Computational Accelerator Physics: Looking forward from a brief history

JOHN R CARY

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Thanks

Svetlana Shasharina Cary, my lifelong partner and co-founder of Tech-X

Thanks to Sandra Biedron for nominating me

Thanks to the committee. I am genuinely sorry to not see Ilan Ben Zvi here.

Thanks to IEEE for creating this award.

Apologies for not being comprehensive in this 12 minutes.

Evolution, Future, Lessons Learned

- Early days: separation, tracking and EM
- More recent: accurate particles + fields combination
- Current: High accuracy, self-consistent beams
- Future: Exascale (device based computing), more scale coverage, new algorithms, self-consistent, nonlinear beams, ease of use

But why?

Discovery
Diagnosis
Prediction
Design

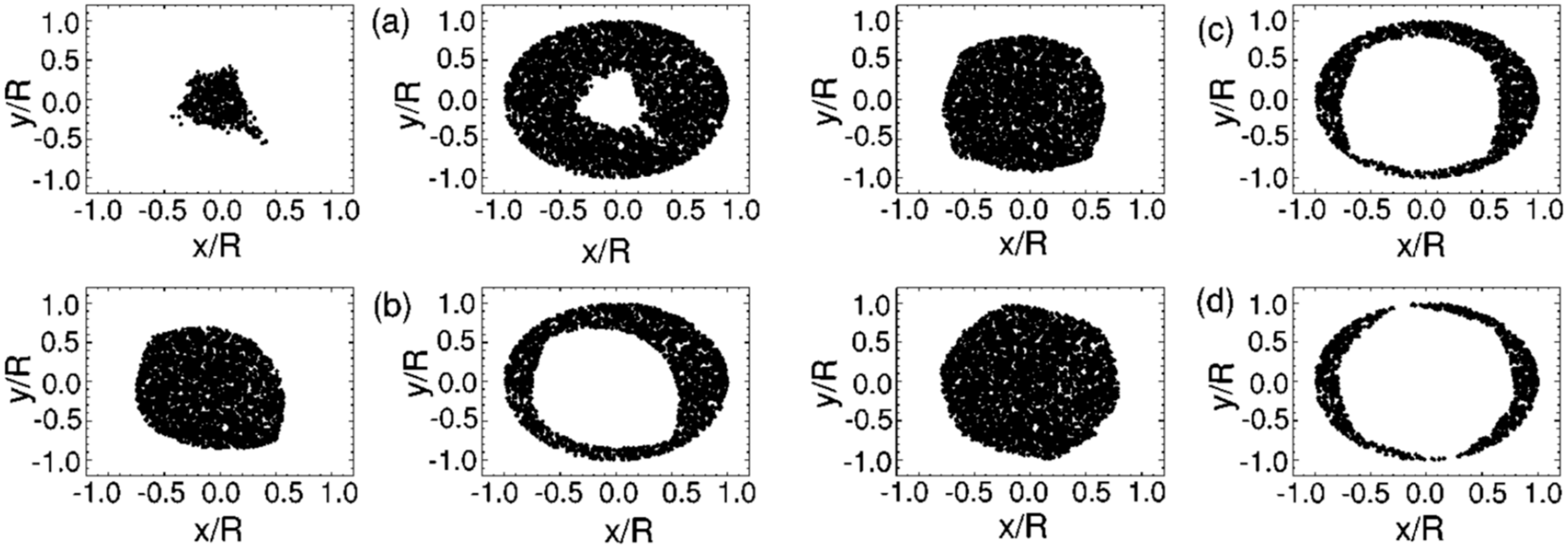
No modern accelerator is built without extensive advance simulation

Accelerator modeling 60’s-90’s: mostly separated physics

- Tracking
  - Are the single-particle trajectories long-time confined?
  - At least one for every lab, and some had two (SixTrack+MAD at CERN)
  - Simple enough (few k lines) that many recreated rather than learn someone else’s software
  - Invariants important! (symplectic integration)
- EM
  - MAFIA (10.1109/ICCEA.1999.825246)
  - CST: The interface is important!

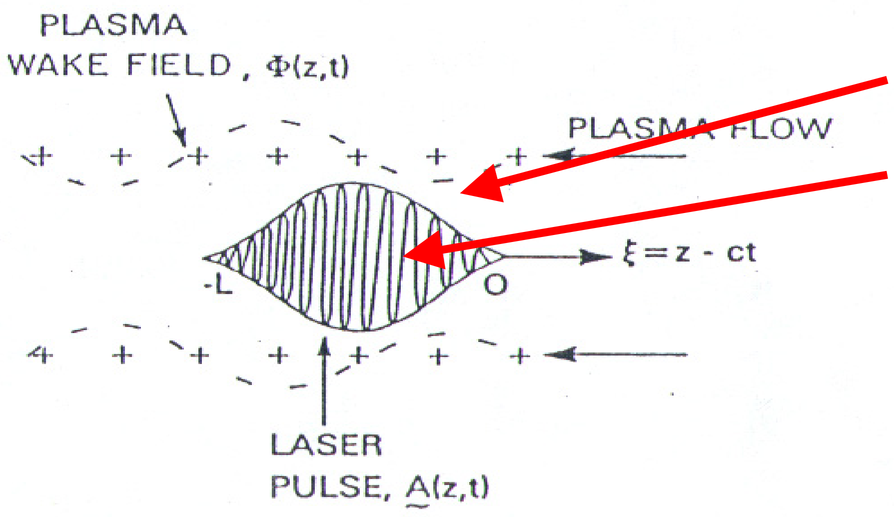
Accelerator modeling 60's-90's: mostly separated physics

- Tracking shows improved lattices: https://doi.org/10.1103/PhysRevE.69.056501



The 2000's gave rise to self-consistent, distributed-memory, parallel computing

Motivation: plasma acceleration, 50x disparity causes 2500x computational requirements.



$$\gamma_L \equiv \omega_L/\omega_p$$

$$\gamma_F = 2\gamma_L^2$$

Computation used to determine what went on

- Like hitting a brick wall with a cannon ball and seeing a nice, coherent beam come out
- Theorem: uniformly moving wavepacket cannot trap particles (to accelerate them)
- Simulations showed that in initial evolution, the breathing of the pulse due to nonlinear laser-plasma interaction led to particle trapping.

High-quality electron beams from a laser wakefield accelerator using plasma-channel guiding

C. G. R. Geddes[1,2], Cs. Toth[1], J. van Tilborg[1,3], E. Esarey[1], C. B. Schroeder[1], D. Bruhwiler[4], C. Nieter[4], J. Cary[4,5] & W. P. Leemans[1]

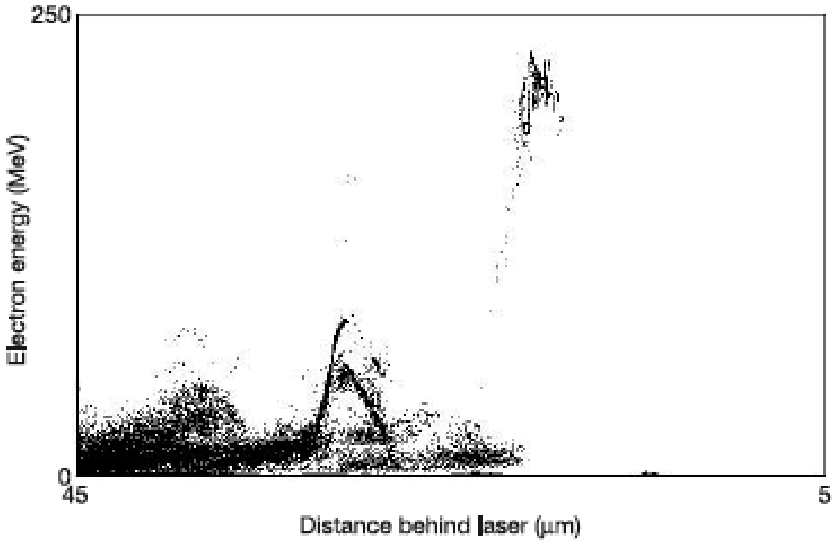


Figure 4 Particle in cell simulations, here displaying the phase space of the electrons, show an energy distribution similar to that in the experiments. A high-quality electron bunch is formed when the acceleration length is matched to the dephasing length, and when the laser strength is such that beam loading is sufficiently strong to turn off injection after the initial bunch of electrons is loaded. The peak energy observed in the simulations is 200 MeV, close to the experimental result.

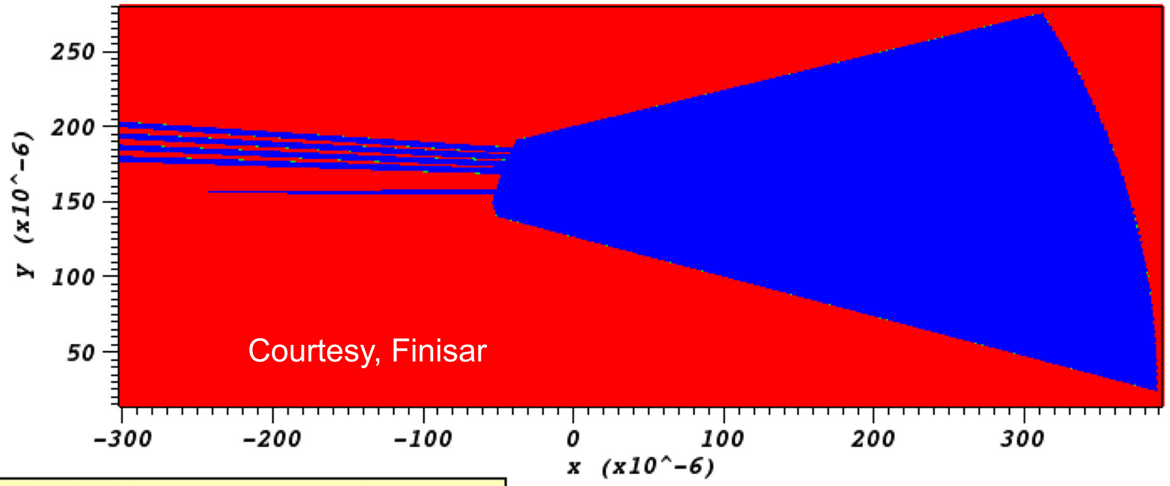
Current: large (distributed memory) parallel computing

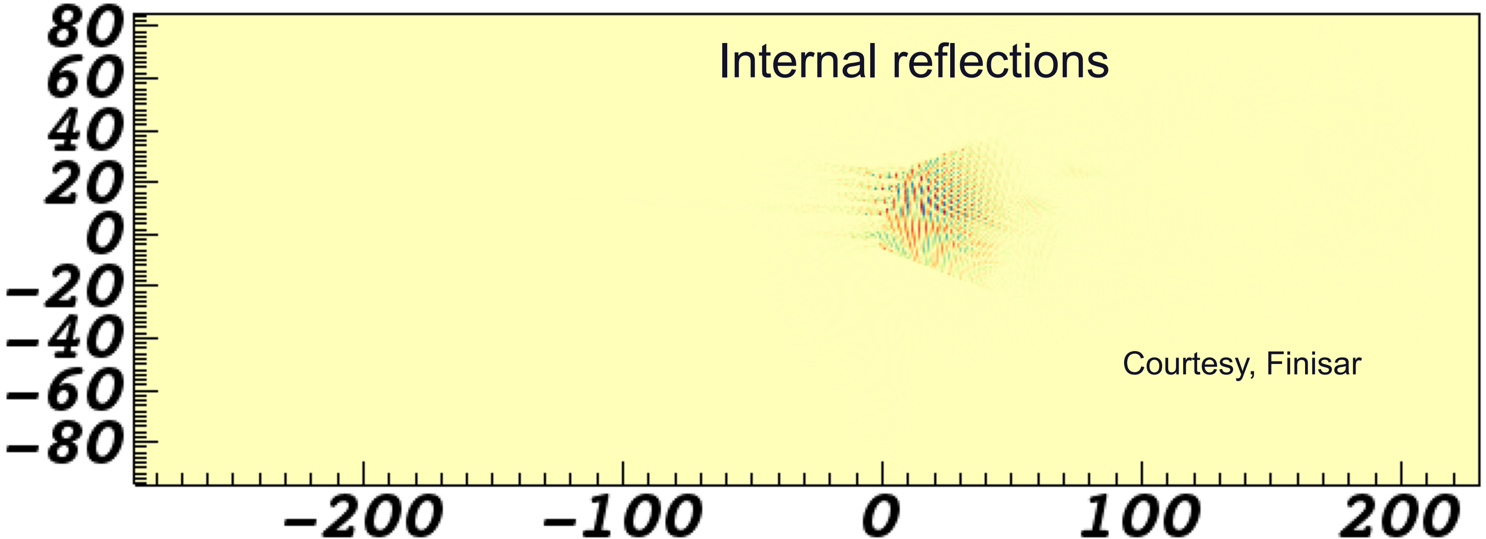
Many-core platforms (theta.alcf.anl.gov, cori.nersc.gov)

Billion-cell calculations routine but expensive

Example: photonics

- Some Photonics devices are computationally large (even if physically small)
- $\lambda = \lambda_0/n = 1310/1.914 = 684$ nm
- 783k λ^2
- At 20 cells/λ, this is 3.1e8 cells in horizontal plane
- 100 cells vertical $\Rightarrow$ 30B cells
- Requires 170,000 steps for analysis

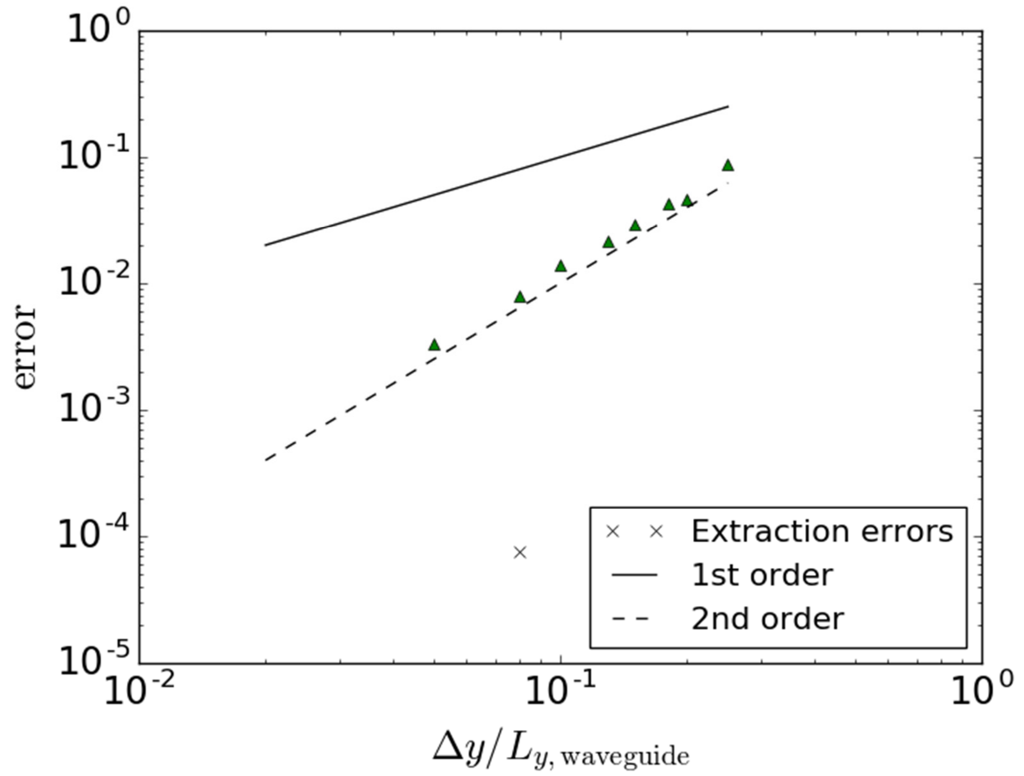




Actual sim

- 518x181x4μm
- # of 3D cells: 6.2B
- Time steps: 82,000
- Cores: 8,192
- Clock time: 5 hours

Algorithms: second-order dielectric updaters relevant

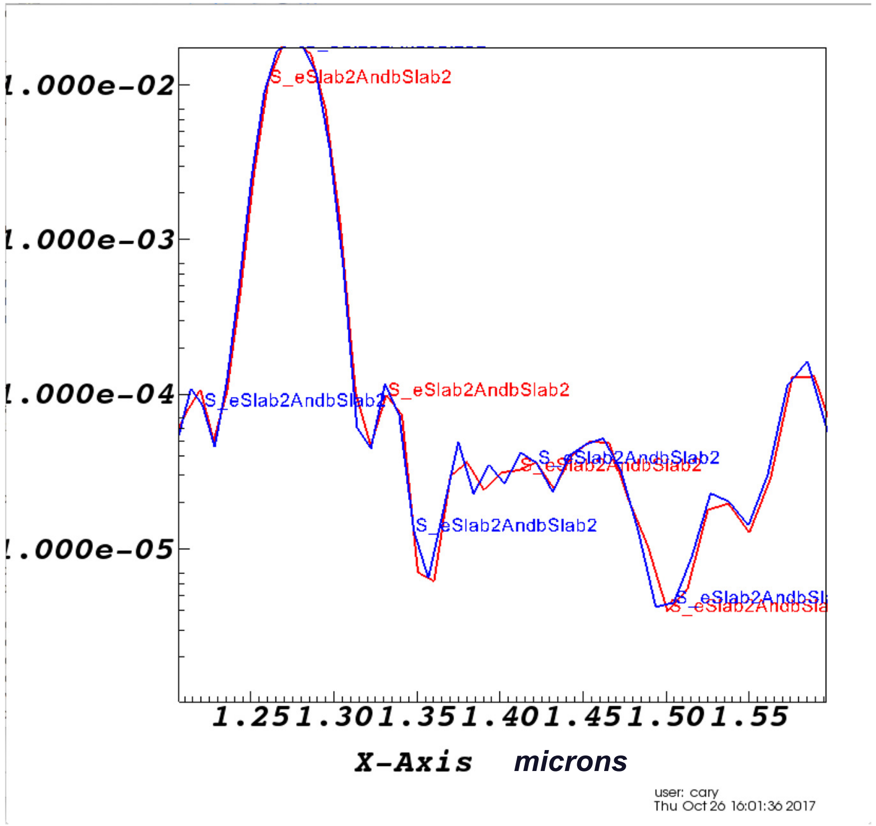


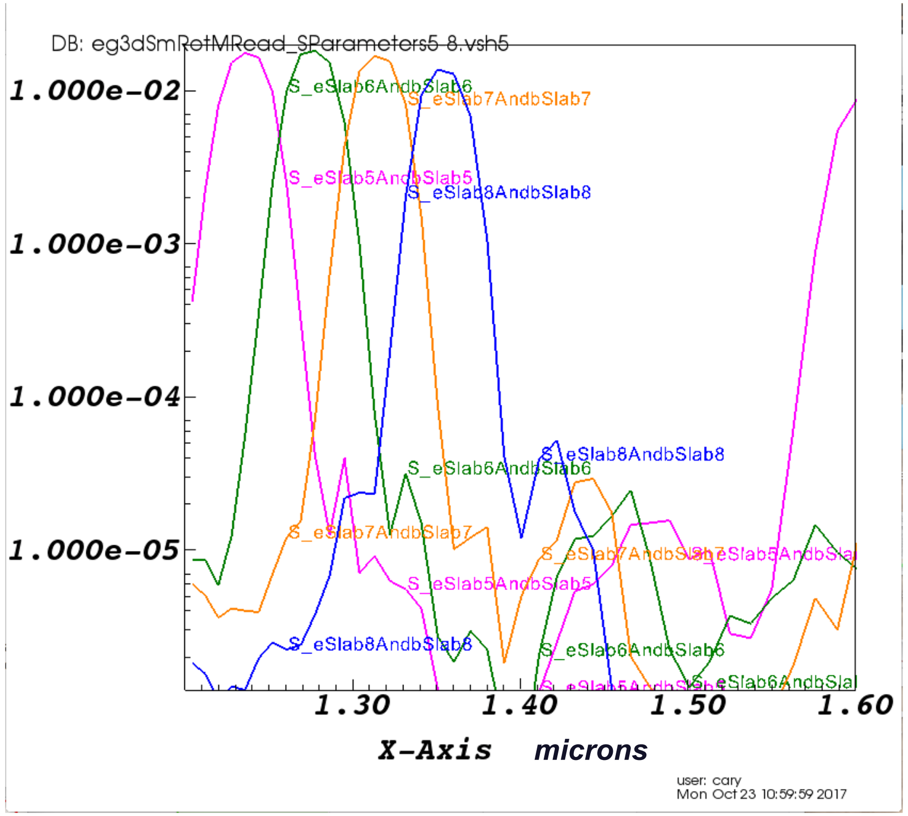
- ACHIP
- THz at FLASHForward
- Dielectric lined wakefield accelerators
- BELLA Dielectric kicker

G. R. Werner and J. R. Cary, “A Stable FDTD Algorithm for Non-diagonal, Anisotropic Dielectrics,” J. Comp. Phys. **226,** 1085-1101 (2007), doi:10.1016/j.jcp.2007.05.008.

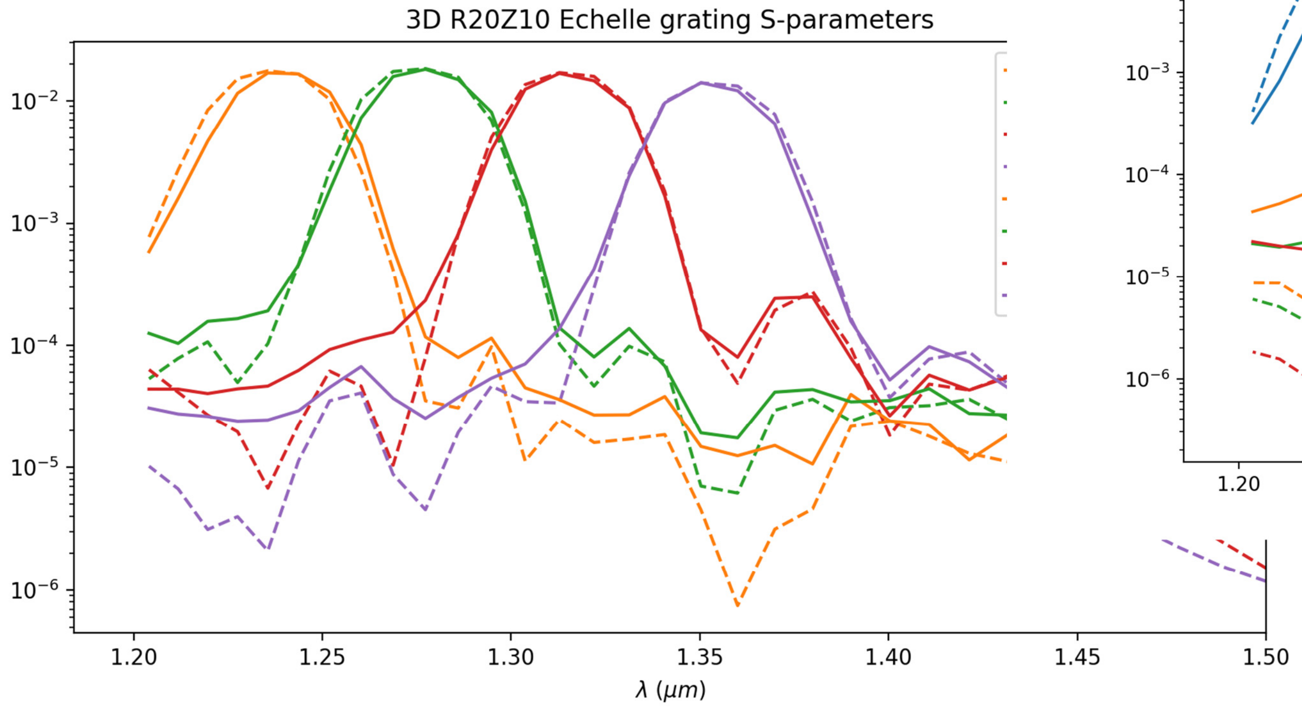
Bauer, Carl A., Gregory R. Werner, and John R. Cary. "A second-order 3D electromagnetics algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh." *Journal of Computational Physics* 230.5 (2011): 2060-2075.

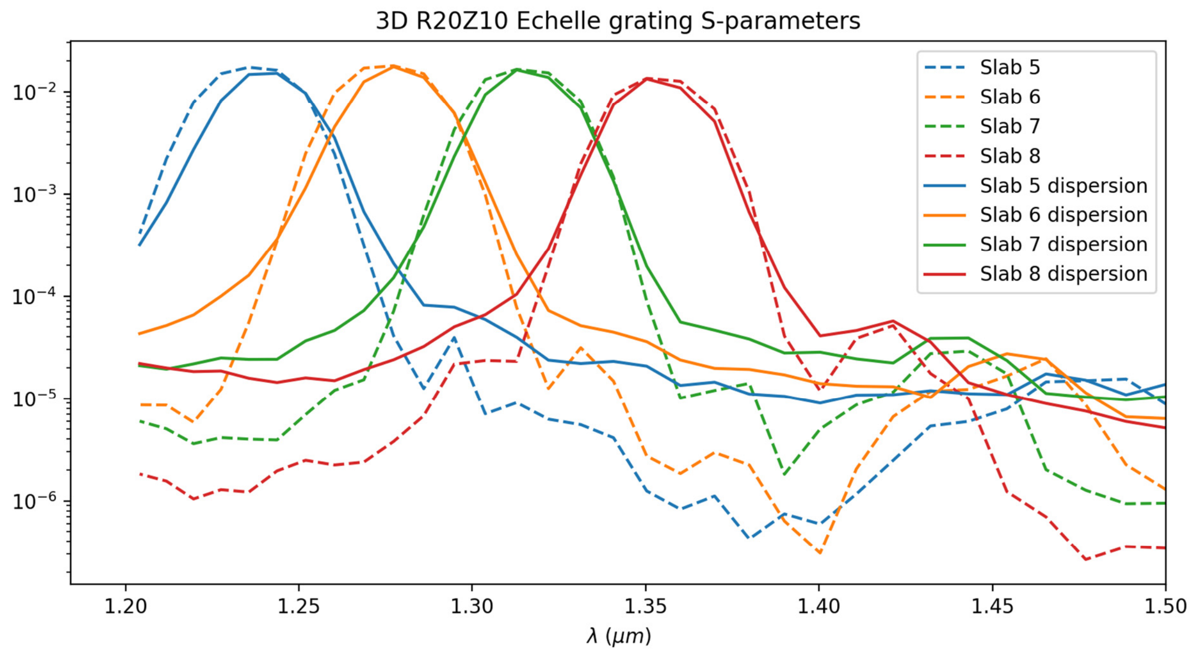
Goal: S parameters in Echelle Grating, convergence shown





Our newest algorithm (not yet published) gives accurate, conformal boundary results in the presence of dispersion





Some things to think about moving forward (what I am excited about)

Exascale

Democratization

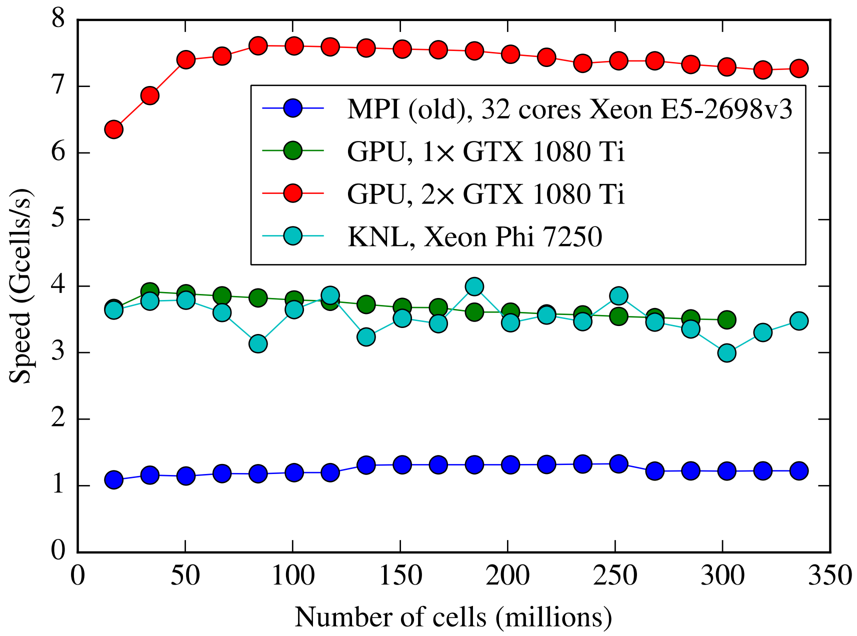
Algorithms

New DOE supercomputers all rely on multi- and heterogeneous device computing

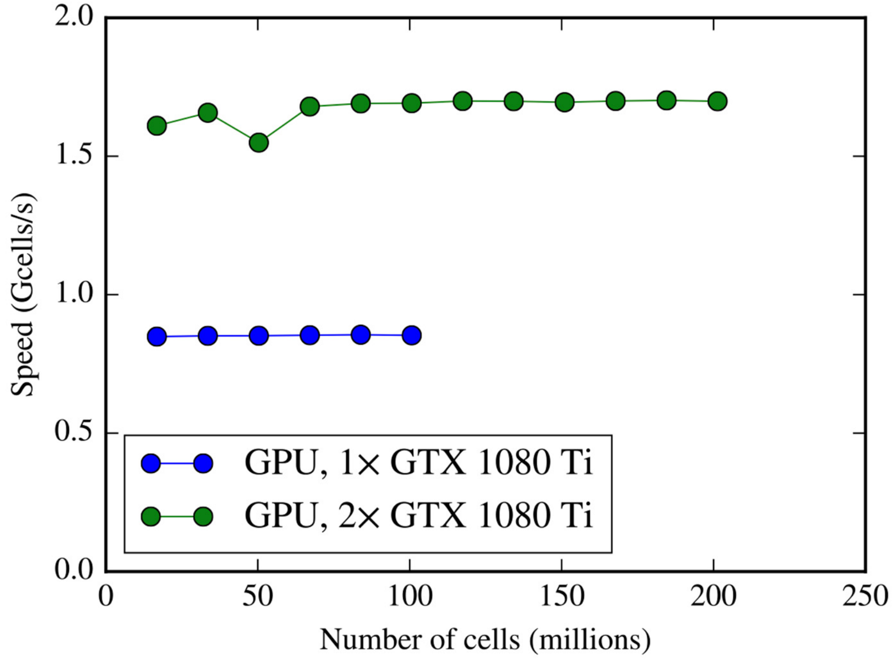
- Summit (2018)
  - 2 IBM Power 9 CPUs/node
  - 6 Nvidia Volta GPUs/node
  - Code via CUDA
  - https://www.olcf.ornl.gov/summit/
- Perlmutter (2020)
  - AMD Epyc CPUs
  - 4 NVidia GPUs per node
  - Code via CUDA
  - https://www.nersc.gov/systems/perlmutter
- Frontier (2021)
  - AMD Epyc CPUs
  - 4 Radeon Instinct GPUs per node
  - Code via HIP (designed to be CUDA compatible)
  - https://www.olcf.ornl.gov/frontier
- Aurora (2021)
  - Intel Xeon
  - Intel's Xe compute architecture (vapor at present)
  - Code via SYCL (also vapor)
  - https://aurora.alcf.anl.gov

All require multiple-device coding as is available in VSim
Exascale really means performance at all scales!
Forget wakefields, just do full EMPIC

Proper restructuring shows near-perfect scaling



Vacuum FDTD updater

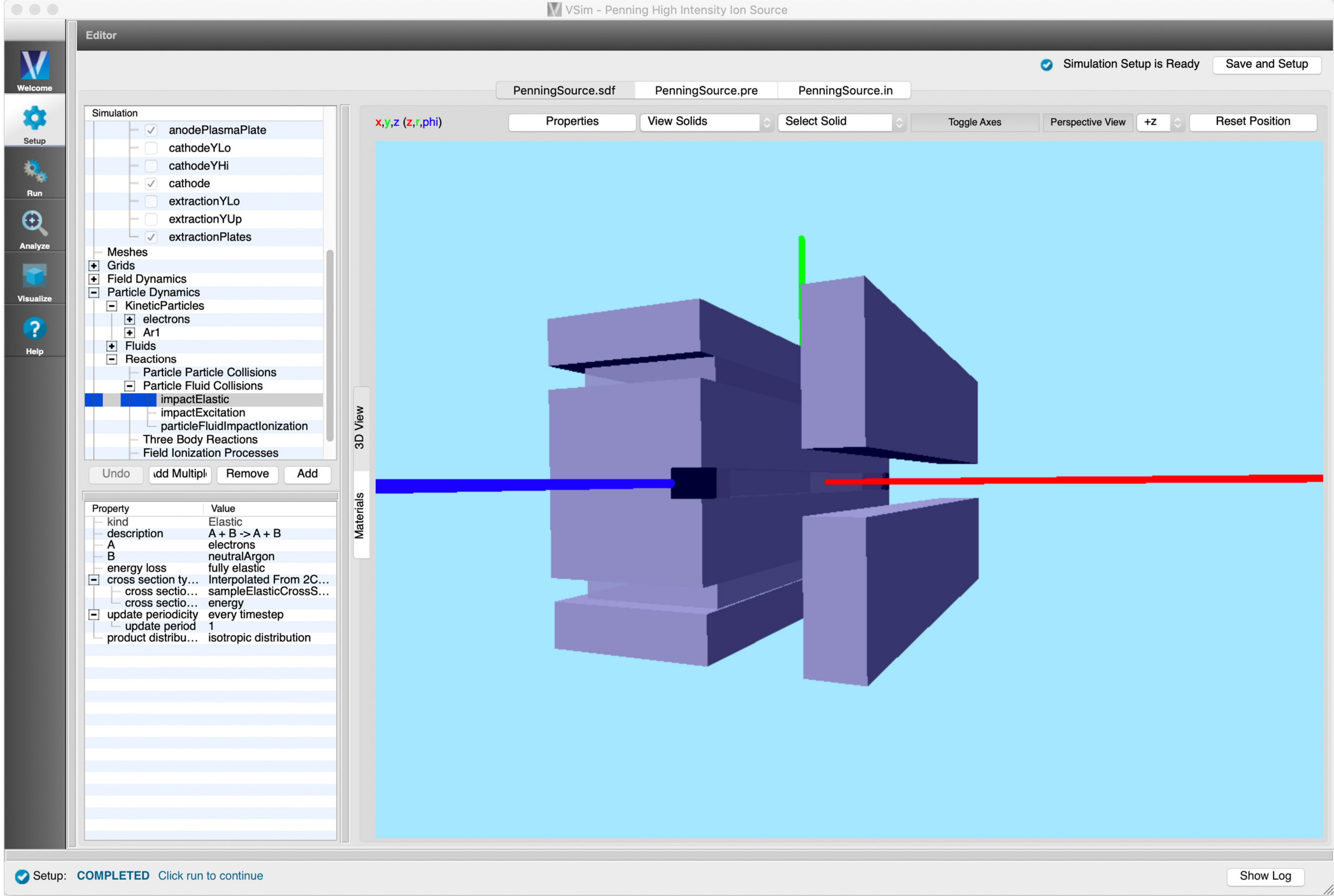


Cut-cell dielectric updater
(applied everywhere)

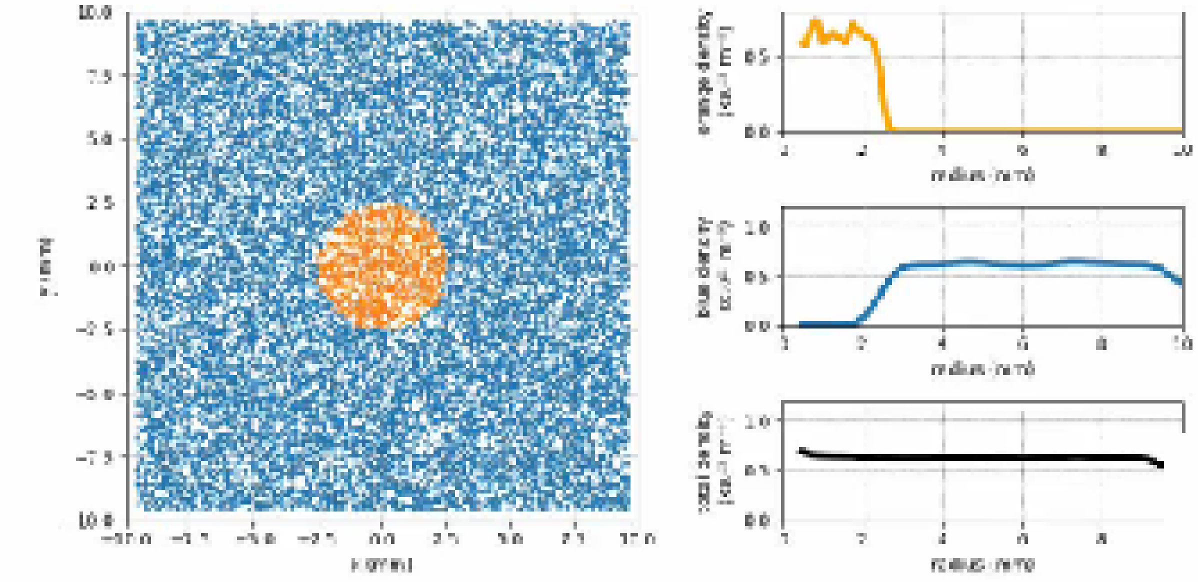
TECH-X SIMULATIONS EMPOWERING YOUR INNOVATIONS

Democratization: make simulation available to all

- Constants, parameters and expressions useful for setting geometries, sources, boundary conditions and diagnostics (we call them “histories” as they collect data from all time steps)
- Geometries
  - Constructive Solid Geometry primitives, booleans and 1d, 2d and 3d arrays
  - GDS, STL and STEP import
- Sources:
  - Gaussian, dipole and from arbitrary currents (visible geometry in the setup)
  - Sources from external profiles
- 2d order mode solver and source from it
- Point, surface and volume diagnostics (2d and 3d visible as well)
- Absorbing layers
- Background permittivity
- Choice of 1st and 2d order solvers
- Dimensionality (3d or 2d)
- Creating surface meshes in the setup
- 3D visualization with analysis
- Post-processing (S params, Poynting flux, Far-fields). Extendable
- Choice of number of cores to run

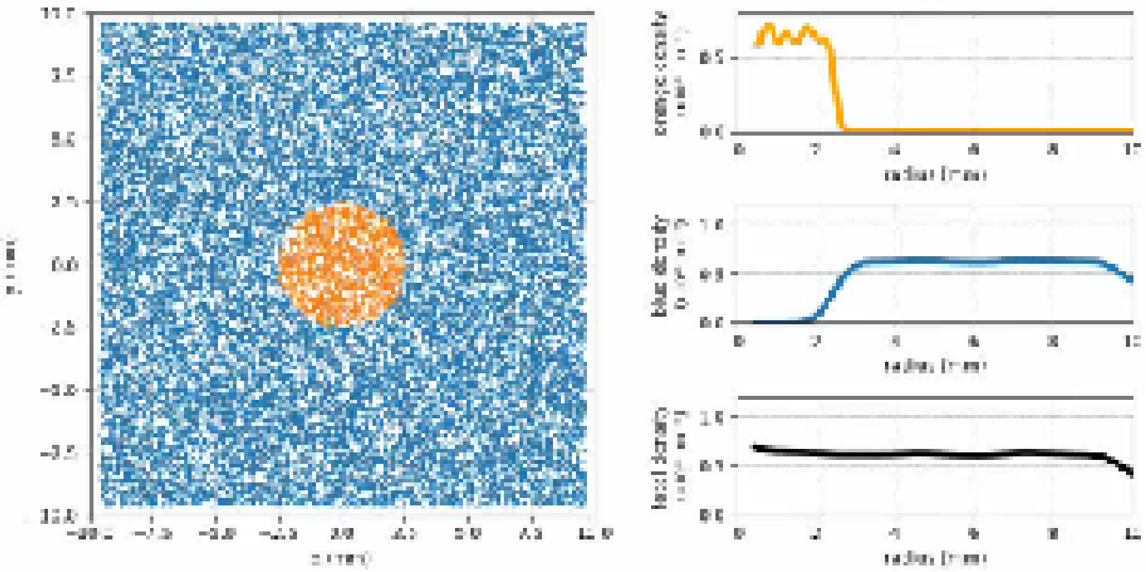


Collisional PIC predicts low-density plasma dynamics



- Thanks to Jarrod Leddy, Scott Sides, Ben Cowan, Greg Werner
- Rayleigh-Taylor

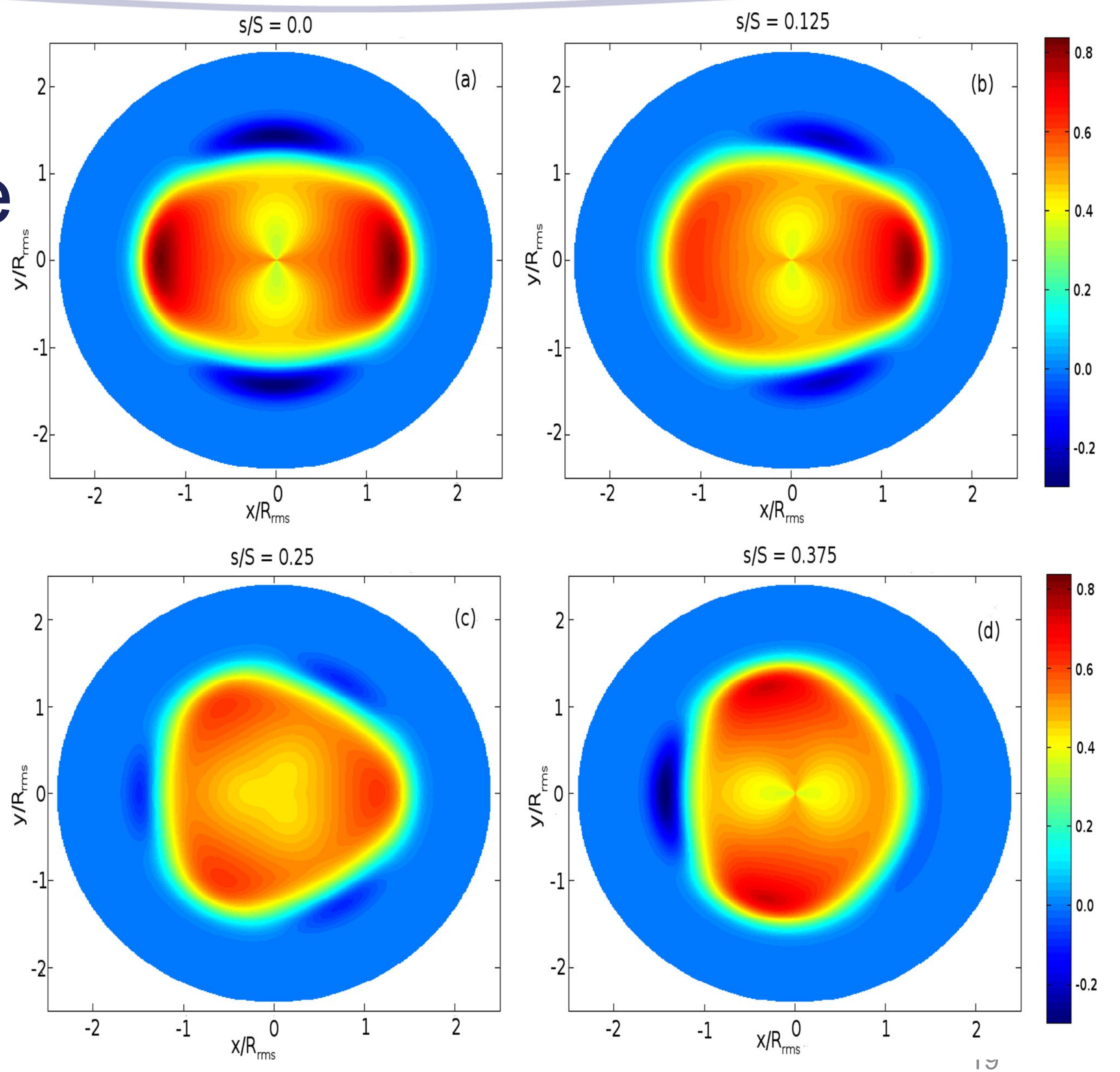
Collisionless



Collisional:

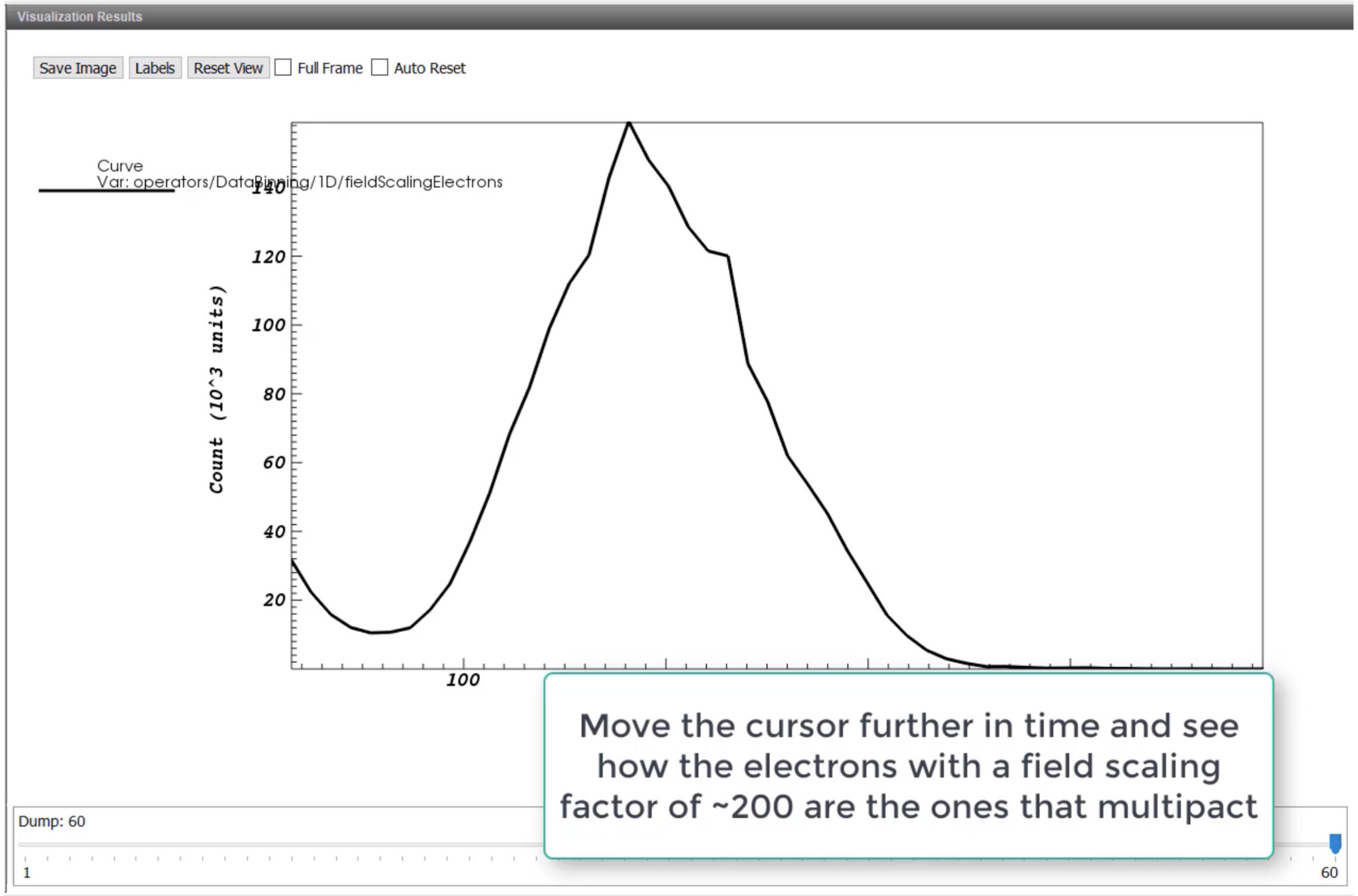
Equilibria of beams in nonlinear lattices with space charge

- Sonnad
- Restarting this work



Multipacting: multiple field values in one simulation

- Import fields from your favorite software
- Load variable interactivity particles
- Get answer for all field values!



Summary

- Computational accelerator physics has evolved from
  - Separate particle tracking (a code for every lab!)
  - Separate O(Dx) field calculations
- To
  - Unified particle-em on large systems
- High-performance computing brings possibility of much greater fidelity
  - 10B's of cells, 100B's of particles
  - Full EMPIC simulations instead of wakefield + particles
  - Kinetic simulations of plasmas for AA targets, plasma cleaning, along with beam interactions
- Allowing direct simulations of many accelerator problems