Introduction to Particle-in-Cell Methods in Plasma Simulations

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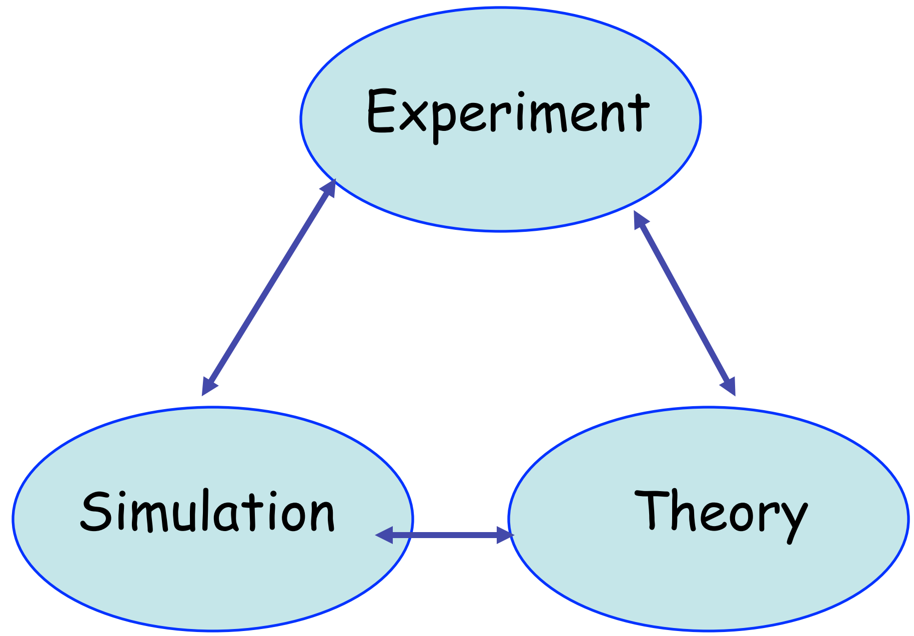
Simulations are an important tool in scientific research

- Computer simulations are carried out to
  - Understand the consequences of fundamental physical laws
  - Help interpret experiments
    - Can provide detailed information which is difficult to measure
  - Design and predict new experiments



PIC simulations are indispensible in HEDP research

- Outline
  - What is PIC method?
  - Numerical algorithm for 2-1/2D EM code
  - An example: two-plasmon-decay instabilities

There are various ways to describe a plasma

- The complete description is to specify x(t) & v(t) of each particle
  - Klimontovich formalism

- Neglecting particle-correlation (collisions), we get the Vlasov equation
  - Closed Vlasov-Maxwell eqs.

- The fluid description describes macroscopic quantities
  - Closure problem

(For details see textbooks, e.g. Krall & Trivelpiece)

$$[\frac{\partial}{\partial t} + v \cdot \nabla + \frac{q_\alpha}{m_\alpha}(E + \frac{v \times B}{c}) \cdot \nabla_v] f_\alpha(\vec{x},\vec{v},t) = 0$$

$$\nabla \cdot E = 4\pi \sum_\alpha q_\alpha \int f_\alpha d\vec{v}$$

$$\nabla \times B = \frac{1}{c}\frac{\partial E}{\partial t} + \frac{4\pi}{c}\sum_\alpha q_\alpha \int \vec{v} f_\alpha d\vec{v}$$

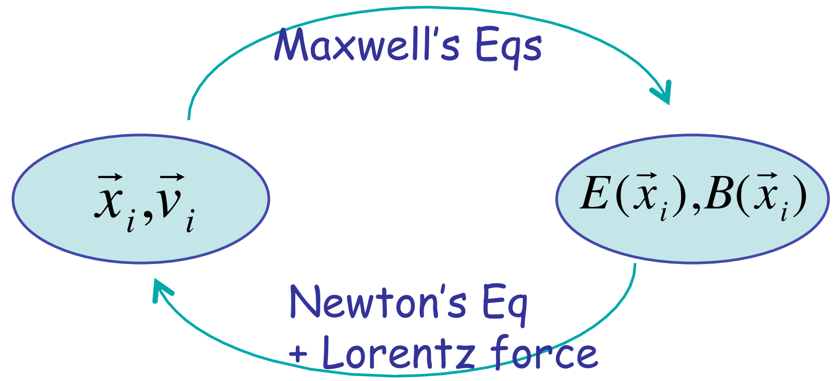
$$\nabla \times E = -\frac{1}{c}\frac{\partial B}{\partial t}$$

$$\frac{\partial n_\alpha(\vec{x},t)}{\partial t} + \nabla \cdot (n_\alpha V_\alpha(\vec{x},t)) = 0$$

$$n_\alpha m_\alpha \frac{\partial}{\partial t} V_\alpha + n_\alpha m_\alpha V_\alpha \cdot \nabla V_\alpha - n_\alpha q_\alpha (E + \frac{V_\alpha \times B}{c}) + \nabla \cdot \vec{P}$$
$$= -\sum_\beta n_\alpha m_\alpha (V_\alpha - V_\beta) < \nu_{\alpha\beta} >$$

Particle simulations take the Klimontovich approach

- Particle methods simulate a plasma system by following a number of particle trajectories
- Essential physics can be captured with a much smaller number of particles than that in a real plasma
  - The charge/mass ratio and charge density remain the same
  - $10^3 \sim 10^{11}$ particles used
- Statistics of the model system is different from a real plasma
- The detailed description is computation-intensive



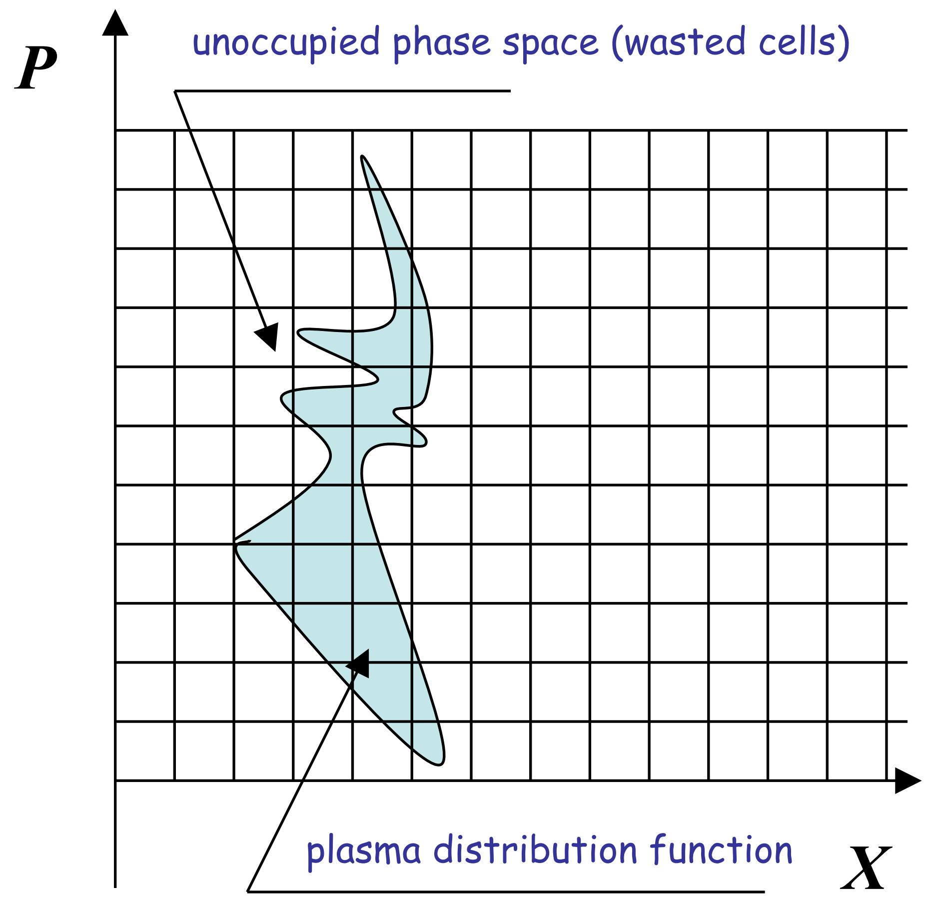
$$\omega_p^2 = \frac{4\pi n e^2}{m}$$

Invariant e/m and ne -> invariant ω_p

The phase-space is efficiently represented in particle methods

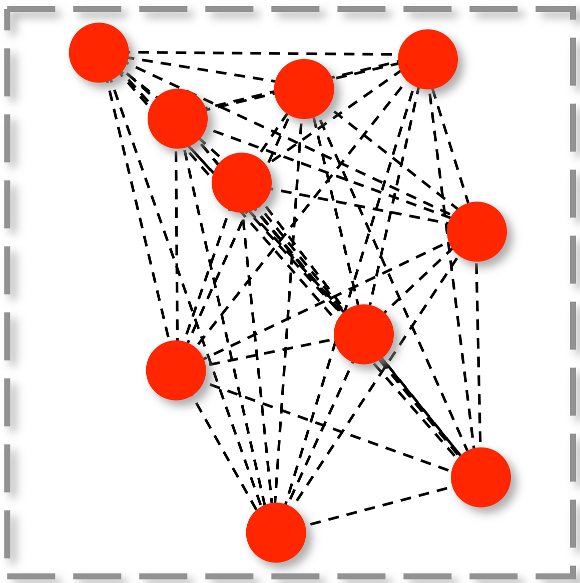
- It is difficult to sample a 6D-phase space by cells
    - o Difficult to solve Vlasov equations in high dimensions

- o PIC codes use particles to efficiently sample the phase space distribution



Calculating inter-particle forces directly is expensive

- number of calculations ~ 100 N_p^2

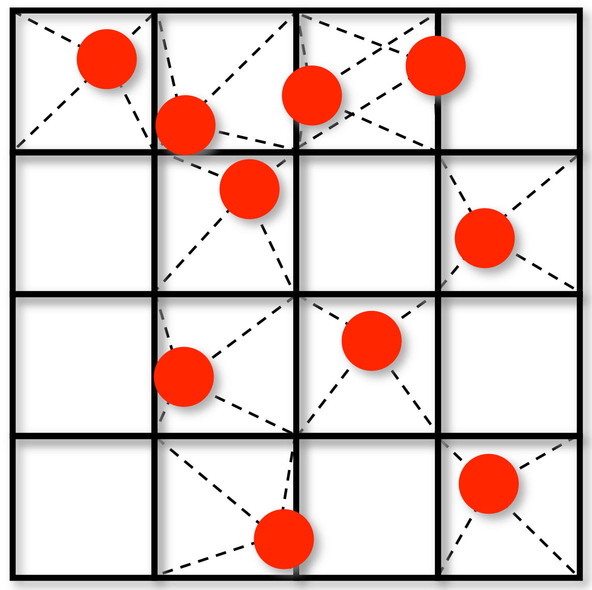


10^8 particles, 100 Tflop/s

- 1 time step ~ **3 hrs**
- 10000 time step sim. ~ **3 yrs**

Particle-in-Cell Algorithms

- Find (ρ_{ij}, J_{ij}) from (x_k, v_k)
- Solving Maxwell's eqs on grid to obtain (E_{ij}, B_{ij})
- Find F_k from (E_{ij}, B_{ij})
- Number of calculatons for 1 step
  - Deposit charge/current $\propto N_p$
  - Advance fields $\propto N_{cells}$
  - Interpolate forces and advance particles $\propto N_p$
  - Total ~ $\alpha N_p + \beta(N_{cells})$



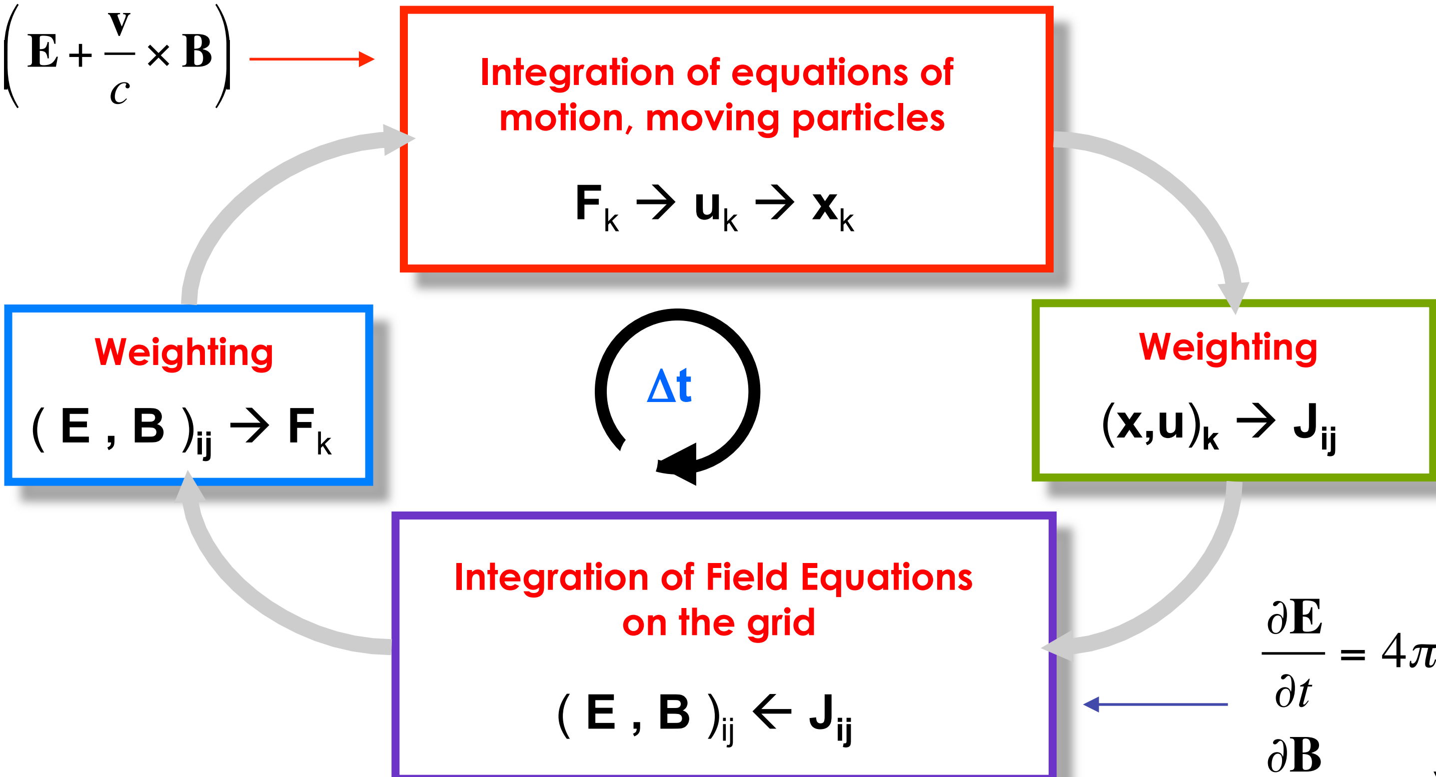
10^8 particles, 100 Tflop/s

64 x 64 x 64 cells

- 1 time step ~ **0.3 ms**
- 10000 time step sim. ~ **3 s**

The Simple & Straightforward PIC Scheme

$$\frac{d\mathbf{p}}{dt} = q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$

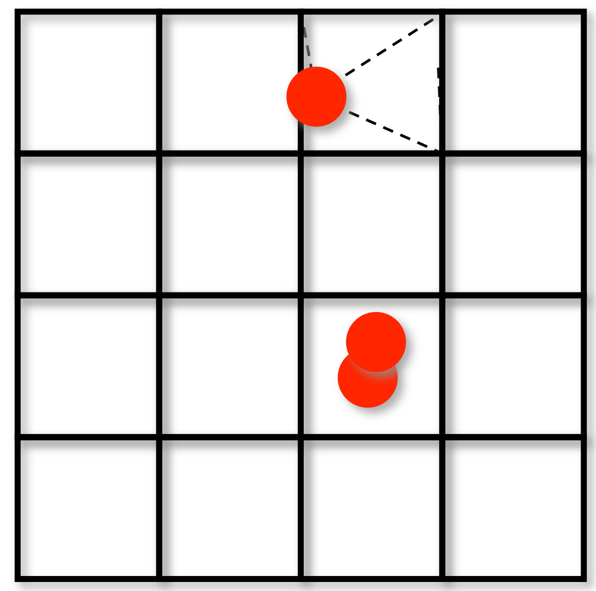


$$\frac{\partial \mathbf{E}}{\partial t} = 4\pi \mathbf{j} - c\nabla \times \mathbf{B}$$

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

Finite-size particles reduce collision

- Close-range collisions are much reduced by using the finite-size particles
- This compensates for the smaller number of particles used
  - $\nu/\omega_p \sim (n\lambda_D^3)^{-1}$
- We are interested in $n\lambda_D^3 \gg 1$ regime
- PIC models are not collisionless
  - Can be used to test collision operators



- References on PIC methods
  - J. M. Dawson, 'Particle simulation of plasmas,' Rev. Mod. Phys. **55**, 403-447 (1983)
  - R. W. Hockney and J. W. Eastwood, **Computer Simulation Using Particles**, McGraw-Hill, New York (1981)
  - C. K. Birdsall and A. B. Langdon, **Plasma Physics via Computer Simulation**, Institute of Physics Publishing, Bristol, UK (1991)

Numerical Algorithms for a 2-1/2D Electromagnetic PIC Code

no spatial variation in z (half-dimension)

Advancing EM Fields

- The EM fields are advanced by Maxwell's Equations
  - The other 2 Maxwell's eqs are satisfied as initial conditions

$$\partial_t B = -\nabla \times E,$$
$$\partial_t E = \nabla \times B - J.$$

$$\nabla \cdot E = \rho,$$
$$\nabla \cdot B = 0.$$

- In 2D, the field components can be decomposed into 2 independent modes
  - TE mode (k·E=0): E_z, B_x, B_y.
  - TM mode (k·B=0): B_z, E_x, E_y.

$$\partial_t B_x = -\partial_y E_z, \partial_t B_y = \partial_x E_z, \partial_t E_z = \partial_x B_y - \partial_y B_x - J_z.$$

$$\partial_t B_z = -(\partial_x E_y - \partial_y E_x), \partial_t E_x = \partial_y B_z - J_x, \partial_t E_y = -\partial_x B_z - J_y.$$

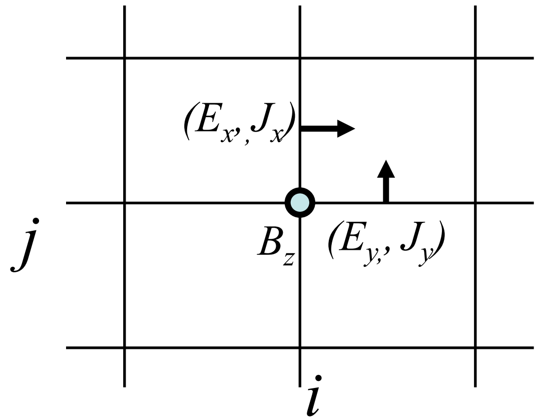
Centered difference can be used in both time & space domain

For TM mode

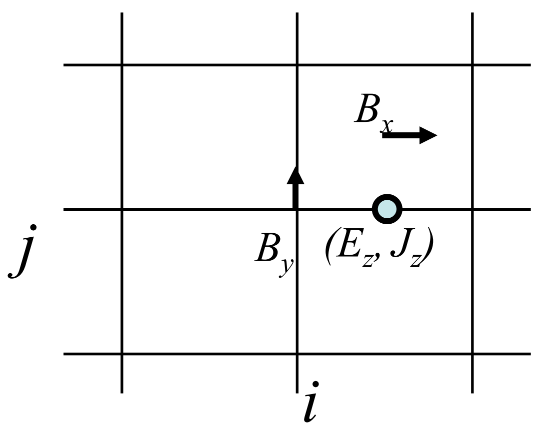
$$\frac{B_{z_{i,j}}^{n+1/2} - B_{z_{i,j}}^{n-1/2}}{\Delta t} = -\frac{E_{y_{i+1/2,j}}^{n} - E_{y_{i-1/2,j}}^{n}}{\Delta x} + \frac{E_{x_{i,j+1/2}}^{n} - E_{x_{i,j-1/2}}^{n}}{\Delta y}$$

$$\frac{E_{x_{i,j+1/2}}^{n+1} - E_{x_{i,j+1/2}}^{n}}{\Delta t} = \frac{B_{z_{i,j+1}}^{n+1/2} - B_{z_{i,j}}^{n+1/2}}{\Delta y} - j_{x_{i,j+1/2}}$$

$$\frac{E_{y_{i+1/2,j}}^{n+1} - E_{x_{i+1/2,j}}^{n}}{\Delta t} = -\frac{B_{z_{i+1,j}}^{n+1/2} - B_{z_{i,j}}^{n+1/2}}{\Delta x} - j_{y_{i+1/2,j}}$$

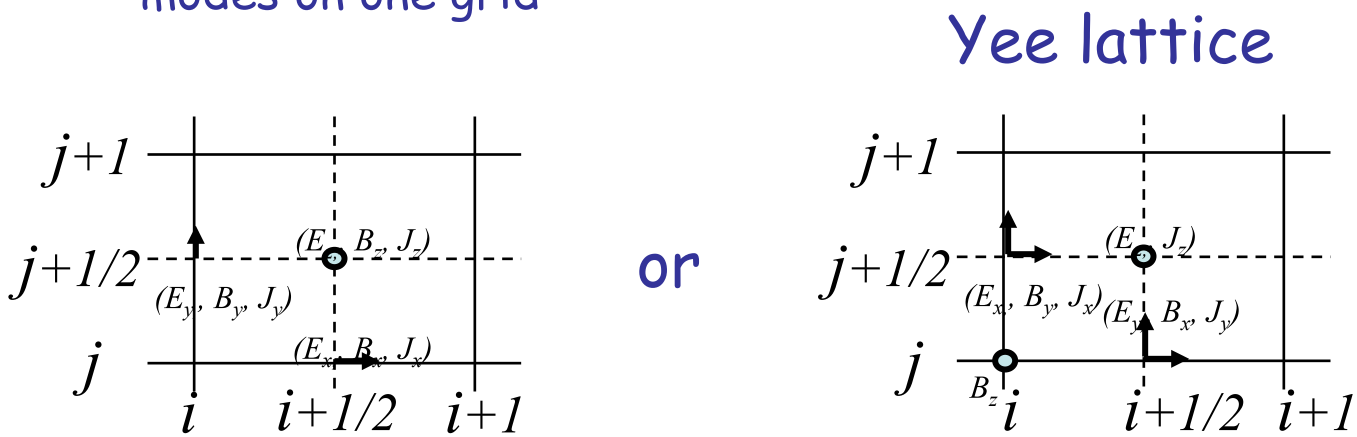


TE mode is similar

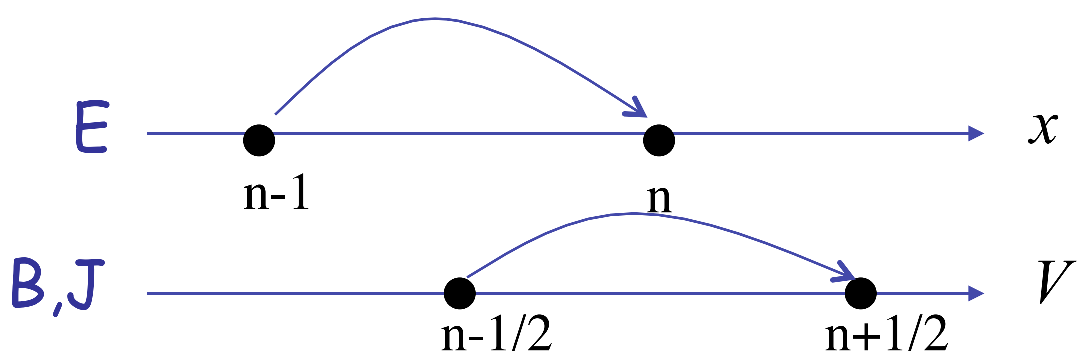


Combining the Two Sets of Fields

- Two equal ways of putting both modes on one grid



- Leapfrog in time domain



Time step is limited by the Courant condition

FSC

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- Plane EM Waves in Vacuum
  - $(E,B)=(E_0,B_0)\exp(ik\cdot x-i\omega t)$
- Dispersion relation from difference scheme
- Small Δt is required for stability in explicit schemes
- Large Δt can be achieved with implicit schemes
  - Still need to resolve relevant physics

$$\Omega B = \kappa \times E$$

$$\Omega E = -\kappa \times B$$

$$\Omega = \omega \frac{\sin(\omega \Delta t/2)}{\omega \Delta t/2}$$

$$\kappa_x = k_x \frac{\sin(k_x \Delta x/2)}{k_x \Delta x/2}$$

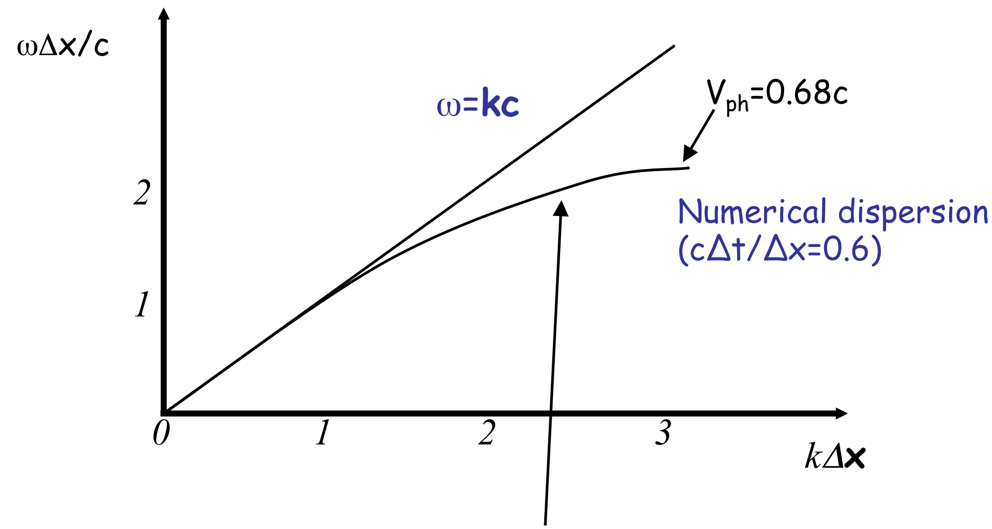
$$\Omega^2 = c^2\kappa^2 \Rightarrow \left(\frac{\sin\frac{\omega\Delta t}{2}}{c\Delta t}\right)^2 = \left(\frac{\sin\frac{k_x\Delta x}{2}}{\Delta x}\right)^2 + \left(\frac{\sin\frac{k_y\Delta y}{2}}{\Delta y}\right)^2$$

$$\frac{1}{c^2\Delta t^2} > \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}$$

Courant Condition for Numerical Stability

The numerical dispersion relation contains modes with V_{ph}<C

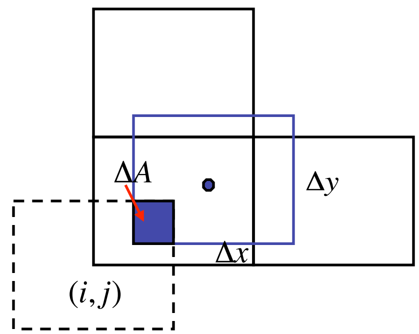
- For relativistic particles with $V > V_{ph}$, unwanted Cerenkov emission can occur.



$$\left(\frac{\sin\frac{\omega\Delta t}{2}}{c\Delta t}\right)^2 = \left(\frac{\sin\frac{k_x\Delta x}{2}}{\Delta x}\right)^2 + \left(\frac{\sin\frac{k_y\Delta y}{2}}{\Delta y}\right)^2$$

Pushing Particles

- To update p, EM fields have to first be interpolated from the grid to the particle locations
  - Linear (area) weighting



$$E(\vec{x}_k) = \sum_{i,j} E_{ij} S(\vec{x}_k - \vec{X}_{ij})$$

$$S(\vec{x}_k - \vec{X}_{ij}) = \frac{\Delta A}{\Delta x \Delta y}$$

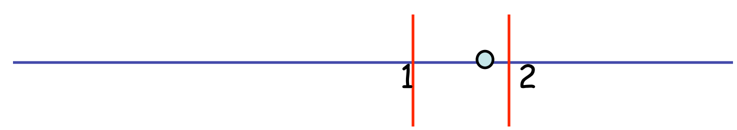
$$\sum_{i,j} S(\vec{x}_k - \vec{X}_{ij}) = 1$$

- The same S should be used in charge deposition to ensure momentum conservation
  - dP/dt=0 for 1 particle, independent of S.

$$\rho_{ij} = \sum_k q_k S(\vec{x}_k - \vec{X}_{ij})$$

$$\frac{dP}{dt} = \sum_k q_k E(\vec{x}_k) = \sum_k q_k \sum_{i,j} E_{ij} S(\vec{x}_k - \vec{X}_{ij})$$

$$= \sum_{i,j} E_{ij} \rho_{ij}$$



$$E_1 = -\frac{\rho_2}{2}, E_2 = \frac{\rho_1}{2} \Rightarrow E_1\rho_1 + E_2\rho_2 = 0$$

Pushing Particles (Boris Pusher)

$$\frac{p^{n+1/2} - p^{n-1/2}}{\Delta t} = \frac{q}{m}\left(E^n + \frac{1}{c}\frac{p^{n+1/2} + p^{n-1/2}}{2\gamma^n} \times B^n\right)$$

$$\left(B^n = \frac{B^{n+1/2} + B^{n-1/2}}{2}\right)$$

- Differencing Relativistic Newton's Eq.

- Separating f_E & f_B

$$p^- = p^{n-1/2} + \frac{\Delta t}{2}\frac{q}{m}E^n$$

$$p^{n+1/2} = p^+ + \frac{\Delta t}{2}\frac{q}{m}E^n$$

- The magnetic force causes a pure rotation

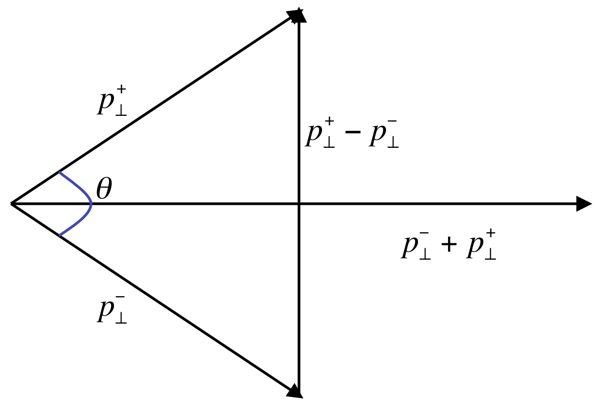
$$\frac{p^+ - p^-}{\Delta t} = \frac{q}{mc}\frac{p^+ + p^-}{2\gamma^n} \times B^n$$

$$[(p^+)^2 - (p^-)^2 = 0]$$

v×B Rotation

Eq. for v×B rotation

$$\frac{p^+ - p^-}{\Delta t} = \frac{q}{mc}\frac{p^+ + p^-}{2\gamma^n} \times B^n$$

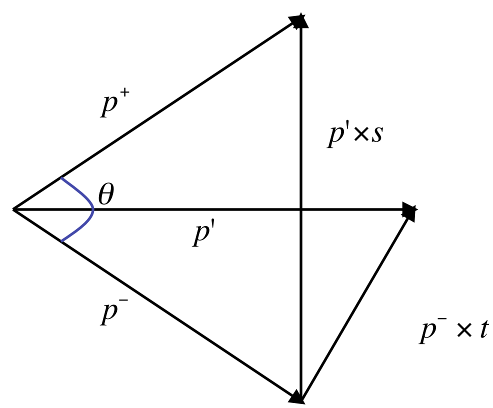


$$\boxed{\tan\frac{\theta}{2} = -\frac{qB}{2mc\gamma}\Delta t}$$

In practice, this is used

$$p' = p^- + p^- \times t, \quad (t = qB\Delta t/2\gamma mc = -\tan\frac{\theta}{2})$$

$$p^+ = p^- + p'\times s, \quad (s = 2t/(1+t^2) = -2\sin\frac{\theta}{2}\cos\frac{\theta}{2})$$



Current Deposition & Charge Conservation

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- Updating positions
- Current deposition needs both V & x defined at different times
  - ∂ρ/∂t+∇·j=0 may not be satisfied
- Charge conservation is critical to guarantee solutions satisfying all Maxwell's eqs.
- Two ways to achieve charge conservation
  - Adjusting longitudinal E
  - Using charge-conserving current deposition schemes
  - Spectral method

$$x^{n+1} = x^n + \frac{p^{n+1/2}}{\gamma^{n+1/2}}\Delta t$$

$$j_{ij}^{n+1/2} = \sum_k q_k v_k^{n+1/2} S\left(\frac{\vec{x}_k^n + \vec{x}_k^{n+1}}{2} - \vec{X}_{ij}\right)$$

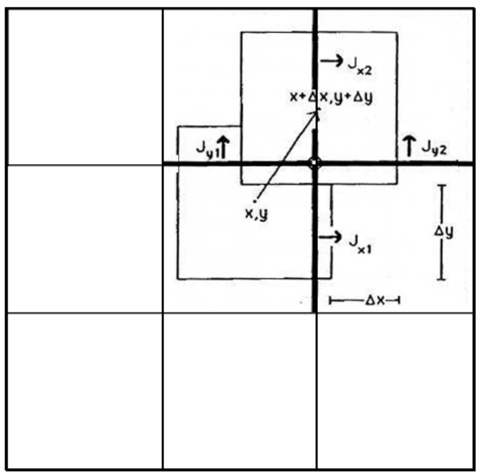
or

$$j_{ij}^{n+1/2} = \sum_k q_k v_k^{n+1/2} \frac{S(\vec{x}_k^n - \vec{X}_{ij}) + S(\vec{x}_k^{n+1} - \vec{X}_{ij})}{2}$$

$$\partial_t B = -\nabla \times E \Rightarrow \partial_t \nabla \cdot B = 0$$

$$\partial_t E = \nabla \times B - J \Rightarrow \partial_t \nabla \cdot E = -\nabla \cdot J \xrightarrow{?} \partial_t \rho$$

Charge-Conserving Current Deposit Scheme



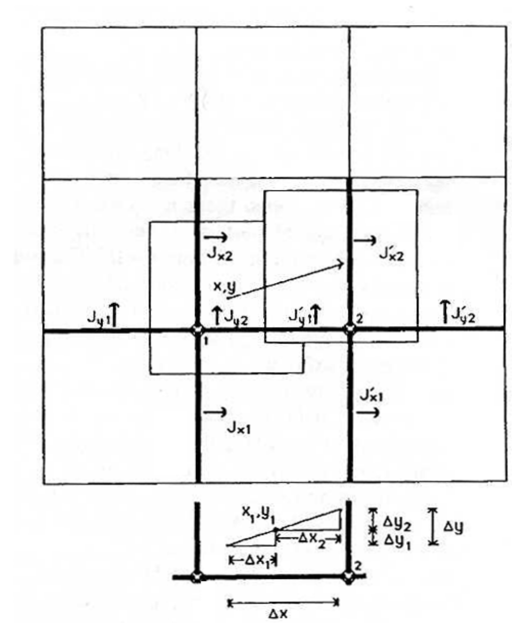
For unit grid & unit charge

$$J_{x1} = \Delta x \frac{(0.5-y)+(0.5-y-\Delta y)}{2} = \Delta x(0.5 - y - \frac{1}{2}\Delta y)$$

$$J_{x2} = \Delta x(0.5 + y + \frac{1}{2}\Delta y)$$

$$J_{y1} = \Delta y(0.5 - x - \frac{1}{2}\Delta x)$$

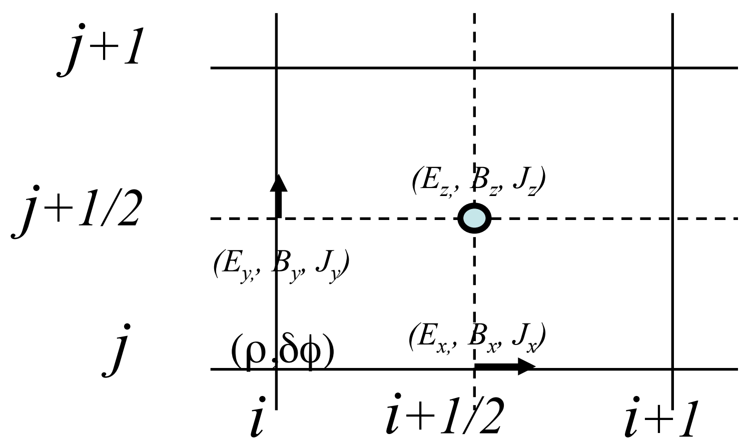
$$J_{y2} = \Delta y(0.5 + x + \frac{1}{2}\Delta y)$$



For more complicated crossing, the current can be calculated in stages [see Villasenor & Buneman, Computer Phys. Comm. **69**, 306 (1992).]

Adjusting E to Satisfy $\nabla\cdot E=\rho$

- E′ obtained from a non-CC j does not satisfy $\nabla\cdot E'=\rho$
- Find $\delta\phi$ so that $\nabla^2\delta\phi=\nabla\cdot E'-\rho$
- The corrected field is $E=E'-\nabla\delta\phi$

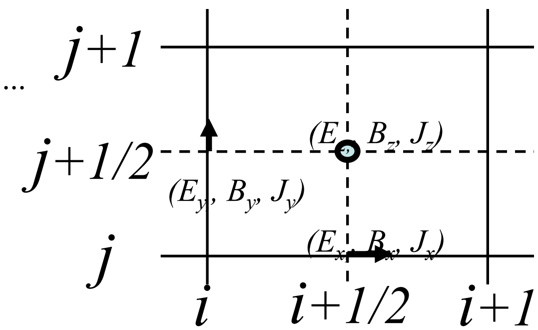


Boundary conditions are important to model reality

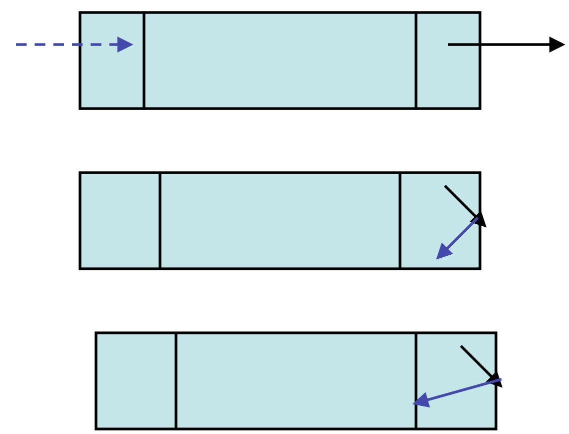
- For fields
  - Periodic
  - Conducting
  - Open, absorbing,…

$$E^z_{-1/2,j} = E^z_{Nx-1/2,j}, E^z_{Nx+1/2,j} = E^z_{1/2,j}, \ldots$$

$$E^y_{0,j} = 0, \frac{E^z_{-1/2,j} + E^z_{1/2,j}}{2} = 0$$



- For particles
  - Periodic
  - Reflecting
  - Thermal bath

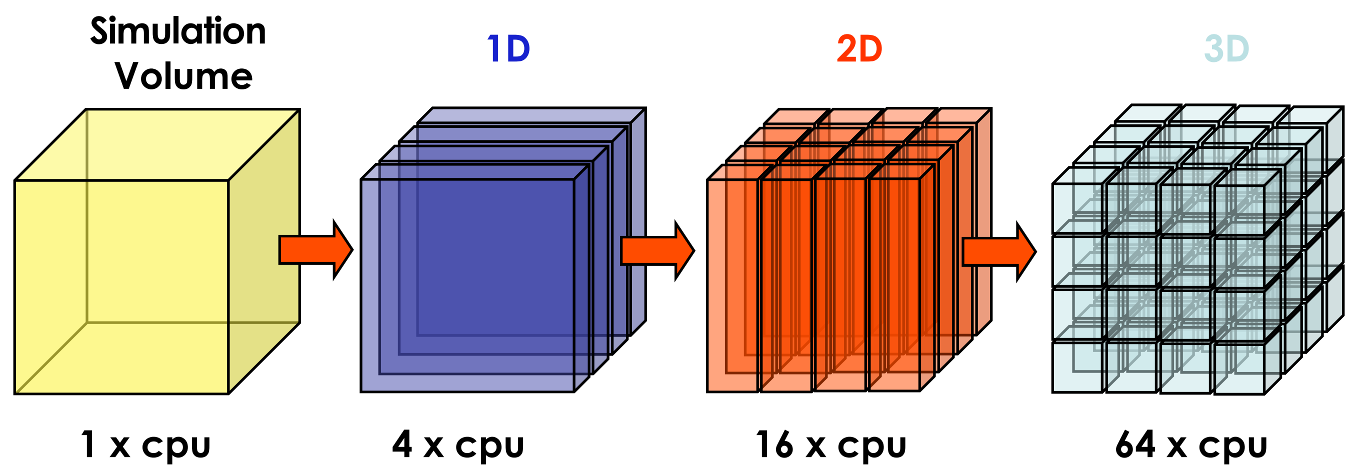


Grid Instability

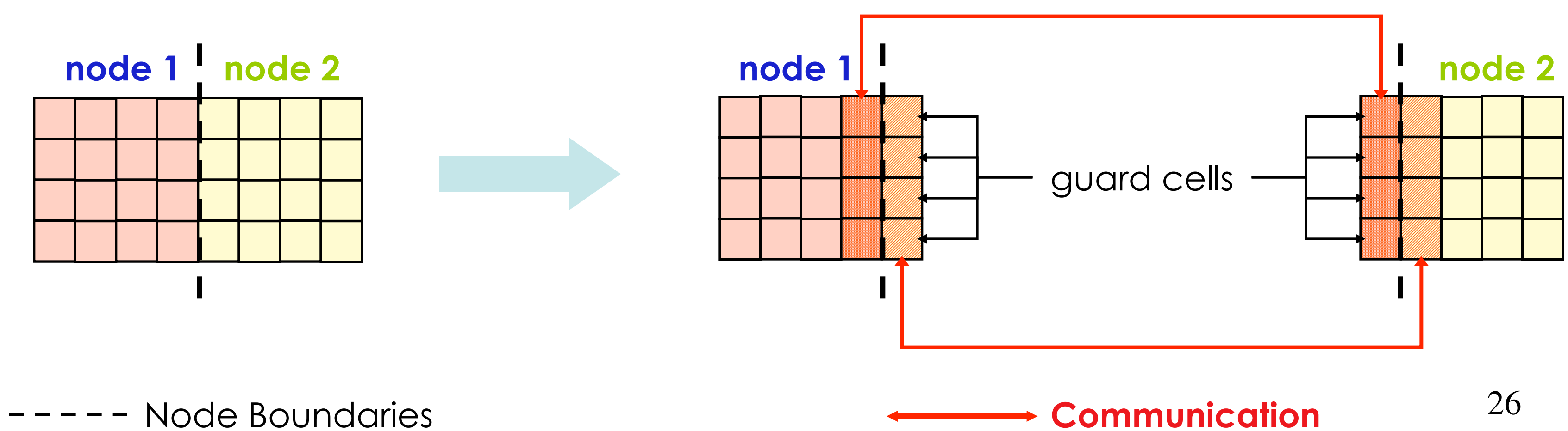
- Since particle positions are continuous, δn can have high-k modes
  - Dominated by $k_n \sim \omega_p / v_t$
- Due to aliasing, $\delta\rho$ can have modes with $k = k_n - p(2\pi/\Delta x)$
- $\delta\rho$ can resonantly interact with E of the same k, causing instability
- In practice, if $\Delta < 3\lambda_D$, the grid instability is largely suppressed
  - Smoothing also helps

Parallelization: Domain Decomposition

Divide simulation space between multiple cpu's



Use guard cells to store needed information from neighboring nodes



PIC codes have good scalability (10^5 processors)

- Distributed memory systems using MPI
- Field solver is local:
  - Communication only with neighboring nodes
  - For parallelizing the global FFT, see Decyk, Comp. Phys. Comm., 1994
- Same decomposition for particles and fields
  - Each computing node acts as a section of the global physical space
- All parallelization is encapsulated in boundary condition routines
  - Developers can focus on local physics

The latest generation supercomputers use GPU's

• 3 out of the top 5 fastest computer in the world use Nvidia GPU's.

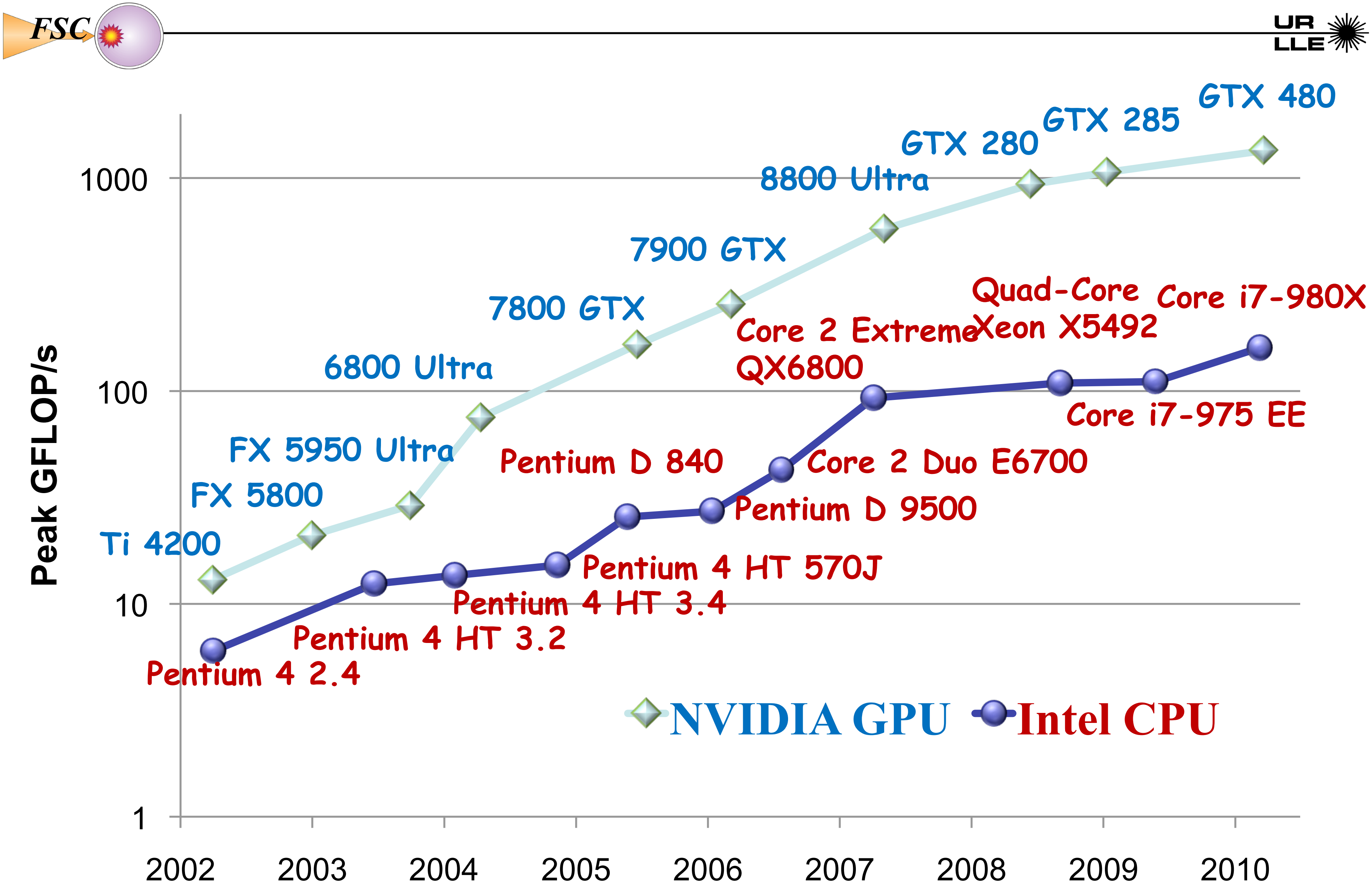
• Tianhe-1A (2.507 petaflops, China) is equipped with 14,336 Xeon X5670 processors and 7,168 Nvidia Tesla M2050 general purpose GPUs (two CPUs and one GPU for each node)

• A 2.507 petaflop system built entirely with CPUs would consume more than 12 megawatts. Tianhe-1A consumes only 4.04 megawatts. GPUs make it 3 times more power efficient.

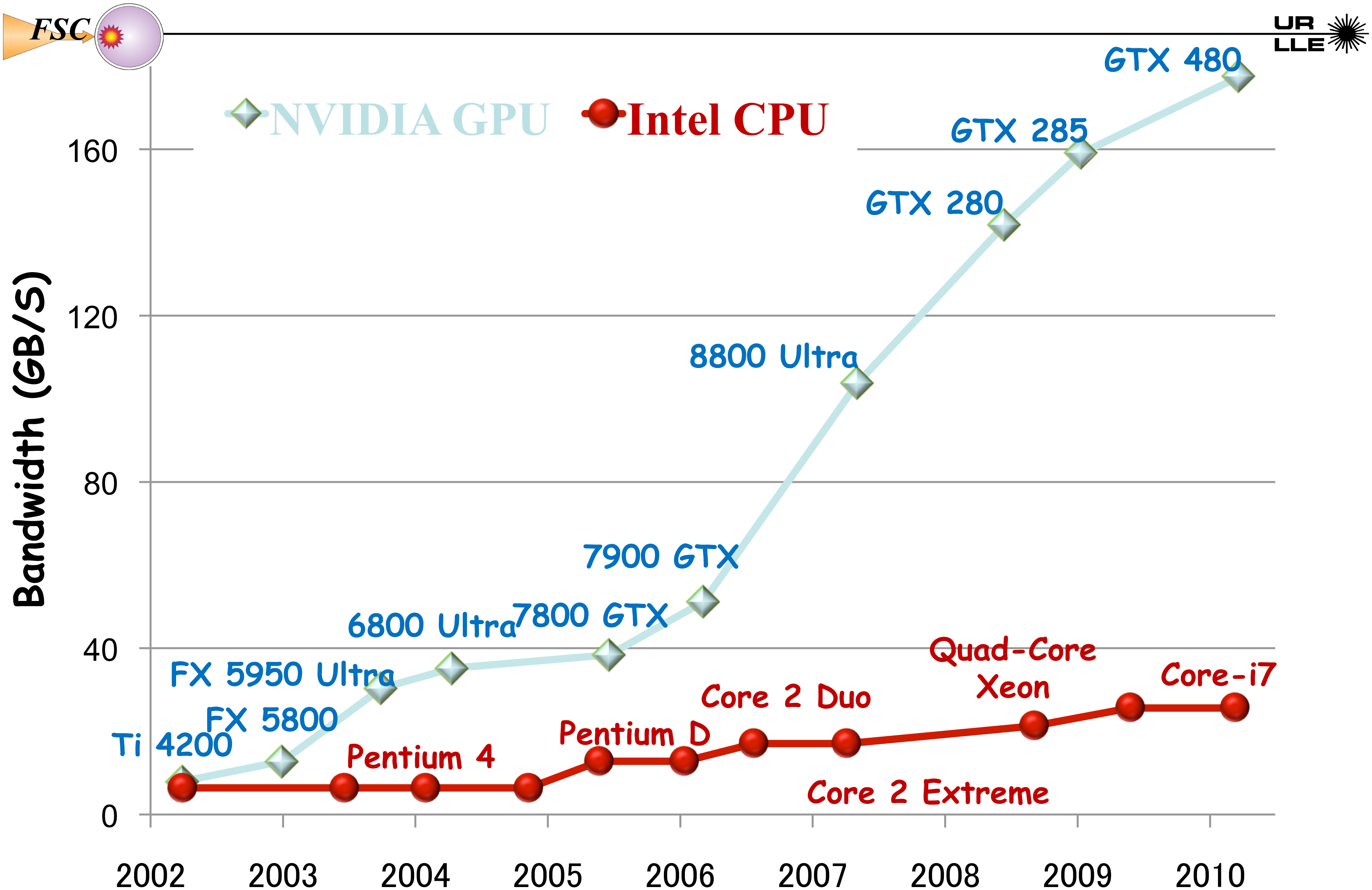
•Exa-scale cluster: 1M GPU's?

	X5670	M2050
# of cores	6	448
Clock speed	2.93GHz	575MHz
Bandwidth	32GB/s	148GB/s
Max power	95W	225W
Price	$1440	$2500

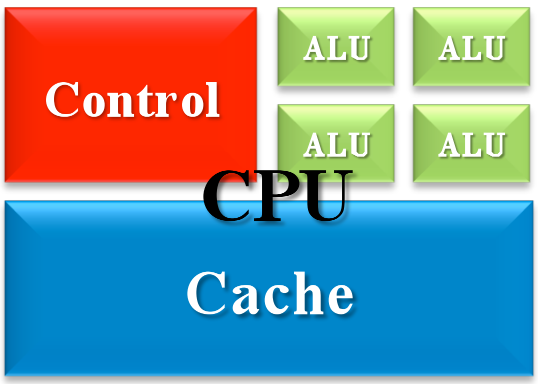
GPU's have ~10x computing power of CPUs



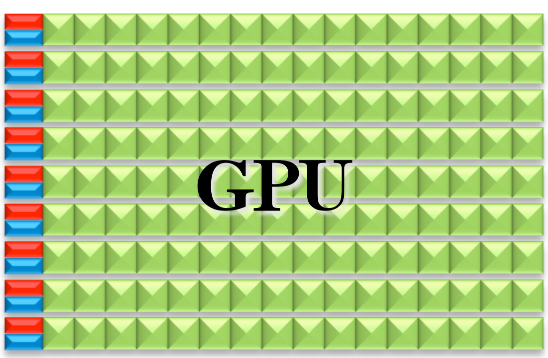
GPU's have very high memory bandwidth



Why are GPU's so powerful for computing?



- CPU dedicates large chip area for the control logic and cache
- High performance on a single thread of execution

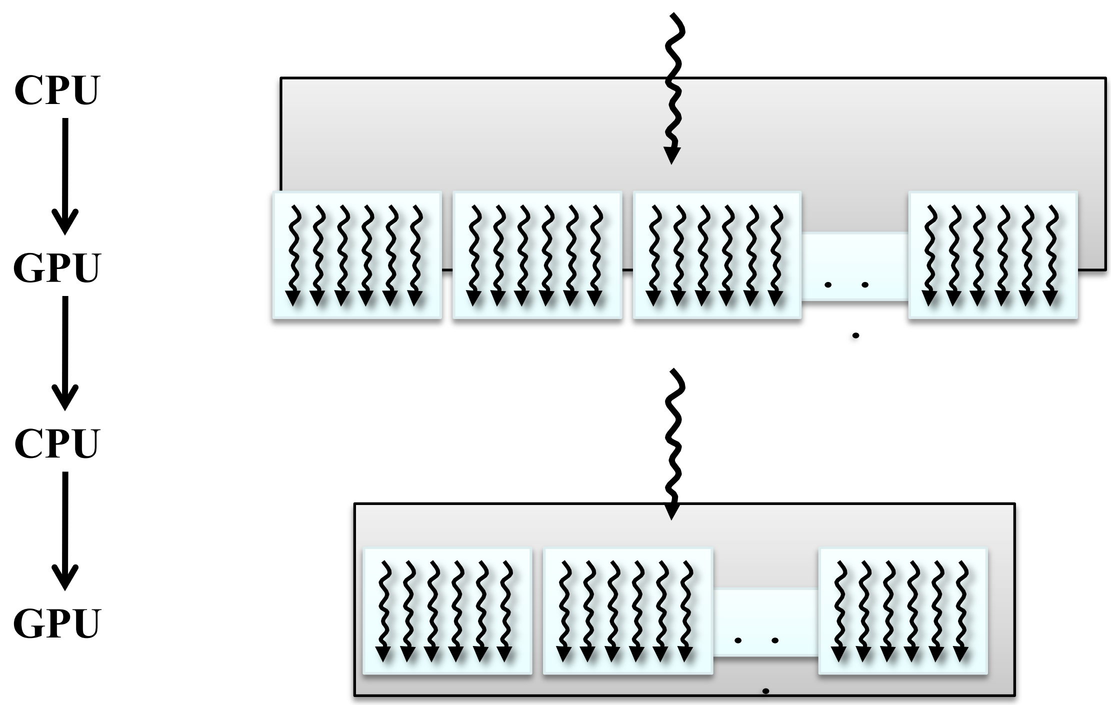


- GPUs spend almost all silicon on the actual computing
- specialized for compute intensive, highly parallel computations

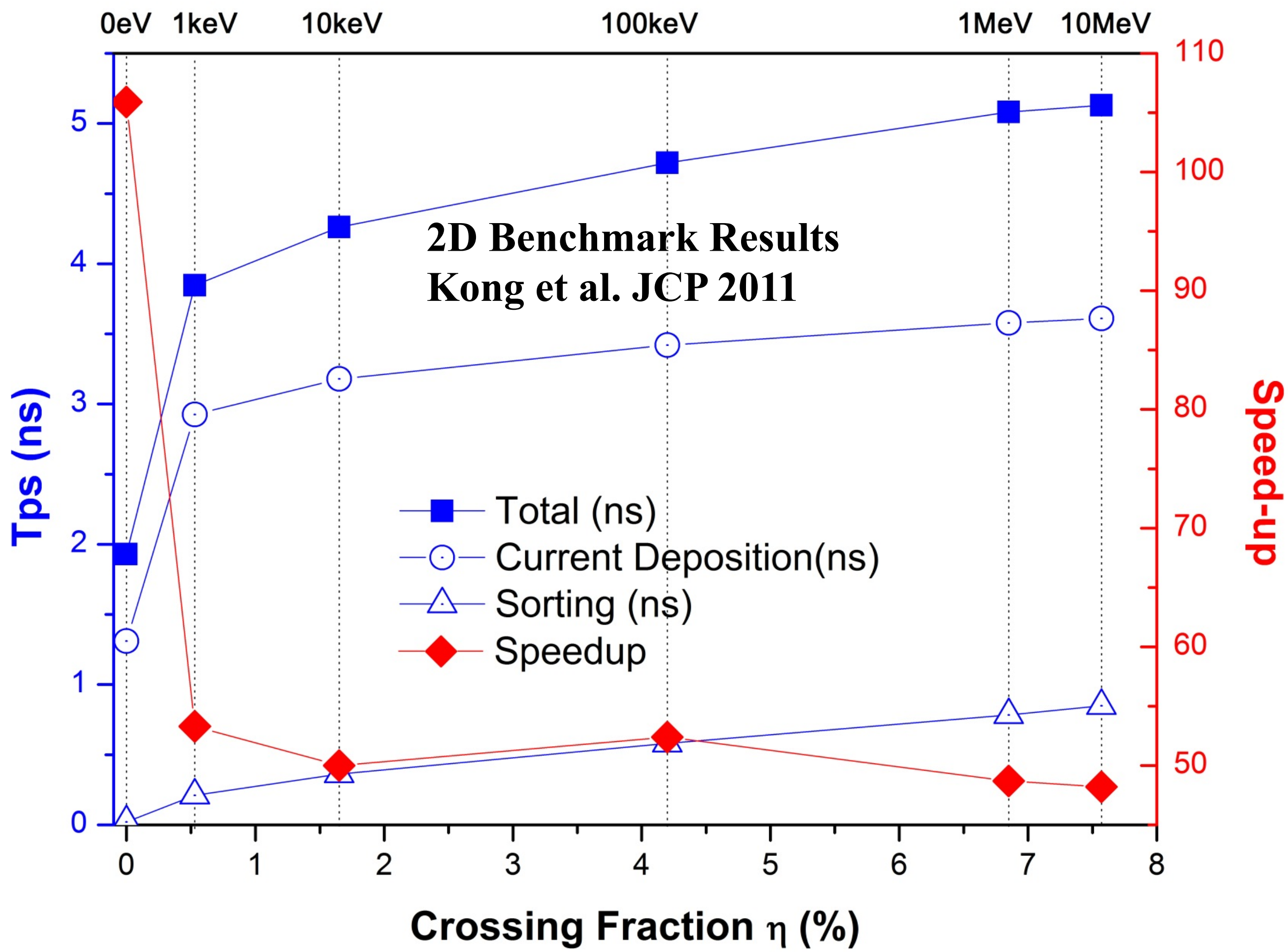
Heterogeneous serial-parallel programming model

CUDA application = serial program executing parallel kernels

- Serial code executed by a CPU thread
- Parallel code executed by GPU, in threads (grouped in blocks)
- Syntax similar to C or Fortran



A GPU-PIC code can be developed with a current deposition scheme with almost no branch and parallel sorting



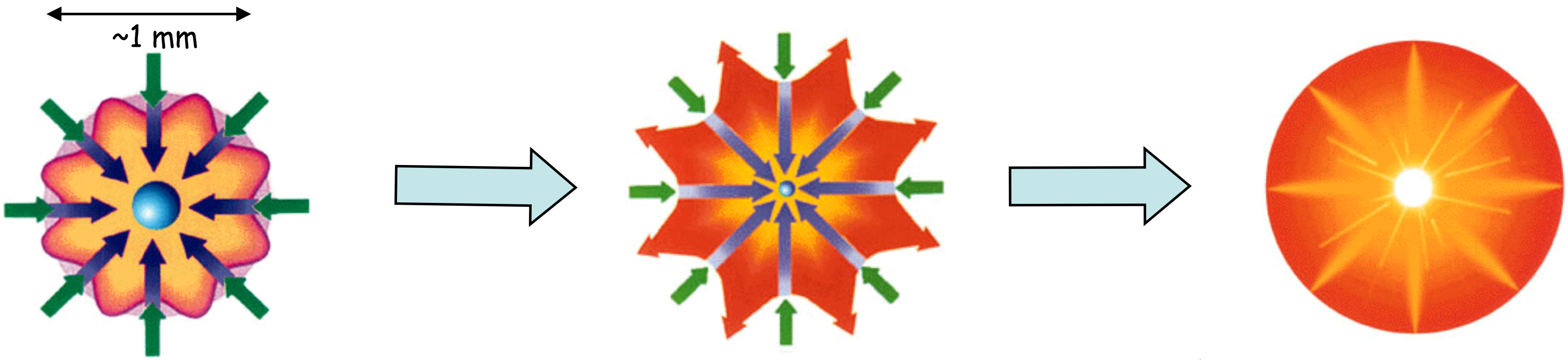
- Other kinds of PIC codes
  - Hybrid codes
    - Fluid description for background plasma + kinetic description for energetic particles
  - Implicit field solver
    - Allows larger Δt
    - Not resolving physics $<\Delta t$
  - More difficult to scale up to large # of processors

Summary on PIC codes

- The PIC model is a first-principle kinetic model for plasma physics
- It efficiently tracks particle trajectories to sample particle phase space
- Its structure is scalable to massively parallel computer systems

PIC Simulations for Two-plasmon-decay instabilities in ICF

Inertial confinement fusion aims to make fusion a clean and boundless energy source

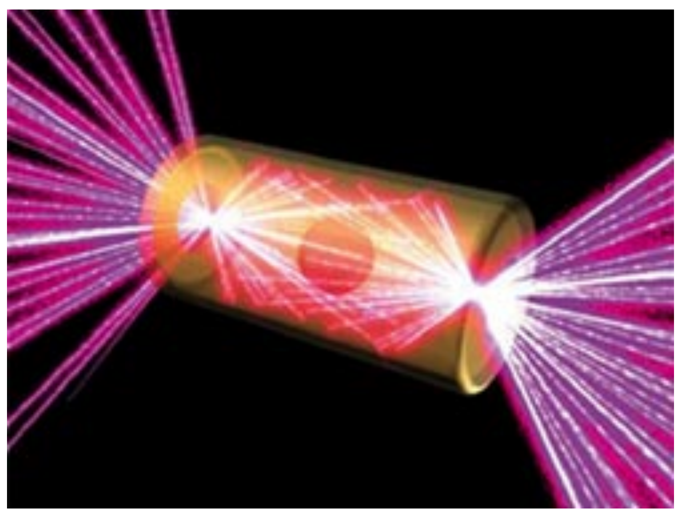


Laser heating pellet surface

rocket liftoff of ablator
-> inward shock wave

A hot spot is created in the dense
core and reaction starts

- The National Ignition Facility aims to achieve ignition in the next two years



What can happen to a laser propagating in a plasma?

- Dispersion relation for EM waves in a plasma

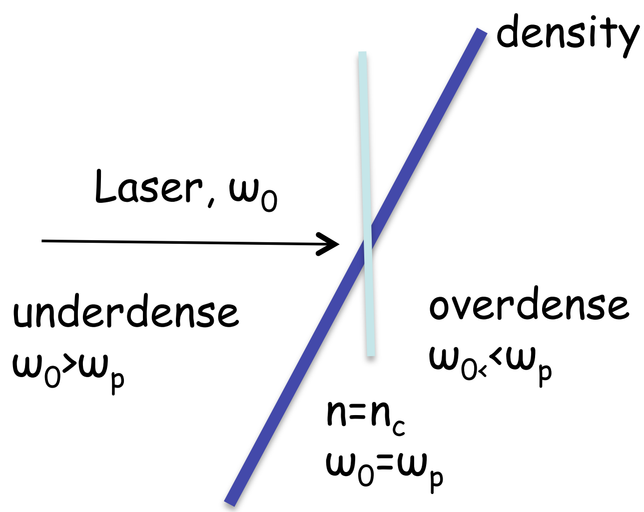
$$\omega^2 = k^2c^2 + \omega_p^2$$

$$\omega_p^2 = \frac{4\pi n e^2}{m}$$

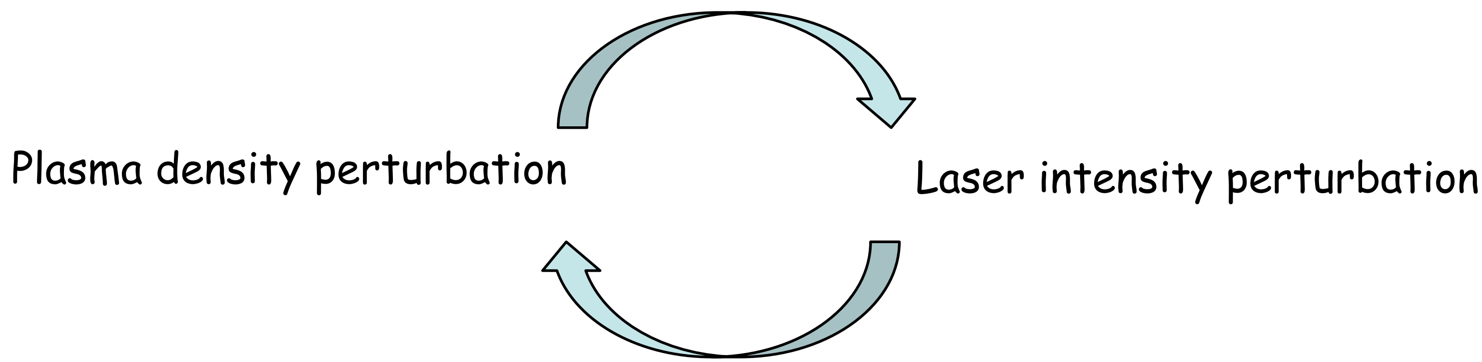
- There is a critical density n_c beyond which a laser cannot propagate

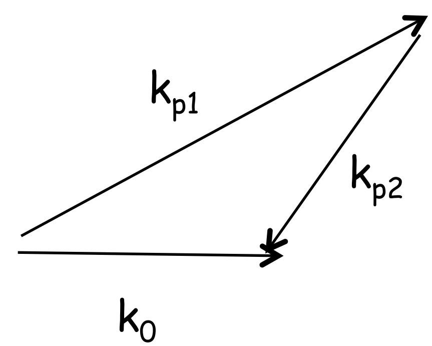
$$\frac{\partial \mathbf{E}}{\partial t} = 4\pi \mathbf{j} - c\nabla \times \mathbf{B}$$

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



Many instabilities can happen in the laser-plasma interactions

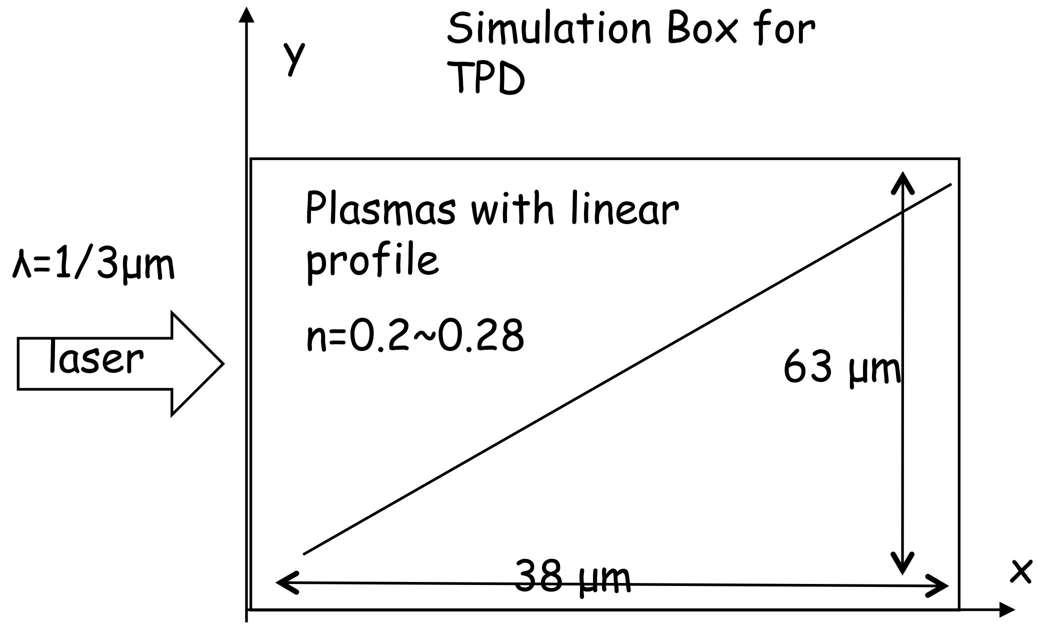




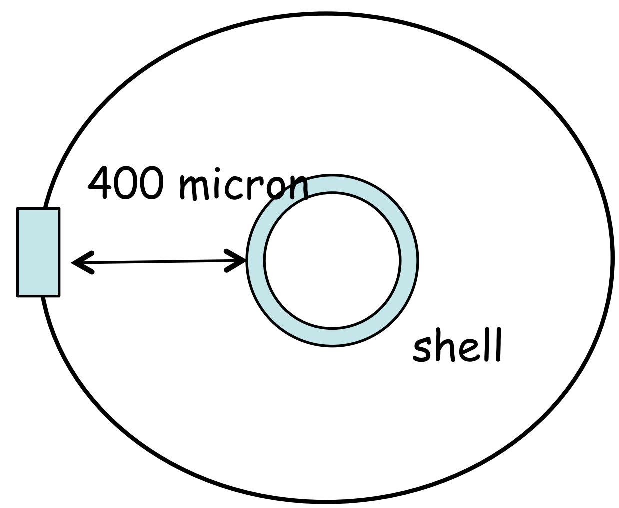
- Two plasmon decay: laser drives two plasma waves
- TPD happens near $n=1/4n_c$ or $\omega_0 \approx 2\omega_p$
- TPD can generate non-thermal electrons that can preheat an ICF target
- The physics is kinetic and nonlinear

Vast scale disparities in PIC simulations demand high performance computing

dx=1/90 micron
Grid: 3600 x 6000, 100ppc
2.2 billion particles
dt=0.025 fs
400,000 steps for 10 ps
230 ns per particle-step per core ----> 56000 cpu-hour
This is only 2D!



Typical target parameters:
mm underdense region and ns-long pulse

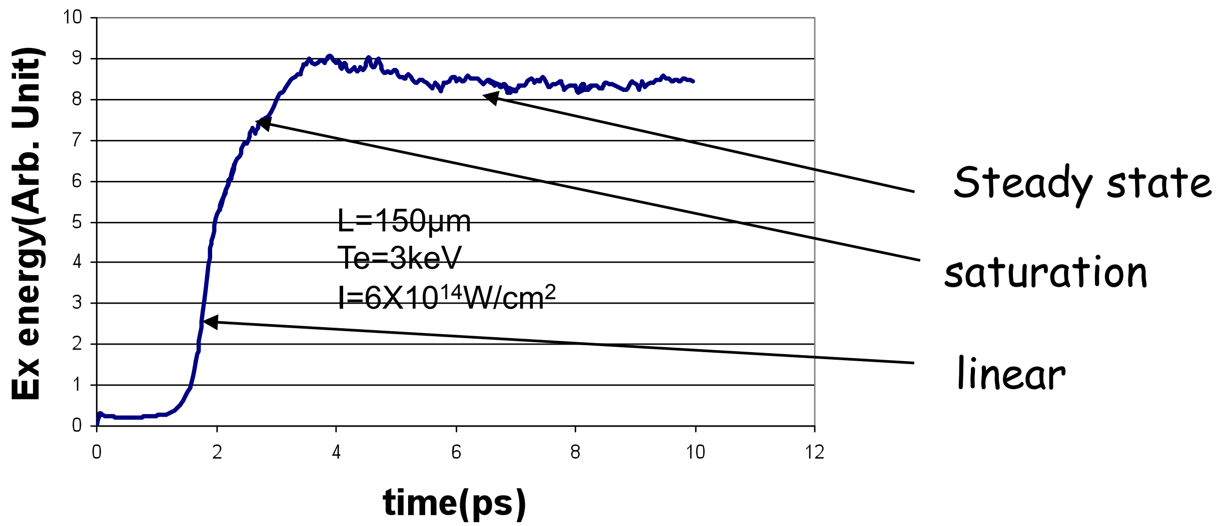


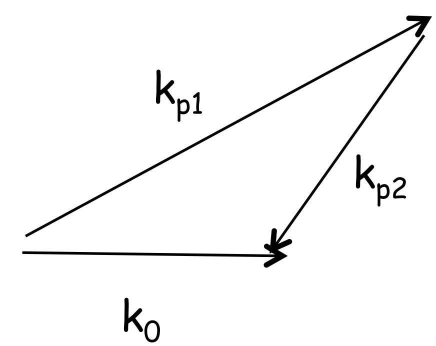
TPD converts an EM wave (E_y) into plasma waves (E_y & E_x)

FSC

UR LLE

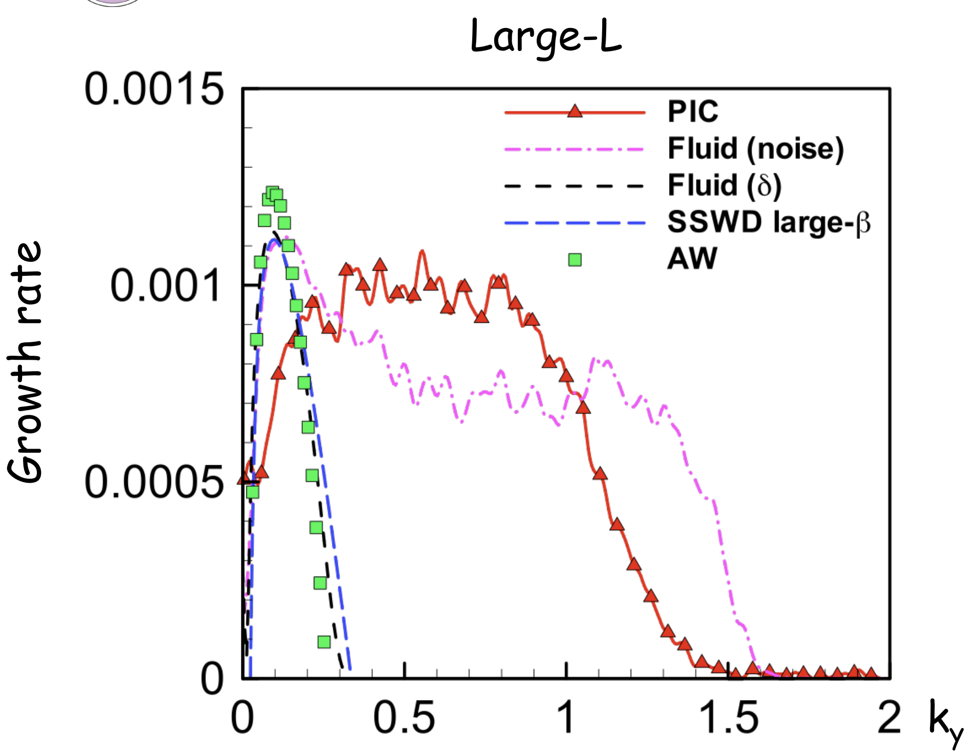
OSIRIS[1] simulation results





1, R. A. Fonseca, L. O. Silva, F. S. Tsung et al., Lect Notes Comput Sc 2331, 342 (2002)

There is general agreement for linear growth among theory, PIC, and fluid simulations

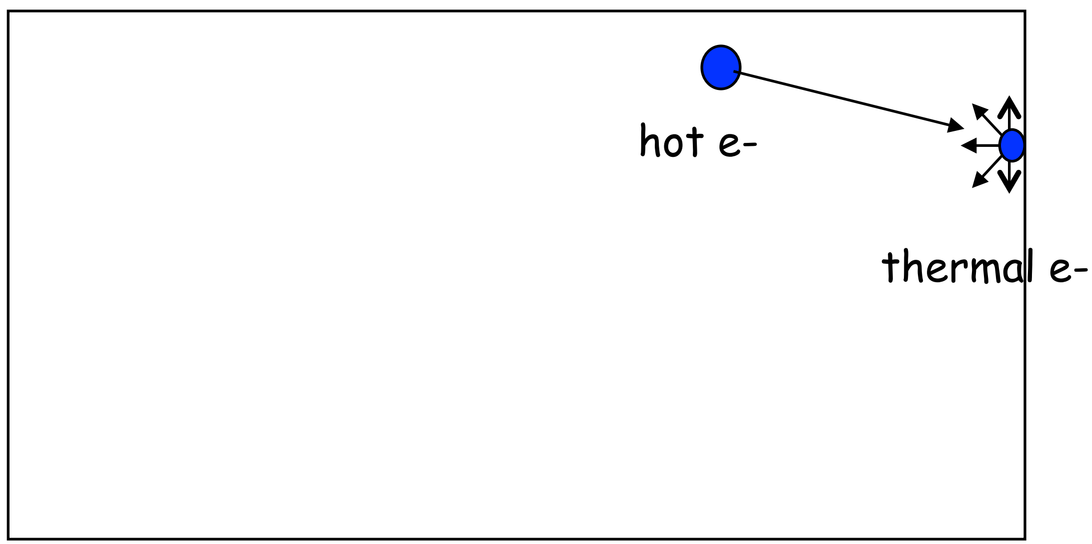


$I=10^{15}$ W/cm^2, L=150 micron
$T_e=T_i=2$ keV, $M_i/m_e=3410$
(Yan et al., PRL'09)

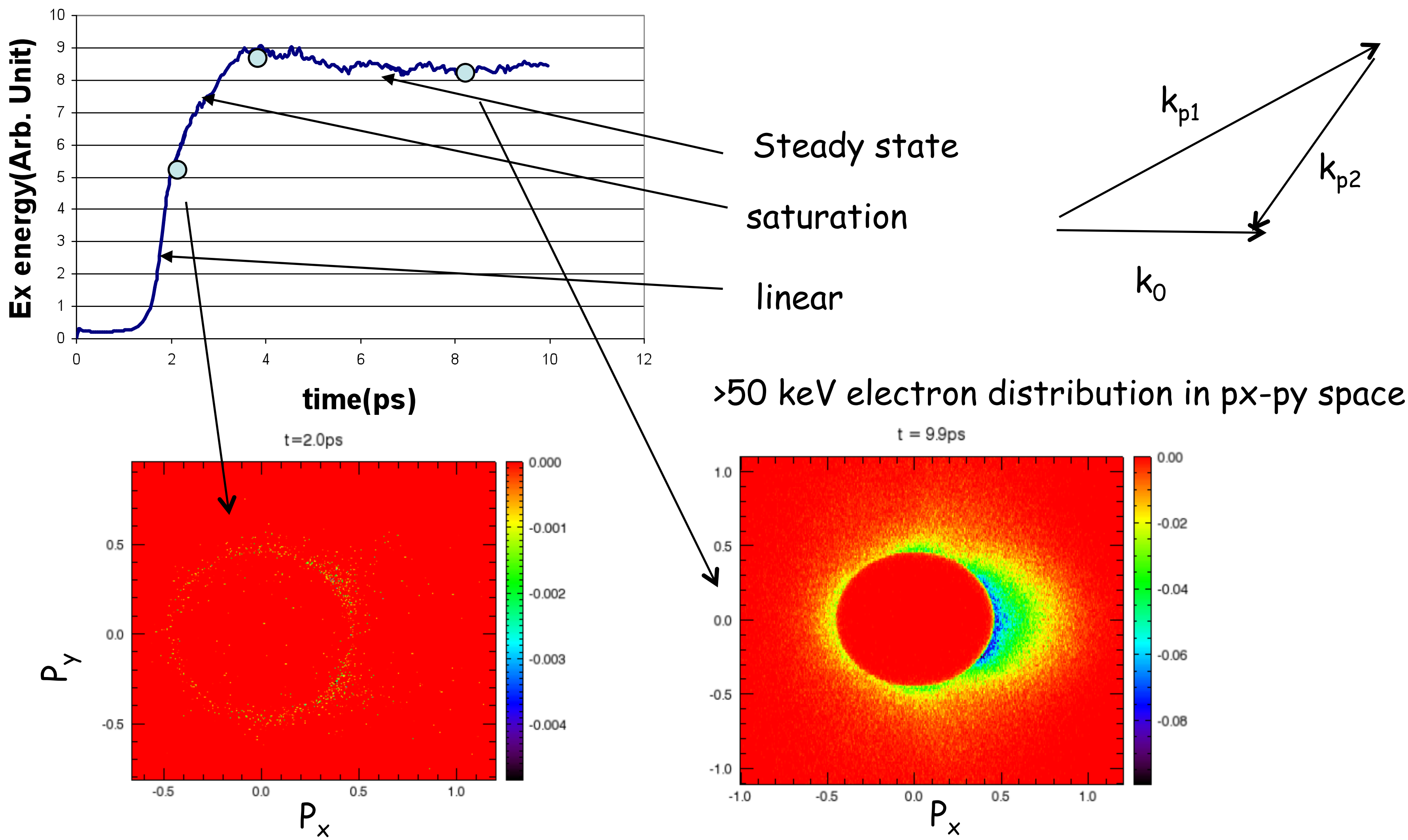
- Both PIC and fluid simulations saw absolute and convective modes
- The lower PIC growth rates in low k_y were due to pump depletion

Diagnostics in PIC simulations

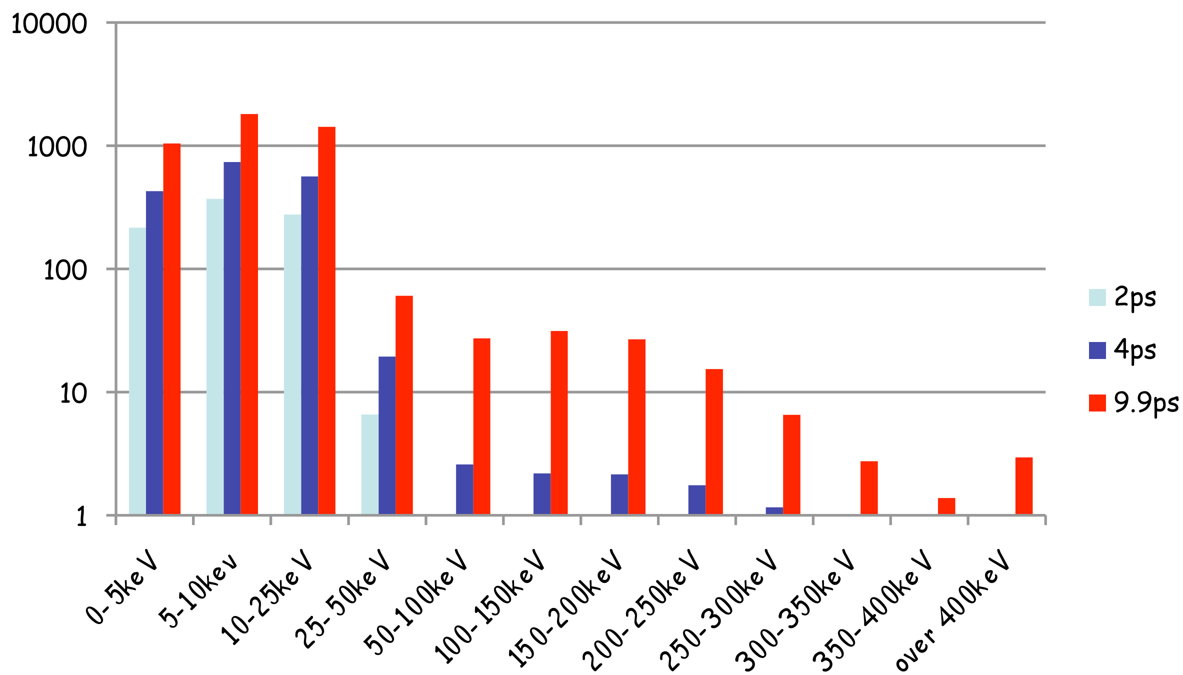
- The boundary diagnostic records the energy difference of the particles going out of and coming into the box.
- It also records the energy distribution of the particles going out of the rear boundary.



Most hot e- are produced in the nonlinear stage

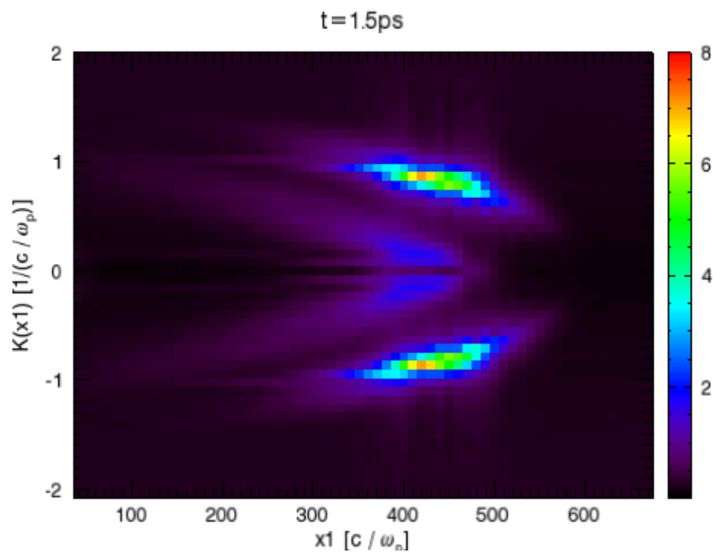


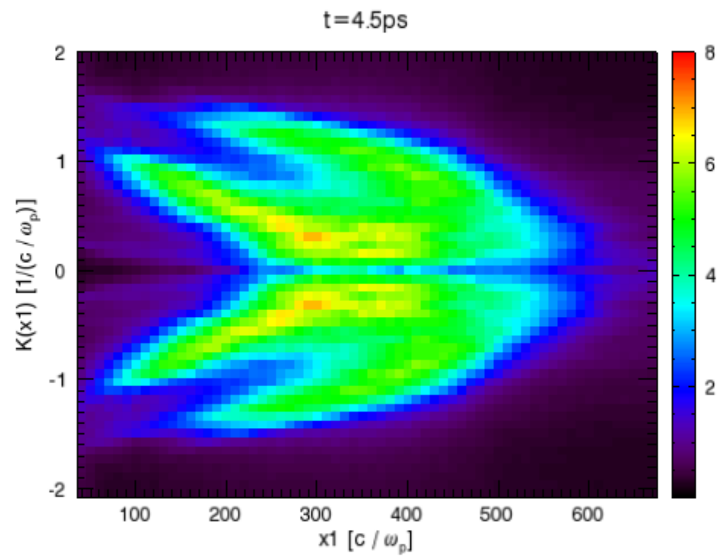
Most hot e- are generated in the nonlinear stage

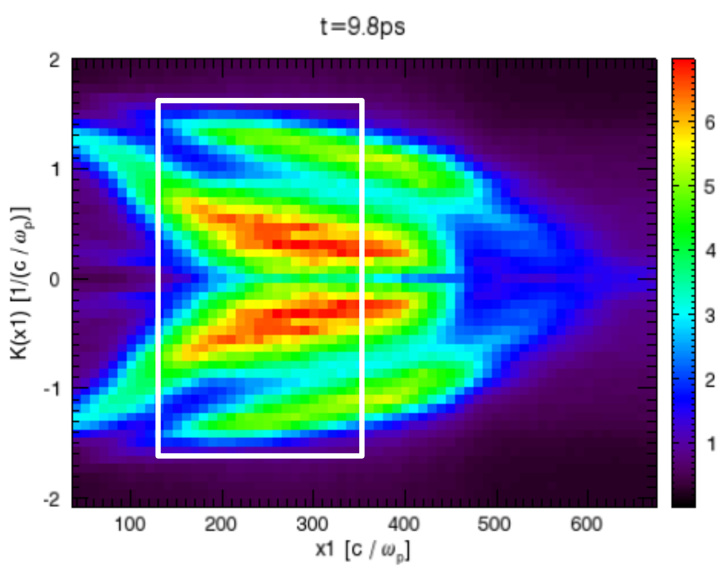


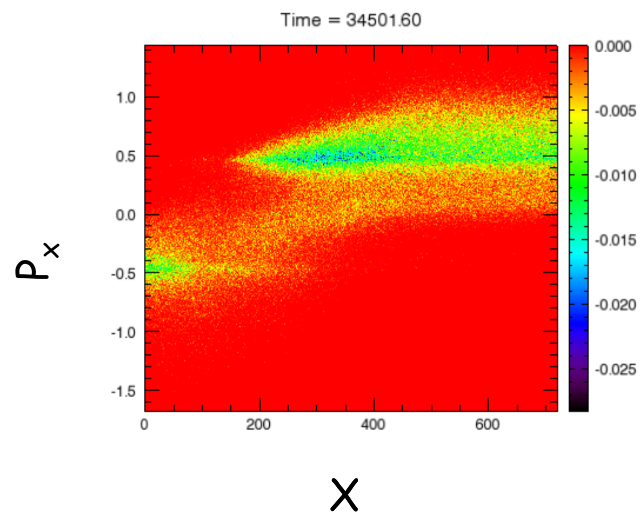
The existence of >100 keV e- is consistent with hard X-ray diagnostic

The appearance of hot e- (>100 keV) is correlated to new modes that are not seen in the linear stage









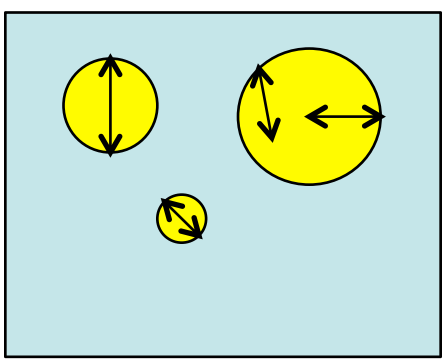
Plane-wave, 2D PIC simulations gave 10-100X more hot electrons than HXR measurements

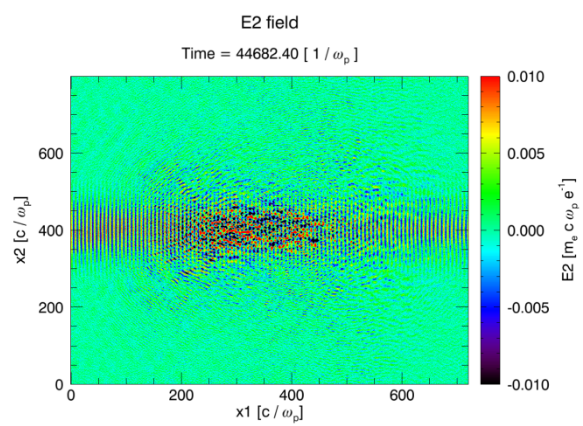
Max I_{14}	T_e(keV)	Ti(kev)	$L_{\mu m}$	Mi/me	Run time	Forward Hot e-(>50kev)	Abs	η
4	3	1.5	150	3410	5ps	~0 (100 ptc per cell)	~0	0.8
6	3	1.5	150	3410	10ps	17% (100 ptc per cell)	42%	1.2

B. Yaakobi et al., Phys. Plasmas **16**, 102703 (2009):
hot e- <1% of laser energy

Comparing the simulations with the experiments is usually challenging

- Are the hydro conditions used in PIC simulations right?
  - Large absorption indicates better coupling between PIC and hydro simulations is needed
- Speckles
  - Polarization smoothing changes laser polarization even within a single speckle
  - Simulation with a narrow beam has shown a reduced hot electron generation





Acknowledgement

V. K. Decyk, R. Fonseca, M. C. Huang, X. Kong, W. B. Mori,, J. Tonge, F. Tsung, L. O. Silva, R. Yan