High-Fidelity Injector Modeling with Parallel Finite Element 3D PIC Code Pic3P

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SciDAC – Finite Element Electromagnetics

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Parallel Finite Element EM Code Suite ACE3P

SLAC has developed the conformal, higher-order, C++/MPI-based parallel EM code suite ACE3P for high-fidelity modeling of large, complex accelerator structures.

ACE3P: Parallel Finite Element EM Code Suite

(Advanced Computational Electromagnetics, 3D, Parallel)

	ACE3P Modules		Accelerator Physics Application
***Frequency Domain*:**	**Omega3P**	**–**	**Eigensolver (nonlinear, damping)**
	S3P	**–**	**S-Parameter**
***Time Domain*:**	**T3P**	**–**	**Transients & Wakefields**
	Pic3P	**–**	**EM Particle-In-Cell** *(this talk)*
***Particle Tracking*:**	**Track3P**	**–**	**Dark Current and Multipacting**
	Gun3P	**–**	**Space-Charge Beam Optics**
***Multi-Physics*:**	**TEM3P**	**–**	**EM-Thermal-Mechanical**

***Visualization*:** **ParaView – Meshes, Fields and Particles**

Funded by SciDAC1 (2001-2006) and continuing under SciDAC2 (in black)
Under development for ComPASS (2007-2011) (in blue)

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Electromagnetic Particle-In-Cell Method

Self-consistent Loop:

1) Push (Macro-)Particles $$\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

2) Deposit Charges $$\mathbf{J} = \rho \mathbf{v}$$

3) Calculate Fields

$$\left\{ \begin{aligned} \oint_{\partial A} \mathbf{E} \cdot \mathbf{ds} &= -\int_A \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{A} \\ \oint_{\partial A} \mathbf{H} \cdot \mathbf{ds} &= \int_A \left(\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \right) \cdot \mathbf{dA} \\ \oint_{\partial V} \mathbf{D} \cdot \mathbf{dA} &= \int_V \rho \, dV \\ \oint_{\partial V} \mathbf{B} \cdot \mathbf{dA} &= 0 \\ \mathbf{B} = \mu \cdot \mu_0 \mathbf{H} \, , &\qquad \mathbf{D} = \epsilon \cdot \epsilon_0 \mathbf{E} \end{aligned} \right.$$

- Fields are discretized on structured or unstructured grid
- Typically, particles are points: $\mathbf{J}(\mathbf{x}, t) = \sum_i q_i \cdot \delta(\mathbf{x} - \mathbf{x}_i(t)) \cdot \mathbf{v}_i(t)$
- Charge conserved if discrete continuity equation fulfilled: $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = \mathbf{0}$

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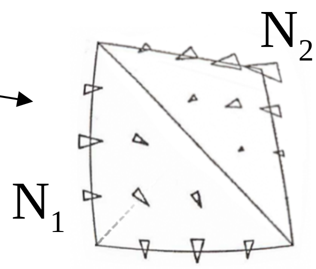
Pic3P – Finite Element Particle-In-Cell Code

Pic3P uses ACD's proven

Parallel Finite Element Time-Domain Methods:

- **Unstructured mesh** with tetrahedral elements (order ***q***=1,2)
- **Higher-order** (Whitney) **vector basis functions** $\mathbf{N_i}$ (order ***p***=1…6)

Quadratic (curved) tetrahedral element



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

For order *p*=2: 20 different $\mathbf{N}_i$'s

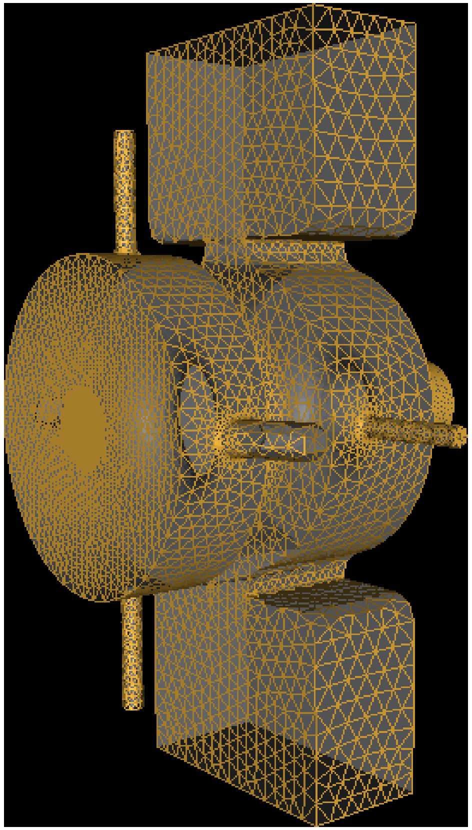
For order *p*=6: 216 different $\mathbf{N}_i$'s

- **Vector wave equation** (combine Faraday's and Ampere's laws)

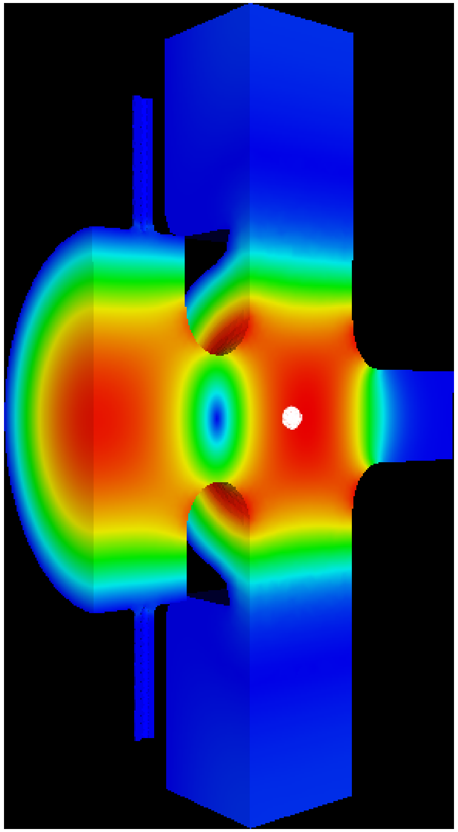
$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times \nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{J}}{\partial t}$$

- **Unconditionally stable** time integration, implicit method (Ax=b)

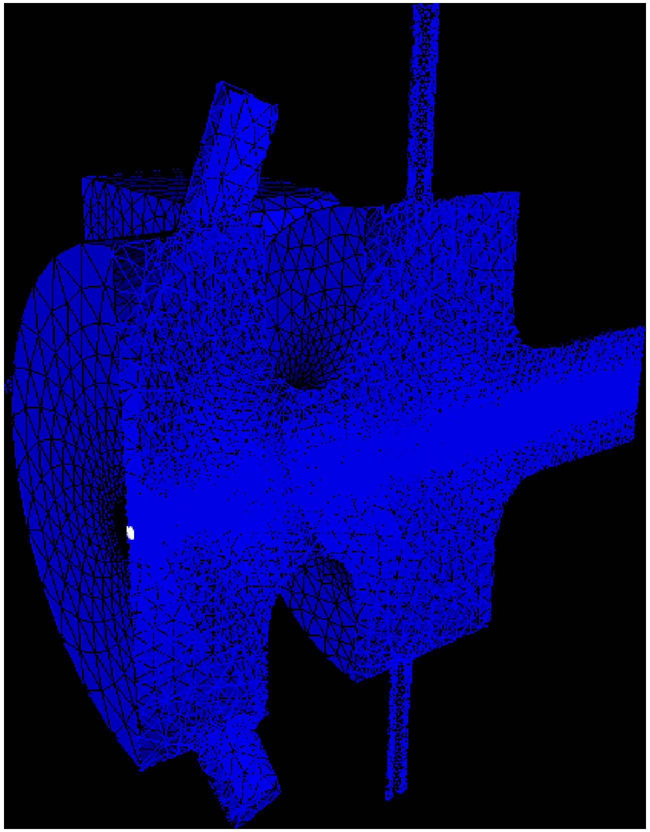
Pic3P Application – LCLS RF Gun



Unstructured mesh model of LCLS RF Gun



Load RF drive fields from Omega3P



Temporal evolution of electron bunch and scattered self-fields

Unprecedented Accuracy thanks to Higher-Order Particle-Field Coupling and Conformal Boundaries

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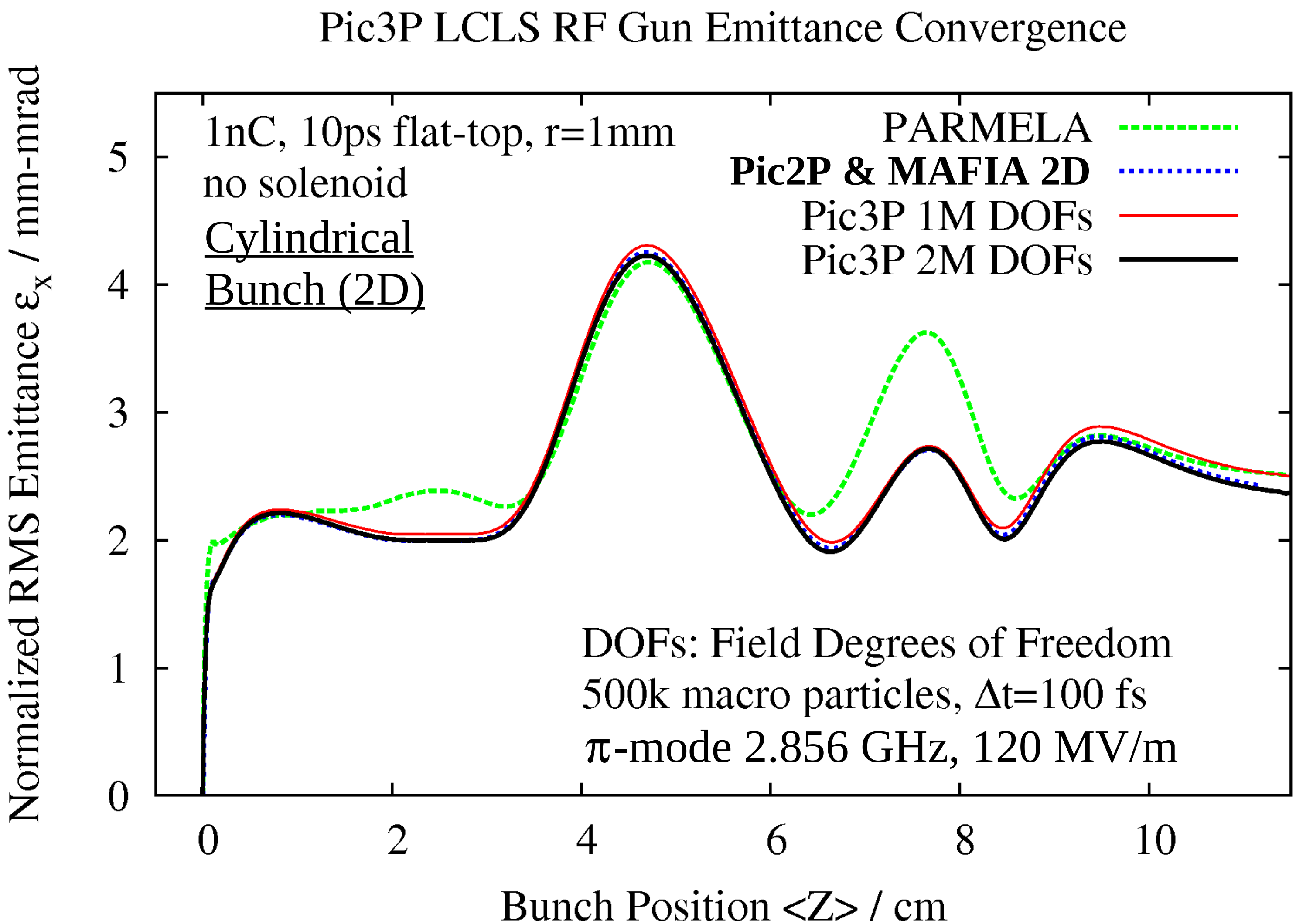
Pic3P – Results and Validation

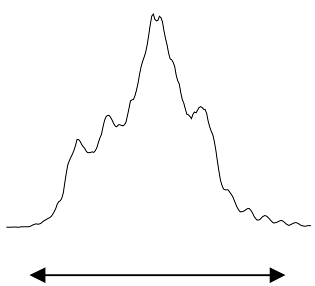


Pic3P – Realistic Particle Distributions

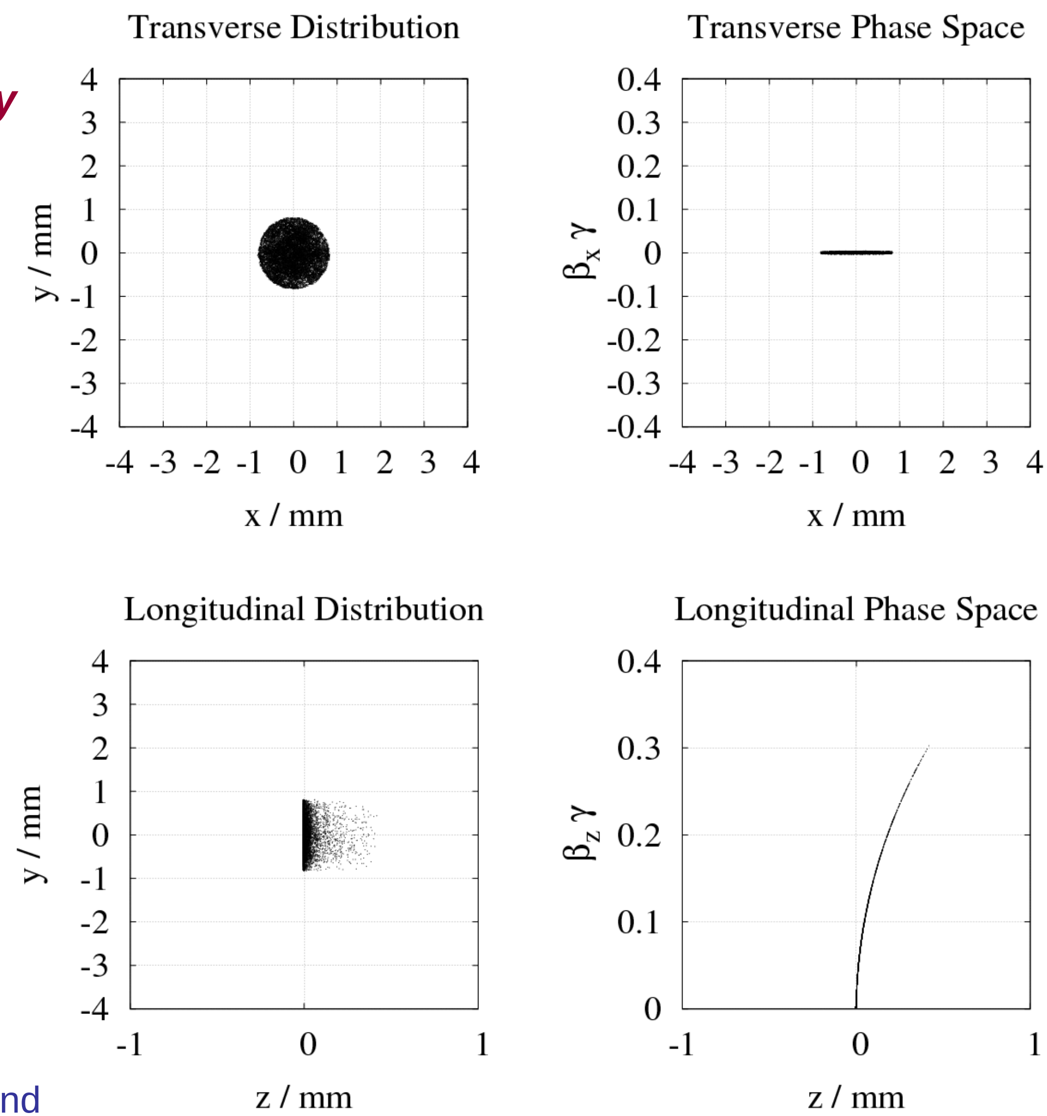
Measured transverse distribution*: *not cylindrically symmetric*

4M macro-particles
initial radius: ~1 mm

Measured temporal laser profile*: *not flat-top*

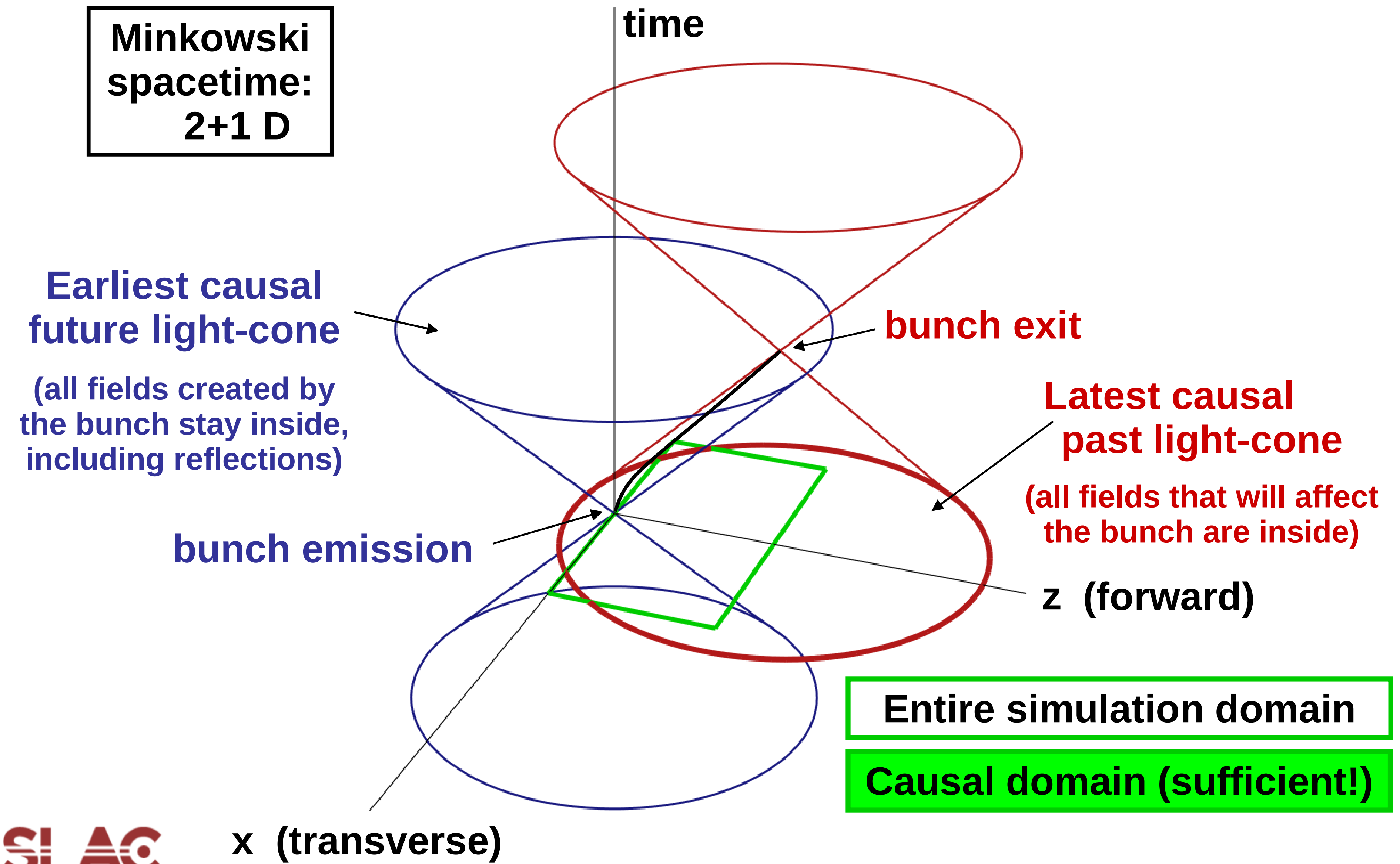


~ 20 ps



* courtesy Cecile Limborg and LCLS Commissioning Team

Physics – Causality in RF Gun



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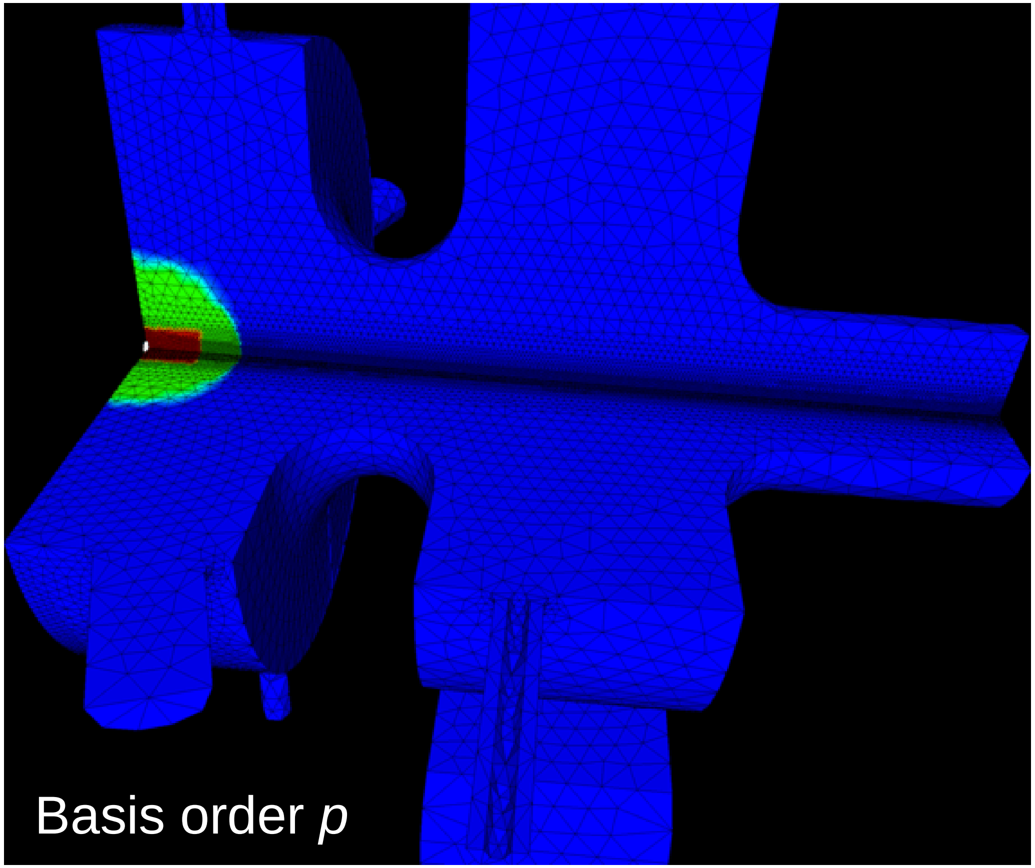
Visualization courtesy Greg Schussman

Pic3P – Causal Adaptive *p*-Refinement



Blue: 0th order | Green: 1st order | Red: 2nd order

Causal "Moving Window":

1. **Enables accurate 3D emittance calculation on workstations in hours**

2. **Allows the solution of large problems on supercomputers**

   (however, localized charge distribution requires sophisticated parallel load balancing scheme)

Restrict calculations onto causal domain:
0th order means no field calculations… Same Results!

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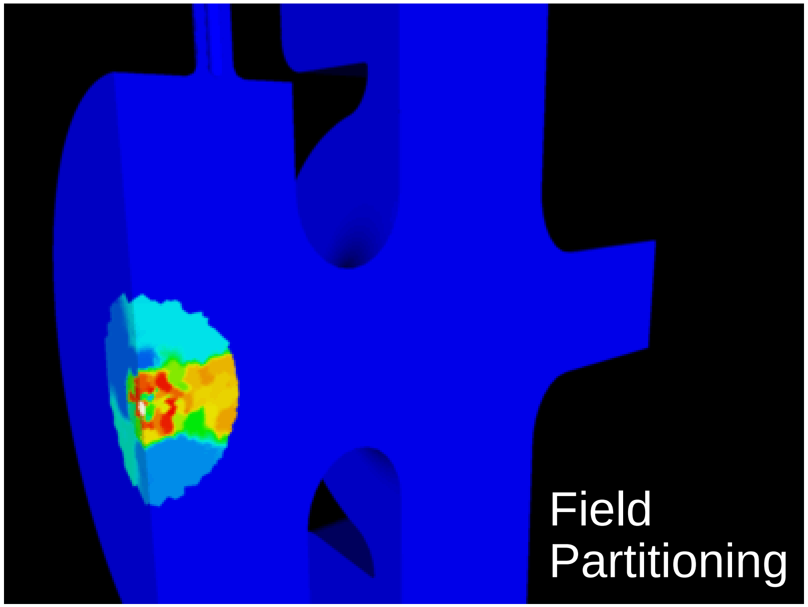
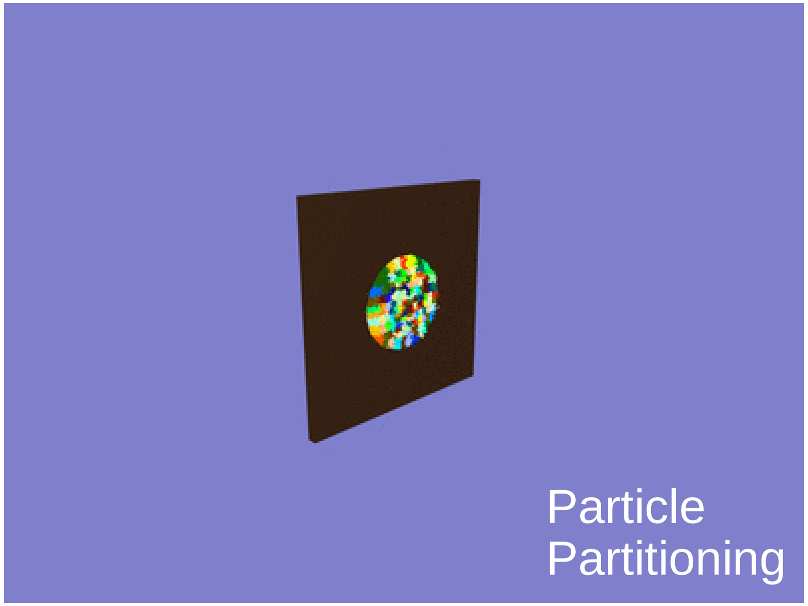
Dynamic Load Balancing using SciDAC Tools

Enhanced Pic3P simulation capability with advanced partitioning scheme

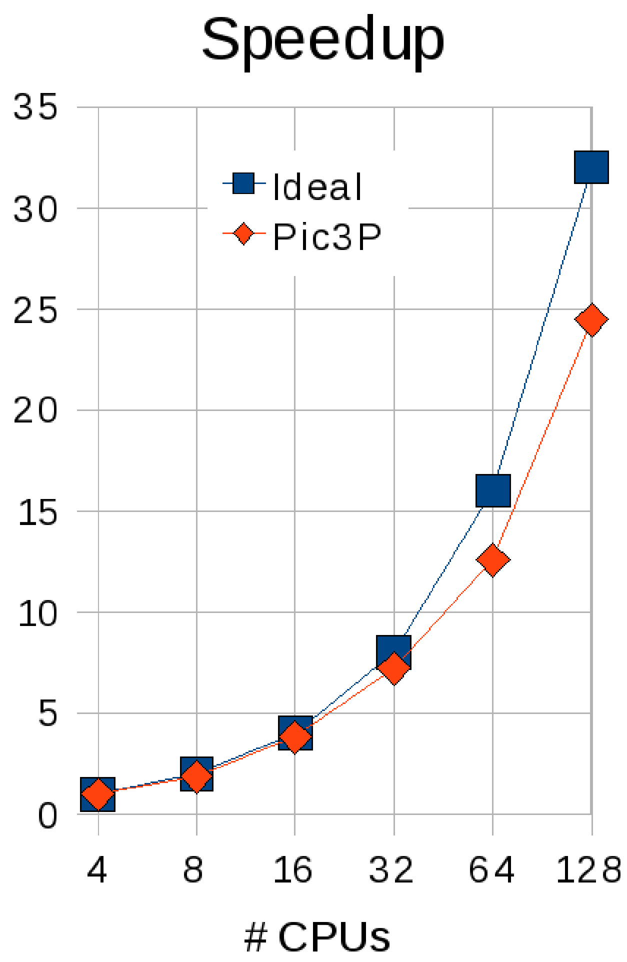
- Fields partitioned with graph-based methods (ParMETIS)
- Particles partitioned geometrically (Zoltan RCB 3D)
- Optimized communication pattern of fields and particle currents
- Enables solution of large problems: 24k CPUs, 750M DOFs, 5B particles



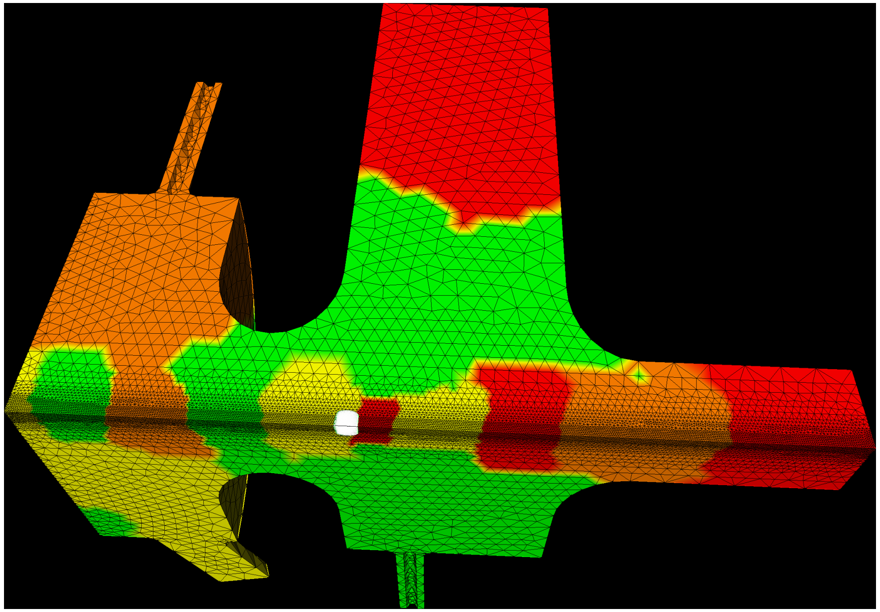


Example: LCLS RF gun, colors indicate distribution to different CPUs

Pic3P – Strong Scaling (Jaguar XT5)



LCLS RF Gun Emittance Convergence:
305k 2nd-order elements, 2M DOFs,
500k particles, iterative linear solver



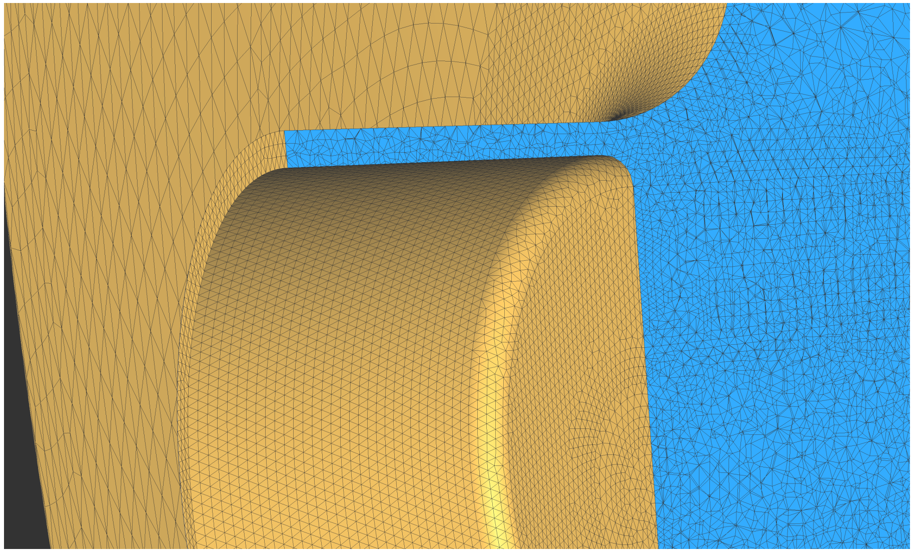
Example Mesh Partitioning on 16 CPUs

Time for fully converged results: ~2h on 128 CPUs

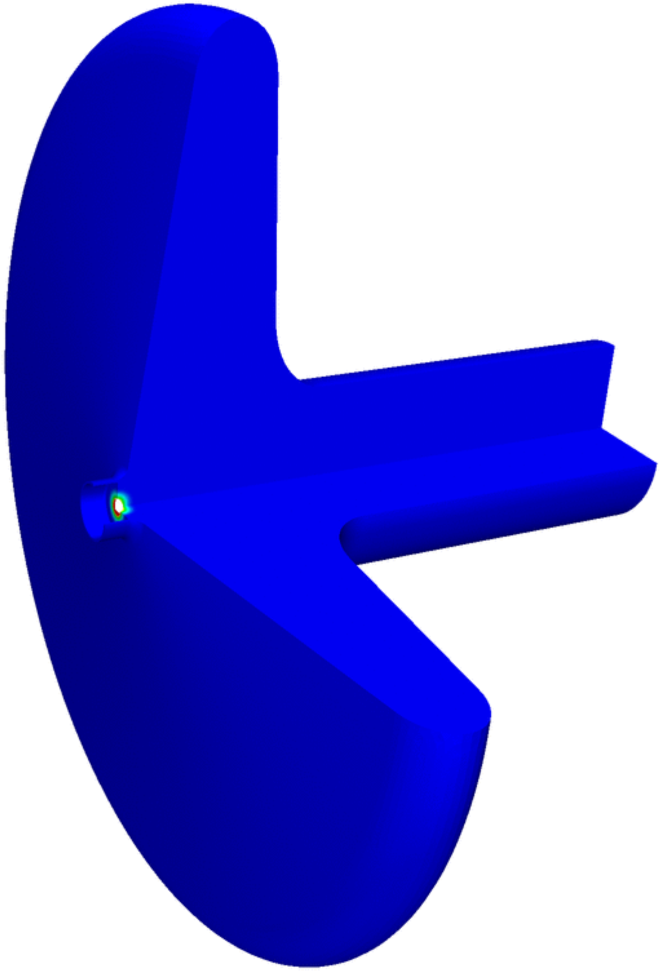
Pic3P – BNL SRF Gun

BNL Polarized SRF Gun:

½ cell, 350 MHz, 24.5 MV/m, 5 MeV, solenoid (18 Gauss), recessed GaAs cathode at T=70K inserted via choke joint, cathode spot size 6.5 mm, Q=3.2 nC, 0.4eV initial energy



Cut-view of unstructured mesh near cathode



Bunch transit through SRF gun (only space-charge fields shown)

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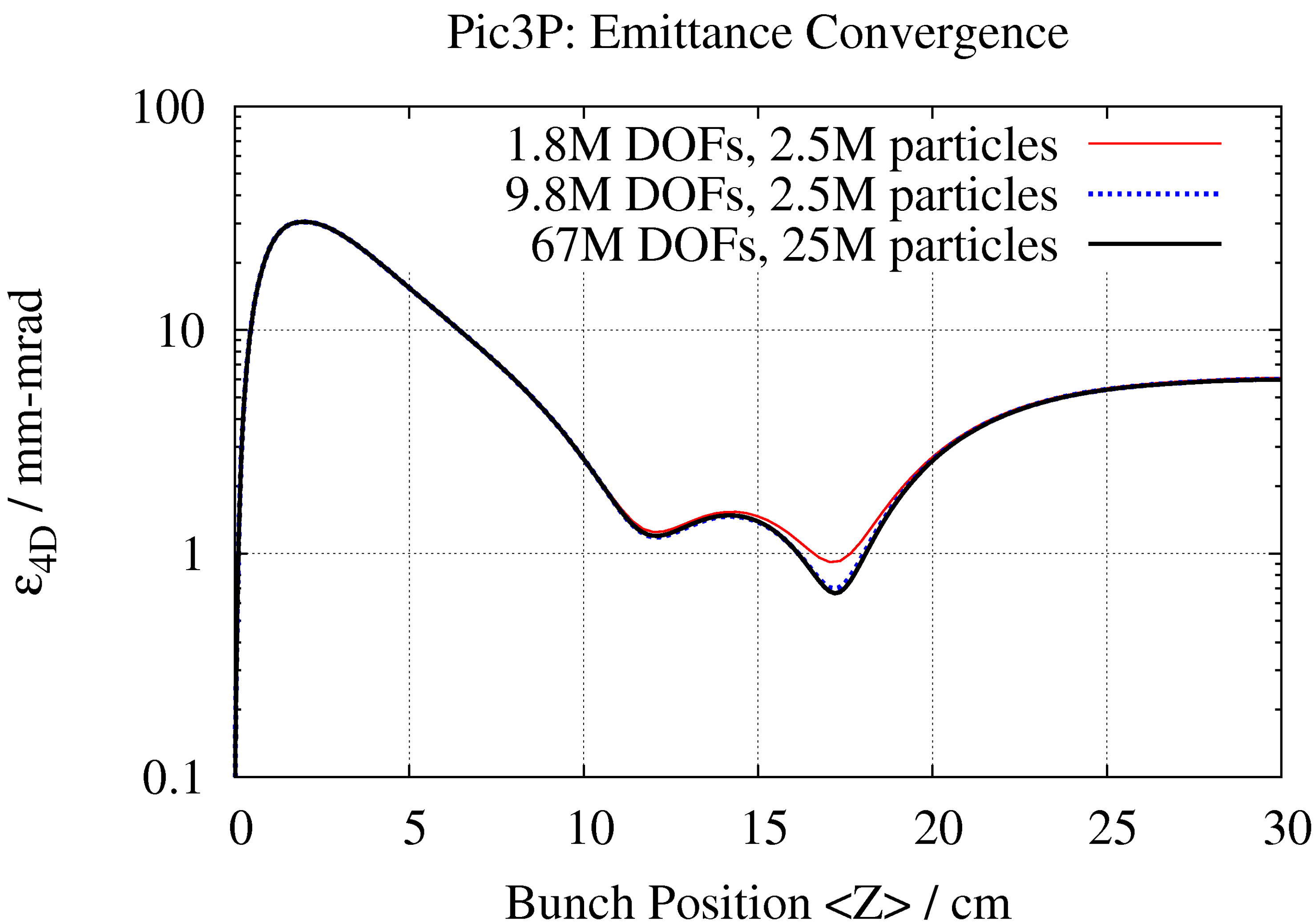
Pic3P – BNL SRF Gun Emittance



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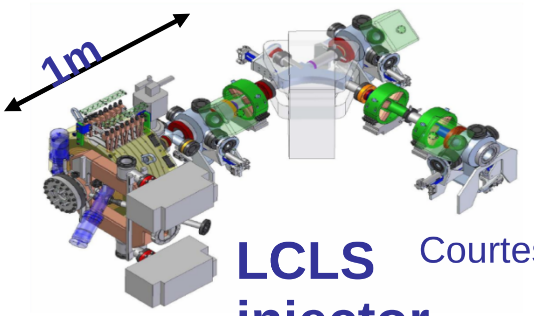
Pic3P – Potential Future Work

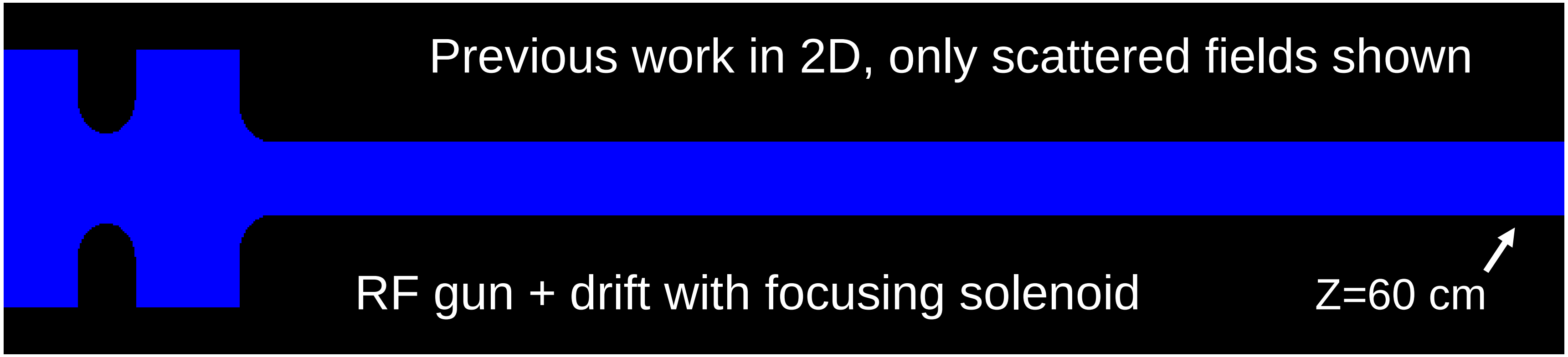
- ***Cathode Physics***
  Photoemission
  Surface roughness
  Laser imperfections

- ***Injector Modeling***
  Gun + drift with solenoid
  Shorter bunches (sub-ps)
  LCLS-2 parameters



LCLS injector

Courtesy LCLS



Summary

- **SLAC's Advanced Computations Department** has developed the **Parallel Finite Element ACE3P Code Suite** for high-fidelity electromagnetic modeling of complex accelerator structures, using conformal geometry and higher-order field representation.
- **ACE3P** modules run on NCCS and NERSC supercomputers and provide state-of-the-art simulation capabilities for accelerator applications.
- **Pic3P** was designed for efficient large-scale self-consistent simulations of beam-cavity interactions in space-charge dominated regimes.
- **Pic3P** was applied to calculate beam emittance in the LCLS RF gun and in the BNL polarized SRF gun and fast solution convergence was observed.

We acknowledge our SciDAC and BNL collaborators