INSTITUTE OF PLASMA PHYSICS
OF THE CZECH ACADEMY OF SCIENCES

PIC modelling used in Magnetic Confinement Fusion Plasmas

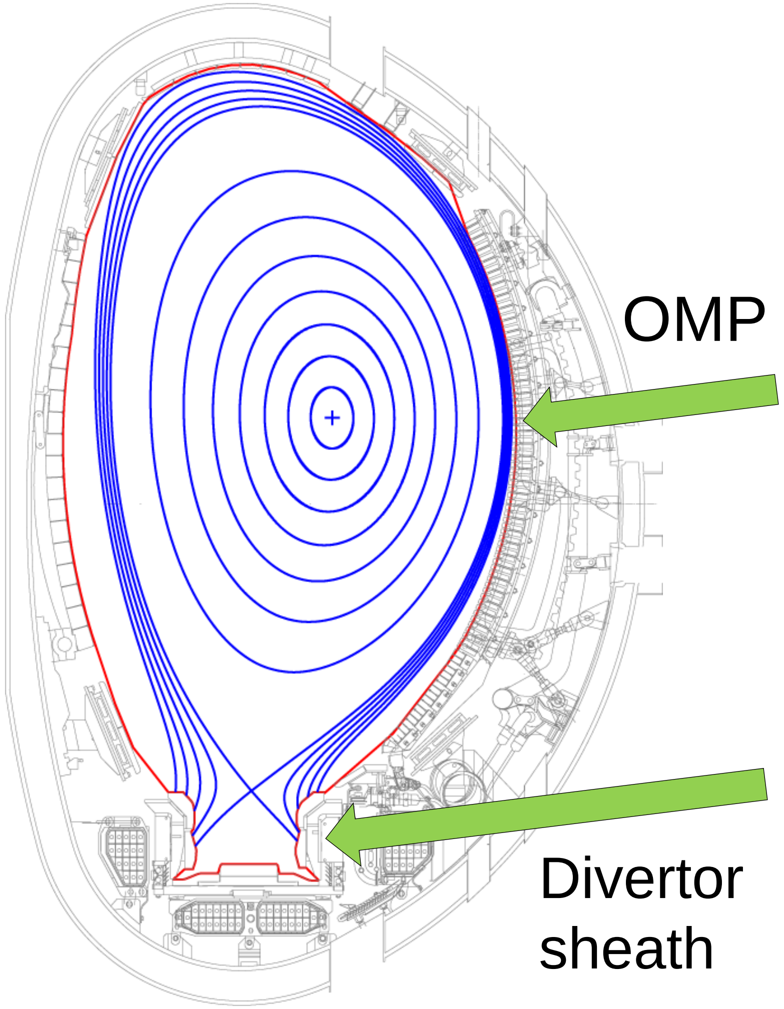
D. Tskhakaya

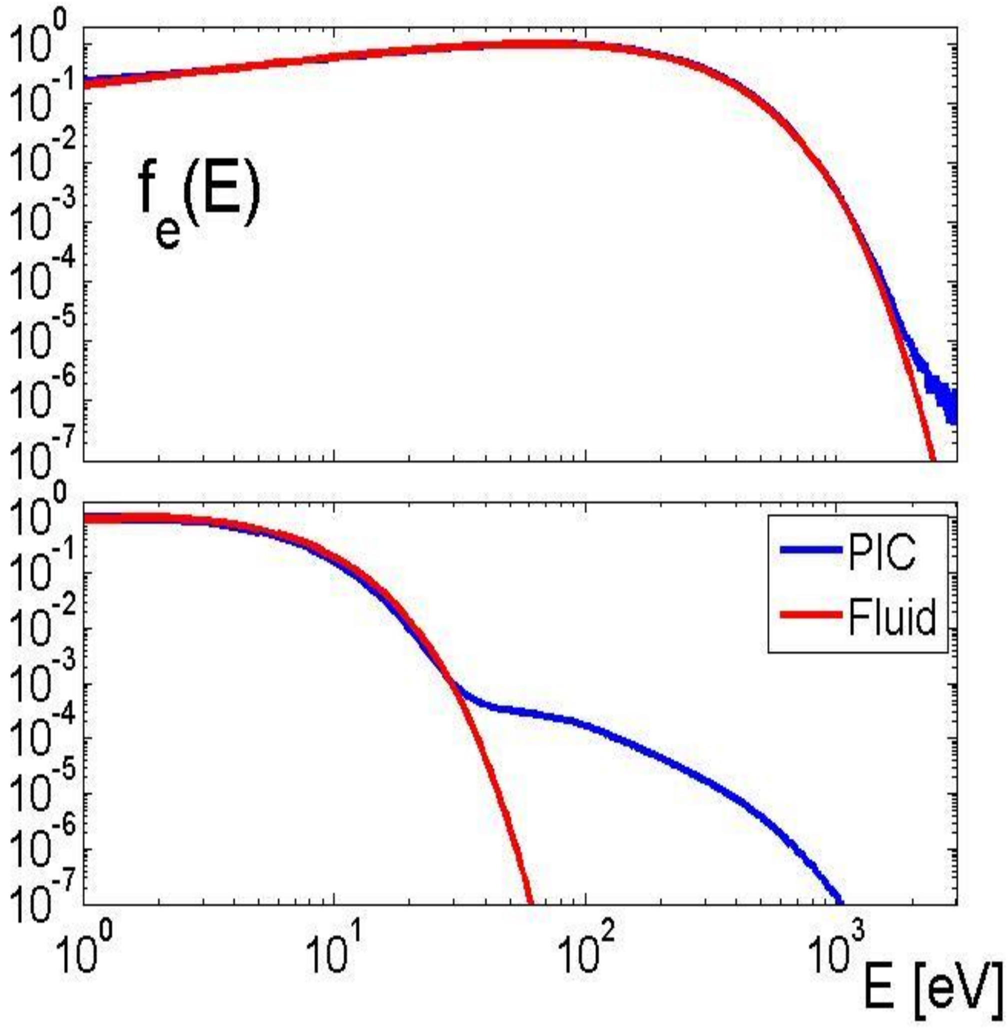
Institute of Plasma Physics of the Czech Academy of Sciences, Prague, Czech Republic

MINISTRY OF EDUCATION,
YOUTH AND SPORTS

Why do we need kinetic modelling?

[1] D. Tskhakaya PSI 2018





Reminder: why PIC?

Direct solution of kinetic equation (Vlasov, Fokker-Plank, Boltzmann codes)

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{e_s}{m_s}\left(\vec{E}+\left[\vec{V}\times\vec{B}\right]\right)\frac{\partial}{\partial \vec{V}}\right)f_s\left(t,\vec{r},\vec{V}\right)=st_s\left(f\right)$$

$$+\quad \text{Maxwell's equations}$$

The advantage: Directly operates with the VDF.

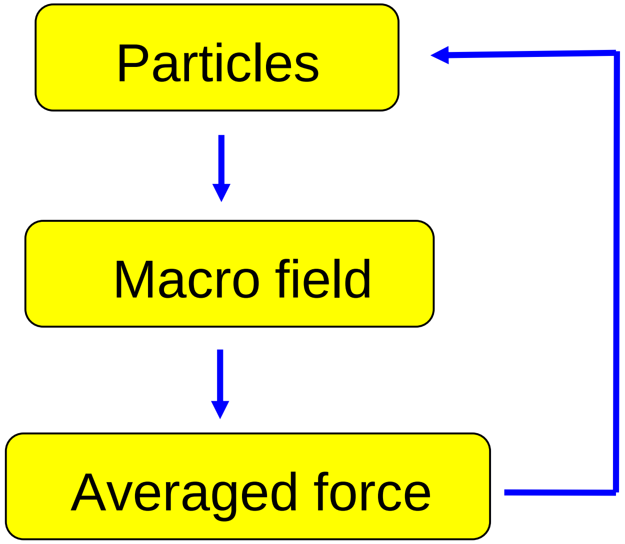
The disadvantage

- Low dimensionality (size of matrix ~ $N_r^3\,N_V^3$, e.g. for , N=100 requires *nxn, n*$=10^{12}$ matrix
- Collision operators are integrals $St\left(f_a\right)\sim\int f_a f_b\ldots$
- Plasma-surface interactions are difficult to implement

Outline

- Introduction
- General scheme of PIC simulation
- Description of different components of the PIC code
- Requirements for PIC simulation
- Numerical heating
- Estimation of the required CPU time

The idea of the PIC



Equations of particle motion

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i\ ,\ i = 1,\dots,N$$

$$\frac{d\mathbf{V}_i}{dt} = \mathbf{F}_i(\mathbf{A})$$

Equations of the macro field

$$\mathbf{A} = \hat{L}_1(\mathbf{B})$$

Macro parameters associated with particles

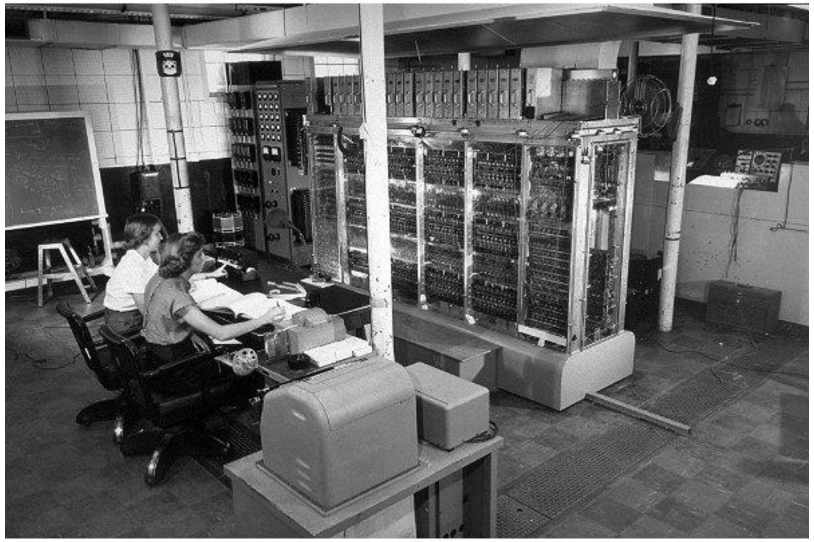
$$\mathbf{B} = \hat{L}_2(\mathbf{r}_1, \mathbf{V}_1, \dots, \mathbf{r}_N, \mathbf{V}_N).$$

In general, PIC codes can be applied in different branches of physics, but usually they are associated with the numerical codes simulating plasma

PIC scaling: ~*M* operations on *N* particles ~ *MN*

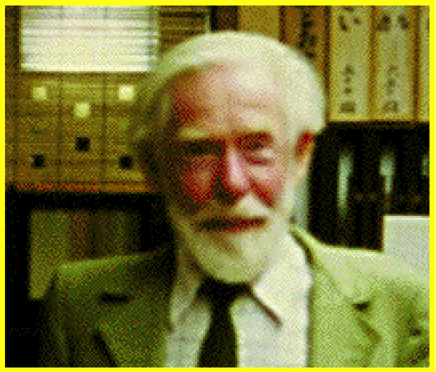
Today: 6-dimensional electromagnetic PIC simulations of up to 10^{12} particles.

First PIC simulations



MANIAC „supercomputer“ at LANL (1953)

F. Harlow, LANL report (1956)



Buneman, PR (1959)

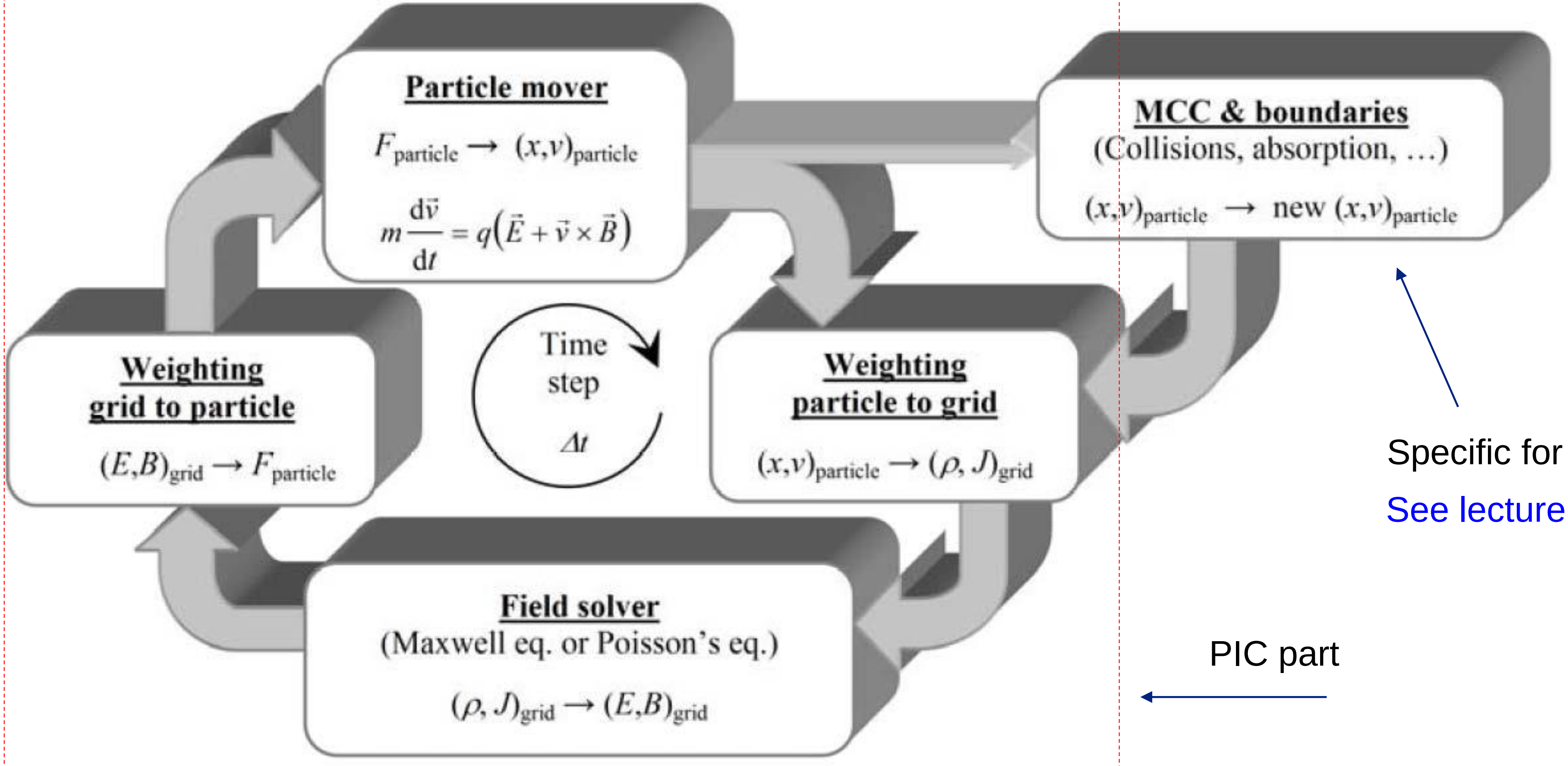
Dawson, PF (1962)

Birdsall, JCP (1969)

Hockney, PF (1966)

[1] D. Tskhakaya PSI 2018

Examples of full PIC + MC codes



Specific for MCFP modelling

See lecture 7 on MC methods

PIC part

PIC codes: general structure

Classification of PIC codes

- **Dimensionality:** 1, 2, or 3D in space, usually 3D in velocity space
- **Fields considered:** electrostatic, or electromagnetic
- **Physical model:** unbounded or bounded plasma, relativistic or classical plasma

Super-particles

$$W = \frac{Number\ of\ real\ particles}{Number\ of\ simulation\ particles} >> 1$$

Invariant of motion

$$\frac{q}{M} = const$$

Field equations

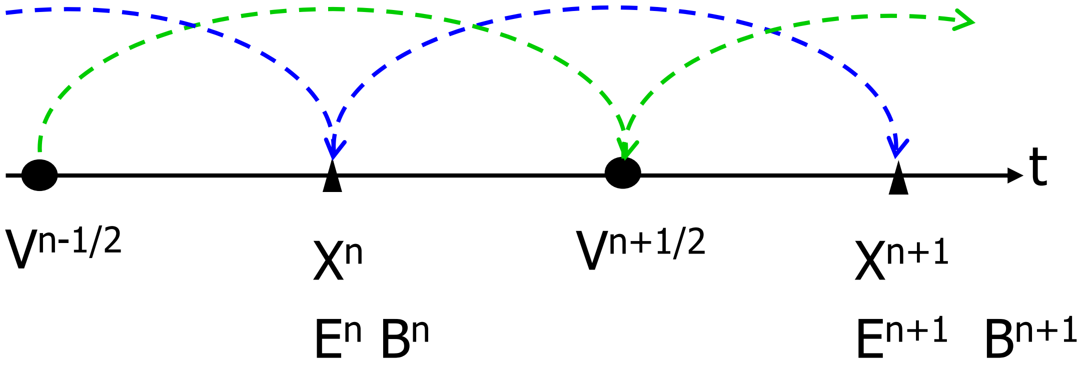
$$q \rightarrow Wq$$

Equations of particle motion

Particle mover: as fast and accurate as possible!

$$\frac{d\mathbf{V}}{dt} = \frac{e}{m}\left(\mathbf{E} + \mathbf{V}\times\mathbf{B}\right)$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{V},$$



$$\frac{\mathbf{V}^{t+\Delta t/2} - \mathbf{V}^{t-\Delta t/2}}{\Delta t} = \frac{e}{m}\left(\mathbf{E}^{t} + \frac{\mathbf{V}^{t+\Delta t/2} + \mathbf{V}^{t-\Delta t/2}}{2}\times\mathbf{B}^{t}\right)$$

$$\frac{\mathbf{r}^{t+\Delta t} - \mathbf{r}^{t}}{\Delta t} = \mathbf{V}^{t+\Delta t/2},$$

← Time-centered

Leap-frog scheme

Coordinates and velocities are shifted in time

Equations of particle motion (ii)

Accuracy

$$\frac{\mathbf{V}^{t+\Delta t/2}-\mathbf{V}^{t-\Delta t/2}}{\Delta t}=F\left(\mathbf{V}^{t+\Delta t/2}+\mathbf{V}^{t-\Delta t/2},\mathbf{E}^{t},\mathbf{B}^{t}\right)$$

$$\mathbf{V}^{t\pm\Delta t/2}=\mathbf{V}^{t}\pm\Delta t/2\dot{\mathbf{V}}^{t}+\left(\Delta t/2\right)^{2}/2\ddot{\mathbf{V}}^{t}+\left(\Delta t/2\right)^{3}/6\dddot{\mathbf{V}}^{t}+\ldots$$

$$\dot{\mathbf{V}}^{t}=F\left(\mathbf{V}^{t},\mathbf{E}^{t},\mathbf{B}^{t}\right)+\underline{\left(\Delta t/2\right)^{2}}\left[F\left(\ddot{\mathbf{V}}^{t},\mathbf{E}^{t},\mathbf{B}^{t}\right)-\dddot{\mathbf{V}}^{t}/6\right]+\ldots$$

$$\sim\Delta t^{2}$$

Stability

$$\frac{d^{2}X}{dt^{2}}=-\omega_{0}^{2}X$$

$$\frac{X^{t+\Delta t}-2X^{t}+X^{t-\Delta t}}{\Delta t^{2}}=-\omega_{0}^{2}X^{t}.$$

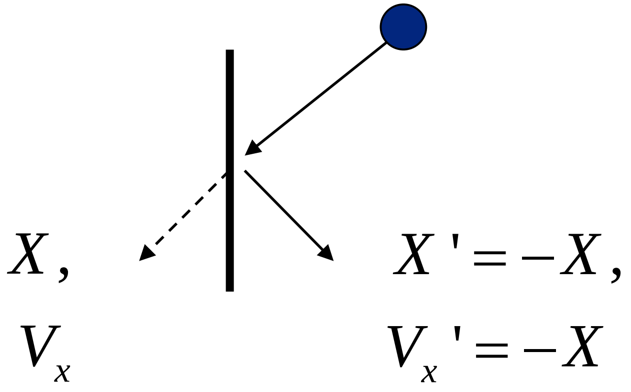
$$X^{t}\propto\exp\left(-i\omega t\right),\quad \sin\left(\omega\Delta t/2\right)=\pm\underline{\omega_{0}\Delta t/2}. \rightarrow$$

$$\Delta t<2/\omega_{0}$$

Boundary conditions

Could be tricky, because **r** and **V** are shifted in time Δt/2

Specular reflection



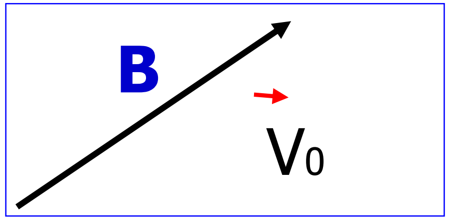
Equations of particle motion (iii)

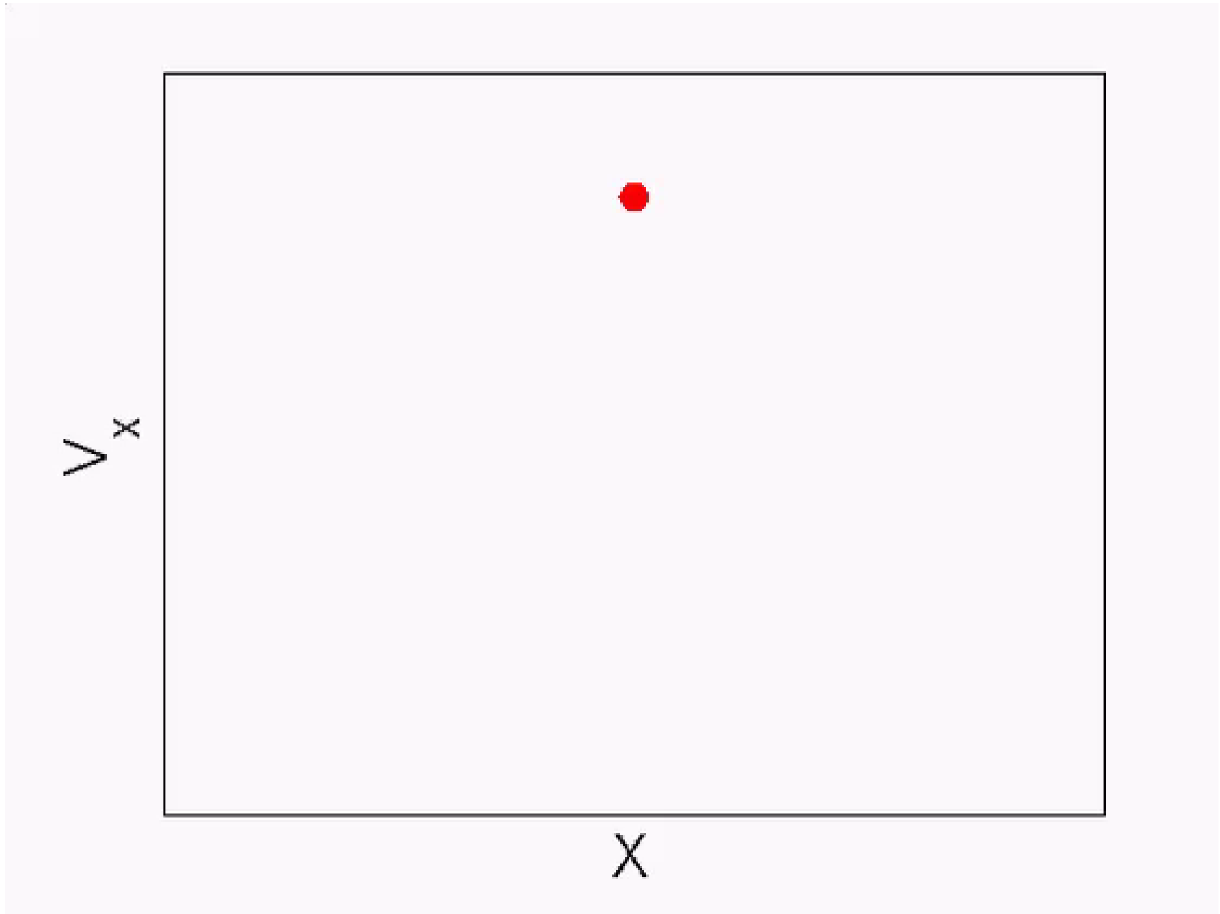
Particle motion in a constant magnetic field

Leap-frog pusher

$$\frac{\mathbf{V}^{t+\Delta t/2}-\mathbf{V}^{t-\Delta t/2}}{\Delta t}=\frac{e}{m}\left(\mathbf{E}^{t}+\frac{\mathbf{V}^{t+\Delta t/2}+\mathbf{V}^{t-\Delta t/2}}{2}\times\mathbf{B}^{t}\right)$$

$$\frac{\mathbf{r}^{t+\Delta t}-\mathbf{r}^{t}}{\Delta t}=\mathbf{V}^{t+\Delta t/2}$$





Questions

Particle weighting

Particle mover

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i\,, \quad k = 1,\ldots,N$$

$$\frac{d\mathbf{V}_i}{dt} = \frac{e_i}{m_i}\left(\mathbf{E} + \mathbf{V}_i \times \mathbf{B}\right)$$

?

→ **Particle weighting** → n, $\mathbf{J}$, T ,…

Simulated particles have finite size:

Weight function $S\left(x - X\right)$

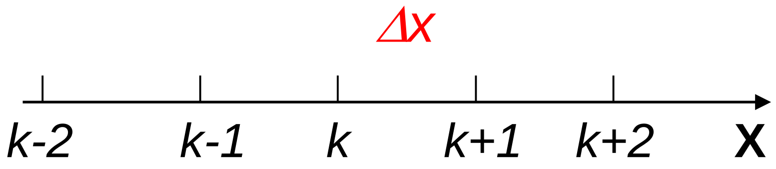
$$n\left(x\right) = \frac{1}{V_{vol}}\sum_{i=1}^{N} S\left(x - X_i\right),$$

$$\mathbf{A}\left(x\right) = \sum_{i=1}^{N} \mathbf{a}_i S\left(x - X_i\right),$$

$$\vec{\mathrm{B}}\left(x\right) = \sum_{i=1}^{N} \vec{b}_i S\left(x - X_i\right),$$

Particle weighting (ii)

Space is “grided”:



Conditions on the shape function:

Space isotropy $S(x) = S(-x)$

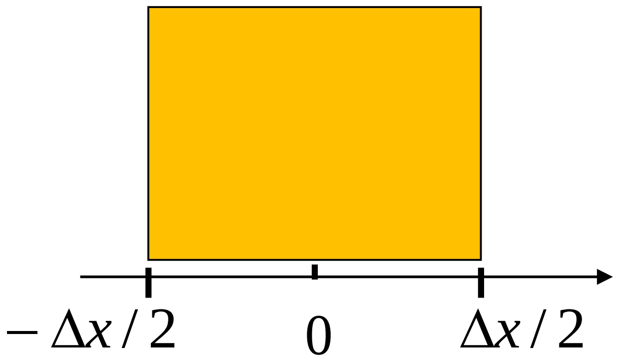
Charge conservation $\sum_{k=1}^{Nc} S(x_k - X) = 1$

Accuracy (field solver) $\sum_{k=1}^{Nc} S(x_k - X)(x_k - X)^n = 0, \;\; n = 1,\dots,n_{\max}$

Particle weighting (iii)

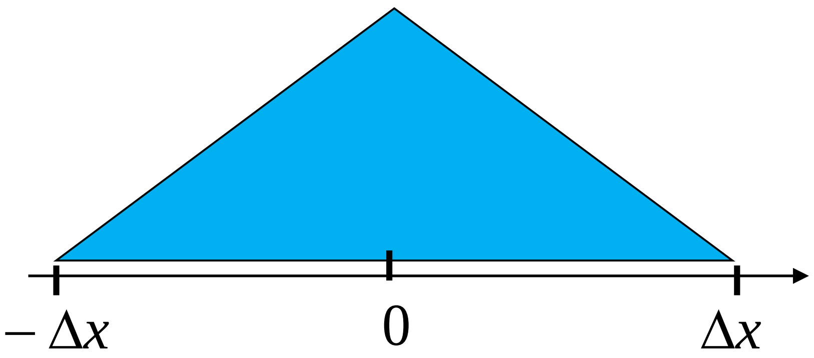
1D:

Zero order (NGP)



$$S_1^0(x-X)=\begin{cases}1, & \text{if } |x-X|\le \Delta x/2\\ 0, & \text{otherwise}\end{cases}$$

First order (CIC)

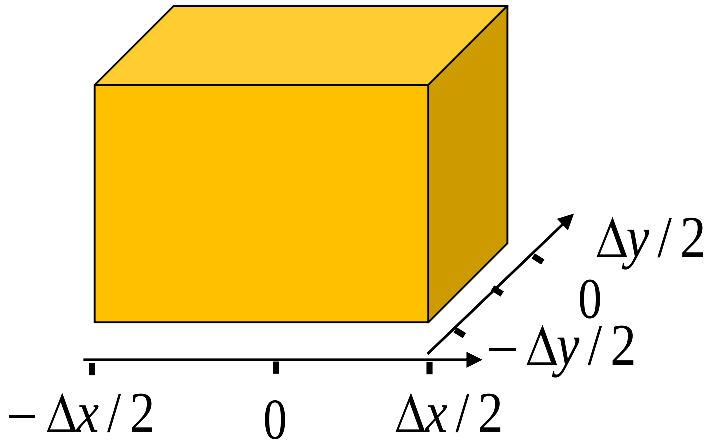


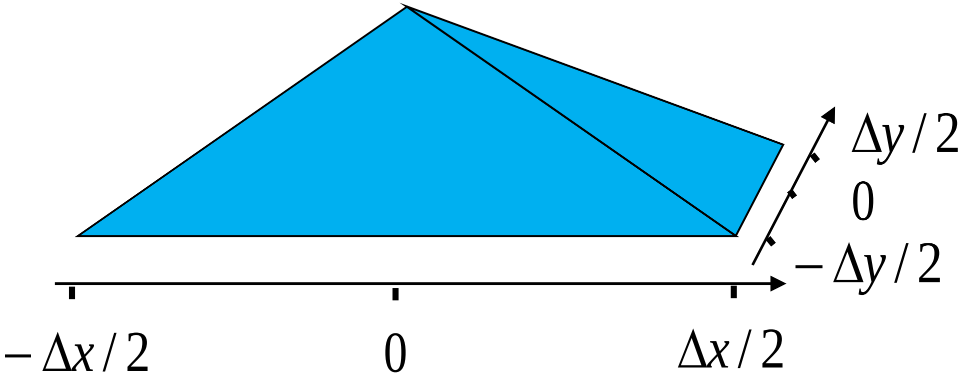
$$S_1^1(x-X)=\begin{cases}1-|x-X|/\Delta x, & \text{if } |x-X|\le \Delta x\\ 0, & \text{otherwise}\end{cases}$$

Particle weighting (iv)

Zero order (NGP) | First order (CIC)

2D:





$$S_2(\mathbf{r}-\mathbf{R}) = S_1(x-X)S_1(y-Y)$$

3D:

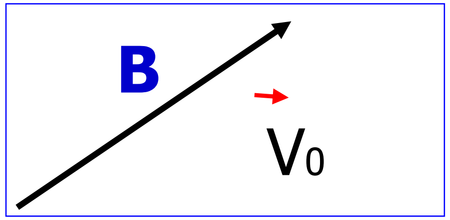
$$S_3(\mathbf{r}-\mathbf{R}) = S_1(x-X)S_1(y-Y)S_1(z-Z)$$

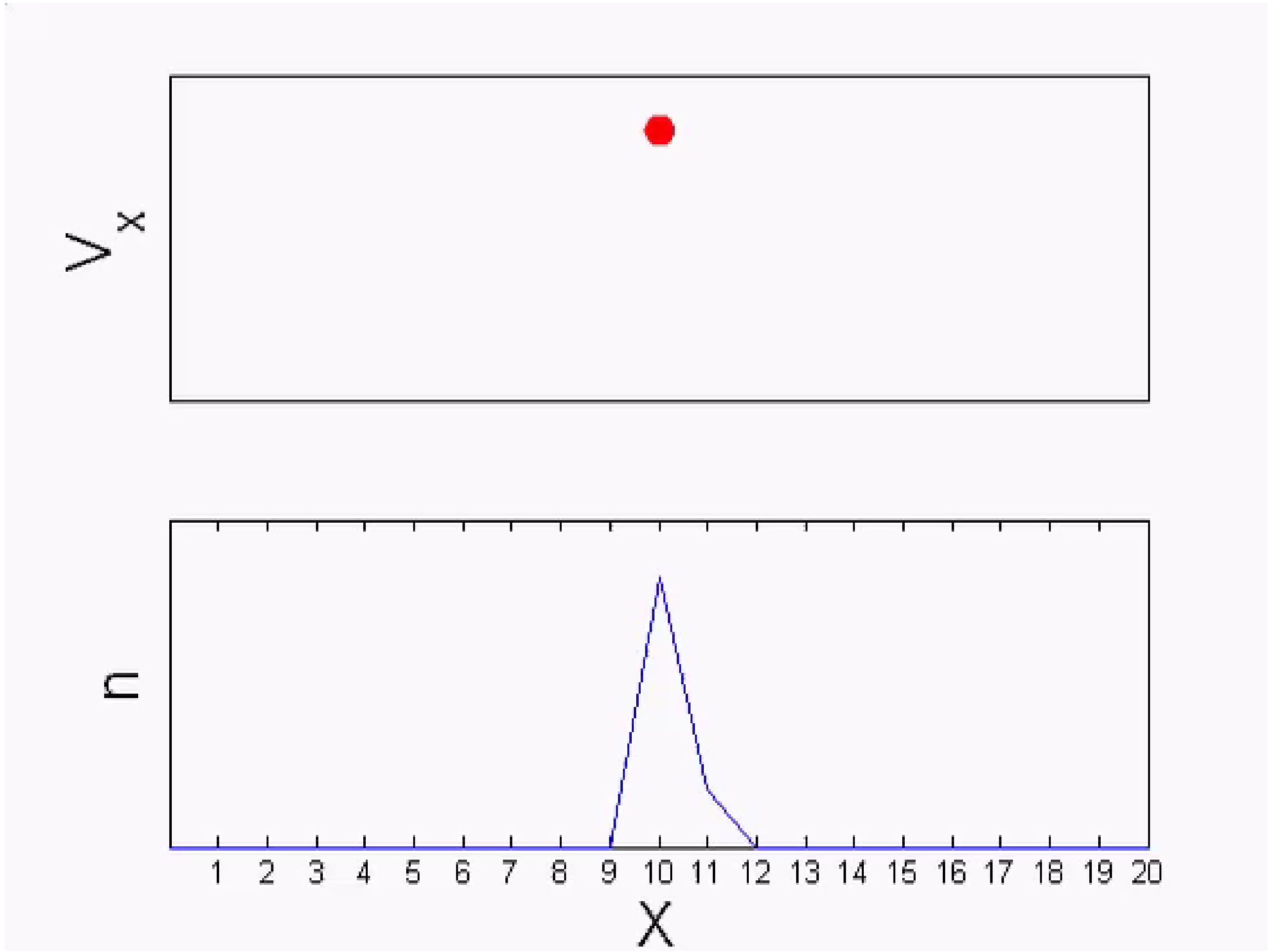
Particle weighting (v)

Particle motion in a constant magnetic field

Leap-frog pusher

Linear weighting





Force interpolation (force weighting)

Particle mover

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i\,, \quad k = 1,\ldots,N$$

$$\frac{d\mathbf{V}_i}{dt} = \frac{e_i}{m_i}\left(\mathbf{E} + \mathbf{V}_i \times \mathbf{B}\right)$$

→

Particle weighting

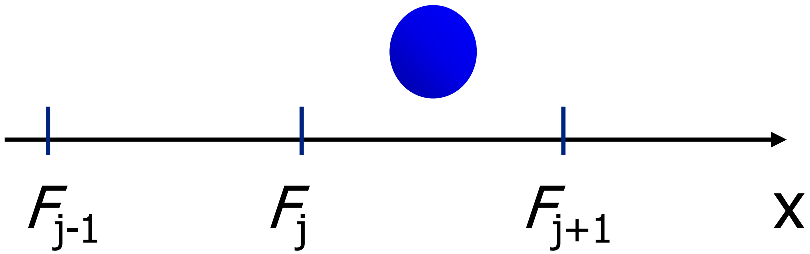
$$n_k\,,\ \mathbf{J}_k$$

→

Solution of the Maxwell's equations

$$\mathbf{E}_k\,,\ \mathbf{B}_k$$

E, B ?



$$F(x) = \sum_{j=1}^{N_c} F_j S_{force}\left(x - x_j\right)$$

Force interpolation (ii)

Conditions for the force "shape function"

$$S_{force}(x) = S_{particle}(x)$$

$$E_k = \sum_{j=1}^{N_c} g_{kj}\rho_j, \quad g_{kj} = -g_{jk}$$

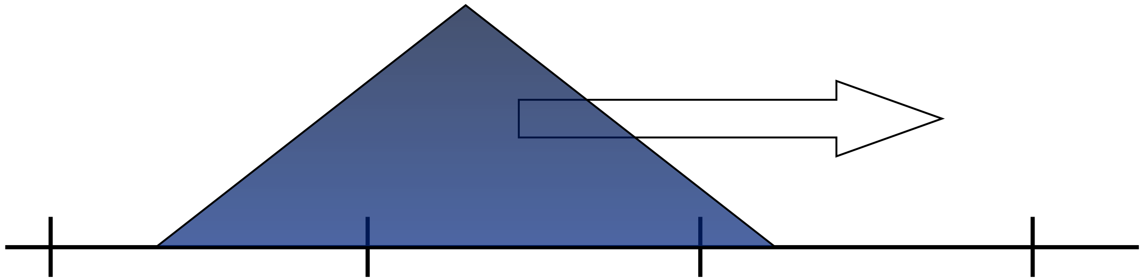
Correctly centered field solver

Momentum conservation is guaranteed, Self-force=0.

Nonuniform grid: the condition in general is not satisfied, which can cause a self-force!

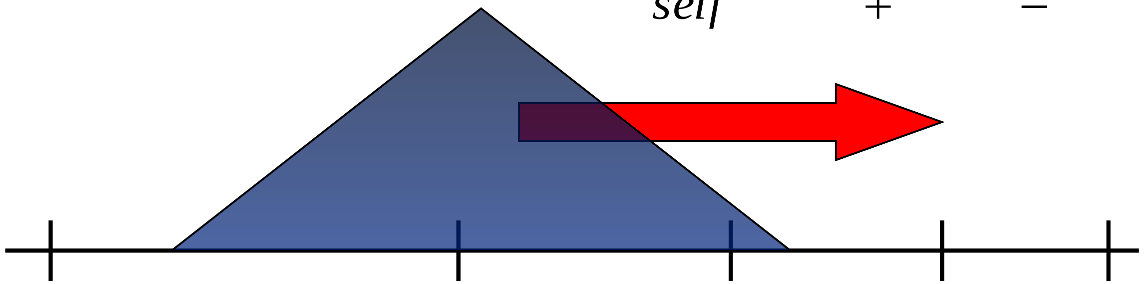
Self-force due to non-uniform mesh

Uniform mesh



$$F_{self} = F_{+} + F_{-} \neq 0$$

Nonuniform mesh[2]



For 1D there exists a solution[3]

No solution has been found for 2D and 3D yet!

Questions

[2] D. Tskhakaya CPP 2007 *[3] Duras, et al., CPP 2014*

Solution of the Maxwell's equations

Maxwell's equations

$$\nabla \mathbf{D} = \frac{\rho}{\varepsilon_0}, \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \mathbf{D} = \varepsilon \mathbf{E},$$

$$\nabla \mathbf{B} = 0, \quad \frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}, \quad \mathbf{B} = \mu \mathbf{H}$$

Types of the field solver[4]

- Mesh-relaxation method
  - Initial "guess": E, B
  - Checking of the divergence
  - Iteration until the desired accuracy is reached
- Matrix solver (too slow)

$$\hat{\mathbf{M}}\mathbf{E},\mathbf{B} = \rho,\ \mathbf{J} \ \rightarrow \ \mathbf{E},\ \mathbf{B} = \hat{\mathbf{M}}^{-1}\rho,\ \mathbf{J}$$

- Solvers using Fourier transformation

$$\rho,\ \mathbf{J}(\mathbf{r}) \rightarrow \rho,\ \mathbf{J}(\mathbf{k}) \rightarrow \mathbf{E},\ \mathbf{B}(\mathbf{k}) \rightarrow \mathbf{E},\ \mathbf{B}(\mathbf{r})$$

- Mixture of methods given above
- Other methods

Electrostatic PIC: 1D

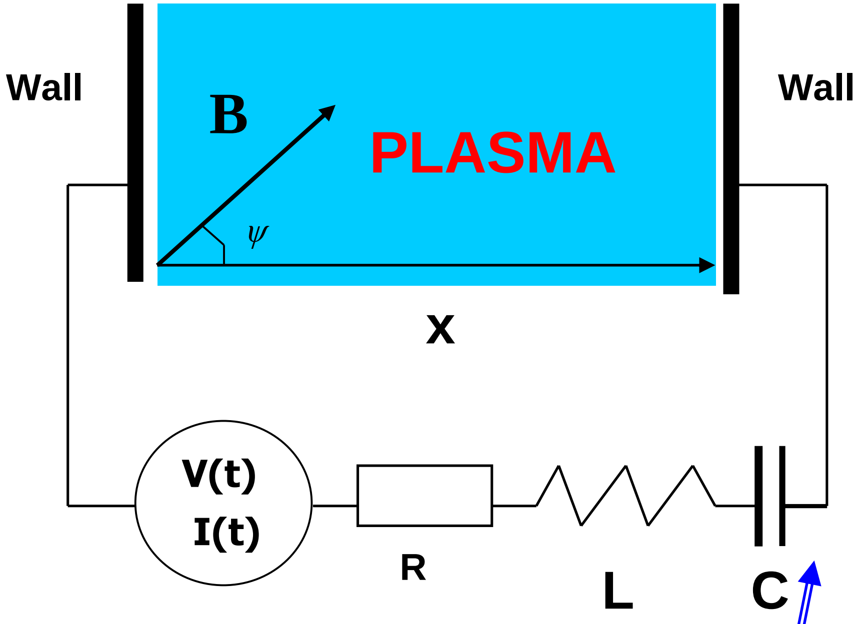
Finite differenced Poisson equation

$$\frac{\partial^2 \varphi}{\partial x^2} = -\frac{\rho}{\varepsilon_0}$$

$$\frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{\Delta x^2} = -\frac{\rho_j}{\varepsilon_0} \quad j = 1,\dots,N_c$$

$$E_j = \frac{\varphi_{j-1} - \varphi_{j+1}}{2\Delta x}$$

Accuracy: $\sim \Delta x^2$



$$L\frac{d^2 Q}{dt^2} + R\frac{dQ}{dt} + \frac{Q}{C} = V(t)$$

Boundary conditions:

$$\varphi_{N_c} = 0,$$

$?$

$$\frac{\phi_0 - \phi_1}{\Delta x} = E_0 + \frac{\Delta x}{2\varepsilon_0}\rho_0$$

$$E_0 = \frac{1}{\varepsilon_0}\left(\sigma_w^{t-\Delta t} + \frac{Q_{pl}^{\Delta t} + Q^{\Delta t}}{S_{area}}\right)$$

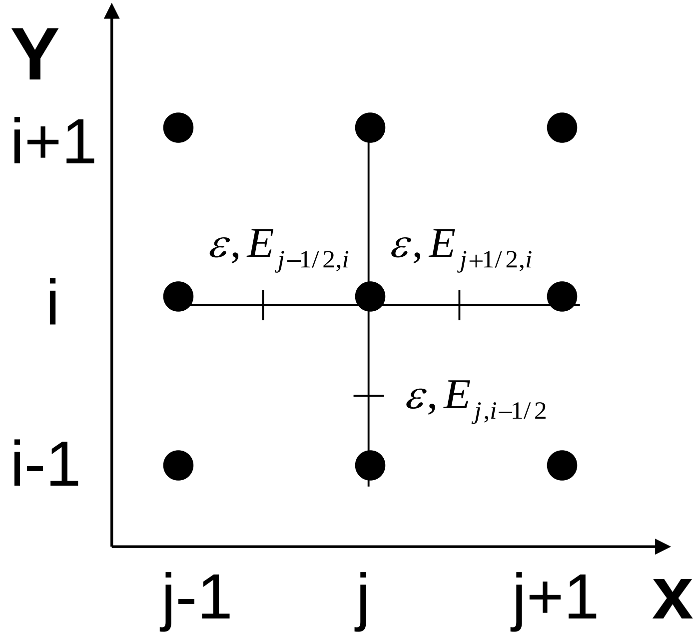
Boundary conditions from XPDP1

Electrostatic PIC: 2D

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi=-\frac{\rho}{\varepsilon_0}$$

$$\frac{\varphi_{j+1,i}-2\varphi_{j,i}+\varphi_{j-1,i}}{\Delta x^2}+\frac{\varphi_{j,i+1}-2\varphi_{j,i}+\varphi_{j,i-1}}{\Delta y^2}=-\frac{\rho_{ji}}{\varepsilon_0},$$

$$E^x_{ji}=\frac{\varphi_{j-1,i}-\varphi_{j+1,i}}{2\Delta x},\quad E^y_{ji}=\frac{\varphi_{j,i-1}-\varphi_{j,i+1}}{2\Delta y}.$$



At the boundaries

$$\oint \varepsilon \vec{E} d\vec{S}=\int \rho dV+\oint \vec{\sigma} d\vec{S},$$

$$\Delta y\Delta z\left(\varepsilon_{j+1/2,i}E^x_{j+1/2,i}-\varepsilon_{j-1/2,i}E^x_{j-1/2,i}\right)+$$

$$\Delta x\Delta z\left(\varepsilon_{j,i+1/2}E^y_{j,i+1/2}-\varepsilon_{j,i-1/2}E^y_{j,i-1/2}\right)=\rho_{ji}\Delta V+\sigma_{ji}\Delta S_{ji}.$$

$$E^x_{j-1/2,i}=\frac{\phi_{j,i}-\phi_{j-1,i}}{\Delta x}$$

$$E^y_{j,i-1/2}=\frac{\phi_{j,i}-\phi_{j,i-1}}{\Delta y}.$$

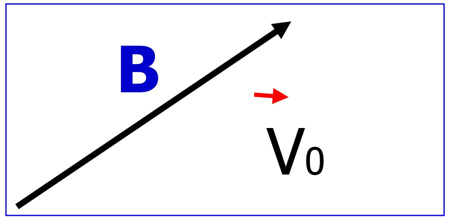
Generalization to 3D is straightforward!

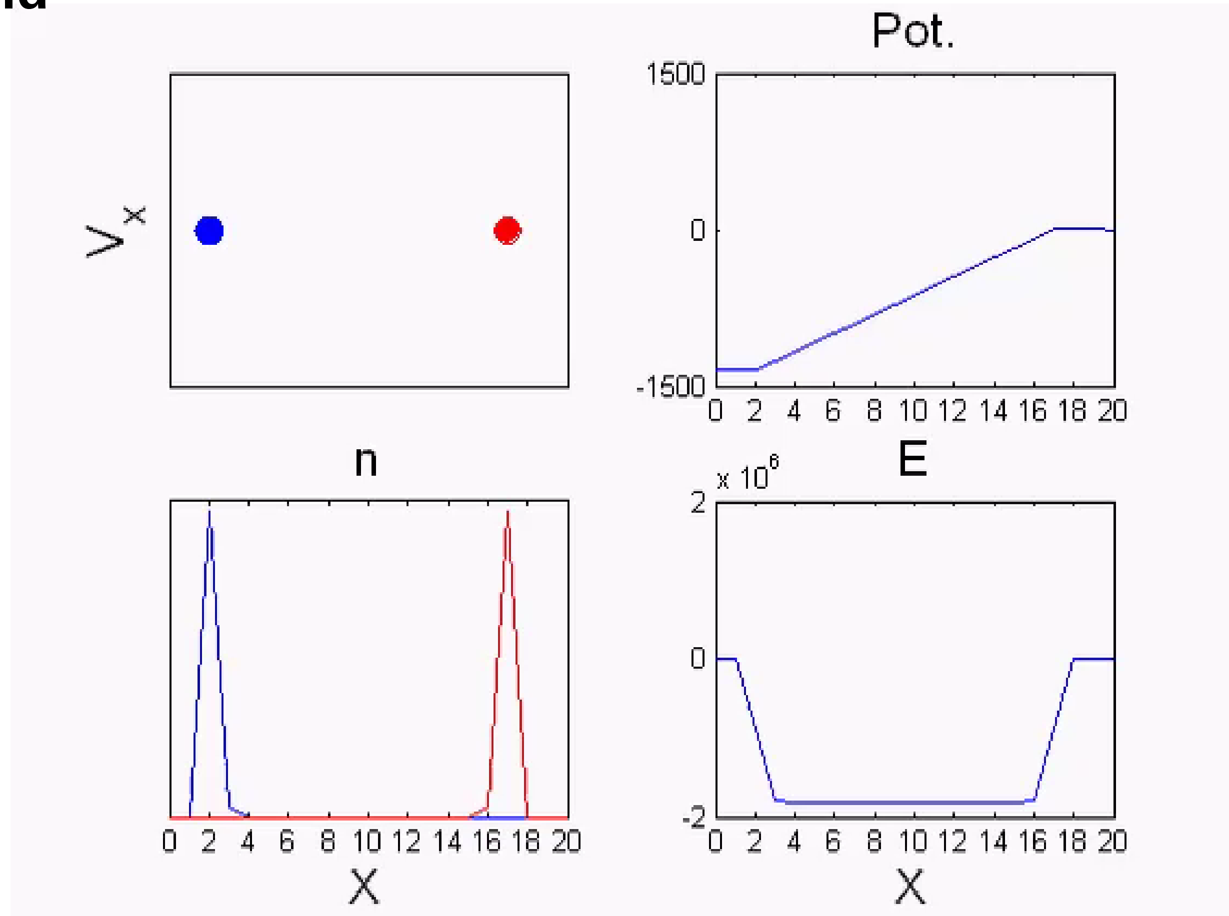
2-particles motion in a constant magnetic field

Leap-frog pusher

Linear weighting

Poisson solver





Questions

Electromagnetic case

$$\nabla \mathbf{D} = \frac{\rho}{\varepsilon_0}, \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \mathbf{D} = \varepsilon \mathbf{E},$$

$$\nabla \mathbf{B} = 0, \quad \frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}, \quad \mathbf{B} = \mu \mathbf{H},$$

In order to reach high accuracy still keeping high simulation speed the differenced equations are centered in space and time

$$\hat{\mathbf{M}} \mathbf{E}, \mathbf{B} = \rho, \mathbf{J} \rightarrow \mathbf{E}, \mathbf{B} = \hat{\mathbf{M}}^{-1} \rho, \mathbf{J}$$

$$D^{i,t}_{i+1/2,j,k}, \quad \rho^{t}_{i,j,k},$$

$$B^{i,t-\Delta t/2}_{i,j+1/2,k+1/2}, \quad J^{i,t-\Delta t/2}_{i+1/2,j,k},$$

Electromagnetic case (ii)

Simplified scheme of the electromagnetic field solver (example)

Initial conditions

$$\nabla \mathbf{D} = \frac{\rho}{\varepsilon_0}, \quad \nabla \mathbf{B} = 0$$

→ $\mathbf{D}(t=0),\ \mathbf{B}(t=0)$ →

Solution of Ampere's and Faraday's laws

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \mathbf{D} = \varepsilon \mathbf{E},$$

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}, \quad \mathbf{B} = \mu \mathbf{H}$$

↓ $\mathbf{D}(t),\ \mathbf{B}(t - \Delta t / 2)$ ↓

Adjusting of E and B to satisfy

$$\nabla \mathbf{D} = \frac{\rho}{\varepsilon_0}, \quad \nabla \mathbf{B} = 0$$

→ $\mathbf{D}'(t,\mathbf{r}),\ \mathbf{B}'(t,\mathbf{r})$ → (back to the solution of Ampere's and Faraday's laws)

Iteration until the both set of equations are not satisfied within the given accuracy.

Electromagnetic case (iii)

Accuracy

Electromagnetic wave in vacuum

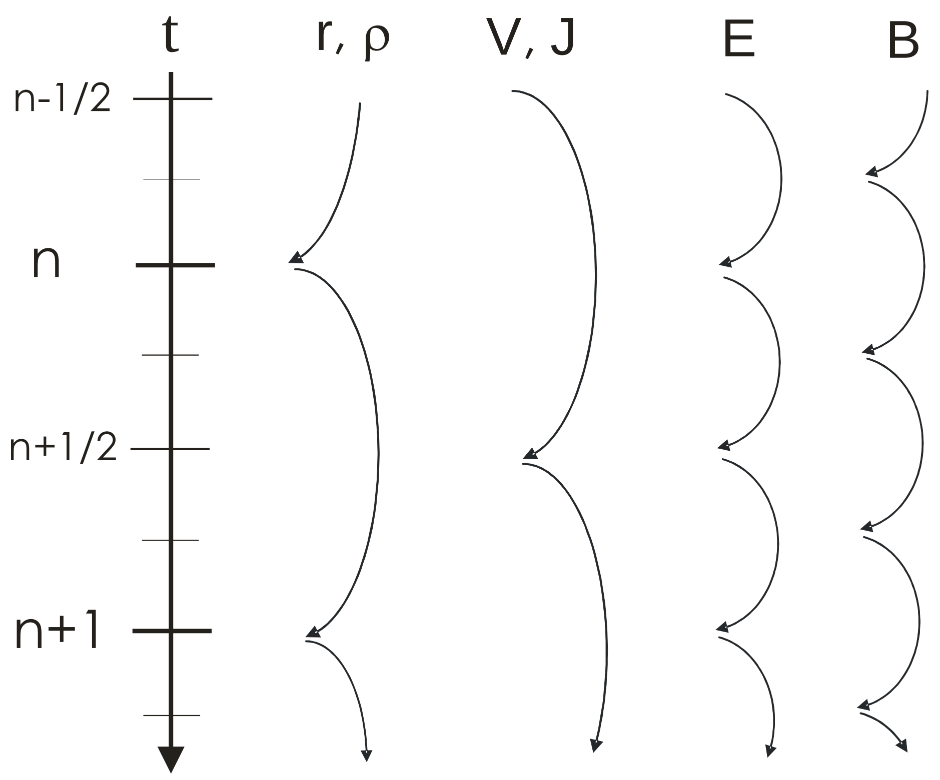
$$A(\vec{r},t) \sim \exp\left(i\left(\vec{k}\vec{r} - \omega t\right)\right)$$

Courant's condition

$$(c\Delta t)^2 < \left(\sum_1^3 \frac{1}{\Delta x^2}\right)^{-1}$$

Different time steps for the field and particles

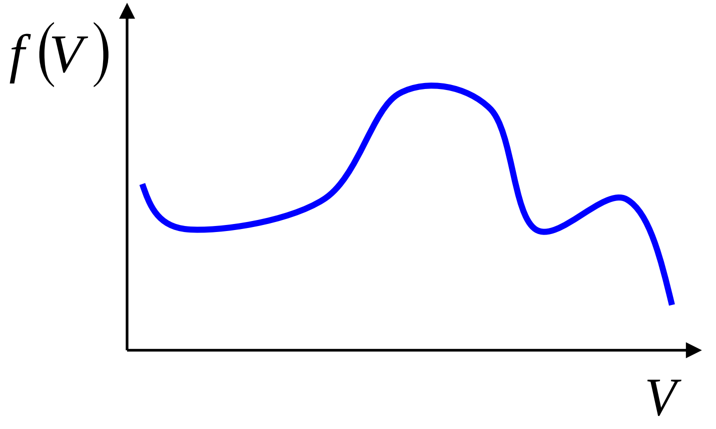
Sub-cycling

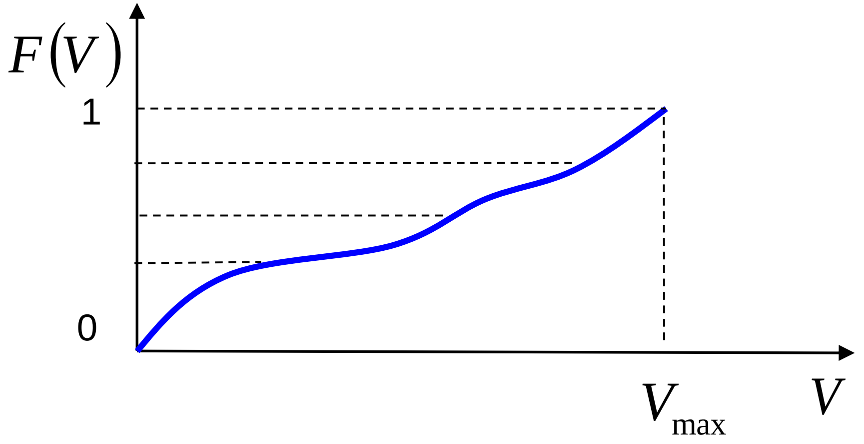


Questions

Particle loading

How to generate particle distribution with a given VDF?





$$F(V) = \frac{\int_{V_0}^{V} f(V)\,dV}{\int_{V_0}^{V_{max}} f(V)\,dV}$$

$$V = F^{-1}(R)$$

R – random number [0, 1]

The probability that the velocity of a particle is lying between V_0 and V

Inversion can be analytic or numerical

Particle loading (ii)

$$V = F^{-1}(R),\ \ R = [0,1] - \text{random number}$$

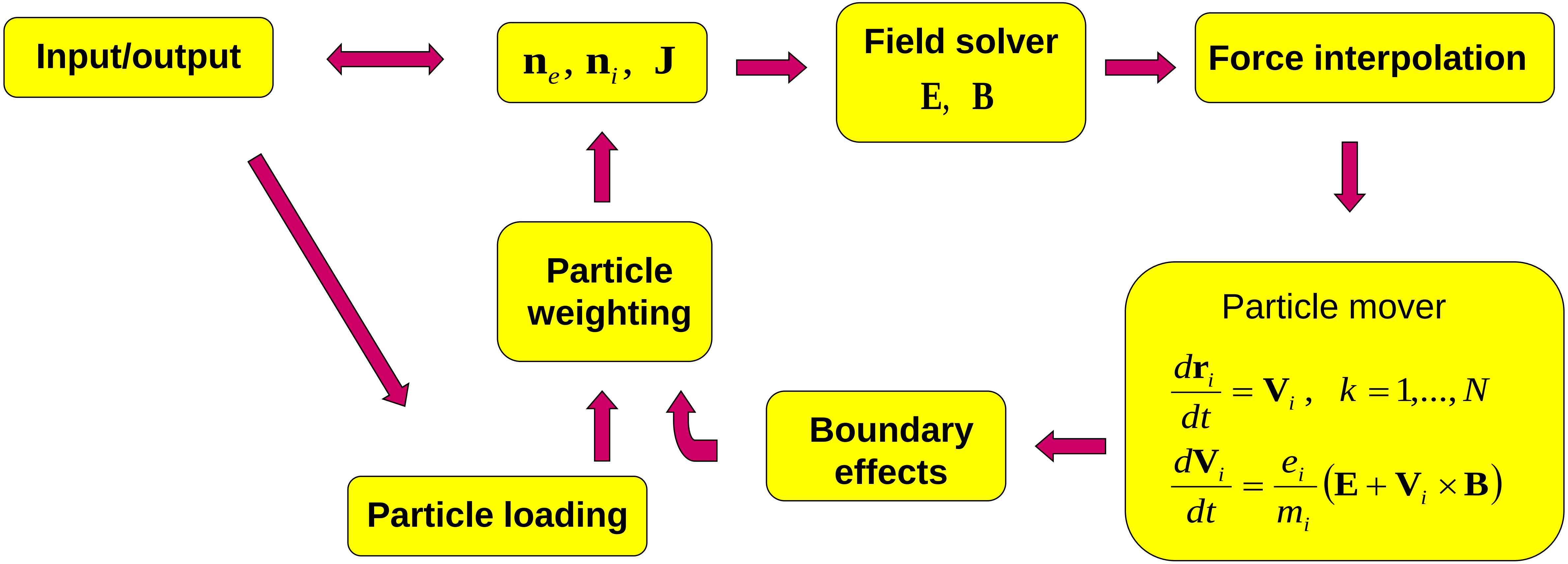
2D Maxwellian distribution

$$f\left(\vec{V}\right) \sim \exp\left(-\frac{V_x^2 + V_y^2}{2V_T^2}\right) = \exp\left(-\frac{V^2}{2V_T^2}\right)$$

$$\int_{-\infty}^{V} \exp\left(-\frac{v^2}{2V_T^2}\right) v\,dv = V_T \exp\left(-\frac{V^2}{2V_T^2}\right), \qquad F\left(V\right) = 1 - \exp\left(-\frac{V^2}{2V_T^2}\right)$$

$$V = F^{-1}\left(R_1\right) = V_T\sqrt{-2\ln\left(1 - R_1\right)} = V_T\sqrt{-2\ln R_1}\,, \quad V_x = V\left(2R_2 - 1\right), \quad V_y = \pm V\sqrt{R_2\left(2 - R_2\right)}$$

A “Simple” PIC


Input/output
$\mathbf{n}_e, \mathbf{n}_i, \mathbf{J}$
Field solver
$\mathbf{E}, \mathbf{B}$
Force interpolation
Particle weighting
Particle mover
$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_i, \quad k = 1, \ldots, N$
$\frac{d\mathbf{V}_i}{dt} = \frac{e_i}{m_i}(\mathbf{E} + \mathbf{V}_i \times \mathbf{B})$
Boundary effects
Particle loading

1D unbounded plasma

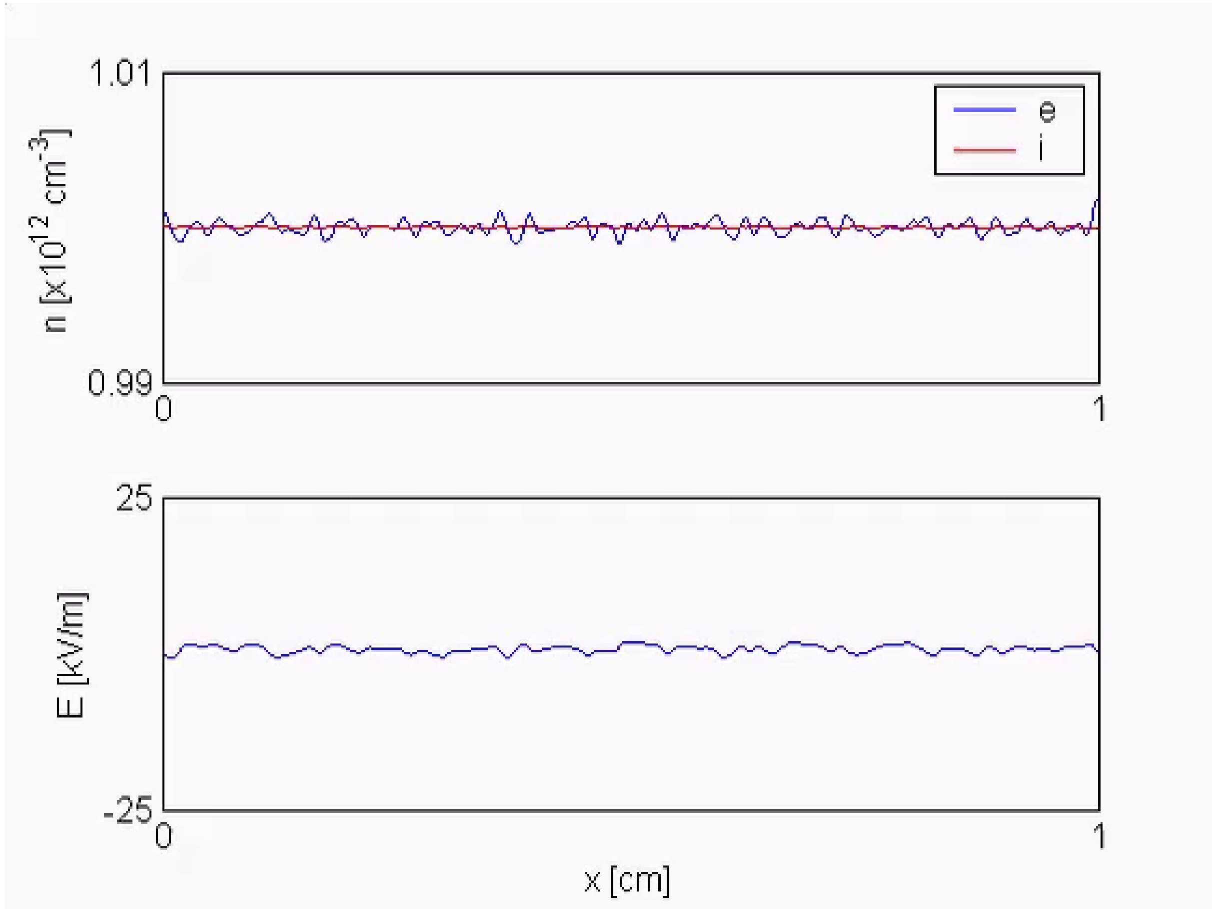
1D plasma in a constant magnetic field

Particle loading

Leap-frog pusher

Linear weighting

Poisson solver



Simulation parameters

Periodic boundary conditions

Number of grid cells: 400

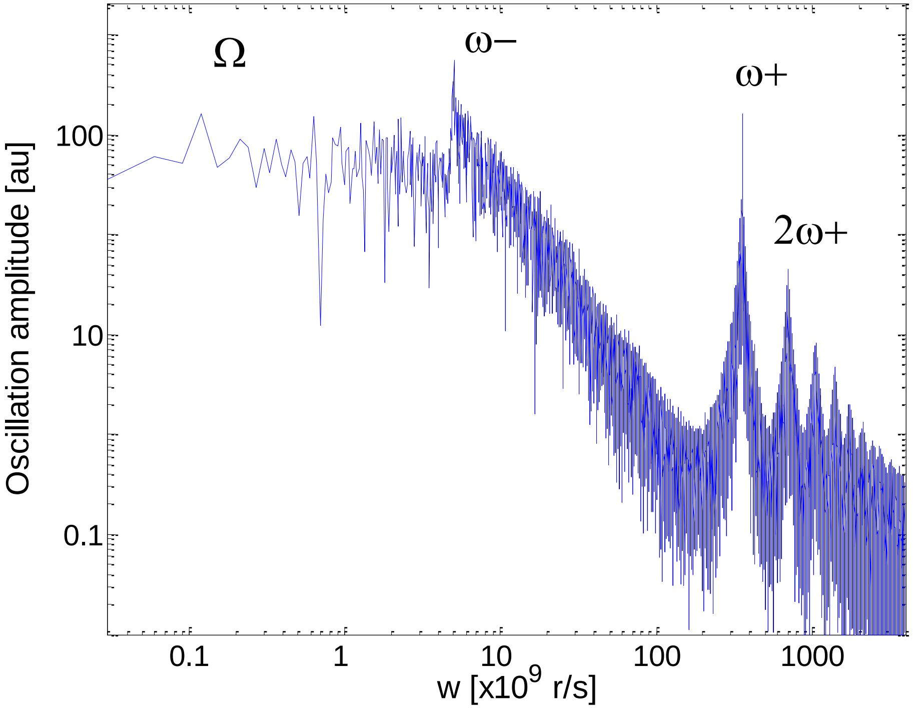
Number of particles: $4x10^5$

Time step: $0.28/W_e$

1D unbounded plasma: results

Expected oscillation modes[5]

$$\omega\pm = \left[\frac{\Omega_e^2 + \omega_p^2}{2} \pm \sqrt{\frac{\left(\Omega_e^2 + \omega_p^2\right)^2}{4} - \omega_p^2 \Omega_e^2 \sin^2\theta}\,\right]^{1/2}, \quad \Omega_i \,.$$



Spectrum of the plasma potential oscillation frequency from the PIC simulation

Questions

[5] Alexandrov, 1984

Analytic theory of finite size particle plasma in a discrete space

Dispersion relation of unmagnetized 1D plasma[6]

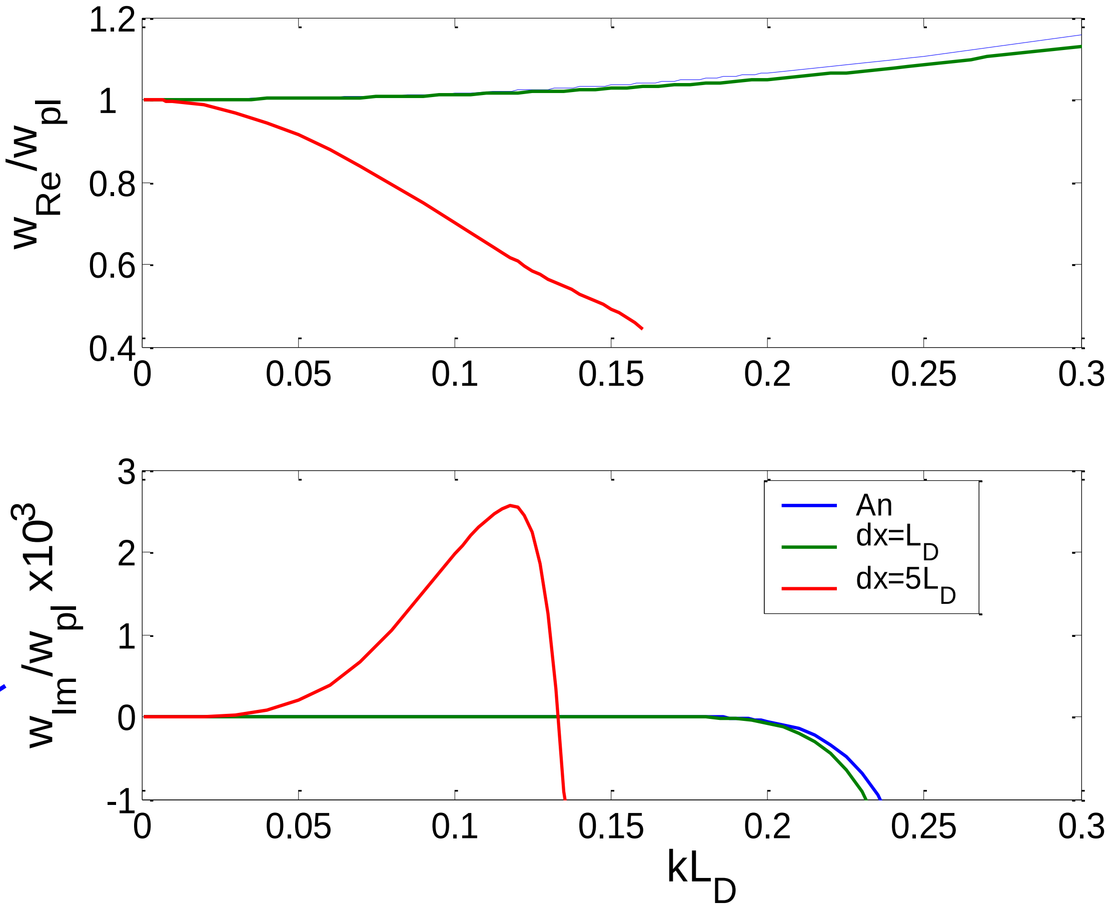
$$\varepsilon(k,\omega) = 1 - \frac{\omega_p^2}{2K^2V_T^2}\sum_{p=\pm\infty}\left|S(k_p)\right|^2\frac{\chi(k_p)}{k_p}Z'\left(\frac{\omega}{\sqrt{2}\left|k_p\right|V_T}\right) = 0;$$

$$K^2 = 4\frac{\sin^2(k\Delta x/2)}{\Delta x^2},$$

$$\chi = \frac{\sin(k\Delta x)}{\Delta x},$$

$$S(k) = \left(\frac{\sin(k\Delta x/2)}{k\Delta x/2}\right)^{m+1},$$

$$k_p = k - p\frac{2\pi}{\Delta x}.$$



$$\Delta x \le \lambda_D$$

[6] C.K. Birdsall, A.B. Langdon 1991

Requirements for PIC simulation

Time scales

$$\Delta t_{field} < \frac{1}{c}\left(\sum_{1}^{3}\frac{1}{\Delta x^2}\right)^{-1/2}$$ Electromagnetic field solver

$$\Delta t < \frac{\Delta x}{V_{\max}}$$ No “jumping” particles

$$\Delta t < \frac{2}{\omega_{pl}}$$ For stability of the leap-frog scheme

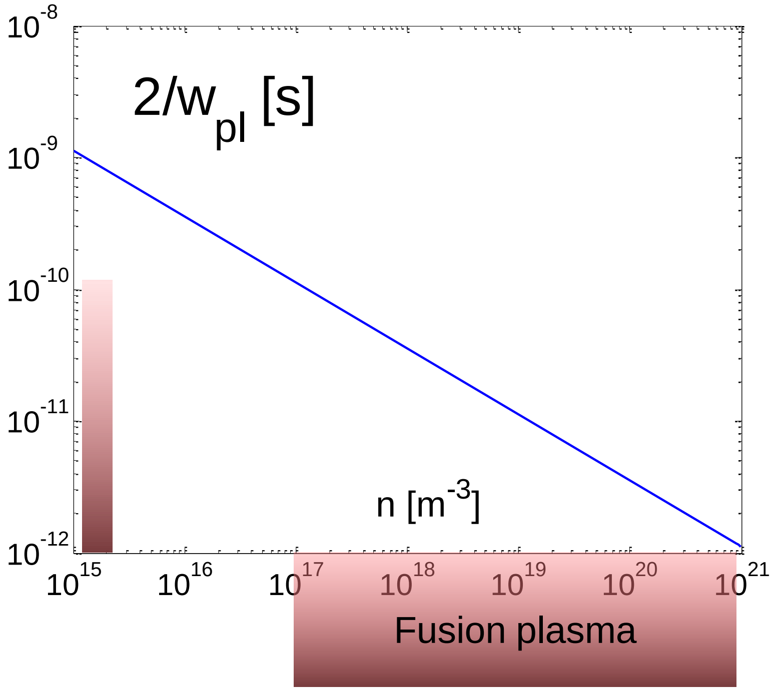
$$\Delta t < \frac{0.35}{\Omega}$$ Ensures 1% accuracy for cyclotron rotation

$$\Delta t << \frac{1}{\nu_{col}}$$ Ensures accuracy for collision operator

Spatial scales

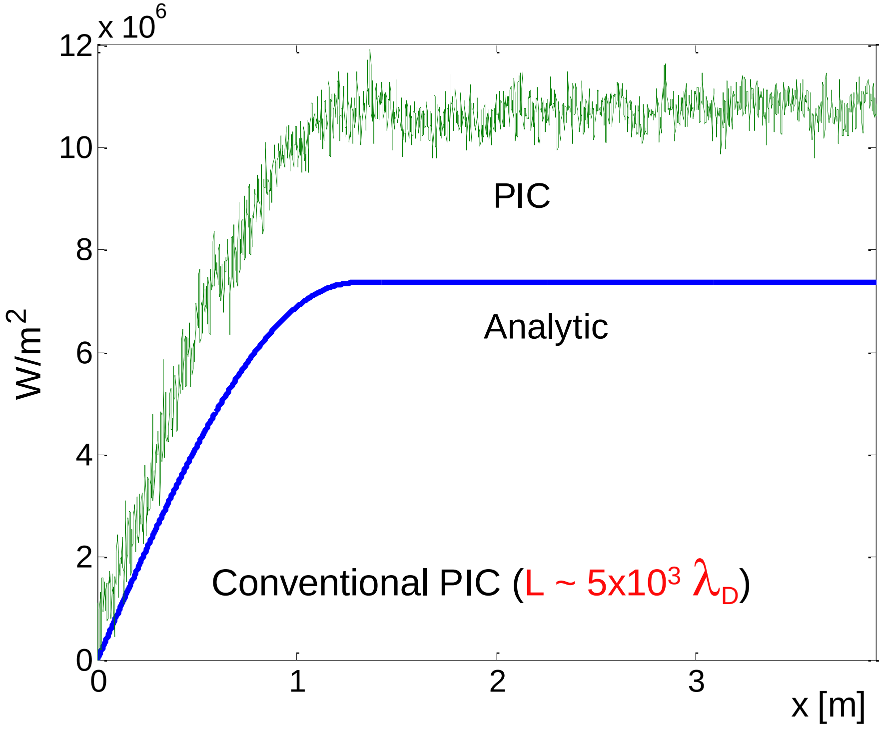
$$\Delta x < \lambda_D = \frac{V_T}{\omega_{pl}}$$ For stability of the Poisson solver

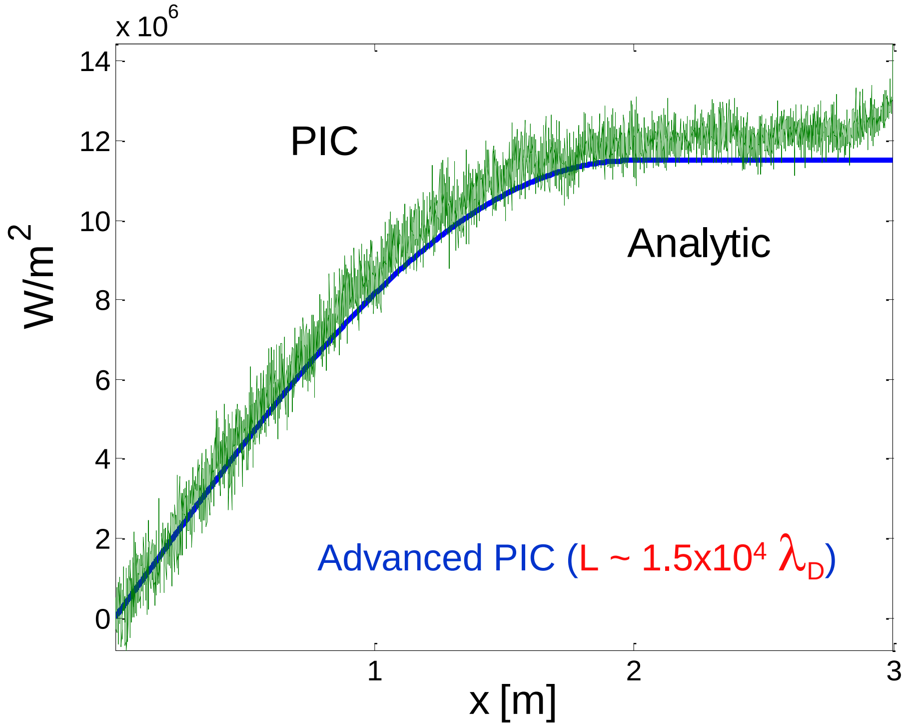
$$\Delta x < l_{geom}$$



Numerical heating

Profile of the energy flux in the tokamak SOL





- ✓ round-off errors
- ✓ numerical diffusion in velocity space, $<\delta E^2>$
- ✓ small number of particles, $\delta E \sim N^{-1/2}$

→

Filters, smoothers

implicit solvers

Numerical heating (ii)

$$\langle \delta E_{kin}(t_H) \rangle = \frac{1}{2} T$$ "Heating" time

$$t_H \approx 500 \frac{N_{pg}}{\omega_{pl}}$$ 2D CIC scheme *[R.W. Hockney 1989]*

Old not applicable

Energy conservation $\delta V \sim \delta E, \quad \langle \delta E \rangle_t = 0, \ \langle \delta E^2 \rangle_t \neq 0$ ➡ $\langle \delta V^2 \rangle_t \neq 0$

$$\langle \delta x \rangle_t = 0, \ \langle \delta x^2 \rangle_t \neq 0$$

⬇

Diffusion in usual space

⬇

Diffusion in velocity space

⬇

Numerical heating