Parallel Higher-Order Finite Element Method for Accurate Field Computations in Wakefield and PIC Simulations

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Outline

- ***SciDAC Parallel FE Time-Domain Codes***
- *Wakefield Simulations with T3P*
- *LCLS RF Gun Modeling with Pic2P*

SciDAC's Accelerator Project

Goal – *To develop next generation simulation tools to improve the performance of present accelerators and optimize the design of future machines using flagship supercomputers at NERSC (LBNL) and NLCF (ORNL)*

NERSC	NLCF
Seaborg IBM SP3	Phoenix Cray X1E
9 TFLOPS, 6 TB+	18 TFLOPS, 2 TB

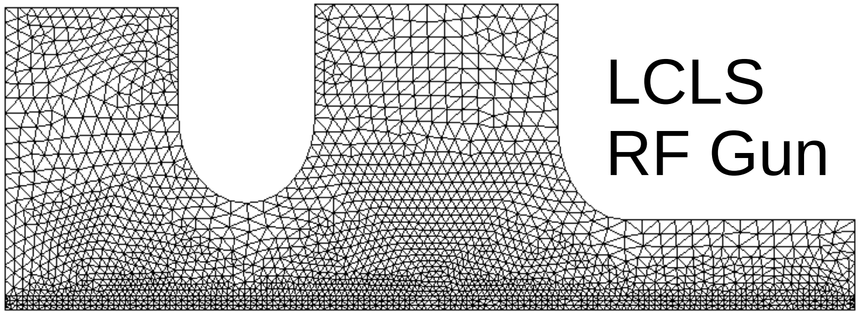
Parallel Finite Element Time-Domain

Maxwell's Equation in Time-Domain:

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times \nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{J}}{\partial t}$$

- ***Spatial discretization*** -

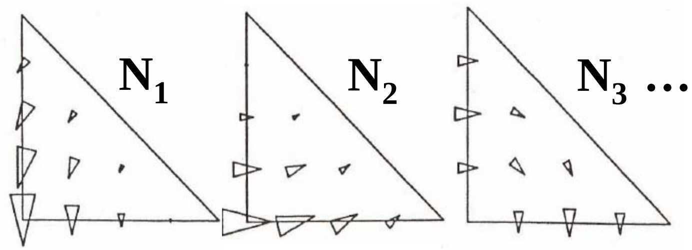
Conformal, unstructured grid with curved surfaces (q=1…2)



LCLS RF Gun

Higher-order (p=1…6) (Whitney) basis functions:

$$\mathbf{E}(\mathbf{x},t) = \sum_i e_i(t) \cdot \mathbf{N_i}(\mathbf{x})$$



- ***Time integration*** - Unconditionally stable implicit Newmark scheme (Matrix inversion)

- ***Parallelization*** - MPI on distributed memory platforms

SciDAC Codes - T3P and Pic2P

- ***T3P*** – **Parallel 3D FE Wakefield Code**

  Rigid beam: Analytical $\mathbf{J}$

- ***Pic2P*** – **Parallel 2.5D FE PIC Code**

1) Compute particle current $\mathbf{J} = \rho \mathbf{v}$

2) Calculate EM fields from Maxwell's eq.

3) Push particles $\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \mathbf{v} \wedge \mathbf{B})$

Higher-order particle-field coupling, no interpolation required

1st successful implementation of self-consistent, charge-conserving PIC code with conformal Whitney elements on unstructured FE grid

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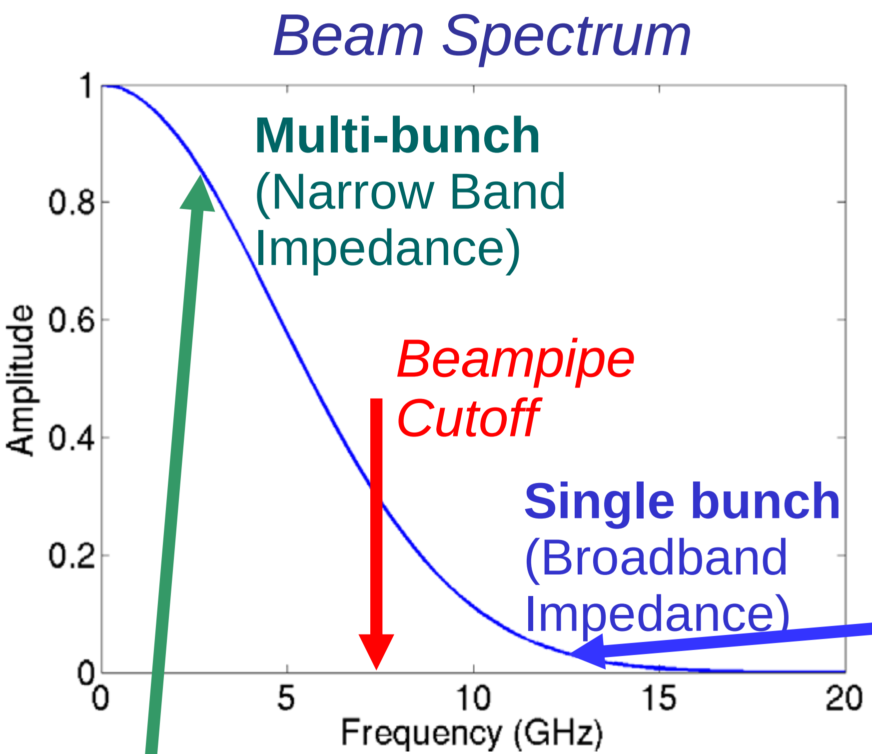
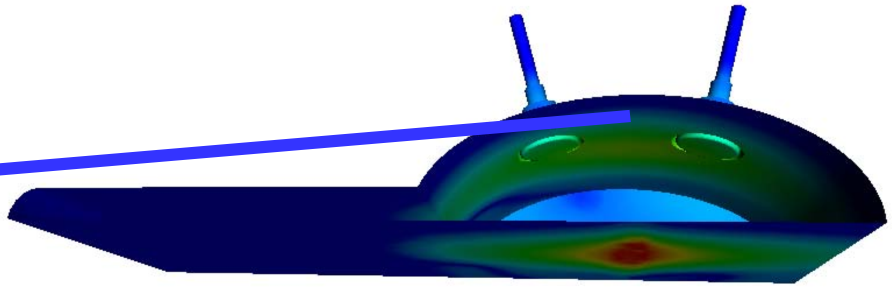
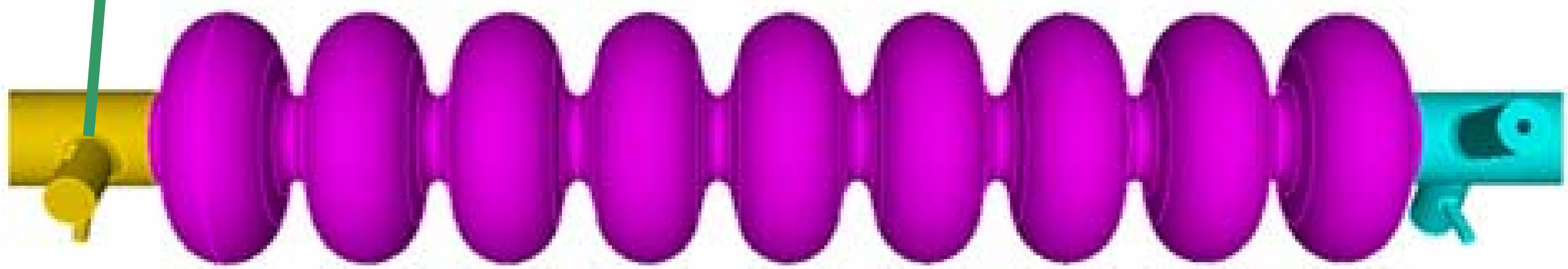
Wakefields on Conformal Grid

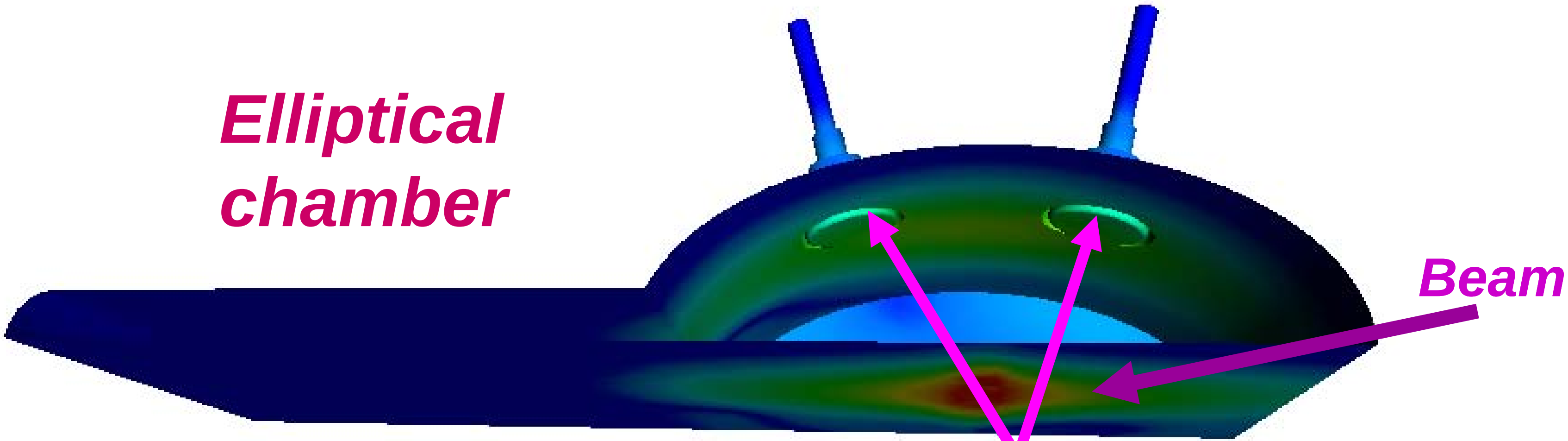


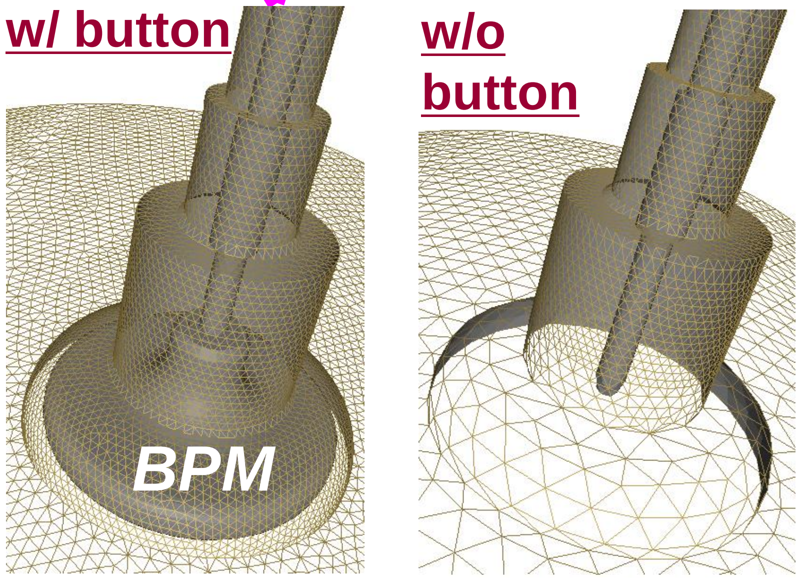
Conformal grid increases accuracy of calculations of single and multi-bunch effects in geometries not modeled well with codes using structured grids





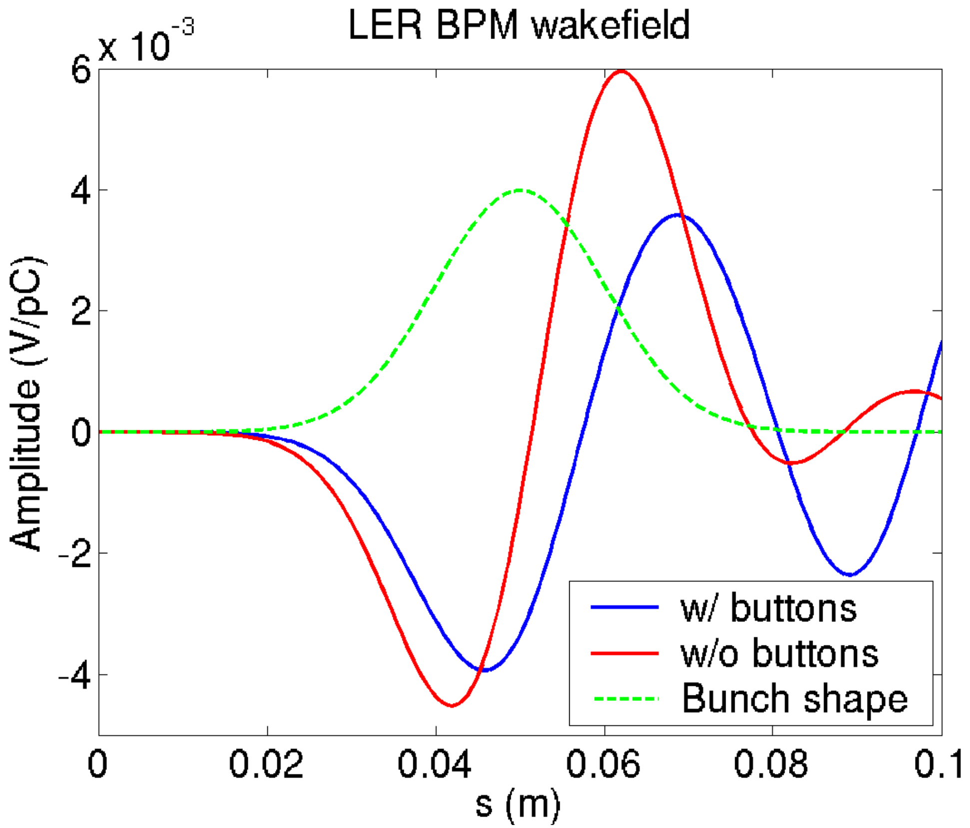
PEP-II LER Arc Chamber

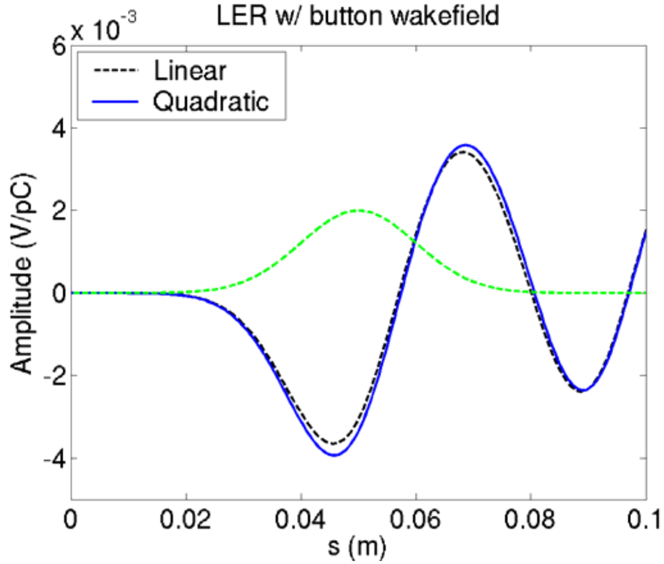


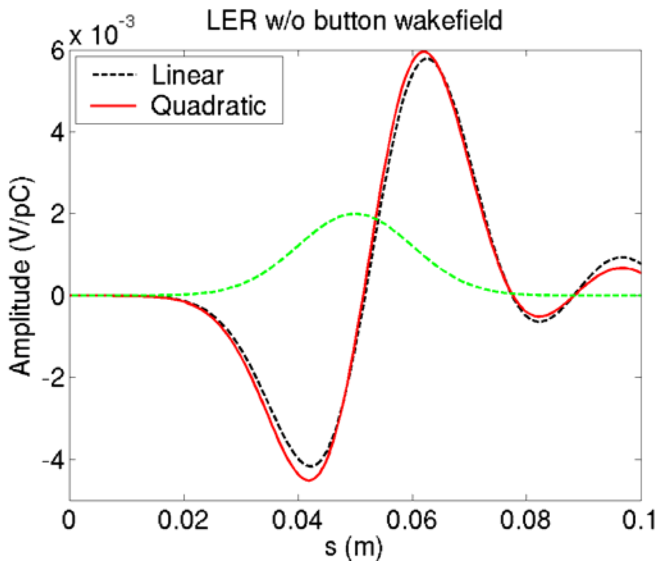


T3P *used to compute the effect of missing buttons in PEP-II LER BPM on storage ring's broadband impedance.*

PEP-II LER BPM Broadband Impedance

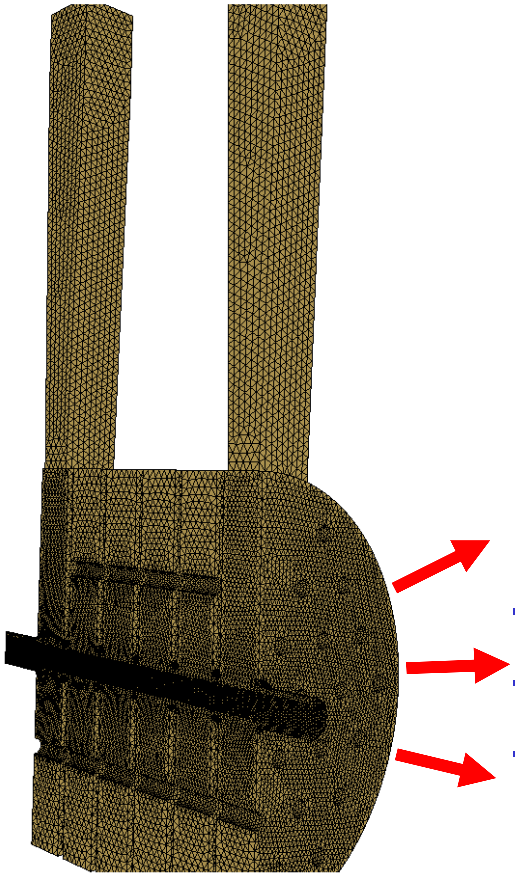






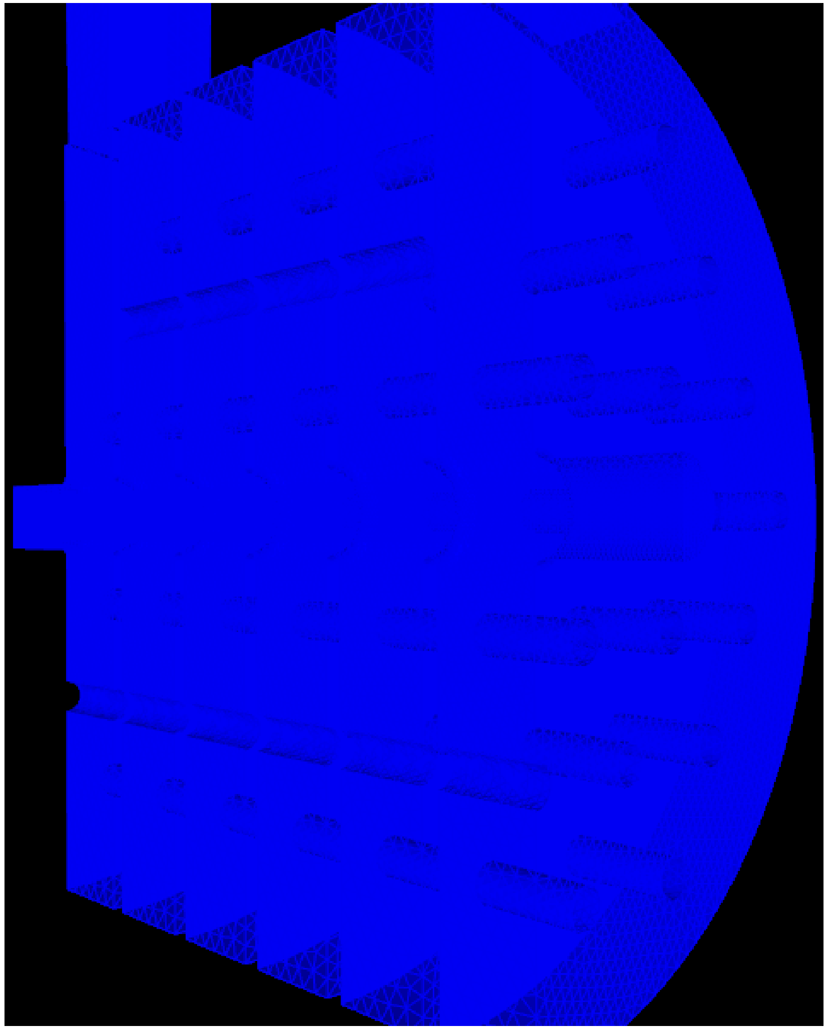
MIT/STAR Photon Band Gap Structure

*Single mode structure by design, **all HOMs can escape***



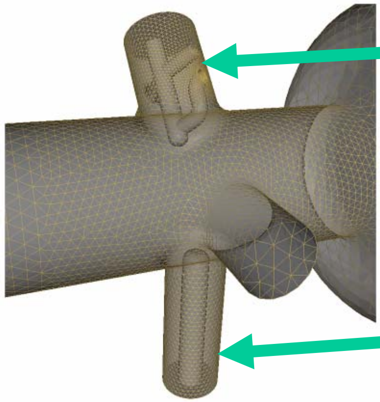
Absorbing Boundary Conditions

35 MV/m accel. gradient demonstrated at MIT.



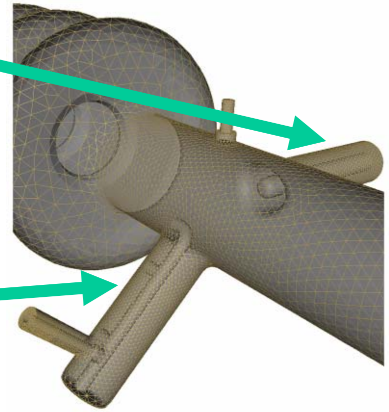
Off-axis transit beam to excite dipole wakefields

ILC Crab Cavity Design



HOM Coupler

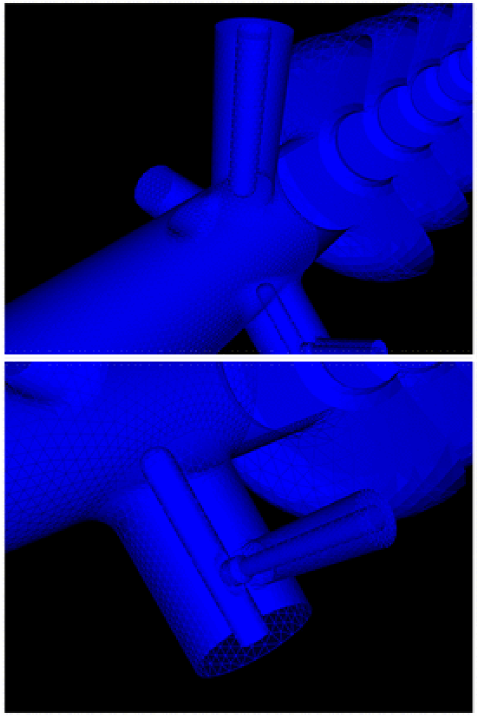
SOM Coupler

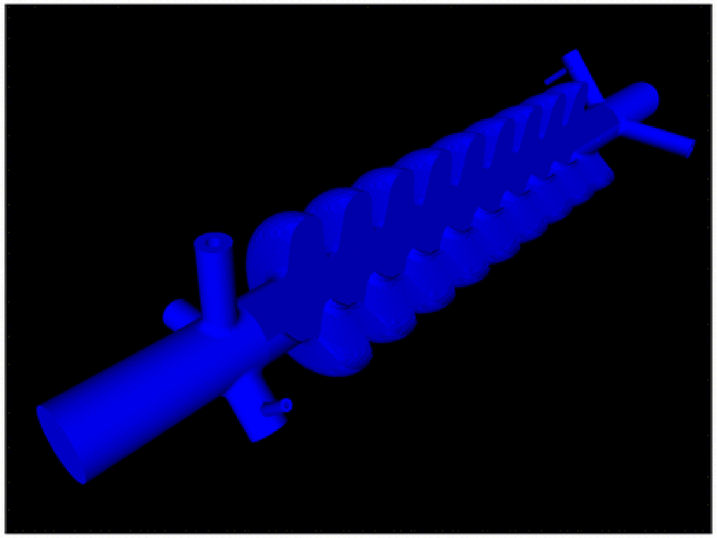


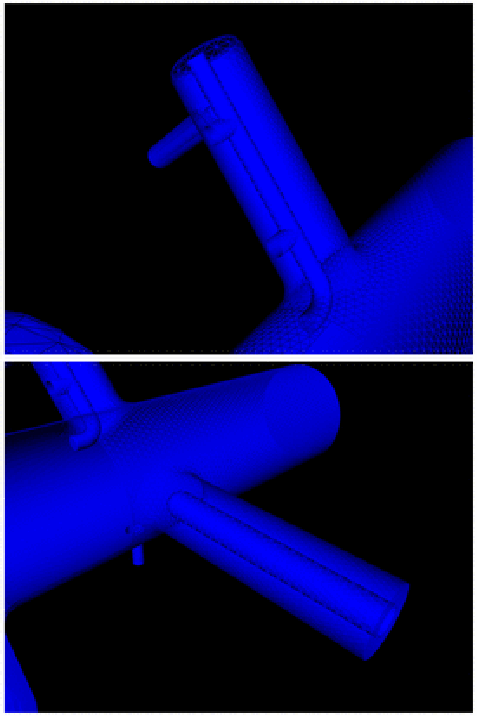
<u>**Port boundary conditions**</u>

Input Coupler

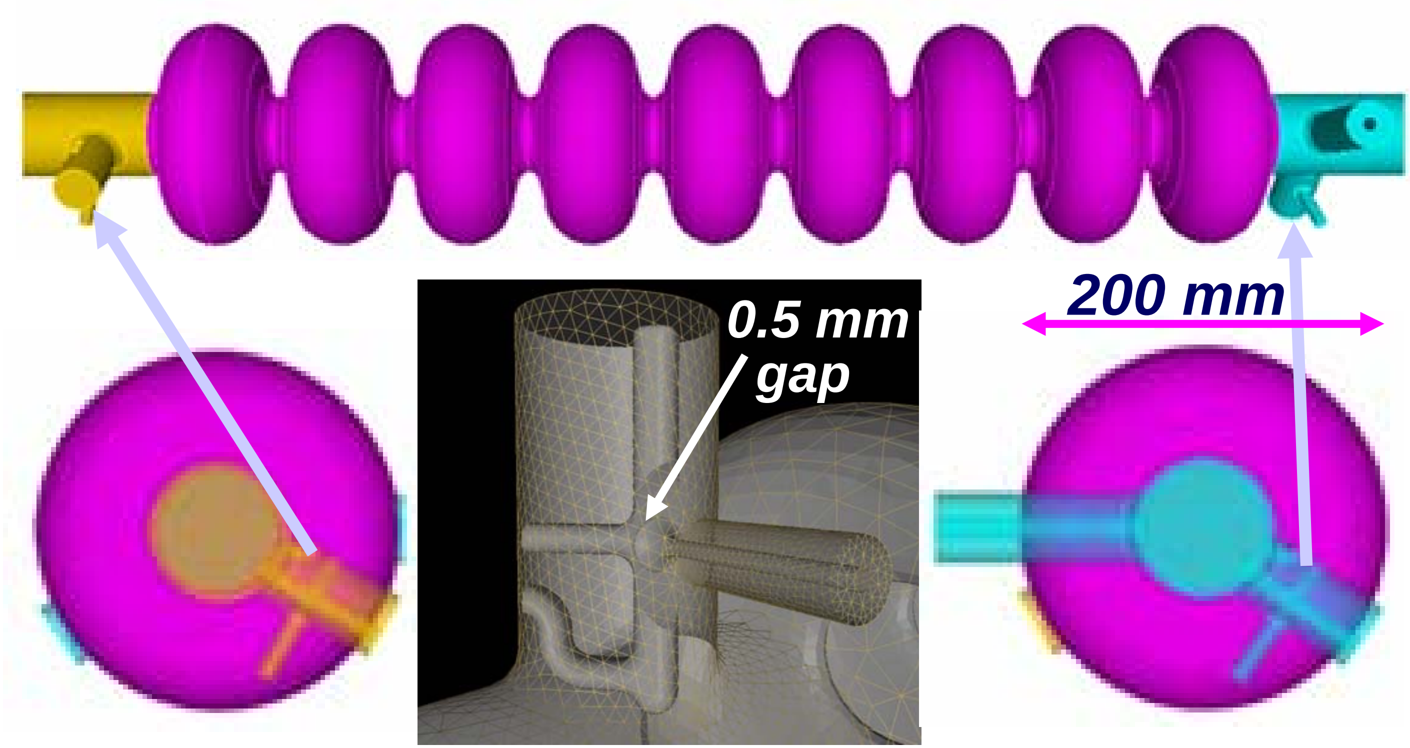
LOM Coupler





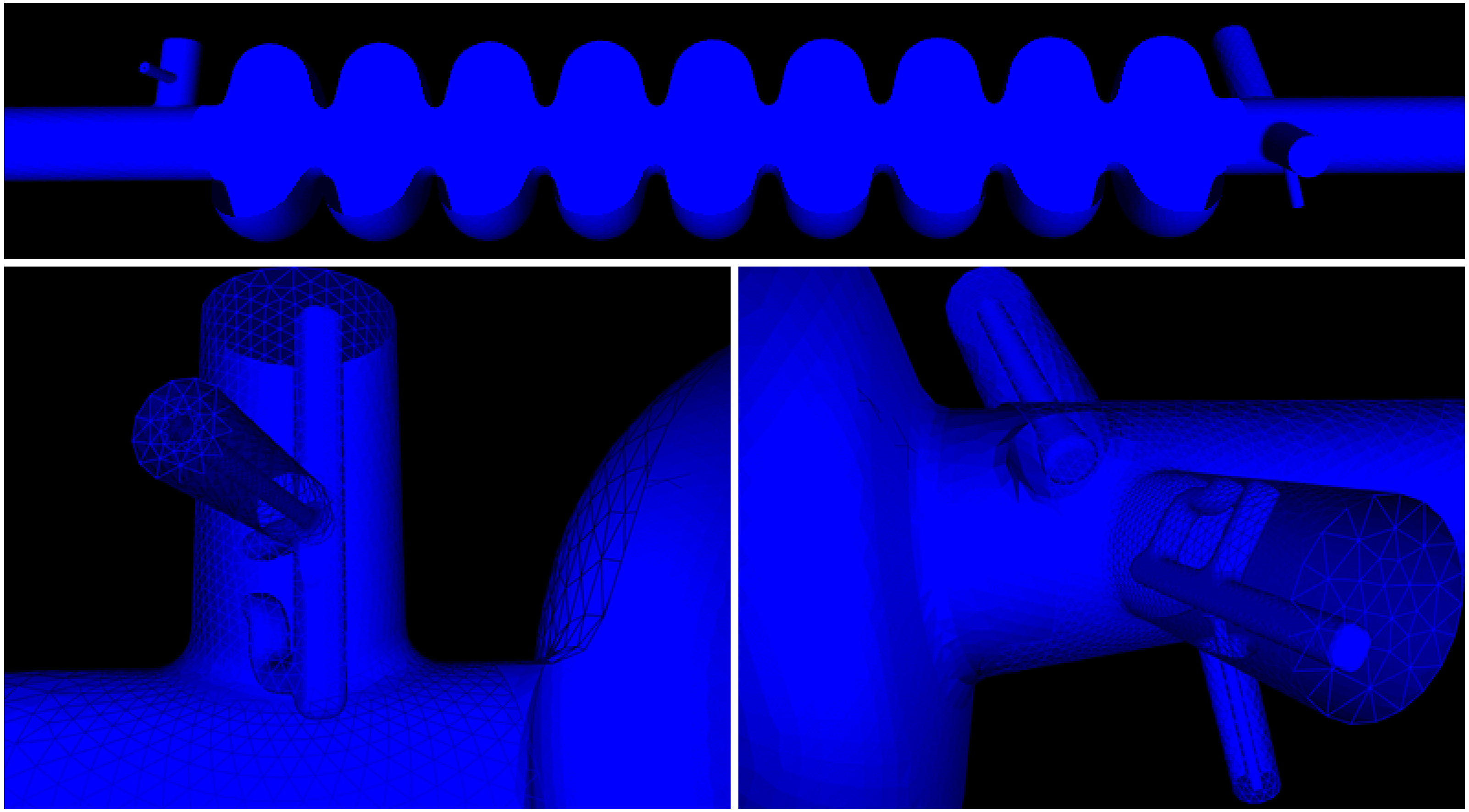


Accurate Modeling of ILC-TDR Cavity



- ***Multi-Scale*** *– HOM coupler notch gap vs cell size*
- ***3D Effects*** *– Short-range wakefields due to couplers*
- ***Fast*** *– Short turn-around time to impact R&D*

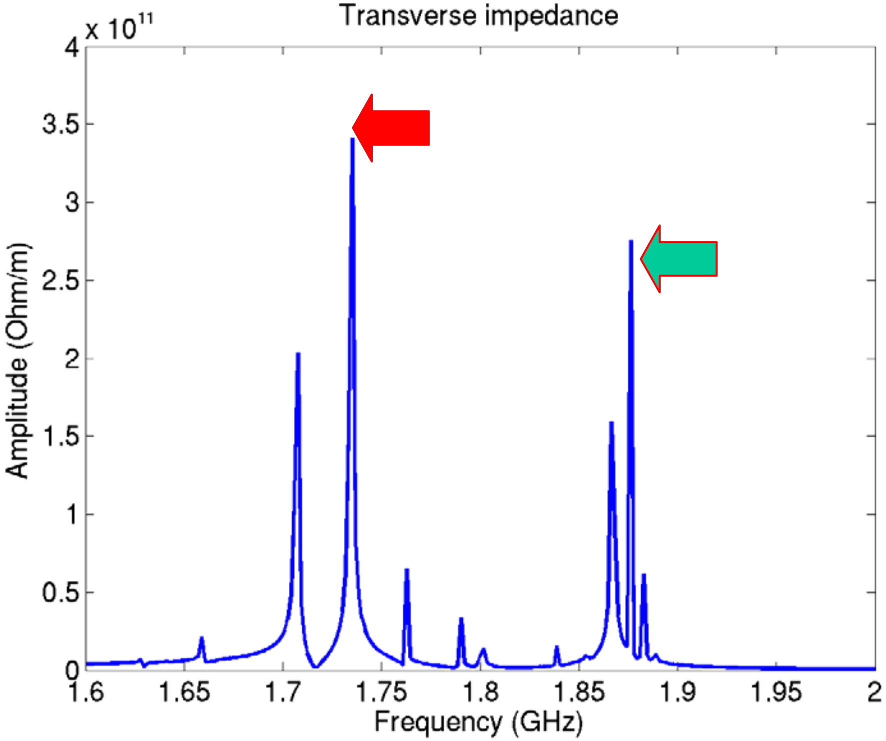
Wakefields in TDR Cavity



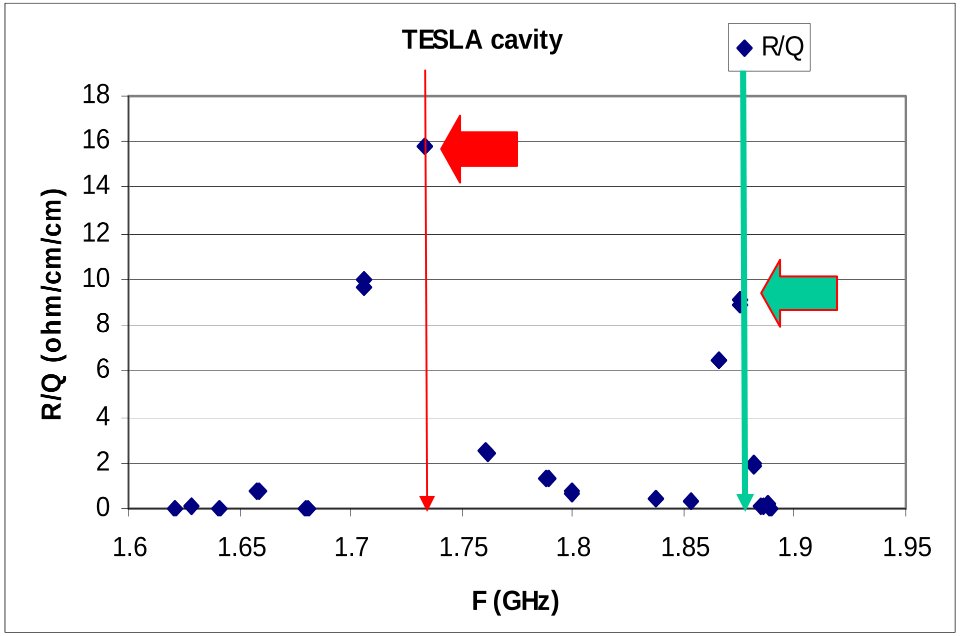
1.75 M quadratic elements, 10 M DOFs, 47 min per nsec on Seaborg 1024 CPUs with 173 GB memory – CG and incomplete Cholesky preconditioner

T3P Comparison with Omega3P

***T3P** transv. impedance (time-domain)*



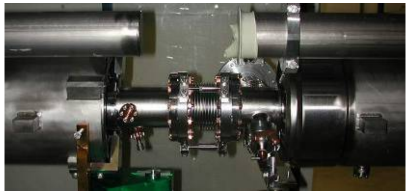
***Omega3P** mode spectrum (frequency-domain)*

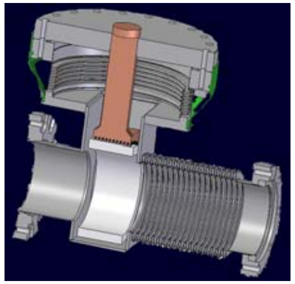


Computational Challenge – ILC Cryomodule

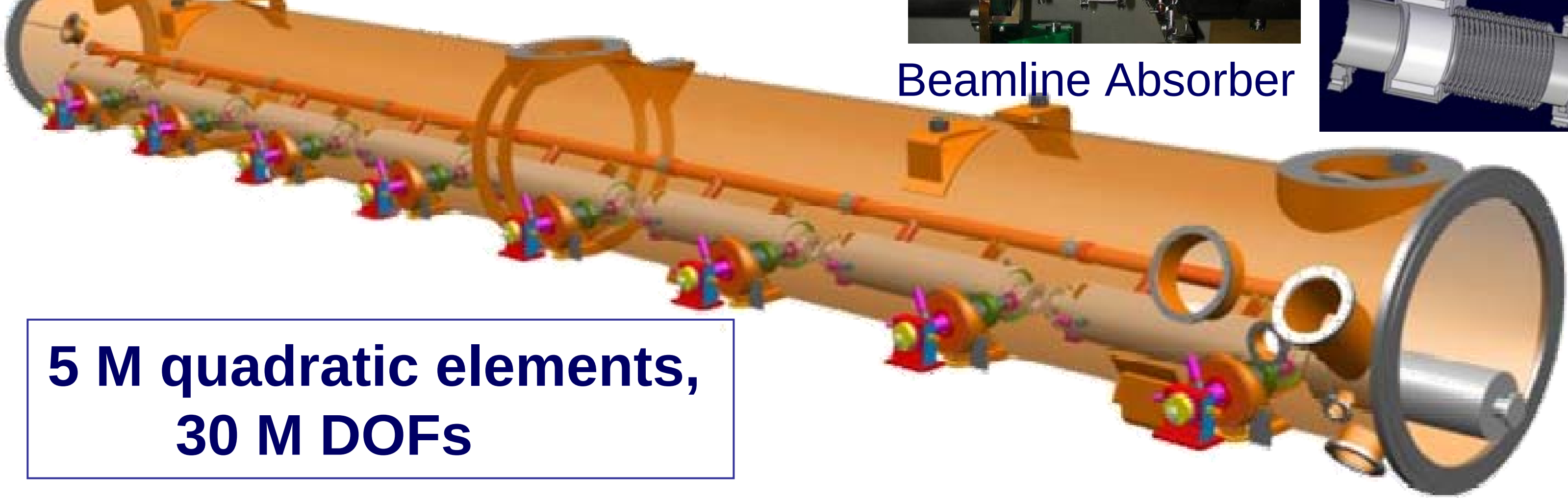
DESY FLASH

Cavity Interconnection



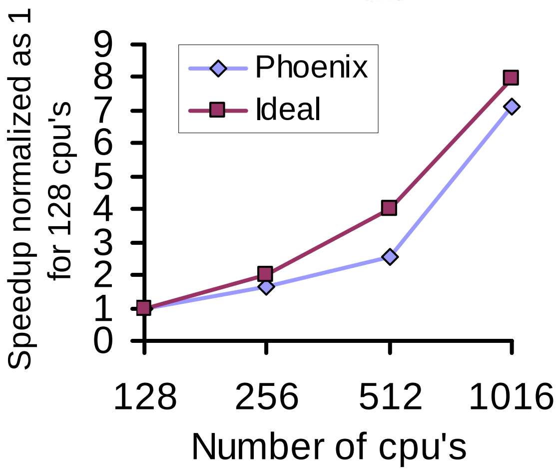


Beamline Absorber



5 M quadratic elements, 30 M DOFs

T3P *will be used to compute the* ***high frequency radiation loss*** *in the* ***ILC cryomodule*** *and assess the effectiveness of the* ***beamline HOM absorber*** *by* ***<u>petascale computing</u>***



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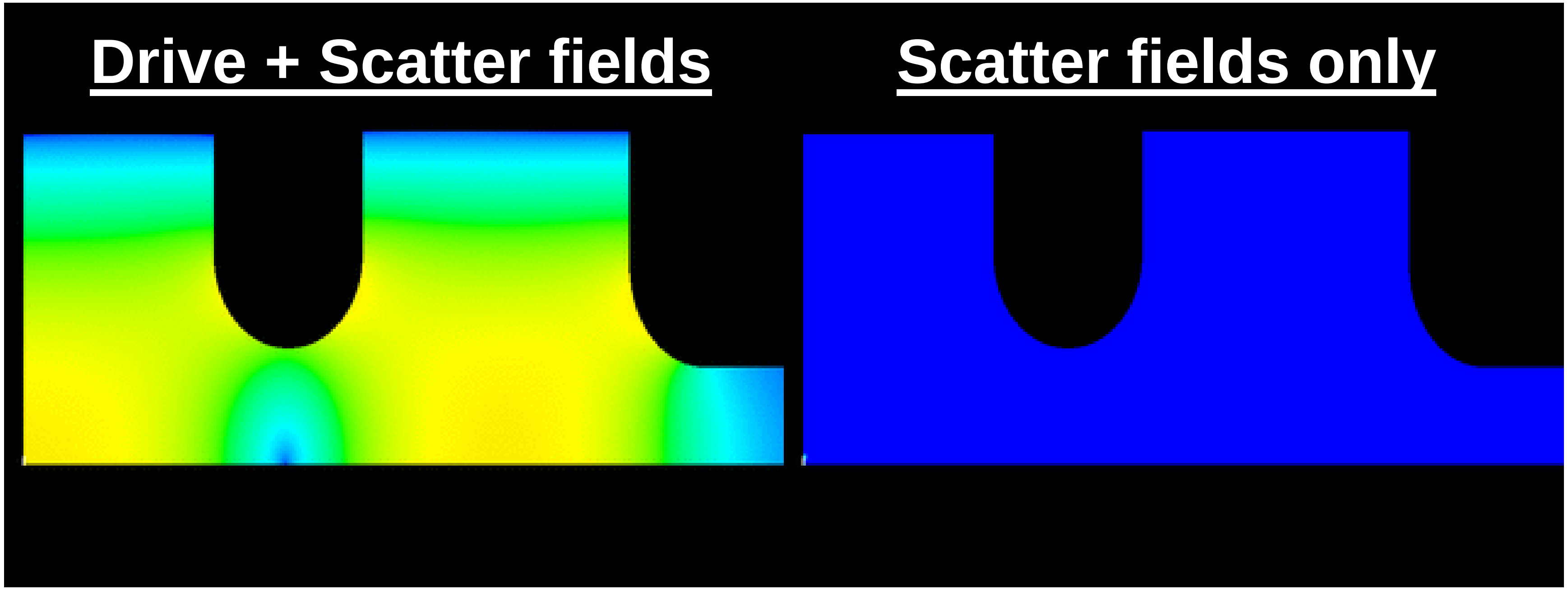
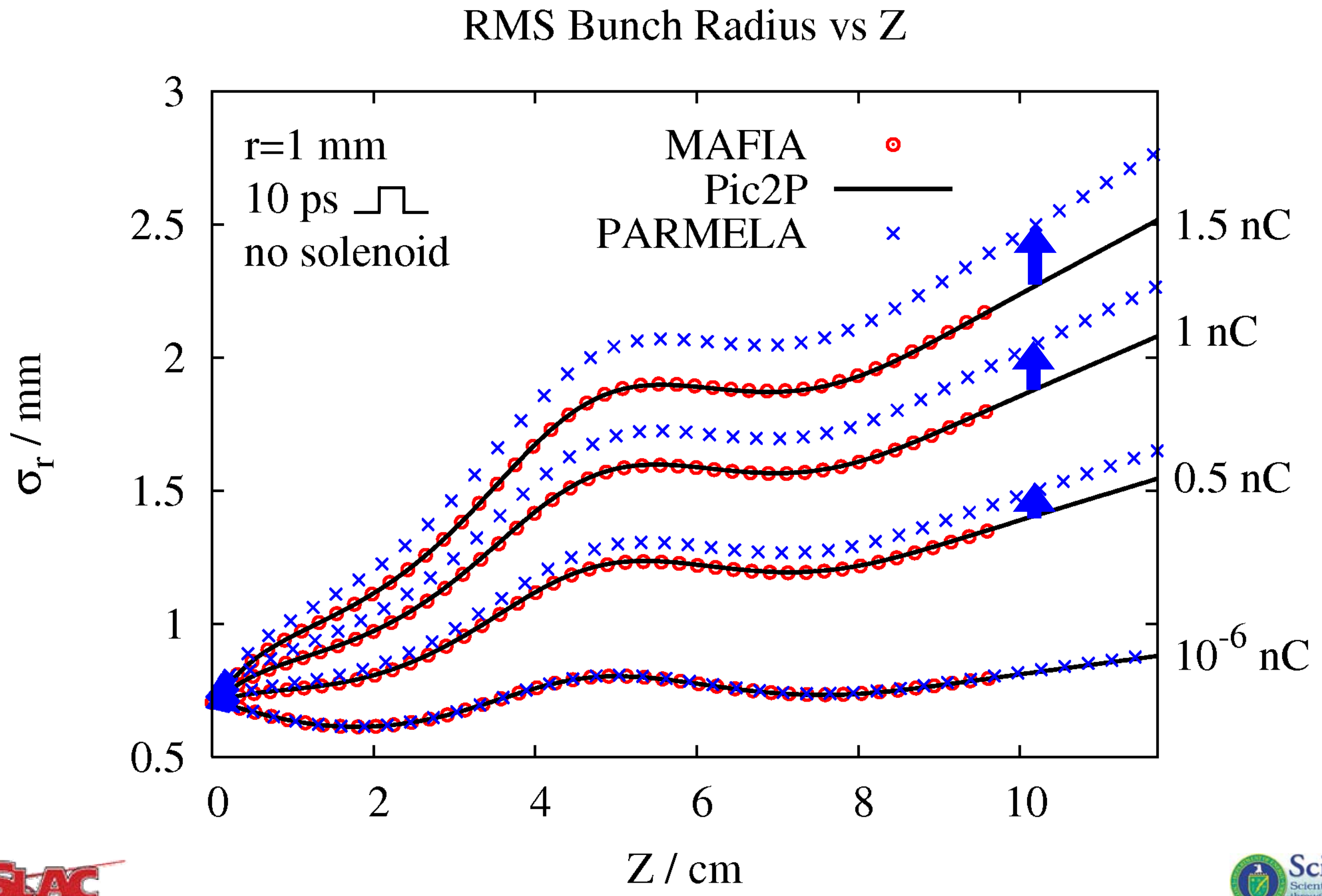
- ***LCLS RF Gun Modeling with Pic2P***

Pic2P Simulation of LCLS RF Gun

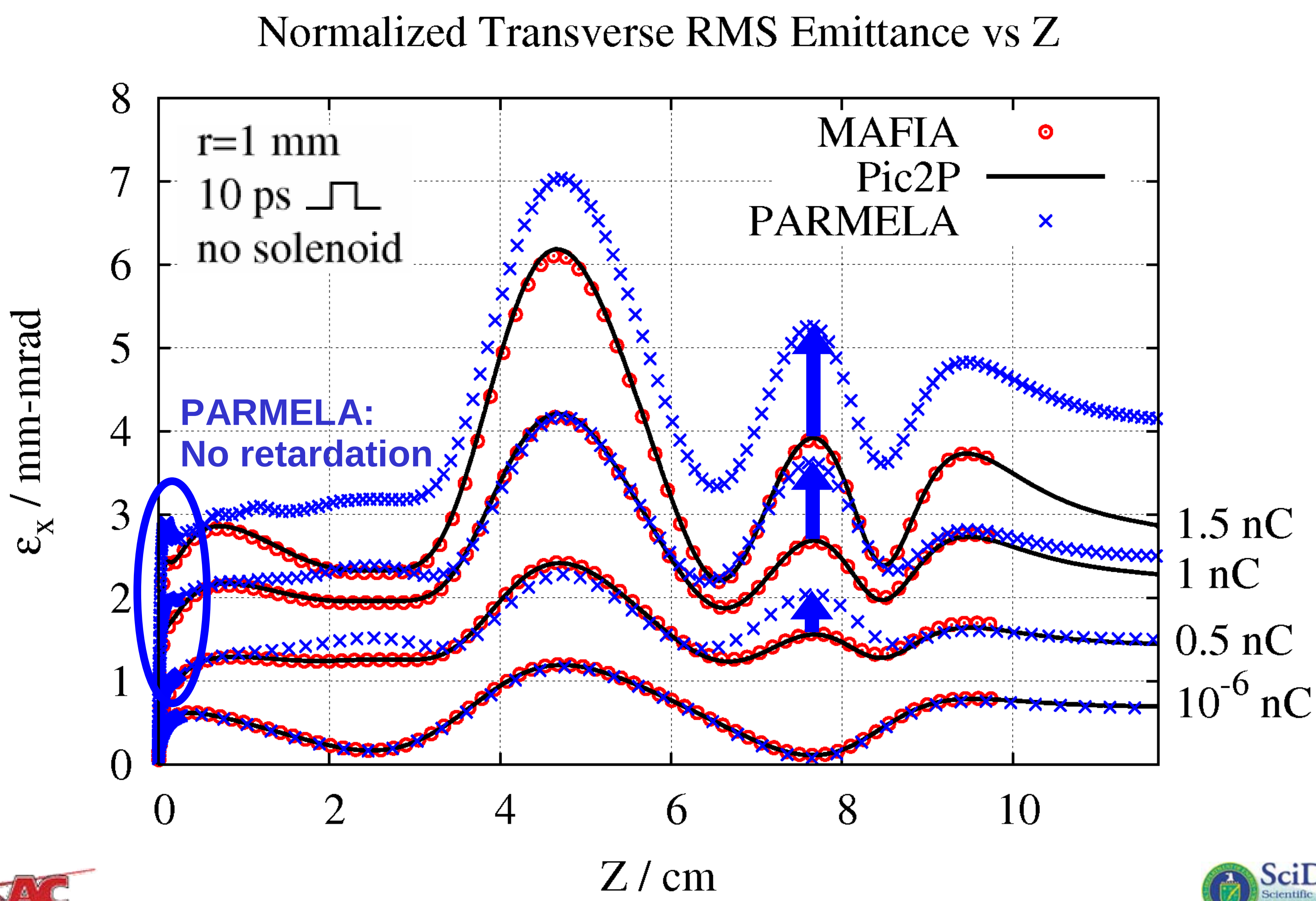


- **Pic2P:** *Code from 1st principles, accurately includes effects of* **space charge, retardation, and wakefields**
- *Extensively benchmarked against analytical solutions and PARMELA / MAFIA*
- *Uses conformal grid, higher-order basis functions and parallel computing for large, fast and accurate simulations*

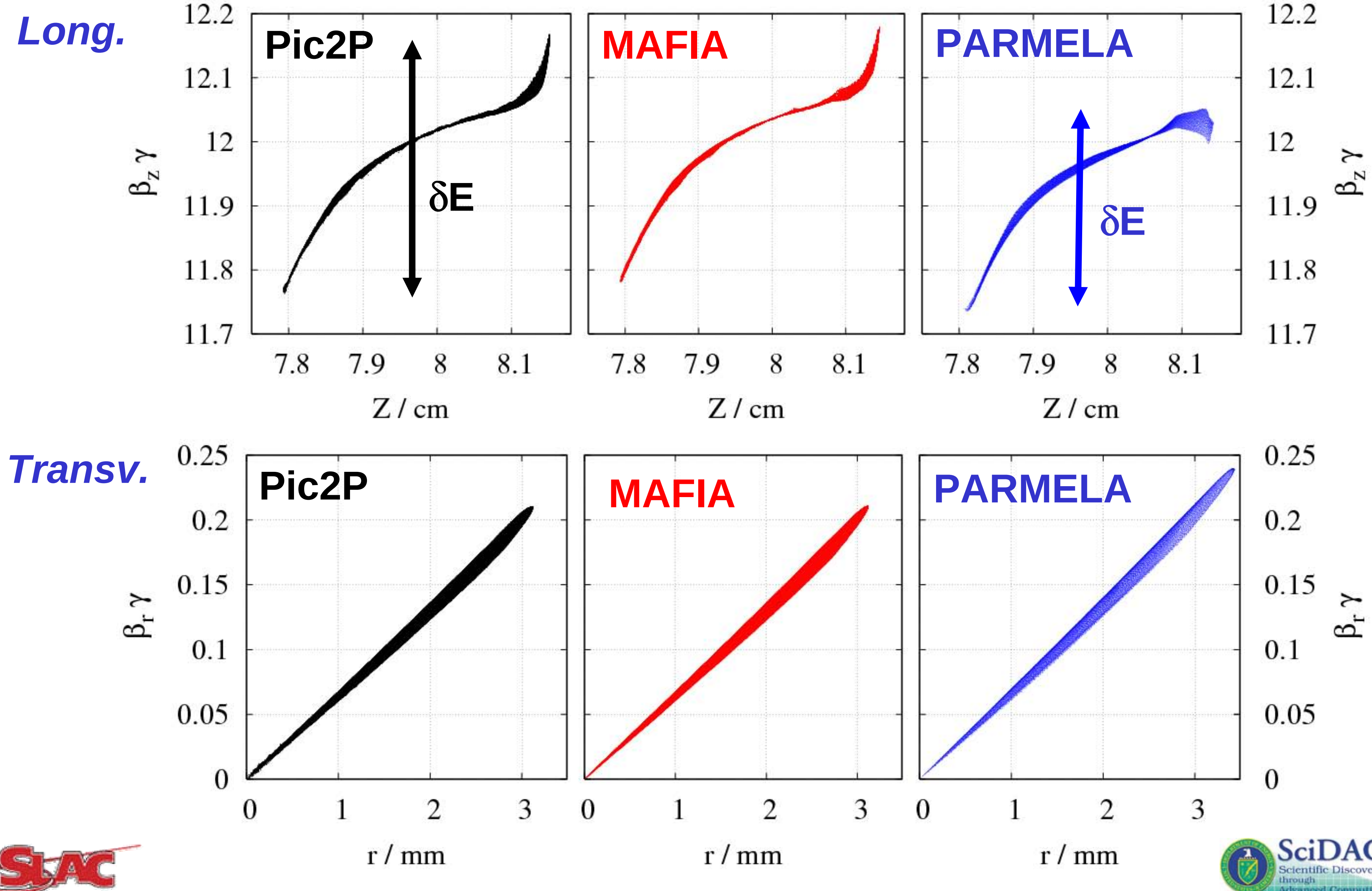
LCLS RF Gun Bunch Radius



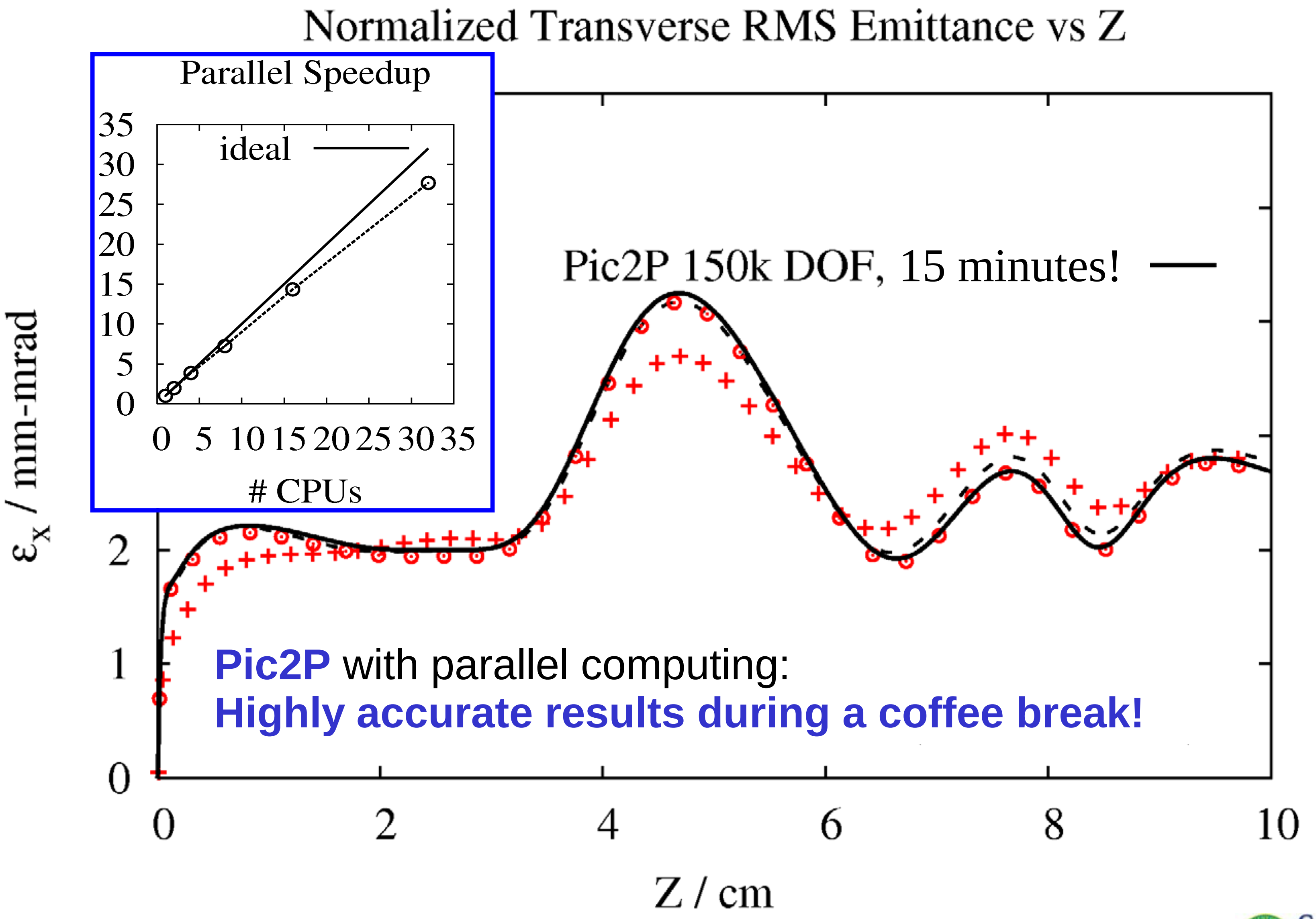
LCLS RF Gun Emittance



LCLS RF Gun Phasespace (1.5 nC)



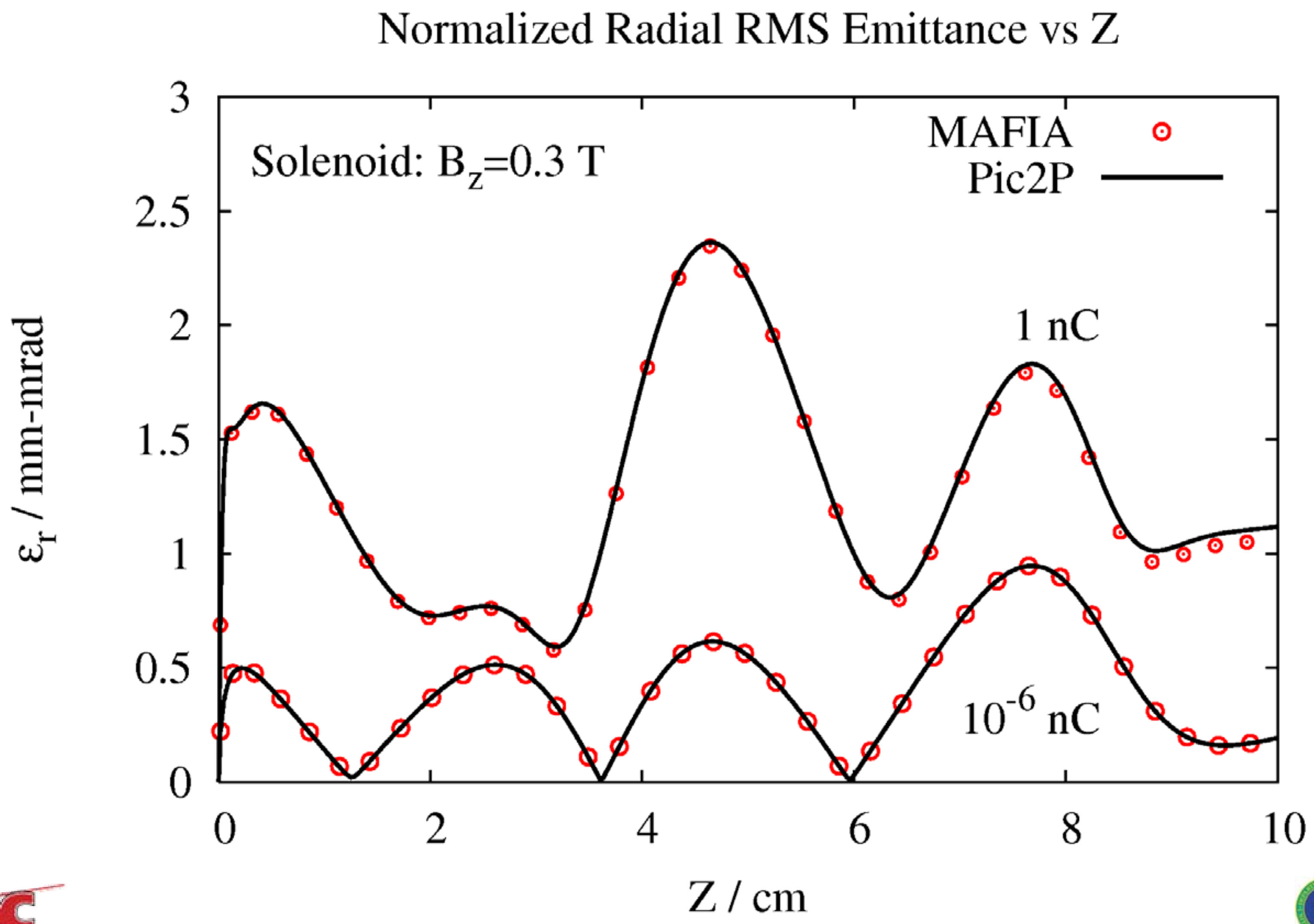
Pic2P - Performance



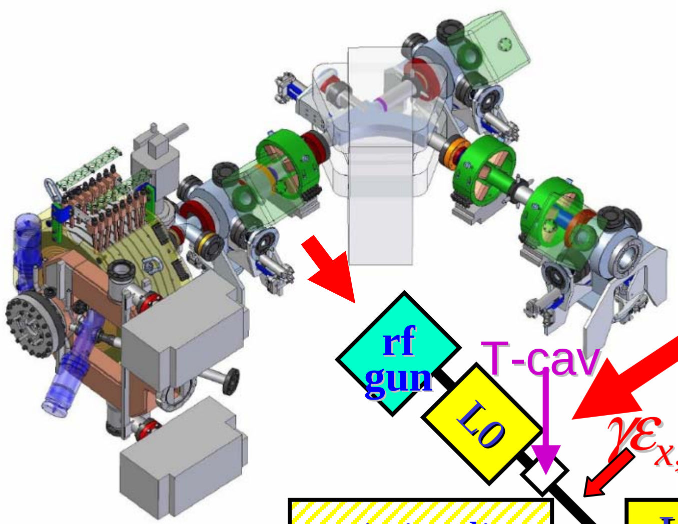
Pic2P with parallel computing:
Highly accurate results during a coffee break!

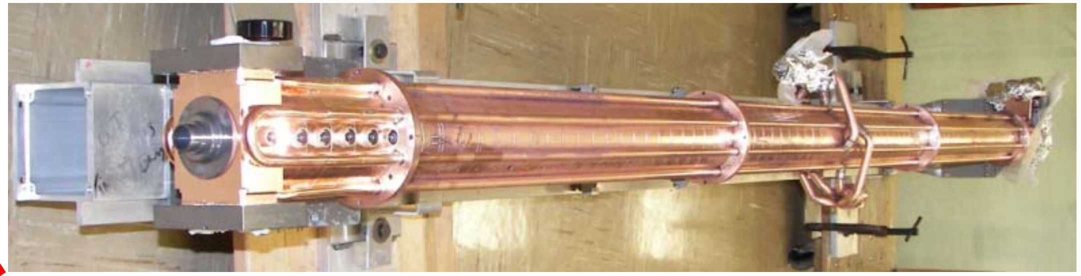
LCLS RF Gun with Solenoid

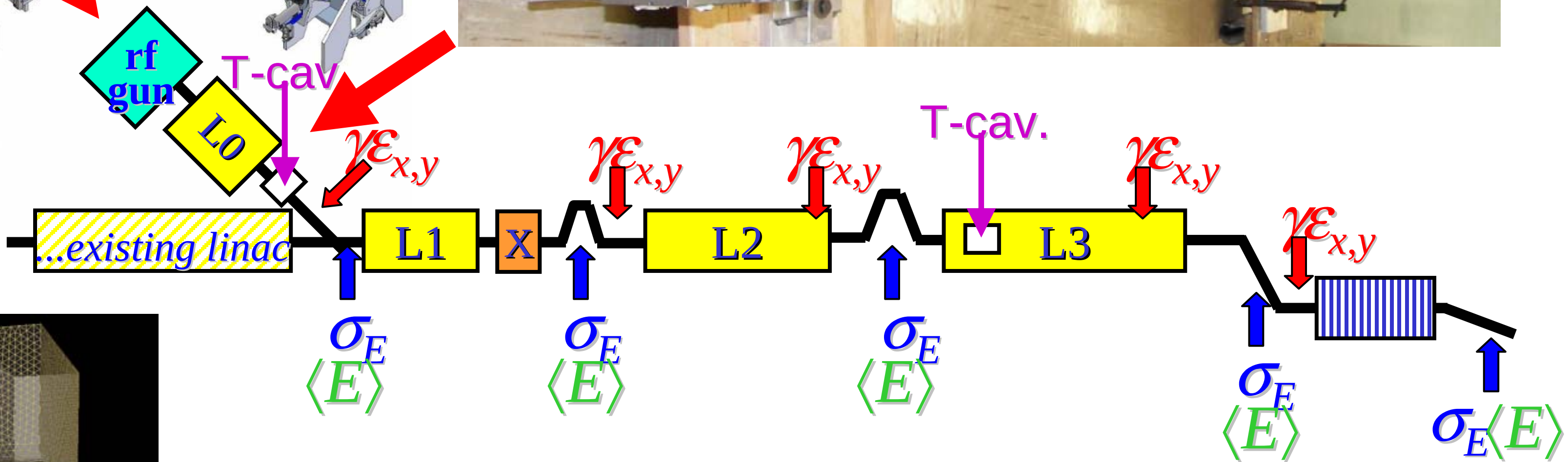
- ✓ **2.5D implemented: Azimuthal dynamics**

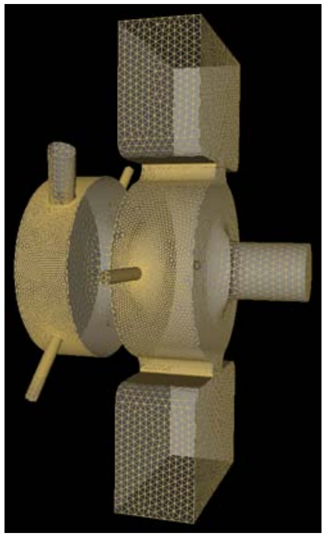


Computational Challenge - LCLS Injector









- *3D RF gun cavity is designed with Omega3P to reduce dipole & quadrupole field components*
- ***3D PIC simulation** is needed for non-uniform laser spot on cathode with emission physics*
- ***Pic3P will be ready** for use in commissioning of the injector*
- *New tool will also benefit the ITF*

Summary

- ➢ SciDAC parallel, conformal, higher-order Finite Element Time-Domain (FETD) codes T3P, Pic2P introduced

- ✓ Wakefield simulations for PEP-II, MIT, ILC (T3P)
- ✓ PIC simulations of LCLS RF gun (Pic2P)

- ➢ Pic3P in development
- ➢ Petascale computing should allow accurate modeling of ILC Cryomodule and LCLS