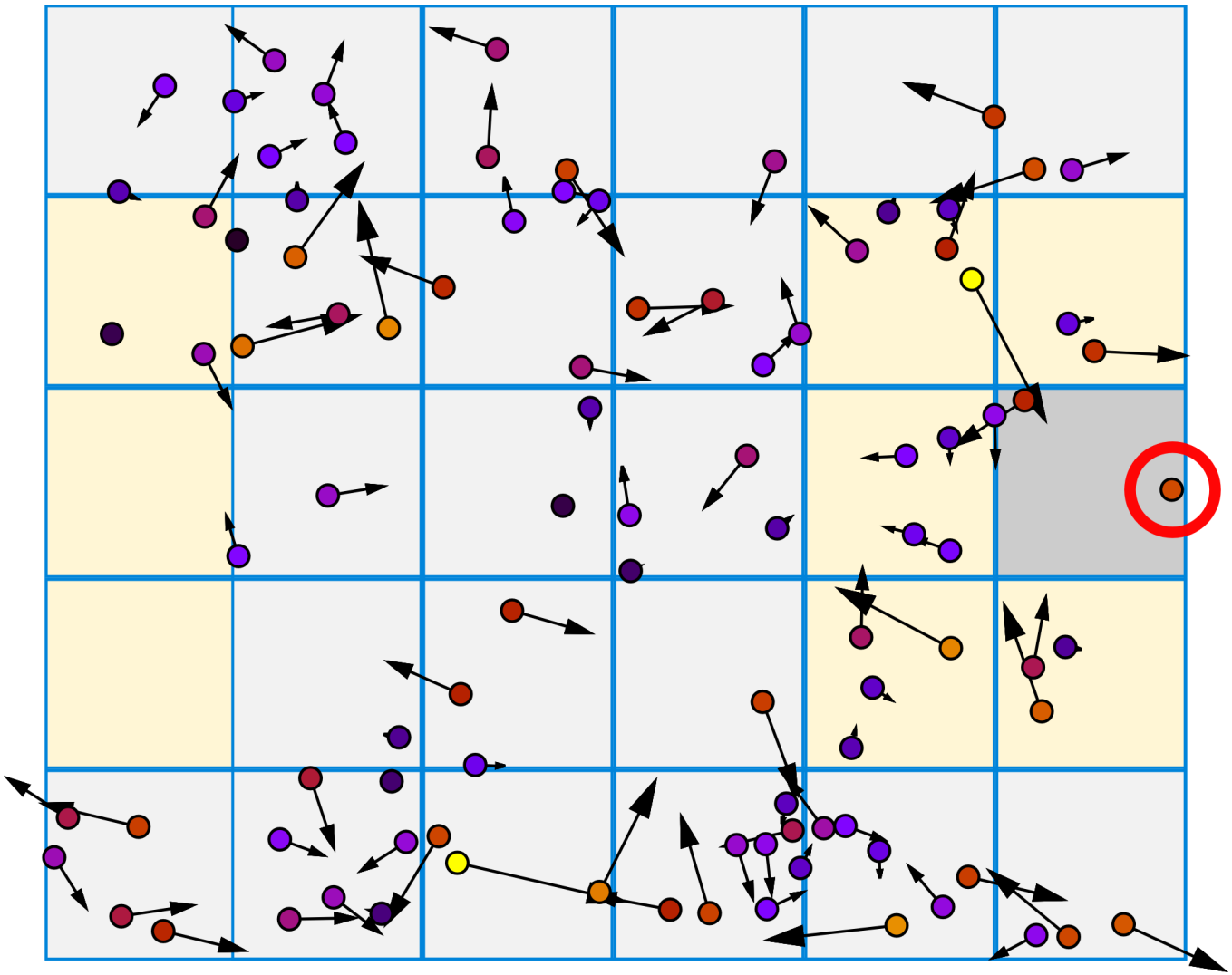
Boundary conditions I

- Periodic boundary conditions



Boundary conditions I

- Periodic boundary conditions

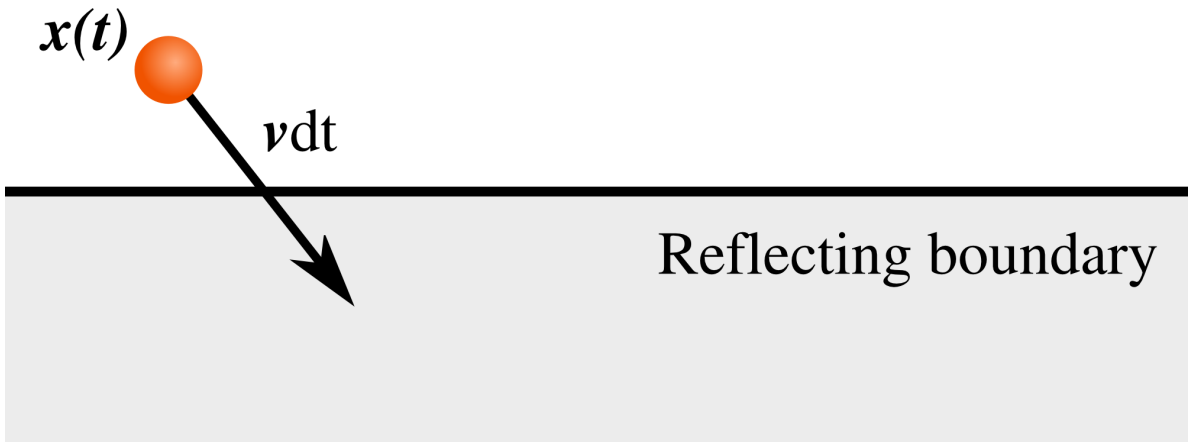


Boundary conditions II

Animation `rbc.gif`

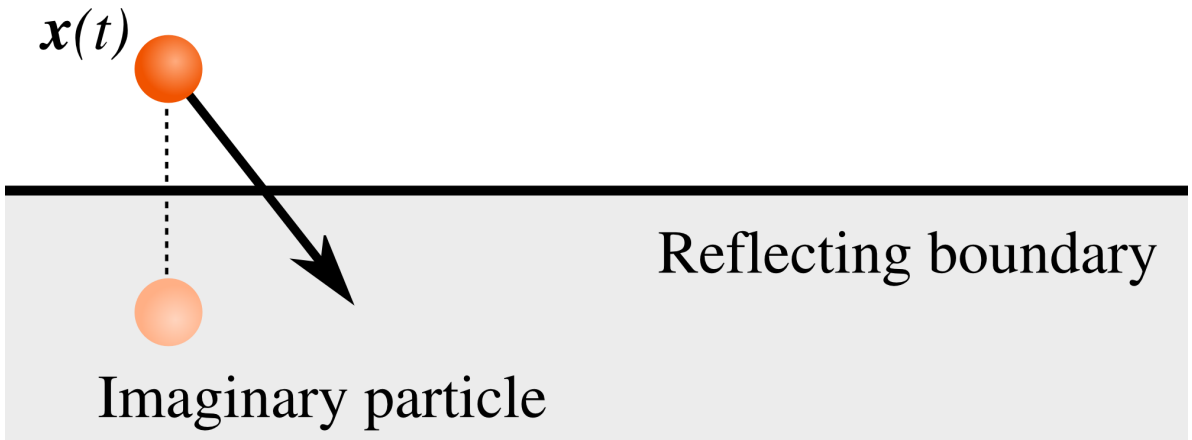
Boundary conditions II

- Reflecting boundary conditions



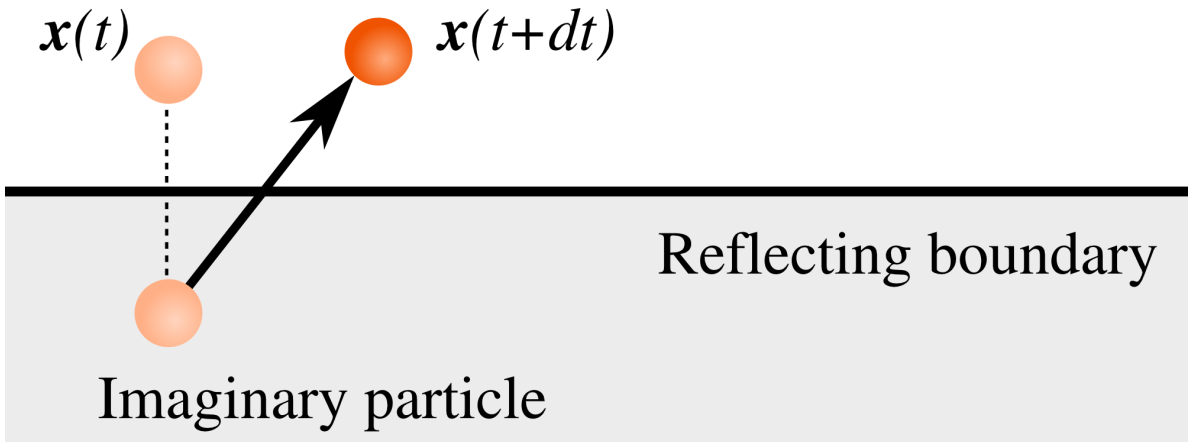
Boundary conditions II

- Reflecting boundary conditions



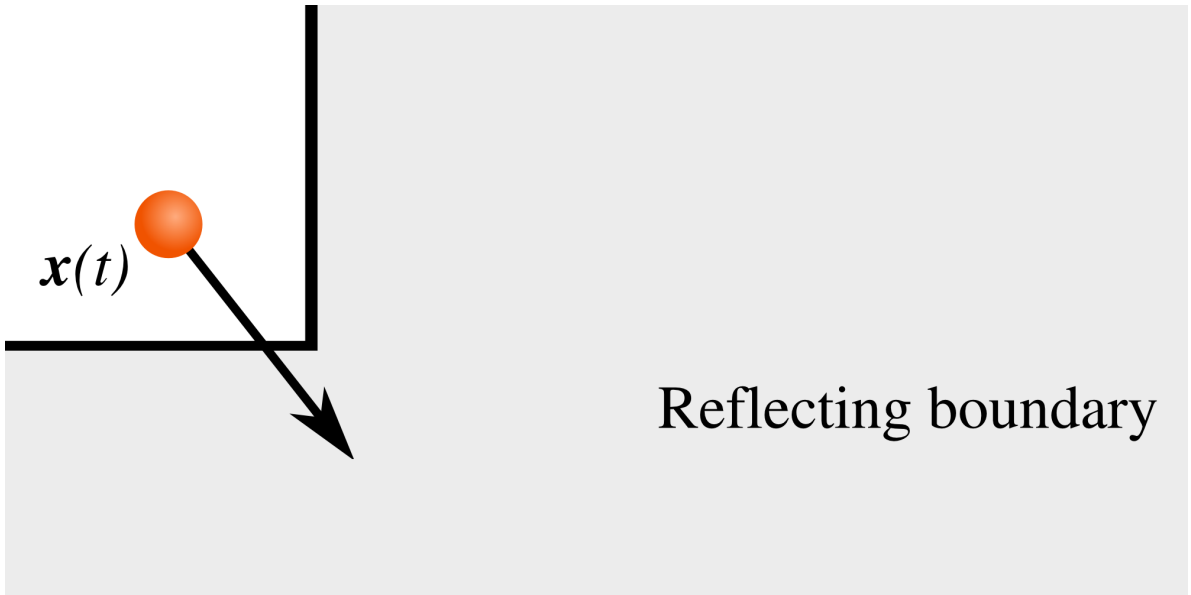
Boundary conditions II

- Reflecting boundary conditions



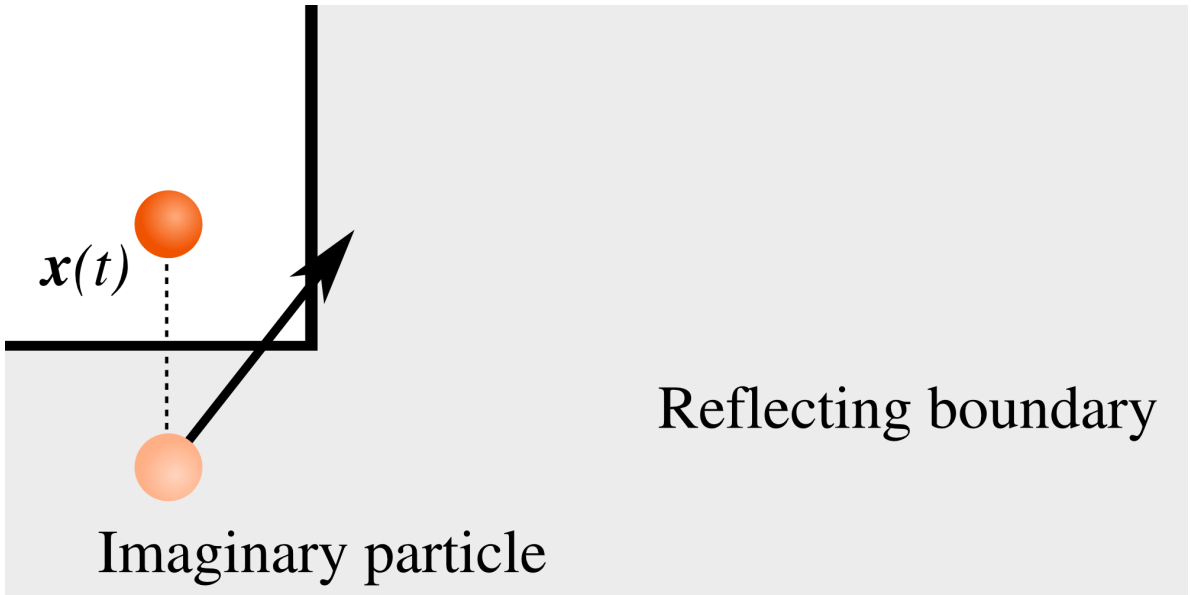
Boundary conditions II

- Reflecting boundary conditions



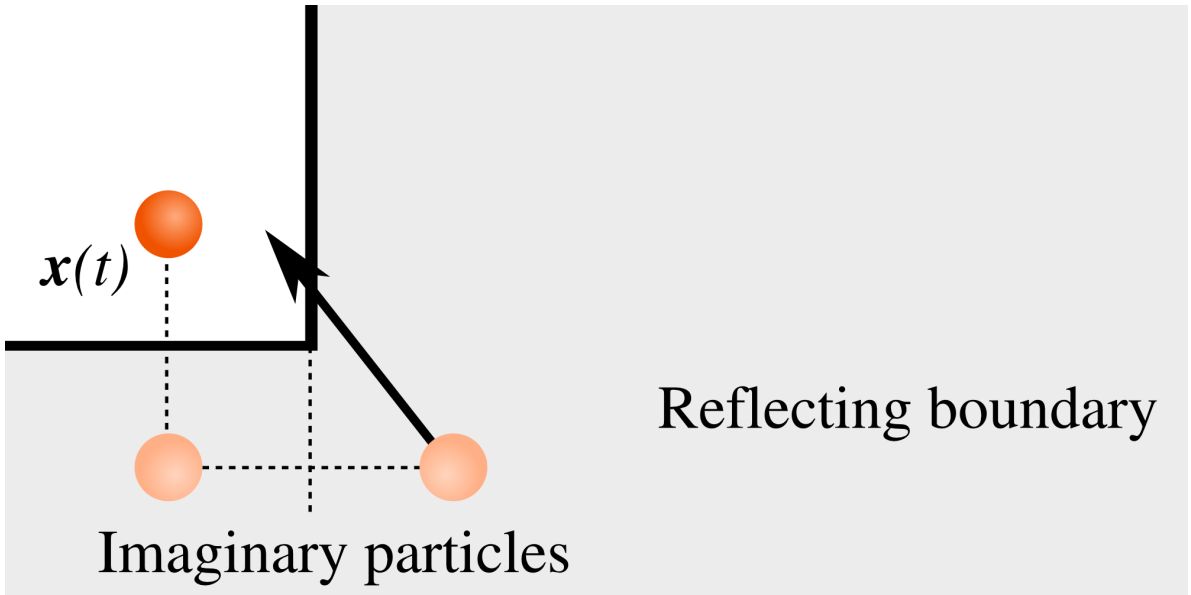
Boundary conditions II

- Reflecting boundary conditions



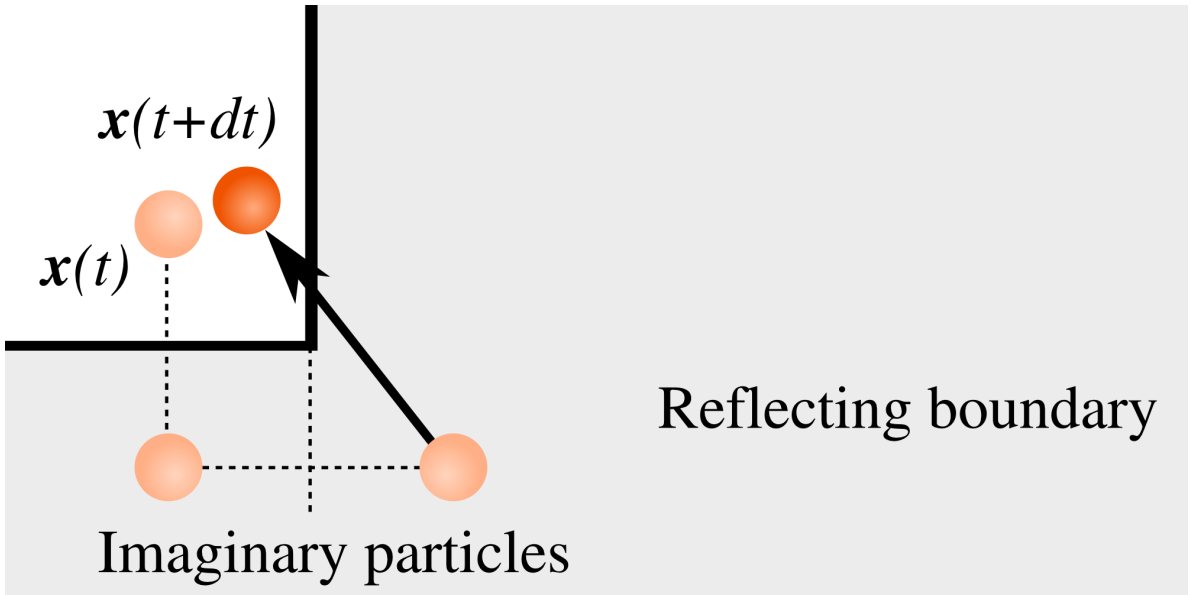
Boundary conditions II

- Reflecting boundary conditions



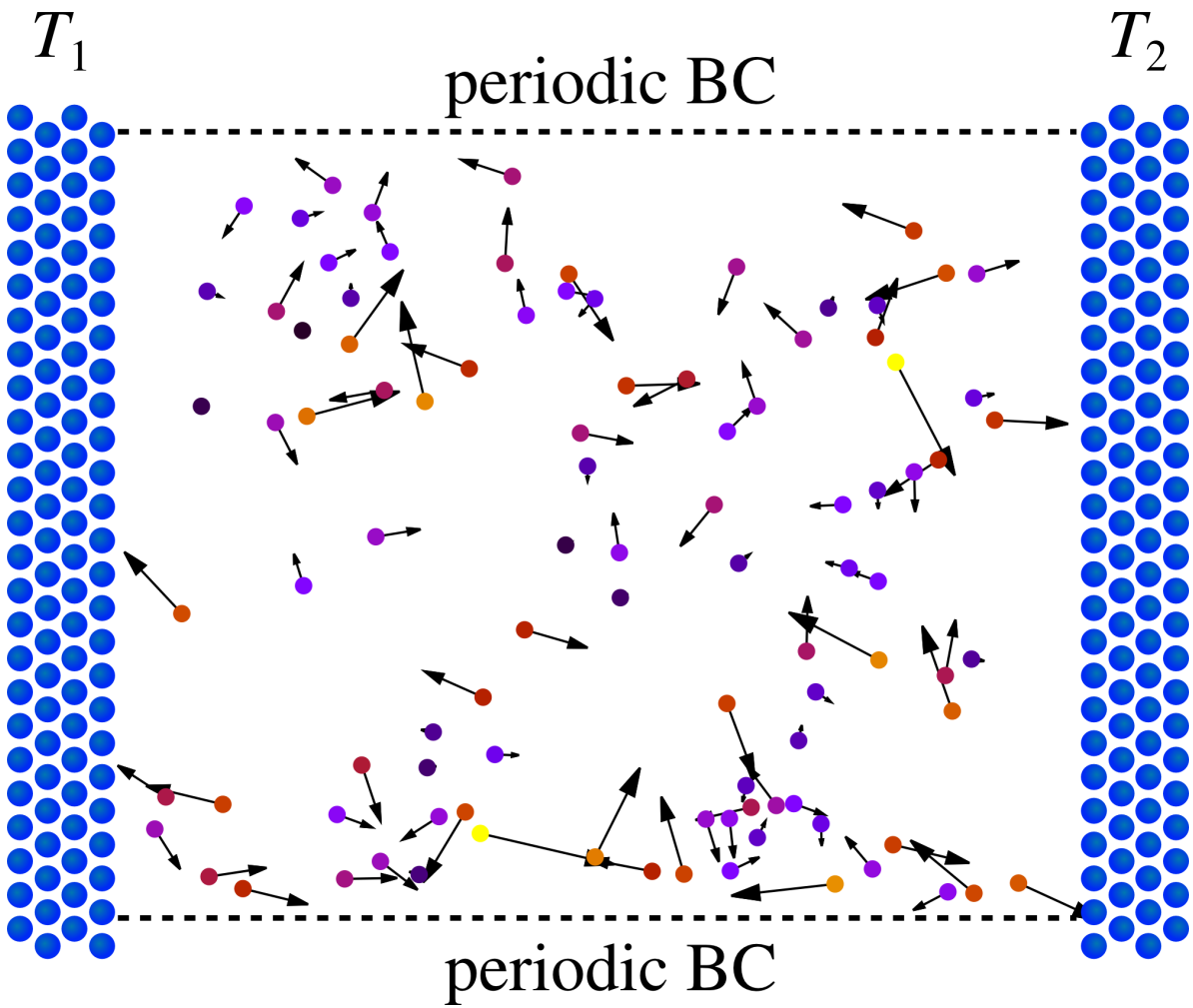
Boundary conditions II

- Reflecting boundary conditions



Boundary conditions II

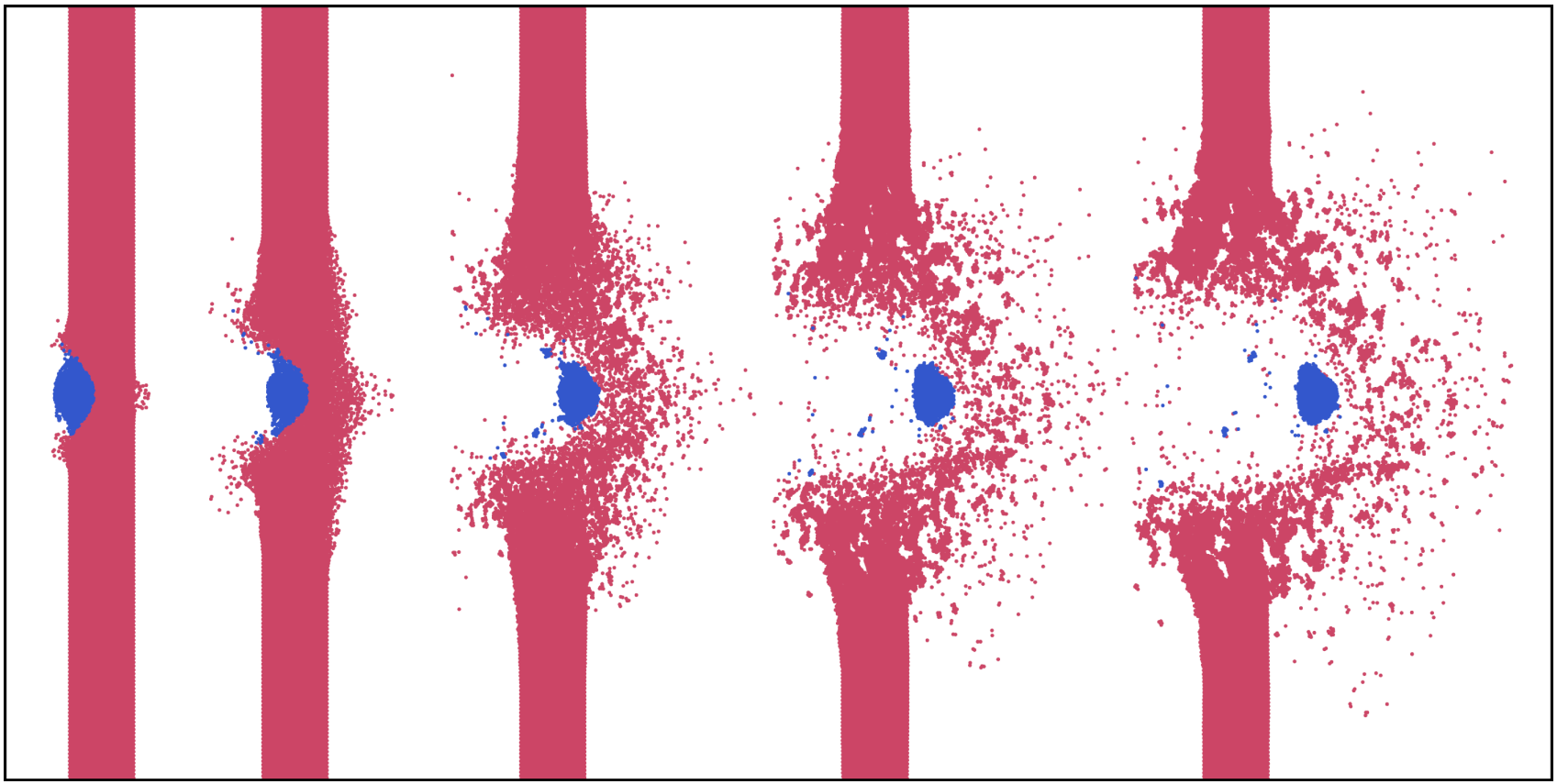
- Reflecting boundary conditions (different approach)



- Rigid walls of immobile atoms (only repulsive or combined action)
- Or walls of moving atoms at certain temperature

Boundary conditions III

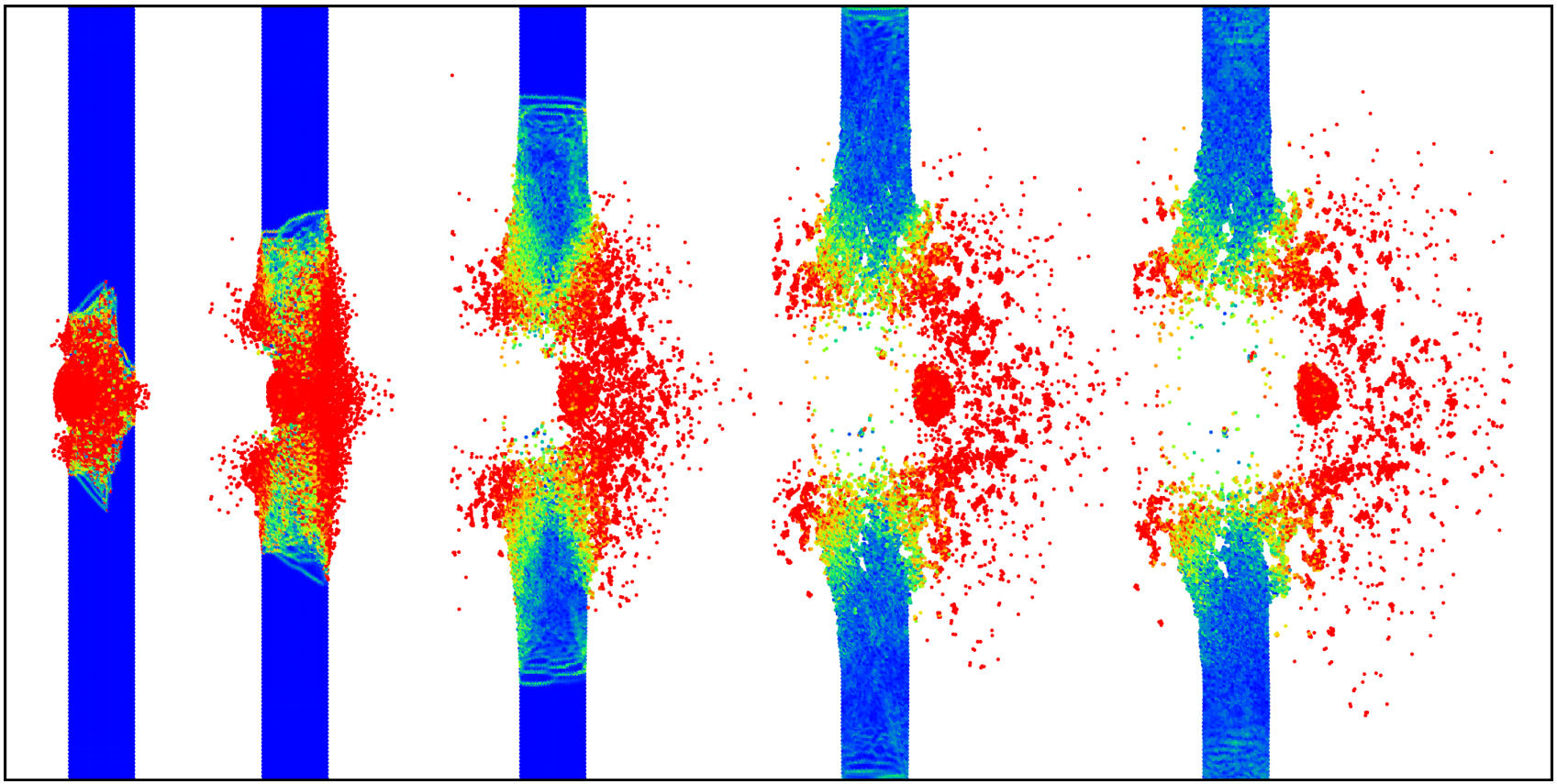
- Initial velocity (initial value problem) : impact, penetration



- Volumetric forces : gravity (additional force $F_i \mathrel{+}= m_i g$)

Boundary conditions III

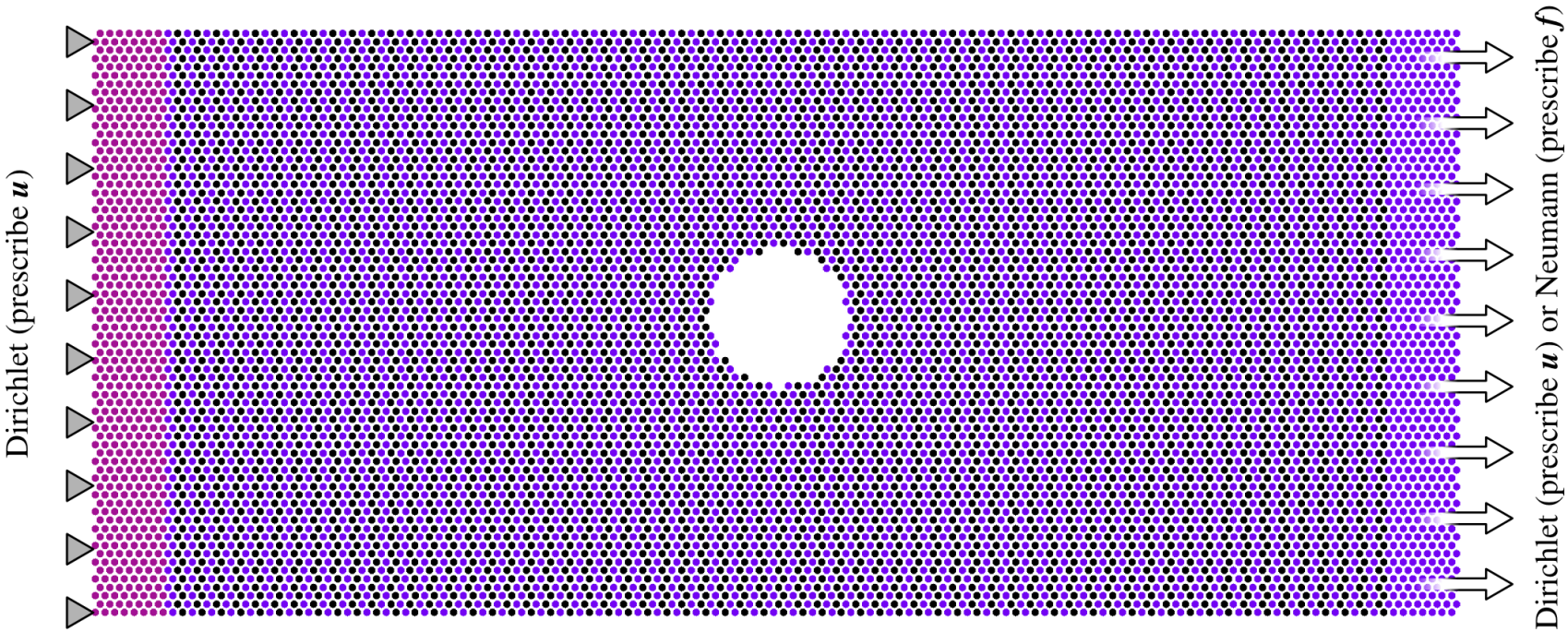
- Initial velocity (initial value problem) : impact, penetration



- Volumetric forces : gravity (additional force $F_i \mathrel{+}= m_i g$)

Boundary conditions IV

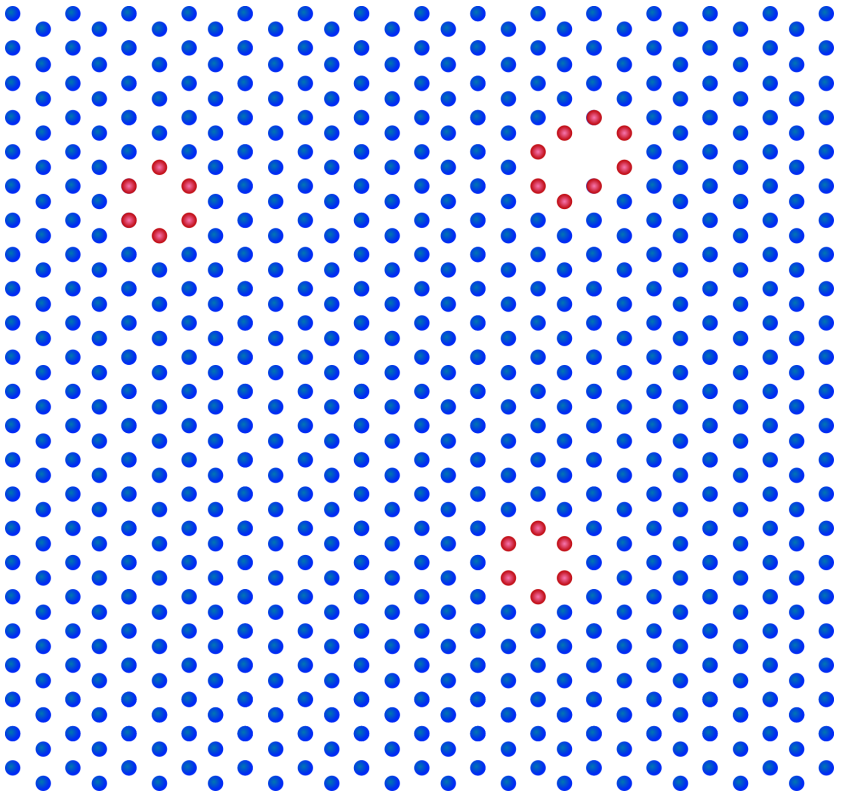
- Mechanical boundary conditions : Dirichlet and Neumann



Initial configuration

Simple configurations :

- Gas/liquid
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
- Stacking faults and dislocations
- Simple geometries
- Long molecules

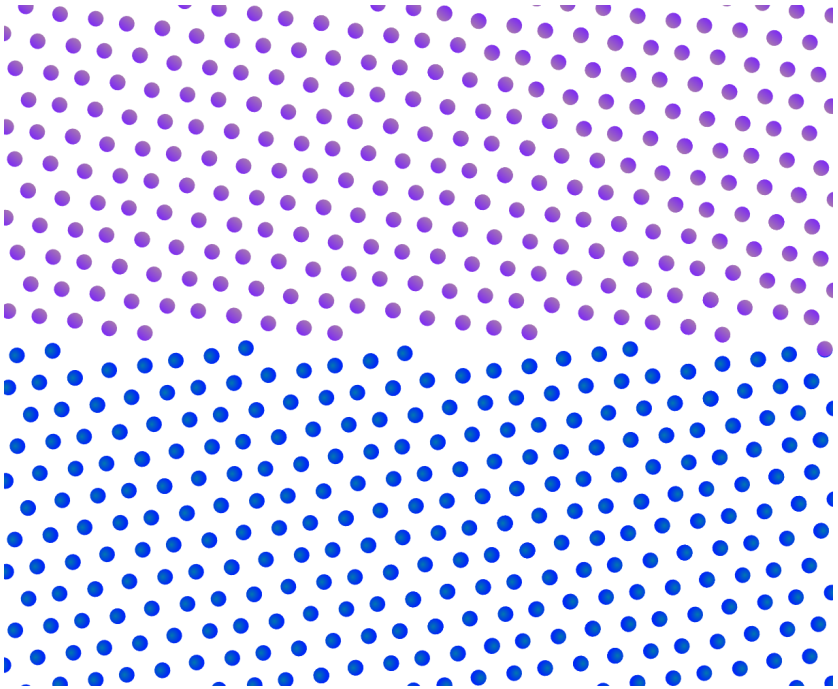


Crystal with vacancy defects (easy to control)

Initial configuration

Simple configurations :

- Gas/liquid
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals[1]
- Stacking faults and dislocations
- Simple geometries
- Long molecules



Bi-Crystal (grain boundary)

[1] Coffman & Sethna. Grain boundary energies and cohesive strength as a function of geometry. Phys Rev B 77 (2008)

Initial configuration

Simple configurations :

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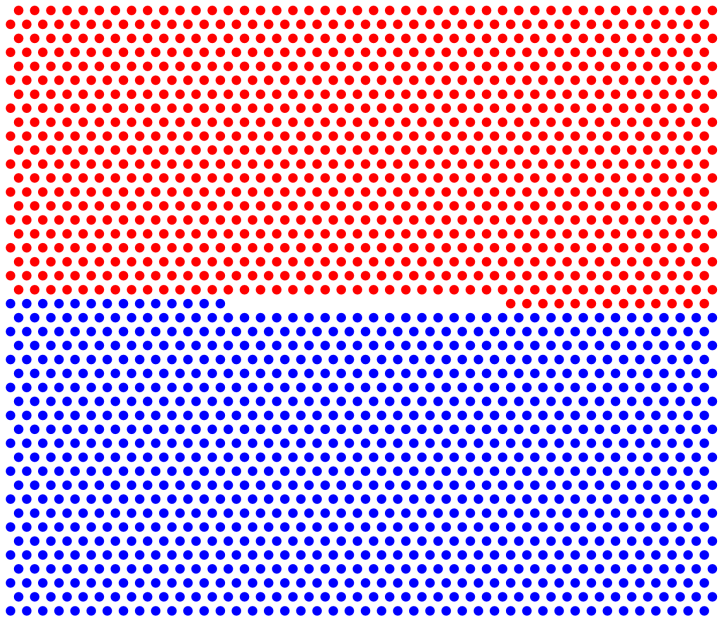
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
- Stacking faults and dislocations
- Simple geometries
- Long molecules



Remove several atoms

Initial configuration

Simple configurations :

- Gas/liquid
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
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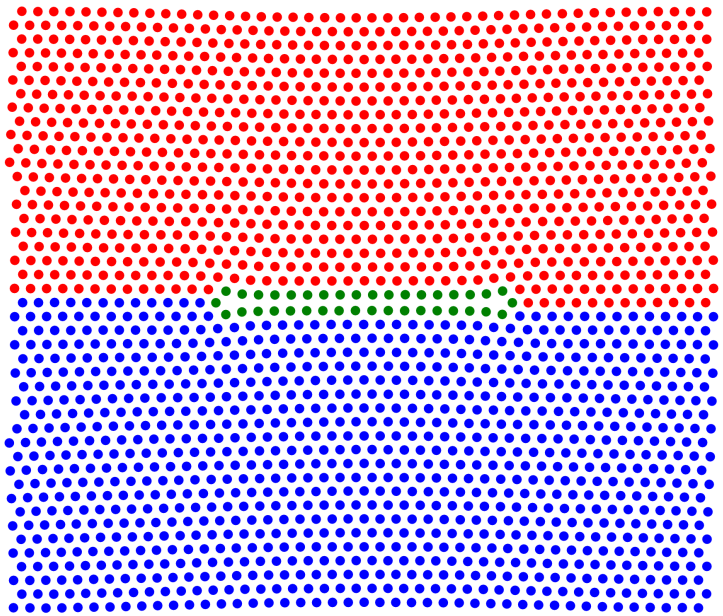
- Simple geometries
- Long molecules

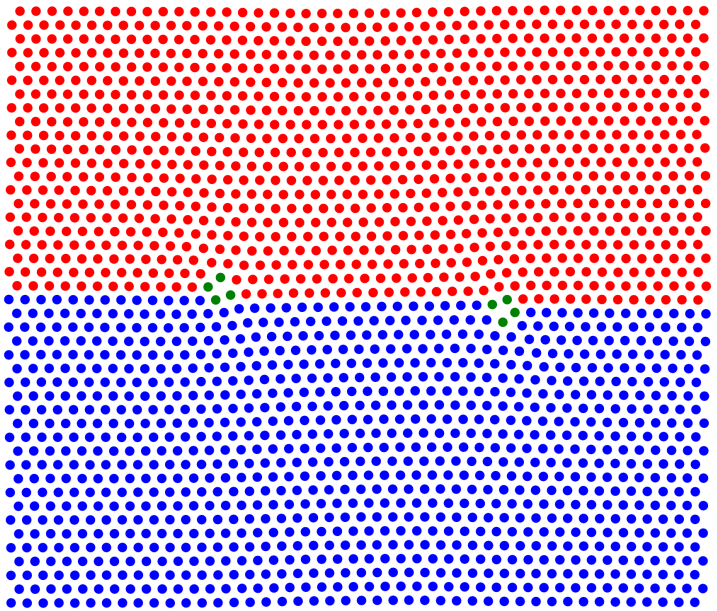


Stacking fault with partial dislocations

Initial configuration

Simple configurations :

- Gas/liquid
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
- Stacking faults and dislocations
- Simple geometries
- Long molecules

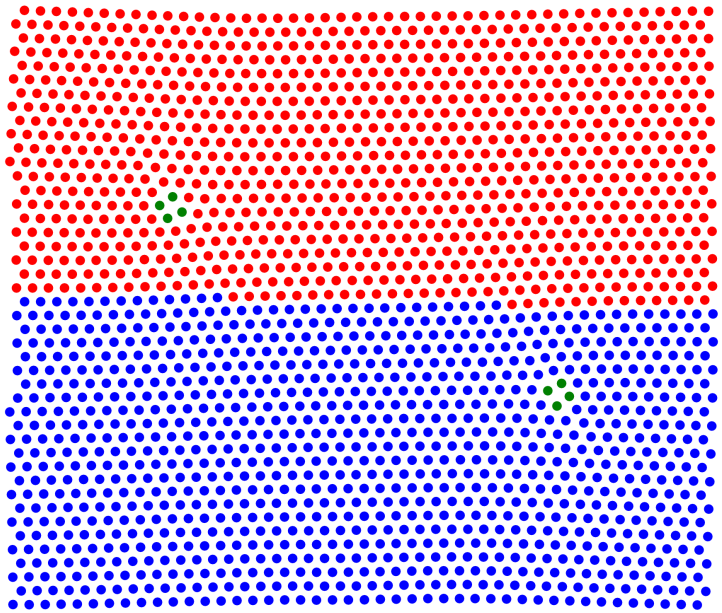


Healing stacking fault forms two perfect edge dislocations

Initial configuration

Simple configurations :

- Gas/liquid
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
- Stacking faults and dislocations
- Simple geometries
- Long molecules



Dislocations glide

Initial configuration

Simple configurations :

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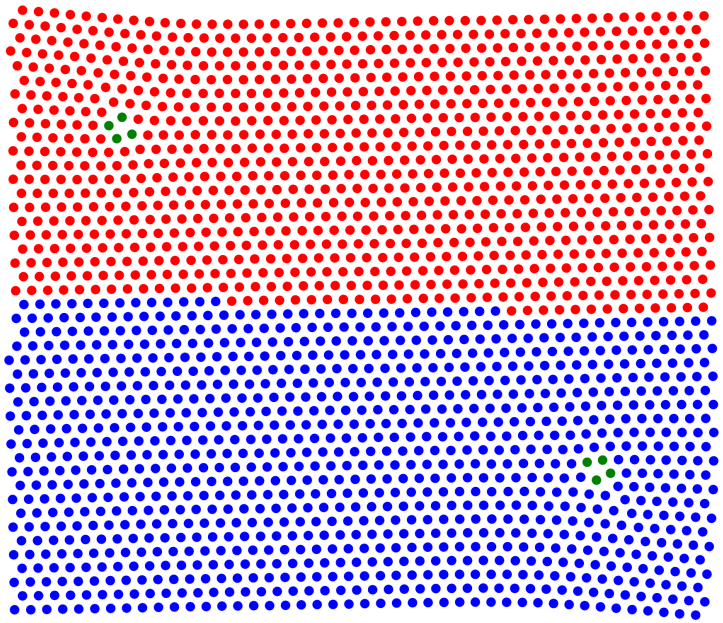
- Simple geometries
- Long molecules



Dislocations glide

Initial configuration

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- Bi-crystals
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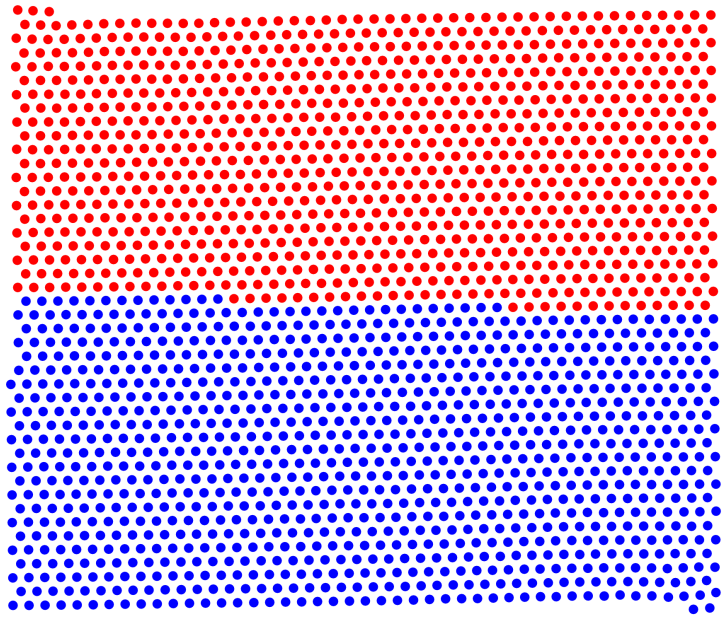

Dislocations form steps on the surface

Initial configuration

Simple configurations :

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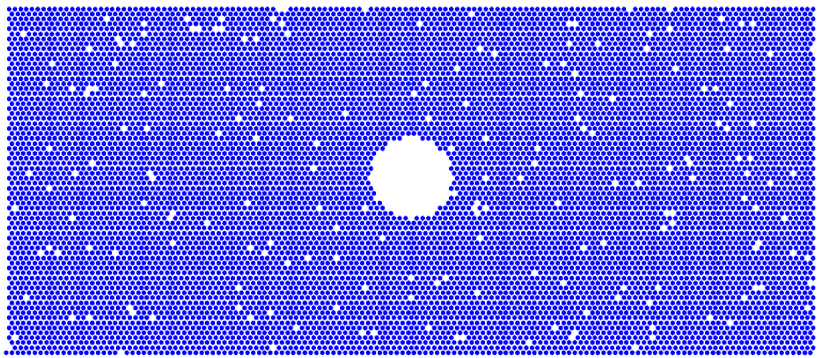
- Perfect crystal
- Crystal with vacancy defects
- Bi-crystals
- Stacking faults and dislocations
- Simple geometries
- Long molecules

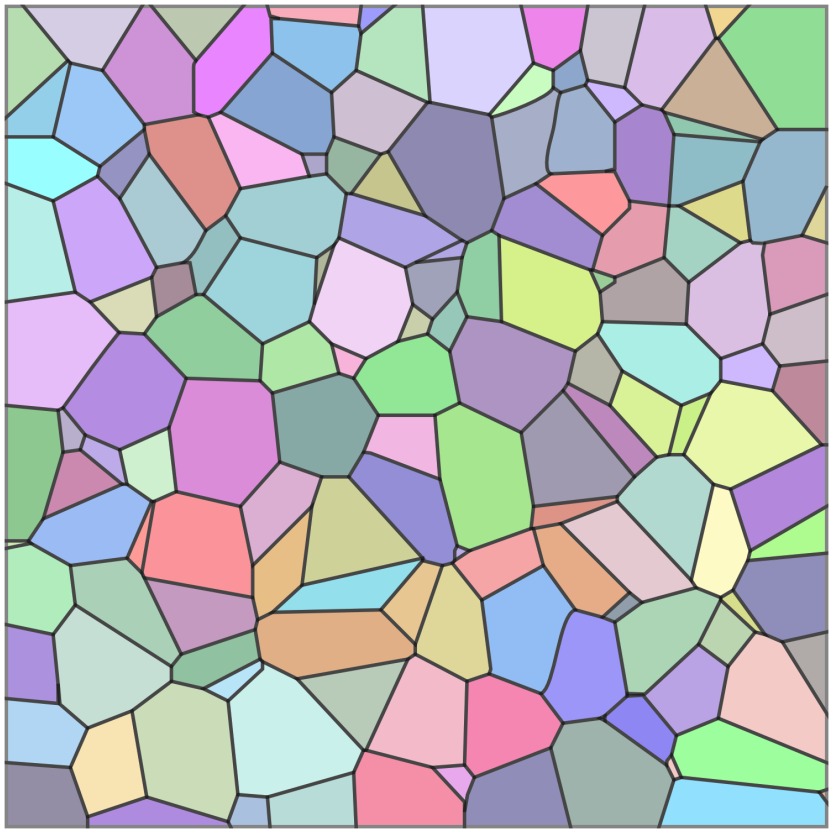


Layer with a circular hole

Initial configuration

Physically based configurations :

- Amorphous solid
  rapidly solidified from a liquid
- Voronoi-based polycrystal
- Polycrystalline solid
  porosity and grain size are controlled by the cooling rate
- Hight-temperature corrosion
  heat up and cool down initial configuration



Voronoi tesselation as a basis for construction of a nano-grained material
(*adapted from Wikipedia*)

Initial configuration

Physically based configurations :

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  rapidly solidified from a liquid
- Voronoi-based polycrystal
- Polycrystalline solid
  porosity and grain size are controlled by the cooling rate
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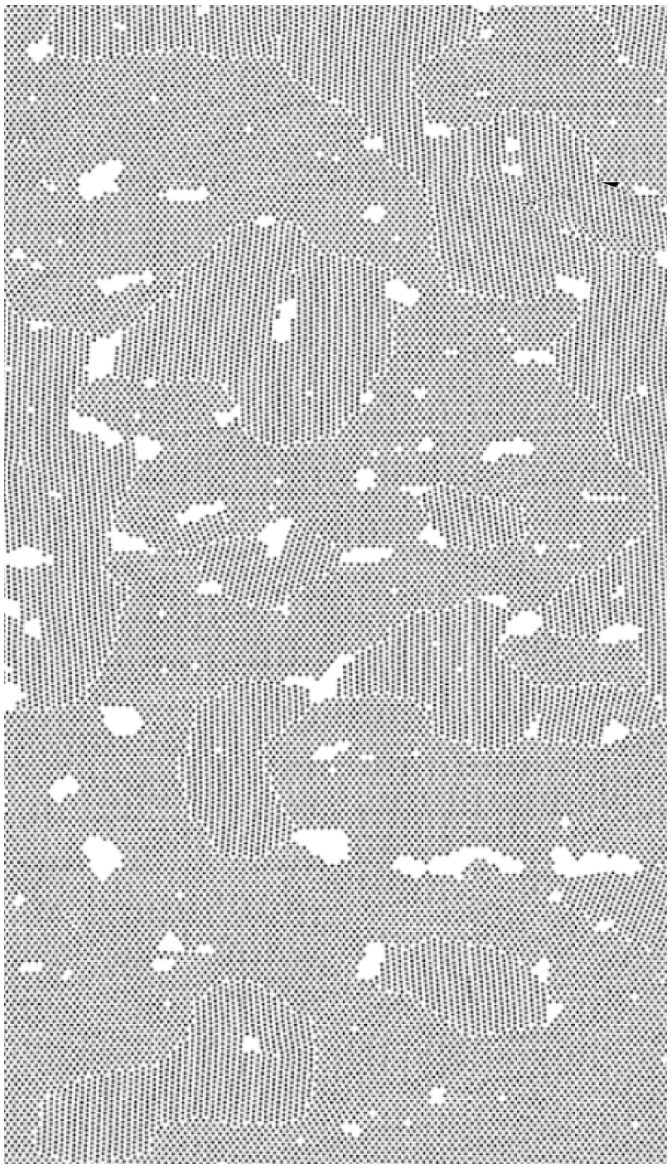

Porous polycrystal obtained from liquid state by relatively fast cooling

General algorithm

- **Initialize :**
  1. distribute particles $x_i(0)$ for $i \in [0, N]$
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  4. store forces $f_i(t)$
  5. evaluate new forces (using, e.g., linked-cell method) $f_i(x(t + \Delta t))$
  6. compute new velocities

     $$\dot{x}_i(t + \Delta t) = \dot{x}_i(t) + \frac{\Delta t}{2m_i} \left[f_i(t) + f_i(t + \Delta t)\right]$$
  7. if needed store data and compute energies.

End of part I