Parallel Finite Element Particle-In-Cell Code for Simulations of Space-Charge Dominated Beam-Cavity Interactions

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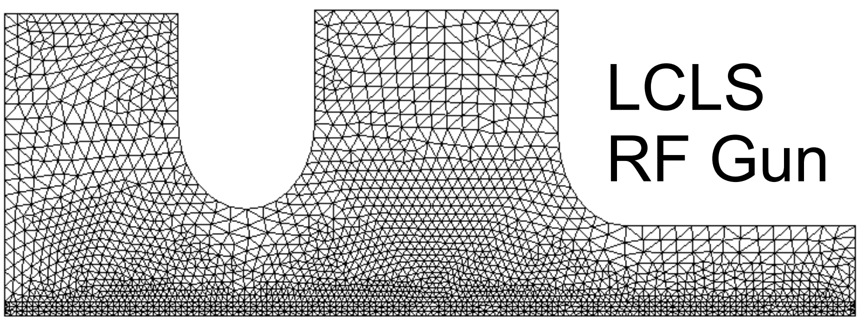
Parallel Finite Element Time-Domain

Maxwell's Wave 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*** -

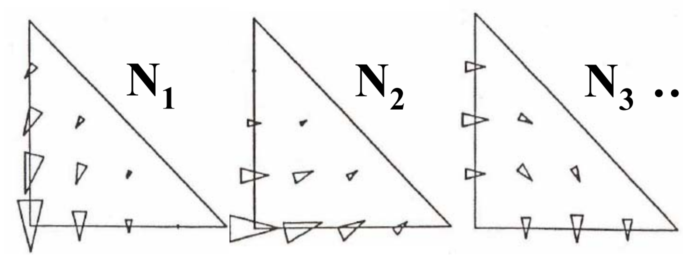
Conformal, unstructured grid with curved surfaces



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 (to do: solve Ax=b)
- ***Parallelization*** - MPI on distributed memory platforms

SciDAC Codes – Pic3P/Pic2P

- ***Pic3P*** **– Parallel 3D FE PIC Code**
- ***Pic2P*** **– Parallel 2.5D FE PIC Code**

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

2) Calculate EM fields from Maxwell's Eqs.

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

SLAC

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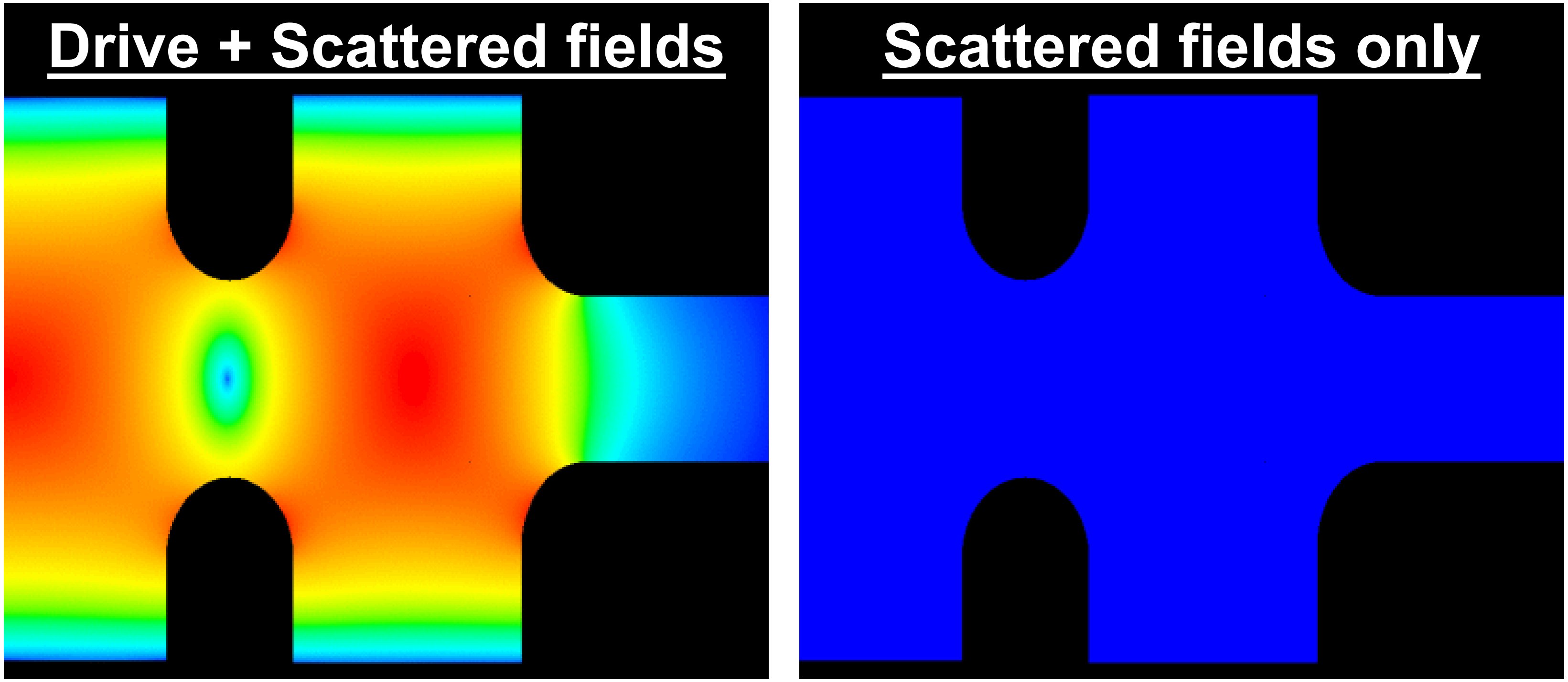
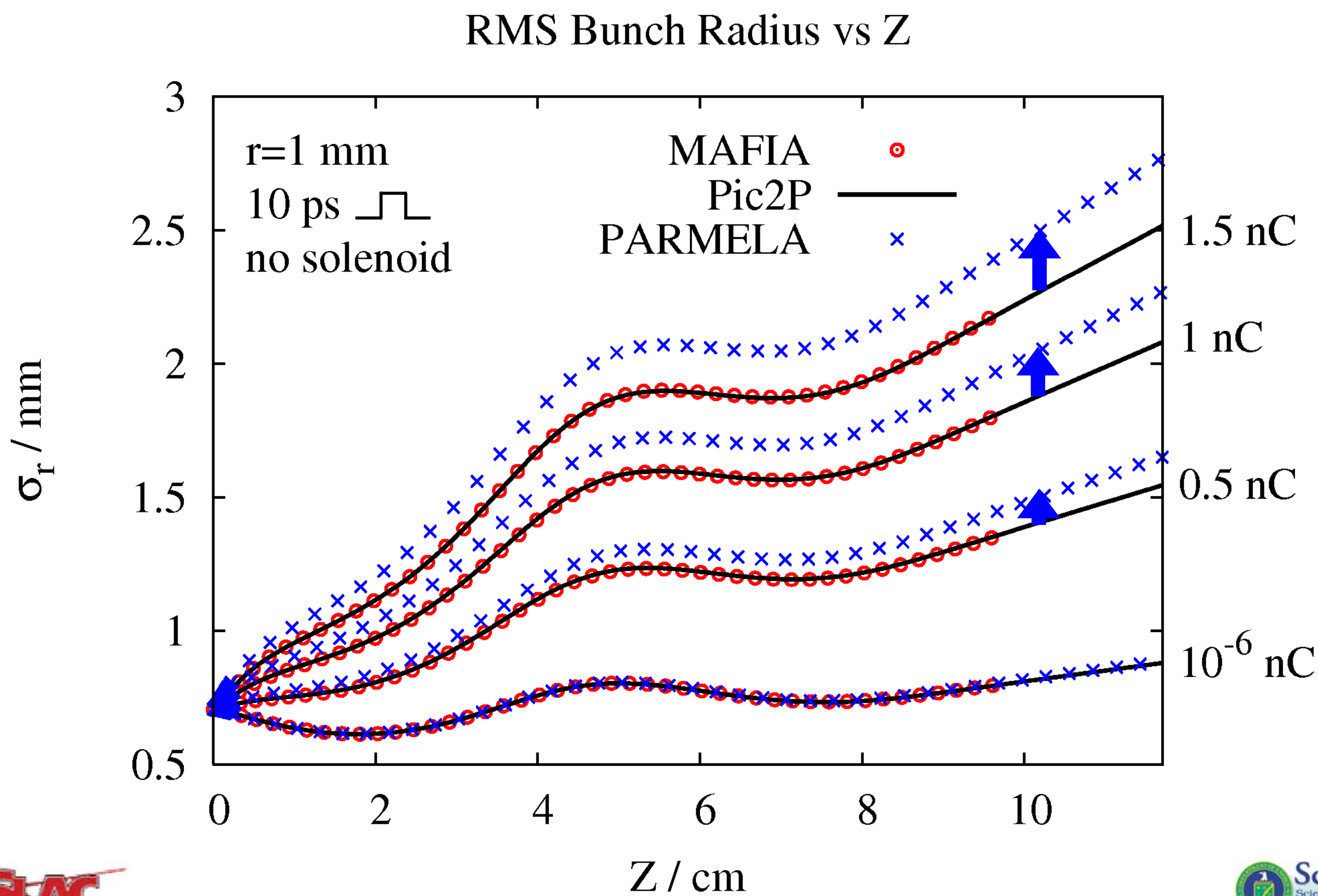
Pic2P Simulation of LCLS RF Gun

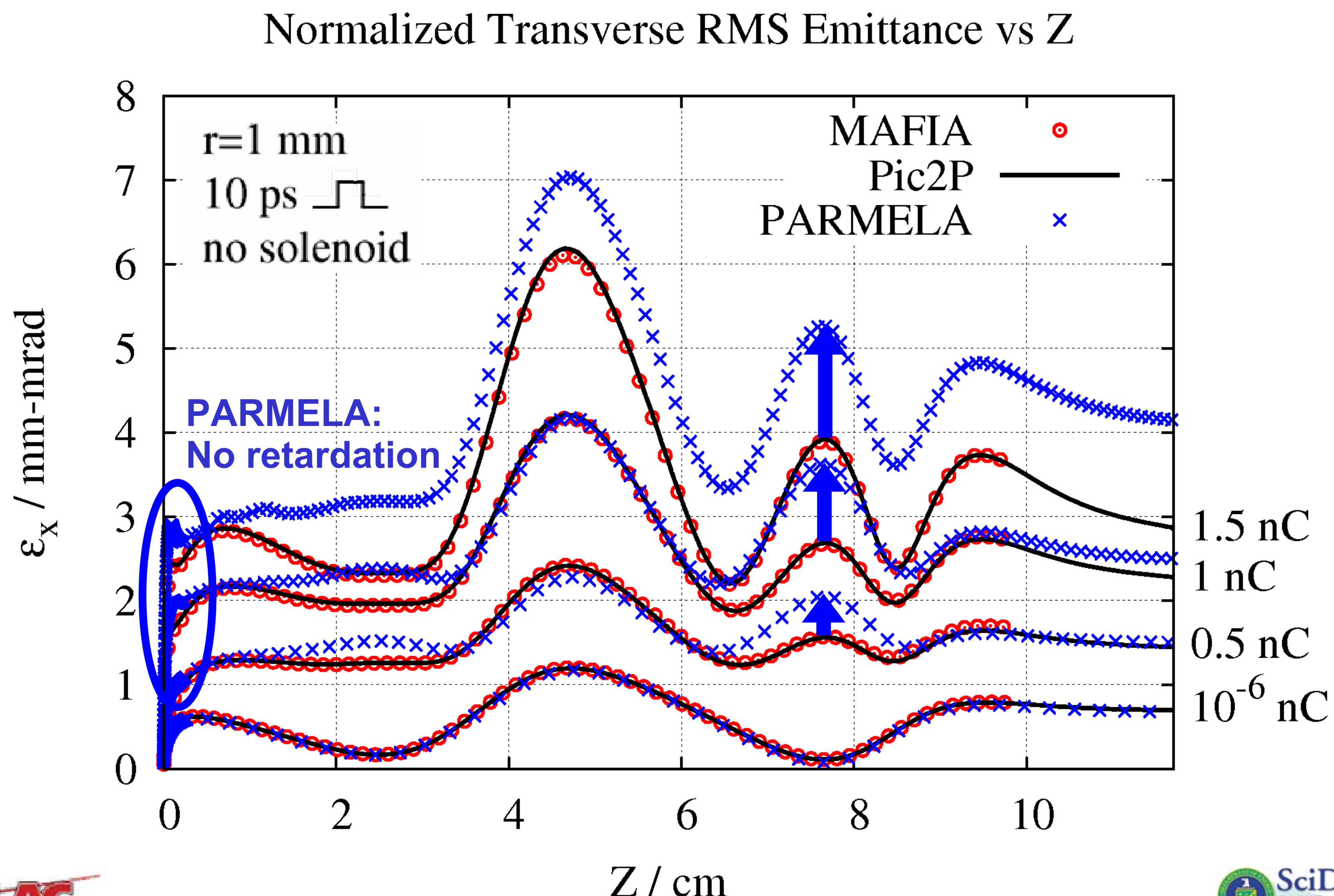


- ***Pic2P*** *– Code from 1st principles, accurately includes effects of* **space charge, retardation, and wakefields**
- *Uses conformal grid, higher-order particle-field coupling and parallel computing for large, fast and accurate simulations*

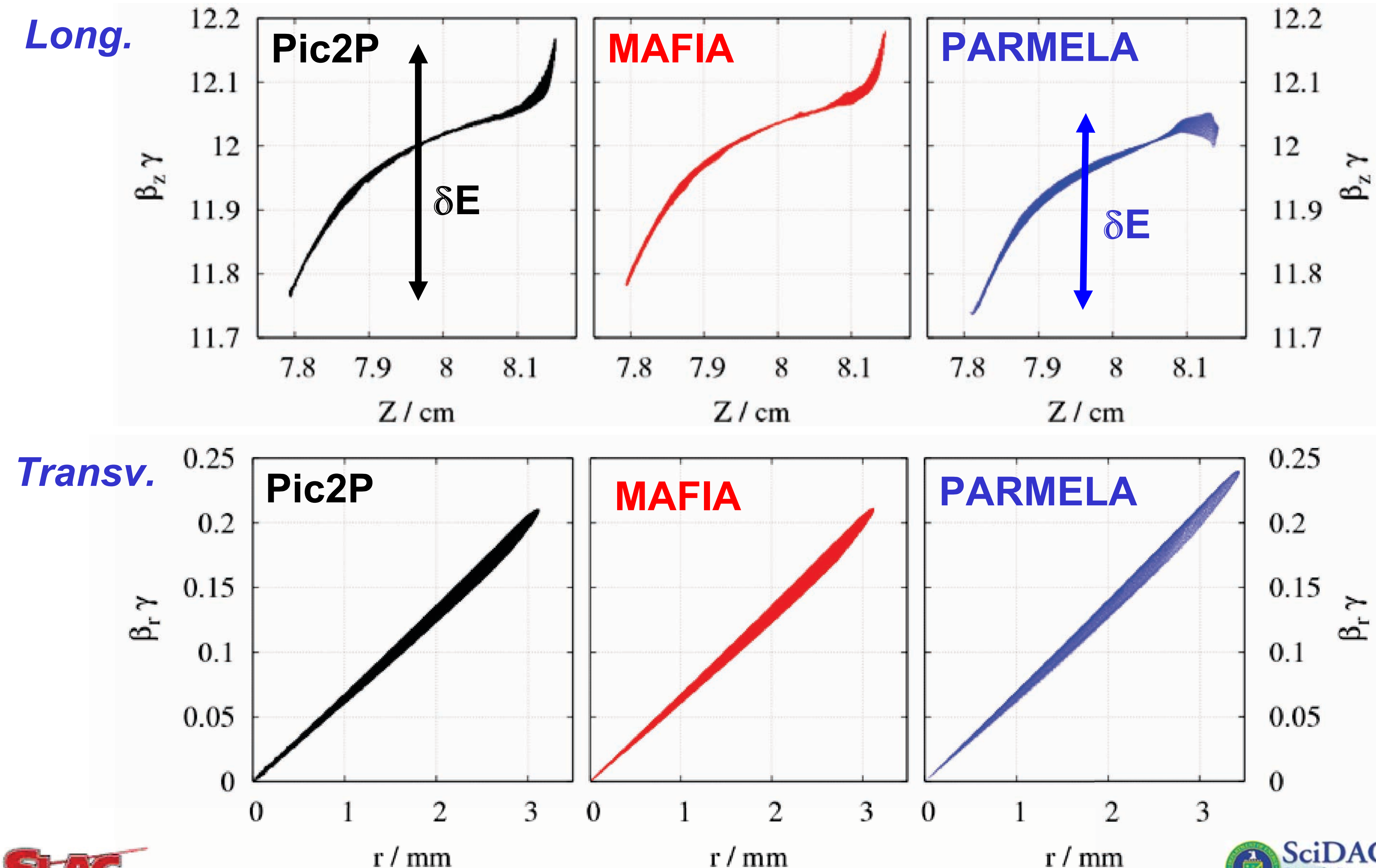
LCLS RF Gun Bunch Radius



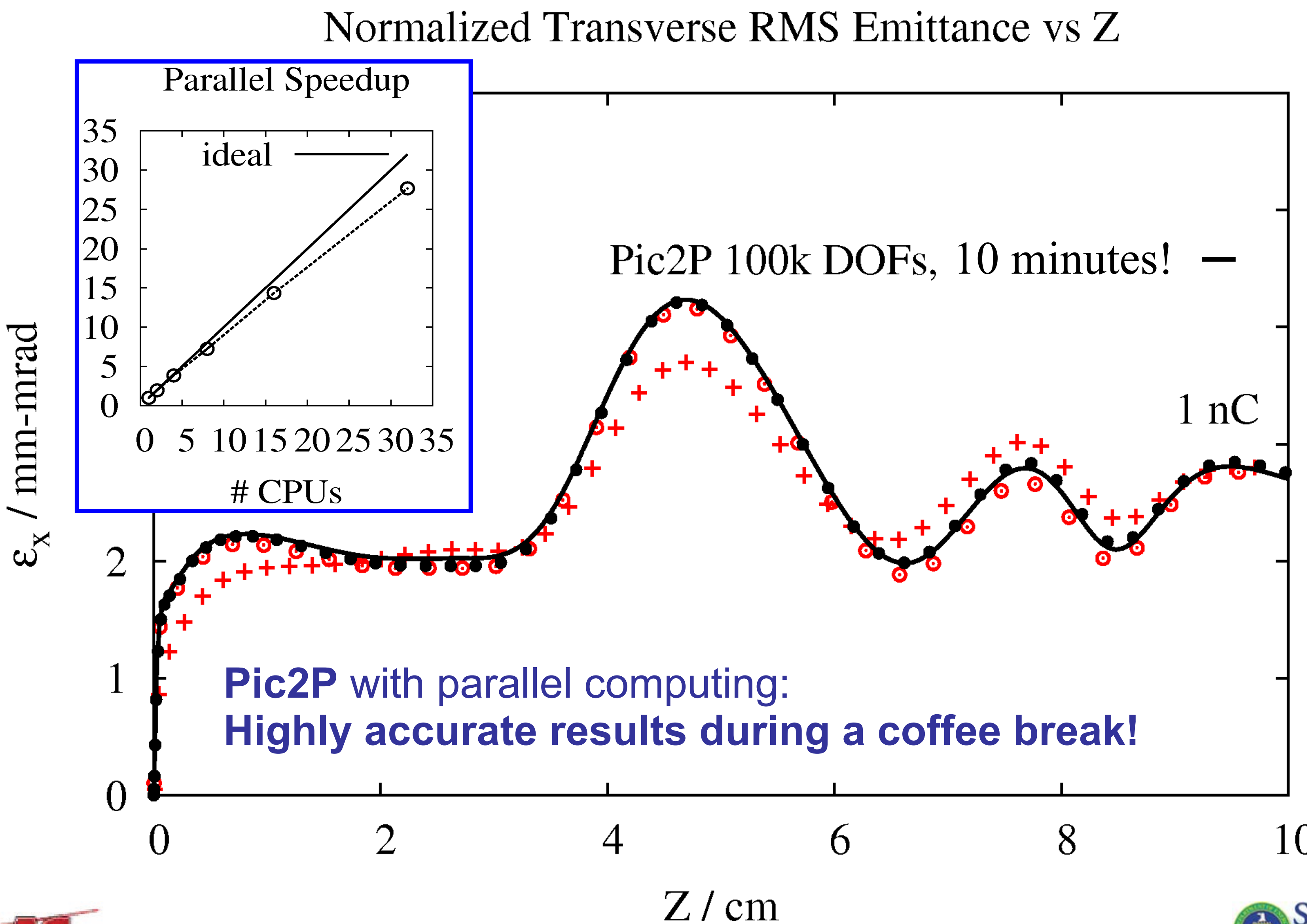
LCLS RF Gun Emittance



LCLS RF Gun Phasespace (1.5 nC)



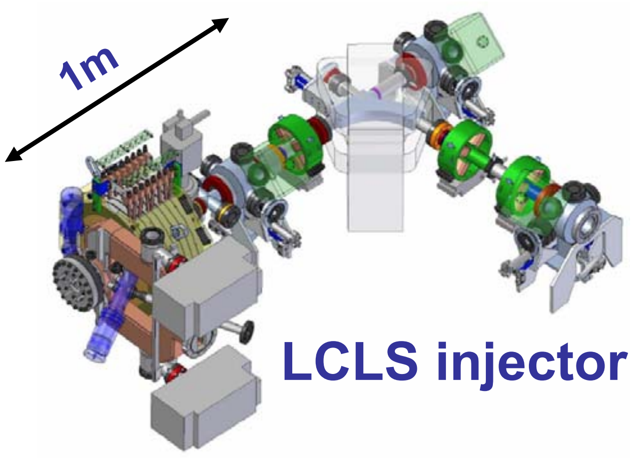
Pic2P - Performance

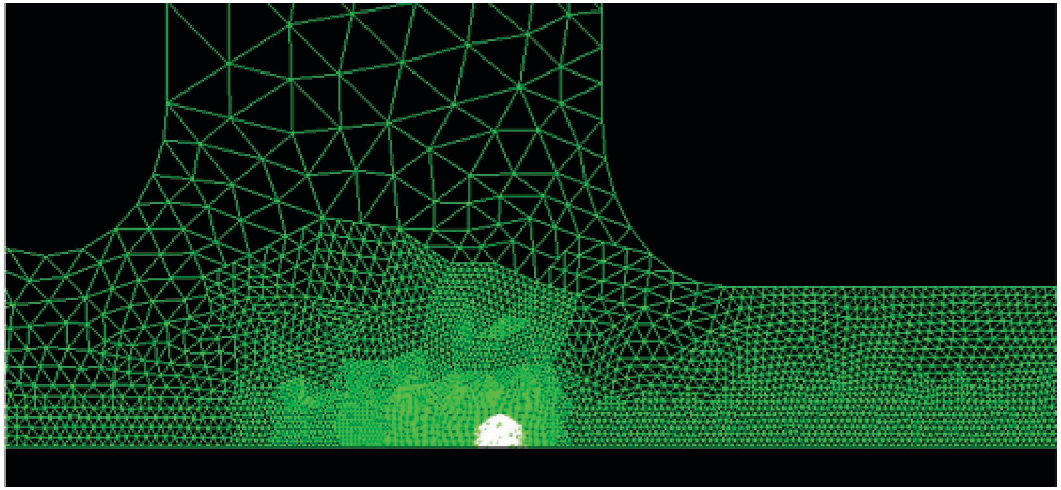


Pic2P with parallel computing:
Highly accurate results during a coffee break!

LCLS Injector Modeling

- ***PIC in long structures*** – Klystrons, injectors, … Active research





- ***Adaptive refinement*** – Efficient simulations of long structures

Summary

- Parallel, conformal, higher-order Finite Element electromagnetic Particle-In-Cell SciDAC codes **Pic3P/Pic2P** introduced

- ✓ PIC simulations of LCLS RF gun (Pic2P)
- ✓ Benchmarked against MAFIA/PARMELA
- ✓ Work in progress: PIC in long structures

- Petascale computing will enable start-to-end 3D modeling of LCLS injector (Pic3P)