Laser plasma acceleration simulations with new code AGASTHII

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Plan of talk

- Development of Particle in Cell (PIC) code AGASTHII

  --- Why one more PIC code?

  --- General PIC method

  --- Code details

  --- Analytical / Simulation Benchmarks

- Future Work

List of parallel 3D EM-PIC codes world wide

Name	Developer	Source code
VORPAL	Tech-X	closed
OSIRIS	UCLA group	via collaboration
VLPL	A Pukhov	via collaboration
ALaDyn	C Benedetti	open
EPOCH	T Arber	via collaboration
PICCANTE	A Sgattoni	open
PICPSI3D	K Patel	via collaboration

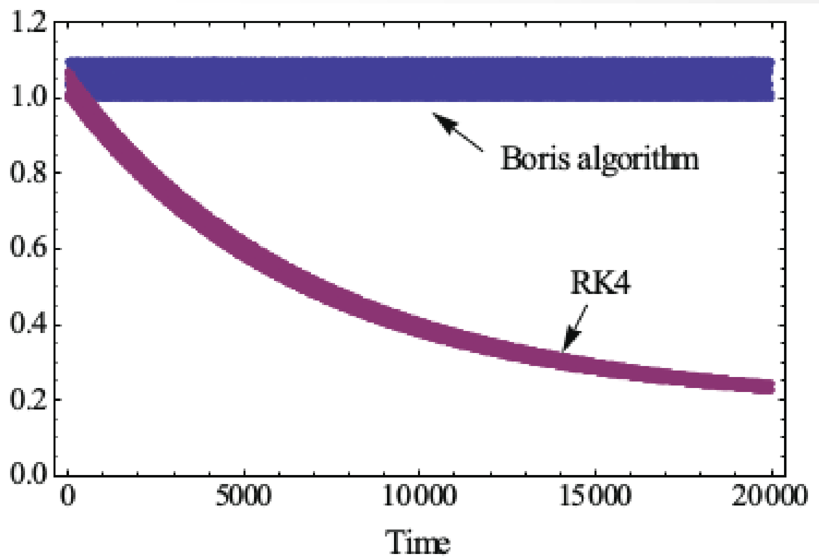
Why reinvent the wheel?

- Modification or addition of extra feature to a close source code is really difficult and sometimes impossible.
- Modification or addition of extra features to a open source code is also difficult unless you know the codes structural and implementations details.
- You do not want to use any code as a black box.

EM-PIC code AGASTHII

Advance General-purpose Accelerator Simulation Toolkit for High Intensity Interaction

- Fully relativistic electromagnetic PIC code – benchmarked with WARP and VORPAL.
- Written in C++ object oriented style.
- 2.5 Dimensional simulation.
- Maxwell equations are solved using FDTD .
- Relativistic Boris algorithm for particle motion.
- Eserkepov algorithm for current deposition.
- Moving window.



- Absorbing boundary conditions for fields and particles.
- Field ionization.
- Run time plotting using Mathgl.
- Parallel simulation on multi-core CPU using OPENMP.
- Conventional Beam transport using matrix approach – benchmarked with TRACEWIN

Particle In Cell (PIC) simulation method

- Developed for weakly coupled system.
- Uses the concept of 'macro' or 'super' or 'computer' particle.
- Works because Lorentz force depends on e/m and not just on e!!!
- Maxwell equations are solved on discrete grid using FDTD or spectral solver.
- Allows statistical representation of general distribution functions in phase space.
- Full nonlinear effects such as space charge and other collective effects can be included.
- The particle treatment allows the incorporation of relativistic effects.
- Parallel algorithm can be implemented.
- Closest to experiments compared to other approaches.

PIC vs Experiment

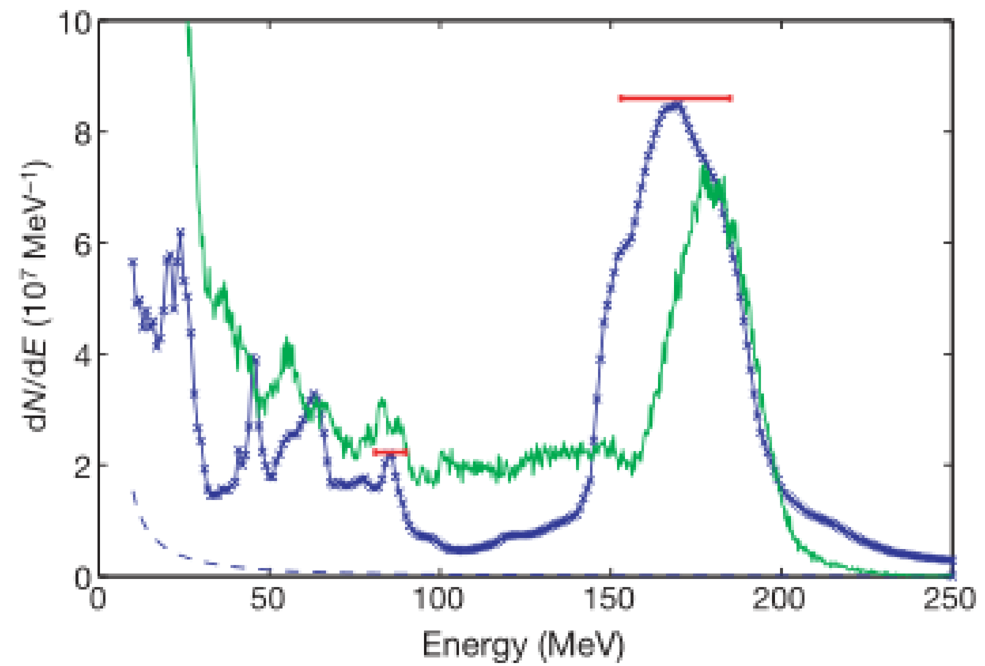


Figure 3 Experimental and simulated electron spectra. Blue line with crosses, electron spectrum corresponding to Fig. 2b, after deconvolution. Dashed line, estimation of the background level. Red horizontal error bars, resolution of the spectrometer. Green line, electron spectrum obtained from 3D PIC simulations. d*N*/d*E* is the number of electrons per MeV (*E* is the electron energy in MeV).

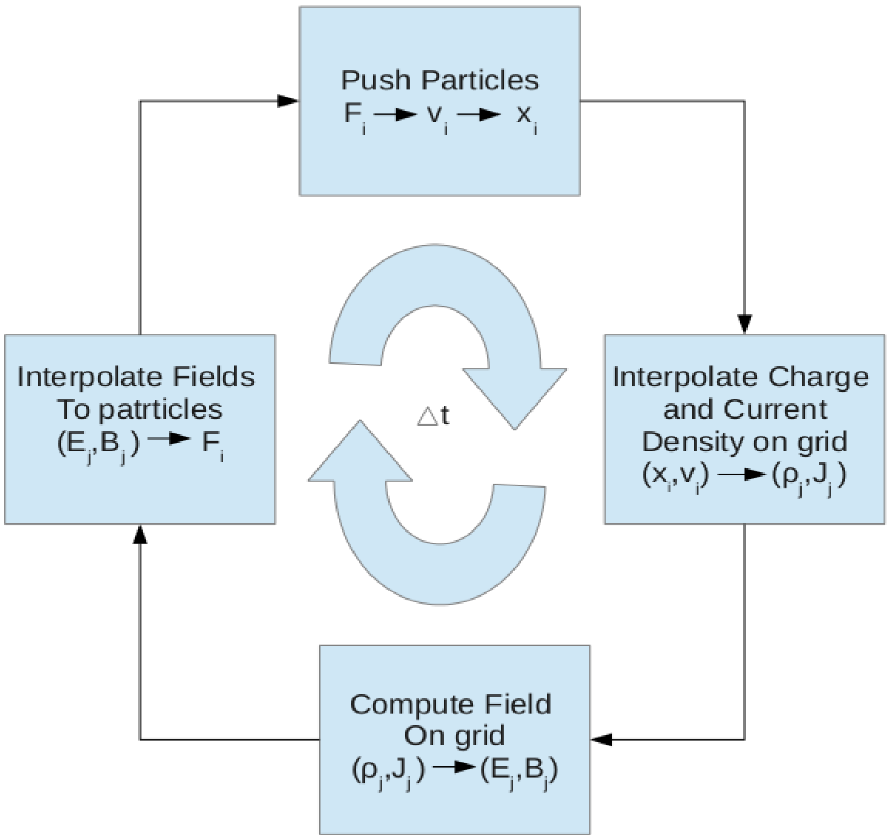
A laser–plasma accelerator producing mono energetic electron beams Letters to Nature 431, 541-544

Electrostatic vs Electromagnetic

- Poisson equation is solved using iterative or FFT base algorithm on grid and particles are push using only the electrostatic field
- No / slowly varying magnetic field
- Self generated magnetic fields are ignored
- Non-relativistic motion
- Low temperature plasmas

- Maxwell curl equations are solved using FDTD or spectral algorithm on grid and particles are push with electromagnetic field
- Slow / fast variation of magnetic field
- Self-consistent fields (external + internal)
- Relativistic motion
- High temperature plasmas

AGASTHII - Particle In Cell (PIC) method flow chart



$$\nabla \cdot \vec{E} = 2\pi\, \rho$$

$$\nabla \cdot \vec{B} = 0$$

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

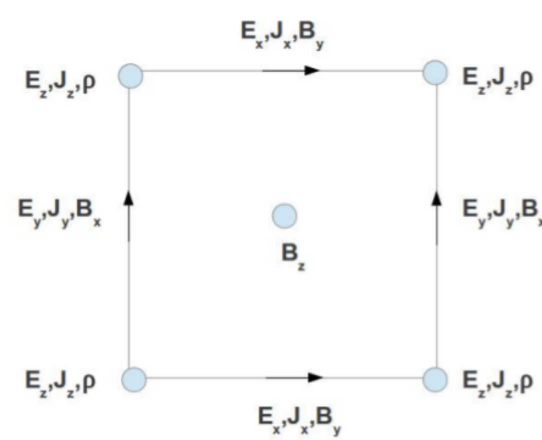
$$\frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{B} - 2\pi \vec{J}$$

$$\frac{d\vec{P}}{dt} = 2\pi \frac{q}{M}(\vec{E} + \vec{v} \times \vec{B})$$

- Smallest length and largest frequency should be well resolved.
- Number of particles per cell should be high.
- Time step should follow Courant limit.
- Some times current/field smoothening is needed

2D Yee mesh discretization for fields

Field quantity	Time location	Space location
E_x, J_x, B_y	$n, n-1/2, n-1/2$	$x+1/2, y$
E_y, J_y, B_x	$n, n-1/2, n-1/2$	$x, y+1/2$
E_z, J_z, ρ	$n, n-1/2, n$	x, y
B_z	$n-1/2$	$x+1/2, y+1/2$



Particle Pusher - Boris algorithm

$$\frac{\mathbf{u}^{t+\Delta t/2} - \mathbf{u}^{t-\Delta t/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}^t + \frac{\mathbf{u}^{t+\Delta t/2} + \mathbf{u}^{t-\Delta t/2}}{2\gamma^t} \times \mathbf{B}^t\right),$$

$$\frac{\mathbf{x}^{t+\Delta t} - \mathbf{x}^t}{\Delta t} = \frac{\mathbf{u}^{t+\Delta t/2}}{\gamma^{t+\Delta t/2}}$$

Half acceleration

$$\mathbf{u}^- = \mathbf{u}^{t-\Delta t/2} + \frac{q\Delta t \mathbf{E}^t}{2m},$$

$$\mathbf{u}' = \mathbf{u}^- + \mathbf{u}^- \times \mathbf{t}^t,$$

Full rotation

$$\mathbf{u}^+ = \mathbf{u}^- + \mathbf{u}' \times \frac{2\mathbf{t}^t}{1 + \mathbf{t}^t \cdot \mathbf{t}^t},$$

Half acceleration

$$\mathbf{u}^{t+\Delta t/2} = \mathbf{u}^+ + \frac{q\Delta t \mathbf{E}^t}{2m}$$

$$\gamma = \sqrt{\frac{1}{1-(v/c)^2}} = \sqrt{1 + \left(\frac{u}{c}\right)^2},$$

$$u = \gamma v.$$

$$\gamma^t = (\gamma^{t-\Delta t/2} + \gamma^{t+\Delta t/2})/2.$$

$$\mathbf{t}^t = \hat{\mathbf{B}} \tan\left(\frac{q\Delta t}{2\gamma^t m} B^t\right)$$

Ref Particle simulation of plasmas: review and advances by J. P. Verboncoeur

Maxwell Solver

Magnetic Field Updater

$$B_{x\,i,j+1/2}^{\,n+1/2} = B_{x\,i,j+1/2}^{\,n-1/2} - \frac{\triangle t}{\triangle y}(E_{z\,i,j+1}^{\,n} - E_{z\,i,j}^{\,n})$$

$$B_{y\,i+1/2,j}^{\,n+1/2} = B_{y\,i+1/2,j}^{\,n-1/2} + \frac{\triangle t}{\triangle x}(E_{z\,i+1,j}^{\,n} - E_{z\,i,j}^{\,n})$$

$$B_{z\,i+1/2,j+1/2}^{\,n+1/2} = B_{z\,i+1/2,j+1/2}^{\,n-1/2} - \frac{\triangle t}{\triangle x}(E_{y\,i+1,j+1/2}^{\,n} - E_{y\,i,j+1/2}^{\,n}) + \frac{\triangle t}{\triangle y}(E_{x\,i+1/2,j+1}^{\,n} - E_{x\,i+1/2,j}^{\,n})$$

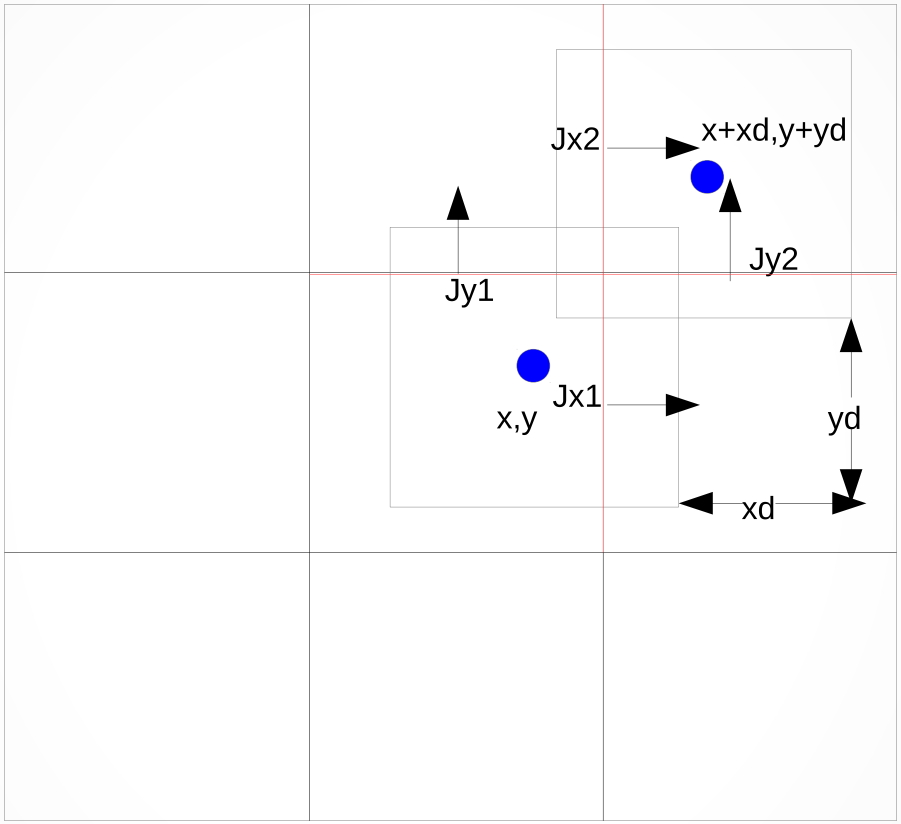
Electric Field Updater

$$E_{x\,i+1/2,j}^{\,n+1} = E_{x\,i+1/2,j}^{\,n} + \frac{\triangle t}{\triangle y}(B_{z\,i+1/2,j+1/2}^{\,n+1/2} - B_{z\,i+1/2,j-1/2}^{\,n+1/2}) - 2\pi J_{x\,i+1/2,j}^{\,n+1/2} \triangle t$$

$$E_{y\,i,j+1/2}^{\,n+1} = E_{y\,i,j+1/2}^{\,n} - \frac{\triangle t}{\triangle x}(B_{z\,i+1/2,j+1/2}^{\,n+1/2} - B_{z\,i-1/2,j+1/2}^{\,n+1/2}) - 2\pi J_{y\,i,j+1/2}^{\,n+1/2} \triangle t$$

$$E_{z\,i,j}^{\,n+1} = E_{z\,i,j}^{\,n} + \frac{\triangle t}{\triangle x}(B_{y\,i+1/2,j}^{\,n+1/2} - B_{y\,i-1/2,j}^{\,n+1/2}) - \frac{\triangle t}{\triangle y}(B_{x\,i,j+1/2}^{\,n+1/2} - B_{x\,i,j-1/2}^{\,n+1/2}) - 2\pi J_{z\,i,j}^{\,n+1/2} \triangle t$$

Current Deposition



$$Jx1 = xd\,(0.5 - y - 0.5yd) \qquad Jy1 = yd\,(0.5 - x - 0.5xd)$$

$$Jx2 = xd\,(0.5 + y + 0.5yd) \qquad Jy2 = yd\,(0.5 + x + 0.5xd)$$

Villasenor, J., and Buneman, O., Computer Physics Communications, 69, 306-316 (1992)

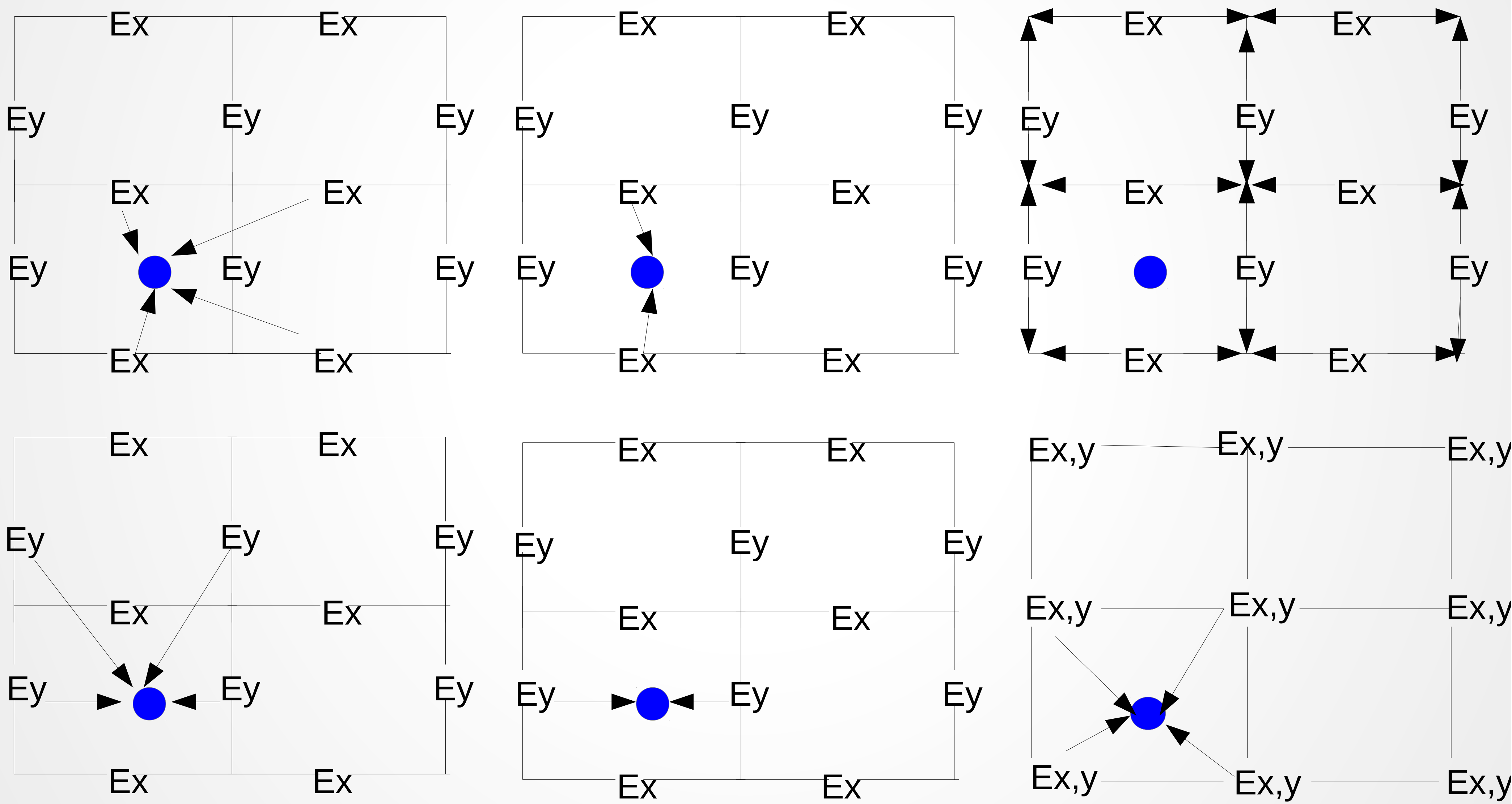
Esirkepov, T. Z., Computer Physics Communications,135,144–153 (2001).

Field interpolation at particle location

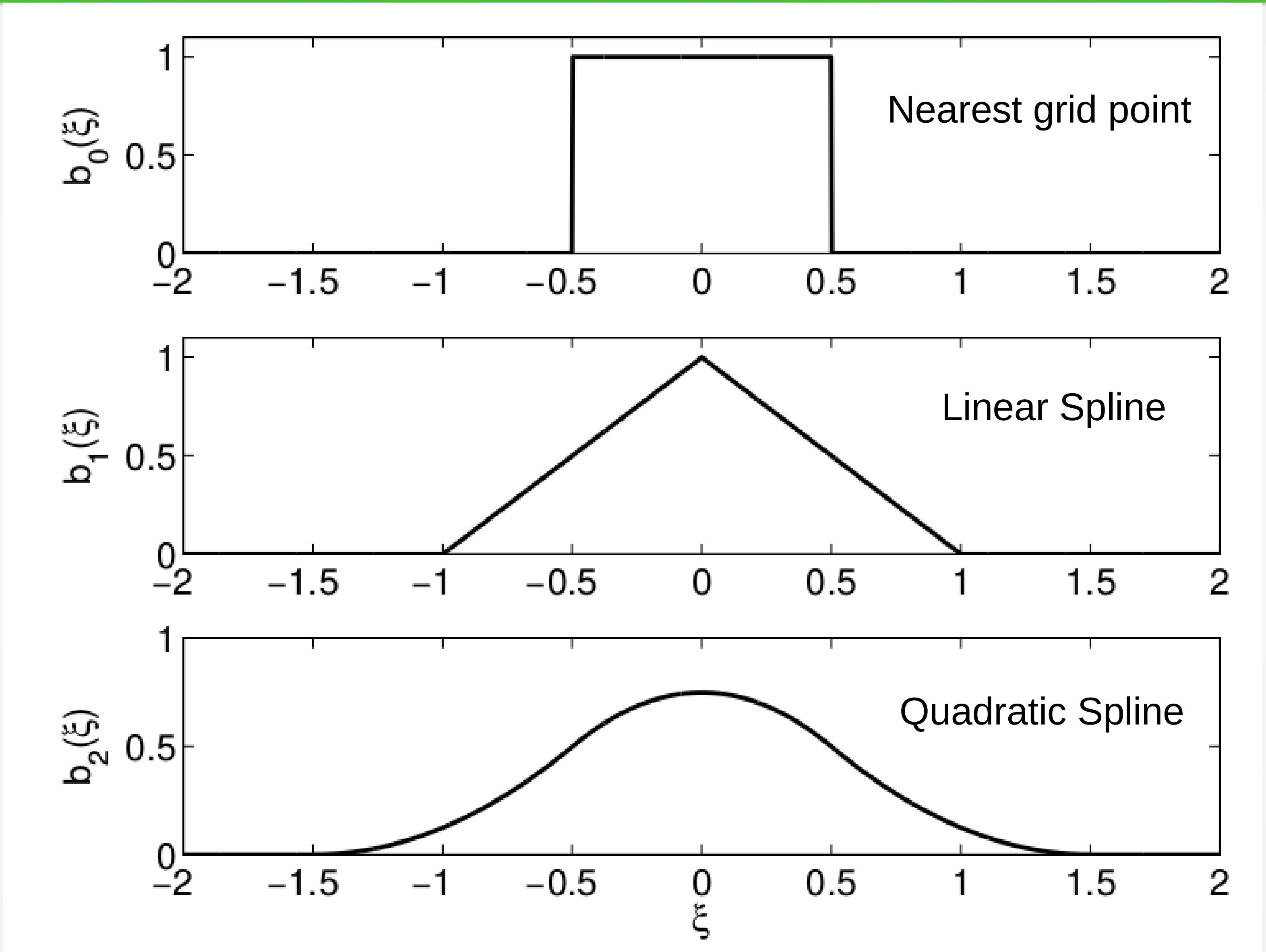
Uniform

Energy conserving

Momentum conserving



Consequence of interpolation : particle shapes



Due to interpolation schemes we dont have point size particles in PIC !

Moving Window for LWFA/PWFA simulations

For a typical 1 GeV controlled acceleration
plasma dimension = 1 cm x 120 μm
If λ = 0.8 μm , dx = $\lambda/32$, dy = $\lambda/4$, particle per cell = 8
nx = 400000 ny = 600
Total Simulation particles = nx*ny*ppc = 192e7
Memory needed for single particle = 5*8 bytes
Total memory needed for particles = 5*8*192e7 / 2^30 = 71 GB !!!!!!!
Time needed to push single particle = 1e-6 s
Total time for pusher = 1920 s = 32 mins
THIS IS ONLY FOR PARTICLES WE HAVE FIELDS ALSO so practically **IMPOSSIBLE**

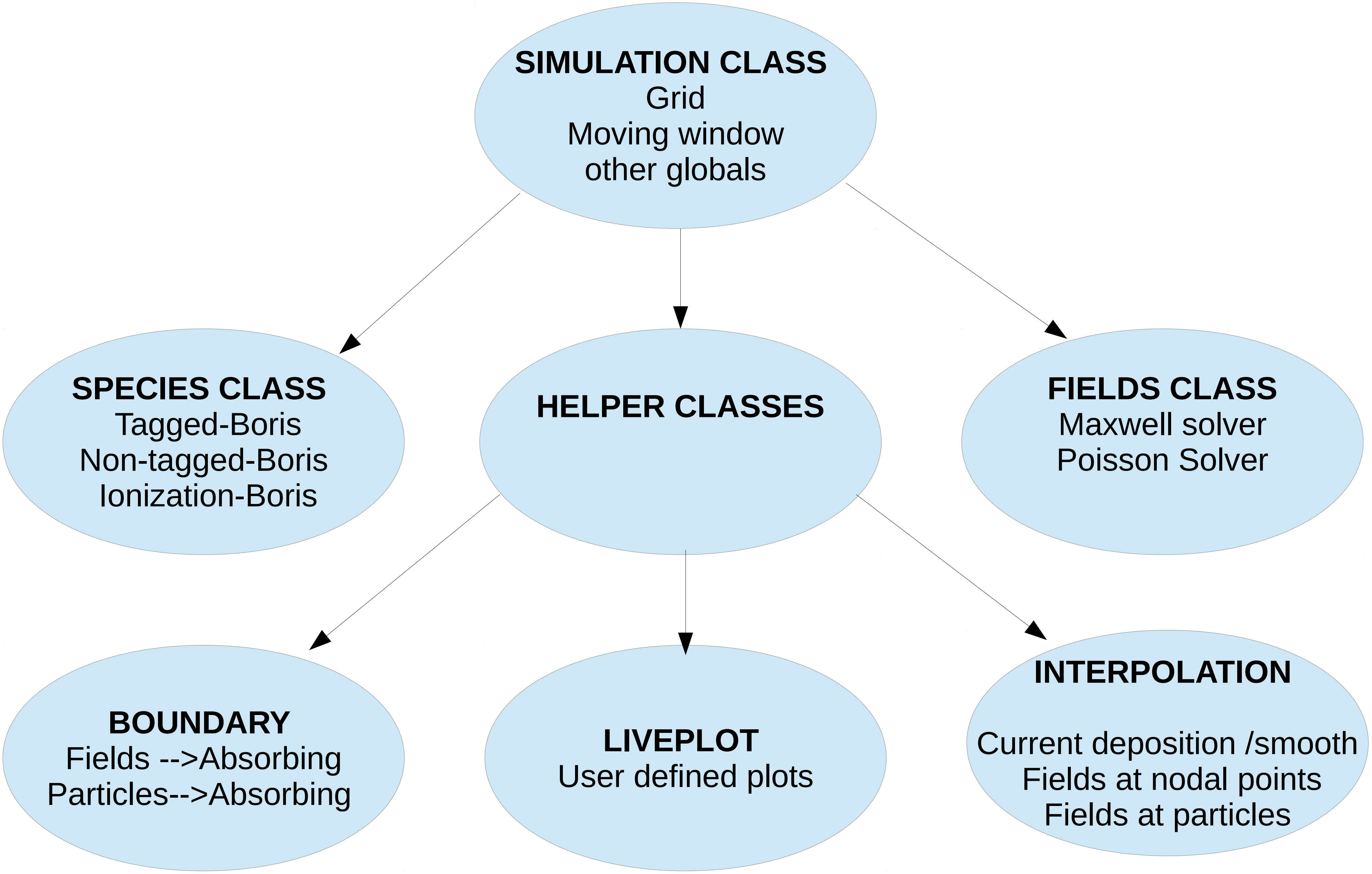
Laser / Beam / Plasma

- Laser pulse can be specified directly inside the simulation box in vacuum by initializing both the laser electric and magnetic field.
- Driver particle beam can specified directly inside the simulation box with arbitrary phase space distribution and charge distribution.
- Speed at which the moving window shifts is based on velocity of driver.
- Plasma can have arbitrary phase space and density distribution.
- Density distribution of the species (plasma / beam) is modeled by giving different weights to the macro particles based on the desired profile.

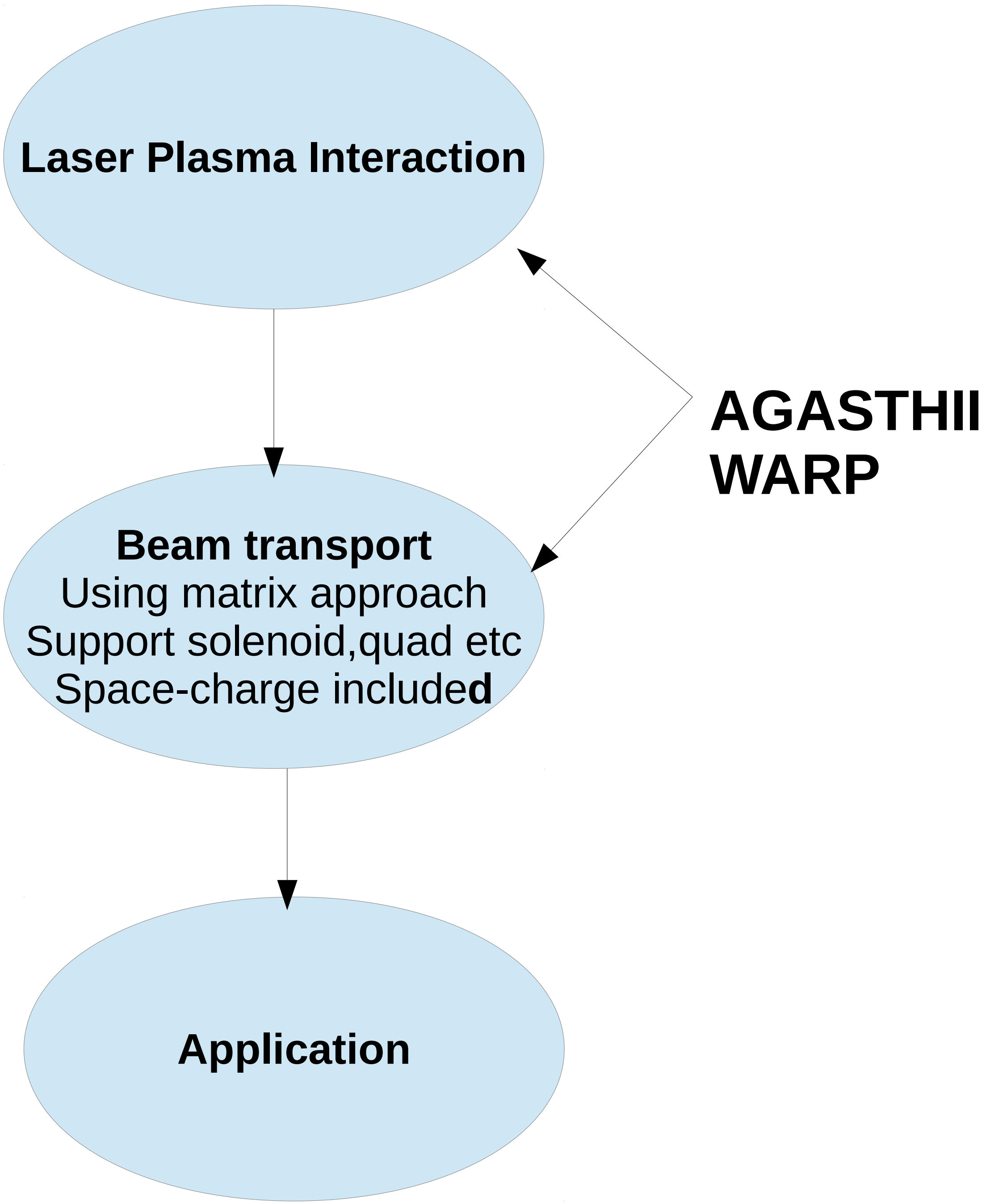
Conventional beam transport module

- Sigma matrix along with individual particles can be tracked.
- Full 6D phase space of the particle can be tracked through different types of focusing elements such as drift, quadrupole, solenoid etc
- Space charge forces are applied using impulse approximation in beam rest frame.
- Space charge can be calculated using any of the following algorithms
  – Linear analytical
  – Iterative Poisson solver
  – Brute force

Code Structure

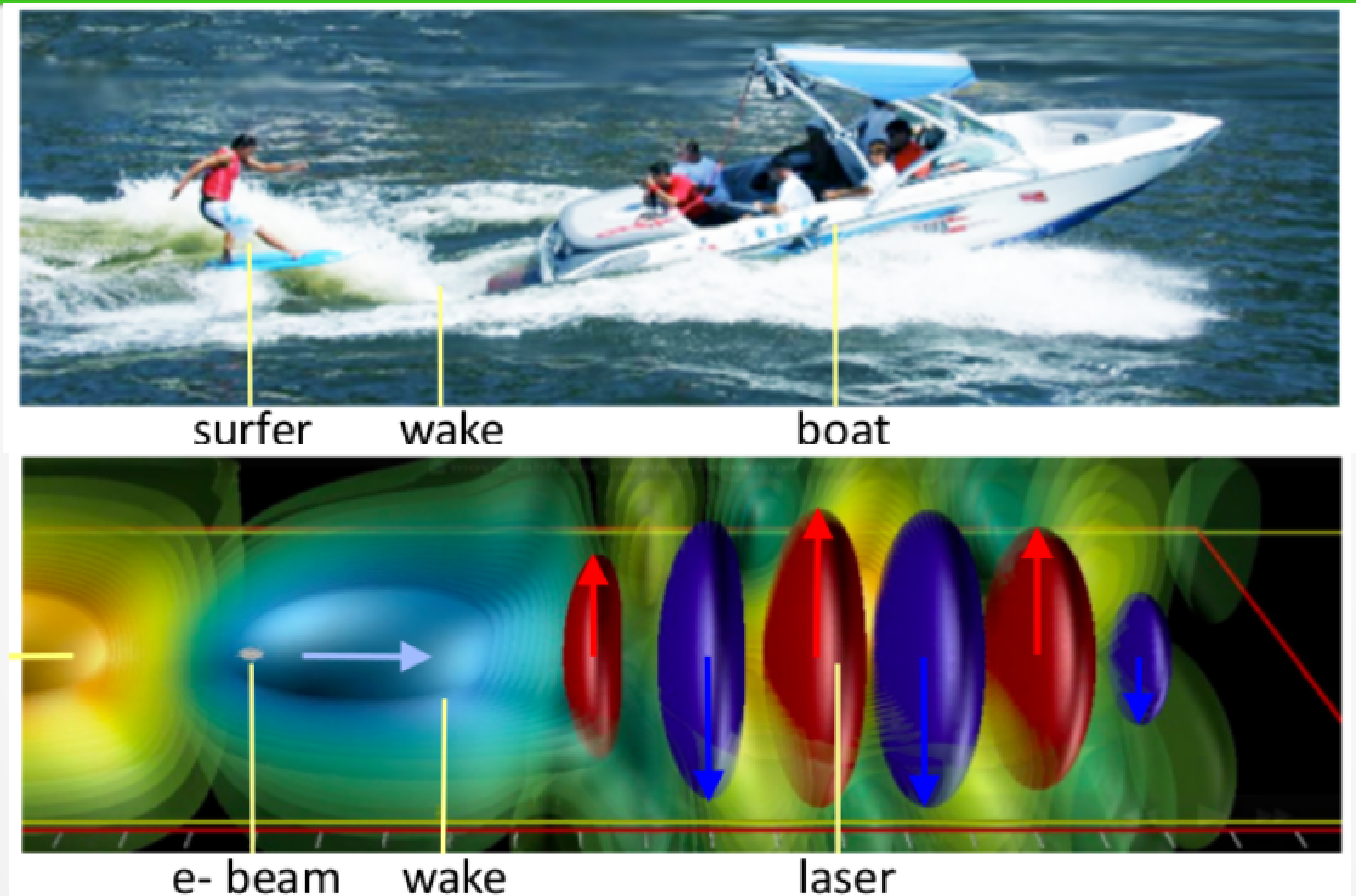


Unique Simulation Feature



Short intro to LWFA

Laser Wake-Field Acceleration (LWFA)



Ref J L Vay PPT

- First proposed by Tajima and Dawson (1979) for a short (< 1ps), high intensity (>10^{17} W/cm^2) laser pulse in under dense plasma $(\lambda/\lambda_p)^2 << 1$
- Wake-Field is most efficient $L \sim \lambda_p$

IMP terms involved in laser-plasma interaction

- **Plasma Density** n_e = *No. electrons/cm*^{3}
- **Debye Length** $\lambda_D = (kT_e/4\pi n_e q_e^2)^{-0.5}$ *cm*
- **Plasma Frequency** $\omega_p = (4\pi n_e q_e^2/m_e)^{0.5}$ *rad/sec*
- **Plasma Wavelength** $\lambda_p = 2\pi c/\omega_p$ μm
- **Laser Strength Parameter** a_0 **:**

$$a_0 = 0.86 \times 10^{-9}\,\lambda(\mu m)\,\mathrm{sqrt}(\,I\,(W/cm^2\,))$$

- **Ponderomotive Force** $F_p = -\nabla I$

– results from the oscillation of the particles in electromagnetic field of laser with spatial or temporal variation in intensity. This force pushes charged particles from high intensity to low intensity region.

Limitations of LWFA

- **Diffraction** length : $Z_R = \pi w_0^2/\lambda$.

- **Depletion** length : $\lambda_{dp} \alpha (\lambda_p^2 / \lambda^2) c\tau_{FWHM}$

- **De-phasing** length : $\lambda_{dph} \alpha \lambda_p^3 / \lambda^2 \alpha n_0^{-3/2}$

Max. Energy = Charge * Peak Electric field * De-phasing length

Electron injection types in LWFA

– **Bubble regime injection**

– **Density transition injection**

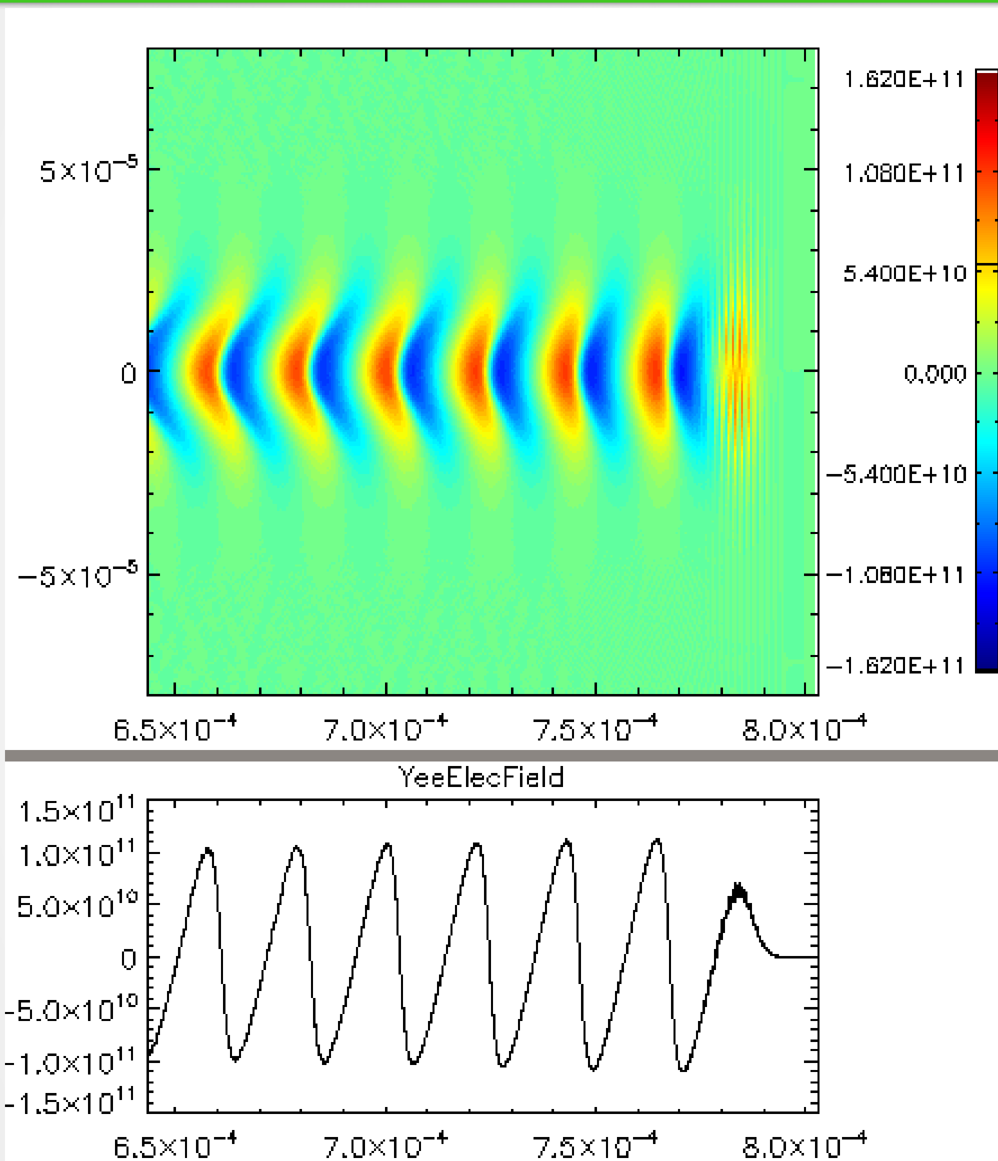
– Other types (External, colliding, ionization induce etc.)

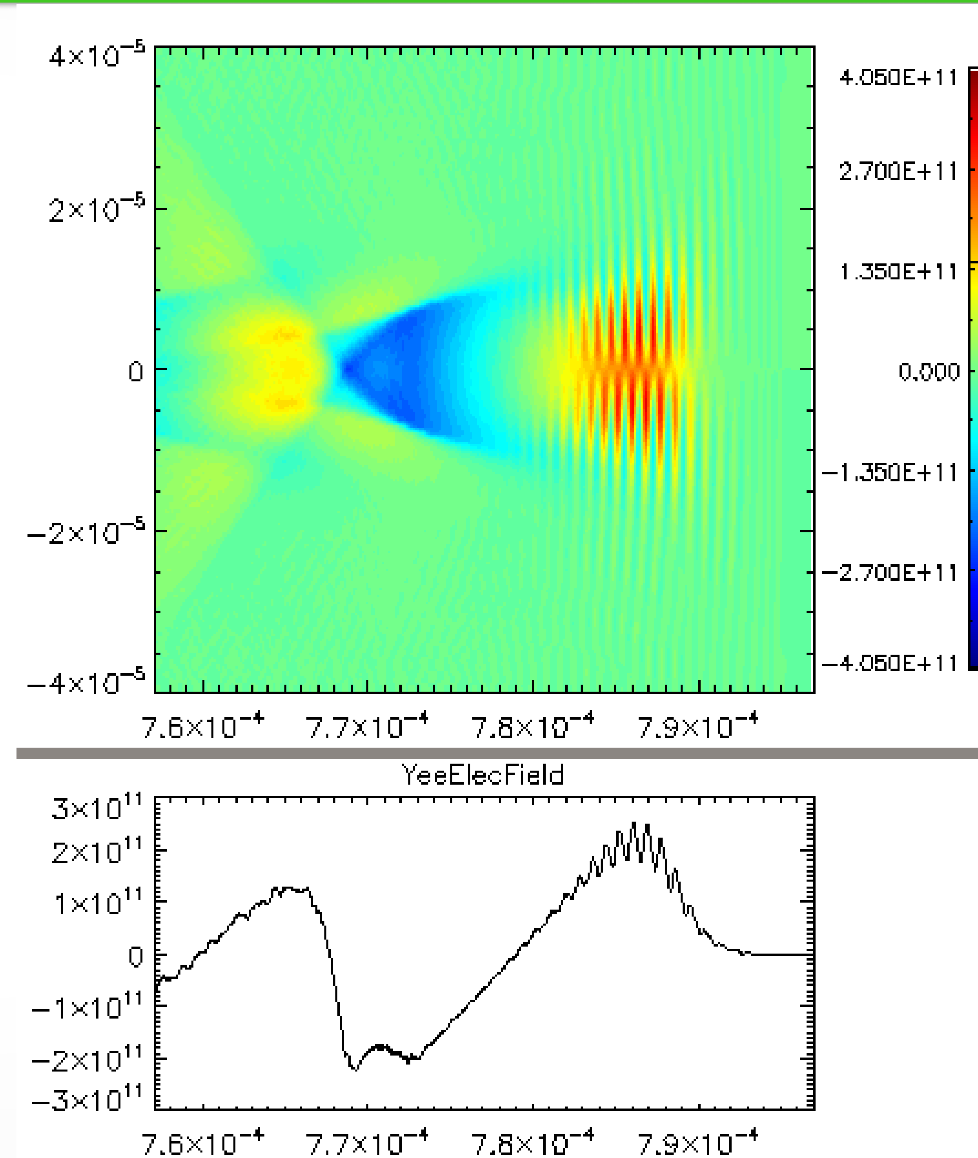
Bubble regime

- High intensity (>10^{18} W/cm^2) laser pulse propagates in under dense plasma, the laser ponder-motive force expels the electrons from the axis, creating a ion cavity like structure free of electrons called as 'Bubble'.
- Small amount of plasma electrons from the background may get trapped in this ion cavity and get accelerated.
- Experimental break throughs :
  – Geddes et al nature 2004.
  – Mangles et al nature 2004.
  – Faure et al in nature 2004.

  – In all electron beam of about 100 MeV energy was obtained

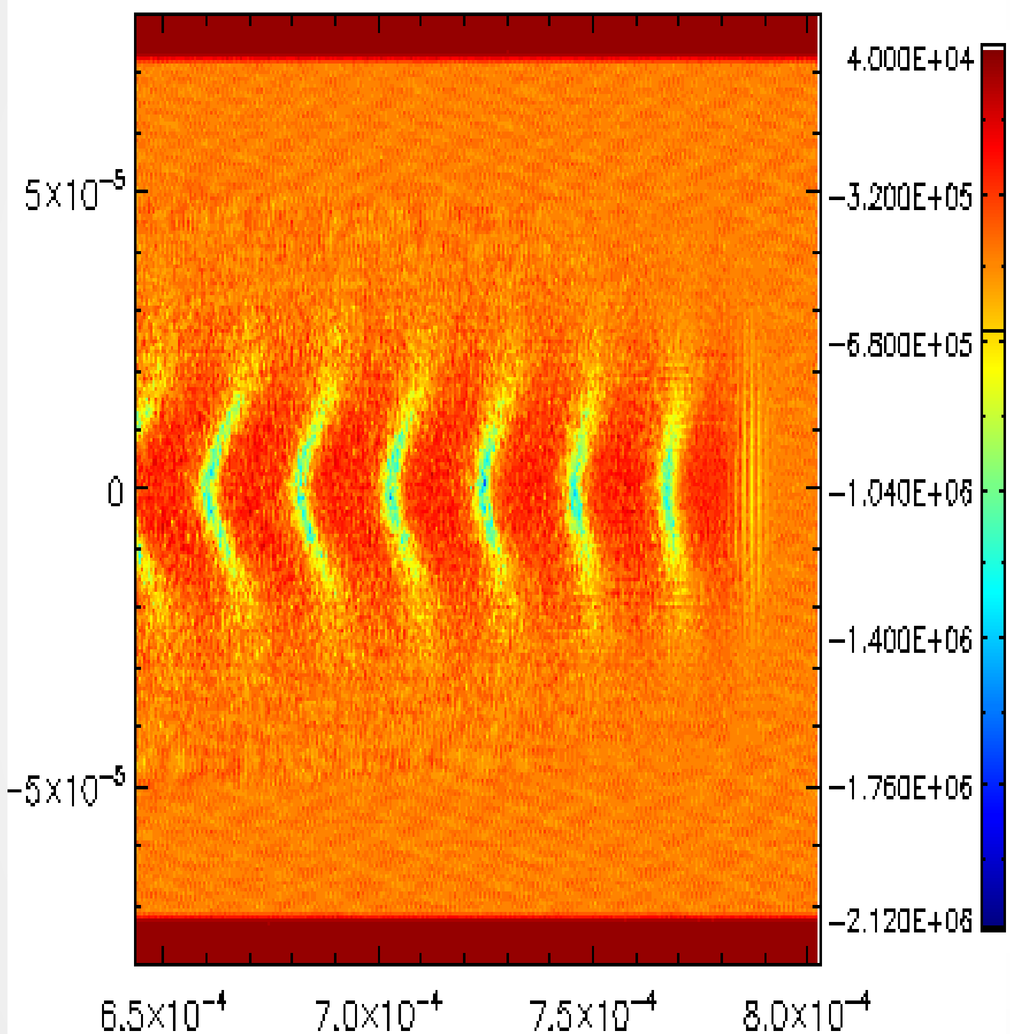
Linear LWFA regime vs Bubble regime

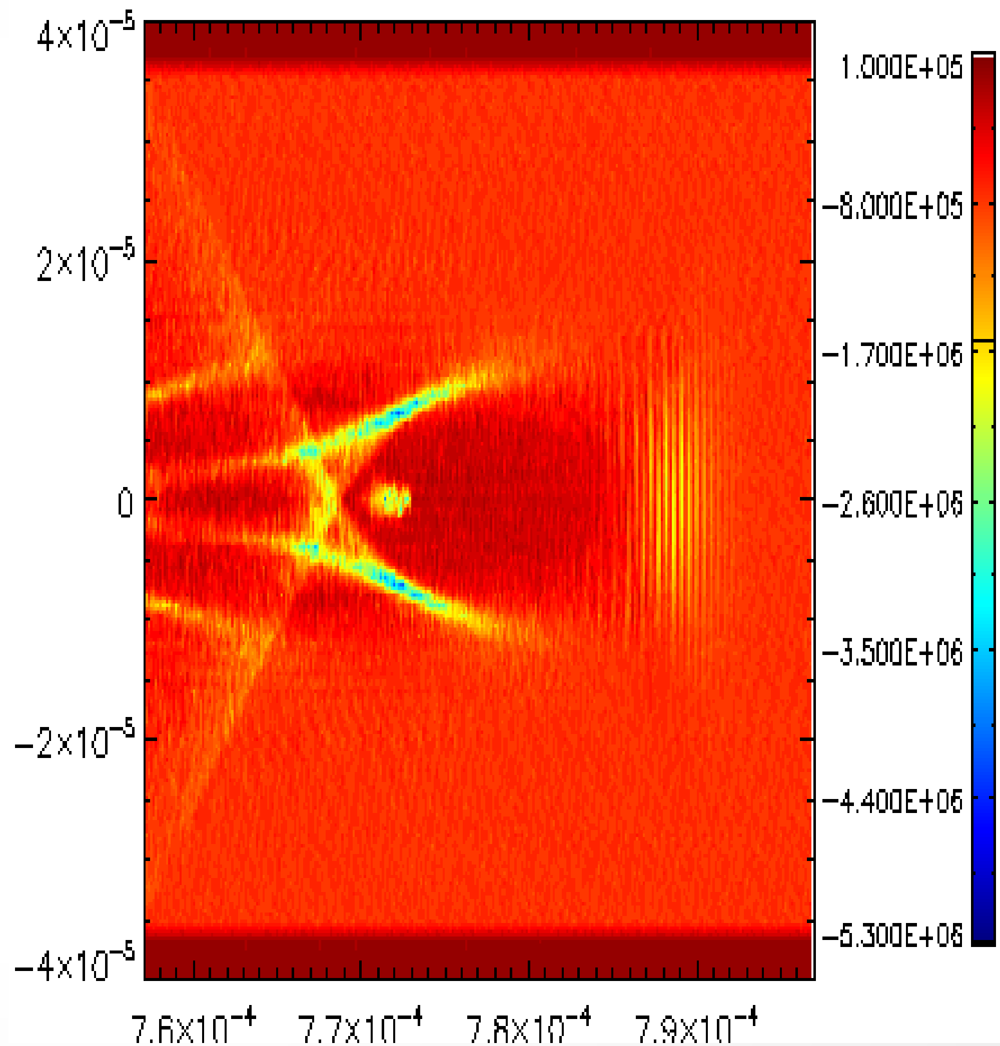




Contour and line out of Wake-Field from VORPAL simulations

Linear LWFA regime vs Bubble regime

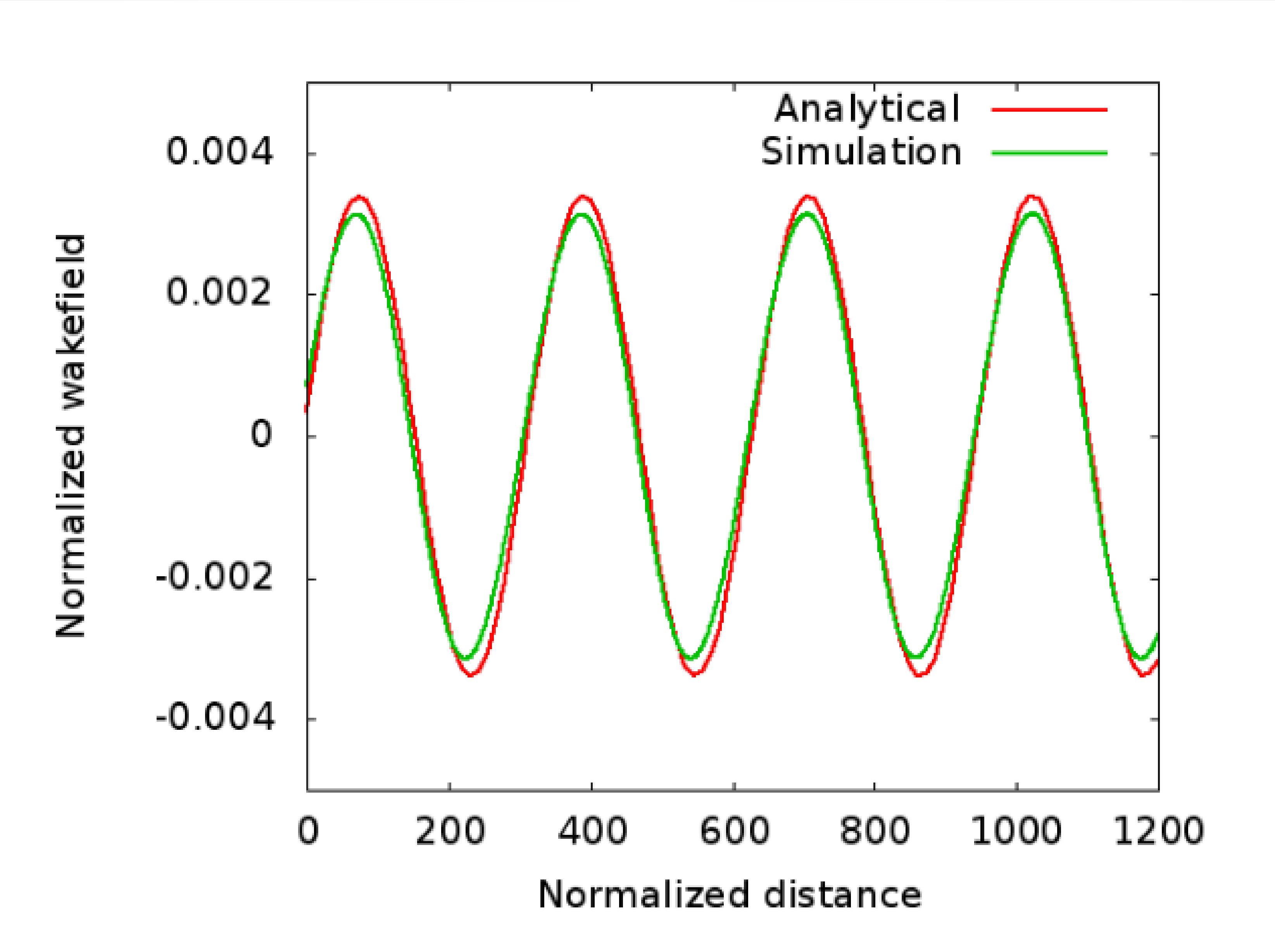




Contour of Charge Density from VORPAL simulations

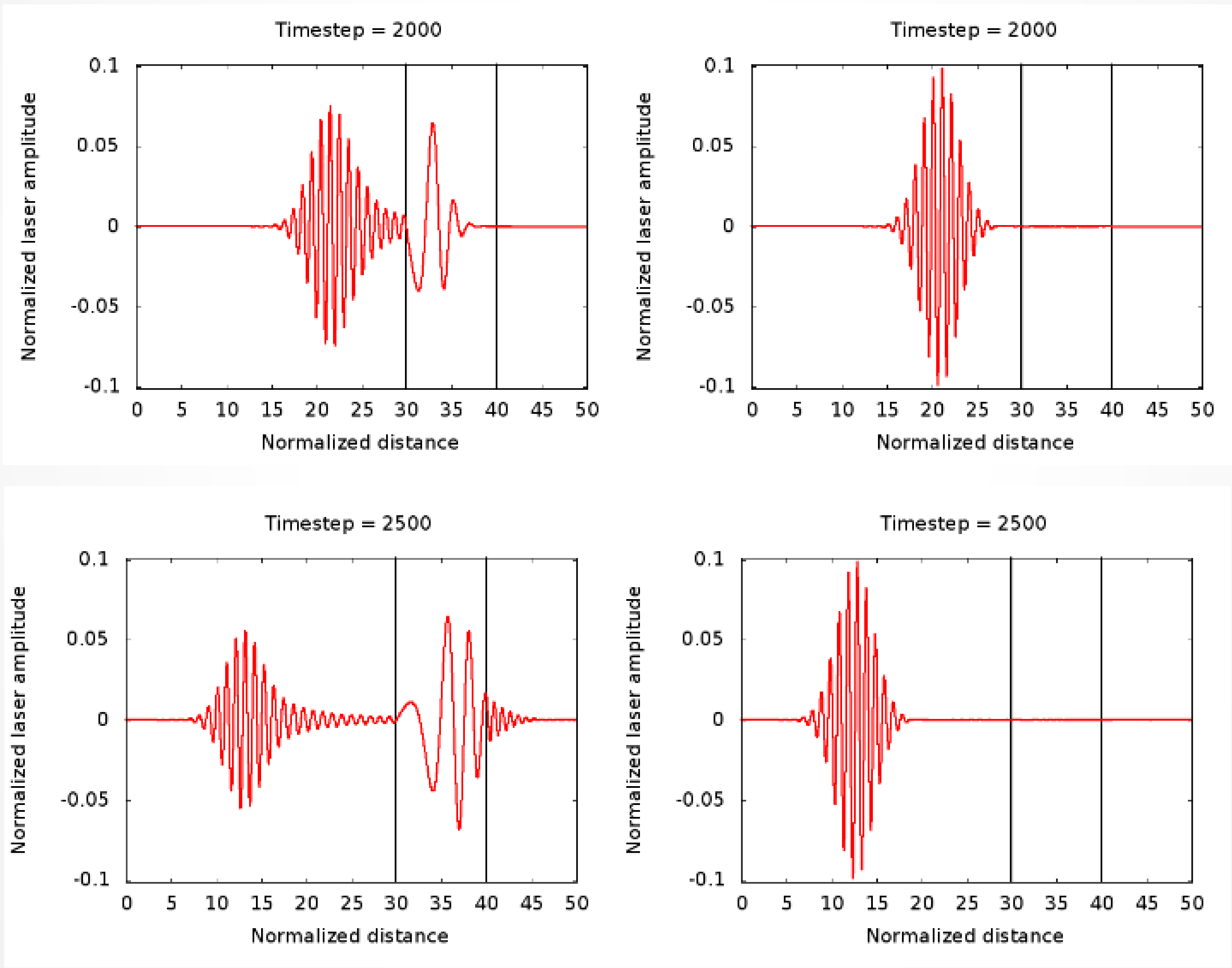
Benchmarking AGASTHII

Linear regime (a_0 = 0.5)



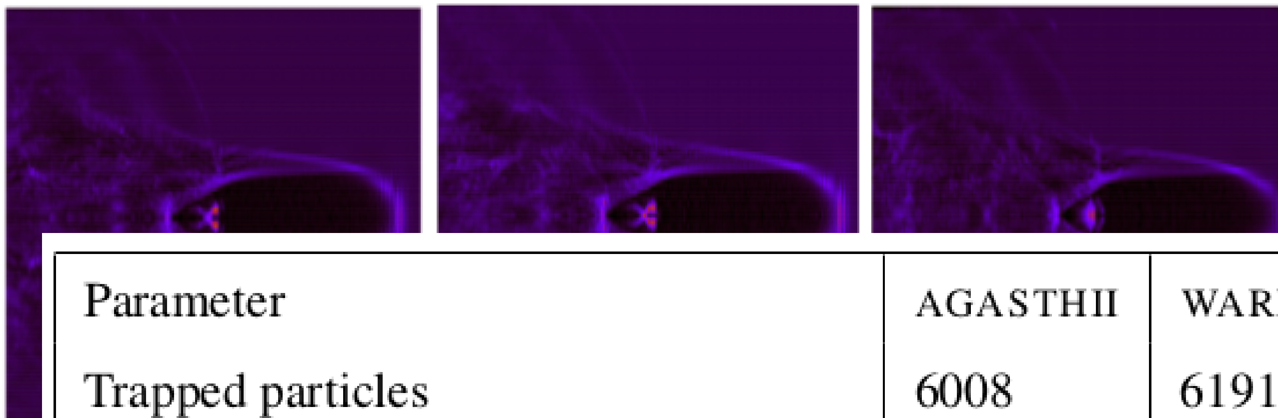
Laser solid interaction

$n_e = n_c$ $\qquad$ $n_e = 10n_c$

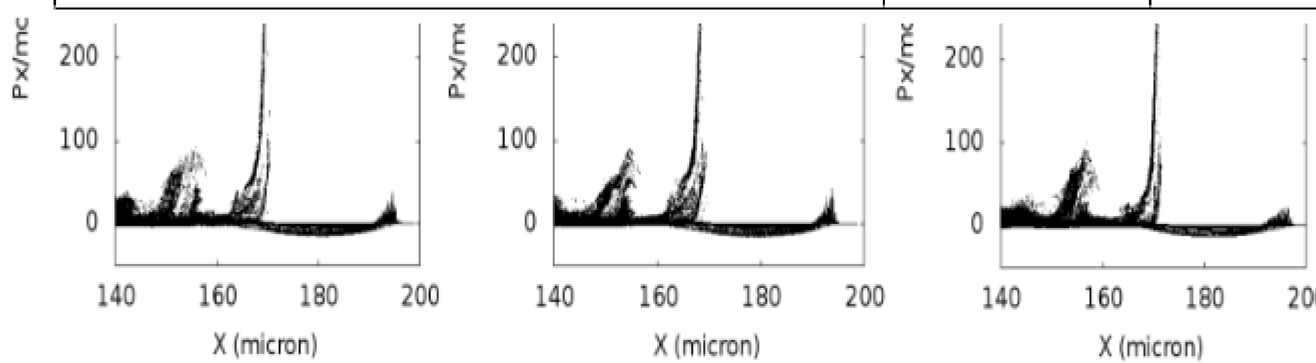


Non-linear bubble regime ($a_0 = 15$)

AGASTHII WARP VORPAL



Parameter	AGASTHII	WARP	VORPAL
Trapped particles	6008	6191	4678
Average energy (MeV)	122	125	118
% rms energy-spread (σ_γ/γ)	30	30	31
Normalized emittance in y (mm-mrad)	22.2	26.8	21.7



(d) (e) (f)

Future work

- PML boundary support
- 3D Parallel AGASTHII using MPI
- Improvement of conventional accelerator beam dynamics module (PIC)
- Reduce dimensional PIC code development
- Monte-Carlo collisions
- Electrostatic modeling

Thanks a lot for your attention!!!

Collaborators :

- Dr. Srinivas Krishnagopal
- Dr. B. Paradkar
- Dr. P. Brijesh
- Abhishek Pathak