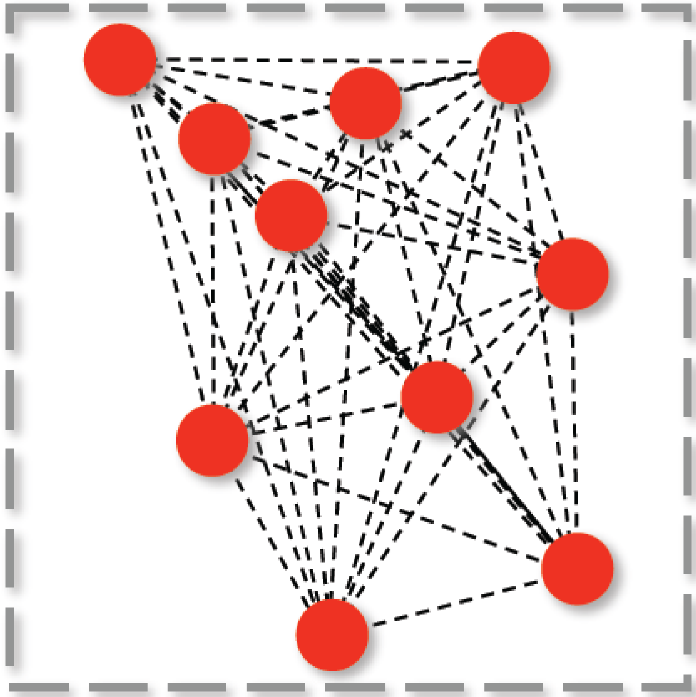
Particle simulation

If interactions particle-particle are included for N particles ⇒ <u>N^2 forces</u>
When two particles get very near to each other – large variation of velocities in small Δt ⇒ short timestep

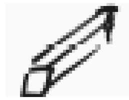


Such approach possible for $N \leq 1000$
For illustration 10^8 částic, 10 Tflop/s,
1 timestep – 3 hours
10^4 timesteps – 3 years
Larger systems

- ***Tree codes*** – interaction particle-cluster
- **<u>Particle-In-Cell</u>** - interaction particle-grid

PIC is very widely applied method
Aim is not accurate description of binary interactions, but oppositely, aim is to obtain equivalent of Vlasov equation.
Thus, macroscopic electromagnetic field and motion of particles in it.
PIC - 1 timestep ~ 0.3 ms, 10^4 steps ~ 3 s

Spatial grid is introduced, field is calculated in nodes and interpolated among them, particles have dimensions equal to cell size - **macroparticles**

In one dimension (1D) – slabs of thickness 1 cell  , 2D –  rods, v 3D cubes, particles have finite dimensions

More velocities than dimensions possible (1D2V,1D3V,2D3V)⇒ currents

Macroparticles may **penetrate** through each other (they are particle clouds)

PIC – illustrative, NL problems solved and limits of analytic models found

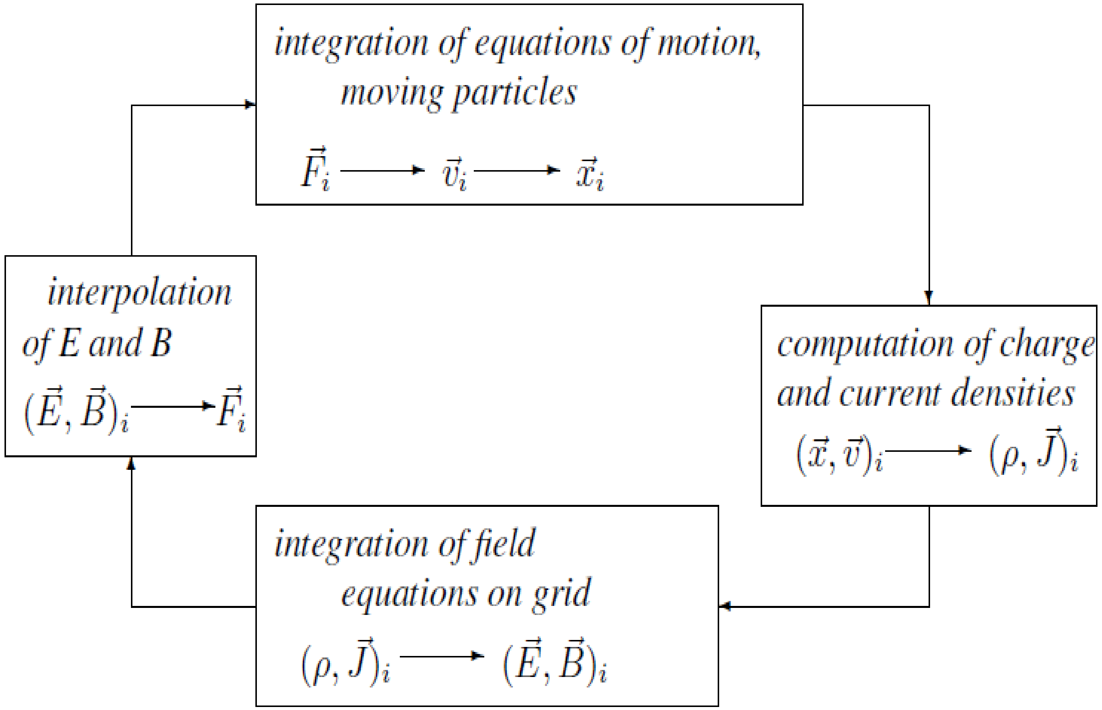
PIC code cycle

Velocities and positions calculated from equations of motion

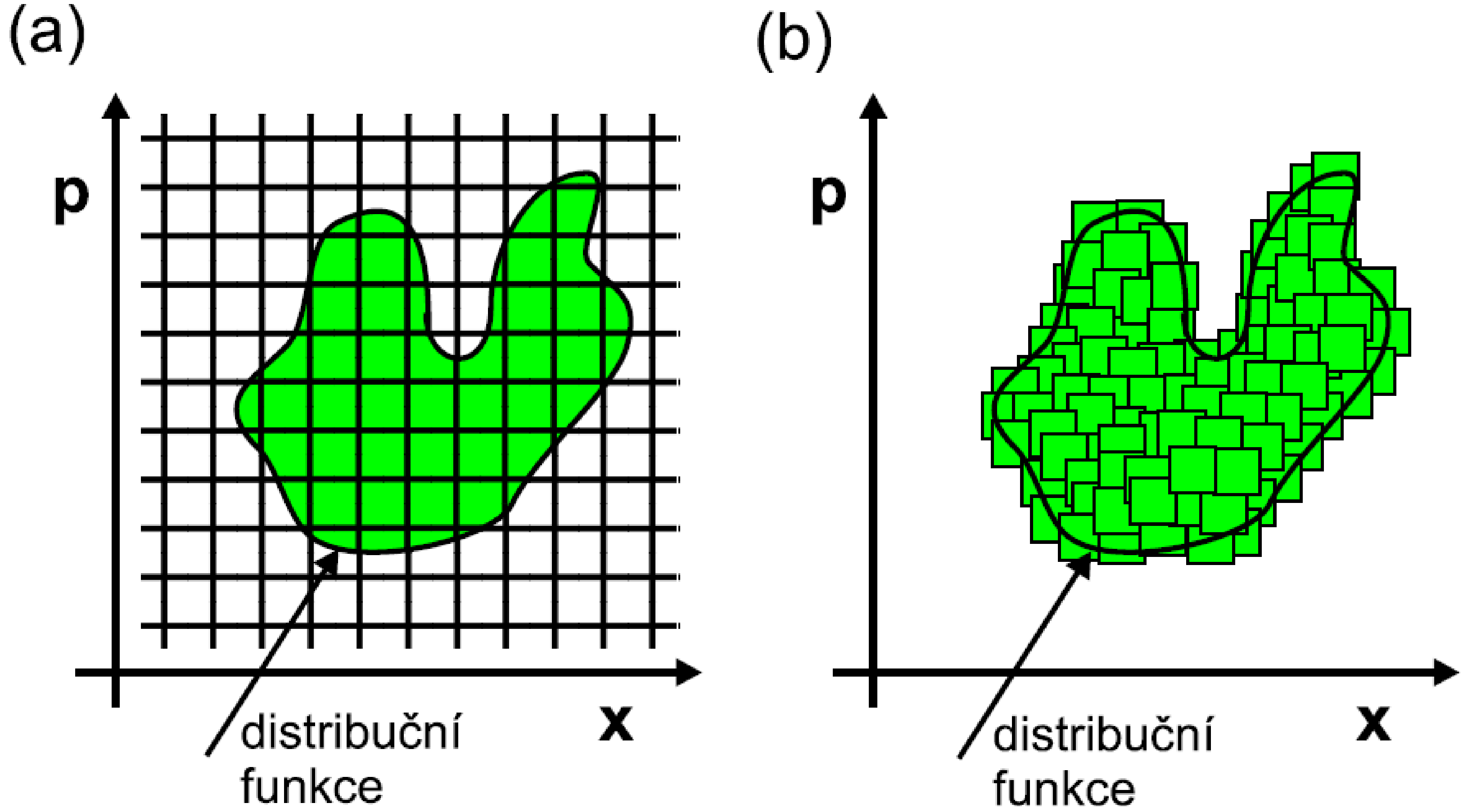
Charge and current densities computed via interpolation to cell nodes

Fields calculated in nodes

Forces via field interpolat-ion to particle positions



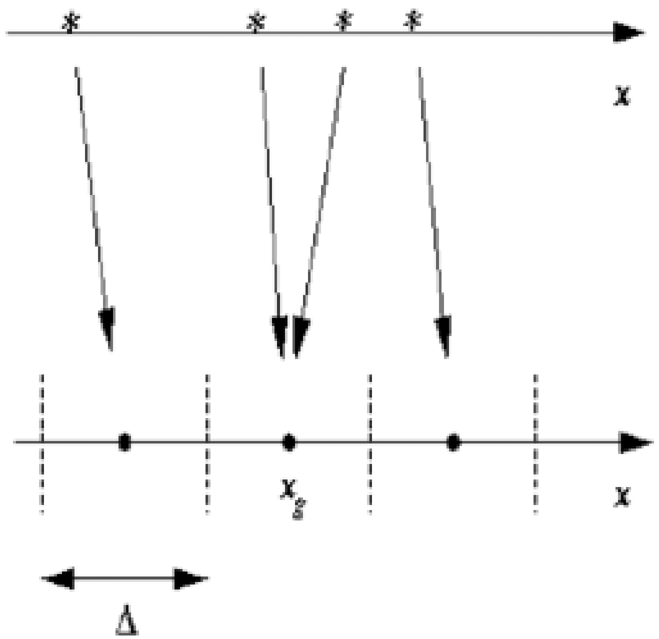
Numerical solving of Vlasov equation – much slower, usually done in less dimensions (often only in 1D), noise-free, favorable for distribution tails
PIC method is in fact solving of Vlasov equation via sampling

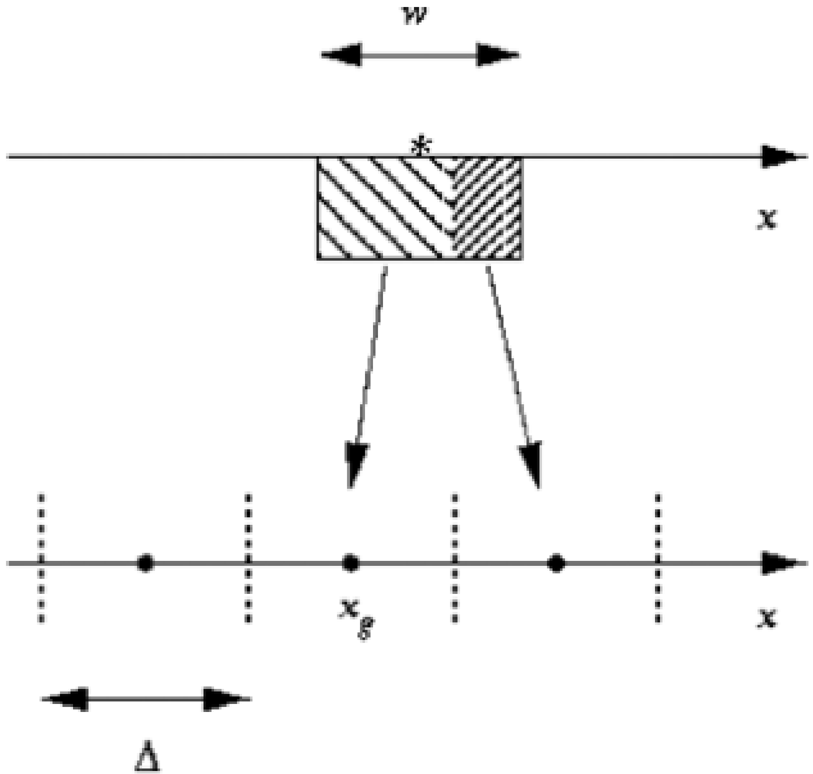


PIC solves Vlasov equation only in places, where particles are present;
it is parallelized easily

Particle assignment and force interpolation

Nearest point assignment (1.order)   Linear interpol. (cloud in cell 2. order)





Maxwell's equations

N cells (length 1) – area length $L=N$, particle number M, length $\delta=1$, particle number per cell $n_{av}=M/L$

Cloud-in-cell – part of charge in $x < (x_i+x_{i+1})/2$ assigned to point i

$$\Delta\rho_i = q(1-\Delta x) \qquad \Delta\rho_{i+1} = q\Delta x$$

Electromagnetic code – Maxwell's equations – charges and currents

In seminars - electrostatic code ES1 $\rightarrow$ Poisson equation

$$\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon_0} \qquad E(i+1) = E(i) + \frac{\rho(i) + \rho(i+1)}{2\varepsilon_0}$$

kód ES1-Fourier transform $\qquad ikE_k = \rho_k / \varepsilon_0$

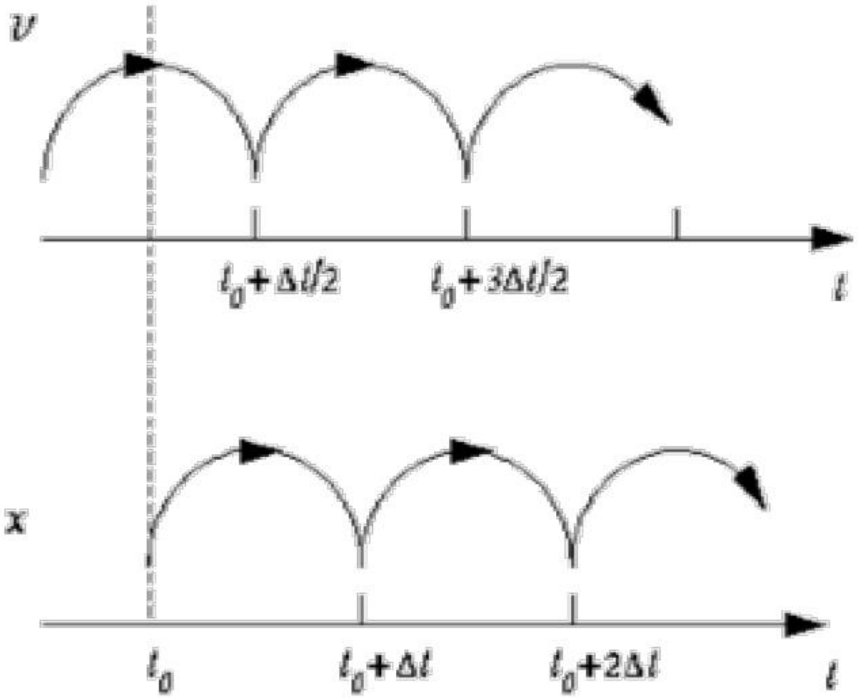
Force acting in $x_i + \Delta x$ $\qquad F = qE_i\left(1 - \Delta x\right) + qE_{i+1}\Delta x$

Leap-frog method often used for particle motion

Equation of motion

$$\mathrm{v}^{n+1/2} = \mathrm{v}^{n-1/2} + F^n \Delta t / m$$

$$x^{n+1} = x^n + \mathrm{v}^{n+1/2}\Delta t$$



Normalization (multiplying by constants takes time)

$$t' = \omega_{pe} t \qquad x' = x/\delta$$

$$\mathrm{v}' = \frac{\mathrm{v}}{\omega_{\mathrm{pe}}\delta} \qquad E' = \frac{\varepsilon_0 E}{eN_{a\mathrm{v}}} = \frac{\varepsilon_0 E}{en_{a\mathrm{v}}\delta}$$

and equations transform into form

$$\frac{\mathrm{d}x'}{\mathrm{d}t'} = \mathrm{v}' \qquad \frac{\mathrm{d}\mathrm{v}'}{\mathrm{d}t'} = -E' \qquad \frac{\mathrm{d}E'}{\mathrm{d}x'} = 1 - \frac{N}{N_{a\mathrm{v}}}$$

simplest case

motion of electrons solved, ions as homogenous neutralizing background

Check – total energy conservation

$$\epsilon = \sum_{j=1}^{M} \frac{m}{2} \mathrm{v}_{\mathrm{j}}^2 + \sum_{i=1}^{N} \frac{\varepsilon_0 E_i^2}{2} \delta = \frac{m\omega_{pe}^2 \delta^2}{2} \left[\sum_{j=1}^{M} \mathrm{v}_{\mathrm{j}}'^2 + N_{a\mathrm{v}} \sum_{i=1}^{N} E_{\mathrm{i}}'^2 \right]$$

ES1 – 1D electrostatic non-relativistic, today for education,

Moving ions, possible $B_0 \perp x$, periodic boundaries *E(N+1)=E(1)*