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Multiscale Simulations of Materials and Structures

Lecture 1. *Molecular Dynamics I*

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@ Centre des Matériaux
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- 2 Chemical bonds
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- 6 General many-body Hamiltonian problem
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- 12 Time integration
- 13 Algorithm
- 14 Boundary and initial conditions

Matter constituents

Standard Model

mass → charge → spin →	$\sim 2.3 \text{ MeV}/c^2$ 2/3 1/2 u up	$\sim 1.273 \text{ GeV}/c^2$ 2/3 1/2 c charm	$\sim 173.37 \text{ GeV}/c^2$ 2/3 1/2 t top	0 1 0 g gluon	$\sim 125 \text{ GeV}/c^2$ 0 0 H Higgs boson
QUARKS	$\sim 4.8 \text{ MeV}/c^2$ -1/3 1/2 d down	$\sim 95 \text{ MeV}/c^2$ -1/3 1/2 s strange	$\sim 4.18 \text{ GeV}/c^2$ -1/3 1/2 b bottom	0 0 1 γ photon	
	$0.511 \text{ MeV}/c^2$ -1 1/2 e electron	$105.7 \text{ MeV}/c^2$ -1 1/2 μ muon	$1.777 \text{ GeV}/c^2$ -1 1/2 τ tau	$81.2 \text{ GeV}/c^2$ 0 1 Z Z boson	
LEPTONS	$< 2.2 \text{ eV}/c^2$ 0 1/2 ν_e electron neutrino	$< 0.17 \text{ MeV}/c^2$ 0 1/2 ν_μ muon neutrino	$< 18.9 \text{ MeV}/c^2$ 0 1/2 ν_τ tau neutrino	$80.4 \text{ GeV}/c^2$ ± 1 0 W W boson	
				GAUGE BOSONS	

Table from Wikipedia

QCD

Neutron



Proton



Quarks are tied by gluons
(strong interaction)

Nuclear physics

Nucleus



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

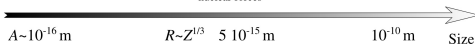
Nucleons are tied by mesons
(quark+antiquark)
nuclear forces

Chemistry (QED)

Atom



Atoms are tied by photons
(electromagnetic forces)



Chemical bonds

Nature of bonds :

- Electrostatic force
- Electrons sharing mechanism

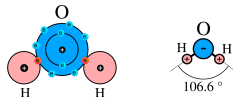
Strength of bonds :

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

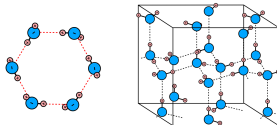
Examples :

- Covalent (H_2O , H_2)
- Hydrogen ($\text{H}_2\text{O}-\text{H}_2\text{O}$, DNA)
- Ionic (NaCl , NaF)
- Metallic (all metals)
- Van der Waals (dipole-dipole e.g. $\text{HCl}-\text{HCl}$, induced dipoles)

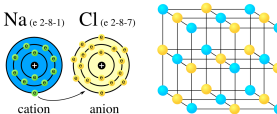
Covalent bond



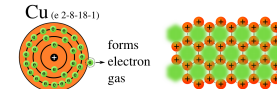
Hydrogen bond



Ionic bond



Metallic bond



Linus Pauling "The Nature of the Chemical Bond"

<http://scarc.library.oregonstate.edu/coll/pauling/bond/index.html>

Assemblies

Lattices

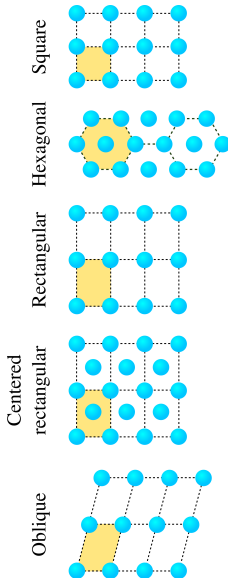
- In 2D : 5 Bravais lattices
- In 3D : 14 Bravais lattices

Molecules

- Diatomic gas (N_2 , O_2)
- Ethanol (C_2H_5OH)
- Macromolecules (rubber, DNA, polyethene, protein)

Amorphous

- Silica SiO_2
- Metallic glass



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

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

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

- For n particles

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

- Time independent form :

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

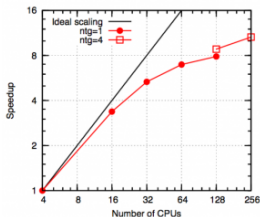
- Modern chemistry can solve Schrödinger equation with up to 40-50 electrons (only!).

Density Functional Theory

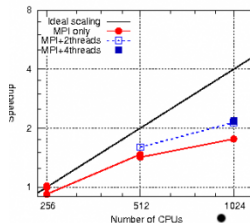
- The DFT is the most successful approach to compute the electronic structure of matter
(Nicely presented in http://www.uam.es/personal_pdi/ciencias/jcuevas/Talks/JC-Cuevas-DFT.pdf)
see also E.A. Carter “Challenges in Modeling Materials Properties Without Experimental Input”, Science 321 (2008)
- Applicable 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, L.J 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 A β -peptide in water containing 838 atoms and 2312 electrons in a 22.1×22.9×19.9 Å³ 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

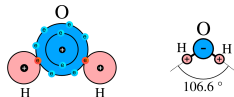
■ Dipole-dipole

■ Induced dipoles

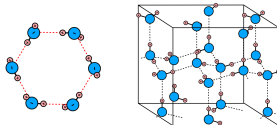
*If electronic structure of the **lattice** is well resolved
(DFT) then feasible :*

■ Metallic bonds

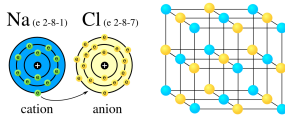
Covalent bond



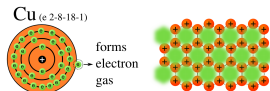
Hydrogen bond



Ionic bond



Metallic bond



MD from the family of Particle Methods

Particle methods

- **SPH**
Smooth-particle hydrodynamics (fluids, solids)
- **DEM**
Discrete element method (granular matter)
- 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)

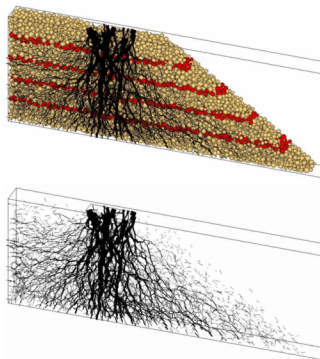
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DEM simulation
Fabio Gabrieli (University of Padova)
geotechlab.wordpress.com

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 : $U(r_{ij}) = -\frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r_{ij}}$

- Elastic (harmonic) potential : $U(r_{ij}) = \frac{k}{2} (r_{ij} - r_0)^2$

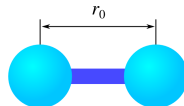
■ Regularization

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

Examples of simple molecular models

- Covalent bonds approximated by harmonic potential

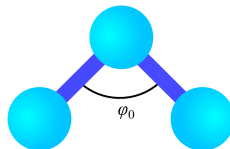
$$V_l(\mathbf{r}_1, \mathbf{r}_2) = \frac{k_l}{2} (|\mathbf{r}_1 - \mathbf{r}_2| - r_0)^2$$



- In-plane angular potential

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

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



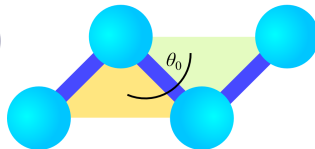
- Torsional potential

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

- Intra-molecular potential

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

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



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

Potentials in LAMMPS

- **pairwise potentials** : Lennard-Jones, Buckingham, Morse, Born-Mayer-Huggins, Yukawa, soft, class 2 (COMPASS), hydrogen bond, tabulated
- **charged pairwise potentials** : Coulombic, point-dipole
- **many-body potentials** : EAM, Finnis/Sinclair EAM, modified EAM (MEAM), embedded ion method (EIM), EDIP, ADP, Stillinger-Weber, Tersoff, REBO, AIREBO, ReaxFF, COMB, SNAP, Streitz-Mintmire, 3-body polymorphic
- **long-range interactions for charge, point-dipoles, and LJ dispersion** : Ewald, Wolf, PPPM (similar to particle-mesh Ewald)
- **polarization models** : QEq, core/shell model, Drude dipole model
- **coarse-grained potentials** : DPD, GayBerne, RESquared, colloidal, DLVO
- **mesoscopic potentials** : granular, Peridynamics, SPH
- **electron force field** : eFF, AWPMD
- **bond potentials** : harmonic, FENE, Morse, nonlinear, class 2, quartic (breakable)
- **angle potentials** : harmonic, CHARMM, cosine, cosine/squared, cosine/periodic, class 2 (COMPASS)
- **dihedral potentials** : harmonic, CHARMM, multi-harmonic, helix, class 2 (COMPASS), OPLS
- **improper potentials** : harmonic, cvff, umbrella, class 2 (COMPASS)
- **polymer potentials** : all-atom, united-atom, bead-spring, breakable
- **water potentials** : TIP3P, TIP4P, SPC
- **implicit solvent potentials** : hydrodynamic lubrication, Debye
- **hybrid potentials** : multiple pair, bond, angle, dihedral, improper potentials can be used in one simulation
- **overlaid potentials** : superposition of multiple pair potentials

Many-body Hamiltonian system

General algorithm

- Potential :

$$U(r_{ij})$$

- System pair potential :

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

- Compute force \mathbf{f}_0 on particle \mathbf{r}_0 :

$$\mathbf{F}_0 = -\nabla_{\mathbf{r}_0} V(\mathbf{r}) = -\sum_{j \neq 0} \nabla_{\mathbf{r}_0} U(|\mathbf{r}_0 - \mathbf{r}_j|)$$

- 2nd Newton's law :

$$\ddot{\mathbf{r}}_0 = \frac{1}{m_0} \mathbf{F}_0$$

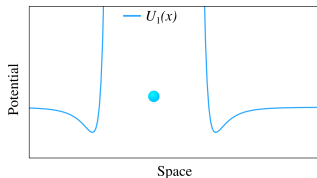
- Integrate in time :

$$\mathbf{r}_0(t) \rightarrow \mathbf{r}_0(t + \Delta t)$$

Properties :

- Energy conservation

$$E = \underbrace{\frac{1}{2} \sum_i m_i \dot{\mathbf{r}}_i^2}_{\text{Kinetic}} + \underbrace{V(\mathbf{r})}_{\text{Potential}}$$



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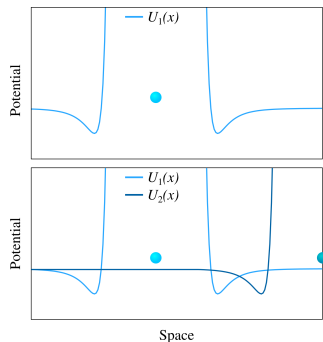
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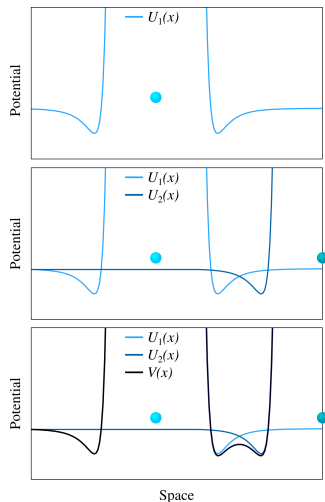
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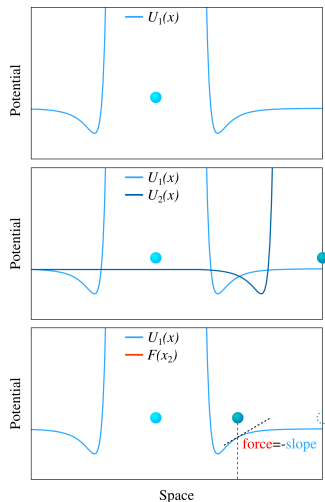
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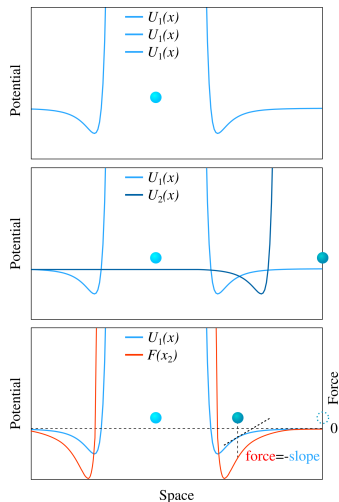
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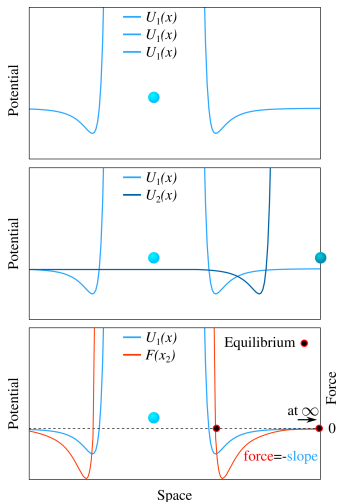
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Example : Lennard-Jones potential

Example :

- 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 :

$$\begin{aligned} F_i(\mathbf{r}_i, \mathbf{r}_j) &= -\nabla U(r_{ij}) = \\ &= 24\varepsilon \left(\frac{\sigma}{r_{ij}} \right)^6 \left[1 - 2 \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \frac{\mathbf{r}_j - \mathbf{r}_i}{r_{ij}^2} \end{aligned}$$

- Equilibrium :

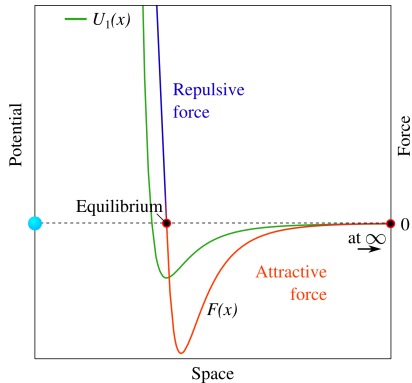
- At $T = 0$ K : $r_{ij}^e = 2^{1/6}\sigma$
- At $T > 0$: $r_{ij}^e(T) > 2^{1/6}\sigma$

- Stable lattice : hcp (or fcc (111))

- Parameters :

σ - length units \sim lattice spacing

ε - energy units \sim bonding energy.



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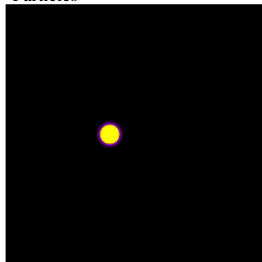
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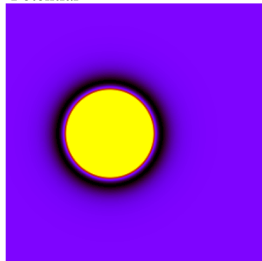
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Particles



Potential



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- At $T = 0$ K : $r_{ij}^e = 2^{1/6}\sigma$
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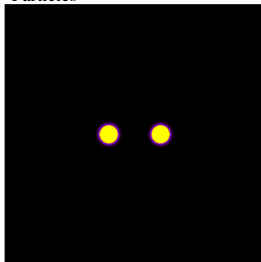
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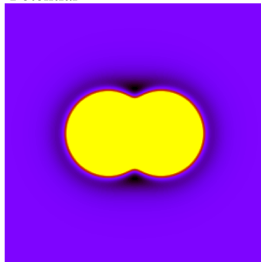
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Particles



Potential



Example : Lennard-Jones potential

Example :

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

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

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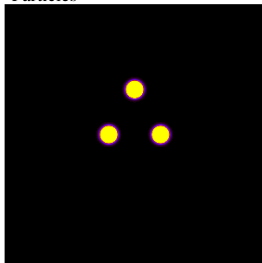
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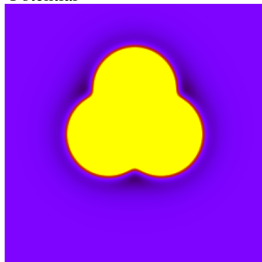
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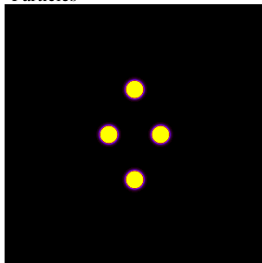
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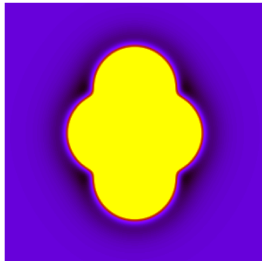
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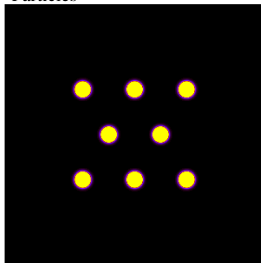
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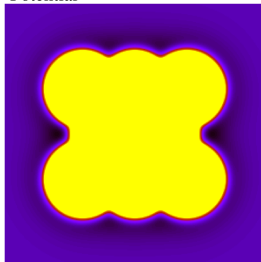
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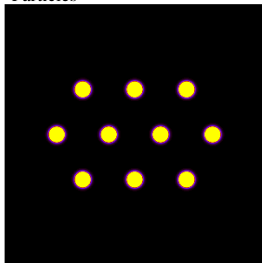
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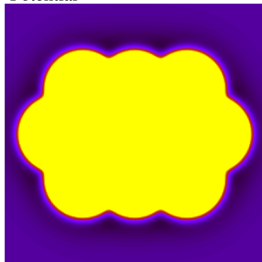
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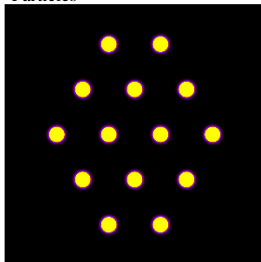
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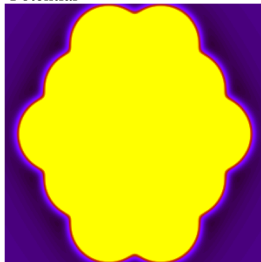
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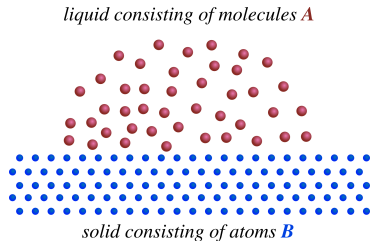
Mixing rule

- 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] :

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

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

- 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



Parameters of interactions:



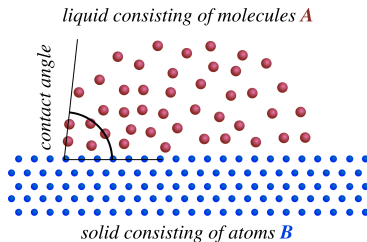
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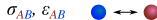
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Parameters of interactions:



Short-range potentials and a cutoff

- Short-range potential

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

- System pair potential :

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

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

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

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

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

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

Multi-body potentials

Example **EAM** : Embedded-Atom Model/Method

- Pair-potential does not work for defects, free surfaces and fracture surfaces, impurities (hydrogen embrittlement), etc.
- In the EAM, each atom in a solid is considered as an impurity embedded in a host made of other atoms (like in Eshelby problem and self-consistent homogenization)
- Multi-body potential EAM :

$$E_{tot} = \sum_i F(\rho_{h,i}) + \sum_{i,j,i \neq j} \phi_{ij}(R_{ij})$$

- With electron densities assumed to be $\rho_{h,i} = \sum_{j \neq i} \rho_j^a(R_{ij})$
- Force acting on atom i :

$$F_i = -\nabla E_i = -\sum_j \frac{\partial F}{\partial \rho_j} \frac{\partial \rho_j}{\partial R_{ij}} - \sum_j \frac{\partial \phi_{ij}}{\partial R_{ij}}$$

[A] Daw, M. S., & Baskes, M. I. (1984). Embedded-atom method . . . Phys Rev B, 29(12), 6443.

[B] Foiles, S. M., Baskes, M. I., & Daw, M. S. (1986). Embedded-atom-method functions . . . Phys Rev B, 33(12), 7983.

Multi-body potentials II

Define functions $F(\rho)$, $\rho(R)$, $\phi(R)$

- Functions are defined in top-bottom fashion, to fit macroscopic quantities
- The lattice constants are

$$A_{ij} = -F'(\bar{\rho})V_{ij}, V_{ij} = \sum_m \rho'_m a_i^m a_j^m / a^m, A_{ij} = 0.5 \sum_m \phi'_m a_i^m a_j^m / a^m$$

where a^m are distances between atoms and a_i^m is the i th-component of the vector-distance

- Elastic constants

$$C_{ijkl} = (B_{ijkl} + F'(\bar{\rho})W_{ijkl} + F''(\bar{\rho})V_{ij}V_{kl})/\Omega_0$$

$$\text{with } B_{ijkl} = 0.5 \sum_m (\phi''_m - \phi'_m/a^m) a_i^m a_j^m a_k^m a_l^m / (a^m)^2$$

$$W_{ijkl} = \sum_m (\rho''_m - \rho'_m/a^m) a_i^m a_j^m a_k^m a_l^m / (a^m)^2$$

- Sublimation energy

$$E_s = -(F(\bar{\rho}) + \bar{\phi}/2)$$

- Vacancy-formation energy is

$$E_{1V}^V = -\bar{\phi}/2 + \sum_m (F(\bar{\rho} - \rho_m) - F(\bar{\rho})) + E_{relax}$$

Multi-body potentials III

- From pure metal to alloy
- Need to compute ϕ_{ij} if we know ϕ_{ii} as :

$$\phi_{ij}(r) = Z_i(r)Z_j(r)/r,$$

with Z being an effective charge of the atom

Testing of resulting properties^[B,C]

- Fracture toughness
- Formation volume and migration density of vacancies / divacancies / self-interstitials
- Surface energies of different faces
- Segregation energy of substitutional impurities
- Phonon frequencies
- Gibbs free energy (T)
- Dislocation properties

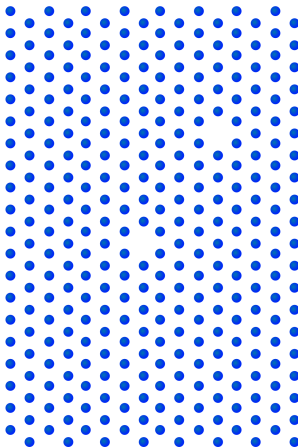
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[C] Daw, M. S., Foiles, S. M., & Baskes, M. I. (1993). The embedded-atom . Materials Science Reports, 9(7-8), 251-310.

Algorithms

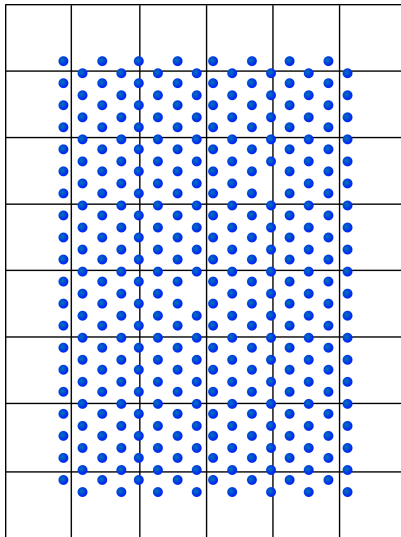
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- Create a spatial grid $d \geq r_{\text{cut}}$
 - Every cell contains a list of particles and a list of neighbouring cells
 - Forces are evaluated in the cell and with respect to the neighbouring cells
 - 3rd Newton's law is used
- Instead of checking 8 neighbouring cells, we check only 4.*



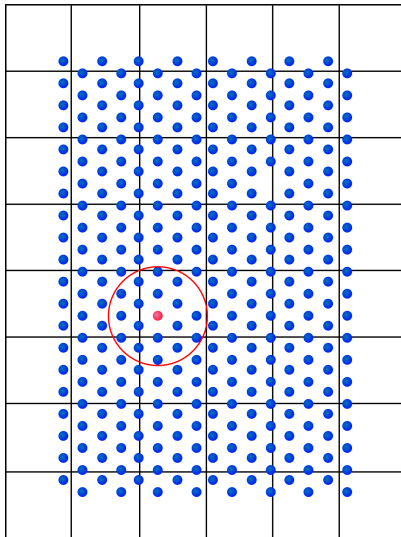
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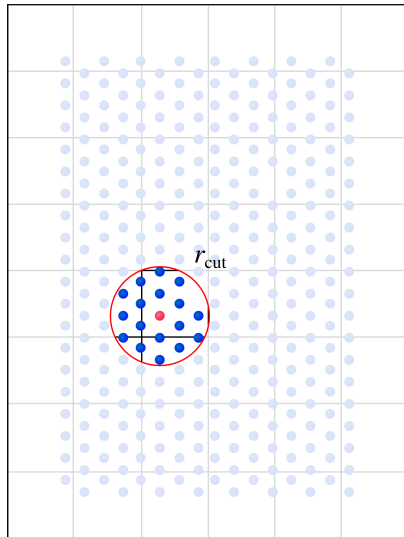
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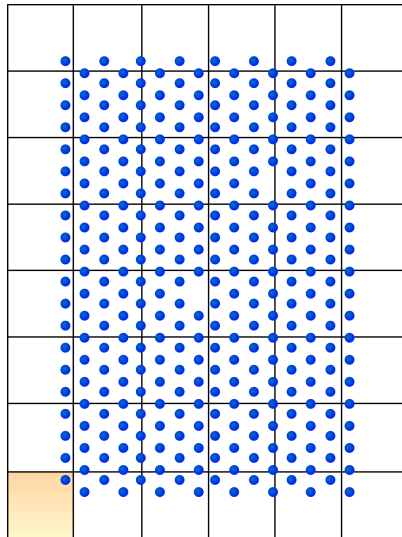
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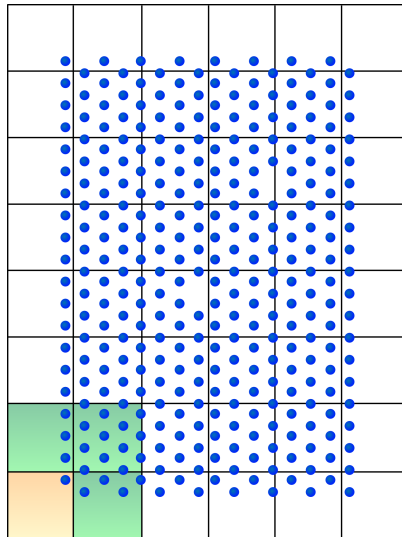
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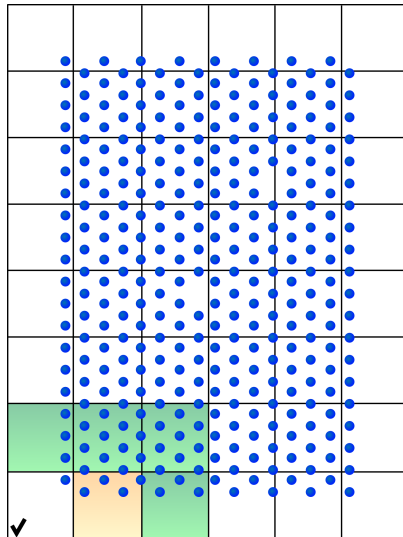
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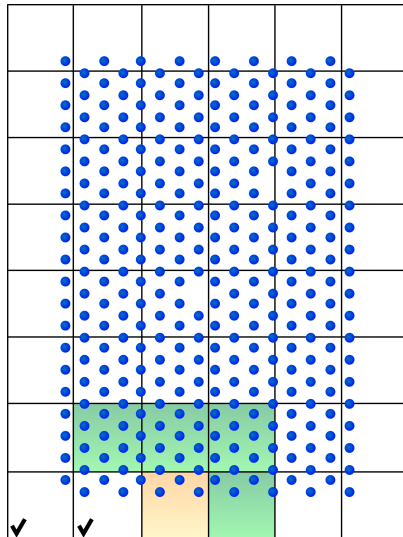
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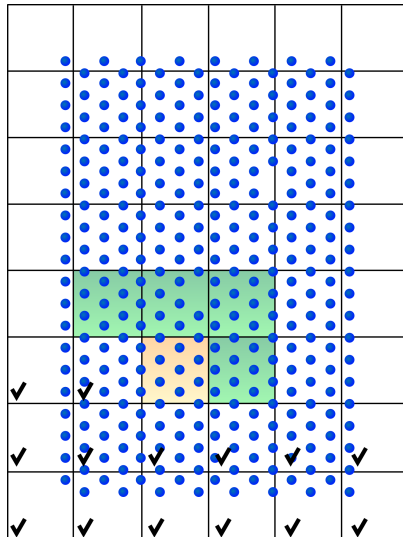
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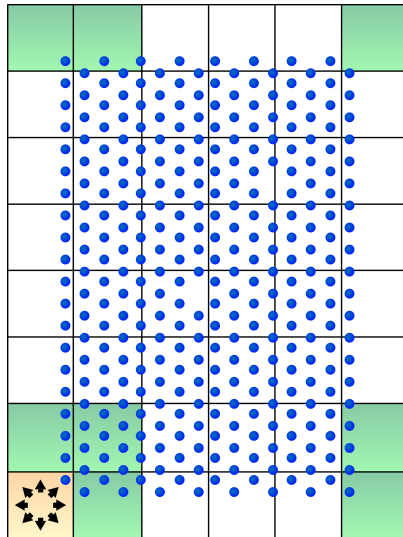
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- Case of periodic BC



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 :

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

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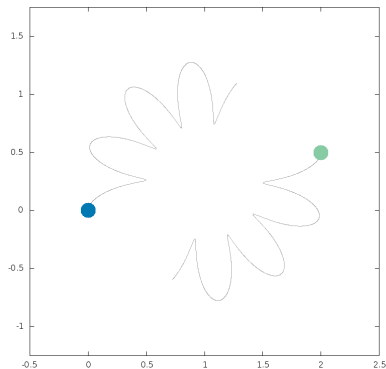
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$$x_i(t + \Delta t) = x_i(t) + \dot{x}_i(t)\Delta t$$

■ 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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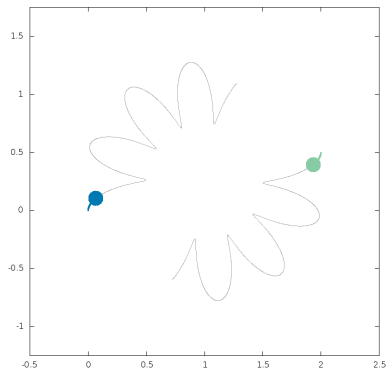
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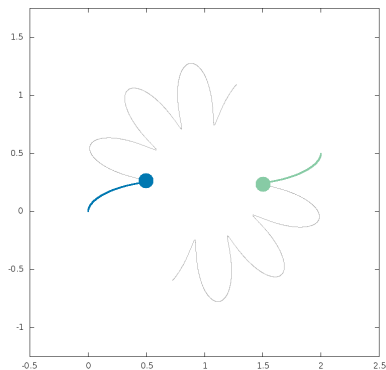
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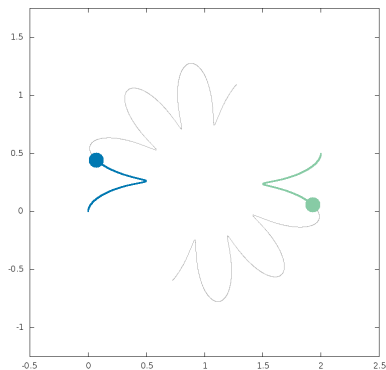
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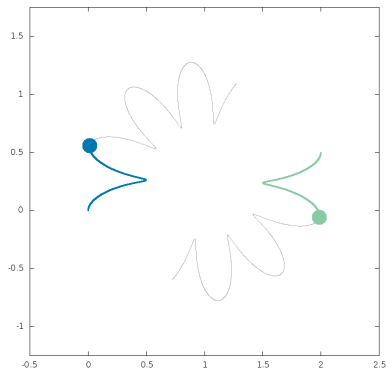
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■ Let's see how fast it diverges

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

$\Delta t = 0.00001$



Time integration : explicit Euler

■ Initial value problem

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

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Compute : $f_i(x(t))$

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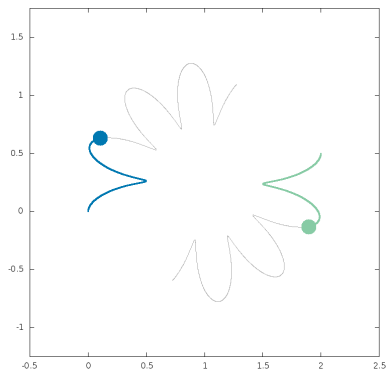
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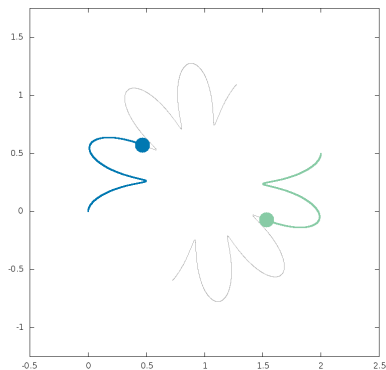
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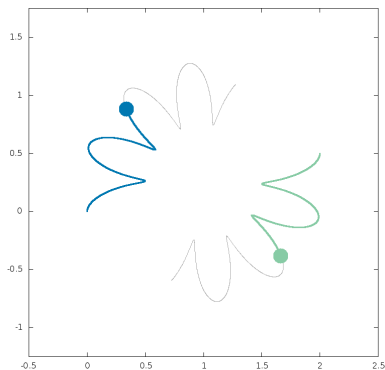
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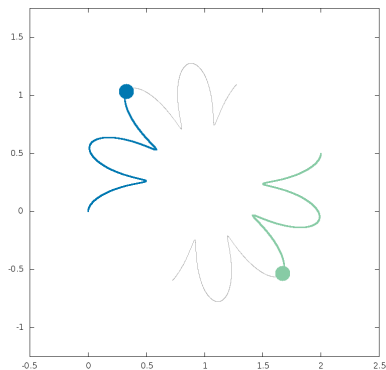
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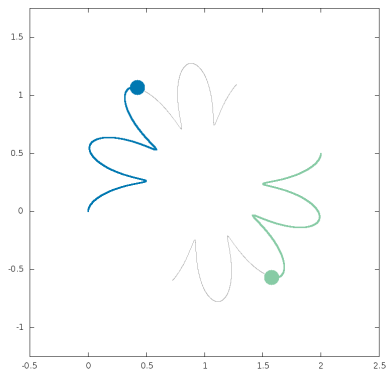
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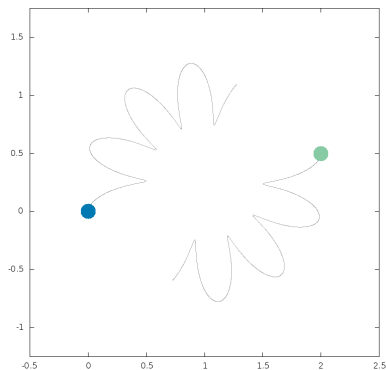
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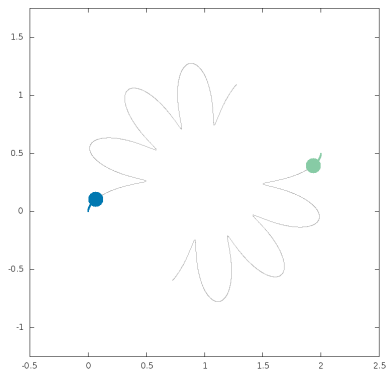
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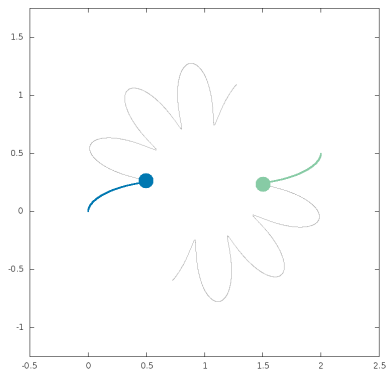
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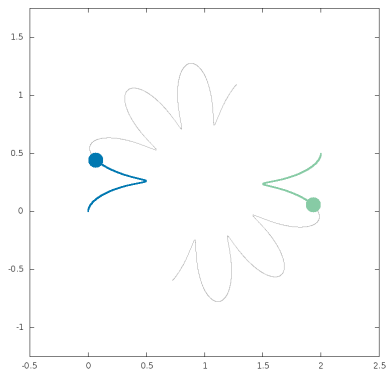
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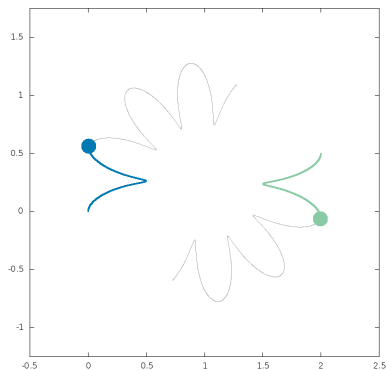
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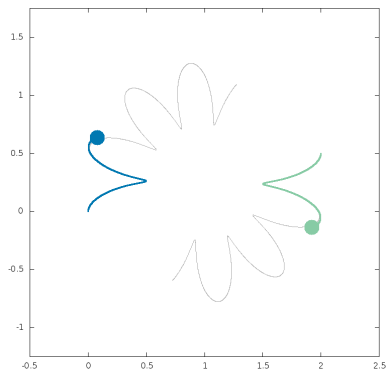
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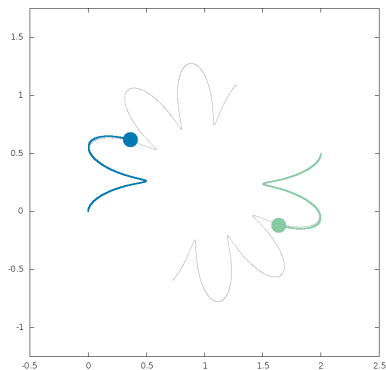
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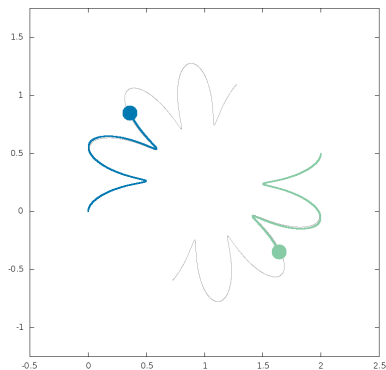
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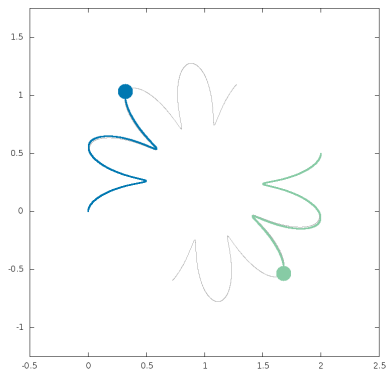
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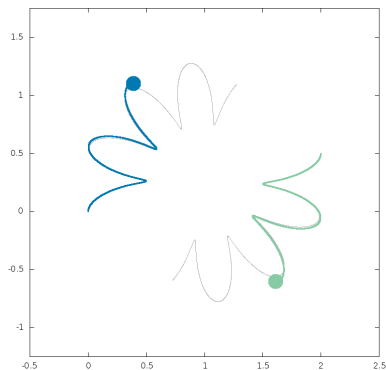
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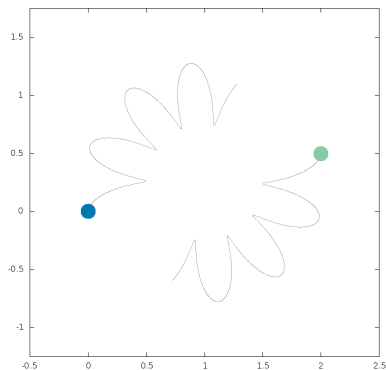
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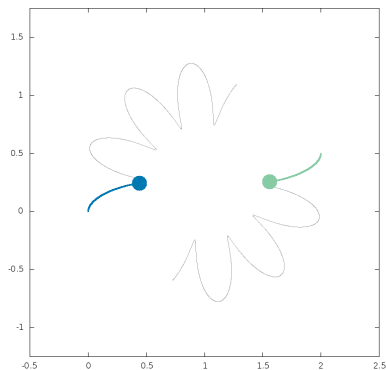
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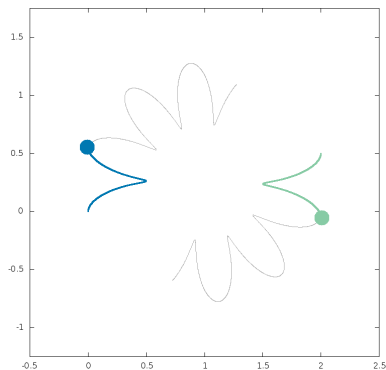
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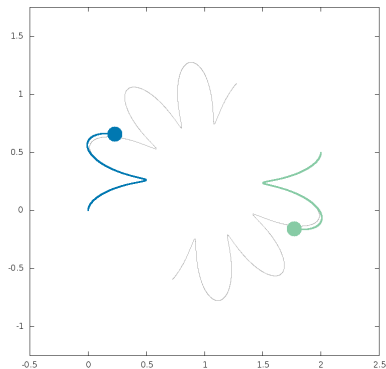
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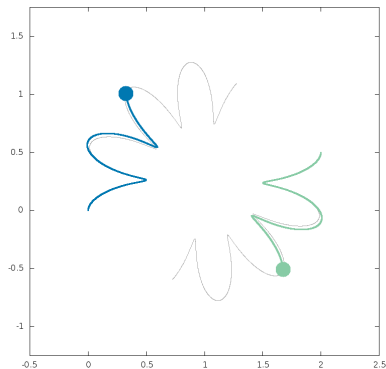
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■ Straight forward approach (**explicit Euler**)

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 :

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

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

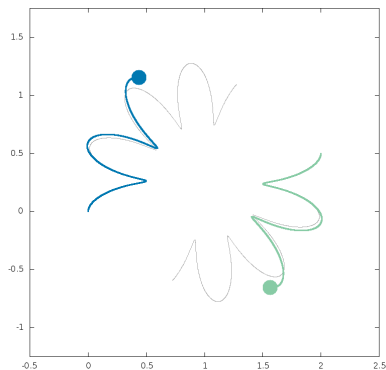
Compute :

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

■ Let's see how fast it diverges

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

$\Delta t = 0.00010$



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**)

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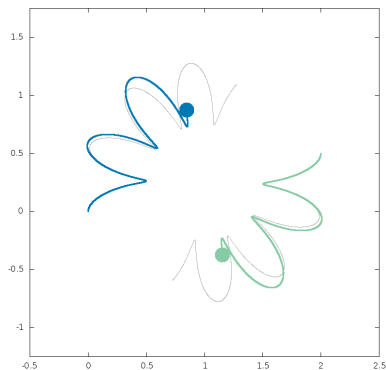
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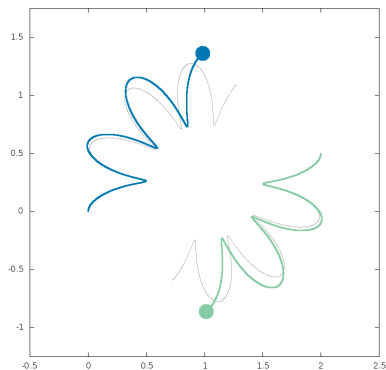
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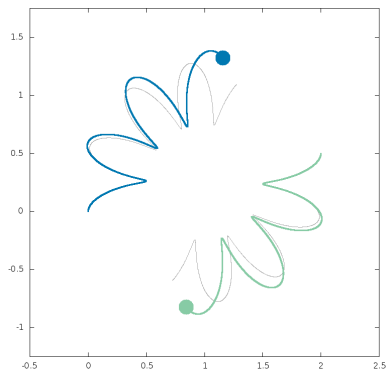
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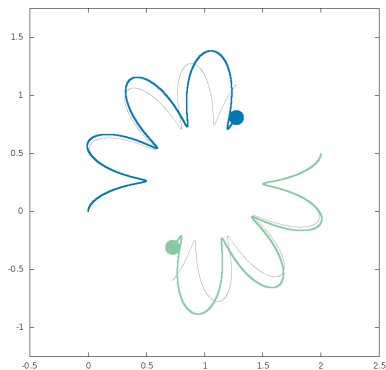
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Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.00010$



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

$\Delta t = 0.01$

■ 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 :

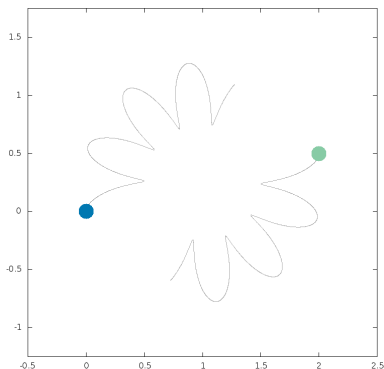
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Compute :

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

■ Symplectic integrator! In average it preserves the energy.



Time integration : semi-implicit Euler

■ Initial value problem

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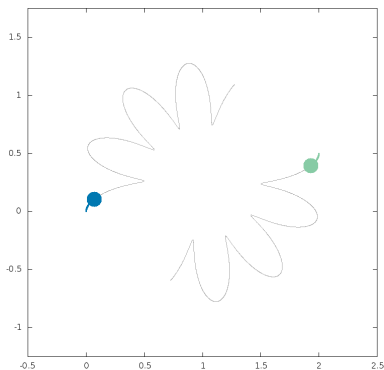
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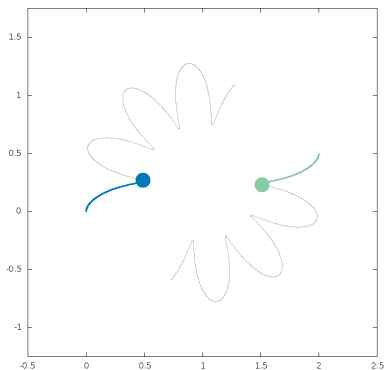
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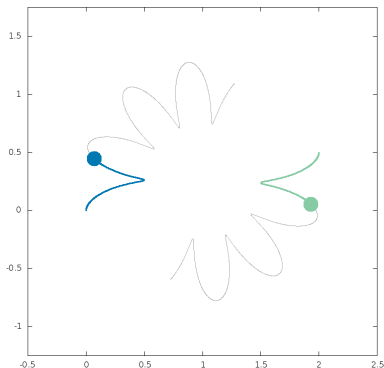
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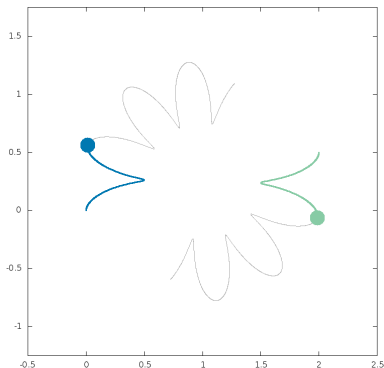
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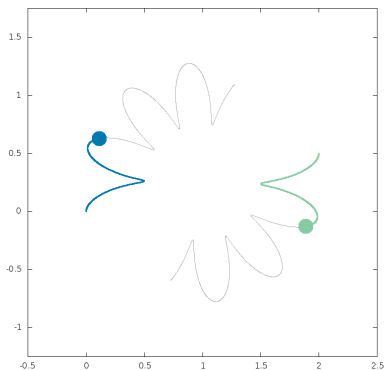
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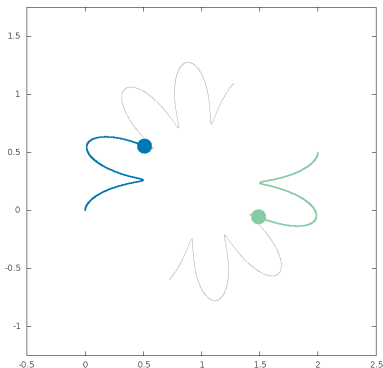
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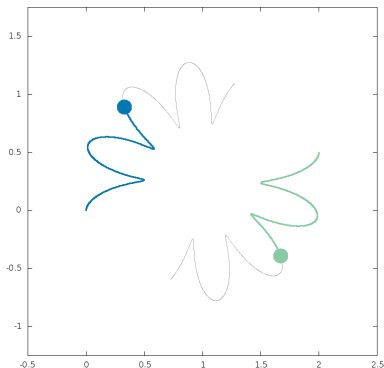
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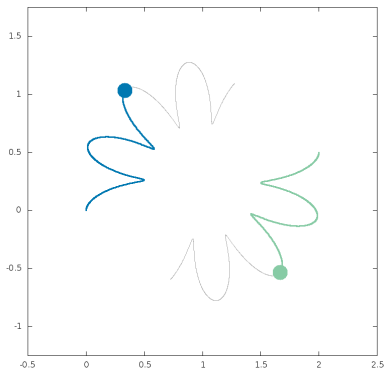
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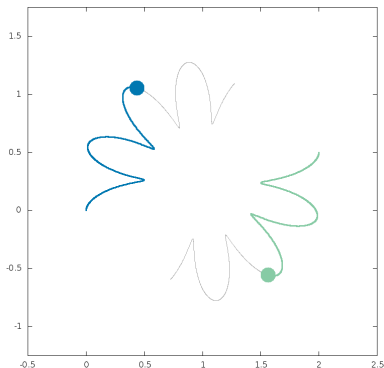
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$\Delta t = 0.02$

■ A better approach

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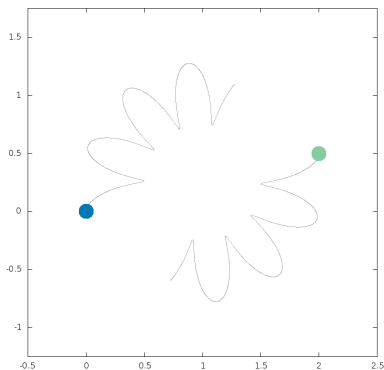
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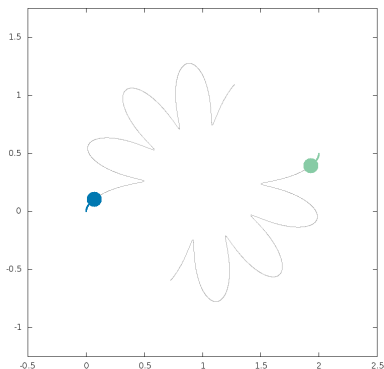
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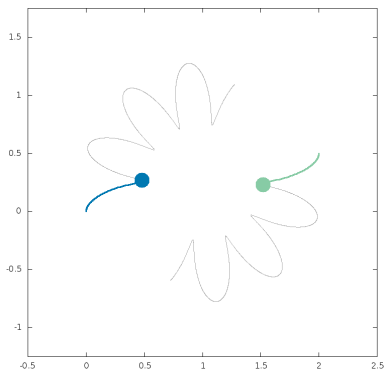
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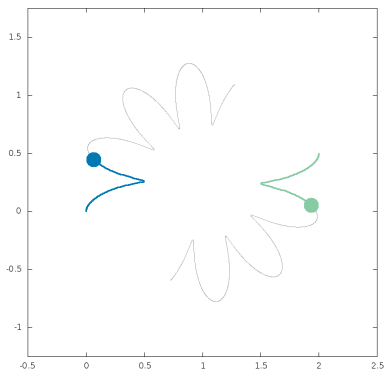
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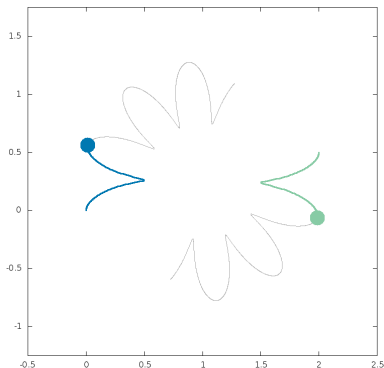
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Example : $\sigma = 1, \varepsilon = 1, m = 1, v_0 = 0.2$

$\Delta t = 0.02$

■ A better approach

(**semi-implicit Euler**)

Compute : $f_i(x(t))$

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

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Compute :

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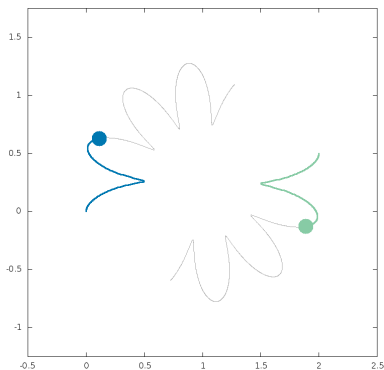
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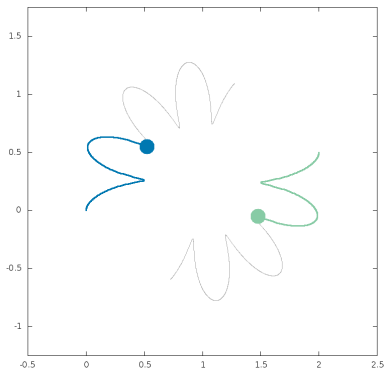
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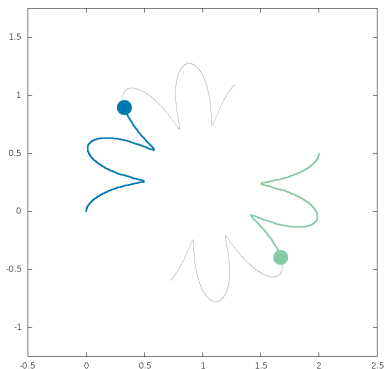
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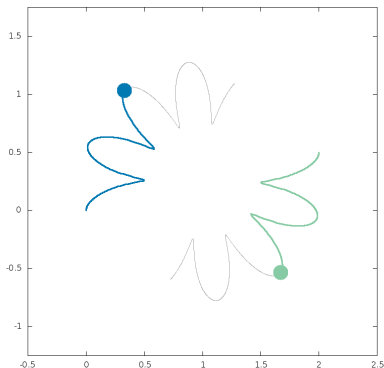
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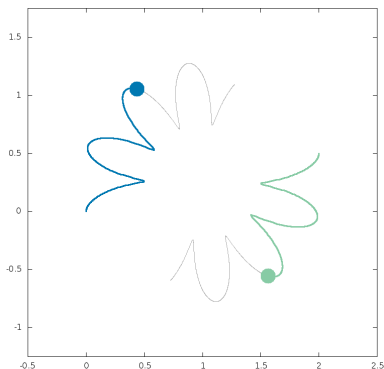
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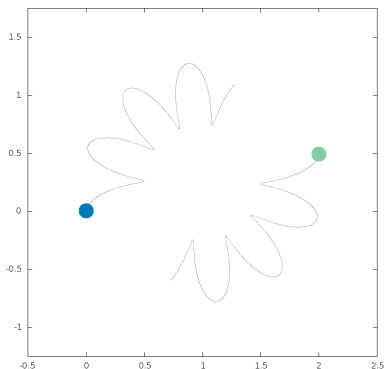
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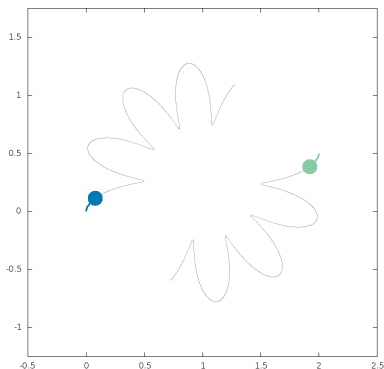
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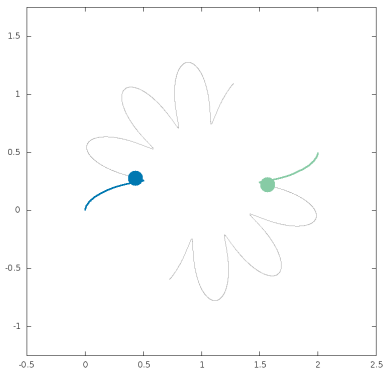
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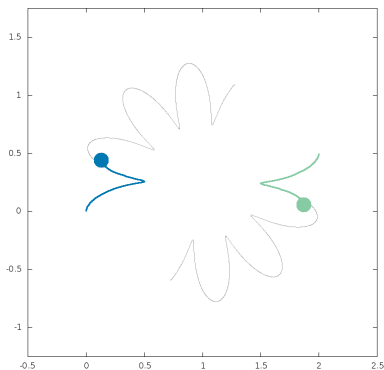
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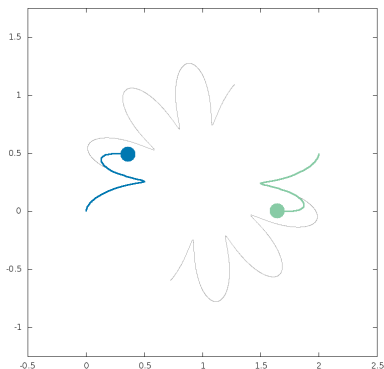
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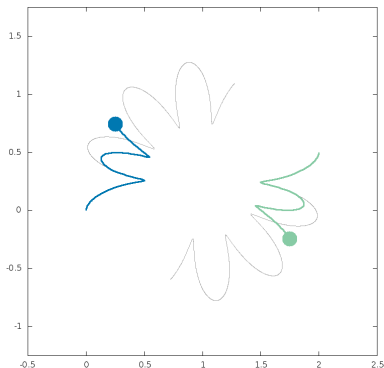
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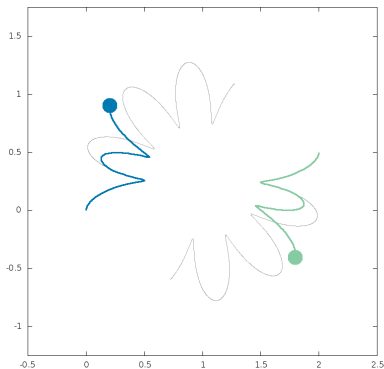
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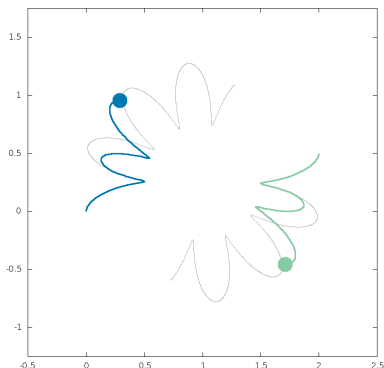
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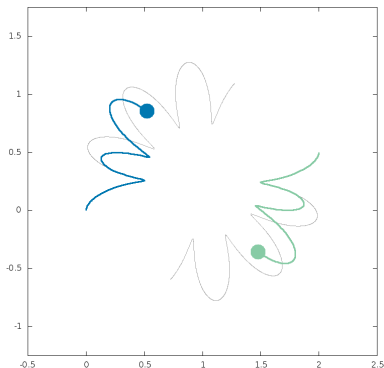
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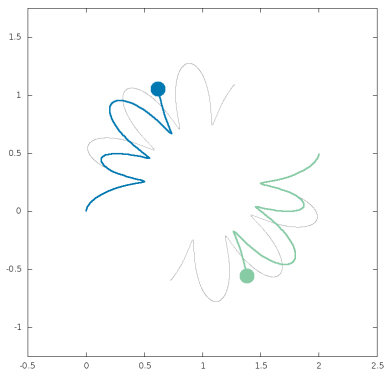
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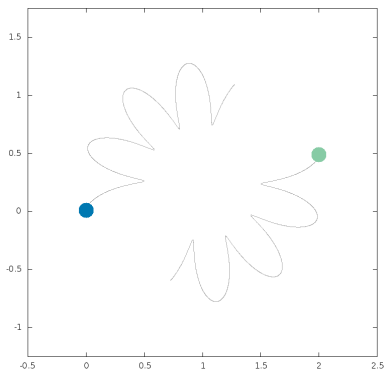
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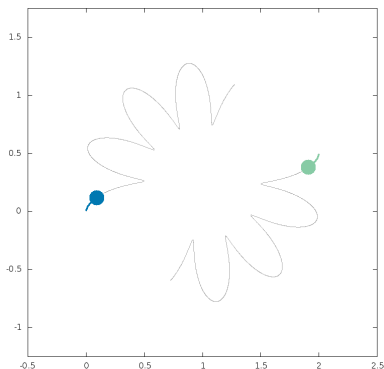
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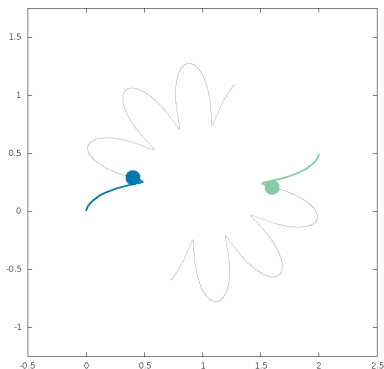
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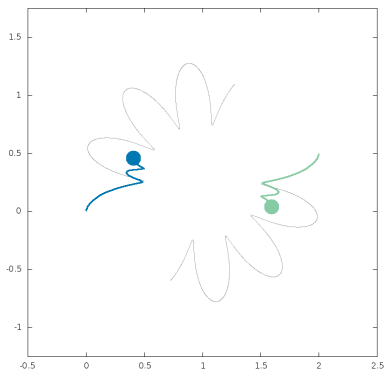
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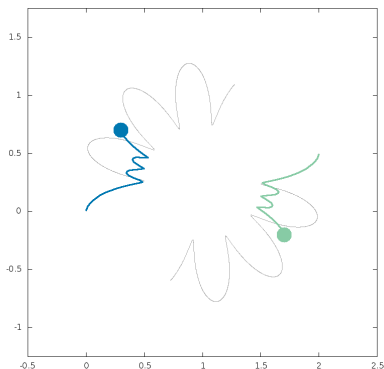
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■ Symplectic integrator! In average it preserves the energy.



Time integration : semi-implicit Euler

■ Initial value problem

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

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

$\Delta t = 0.10$

■ 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 :

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

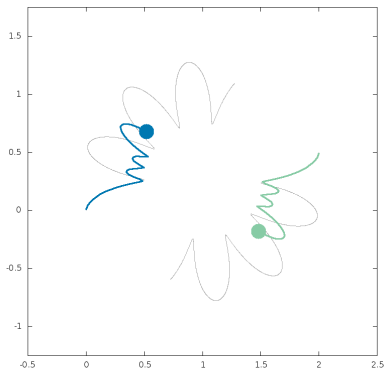
$$\dot{x}_i(t + \Delta t) = \frac{x_i(t+\Delta t) - x_i(t)}{\Delta t}$$

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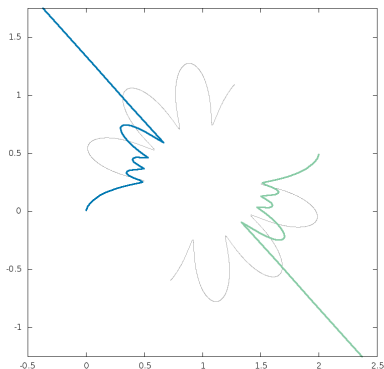
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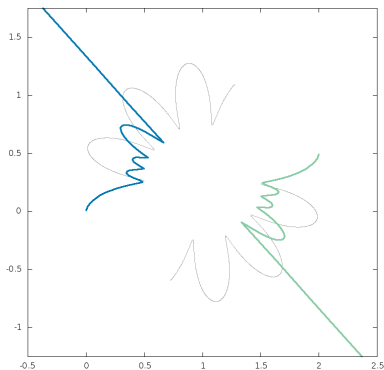
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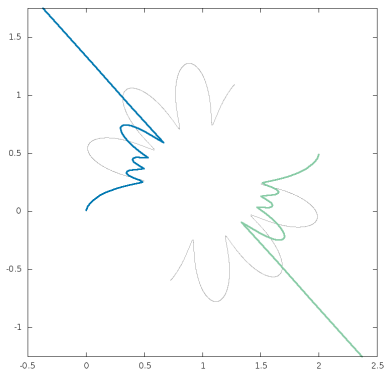
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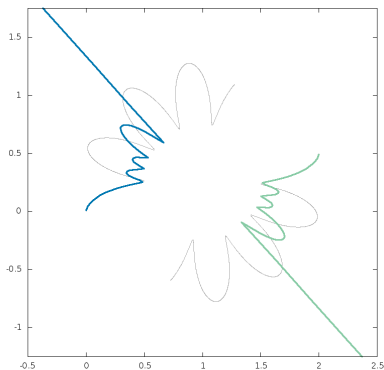
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■ Symplectic integrator!

In average it preserves the energy.



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

Store $f_i(t)$

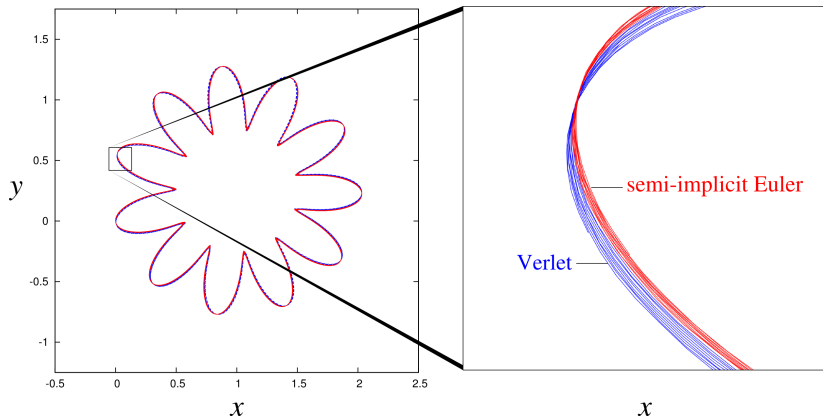
Compute : $f_i(t + \Delta t) = f_i(x(t + \Delta t))$

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

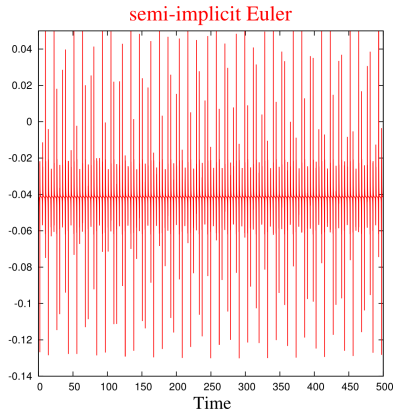
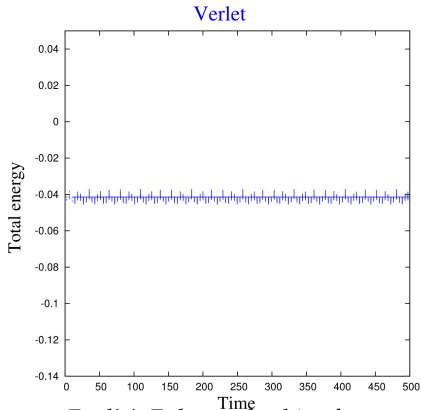
- Requires additional storage for $f_i(t)$.
- Symplectic integrator!
In average it preserves the energy.

[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 symplectic, i.e. in average they preserve the system energy
- *Velocity-Verlet* has better energy preserving properties

■ 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 $t \rightarrow t + \Delta t$
- 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.

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- 1 distribute particles $x_i(0)$ for $i \in [0, N]$
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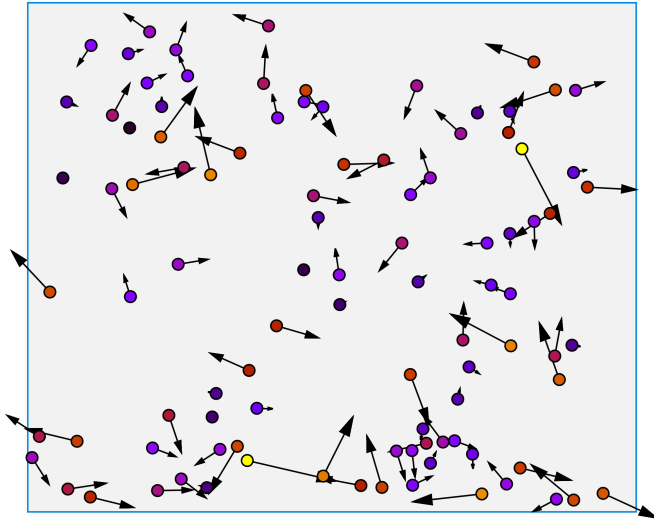
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Animation `pbc.gif`

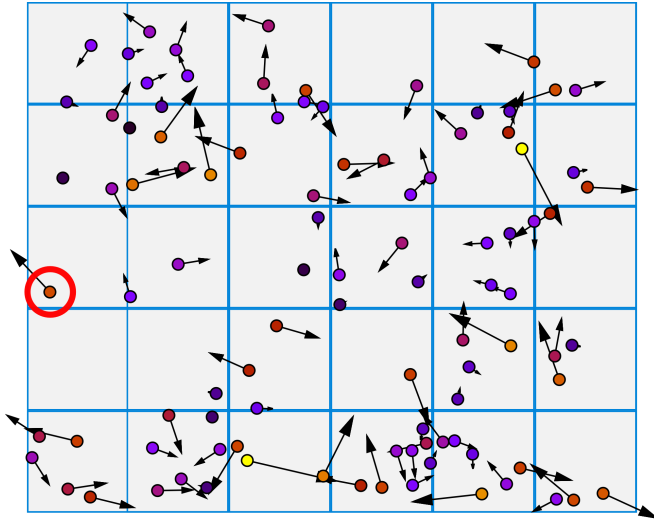
Boundary conditions I

■ Periodic boundary conditions



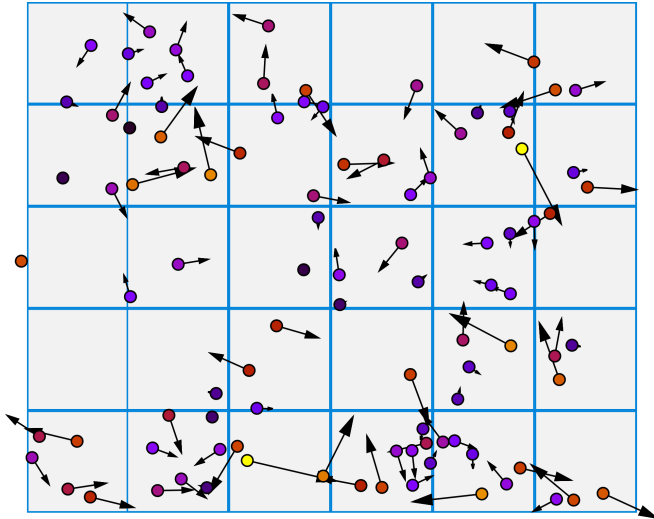
Boundary conditions I

■ Periodic boundary conditions



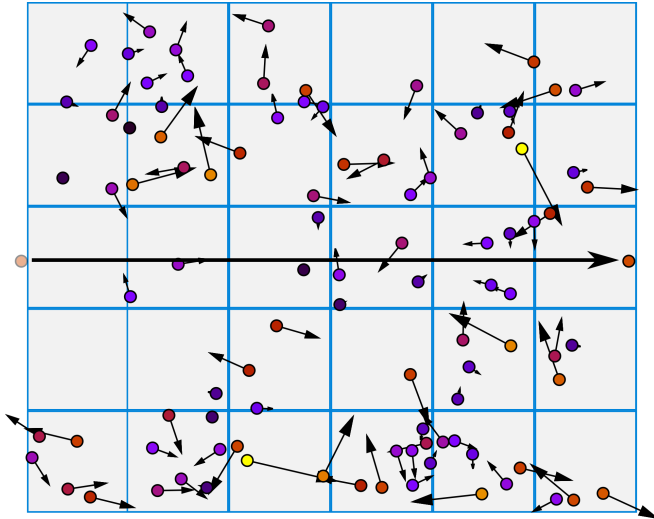
Boundary conditions I

■ Periodic boundary conditions



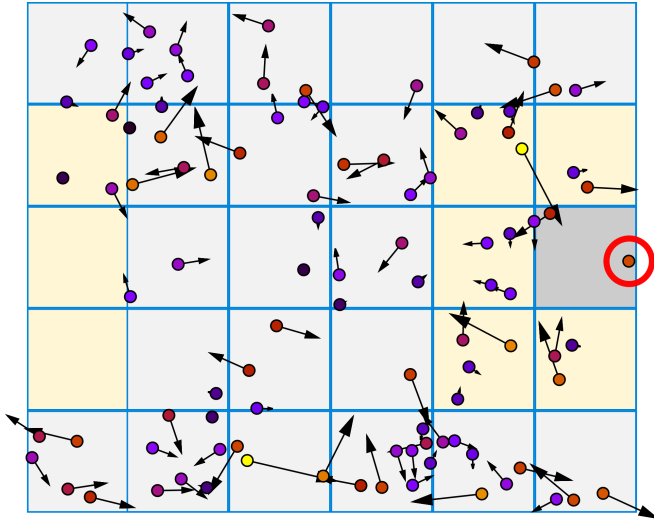
Boundary conditions I

■ Periodic boundary conditions



Boundary conditions I

■ Periodic boundary conditions



Animation `rbc.gif`

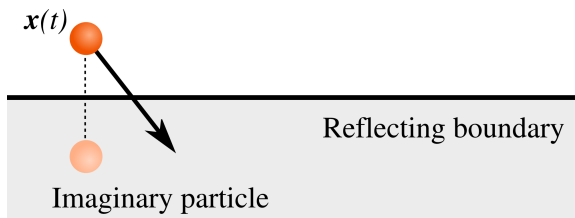
Boundary conditions II

■ Reflecting boundary conditions



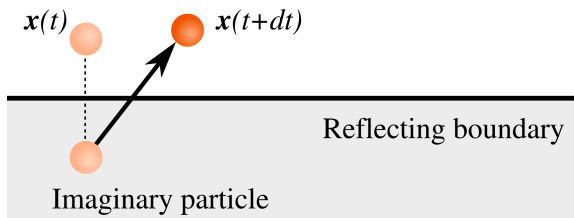
Boundary conditions II

■ Reflecting boundary conditions



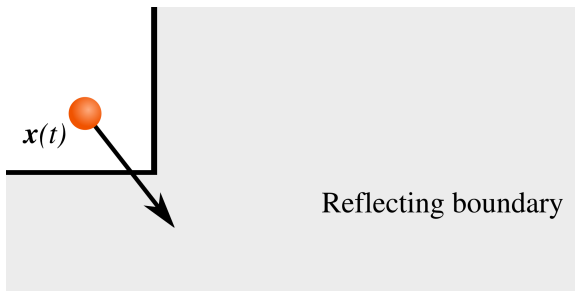
Boundary conditions II

■ Reflecting boundary conditions



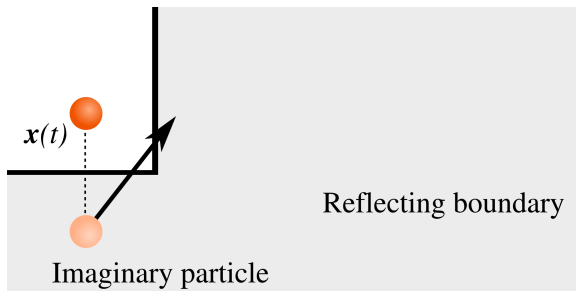
Boundary conditions II

- Reflecting boundary conditions



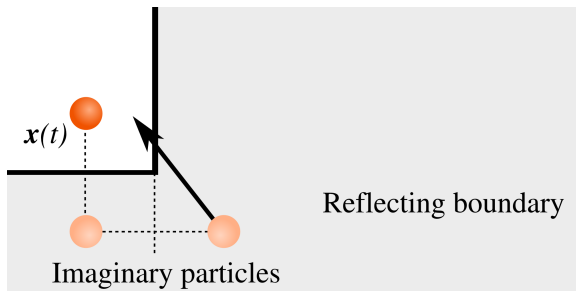
Boundary conditions II

■ Reflecting boundary conditions



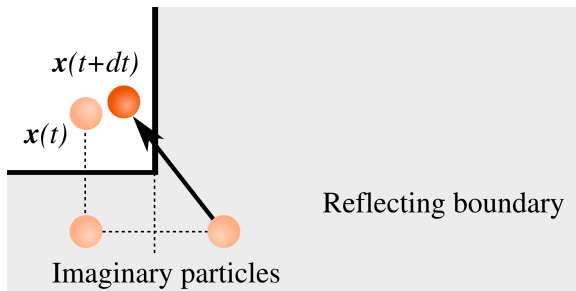
Boundary conditions II

■ Reflecting boundary conditions



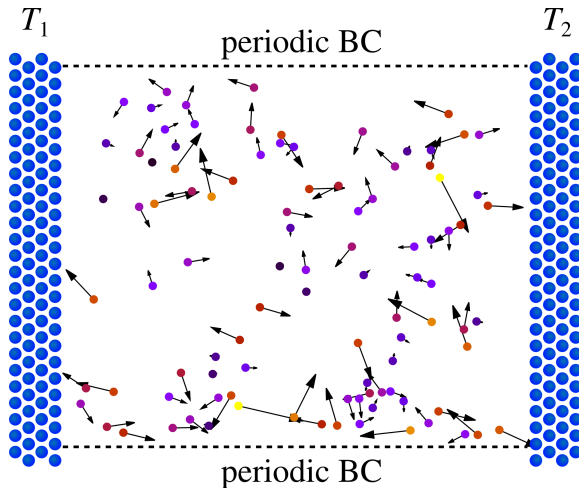
Boundary conditions II

■ Reflecting boundary conditions



Boundary conditions II

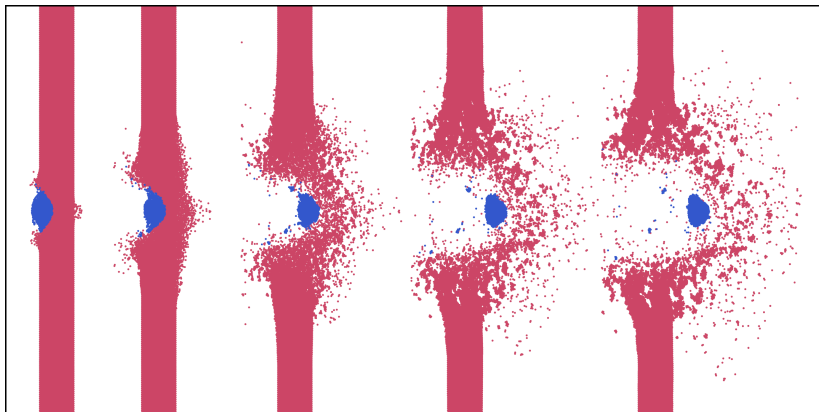
■ Reflecting boundary conditions (different approach)



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

Boundary conditions III

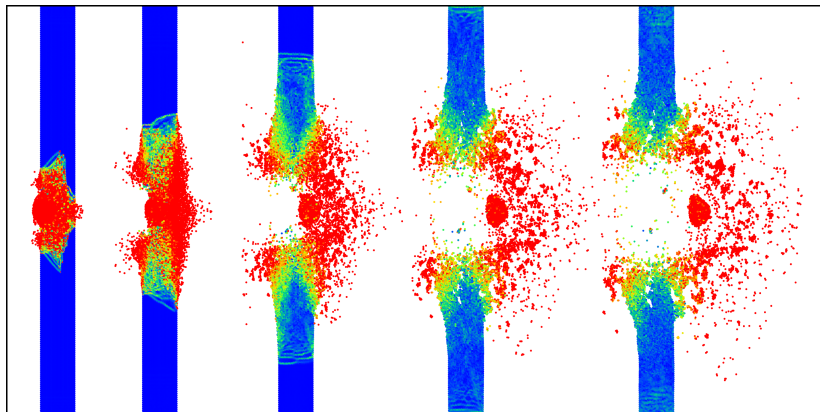
- Initial velocity (initial value problem) : impact, penetration



- Volumetric forces : gravity (additional force $F_i += m_i g$)

Boundary conditions III

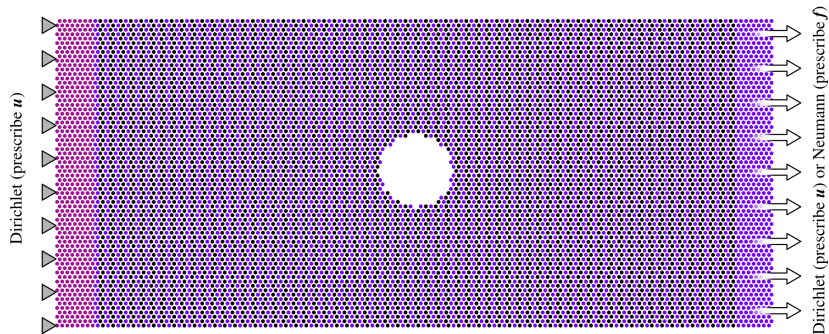
- Initial velocity (initial value problem) : impact, penetration



- Volumetric forces : gravity (additional force $F_i += m_i g$)

Boundary conditions IV

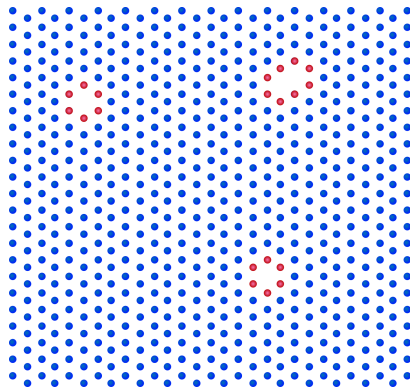
- Mechanical boundary conditions : Dirichlet and Neumann



Initial configuration

Simple configurations* :

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



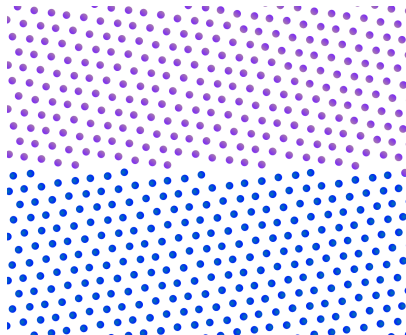
Crystal with vacancy defects (easy to control)

*Stable initial configuration can be produced by minimization of the system potential energy.

Initial configuration

Simple configurations* :

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- Bi-crystals^[1]
- Stacking faults and dislocations
- Simple geometries
- Long molecules



Bi-Crystal (grain boundary)

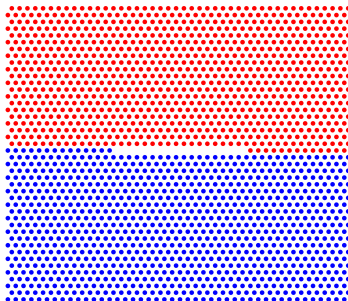
*Stable initial configuration can be produced by minimization of the system potential energy.

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

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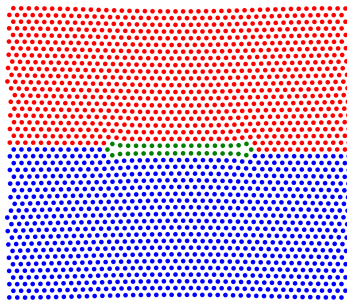
Remove several atoms

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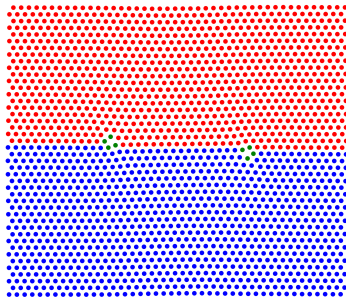
Stacking fault with partial dislocations

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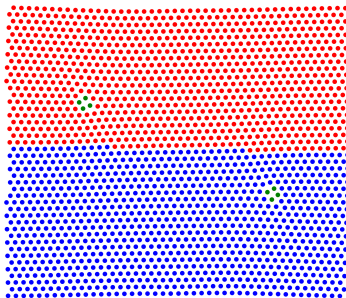
Healing stacking fault forms two perfect edge dislocations

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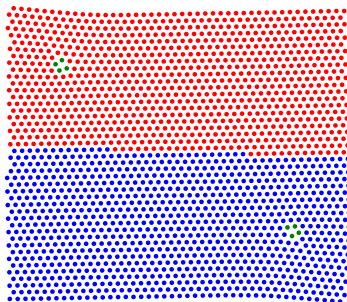
Dislocations glide

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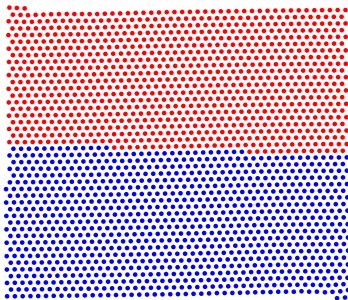
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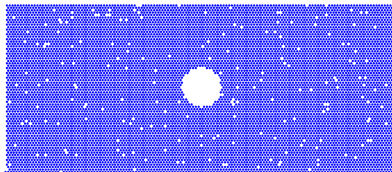
Dislocations form steps on the surface

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- Bi-crystals
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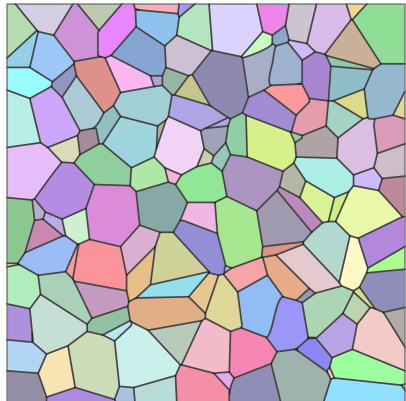
Layer with a circular hole

*Stable initial configuration can be produced by minimization of the system potential energy.

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
- High-temperature corrosion
heat up and cool down initial configuration

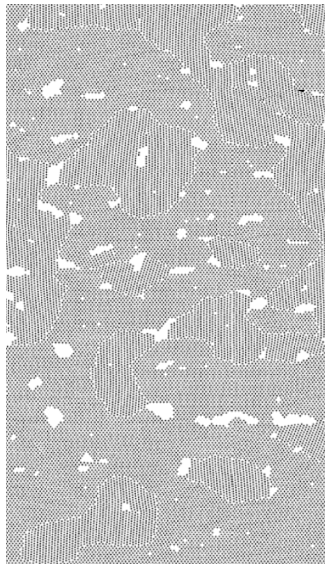


Voronoi tessellation as a basis for construction of a nano-grained material
(adapted from Wikipedia)

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- 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



Porous polycrystal obtained from liquid state by relatively fast cooling

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End of part I