WG1 – Computational Accelerator Physics

Summary

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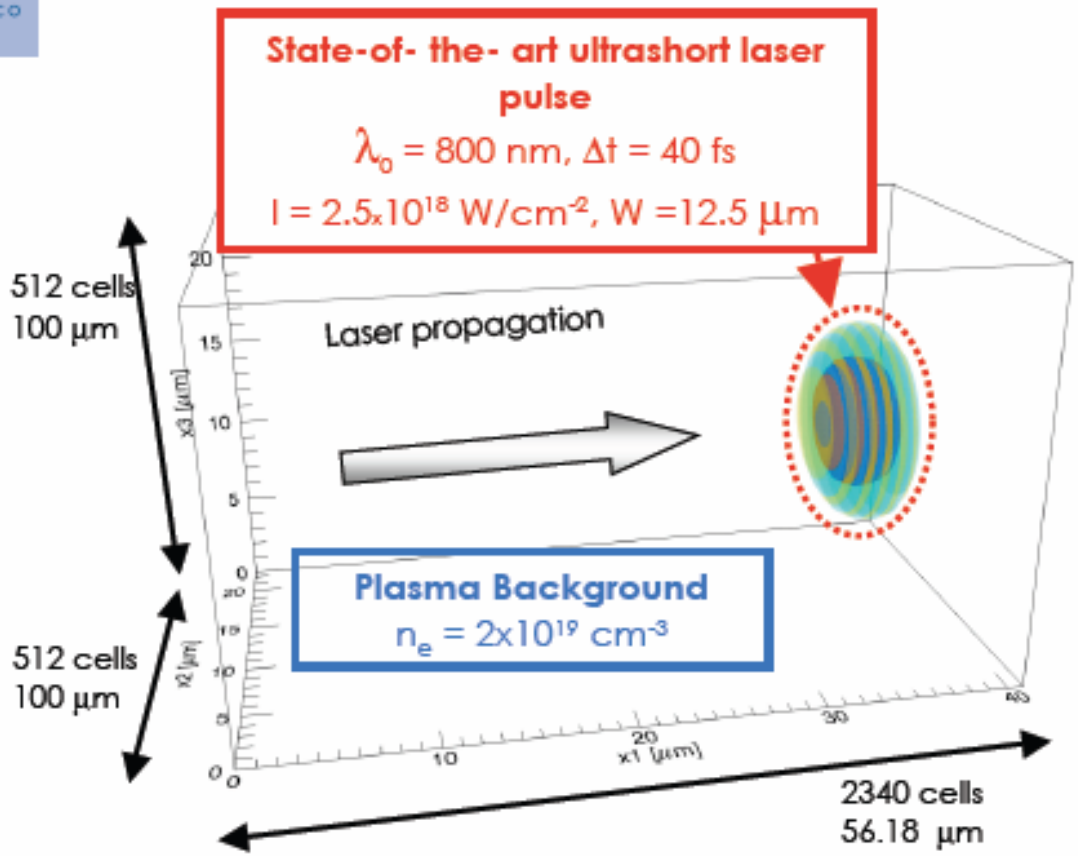
Focus question #1

- What is required for explicit PIC simulations of LWFA expt's to become quantitatively correct, with predictive capability?
  - 3D simulation results are very different from 2D
    - 2D remains useful for parameter scans & qualitative understanding
    - 3D requires 50,000 – 500,000 processor hours for *each* run
  - Recent successes of 3D explicit PIC are amazing
    - Pukhov *et al*. predicted "bubble regime" in 2002
    - Tsung *et al*. saw "monoenergetic" beams with OSIRIS in 2004
  - Fundamental uncertainties and difficulties
    - uncertainties in plasma density, laser pulse energy & shape, etc.
    - instabilities & "threshold" physics are hard to model quantitatively
  - e- beam charge and avg. energy can show good agreement
    - Simulated energy spread and beam emittance do not agree well

Full scale 3D Imperial College Simulation



- Simulation Parameters
  - Laser:
    - $a_0 = 1.1$
    - $W_0 = 12.5\,\mu m$
    - $\omega_l/\omega_p = 10$
  - Particles
    - 1x1x2 particles/cell
    - 600 million total
  - Plasma length
    - L=.12cm
    - 50,000 timesteps

Simulation ran for ~50,000 time steps
(~2 Rayleigh lengths)

The agreements between simulation and experiment is good

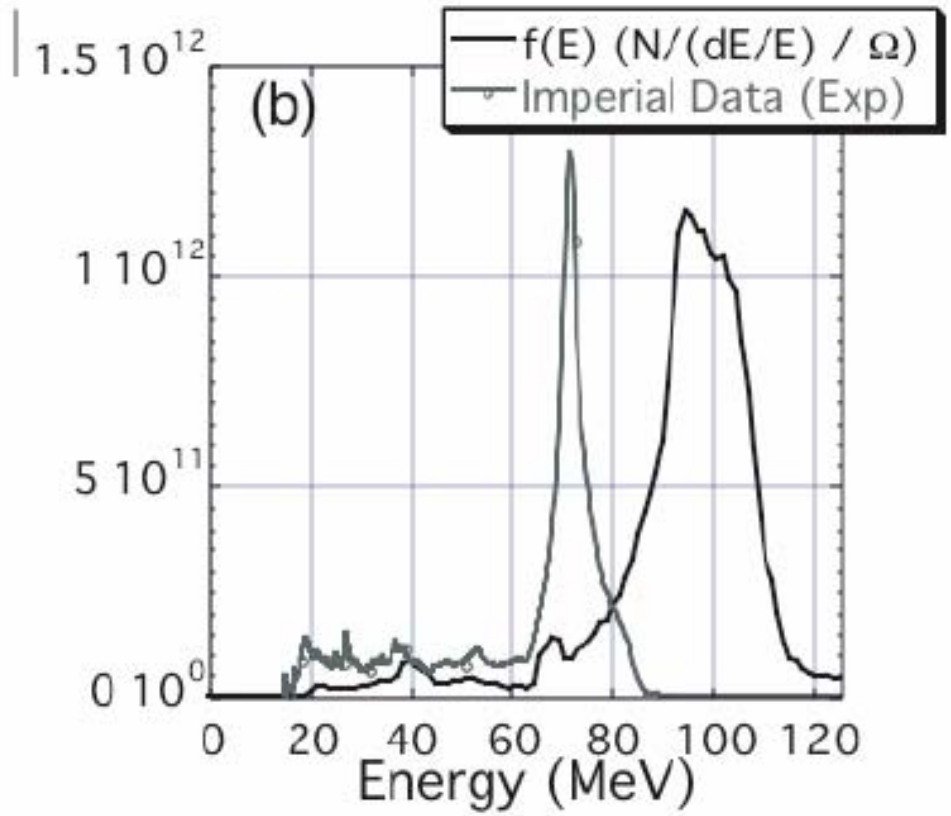
Total # of electrons:
2.3 10^8 (2.0 10^8 reported in *Nature*).

Average Energy ~95 MeV (*Nature* reports [50,80] MeV).

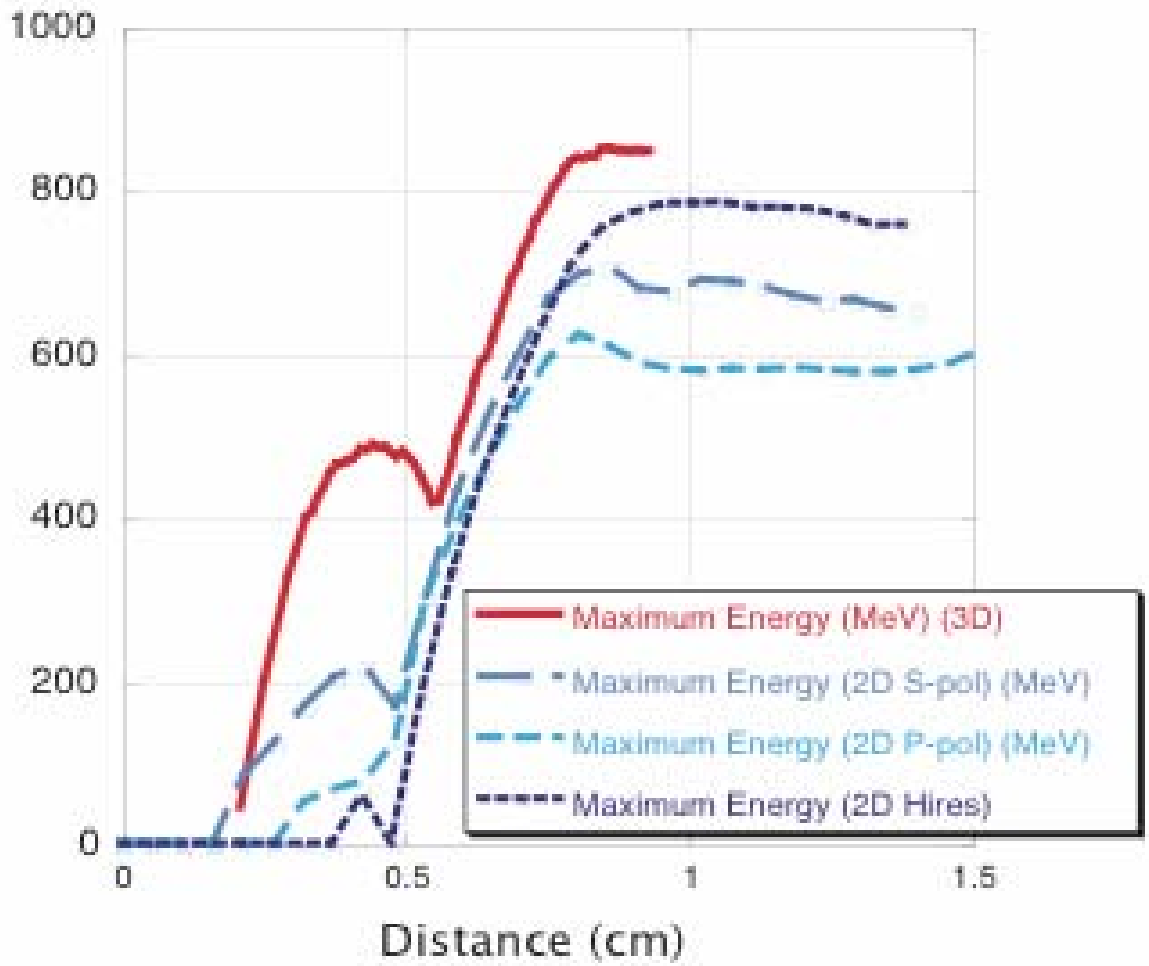
Normalized Emittance:

3.51 μm (in b)

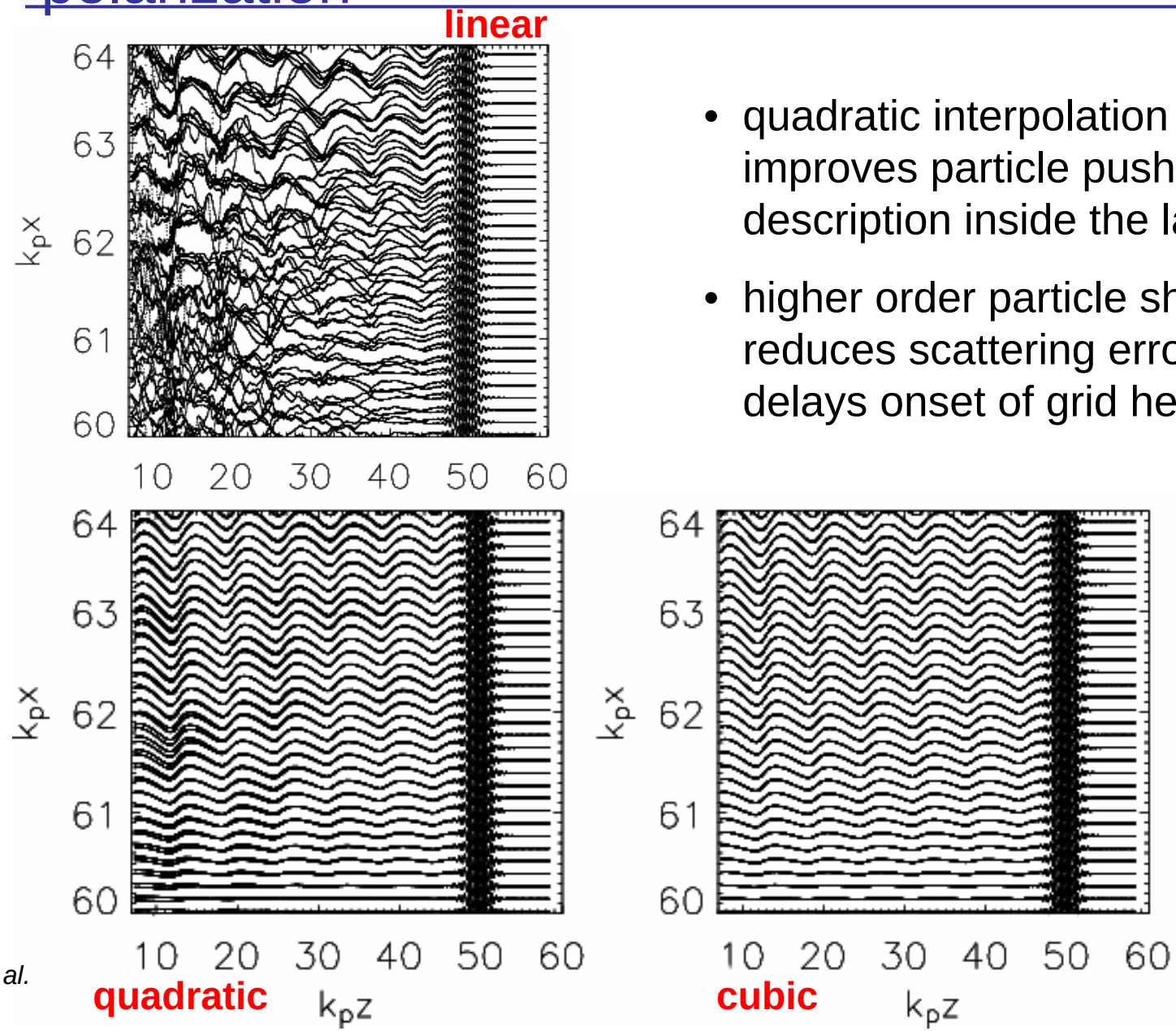
7.61 μm (in e)



2D vs 3D

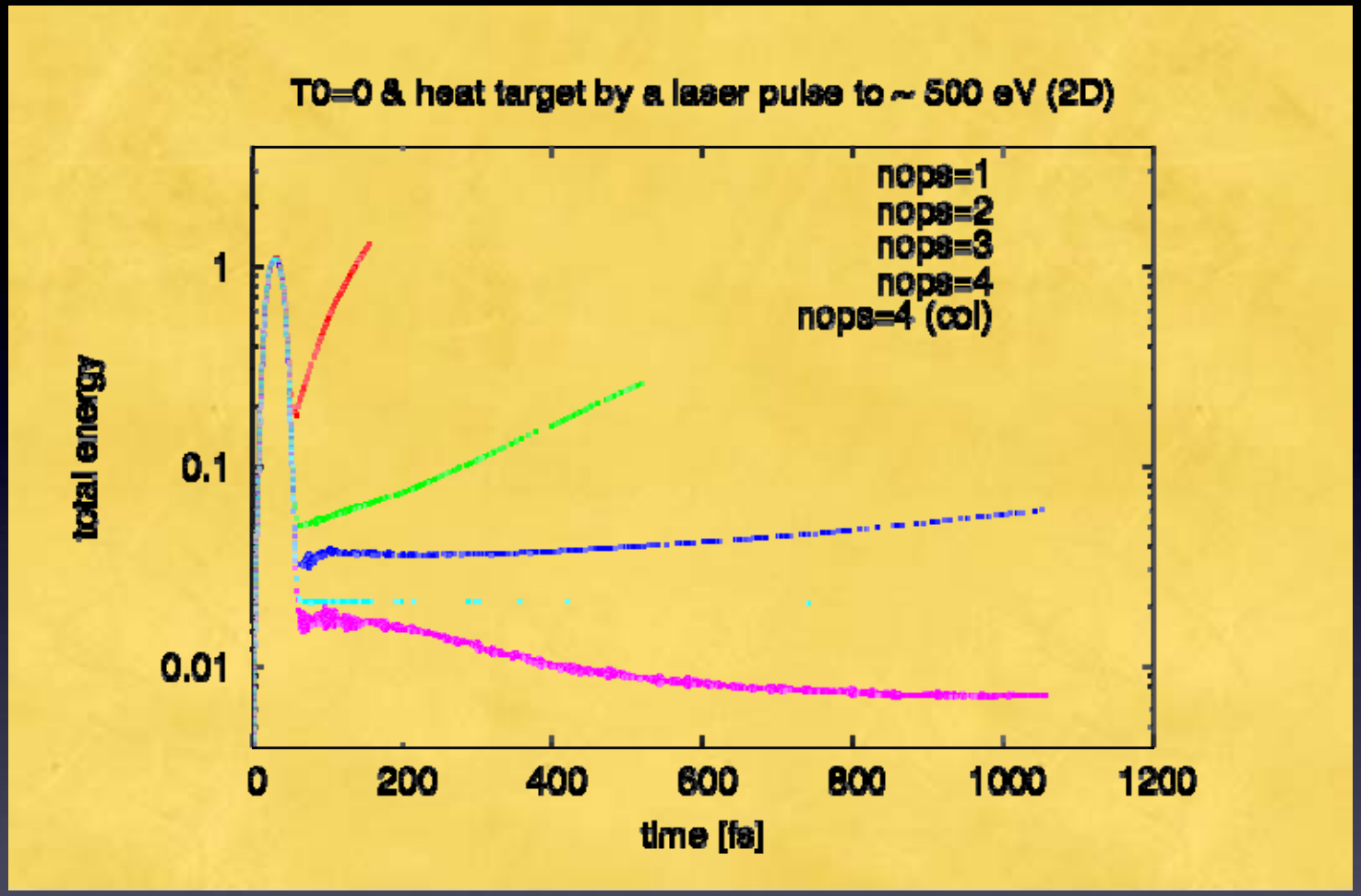

1000
800
600
400
200
0
0
0.5
1
1.5
Distance (cm)
Maximum Energy (MeV) (3D)
Maximum Energy (2D S-pol) (MeV)
Maximum Energy (2D P-pol) (MeV)
Maximum Energy (2D Hires)

Higher order particle shape: in the plane polarization



- quadratic interpolation improves particle push description inside the laser
- higher order particle shapes reduces scattering error and delays onset of grid heating

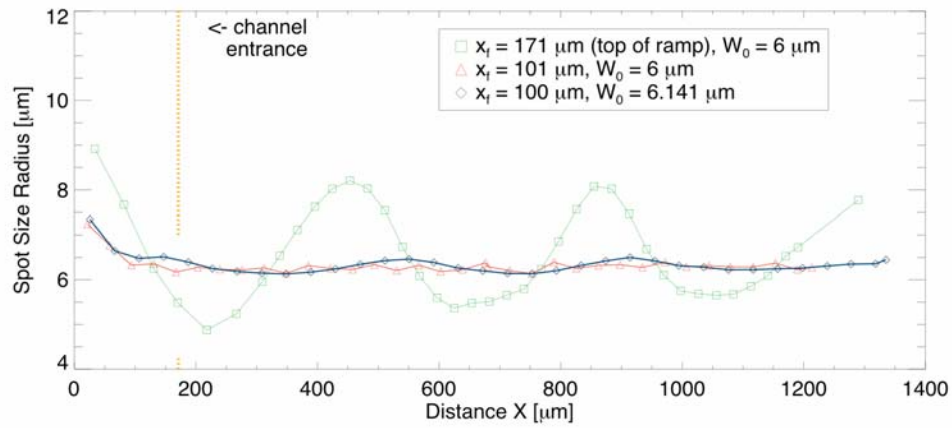
Estelle Michel *et al.*
UNR/LBNL

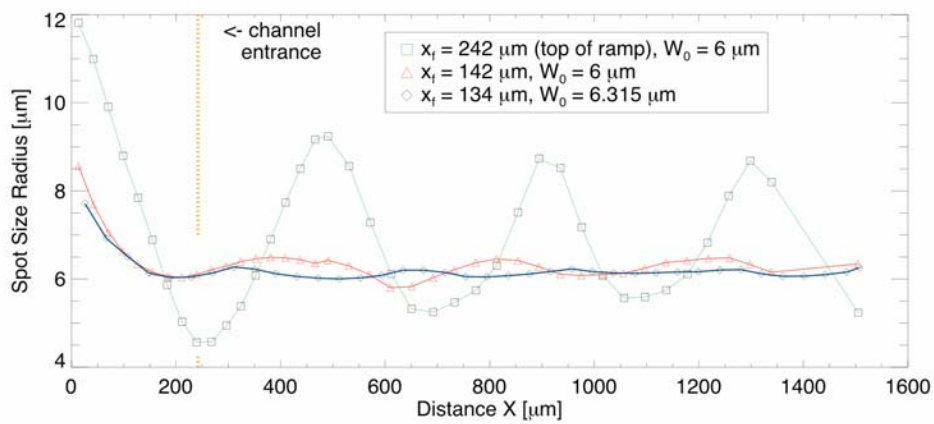


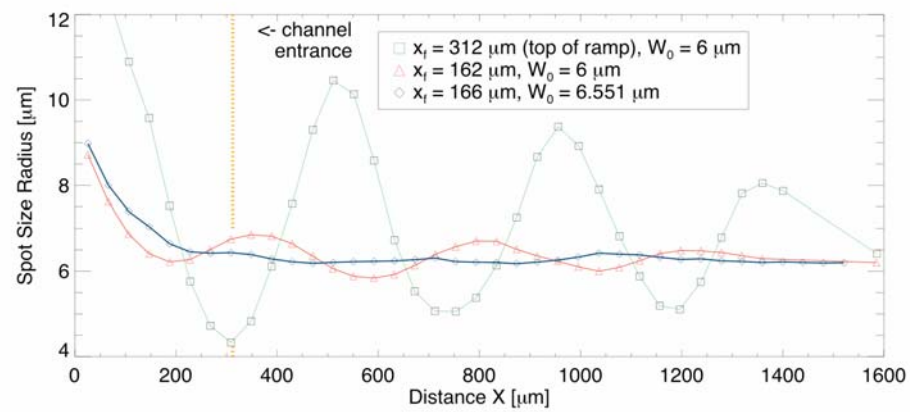
target 40nc, thickness 2 um,
box:10um x 6um
a=2, 30 fs, np=10

The PIC Simulations Confirm the Theoretical Prediction for the Optimal Coupling

- Preionized plasma channel cases with different ramp lengths: Z_R, $1.5Z_R$, $2Z_R$.



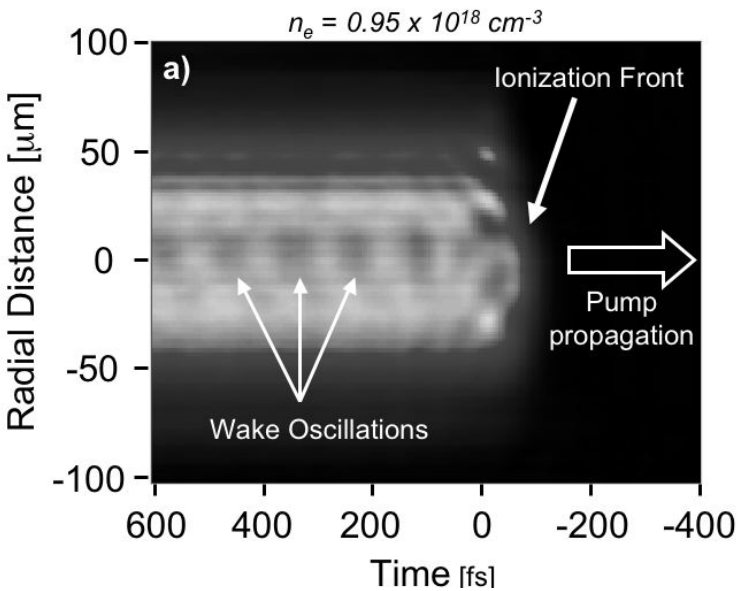


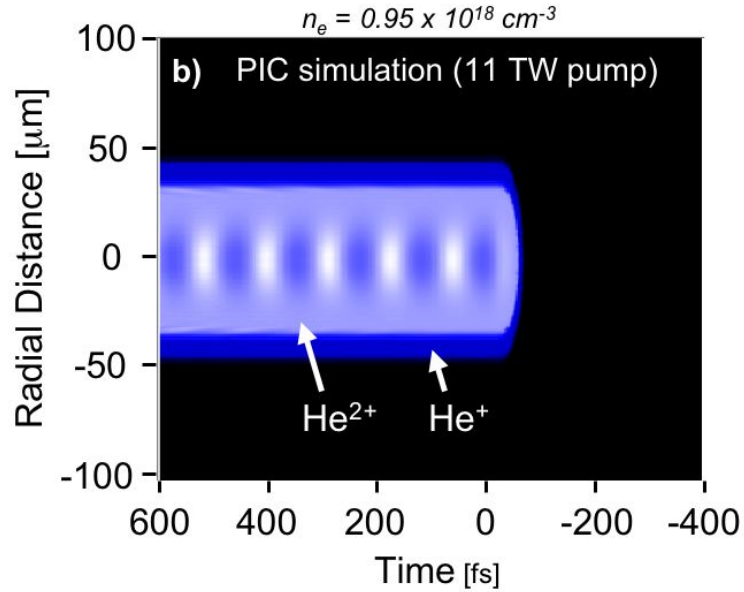


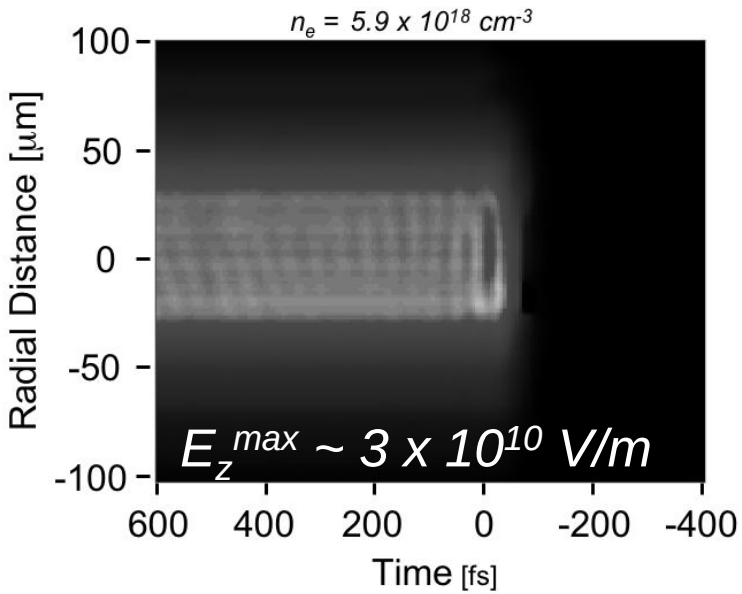
N. H. Matlis et al., submitted to Nature Physics (2006)

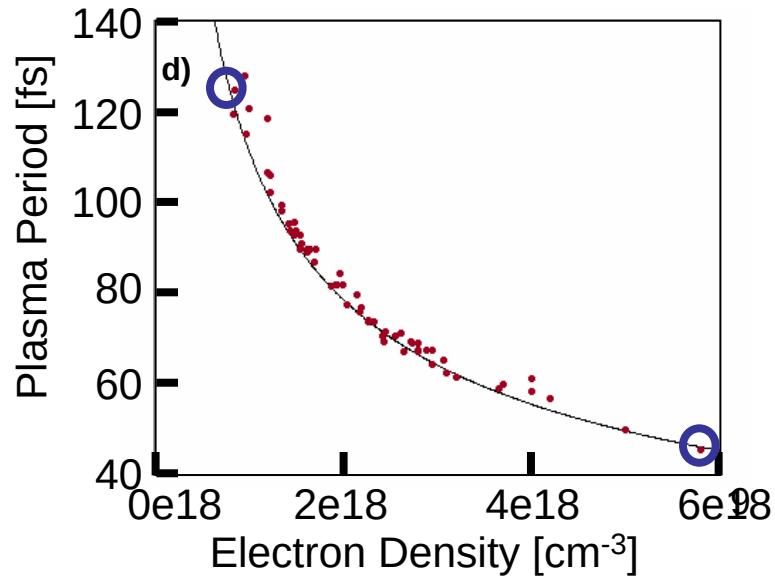
Holographic snapshots of laser wakefields

P ~10 TW, I ~ 10^{18} W/cm^2

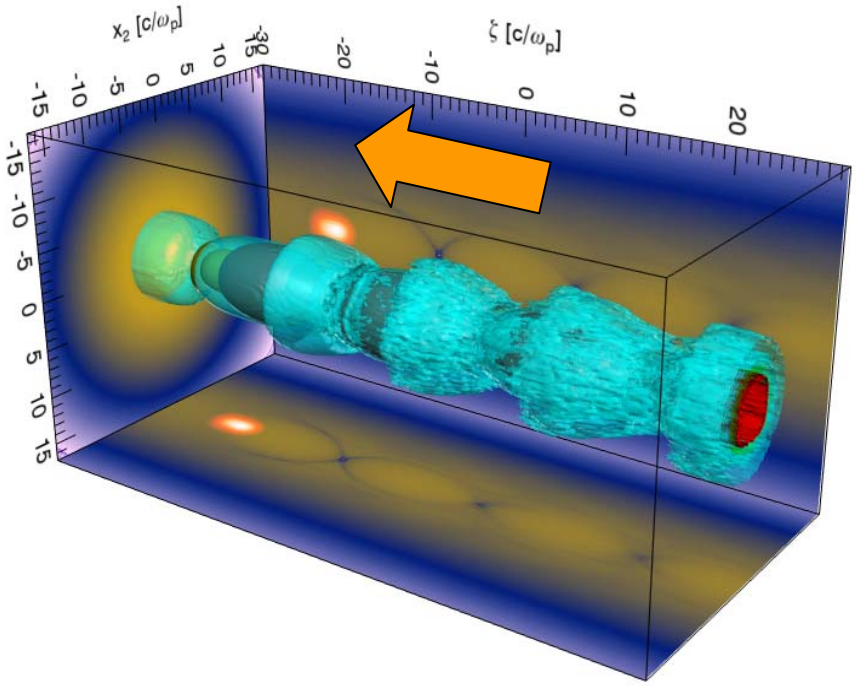


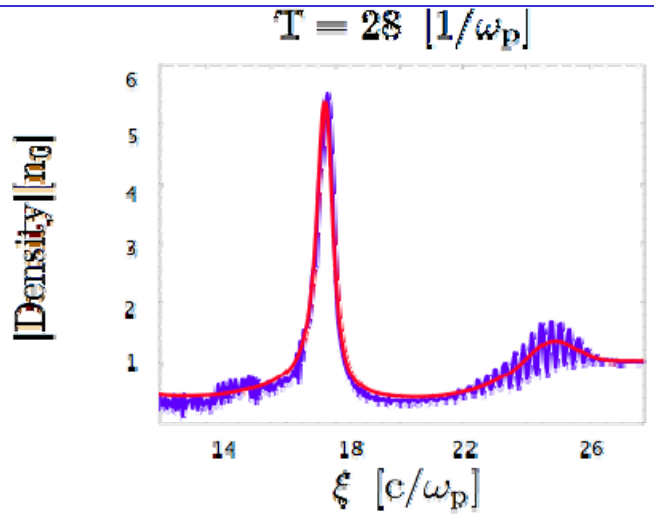


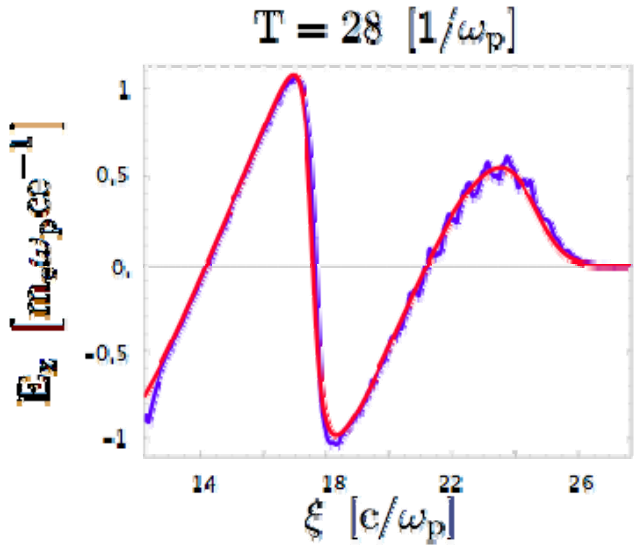




Non linear regime: a_0=2







3D OSIRIS

QUICKPIC

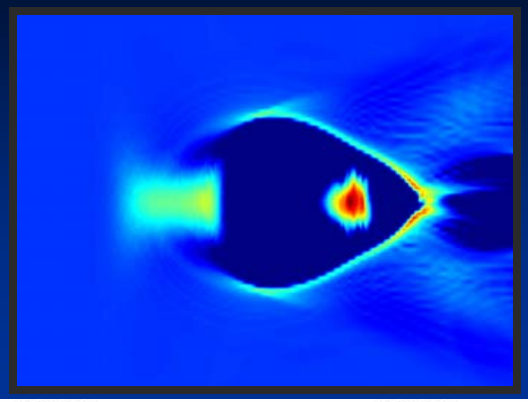
Tev class afterburners

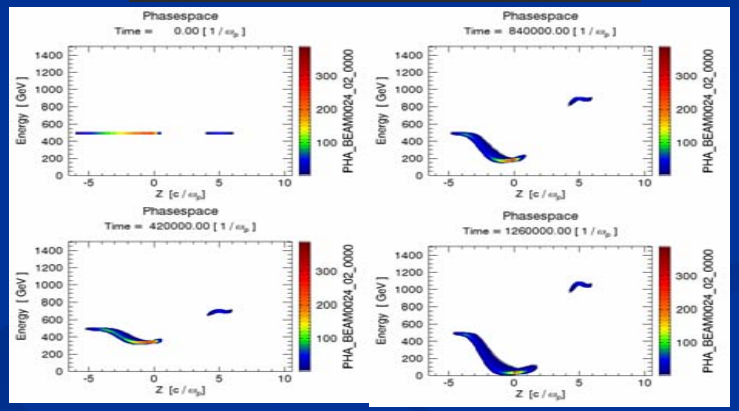
- By taking advantage of the two different time scales in PWFA problem, QuickPIC allows 100 times time-saving for afterburner type simulation compared with full PIC code.

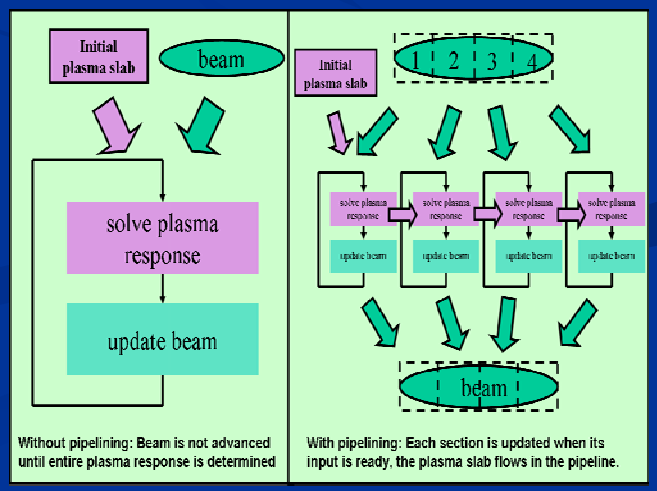
- Full scale simulation studies of TeV class afterburner conceptual designs can now be done using a quasi-static PIC code QuickPIC.

- Simulation shows 500 GeV energy gain in plasma afterburner stage is possible with reasonable beam quality, more study of the hosing and ion motion issues need to done.

- Software pipelining technique can further improve turn-out time of TeV class afterburner simulation.





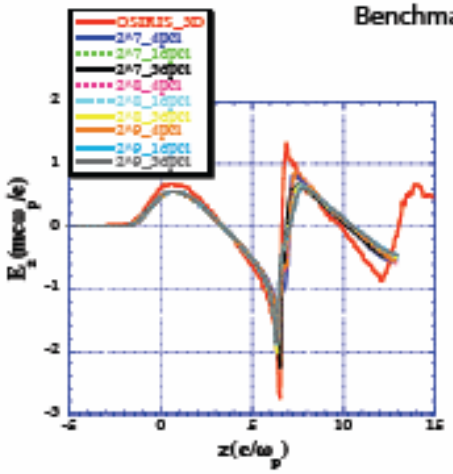


Adding realism into QuickPIC

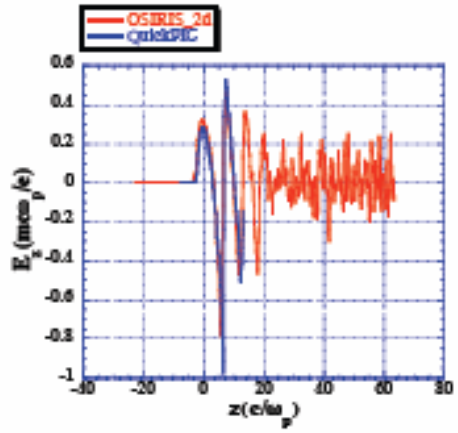
Miaomiao Zhou (UCLA)

Implementation of field-ionization in quasi-static QuickPIC

Benchmark versus OSIRIS



(a) Far above ionization threshold

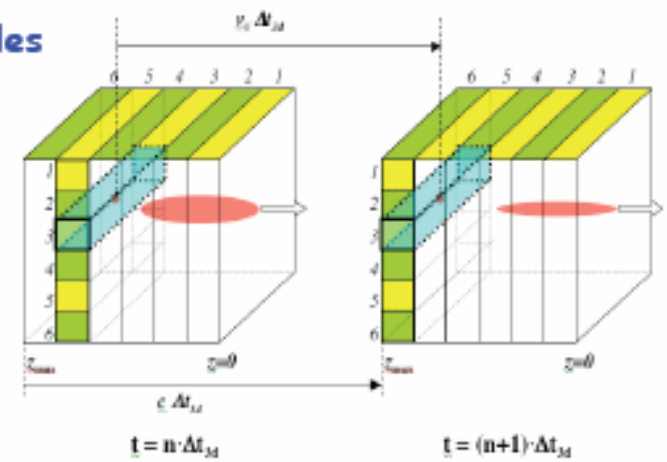


(b) Near ionization threshold

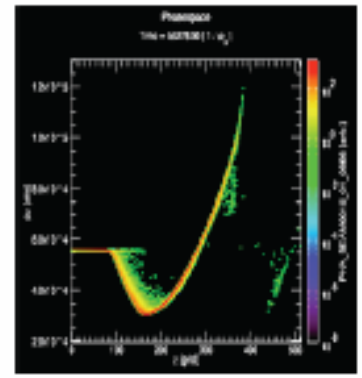
Dealing with trapped particles

"Promote" trapped plasma particles to beam particles.

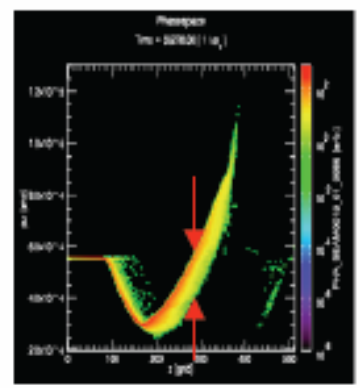
$$z^{n+1} = z^n + (c - v_{//}) \cdot \Delta t_{3d} < z_{max}$$



Modeling synchrotron radiation effects



(a) Without radiation drag



(b) With radiation drag

Broadening agreed well with theoretical estimation.

Electron hosing instability in the blow-out regime

Linear fluid theory (Lampe & Whittum 93)

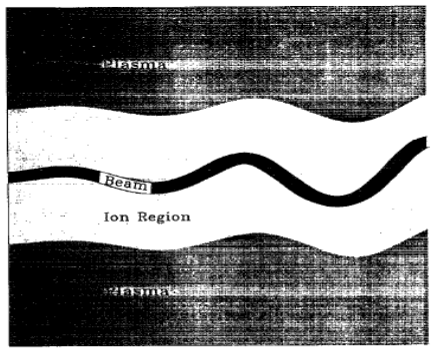
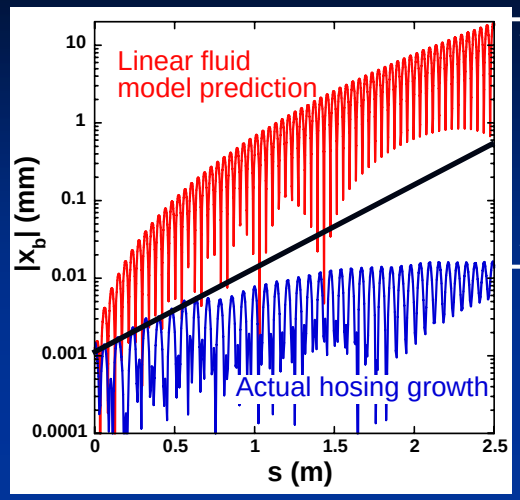


FIG. 2. Schematic of the unstable beam, which is propagating from right to left. The neutralization radius, as well as the beam, experiences growing hoselike oscillations.



3 orders of magnitude

Simulation shows much less hosing

Assumptions: $I_b << I_0 \equiv mc^3/e = 17$kA

Return current sheet not important

Equilibrated channel

Equations:

0th order, adiabatic

Fields

$$\nabla_\perp^2 \phi_e = 4\pi n_e e,$$

$$\nabla_\perp^2 \phi_b = 4\pi n_b e.$$

Plasma

$$\frac{\partial n_e}{\partial \tau} + \nabla_\perp \cdot (n_{e0} \mathbf{v}_e) = 0,$$

$$\frac{\partial \mathbf{v}_e}{\partial \tau} = \frac{e}{m} \nabla_\perp \phi.$$

Beam:

$$\frac{\partial^2 x}{\partial z^2} + k_\beta^2 x = -\frac{eE_{xp}}{mc^2\gamma} = \frac{2\pi n_p e^2}{mc^2\gamma} X_c,$$

Non-relativistic, electro-static

Linear perturbative hosing theory of the relativistic motion is developed

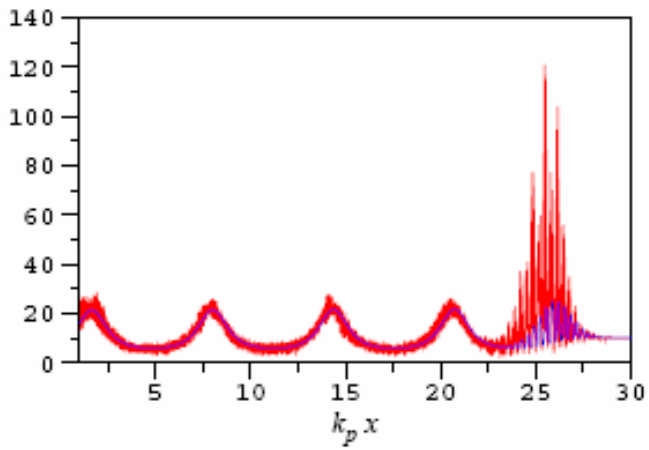
$$\partial_\xi^2 x_c = c_r c_\psi c_l \omega_0^2 (x_b - x_c)$$

c_r, c_ψ, c_l represent effects from channel radius, relativistic motion, plasma shielding respectively. Generally $c_r c_\psi c_l \sim 0.1$-0.2 for the blow-out regime, therefore hosing is reduced. Very good quantitative agreement with simulations.

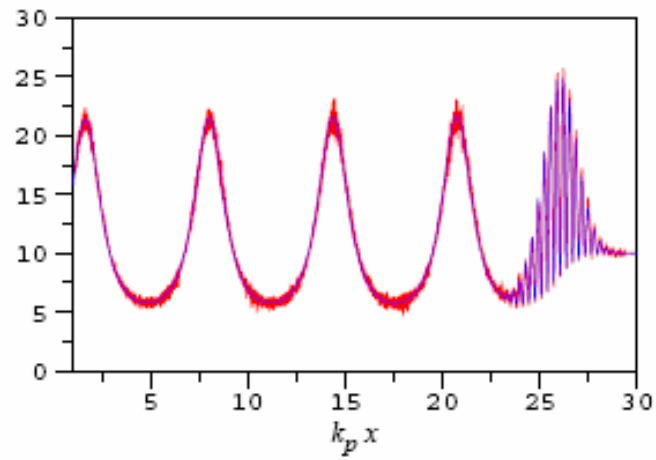
Comparing Vlasov and PIC...

Longitudinal momentum spread (Π_{zz}) in eV

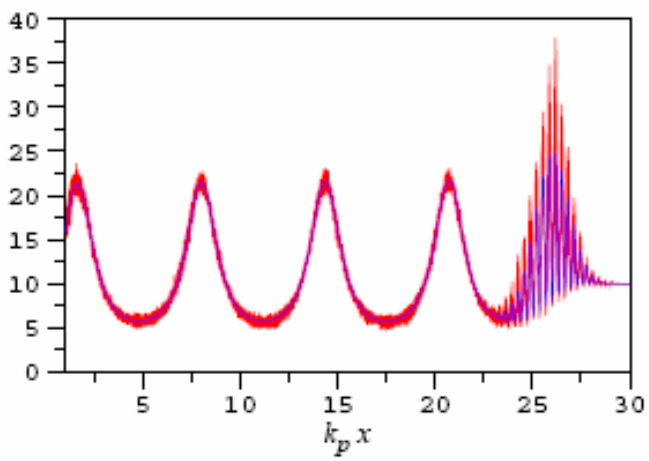
$\lambda_0/\Delta x = 20$ $N_p = 400$



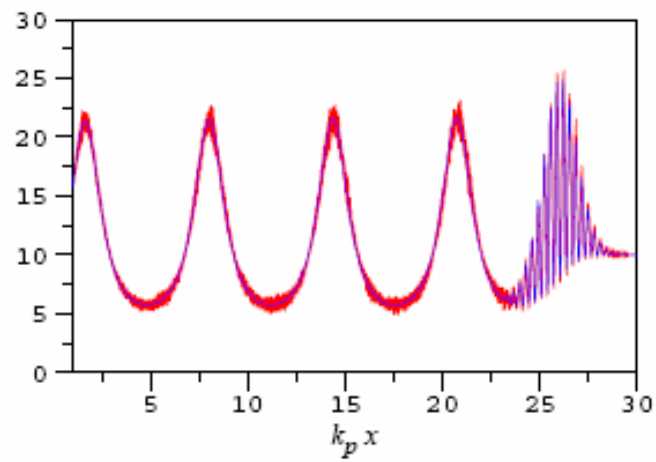
$\lambda_0/\Delta x = 320$ $N_p = 400$



$\lambda_0/\Delta x = 40$ $N_p = 800$



$\lambda_0/\Delta x = 640$ $N_p = 400$



Focus question #2

- Should electron photoinjector simulations be electrostatic or electromagnetic, or both?
- Answer: Both approaches should continue to be used

Electromagnetic

- Some problems require this approach
  - in a SC rf photoinjector with high peak current (> 1 nC) and high avg current (i.e. fill all rf buckets), wakefields could generate large dipole, quad. or higher order modes, which are intrinsically 3D and depend on cavity geometry
  - very high gradient & charge → radiating EM fields at cathode
- Computationally intensive
  - Courant limit sets the time step
  - fine resolution near photocathode
  - requires parallel computing

Electrostatic

- Well-tested and benchmarked
  - Parmela used for many years
- New developments are continuing
  - IMPACT-T (3D, parallel, slices)
  - wavelet-based de-noising
  - benchmarked with Parmela
- Fast
  - No "Courant limit" for stability
- IMPACT-T
  - parallel 3D PIC in beam frame
  - Lorentz transform to lab frame
  - multiple energy slices correctly handle large energy spreads
- Parmela
  - serial, GUI
  - interface to superfish

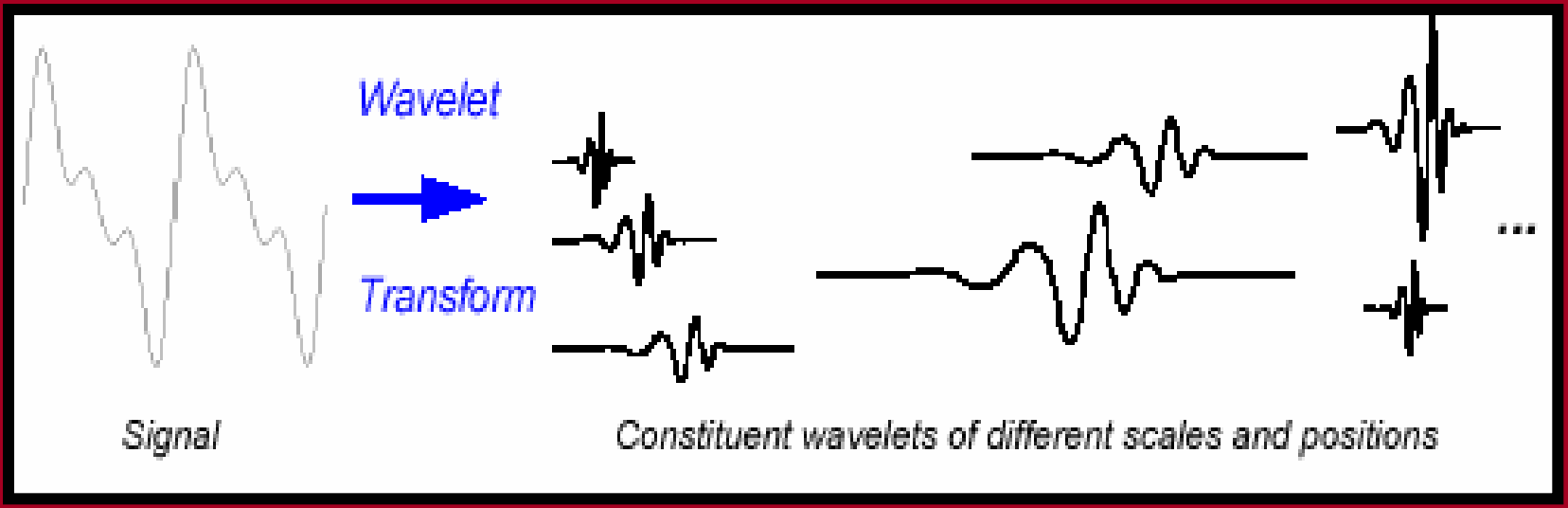
The IMPACT-T code

- 3D Integrated Green method to accurately compute the space-charge forces for a beam with large aspect ratio
- 3D Shifted Green method to efficiently compute the space-charge forces from the image charge
- Multiple slices/bins to handle the beam with large energy spread
- Arbitrary overlap of external fields to allow the modeling of both standing wave and traveling wave structure
- Transverse and longitudinal wakefield effects included (in testing)
- Parallel implementation on high performance computer to allow multiple million, high resolution simulation

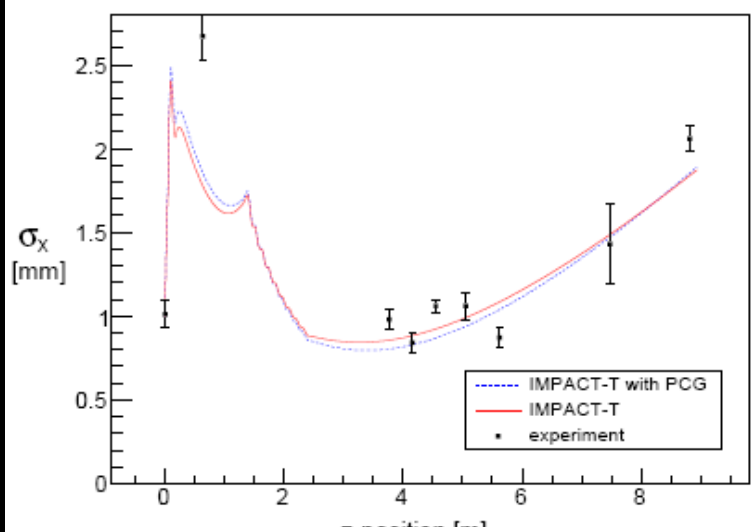
What are Wavelets?

In general, they are a family of representations using:

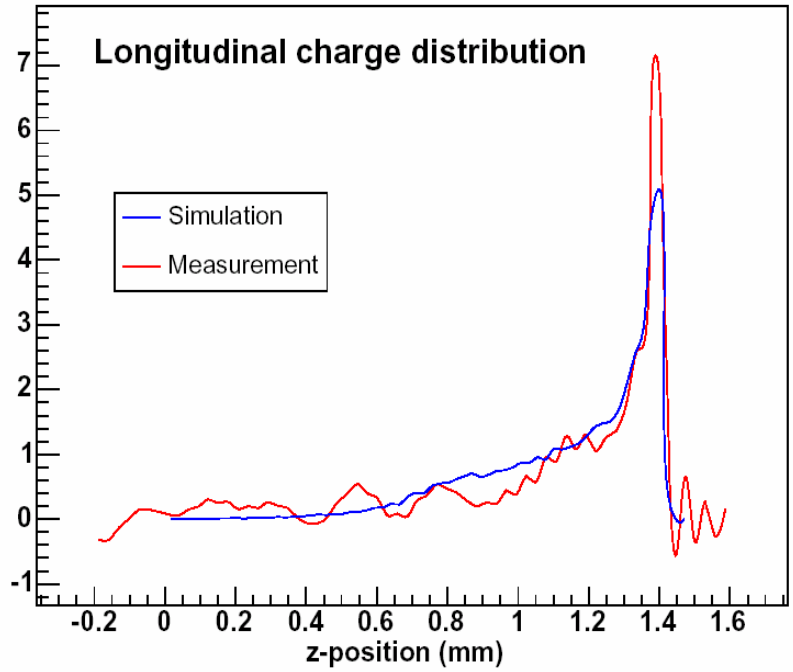
- **hierarchical (nested), often orthogonal basis functions**
- **finite domain ("compact support")**
- **fast transforms (faster than FFT!)**



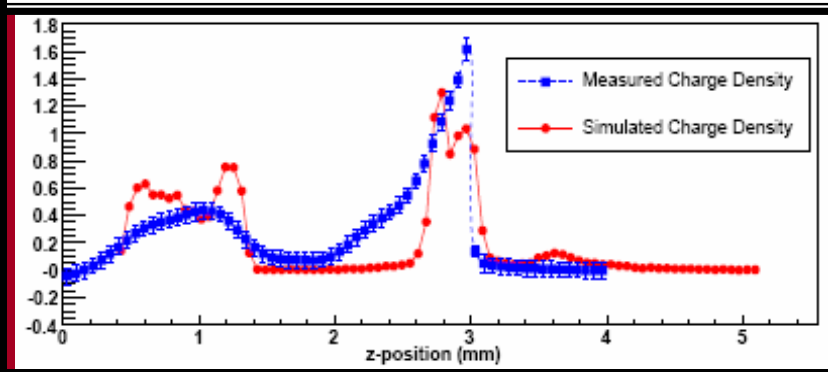
Code Validation: Fermilab/NICADD Photoinjector Data



Transverse rms beam size of 1 nC bunches: measured (·), conventional IMPACT-T (——), Wavelet IMPACT-T (– – –).



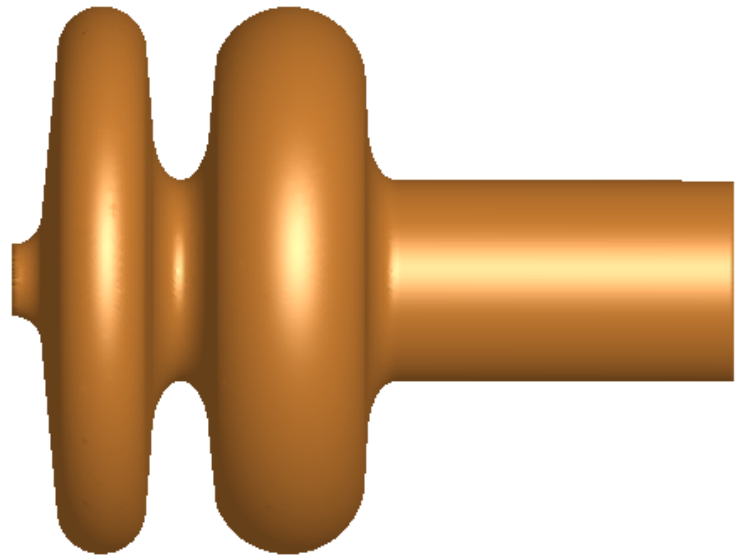
Longitudinal density profile of compressed 3 nC bunches: measured (red) vs. PARMELA with 20,000 particles (blue).

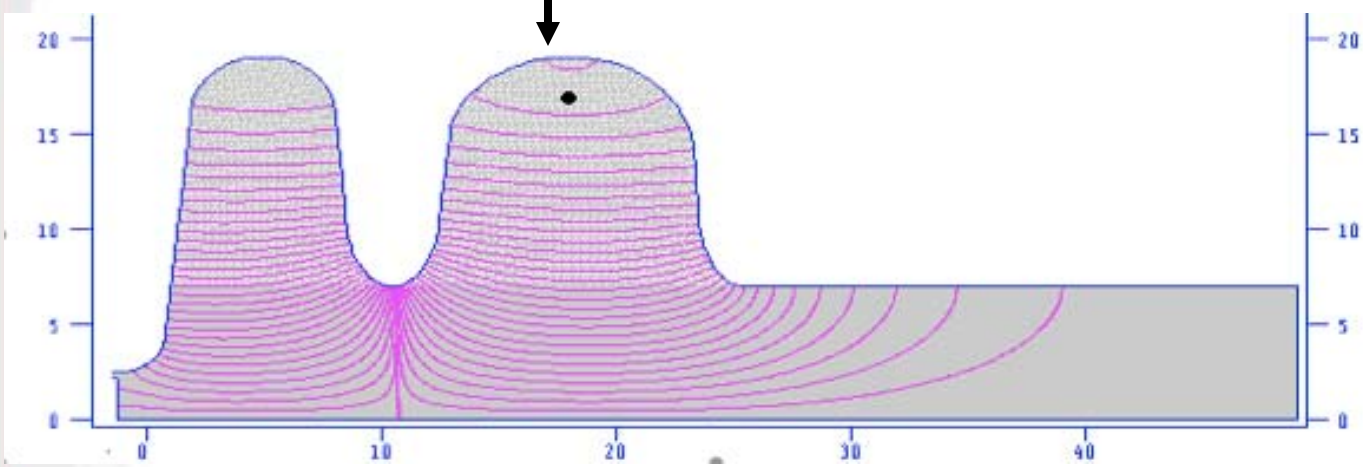


Longitudinal density profile of compressed double-bunch (0.5 nC ea.) configuration: measured , conventional IMPACT-T.

Simulation parameters are for the 1.5 Cell RF Gun Developed in BNL - (1)

- 3D geometry of the gun in VORPAL:
- Based on a SUPERFISH axial symmetry description:





D. A. Dimitrov, *Initial 3D EM RF Gun Simulations with VORPAL*, AAC06, 7/10-15/06.

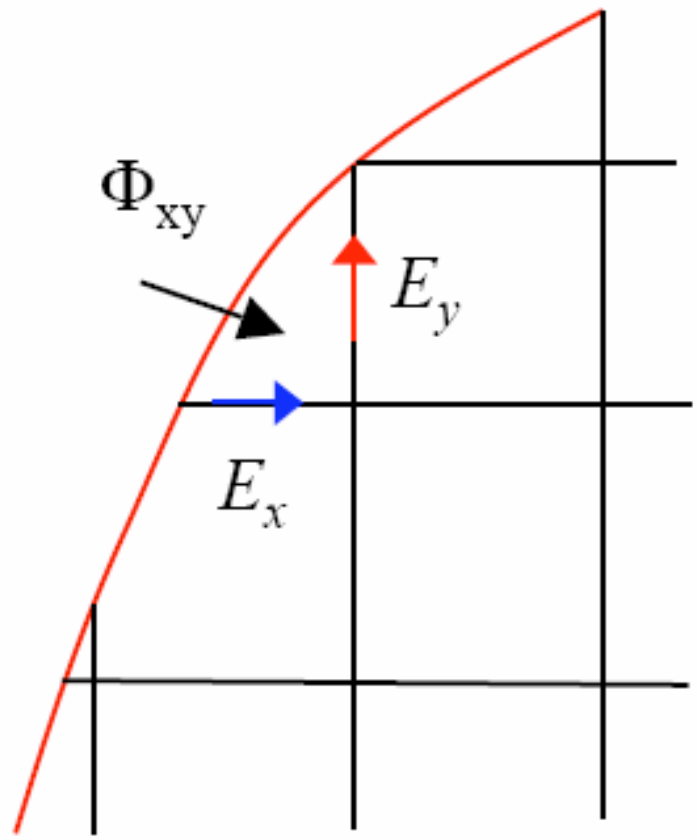
Resurgence of regular grids: cut cells give same accuracy as finite elements

- For cells fully interior, use regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via

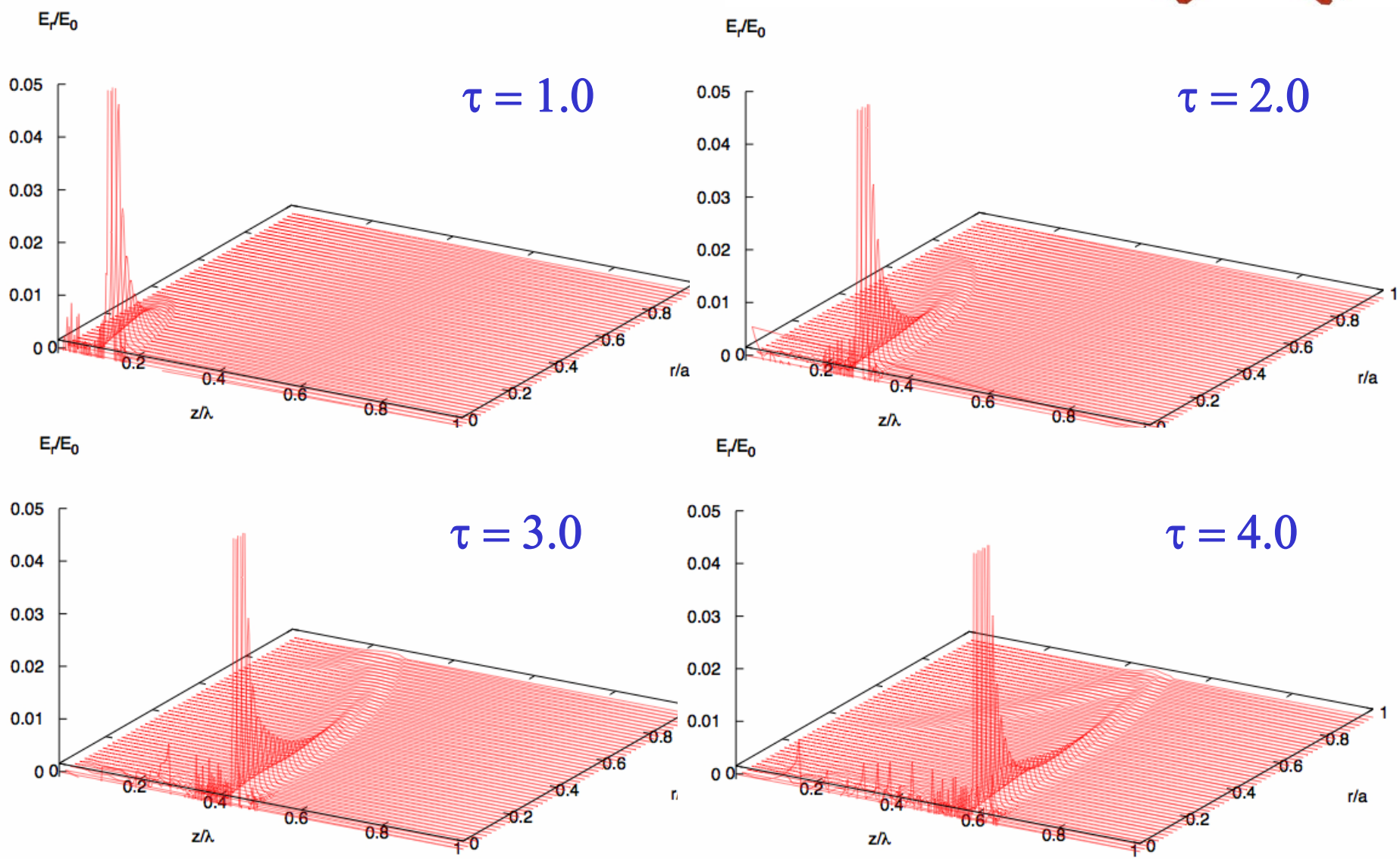
$$\dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y$$

  - Update fields via

$$B_z = \Phi_{xy} / A_{xy}$$



Numerical Solution of E_r (C. S. Park)



Photocathode Modeling

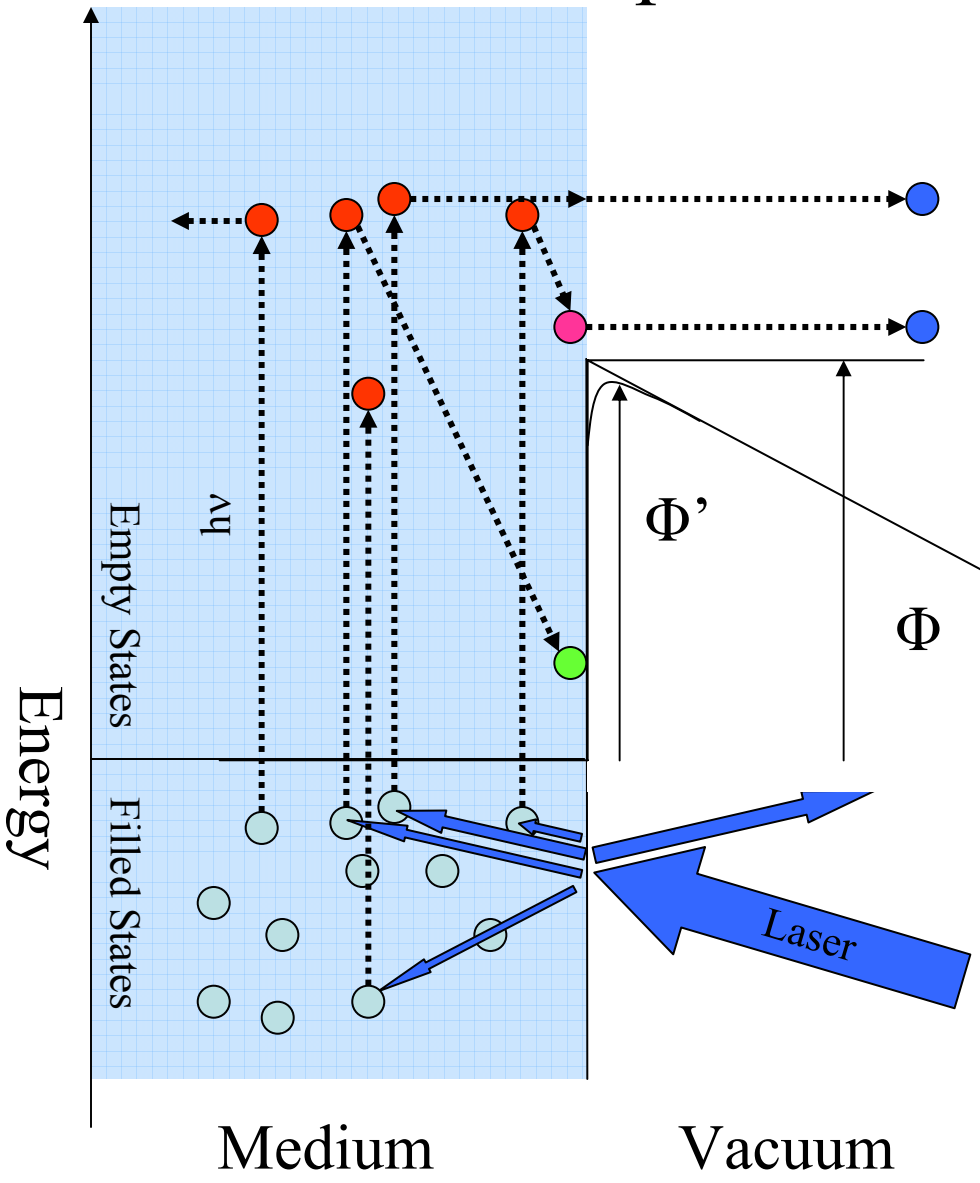
John Smedley

- Modeling should start with the emission process from the cathode, especially for semiconductors
- Detailed theories exist to describe the process of photoemission, and give the quantities of interest for accelerators: QE, initial random energy ('thermal'), temporal response, angular spread
- Numerical implementation of these models is in progress
- An experimental program to characterize cathodes is needed, especially for semiconductors (time for Light Sources to help us)

Thanks to Kevin Jensen (NRL)

BROOKHAVEN NATIONAL LABORATORY

Three Step Model of Photoemission

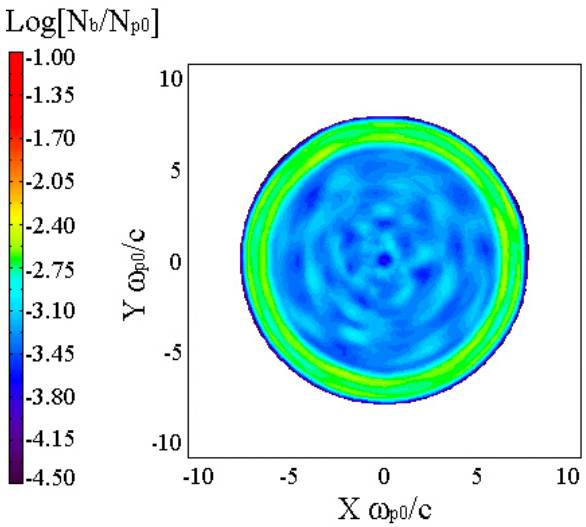


1) Excitation of e^- in metal
   - Reflection
   - Absorption of light
   - Energy distribution of excited e^-
2) Transit to the Surface
   - e^--e^- scattering
   - Direction of travel
3) Escape surface
   - Overcome Workfunction
   - Reduction of Φ due to applied field (Schottky Effect)

Integrate product of probabilities over all electron energies capable of escape to obtain Quantum Efficiency

M. Cardona and L. Ley: Photoemission in Solids 1, (Springer-Verlag, 1978)

Simulating other AA concepts

- High-energy density physics (HEDP)
- High-intensity beams
- Photonic Band Gap (PBG) accelerating structures

Benchmarking with the LSP PIC