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Particle-in-Cell Codes for plasma-based particle acceleration

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Outline

- Relativistic plasmas, acceleration and the simulation tools
- Explicit PIC codes
- Lorentz boost
- Quasi-static approximation
- Hybrid methods

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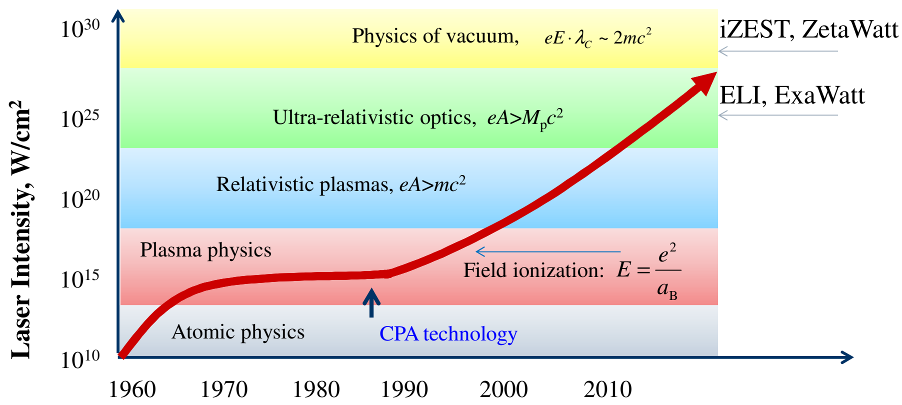
Laser technology and new physics



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Important relativistic laser-plasma parameters

Dimensionless laser amplitude $a=\frac{eA}{mc^2}$

relativistic when $a \approx 1 \leftrightarrow I\lambda^2 = 1.37\times10^{18}$ W μm²/cm²

Critical plasma density $N_c = \frac{\omega_0^2 m}{4\pi e^2} \sim 10^{21}$ cm^{-3}

***S*-number** $S=\frac{N}{aN_c}$

Gordienko & Pukhov
Phys. Plasmas **12**, 043109 (2005)

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A. Pukhov, *J. Plasma Physics*, *vol.* 61, *part* 3, *p*. 425 (1999).

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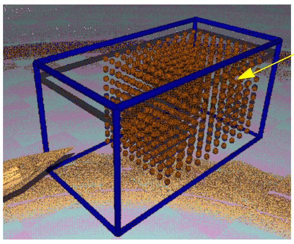
Virtual Laser Plasma Lab

A. Pukhov, J. Plasma Phys. 61, 425 (1999)



Plasma or neutral gas

Gas of an arbitrary element can be used.

The code VLPL is written in C++, object oriented, parallelized using MPI for **Massively Parallel** performance

10^9 **particles and** 10^8 **cells** can be treated

Advanced physics & numerics

- Inelastic processes
- Radiation damping
- QED effects
- hybrid hydro model
- quasi-static approximation

Fields

$$\nabla\times\mathbf{B}=\frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}+\frac{4\pi}{c}\mathbf{j}$$

$$\nabla\times\mathbf{E}=-\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$$

Particles

$$\frac{d\mathbf{p}}{dt}=q\mathbf{E}+\frac{q}{c\gamma}\mathbf{p}\times\mathbf{B}$$

$$\gamma=\sqrt{1+p^2/(mc)^2}$$

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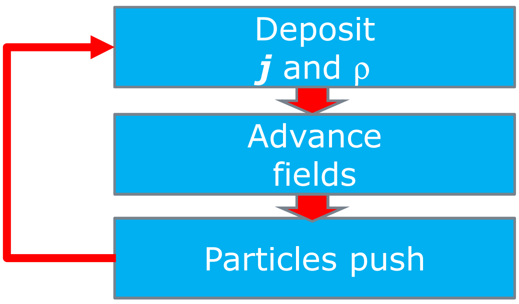
The standard PIC time step cycle



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Equations to solve in full electromagnetic codes

Ampere's law	$\frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c}\mathbf{j}$	Dynamic equations
Faraday's law	$\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$	
Poisson's eq.	$\nabla \cdot \mathbf{E} = 4\pi\rho$	Static equations
No magnetic dipoles	$\nabla \cdot \mathbf{B} = 0$	

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Charge continuity and locality of the equations

Continuity Eq.	$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$	Local equations
Ampere's law	$\frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c}\mathbf{j}$	
Poisson's eq.	$\nabla \cdot \mathbf{E} = 4\pi\rho$	Global initial conditions
No magnetic dipoles	$\nabla \cdot \mathbf{B} = 0$	

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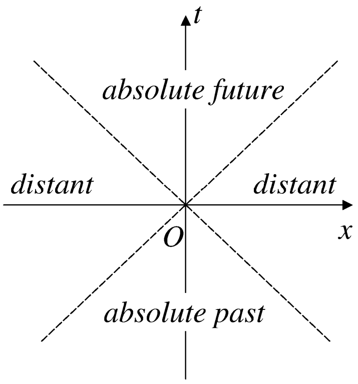
Locality of the equations



Only particles within the radius of cτ communicate to each other at every time step τ.

This allows for efficient parallelization using domain decomposition

Distribution function and kinetic equation

N-particles distribution function: $F_N(t, \mathbf{r}_1, \mathbf{p}_1, \ldots, \mathbf{r}_N, \mathbf{p}_N)$

Nearly ideal plasma:
single particle distribution function: $f(t, \mathbf{r}, \mathbf{p})$

$$\frac{\partial f(t,\mathbf{r},\mathbf{p})}{\partial t} + \frac{\mathbf{p}}{m\gamma} \nabla_{\mathbf{r}} \cdot f(t,\mathbf{r},\mathbf{p}) + \frac{q}{\gamma}\left[\mathbf{E} + \frac{\mathbf{p}}{mc\gamma} \times \mathbf{B}\right] \nabla_{\mathbf{p}} \cdot f(t,\mathbf{r},\mathbf{p}) = St$$

How to solve this equation?

Eulerian approach, FDTD "Vlasov codes"

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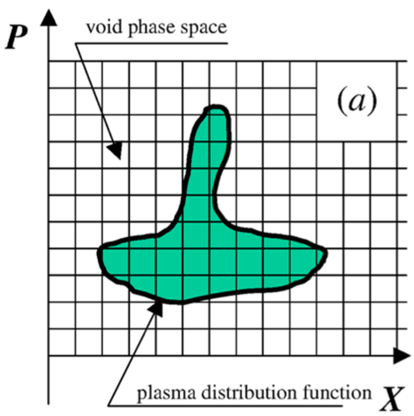

Very inefficient:
a lot of empty phase space
has to be processed.

However, temperature effects
may be described more carefully.
Low noise.
May be subject
to numerical diffusion.

"Finite elements" approach, integrating along characteristics

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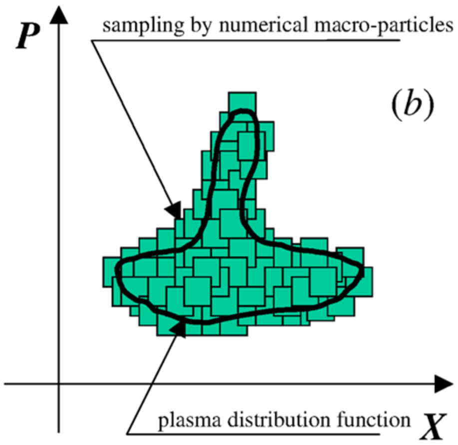
Characteristics of the Vlasov Eq.
coincide with the equations of motion

$$\frac{d\mathbf{p}}{dt} = q\left[\mathbf{E} + \frac{\mathbf{p}}{mc\gamma} \times \mathbf{B}\right] + \mathbf{F}_{st}$$

Thus, we just push
the numerical macroparticles
in self-consistent
electromagnetic fields

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m\gamma}$$

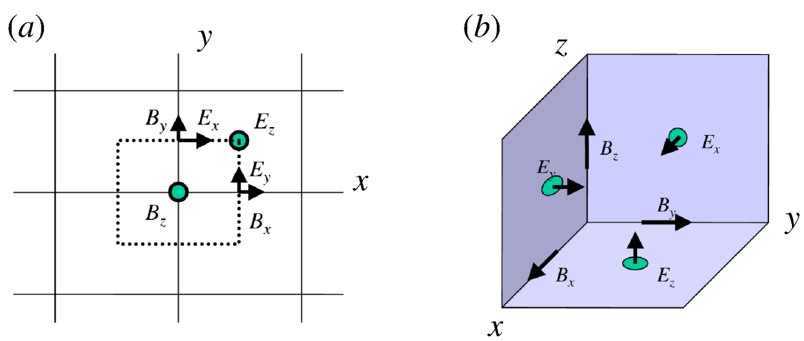
Sampling phase space: numerical macroparticles



Computationally efficient: only filled parts of phase space have to be processed.

However, temperature effects are poorly described, or require very many particles. Noisy as $N^{1/2}$.

Maxwell solver: Yee lattice The conservative scheme



Yee lattice and the continuity equation

The Yee solver conserves div **E** and rot **E**.
In Coulomb gauge, e.g.:

$$\mathbf{E}=\mathbf{E}_{\parallel}+\mathbf{E}_{\perp}=-\nabla\varphi-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t};\qquad \mathbf{E}_{\parallel}=-\nabla\varphi;$$

However, we don't solve the Poisson Eq. $\nabla^2\varphi=-4\pi\rho$

Rather, we solve $\frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}=\nabla\times\mathbf{B}-\frac{4\pi}{c}\mathbf{j}$

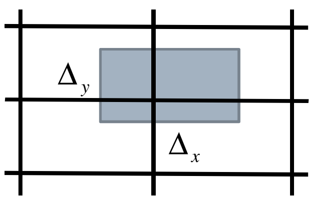
We must define the currents correctly to satisfy the continuity Eq $\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0$

Numerical macro-particles

We define the charge density at the centers of the grid cells

$$\rho_{i+1/2,j+1/2,k+1/2}=\sum_n W_n^\rho S^\rho\left(\mathbf{r}_{i+1/2,j+1/2,k+1/2}-\mathbf{r}_n\right)$$

The macro-particles may have arbitrary shapes *S*.
The most common shapes are bricks

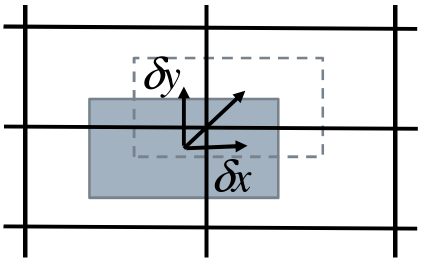


$$S^\rho(\mathbf{r})=S_x^\rho(x)S_y^\rho(y)S_z^\rho(z)$$

$$S_i^\rho(r_i)=1-2\frac{|r_i|}{\Delta_i},\quad |r_i|<\frac{\Delta_i}{2}$$

Pushing macro-particles in a cell

We assume the second order numerical scheme.
Thus, the particle trajectory within the time step τ is a straight line.



$$\mathbf{J}\tau = \oint_{\Omega} d\Omega \int_0^{\tau} \mathbf{V} W^{\rho} S^{\rho} dt$$

$$= \oint_{\Omega} d\Omega \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} W^{\rho} S^{\rho} \left(\mathbf{r}_{i+1/2,\,j+1/2,\,k+1/2} - \mathbf{r}\right) d\mathbf{r}$$

Villacenor, Buneman CPC 69, 306 (1992)

Pushing macro-particles in a cell

For the simple brick shape, the equations are:

$$J^{x}_{i,\,j+1/2,k+1/2} = \delta x W^{\rho}\left(a_y a_z + b_{yz}\right)$$
$$J^{y}_{i+1/2,\,j,k+1/2} = \delta y W^{\rho}\left(a_x a_z + b_{xz}\right)$$
$$J^{z}_{i+1/2,\,j+1/2,k} = \delta z W^{\rho}\left(a_x a_y + b_{xy}\right)$$

$$a_{\alpha} = 1 - 2\frac{|r_{\alpha} + 0.5\Delta_{\alpha}|}{\Delta_{\alpha}}$$

$$b_{\alpha\beta} = \frac{1}{12}\delta x_{\alpha} \delta x_{\beta}$$

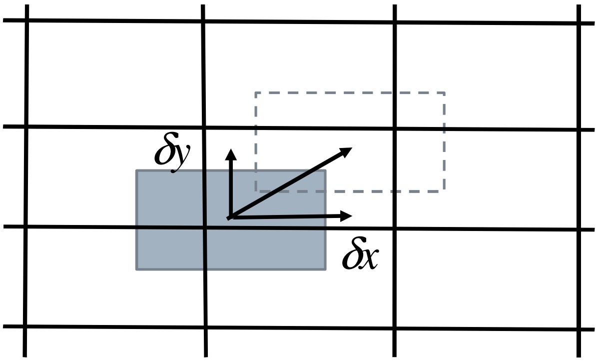
$$\alpha, \beta = \{x, y, z\}$$

Leap-frog field pusher:

$$\mathbf{E}^{n+1} = \mathbf{E}^{n} + c\tau\nabla\times\mathbf{B}^{n+1/2} - 4\pi\tau\mathbf{J}^{n+1/2}$$

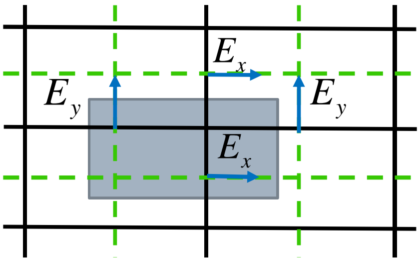
Pushing macro-particles across cells

In its motion within one single time step, the particle can cross several cells. The algorithm must handle all these cases.



Interpolating fields to the particle positions

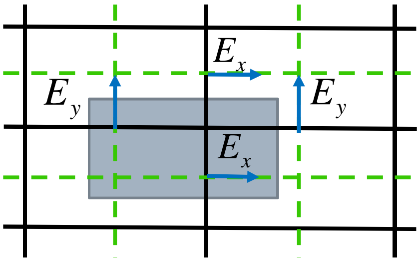
One can interpolate the fields to the centers for the cells first and then interpolate them to the particle center in the same way as one deposits charges



This scheme "conserves" momentum but not energy

Interpolating fields to the particle positions

Alternatively, one can interpolate the electric fields in the same way as one deposits currents

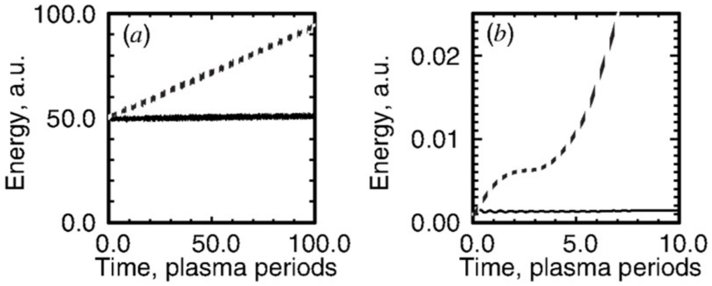


This scheme “conserves” energy, but not momentum

When the particle crosses the cell boundaries, all conservations fail

Energy (in-)conservation in PIC

The total energy: $$\mathcal{E} = \sum_n m_n c^2 (\gamma - 1) + \frac{1}{8\pi}\int_V \left(E^2 + B^2\right) dV$$



Debye length resolved: h=0.5r_D Cold plasma: h=$10^{-3}r_D$

Numerical dispersion in the Yee Maxwell solver

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Numerical waves do not propagate with the speed of light.
Even in vacuum.
The standard Yee dispersion relation is:

$$\frac{1}{\tau^2}\sin^2\frac{\omega\tau}{2} = \frac{\hat{\omega}_p^2}{4} + \frac{1}{h_x^2}\sin^2\frac{k_x h_x}{2} + \frac{1}{h_y^2}\sin^2\frac{k_y h_y}{2} + \frac{1}{h_z^2}\sin^2\frac{k_z h_z}{2}$$

The stability condition is: $$\frac{1}{\tau^2} > \frac{\hat{\omega}_p^2}{4} + \frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}$$

Numerical dispersion in the Yee Maxwell solver

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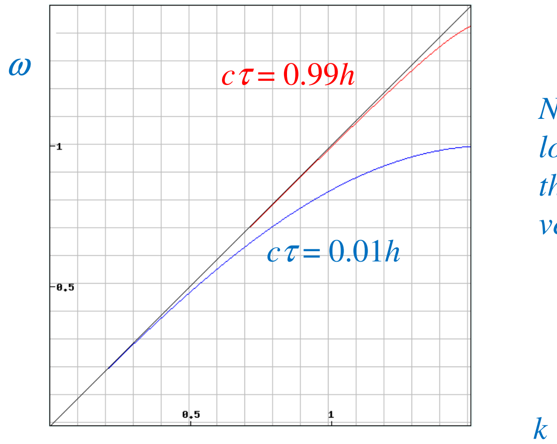
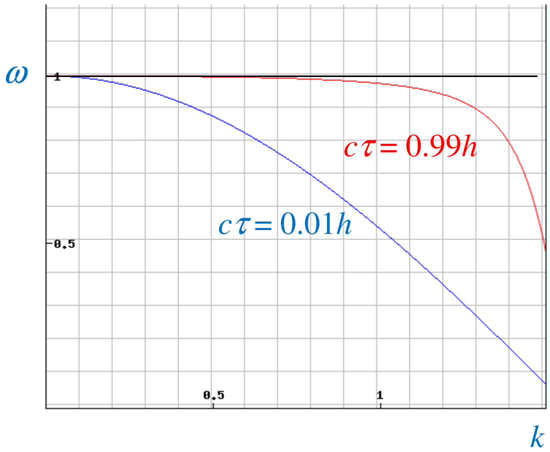


Numerical frequency is lower than the real one this leads to lower phase velocity

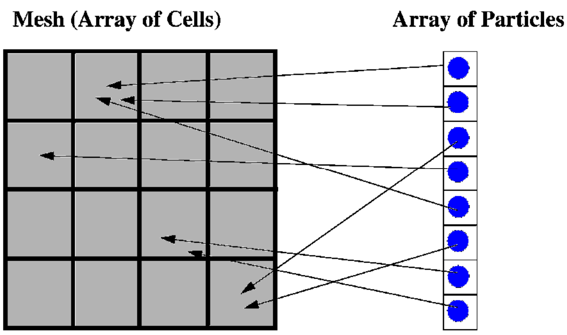
Numerical dispersion in the Yee Maxwell solver



Waves with the shortest wavelengths are very slow!

Small time steps lead to a bad dispersion

Implementation of a PIC code Single processor optimization



The central problem of a PIC code: particles must interact with the array of cells

Implementation of a PIC code
Single processor optimization

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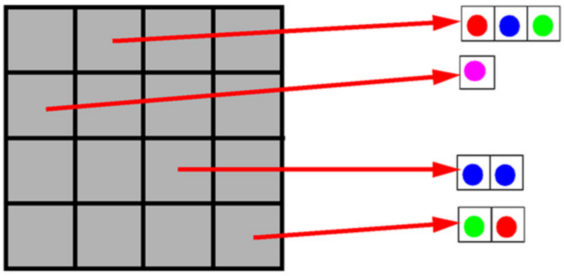
Mesh (Array of Cells) → *points to* → Linked Lists of Particles



The linked list of particles with the bases in the cells help to optimize the cache and memory usage

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Implementation of a PIC code
Parallelization: domain decomposition

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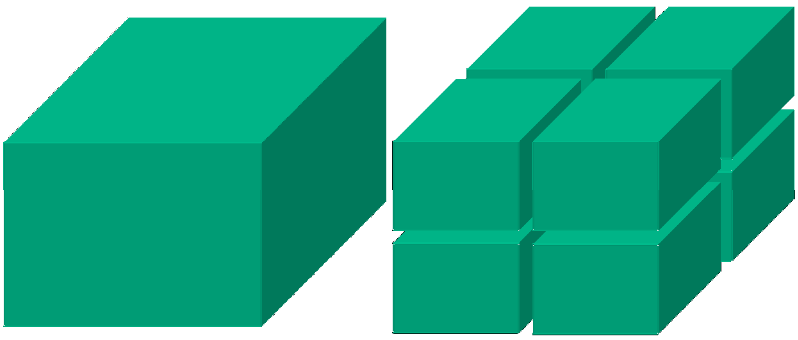

Full simulation domain 3d domain decomposition

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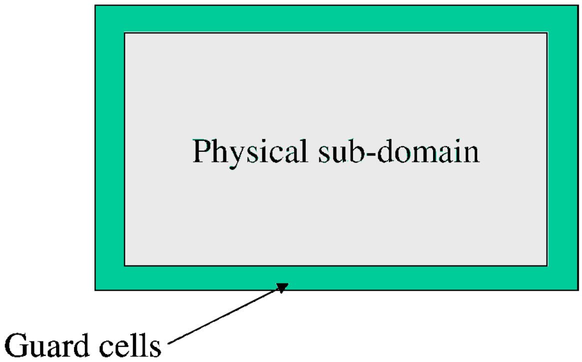
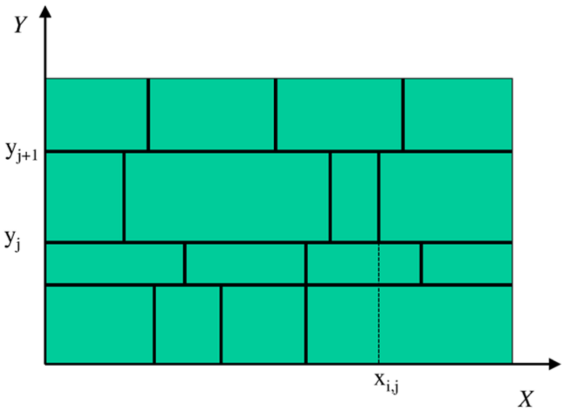
Implementation of a PIC code
Parallelization: domain decomposition



Algorithm locality: only guard cells must communicate between processors.
No global communications

Possibility for load balancing



The adaptive partitioning according to the number of particles per processor

PIC codes for plasma-based acceleration Bubble regime

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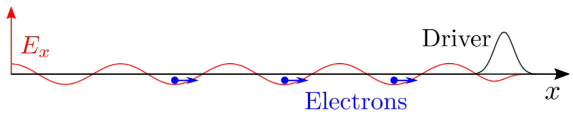
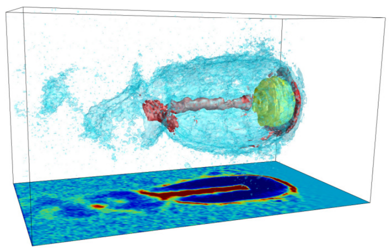
A.Pukhov & J.Meyer-ter-Vehn, *Appl. Phys. B*, **74,** *p*.355 (2002)



- Plasma wake fields offer a promising alternative to conventional particle accelerators



- Ultra-short laser pulse or particle bunch creates driven plasma oscillation
- Secondary particles can become accelerated in the wake
- Accelerating field reaches hundreds of GV/m
- Simulations carried out with Virtual Laser Plasma Lab

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The multi-scale problem

The plasma acceleration has several very disparate scales

1. Small scale: laser wavelength λ or plasma wavelength λ_p
2. Medium scale: driver length
3. Large scale: acceleration length $L_A=10^4\ldots10^7\ \lambda,\ \lambda_p$

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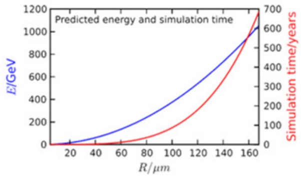
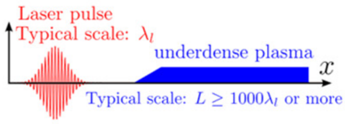
Energy gain and simulation time

- Scaling laws predict possibility of large-scale bubble regime accelerators
- Simulations extremely costly
- Simulations of relativistic interaction show disparity of time scales



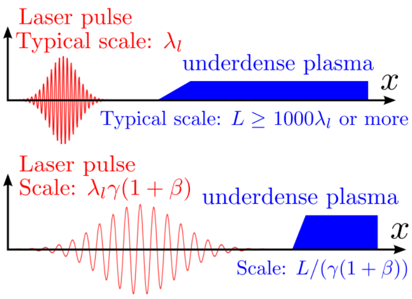


λ_l =Laser wave length, L =plasma length

- Problem: Wake field often behaves quasi-statically, but explicit PIC integrators must resolve smallest scale

Boosted frame

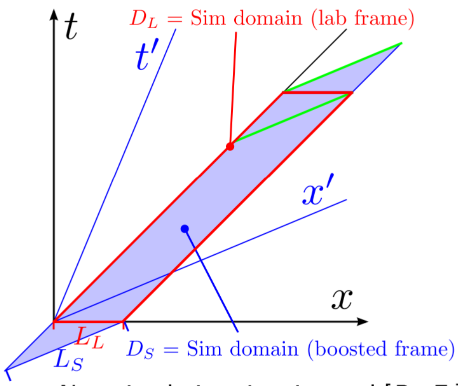
- Solution: Do simulations in a Lorentz-boosted inertial frame moving with velocity β and relativistic factor γ



- Laser wavelength increases, plasma length decreases
- Promises speedup of 10 - 10^6
- Boosted frame module for H-VLPL3D with automatic initialization and back-transform

J.-L. Vay, PRL ***98****, 130405 (2007)*

Boosted frame geometry

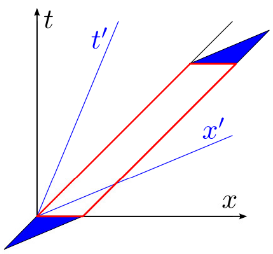


Conventional simulation defined by:
Lab frame Box length L_L, Lab frame simulation time T_L, moving window with $v_{MW} = c$.

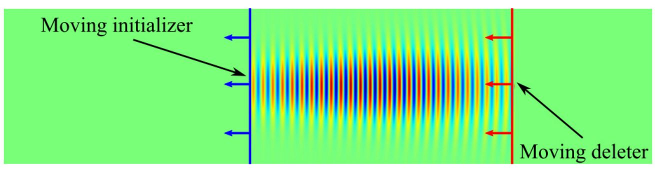
Space-time set D_S covered by boosted frame simulation must contain the lab-frame set D_L
Consequence:
Box length in boosted frame
$L_S = \gamma(1+\beta) L_L$

New simulation time interval: $[B_s, E_s] = [-\gamma\beta L_L, T_L/\gamma(1+\beta)]$
Effect: Box content gets stretched $\Rightarrow \Delta x, \Delta t$ step size larger by $\gamma(1+\beta)$
$\Rightarrow$ Speedup of $\gamma^2(1+\beta)^2$

"Moving window" initialization

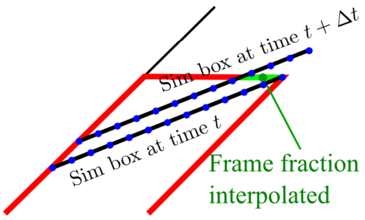


- Problem: Simulating the blue 'wedges' reduces speedup
- Solution: 'Frozen' region in simulation box
- Initialize box content with a backwards-moving plane
- Similarly, delete box content with a second moving plane



Lorentz backtransform

- Problem: How to obtain simulation snapshots in laboratory frame?
- Solution: Assemble the frames piece-by-piece



- Let the frame of interest be located at laboratory frame time t^F
- For each time step interval $[n\Delta t, (n+1)\Delta t]$, find the x positions where the simulation box intersects with the frame
- Get the frame grid points which have passed through the box
- Obtain data by interpolating in space and time

Numerical Cerenkov Instability

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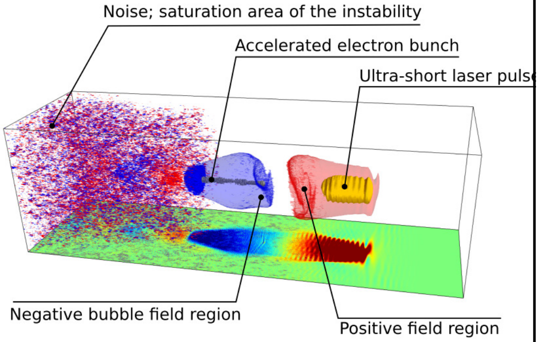
- Full electromagnetic PIC codes cannot simulate relativistic streaming plasmas
  $\rightarrow$ Boosted frame simulations with $\gamma \gtrsim 10$ get destroyed by severe instability



- Instability can be mitigated via filtering and modified solvers

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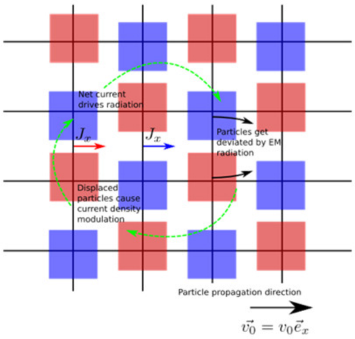
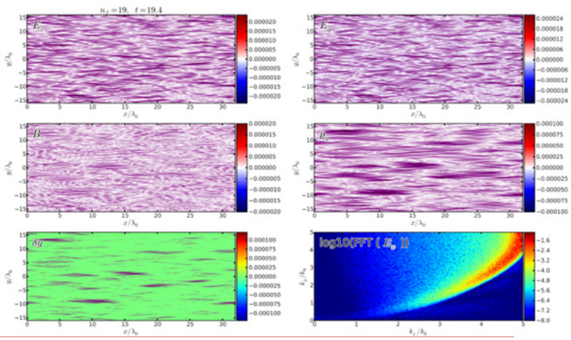
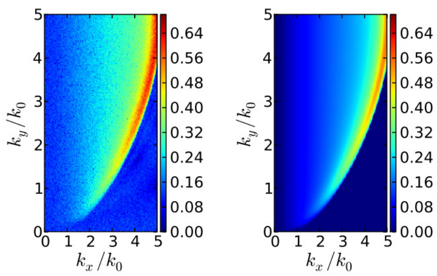
Numerical Cerenkov Instability

- Radiation propagates alongside streaming plasma
  → EM force deviates particles momenta and position
  → net current density drives radiation





Numerical Cerenkov Instability



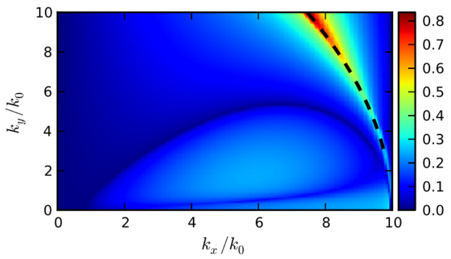
Left: PIC with random perturbation
Right: Analytical growth rate

- Dispersion relation

$$\det(M(\omega, \mathbf{k})) = 0$$

  is 7th order polynomial in $e^{i\omega\Delta t}$
  → numerical solution
- Very good agreement with simulations
- Curve-like area of high growth

Numerical Cerenkov Instability persists even for dispersion-free solvers



Reason:

- Spatial aliasing - interpolation schemes act as signal choppers
- Temporal aliasing - non-resolved frequencies are aliased

$$\omega_{eff} = \pm \left(\sqrt{k_x^2 + k_y^2} - \frac{1}{\Delta t} \right)$$

$\rightarrow$ resonance condition fulfilled

$$k_y\left(k_x\right) = \frac{1}{h}\sqrt{h^2 k_x^2 \left(v_0^2 - 1\right) - 2hk_x v_0^2 + v_0^2}$$

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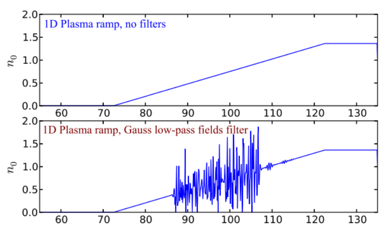
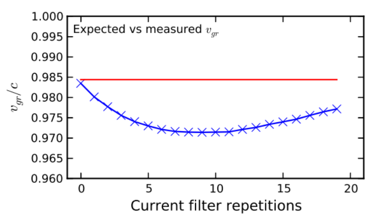
Instability mitigation

- Three possibilities for simple spatial filtering:
  1. filter EM fields periodically
  2. filter the plasma current density
  3. push PIC particle momenta with a filtered copy of the fields

- Fields filtering is dangerous: Cutting low-amplitude plasma oscillations distorts plasma structures
- filtering currents or fields seen by particles reduces pulse group velocity in plasma





- We have designed filters with better frequency separation
- Modified solvers also supress instability (article in preparation)

H-VLPL3D Implementation

A Boosted frame module was implemented into H-VLPL3D

Features:

- Automatic initialization
- Tunable Maxwell solvers
- Filtering
- Moving initializer/deleter
- Versatile particle injection system
- Lorentz back transform

First tests very promising:

- Without any filtering, mm-scale LWFA simulations run 10-20 times faster
- With $\gamma = 10$: 70x speedup

Simulations

- Comparison of scaling laws against Lorentz-boosted PIC simulations shows good match
- Large scale simulations with R_{laser} =80 μm, L_{acc} =40 cm possible
- Tests of scaling laws and simulations of 50 GeV stages running

Movie

Numerical Cerenkov Instability is mitigated by filtering

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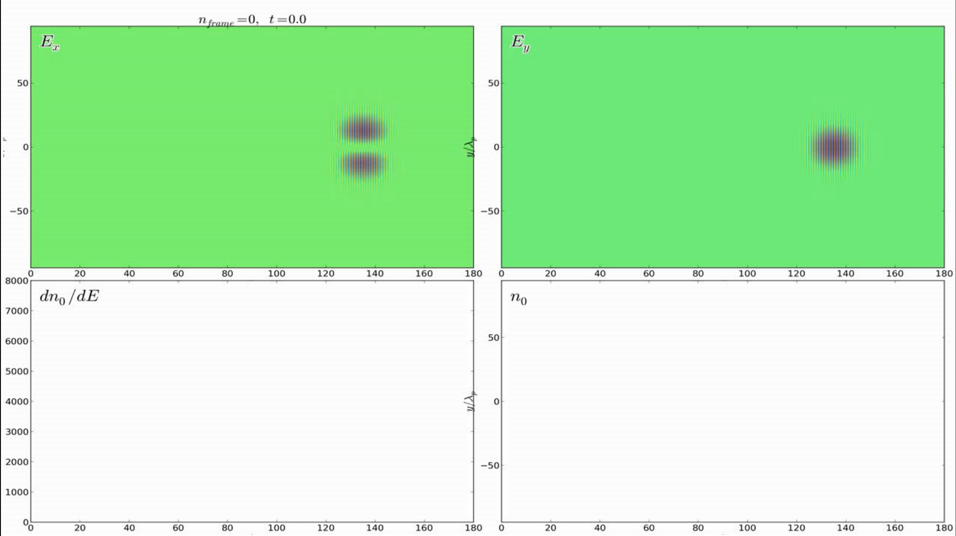

A Pukhov et al. 2014 preprint arXiv:1408.0155, *accepted in PRL*

Electron acceleration in a channel: towards high quality acceleration

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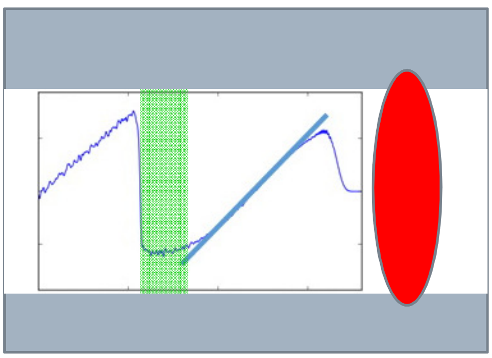

A channel helps to moderate the accelerating field and adjust the laser depletion length

A region of constant accelerating field appears where monoenergetic acceleration is possible

A Pukhov et al. 2014 preprint arXiv:1408.0155, *accepted in PRL*

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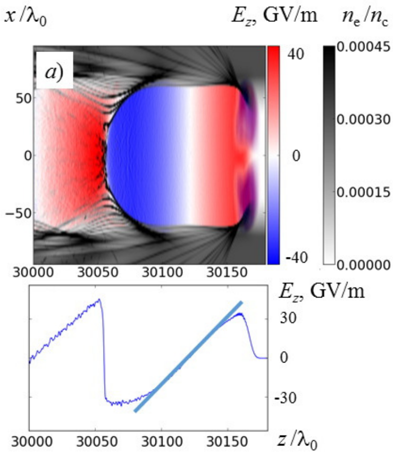
Electron acceleration in a channel: towards high quality acceleration



3D PIC simulation
in a Lorentz-boosted frame

Energy gain: 24 GeV

Laser pulse: 140 J, 16 fs
Plasma: 3×10^{17} $1/cm^3$.

Acceleration distance: 100 cm

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A Pukhov et al. 2014 preprint arXiv:1408.0155, *accepted in PRL*

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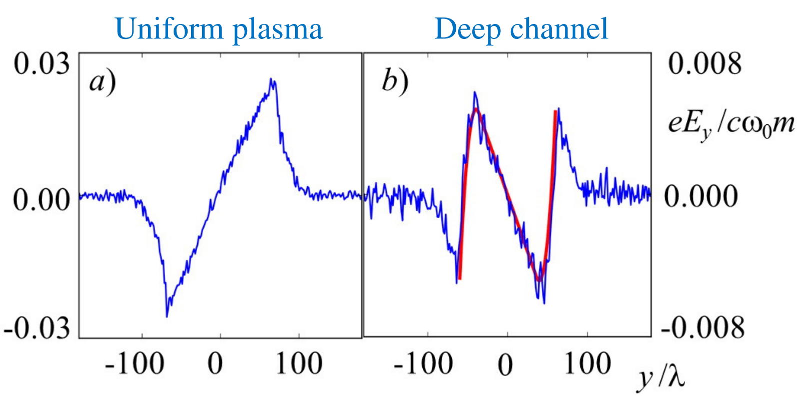
Electron acceleration in a channel: Field Reversed Bubble

The transverse electric field reverses



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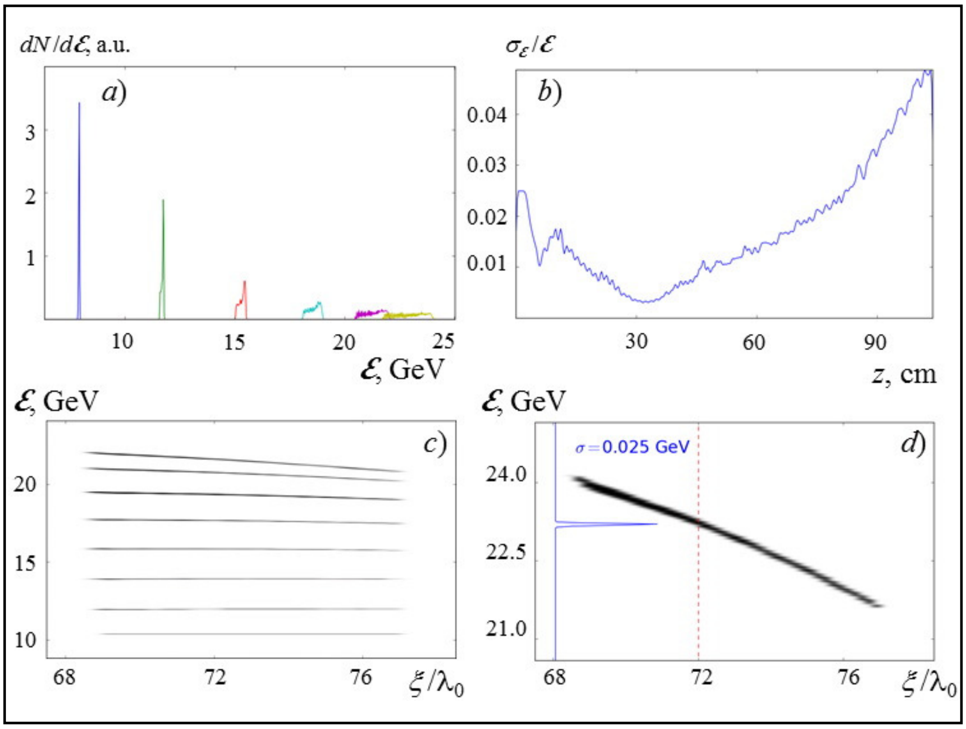

Analytical methods to bridge the scales gap

First-principles PIC codes are universal but computationally expensive. Efficient analytical methods exist to handle the multi-scale problems.

1. Envelope approximation for the laser removes the laser wavelength λ scale

2. Quasi-static approximation explicitly separates the fast coordinate $\zeta = z - ct$ and the slow evolution time $\tau = t$

Any approximation means some physics is neglected though…

Envelope approximation for the laser

When the laser pulse amplitude changes slowly on the laser wavelength scale, the envelope approximation can be used

$$\left[\frac{2}{c}\frac{\partial}{\partial t}\left(ik_0+\frac{\partial}{\partial\varsigma}\right)+\nabla^2\right]\mathbf{A}_L=\frac{4\pi q^2}{mc^2}\left\langle\frac{n}{\gamma}\right\rangle\mathbf{A}_L$$

This approximation excludes, e.g. sharp fronts of laser pulses.

Particle motion in ponderomotive approximation

The laser pulse acts on particles then via its ponderomotive force only

$$\frac{d\mathbf{p}}{dt}=q\left[\mathbf{E}+\frac{\mathbf{p}}{mc\gamma}\times\mathbf{B}\right]-\frac{q^2}{2\gamma m}\nabla|A_L|^2$$

This approximation works only when the particle excursion length is smaller than the laser pulse focal spot.

D.F.Gordon et al. IEEE TPS **28**, 1224 (2000)

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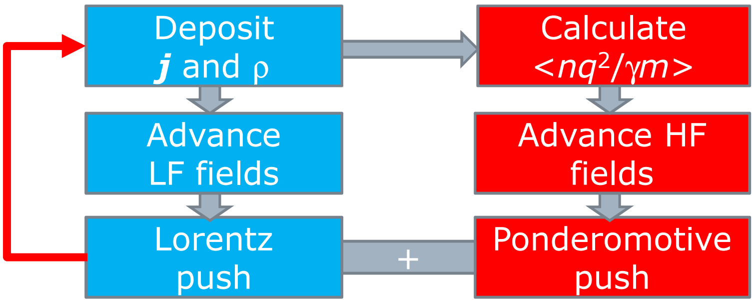
Ponderomotive guiding center PIC

Fields are separated in low frequency and high frequency components. The LF is treated by standard PIC, the HF is treated in envelope approximation



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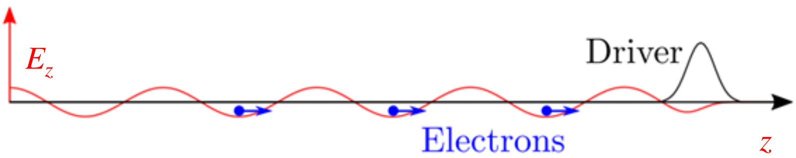
Quasi-static approximation



We separate the fast coordinate $\zeta=z-ct$ and the slow evolution time $\tau=t$.

$$\frac{\partial}{\partial t} << \frac{\partial}{\partial \zeta}$$

It is assumed that the driver does not change during the time it passes its own length

Quasi-static approximation
Integral of motion

Particles have an additional integral of motion in the QS approximation:

$$H = \gamma - p_z + q\psi = 1$$

Where the wake potential is $\psi = \varphi - A_z$

and we use the axial gauge $\varphi = -A_z = \psi / 2$

so that

$$\frac{d\varsigma}{dt} = v_z - 1 = -\frac{1 - q\psi}{\gamma}$$

Quasi-static approximation
Field equations

We change variables to the fast coordinate $\zeta = z - ct$ and the slow evolution time $\tau = t$ in Maxweel Eqs.:

and neglect the time derivatives ∂_τ in (1) and (2), so that

$$\partial_t = -\partial_\xi$$

$$\nabla \times B = j + \partial_t E \quad (1)$$

$$\nabla \times E = -\partial_t B \quad (2)$$

$$\nabla \cdot B = 0 \quad (3)$$

$$\nabla \cdot E = \rho \quad (4)$$

Thus, the quasi-static approximation cannot treat radiation anymore!

Quasi-static approximation
Field equations

It is possible to write the quasi-static equations on the fields only (K.V.Lotov 2007):

$$\nabla_\perp^2 \mathbf{E}_\perp = \nabla_\perp \rho - \nabla_\parallel \mathbf{j}_\perp \qquad \nabla_\perp^2 E_\parallel = \nabla_\perp \cdot \mathbf{j}_\perp$$

$$\nabla_\perp^2 \mathbf{B} = -\nabla \times \mathbf{j}$$

Alternatively, one can use potentials.

In all cases, the quasi-static equations are not local anymore in the transverse planes. This is the result of removing the wave behavior. Instead of the wave equation, we obtain a set of elliptic equations on the fields.

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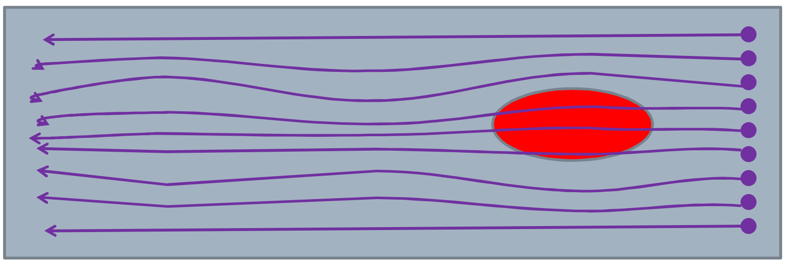
Pushing particles

In quasi-static codes, one seeds a single layer of particles at the leading edge of the simulation box and pushes them through the driver



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Quasi-static approximation
Equations of motion

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We push the particles along the ζ coordinate

$$\frac{d\mathbf{p}}{dt}=\frac{d\mathbf{p}}{d\varsigma}\frac{d\varsigma}{dt}=\left(v_z-1\right)\frac{d\mathbf{p}}{d\varsigma} \qquad \mathbf{v}=\frac{d\mathbf{r}}{dt}=\frac{d\mathbf{r}}{d\varsigma}\frac{d\varsigma}{dt}=\left(v_z-1\right)\frac{d\mathbf{r}}{d\varsigma}$$

so that

$$\frac{d\mathbf{p}}{d\varsigma}=\frac{1}{v_z-1}\left\{q\left[\mathbf{E}+\frac{\mathbf{p}}{mc\gamma}\times\mathbf{B}\right]-\frac{q^2}{\gamma}\nabla|A_L|^2\right\}$$

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Quasi Static Simulation Code WAKE

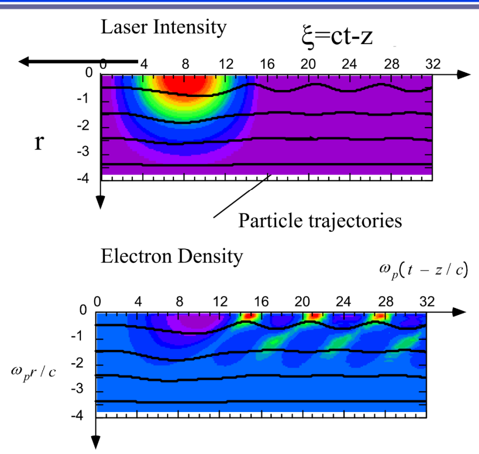
P. Mora and T. M. Antonsen Jr. - Phys Plasma 4, 217 (1997)

Two Time Scales
1. "fast time"
   $t \sim T_D \sim \omega_p^{-1}$

particle trajectories and wake fields determined

2. "slow time"

laser pulse evolves
diffraction
self-focusing
depletion



Compare quasi-static qs-VLPL3D vs explicit VLPL3D

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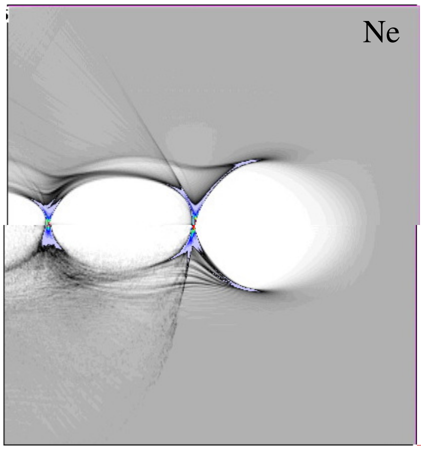

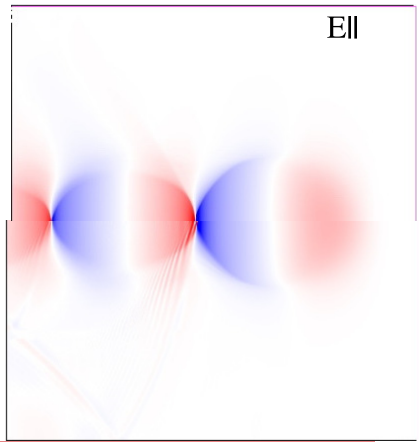

Example
Compare quasi-static VLPL3D vs explicit

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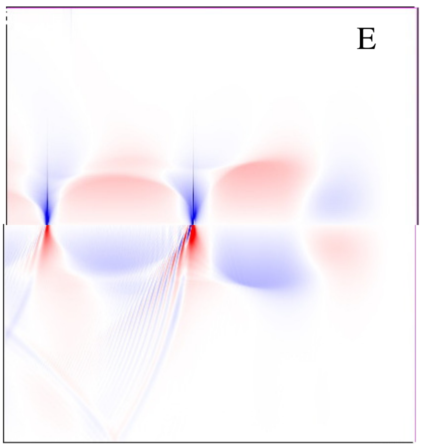
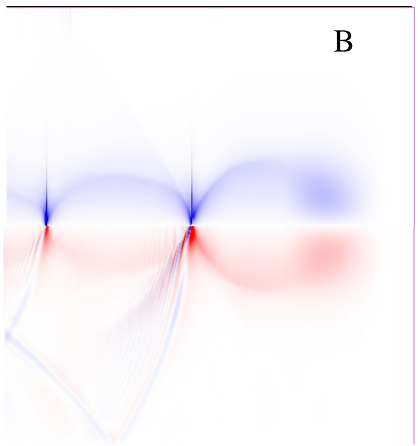




Efficiency of the PIC codes

Explicit PIC effort (number of operations): $N_{op} = N_\tau N_x N_y N_z$

$$\tau << \lambda_0 / c,\ \ h_x << \lambda_0,\ \ h_y, h_z << \lambda_p$$

Lorentz-boost: relativistic gain up to γ^2

Quasi-static codes $\tau << \lambda_p^2 / c\lambda_0,\ \ h_x << \lambda_p,\ \ h_y, h_z << \lambda_p$

gain in performance as $(\lambda_p / \lambda_0)^3$

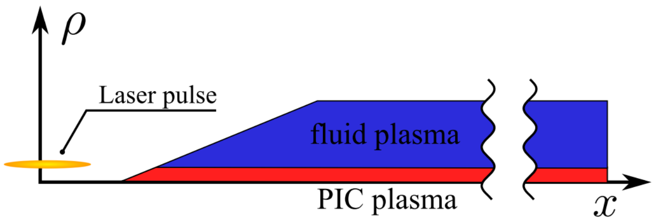
Hybrid PIC/hydro codes

The kinetic PIC description is rather expensive

Alternative: Computational Fluid Dynamics (CFD)
- Euler's equations, Navier-Stokes equations or variants are solved on a grid
- Very established field of research - large number of solvers available
- Faster and more efficient
- Less physics: cannot e.g. model wave breaking

Introduction - Hybrid methods

- Limitations of the PIC method: Stability conditions, noise, interpolation errors
- PIC/Fluid hybrid methods combine advantages of both concepts



- Optimized numerical algorithms for different parts of plasma

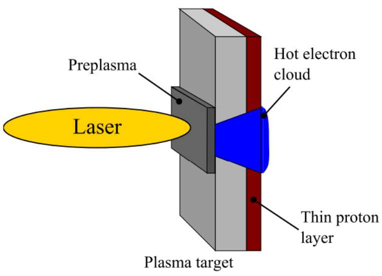
Tuckmantel et al., IEEE TPS **38** (2012)

Hybrid code for high density plasmas

- Problem: High plasma density→ high plasma frequency; stability condition

$$\Delta t \leq \frac{2}{\omega_p}$$

makes PIC simulations inefficient



- Example: Target Normal Sheath Acceleration (TNSA), Simulation difficult because of high density
- Solution: Hybrid code with linearized fluid model.
PIC method for hot, thin plasma; fluid algorithm for cold, dense part

Tuckmantel et al., IEEE TPS **38** (2012)

Hybrid code for high density plasmas

Physical model

Linearized fluid model

$$\begin{aligned} \frac{\partial}{\partial t}\mathbf{E} &= \nabla\times\mathbf{B} - \mathbf{J}^{PIC} - \frac{n_h e}{\gamma_h}\mathbf{p}_h \\ \frac{\partial}{\partial t}\mathbf{B} &= -\nabla\times\mathbf{E} \\ \frac{\partial}{\partial t}\mathbf{p}_h &= e\mathbf{E} \end{aligned}$$

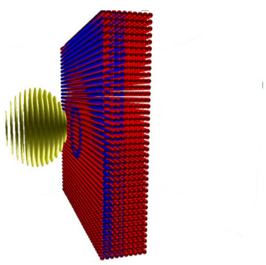
Numerical algorithm

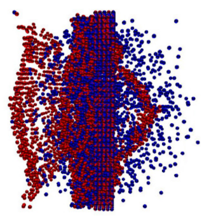
Exponential integrator

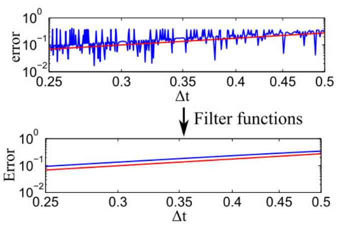
$$\begin{aligned} \mathbf{B}^{n+\frac{1}{2}} &= \mathbf{B}^n - \frac{1}{2}\Delta t\tilde{\nabla}\times\mathrm{sinc}(\frac{\Delta t}{2}\omega_p^n)\mathbf{E}^n \\ \mathbf{E}^+ &= \mathbf{E}^n + \frac{1}{2}\Delta t\,\mathrm{sinc}(\frac{\Delta t}{2}\omega_p^n)\tilde{\nabla}\times\mathbf{B}^{n+\frac{1}{2}} \\ \begin{bmatrix}\mathbf{p}_h^{n+1}\\ \mathbf{E}'\end{bmatrix} &= \begin{bmatrix}\cos\Delta t\omega_h & \Delta t\,\mathrm{sinc}\\ -\omega_h\sin\Delta t\omega_h & \cos\Delta t\omega_h\end{bmatrix}\begin{bmatrix}\mathbf{p}_h^n\\ \mathbf{E}^+\end{bmatrix} \\ \mathbf{E}^{n+1} &= \mathbf{E}' + \frac{1}{2}\Delta t\,\mathrm{sinc}(\frac{\Delta t}{2}\omega_p^n)\tilde{\nabla}\times\mathbf{B}^{n+\frac{1}{2}} \\ \mathbf{B}^{n+1} &= \mathbf{B}^{n+\frac{1}{2}} - \frac{1}{2}\Delta t\tilde{\nabla}\times\mathrm{sinc}(\frac{\Delta t}{2}\omega_p^n)\mathbf{E}^{n+1} \end{aligned}$$

- Mollified impulse method: Three component operator splitting
- Oscillation step for $\mathbf{p}_h^{n+1}, \mathbf{E}$.
- Filtering prevents resonance effects. Second order accuracy, independent of plasma frequency ω_p.

Results







- 2nd order accuracy was numerically shown
- Code was successfully tested on the TNSA scenario

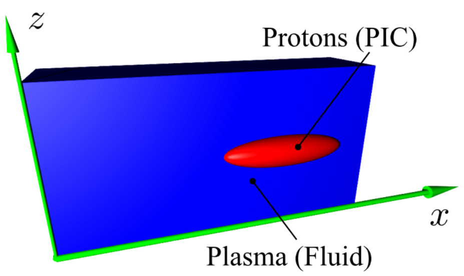
PWFA via self-modulating proton bunches

www.cern.ch/awake

- Idea: Use proton bunches from Super Proton Synchrotron (SPS, CERN) for wake field acceleration
- Bunch is long ($\sigma \approx$12 cm), but self-modulates
  - Problem: Simulation must model 500 plasma oscillations and large propagation lengths
  - Particle-in-Cell simulations very difficult due to interpolation errors and noise

New PIC/Fluid hybrid code H-VLPL3D

- Solution: PIC/Fluid hybridcode
- Fast fluid algorithms with less noise and damping possible
- Can simulate hundreds of plasma oscillations with small losses
- Implementation: Hybrid-Virtual Laser Plasma Lab (H-VLPL3D)-Code



T Tückmantel, A Pukhov Journal of Computational Physics 269, 168-180 (2014)

H-VLPL3D Concept

Cold fluid model for background plasma
Field equations:

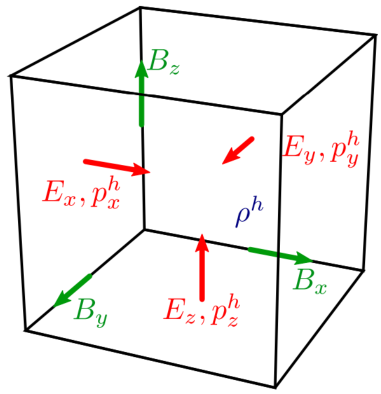
$$\frac{\partial}{\partial t}\mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}^{PIC} - \frac{q}{\gamma^h}\rho^h \mathbf{p}^h$$

$$\frac{\partial}{\partial t}\mathbf{B} = -\nabla \times \mathbf{E}$$

$$\frac{\partial}{\partial t}\mathbf{p}^h = -(\mathbf{v}^h \cdot \nabla)\mathbf{p}^h + q(\mathbf{E} + \mathbf{v}^h \times \mathbf{B})$$

$$\frac{\partial}{\partial t}\rho^h = -\nabla \cdot (\frac{\rho^h}{\gamma^h}\mathbf{p}^h)$$

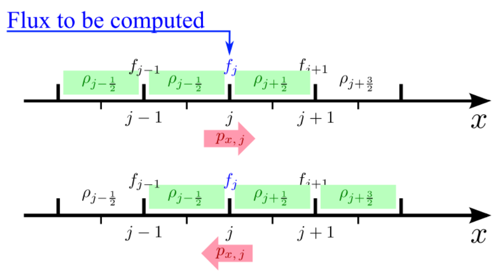
Save interpolations by using staggered grid



T Tückmantel, A Pukhov Journal of Computational Physics 269, 168-180 (2014)

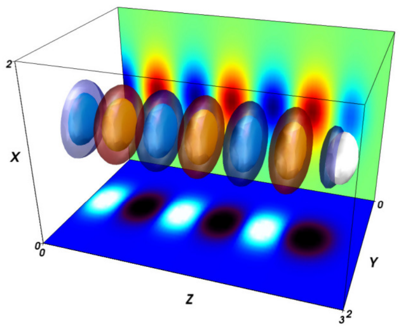
H-VLPL3D fluid integrator

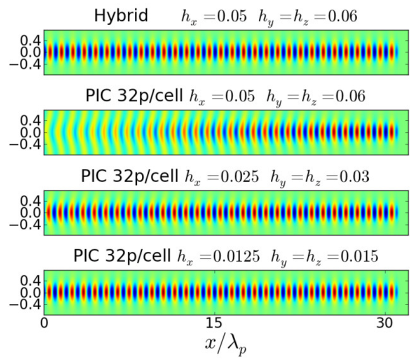
- Finite Volume Method (FVM)
- Long wake fields require accurate ρ^h interpolation: modified QUICK algorithm (3rd order accurate)



- FVM guarantees perfect charge conservation, always satisfying Poisson's equation
- Stable and ripple-free through Flux-Corrected Transport(FCT)

H-VLPL3D test results



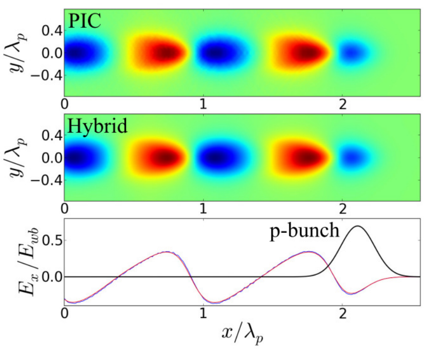


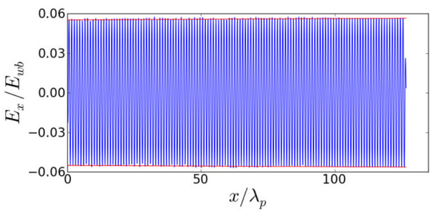
- H-VLPL3D was tested on long p-bunch driven wake fields
- First test: Linear regime

- Comparison of H-VLPL3D hybrid code and PIC for wake field (E_x-Feld)
- PIC needs much higher resolution for same result (CPU time: 250x)

T Tückmantel, A Pukhov Journal of Computational Physics 269, 168-180 (2014)

H-VLPL3D test results





- Comparison in nonlinear regime
- Same result, hybrid code shows less noise

- Unphysical damping of fields makes conventional PIC simulations of SM-PDPWFA difficult
- H-VLPL3D shows very little damping with minimum $1/e$ length $\sim 750\lambda_p$.

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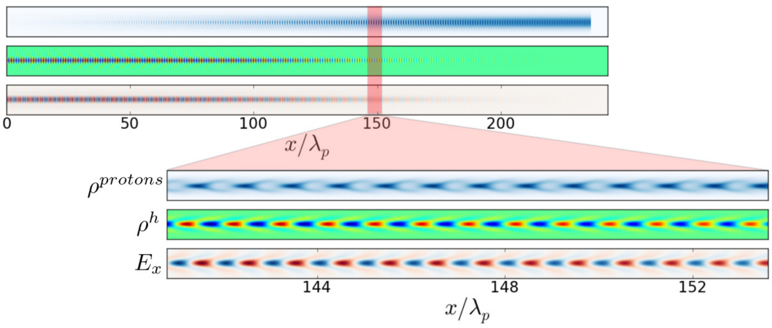
Simulation of long p-bunches

- 450 GeV proton bunch from Super Proton Synchrotron (SPS) was simulated with H-VLPL3D
- Protons (PIC) propagate through plasma (fluid)
- Wake fields cause a modulation of the bunch, further amplifying the fields



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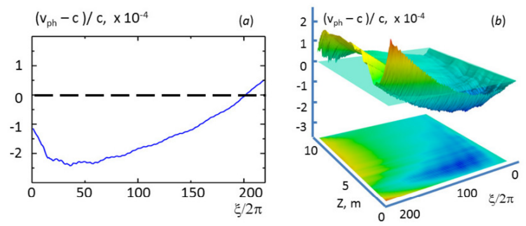
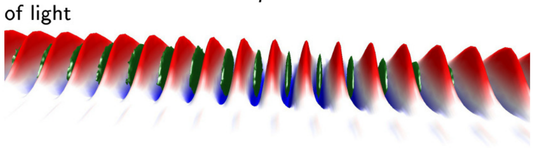
Phase velocity control



Wake field phase velocity v_{ph}; cyan surface shows speed of light



3D visualization of injected electrons

- New approach: Control v_{ph} via plasma density gradients
- Offers possibility to optimize phases of injected particles
- Multi-staged test particle simulations of side injection promising: Electrons get drawn into accelerating phases

Pukhov, A., Kumar, N., Tückmantel, T., et al., PRL ***107*** *(2011) 145003.*

Summary

- PIC codes are the established tools for plasma simulation
- Lorentz boost can bridge the gap of scales in plasma acceleration still keeping the first principles. Unfortunately, it is subject to numerical instabilities.
- Quasi-static codes use analytic approaches to separate the scales
- Hybrid hydro-PIC codes help to improve the numerical dispersion and stability