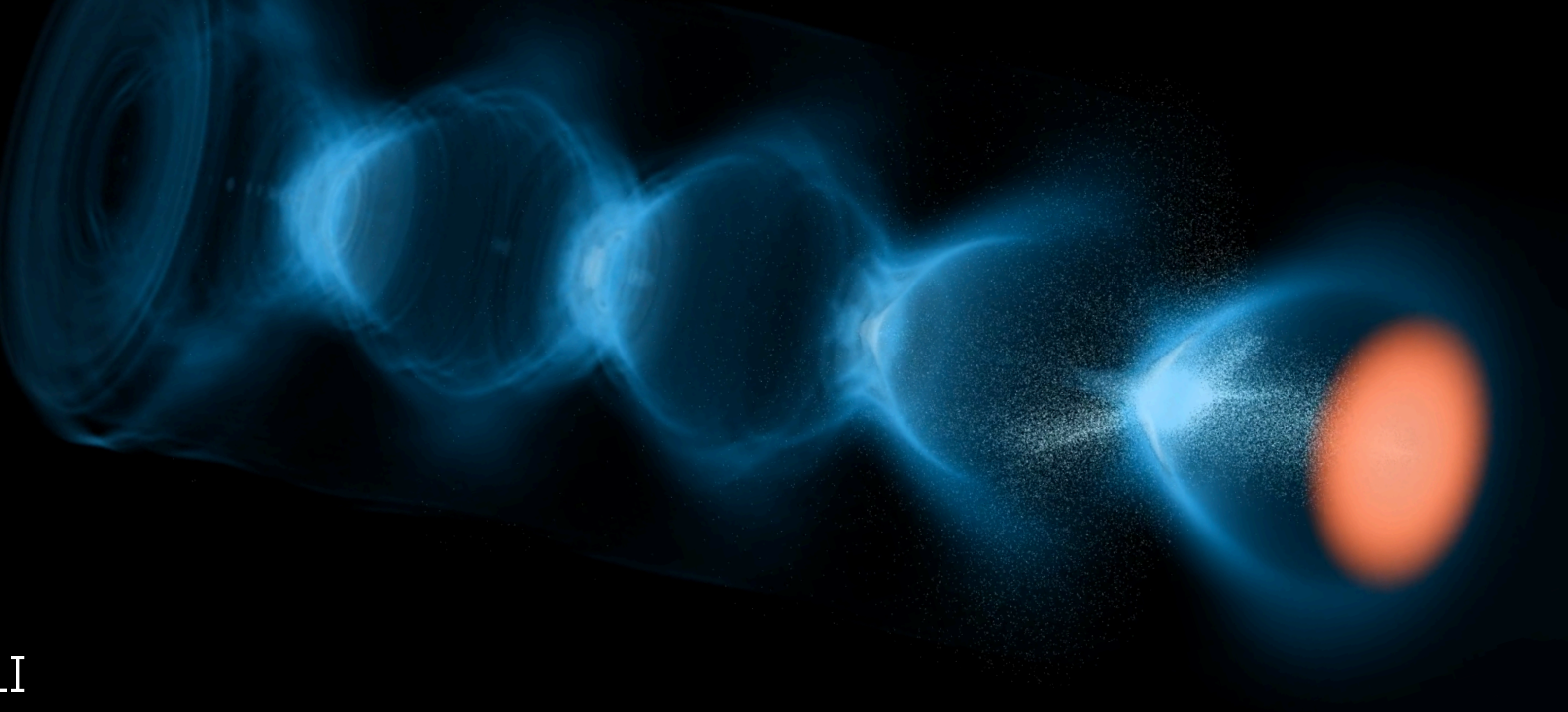
The Particle-In-Cell (PIC) Simulation of Plasmas



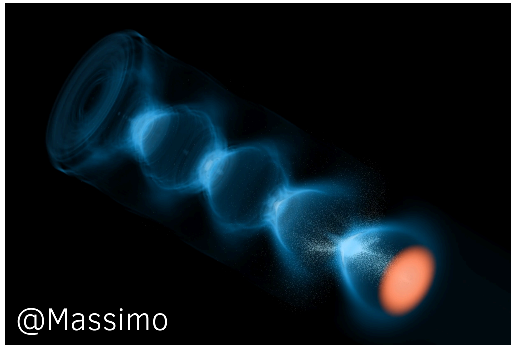
Mickael Grech, LULI

SCIPAC • Atelier Calcul • IJClab, Orsay • October 16-18, 2024

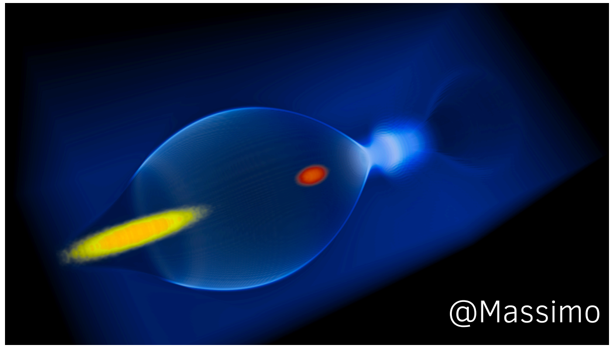
The Particle-In-Cell (PIC) simulation of plasmas

from Laboratory Plasmas ...

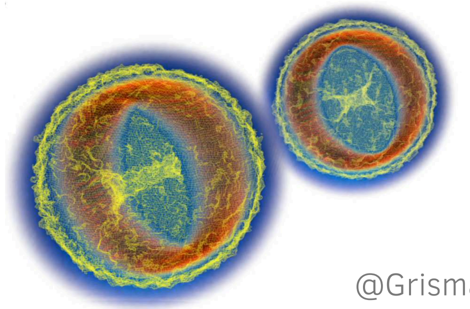
Laser Wakefield Acceleration



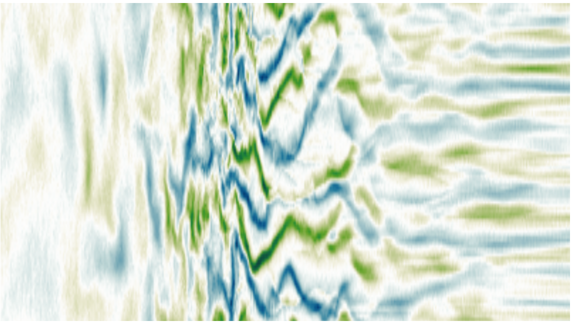
Particle-driven Wakefield Acceleration



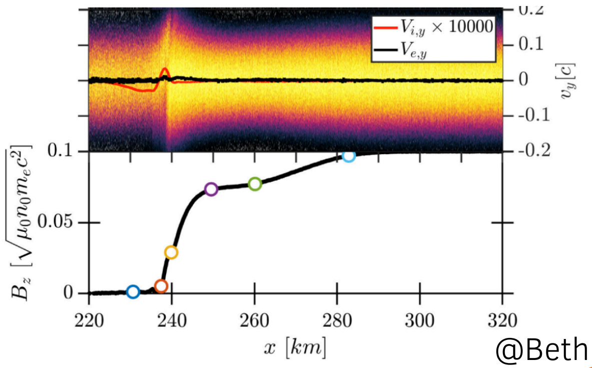
Beam-beam collision



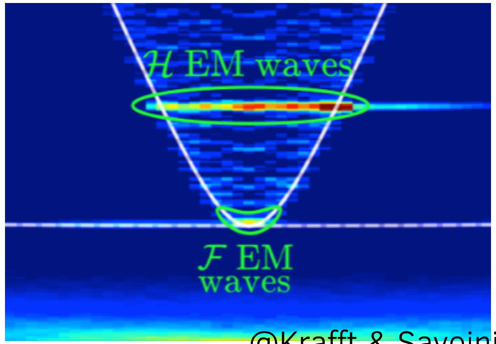
Collisionless shocks & Cosmic Rays



Comet boundaries



Solar radio-burst



... to Space & Astrophysical Plasmas

The Vlasov-Maxwell description

Vlasov Eq - Species of the plasma

$$\partial_t f_s + \frac{\mathbf{p}}{m_s \gamma} \cdot \nabla f_s + \mathbf{F}_L \cdot \nabla_p f_s = 0$$

$$\mathbf{F}_L = q_s \left(\mathbf{E} + \frac{\mathbf{p}}{m_s \gamma} \times \mathbf{B} \right)$$

$$\rho(t, \mathbf{x}) = \int d\mathbf{p} f_s(t, \mathbf{x}, \mathbf{p})$$

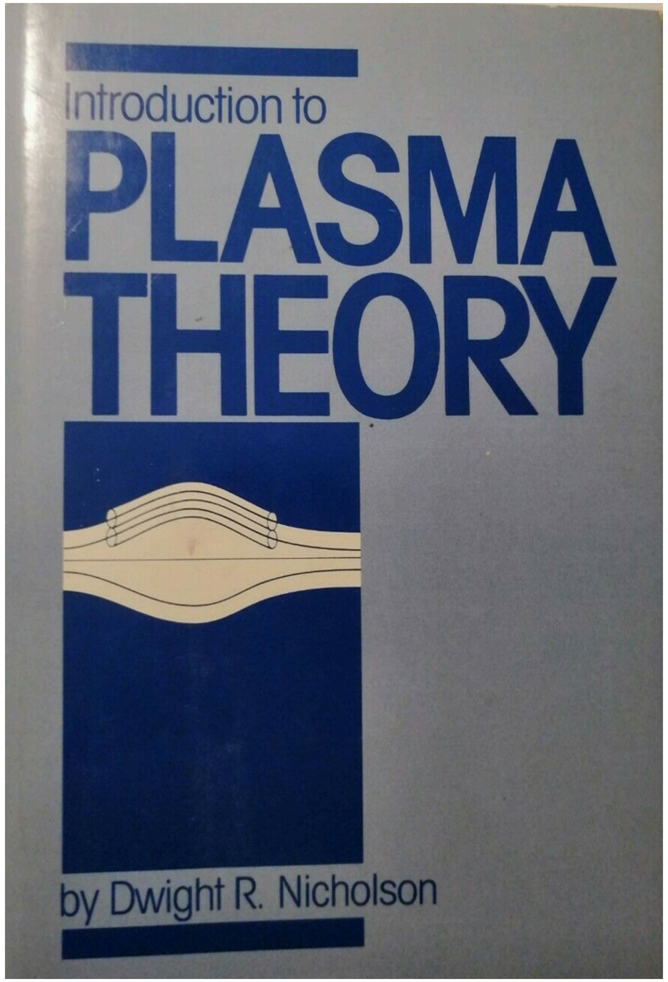
$$J(t, \mathbf{x}) = q_s \int d\mathbf{p} \frac{\mathbf{p}}{m_s \gamma} f_s(t, \mathbf{x}, \mathbf{p})$$

Maxwell Eqs - Electromagnetic Fields

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \partial_t \mathbf{E} = -\frac{1}{\epsilon_0} \mathbf{J} + c^2 \nabla \times \mathbf{B}$$

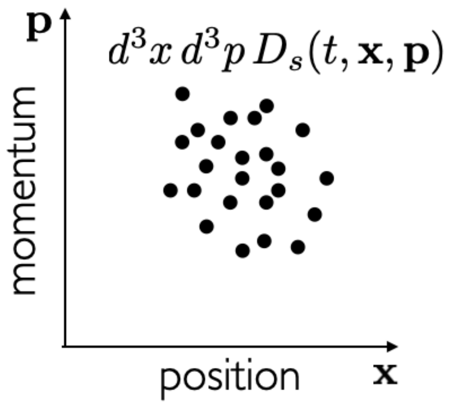
$$\nabla \cdot \mathbf{B} = 0 \qquad \partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Introduction to plasma theory, D. R. Nicholson (1983)



Vlasov equation in a nutshell

Starting point : Klimontovich's exact picture



If the exact state of the system is know at a time t_0

$$D_s(t_0, \mathbf{x}, \mathbf{p}) = \sum_p \delta(\mathbf{x} - \mathbf{x}_p(t_0))\, \delta(\mathbf{p} - \mathbf{p}_p(t_0))$$

the evolution of the system at later times is known exactly and satisfies the **Klimontovich equation**:

$$\boxed{\partial_t D_s + \mathbf{p} \cdot \nabla D_s + q_s(\mathbf{E}_{\text{tot}} + \mathbf{v} \times \mathbf{B}_{\text{tot}}) \cdot \nabla_p D_s = 0\,.}$$

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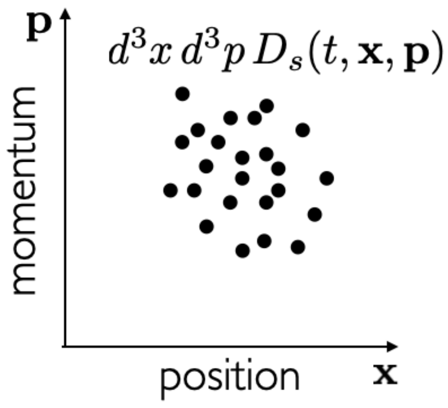

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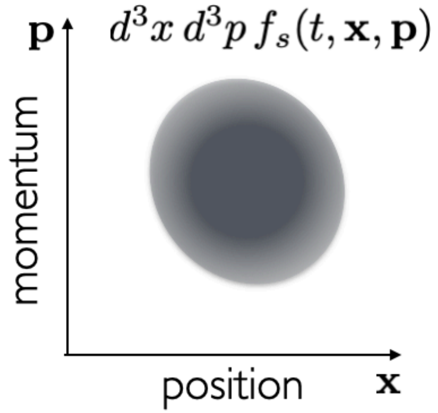
Ensemble averaging : towards the plasma kinetic equation and Vlasov equation



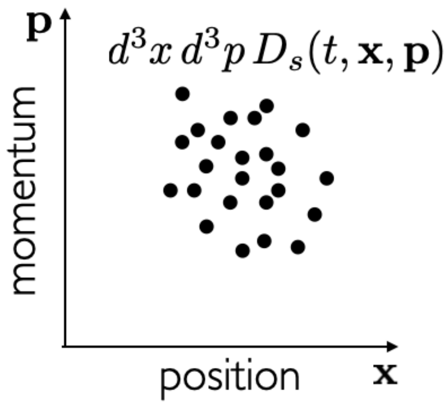
$$\begin{aligned}
\overbrace{D_s(\mathbf{x}, \mathbf{v}, t)}^{\text{total}} &= \overbrace{f_s(\mathbf{x}, \mathbf{v}, t)}^{\text{smooth, average}} + \overbrace{\delta D_s(\mathbf{x}, \mathbf{v}, t)}^{\text{microscopic fluctuations}} \\
\mathbf{E}_{\text{tot}}(\mathbf{x}, t) &= \mathbf{E}(\mathbf{x}, t) + \delta\mathbf{E}(\mathbf{x}, t) \\
\mathbf{B}_{\text{tot}}(\mathbf{x}, t) &= \mathbf{B}(\mathbf{x}, t) + \delta\mathbf{B}(\mathbf{x}, t))
\end{aligned}$$

Pluging this in Klimontovich equation and ensemble averaging leads:

$$\partial_t f_s + \mathbf{p} \cdot \nabla f_s + q_s(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_p f_s = -q_s \left\langle (\delta\mathbf{E} + \mathbf{v} \times \delta\mathbf{B})\, \delta f_s \right\rangle\,.$$

Vlasov equation in a nutshell

Starting point : Klimontovich's exact picture



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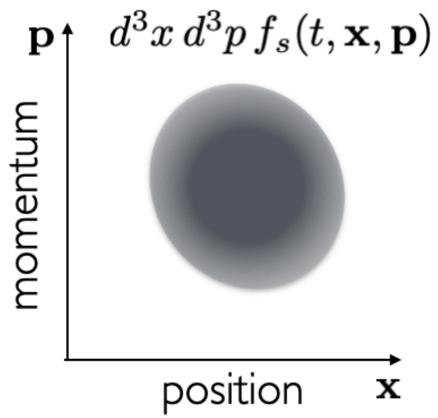
Ensemble averaging : towards the plasma kinetic equation and Vlasov equation



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collective behavior **microscopic/collisions**

Solving Vlasov-Maxwell with the PIC method

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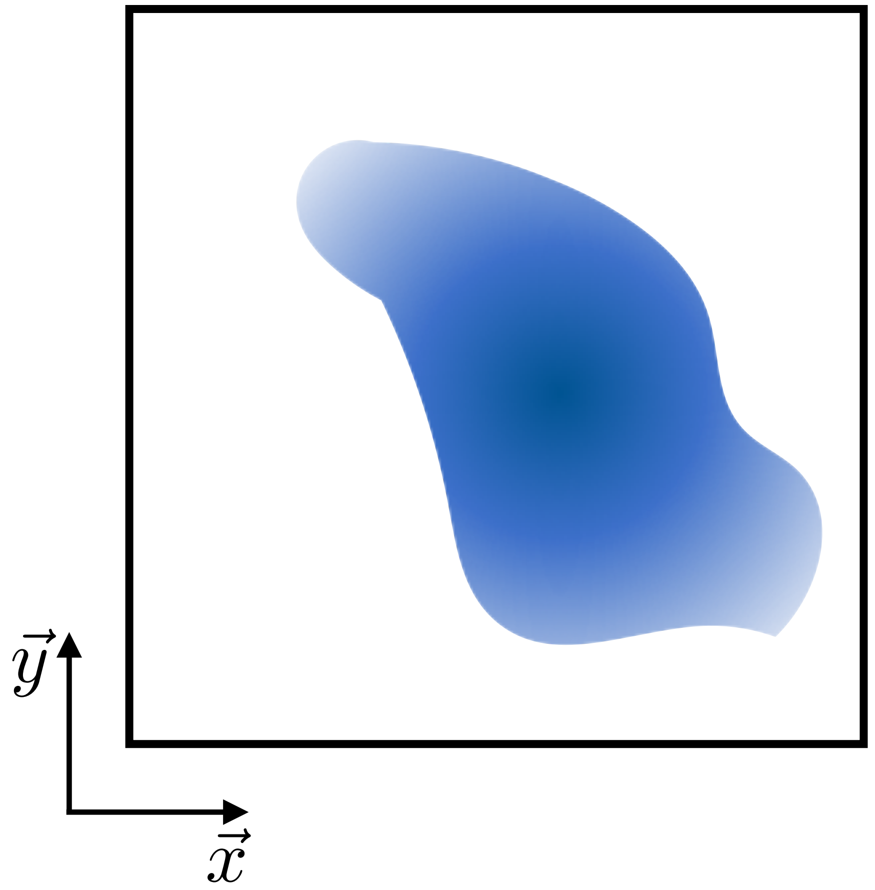

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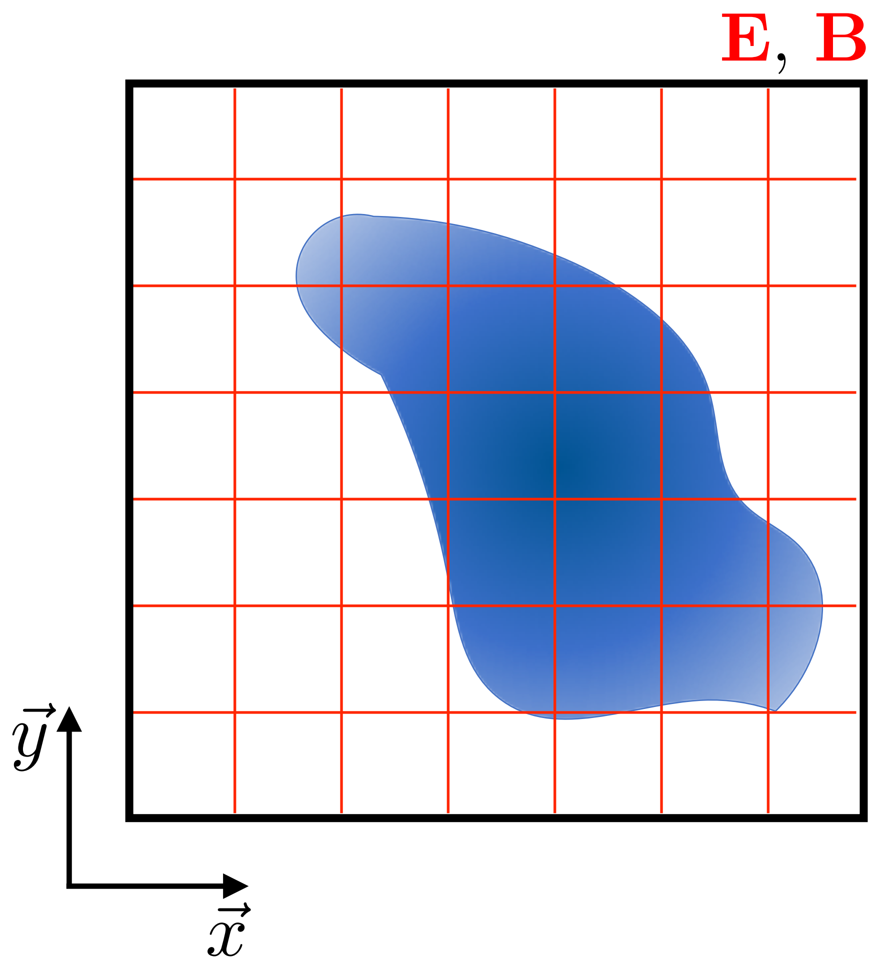

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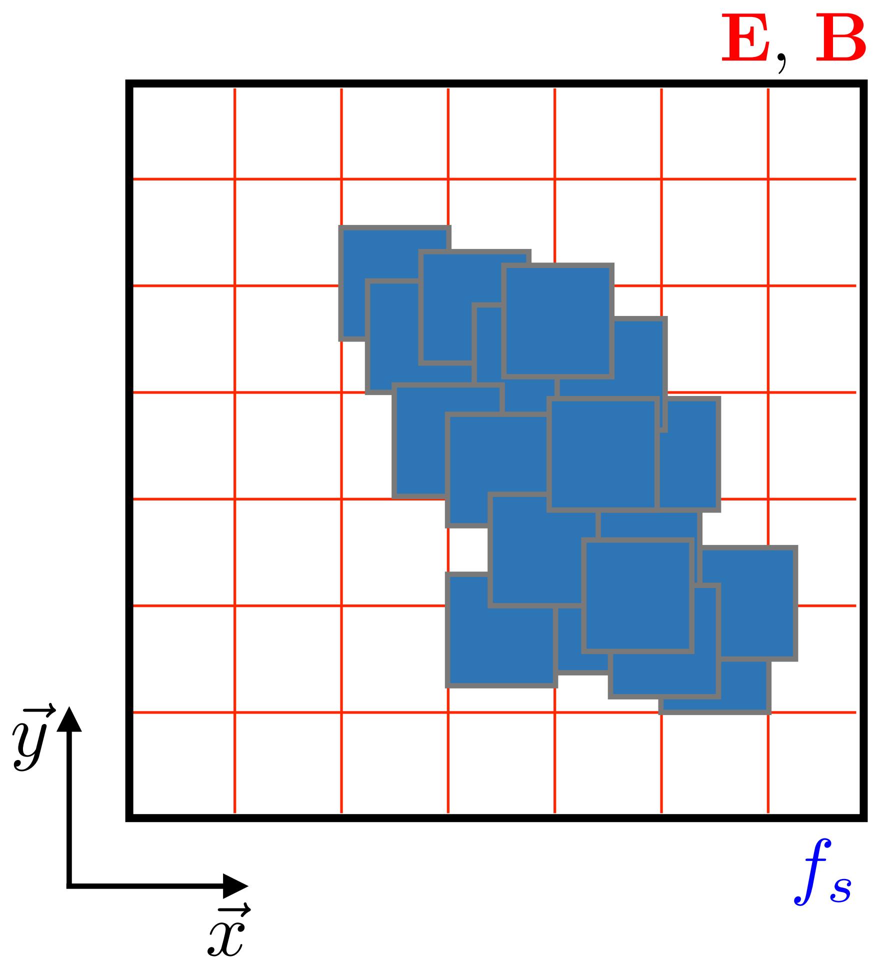
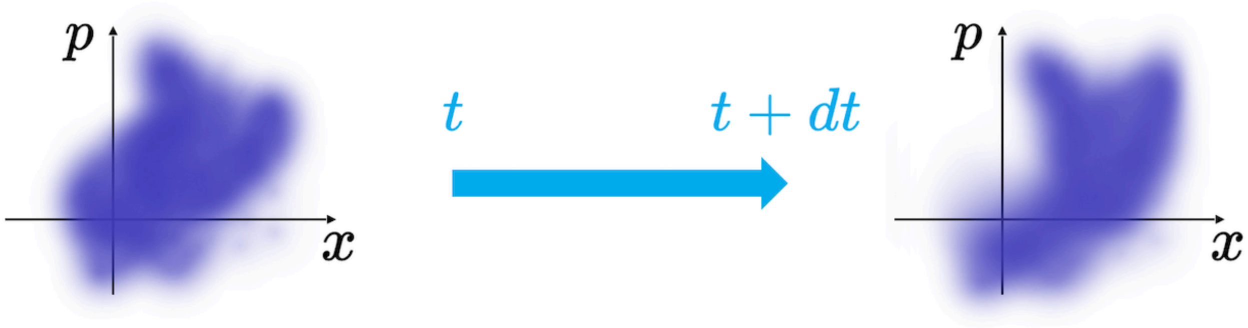


The PIC ansatz

We want to solve a discretized version of Vlasov equation:

$$\partial_t f_s + \frac{\mathbf{p}}{m_s \gamma} \cdot \nabla f_s + \mathbf{F}_L \cdot \nabla_p f_s = 0$$



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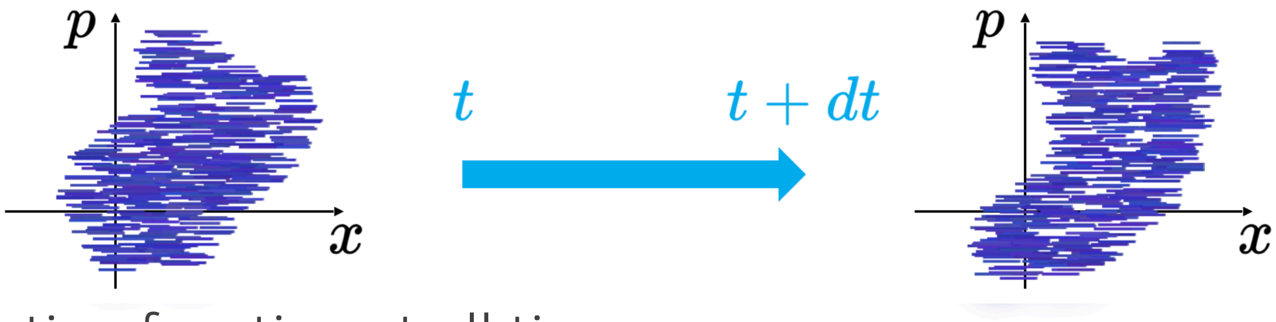

This is done using approximating the distribution function at all times as a sum of quasi/macro/pseudo-particles:

$$f_s(t, \mathbf{x}, \mathbf{p}) \stackrel{!}{=} \sum_{p=1}^{N} w_p \, S(\mathbf{x} - \mathbf{x}_p(t)) \, \delta(\mathbf{p} - \mathbf{p}_p(t))$$

numerical weight — shape-function

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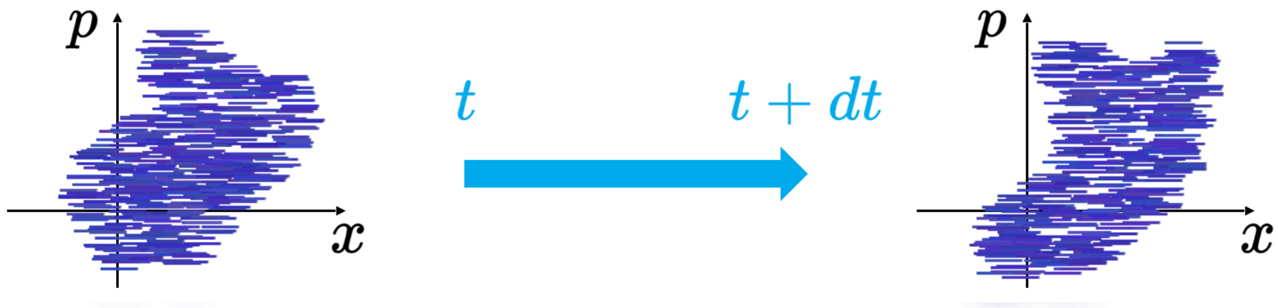

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numerical weight — shape-function

Solving Vlasov then reduces to solving the (relativistic) equations of motion of the macro-particles:

$$\partial_t \mathbf{p}_p = q_s\left(\mathbf{E}_p + \mathbf{v}\times\mathbf{B}_p\right) \quad \text{with} \quad (\mathbf{E},\mathbf{B})_p \equiv \int d\mathbf{x}\,(\mathbf{E},\mathbf{B})(\mathbf{x})\,S(\mathbf{x}-\mathbf{x}_p)$$

The PIC loop: (1) Field interpolation

Field Interpolation

$[\mathbf{E},\mathbf{B}] \rightarrow [\mathbf{E}_p,\mathbf{B}_p]$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Particle Pusher

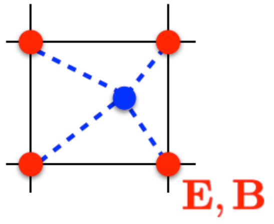
$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p\right)$$

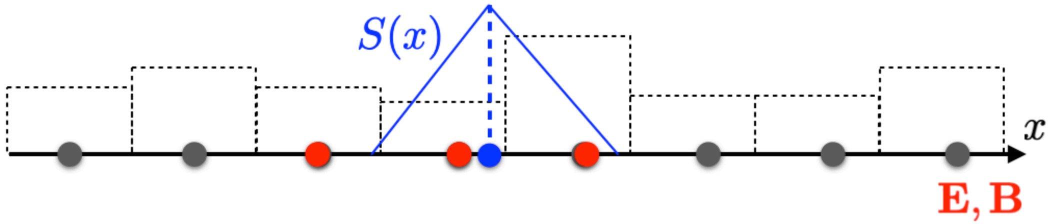
$$d_t \mathbf{x}_p = \mathbf{p}_p / \left(m_s \gamma\right)$$

Current Projection

$[\mathbf{x}_p,\mathbf{p}_p] \rightarrow [\rho_s,\mathbf{J}_s]$

$$(\mathbf{E},\mathbf{B})_p \equiv \int d\mathbf{x}\,(\mathbf{E},\mathbf{B})(\mathbf{x})\,S(\mathbf{x}-\mathbf{x}_p)$$





The PIC loop: (2) Particle pusher

Field Interpolation

$$[\mathbf{E}, \mathbf{B}] \rightarrow [\mathbf{E}_p, \mathbf{B}_p]$$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Particle Pusher

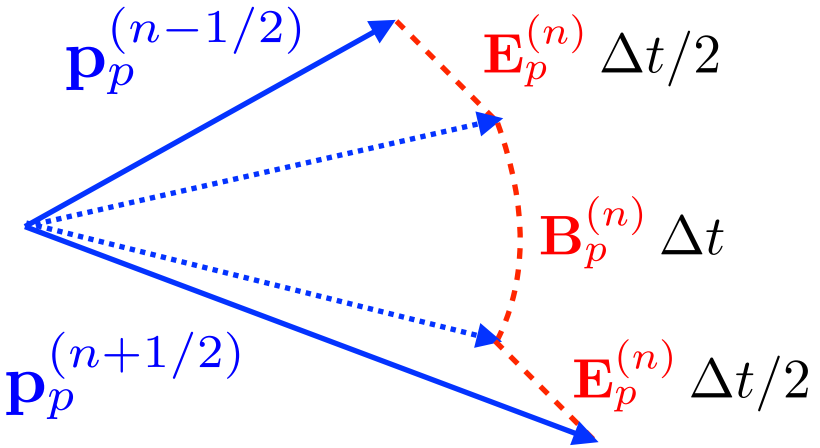
$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p \right)$$

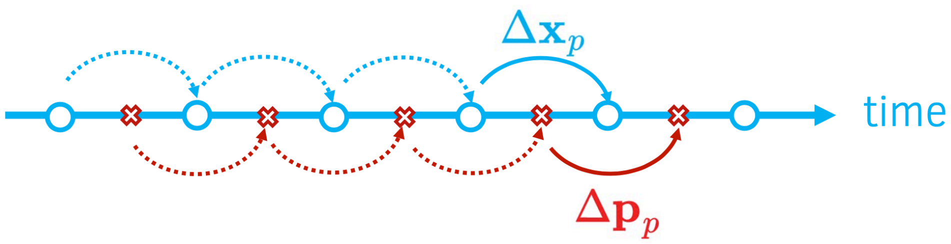
$$d_t \mathbf{x}_p = \mathbf{p}_p / \left(m_s \gamma \right)$$

Current Projection

$$[\mathbf{x}_p, \mathbf{p}_p] \rightarrow [\rho_s, \mathbf{J}_s]$$

the Boris (leap-frog) Pusher





The PIC loop: (3) Current deposition

Field Interpolation

$[\mathbf{E}, \mathbf{B}] \rightarrow [\mathbf{E}_p, \mathbf{B}_p]$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Particle Pusher

$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p \right)$$

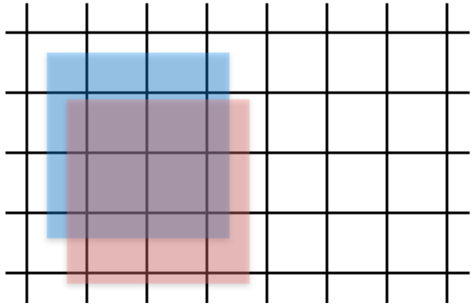
$$d_t \mathbf{x}_p = \mathbf{p}_p / \left(m_s \gamma \right)$$

Current Projection

$[\mathbf{x}_p, \mathbf{p}_p] \rightarrow [\rho_s, \mathbf{J}_s]$

the Esirkepov method for

charge-conserving current deposition



$$(J_{x,p})^{(n+\frac{1}{2})}_{i+\frac{1}{2},j} = (J_{x,p})^{(n+\frac{1}{2})}_{i-\frac{1}{2},j} + q_s\, w_p\, \frac{\Delta x}{\Delta t} (W_x)^{(n+\frac{1}{2})}_{i+\frac{1}{2},j}$$

$$(J_{y,p})^{(n+\frac{1}{2})}_{i,j+\frac{1}{2}} = (J_{y,p})^{(n+\frac{1}{2})}_{i,j-\frac{1}{2}} + q_s\, w_p\, \frac{\Delta y}{\Delta t} (W_y)^{(n+\frac{1}{2})}_{j,i+\frac{1}{2}}$$

Esirkepov, Comp. Phys. Comm. **135**, 144 (2001)

The PIC loop: (4) Maxwell solver

Field Interpolation

$[\mathbf{E},\mathbf{B}] \rightarrow [\mathbf{E}_p,\mathbf{B}_p]$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Particle Pusher

$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p\right)$$

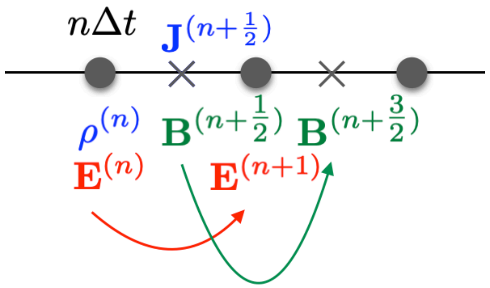
$$d_t \mathbf{x}_p = \mathbf{p}_p / \left(m_s \gamma\right)$$

Current Projection

$[\mathbf{x}_p,\mathbf{p}_p] \rightarrow [\rho_s,\mathbf{J}_s]$

the Finite-Domain Time-Difference

Maxwell solver



$$\left(\frac{dE_y}{dt}\right)_i^{(n)} = -(J_y)_i^{(n)} + \frac{(B_z)_{i+1/2}^{(n+1/2)} - (B_z)_{i-1/2}^{(n+1/2)}}{\Delta x}$$

Taflove, *Computation Electrodynamics* (2005)
Nuter et al., EPJD **68**, 1 (2014)

The PIC loop: (4) Maxwell solver

Field Interpolation

$[\mathbf{E}, \mathbf{B}] \rightarrow [\mathbf{E}_p, \mathbf{B}_p]$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Particle Pusher

$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p \right)$$

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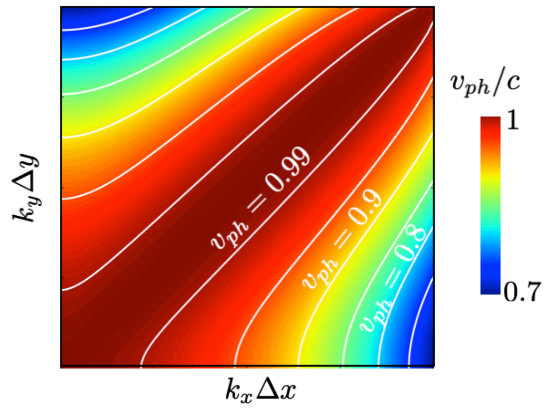
Current Projection

$[\mathbf{x}_p, \mathbf{p}_p] \rightarrow [\rho_s, \mathbf{J}_s]$

the Finite-Domain Time-Difference

Maxwell solver



Taflove, *Computation Electrodynamics* (2005)
Nuter et al., EPJD **68**, 1 (2014)

The PIC loop: (4) Maxwell solver

Field Interpolation
$[\mathbf{E}, \mathbf{B}] \rightarrow [\mathbf{E}_p, \mathbf{B}_p]$

Maxwell Solver
$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$
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Particle Pusher
$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p \right)$$
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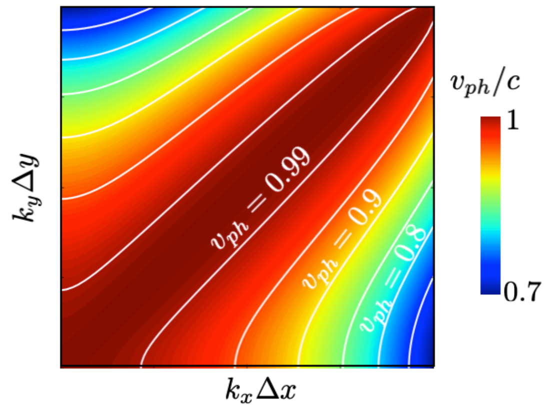
Current Projection
$[\mathbf{x}_p, \mathbf{p}_p] \rightarrow [\rho_s, \mathbf{J}_s]$

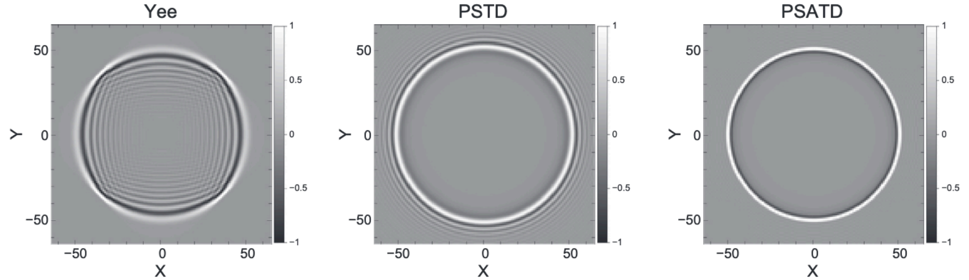
the Finite-Domain Time-Difference

Maxwell solver



Taflove, *Computation Electrodynamics* (2005)
Nuter et al., EPJD **68**, 1 (2014)

Spectral methods are also interesting



Vay et al., J. Comp. Phys. **243**, 260 (2013)

Around the PIC loop: Initialization, Boundary Conditions, Parallelization

Field Interpolation

$$[\mathbf{E},\mathbf{B}] \rightarrow [\mathbf{E}_p,\mathbf{B}_p]$$

Maxwell Solver

$$\partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

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Particle Pusher

$$d_t \mathbf{p}_p = q_s \left(\mathbf{E}_p + \mathbf{v} \times \mathbf{B}_p\right)$$

$$d_t \mathbf{x}_p = \mathbf{p}_p / \left(m_s \gamma\right)$$

Current Projection

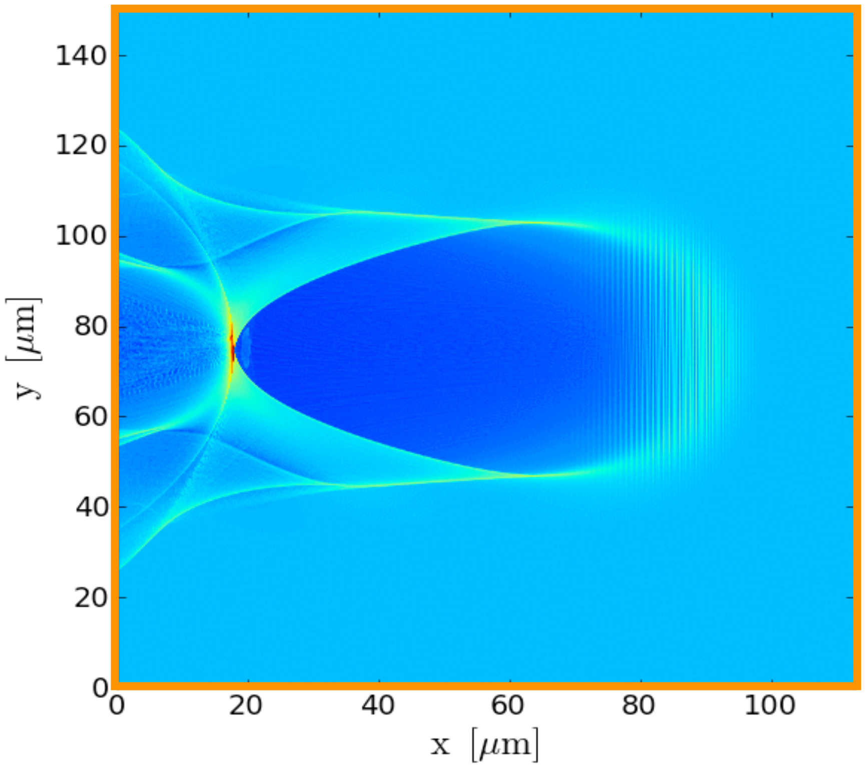
$$[\mathbf{x}_p,\mathbf{p}_p] \rightarrow [\rho_s,\mathbf{J}_s]$$

Initialization: entering the PIC loop

- initialize your macro-particles
- solve Poisson equation(s)
- add divergence-free fields

Around the PIC loop: Initialization, Boundary Conditions, Parallelization

My Simulation (LWFA)



Initialization: entering the PIC loop

- initialize your macro-particles
- solve Poisson equation(s)
- add divergence-free fields

Boundary conditions:

- on electromagnetic fields (reflecting, injecting, absorbing, etc)
- on macro-particles (reflecting, injecting, thermalizing, etc)

Around the PIC loop: Initialization, Boundary Conditions, Parallelization

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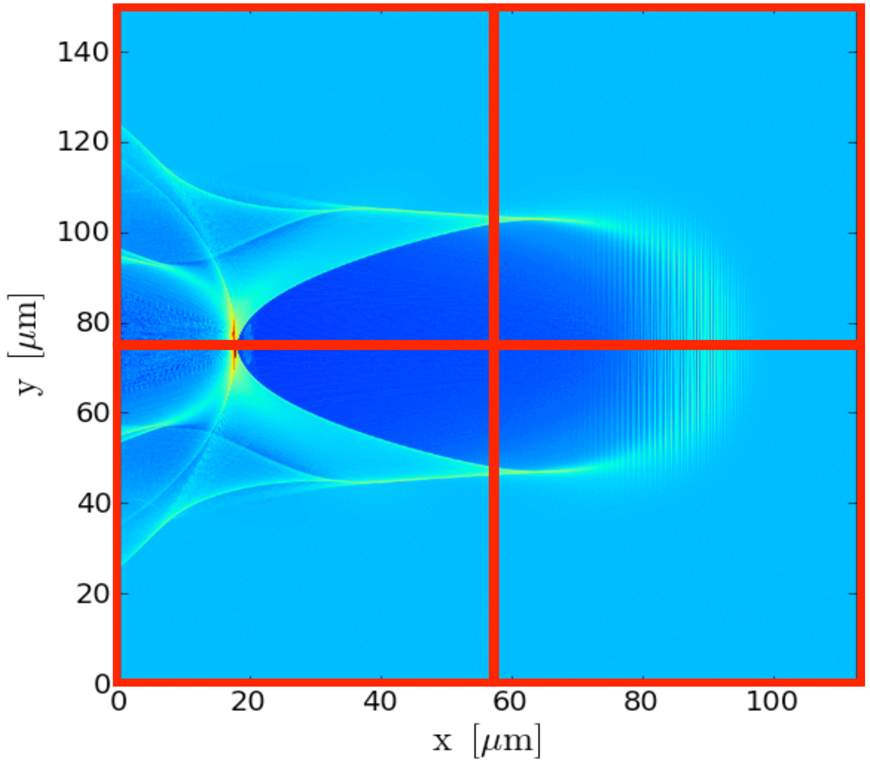

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Boundary conditions:

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- on macro-particles (reflecting, injecting, thermalizing, etc)

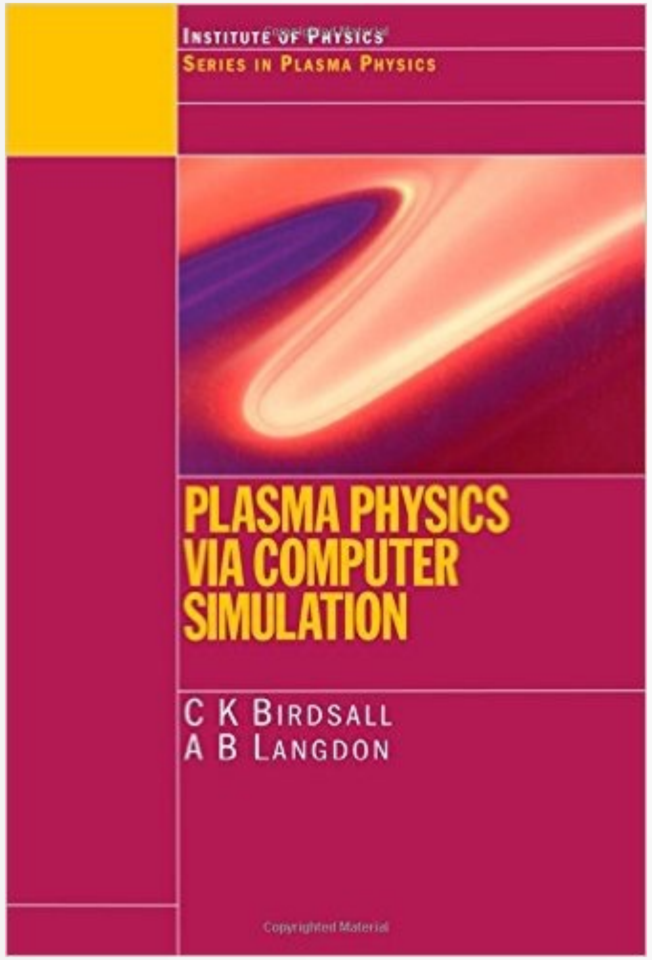
Parallelization:

- domain decomposition
- (dynamic) load balancing
- vectorization & much more

References to go beyond this introduction

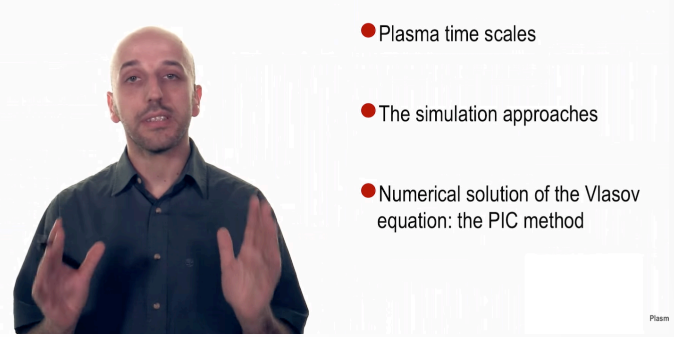
Plasma Physics via Comp. Sim.

Birdsall & Langdon



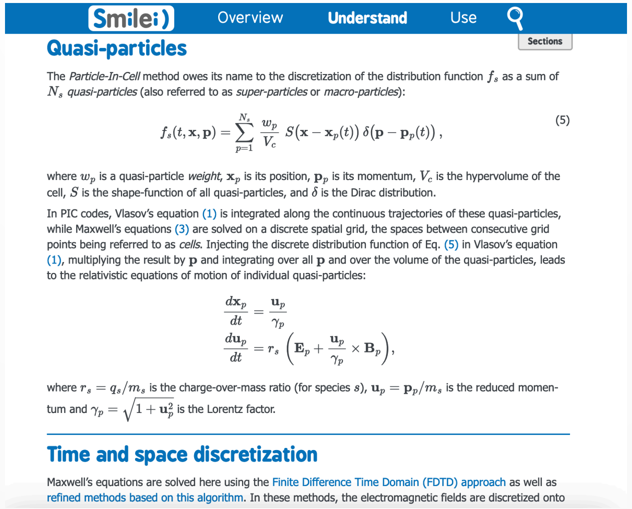
Series of online lectures by Paolo Ricci

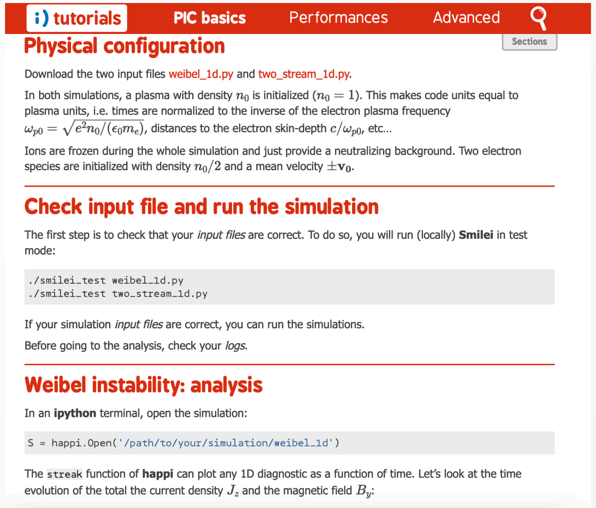
EPFL lectures, available on youtube



The Smilei PIC code website

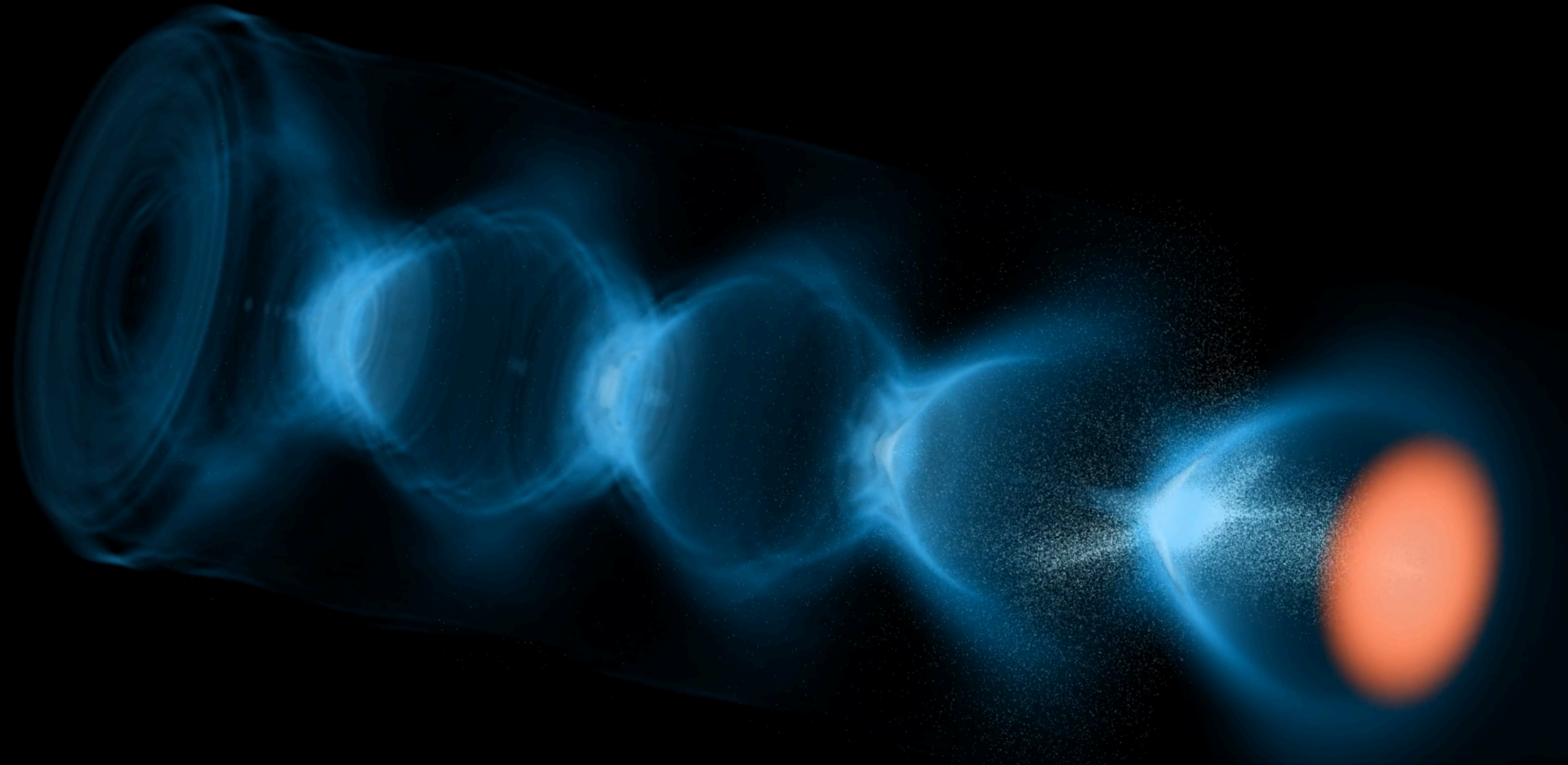
Extensive documentation & tutorials





Derouillat et al., Comp. Phys. Comm. **222**, 351 (2018)

Thanks for your attention!



mickael.grech@polytechnique.edu