Pic3P – Electromagnetic Particle-In-Cell

SLAC National Accelerator Laboratory

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Pic3P: Parallel EM PIC Code

Self-consistent Loop:

1) Push (Macro-)Particles

2) Deposit Charges

3) Calculate Fields

$$\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$\mathbf{J} = \rho\mathbf{v}$$

$$\oint_{\partial A} \mathbf{E} \cdot \mathbf{ds} = -\int_A \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{A}$$

$$\oint_{\partial A} \mathbf{H} \cdot \mathbf{ds} = \int_A \left(\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}\right) \cdot \mathbf{dA}$$

$$\oint_{\partial V} \mathbf{D} \cdot \mathbf{dA} = \int_V \rho \, dV$$

$$\oint_{\partial V} \mathbf{B} \cdot \mathbf{dA} = 0$$

$$\mathbf{B} = \mu \cdot \mu_0 \mathbf{H} \,, \qquad \mathbf{D} = \epsilon \cdot \epsilon_0 \mathbf{E}$$

Full-wave "EM" PIC, in contrast to electrostatic PIC

Pic3P is charge-conserving, and typically uses point particles:

$$\mathbf{J}(\mathbf{x}, t) = \sum_i q_i \cdot \delta(\mathbf{x} - \mathbf{x}_i(t)) \cdot \mathbf{v}_i(t)$$

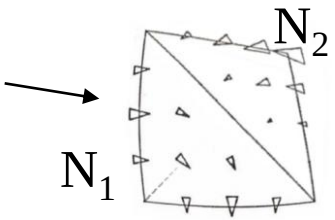
High-Fidelity Through Higher-Order FEM

Pic3P is based on SLAC's ACE3P

Parallel Finite Element Time-Domain Method:

- **Conformal unstructured mesh** (order ***q***=1,2)
- **Higher-order vector basis functions** (order ***p***=1…6)

Quadratic curved (*q*=2) 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** (Faraday & Ampere & time-integral)

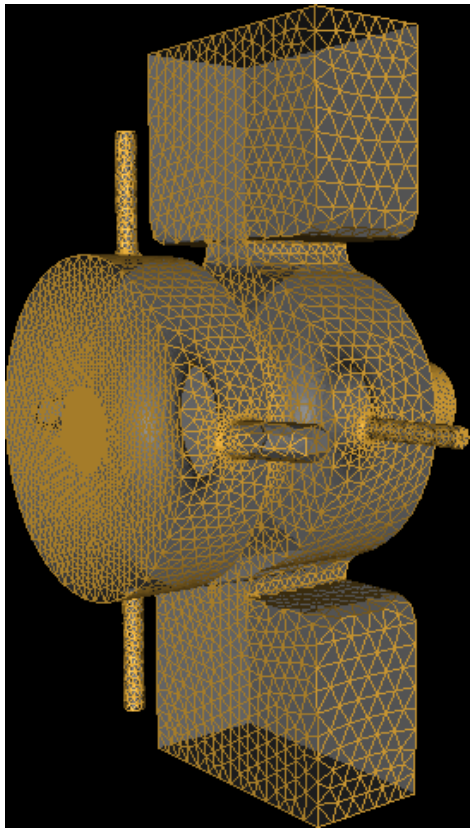
$$\left(\varepsilon\frac{\partial^2}{\partial t^2} + \sigma\frac{\partial}{\partial t} + \nabla\times\mu^{-1}\nabla\times\right)\int^t \mathbf{E}(\mathbf{x},\tau)\,\mathrm{d}\tau = -\mathbf{J}(\mathbf{x},t)$$

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

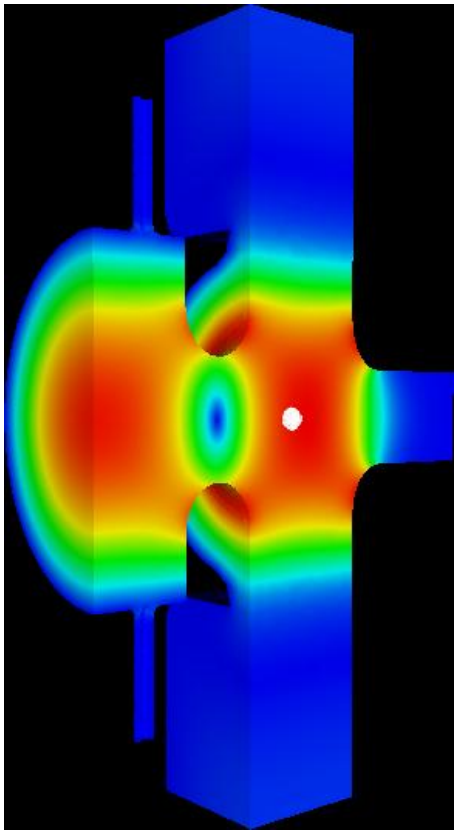
Pic3P Capabilities

- **Low-energy space-charge calculations**
  - Self-consistent modeling of RF guns up to ~ 10 MeV
  - Space-charge, image charge effects, time retardation and wakefield effects included
  - Read RF map (Omega3P or ASCII file) and/or solenoid map (ASCII)
  - Causal moving window technique for efficiency
- **Particle distributions**
  - Simple distribution generator:
    - Longitudinal: Flat-top (with risetime) or Gaussian
    - Transverse: Uniform
    - Initial momentum: Uniform
  - Read-in of arbitrary distributions:
    - Read NetCDF file (can convert from ASCII)
- **Diagnostics**
  - Full 6D phase space dump at given times or z-positions
  - Automatic calculation of moments (1st & 2nd order) and emittances
  - Flat screen “Observerplanes” record particle transit position and time

Pic3P Example Case – LCLS RF Gun



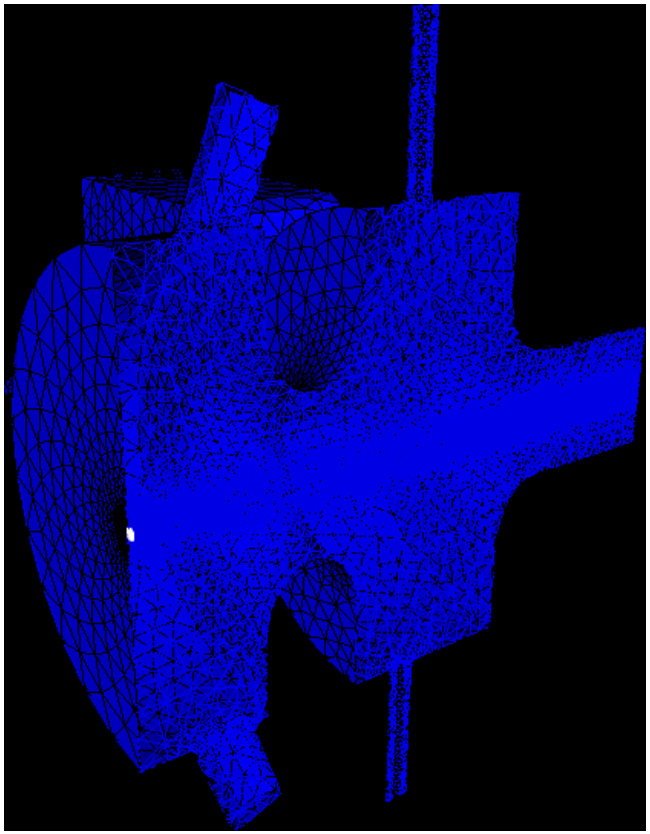
Unstructured mesh model of LCLS RF gun, generated with Cubit



Omega3P calculates RF drive fields, directly imported into Pic3P

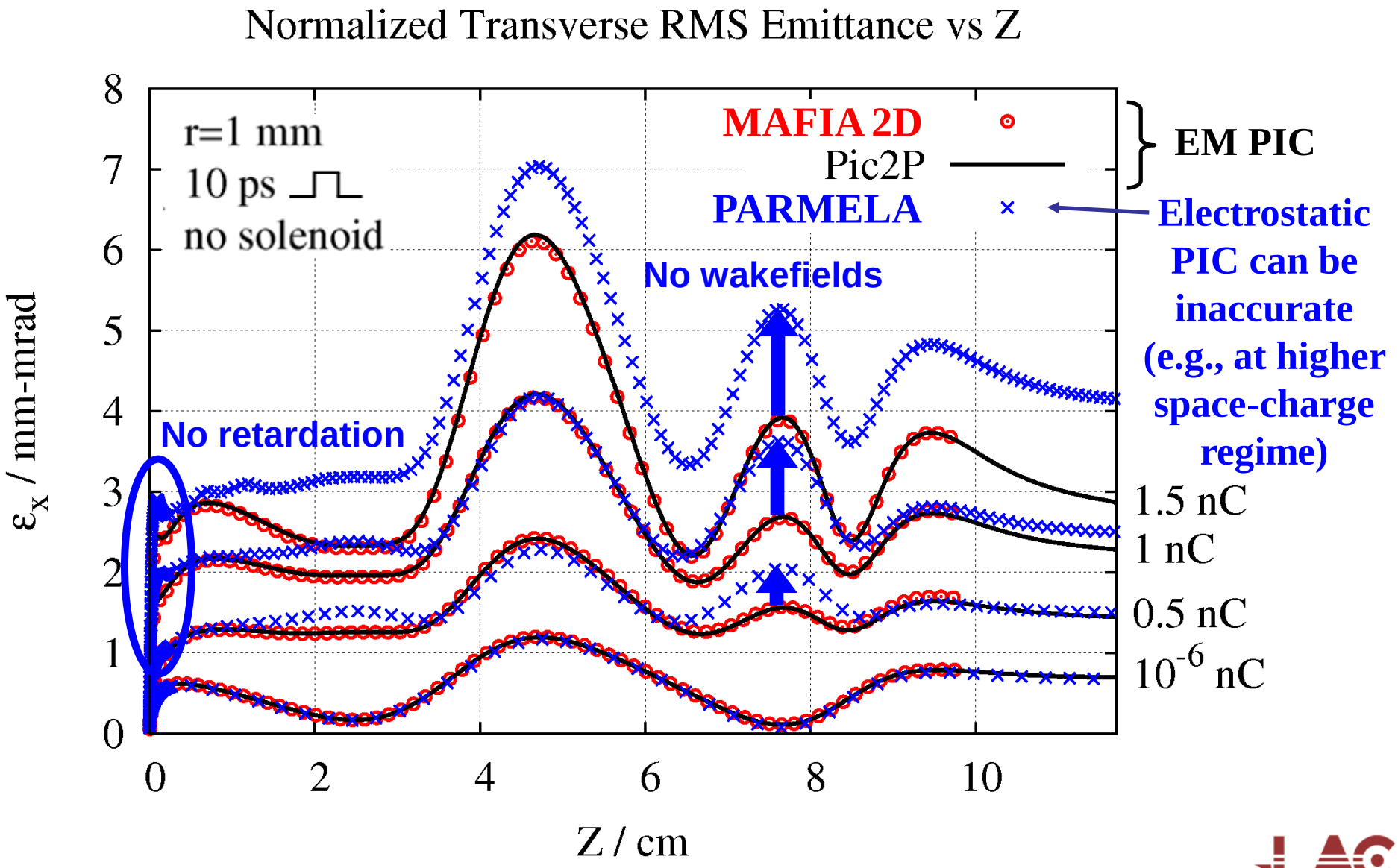
π-mode 2.856 GHz

120 MV/m



Temporal evolution of electron bunch and scattered self-fields as modeled with Pic3P

LCLS RF Gun – Why use EM PIC Code?



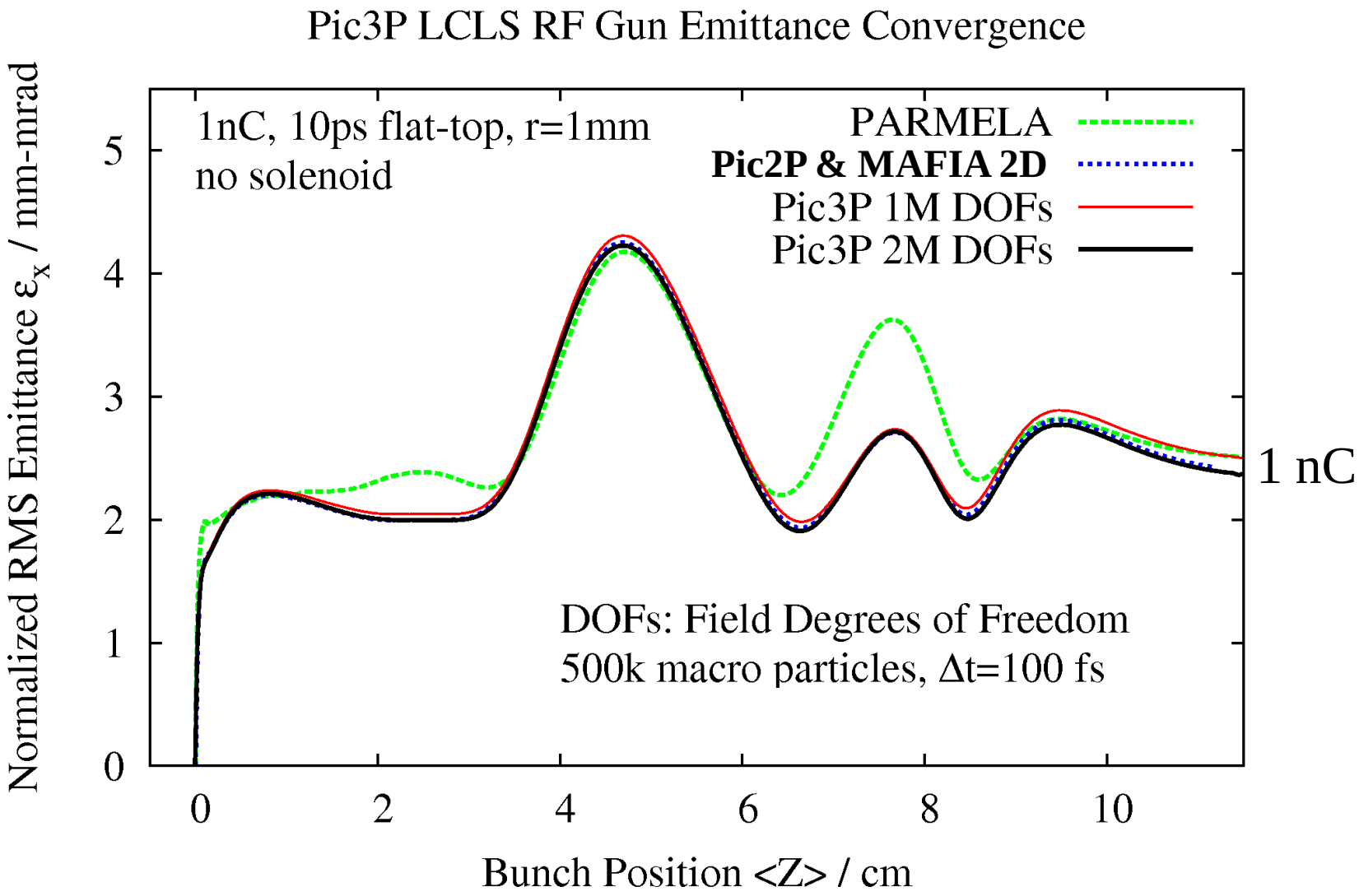
Pic3P Example Input – LCLS RF Gun

```
Loading:
{
  Type: PICLoading
  SymmetryFactor: 4            // typical: ¼ structure modeled (if no solenoid)
  SymmetryOrigin: 0 0 0        // reflections at magnetic symmetry planes

  Particles:
  {
    NumberOfParticles: 1e5              // total number of particles
    TotalCharge: -1e-9                  // charge in C
    Beta: 0 0 0.03                      // uniform initial v/c
    CathodeCenter: 0 0 -6.0325e-2       // center of emission

    Flattop: 1                          // for beer-can bunch distribution
    DeltaT: 10e-12                      // bunch length in s
    rMax: 1e-3                          // bunch radius in m

    …
```

Pic3P Example Input – LCLS RF Gun

```
 …
 Monitors: {
   DumpTimeStart: 0          // start time for dumping 6D phase space
   DumpTimeEnd: 1e-9         // end time for dumping 6D phase space
   DumpTimeStep: 1e-11       // time interval for dumping 6D phase space
   DumpPositions: .01 .05    //<z>-positions where to dump the phase space
   ObserverPlane Z-Positions: 1e-2 2e-2 // record transiting particles phase space (&time)
 }
 EigenMode: {      // use multiple of these EigenMode containers for multiple drive modes
    ModeNumber: 1                    // which Eigenmode to load?
    FieldComponent: 2                //Z
    FieldValueAtPhase0: -120e6       // E field (component) value at GradientPoint at phase=0
    SamplePoint: 0 0 -6.0325e-2      // Point at which to specify the gradient
    CentroidPhaseBeforeCrest: -58  // injection rf phase of bunch centroid

   Omega3PMap: {
      Directory: EigenMode // path to directory that contains the Omega3P run data
      InputFile: in.o3p          // name of the input file used for Omega3P run (without path)
      StartPoint: -1e-2 -1e-2 -6.0325e-2   //min corner of bounding box where to load Omega3P map
      EndPoint: 1e-2  1e-2 0.1  // max corner of bounding box where to load Omega3P map
    }
 }  // EigenMode
}  // Particles
```

LCLS RF Gun: Emittance Convergence

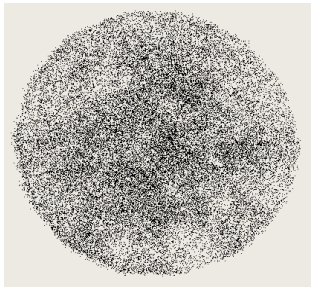


1 nC

InitialDistributionFile: PhaseSpace6D.ncdf

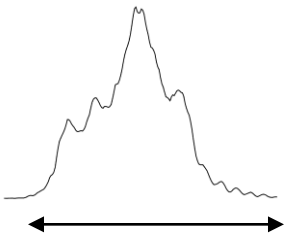
Please contact Arno Candel for instructions

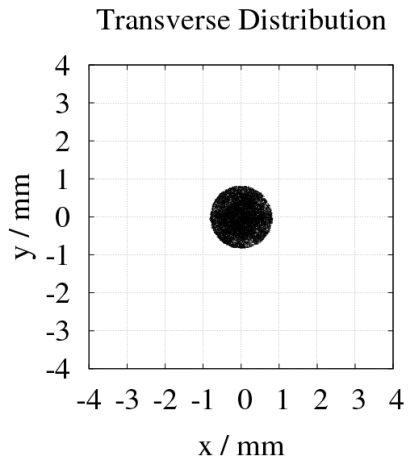
Measured transverse distribution*: ***not cylindrically symmetric***

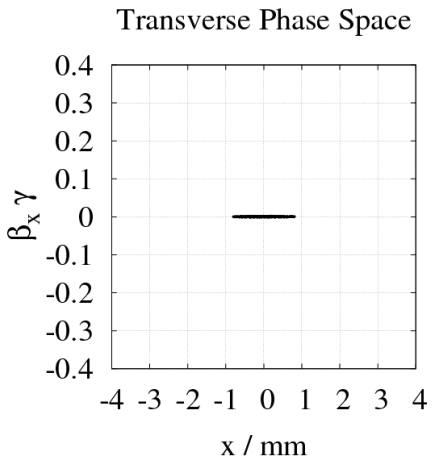


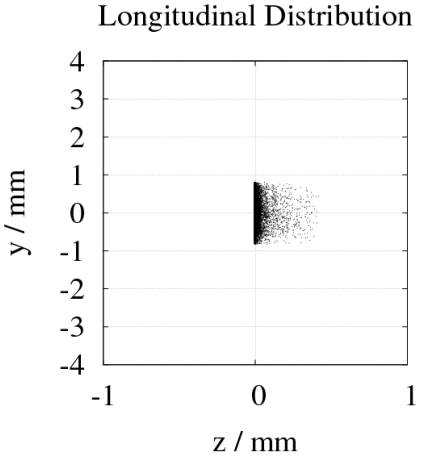
4M macro-particles
initial radius: ~1 mm

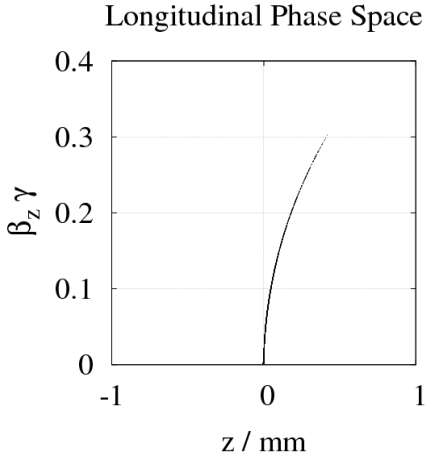
Measured temporal laser profile*: ***not flat-top***







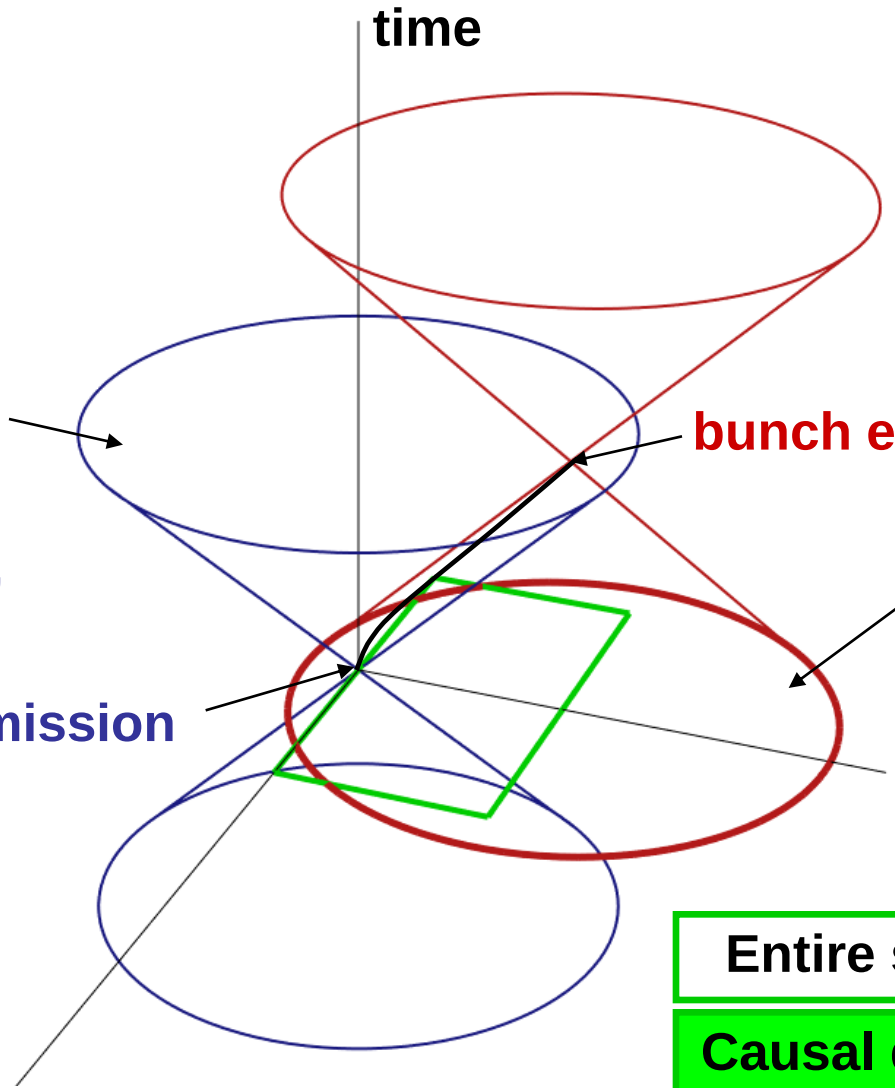




* courtesy Cecile Limborg and LCLS Commissioning Team

Physics - Causality in RF Gun

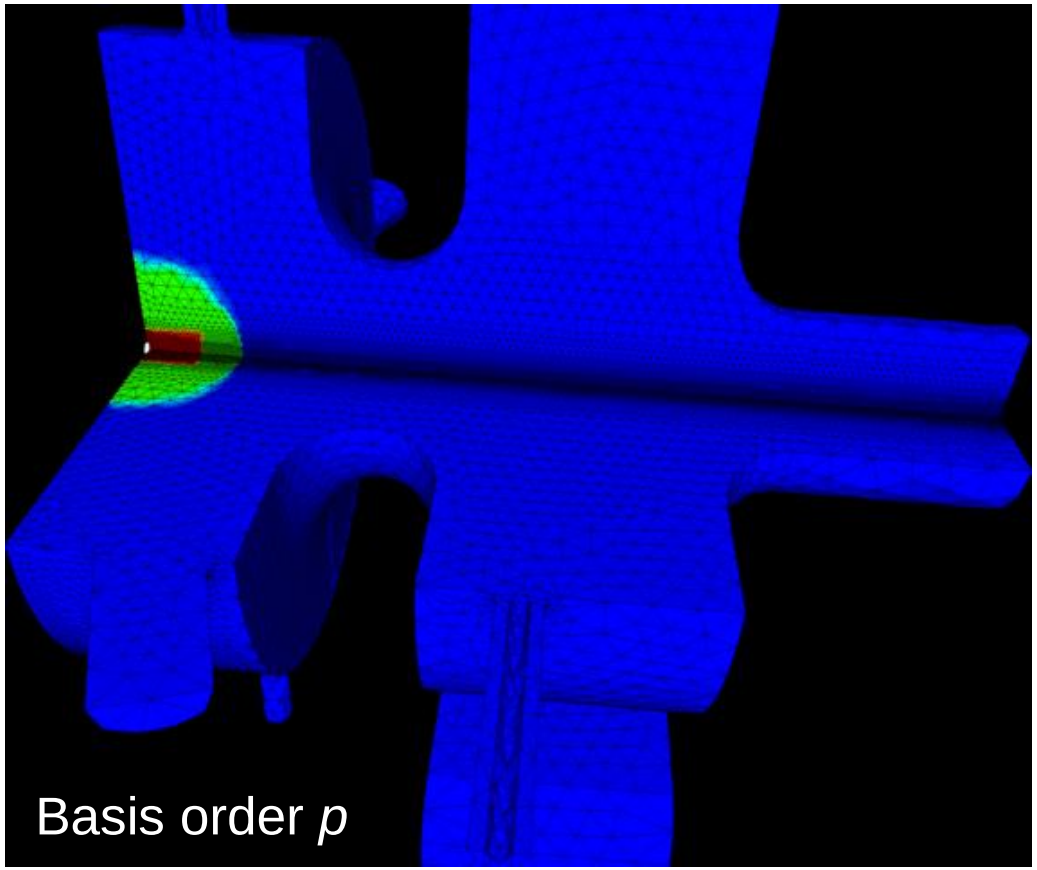
Minkowski spacetime: 2+1 D



Entire simulation domain

Causal domain (sufficient!)

Causal Adaptive *p*-Refinement: Specify *p*



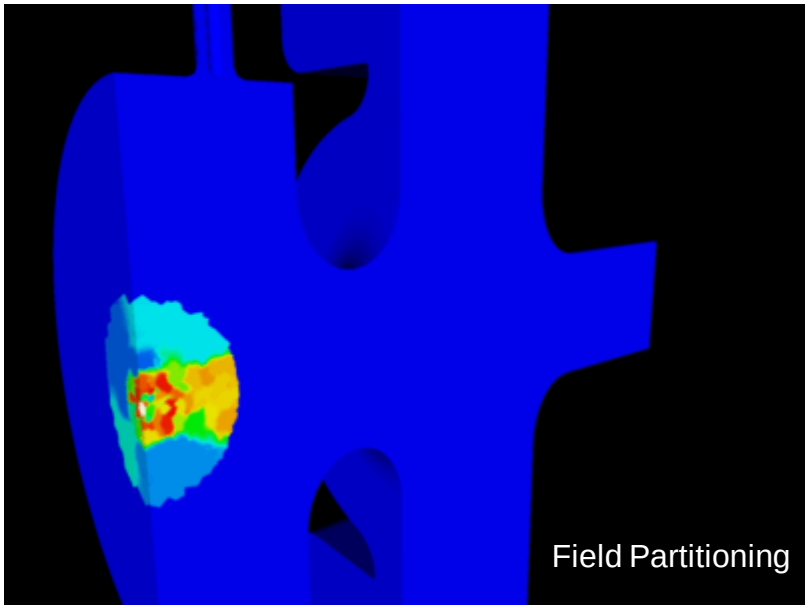
Blue: 0th order | Green: 1st order | Red: 2nd order

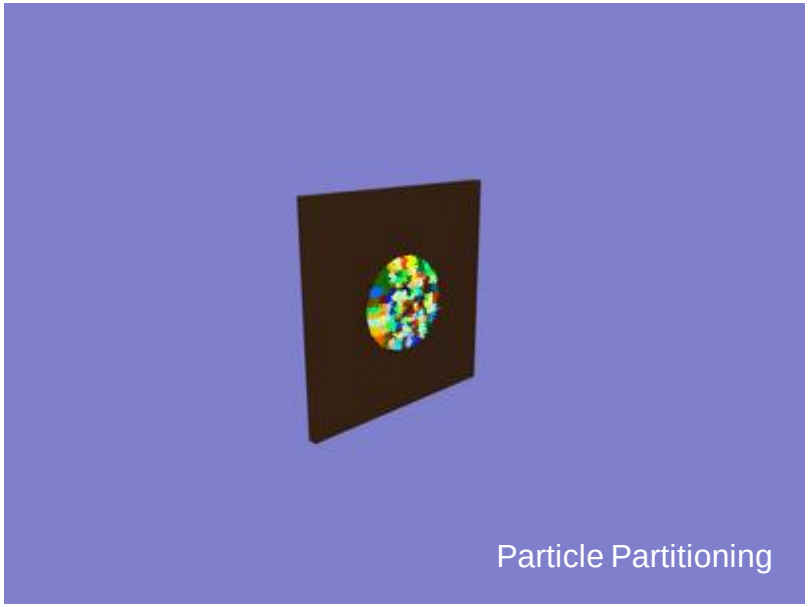
```
FiniteElement: {
  Order: 0
  Curved Surfaces: on
}

PRegion: {
  Type: PICCausality
  Order: 1
}

PRegion: {
  Type: PICDomain
  Order: 2
}
```

LCLS RF gun: Causal moving window reduces computational resource requirements *by orders of magnitude*

Ready for Supercomputers at NERSC

- Fields partitioned with graph-based methods (ParMETIS)
- Particles partitioned geometrically (Zoltan RCB 3D, SciDAC collaboration)
- Collective MPI on sub-communicators in disjoint regions, with optimized ordering to allow higher concurrency of communication





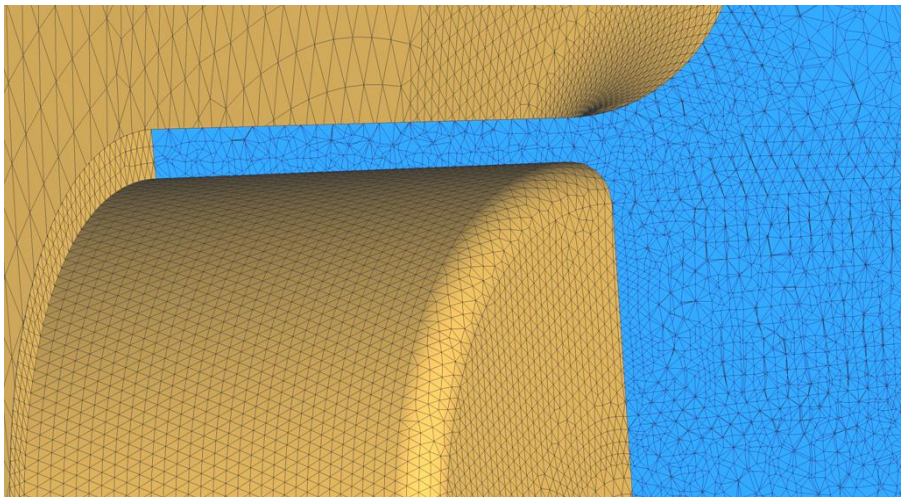
Example: LCLS RF gun, colors indicate distribution to different CPUs

Pic3P was tested on 24k CPUs: 750M DOFs, 5B particles

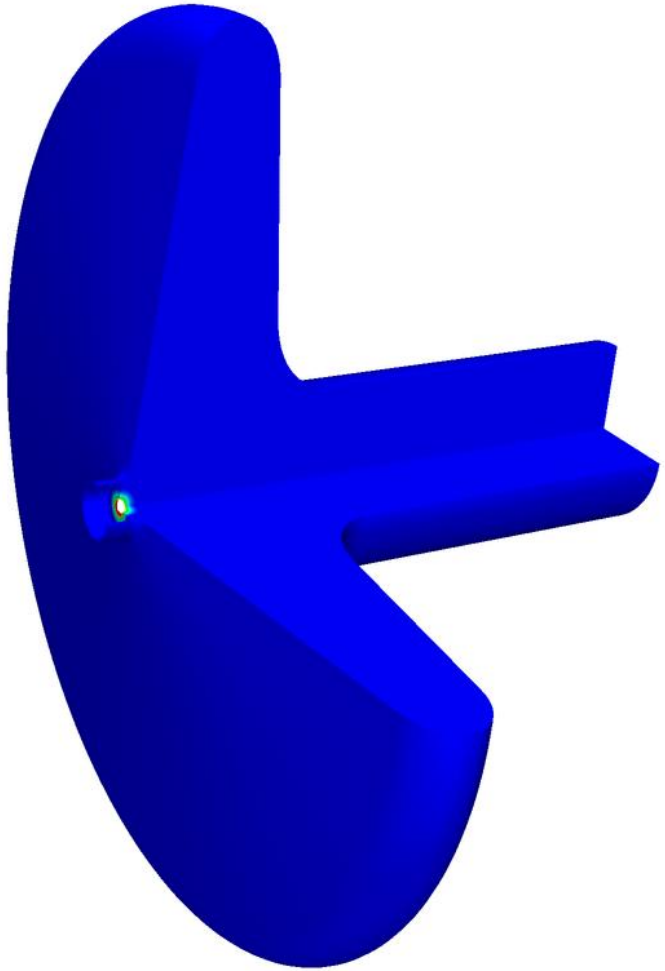
Larger problem: BNL Polarized SRF Gun

BNL Polarized SRF Gun (J. Kewisch)

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

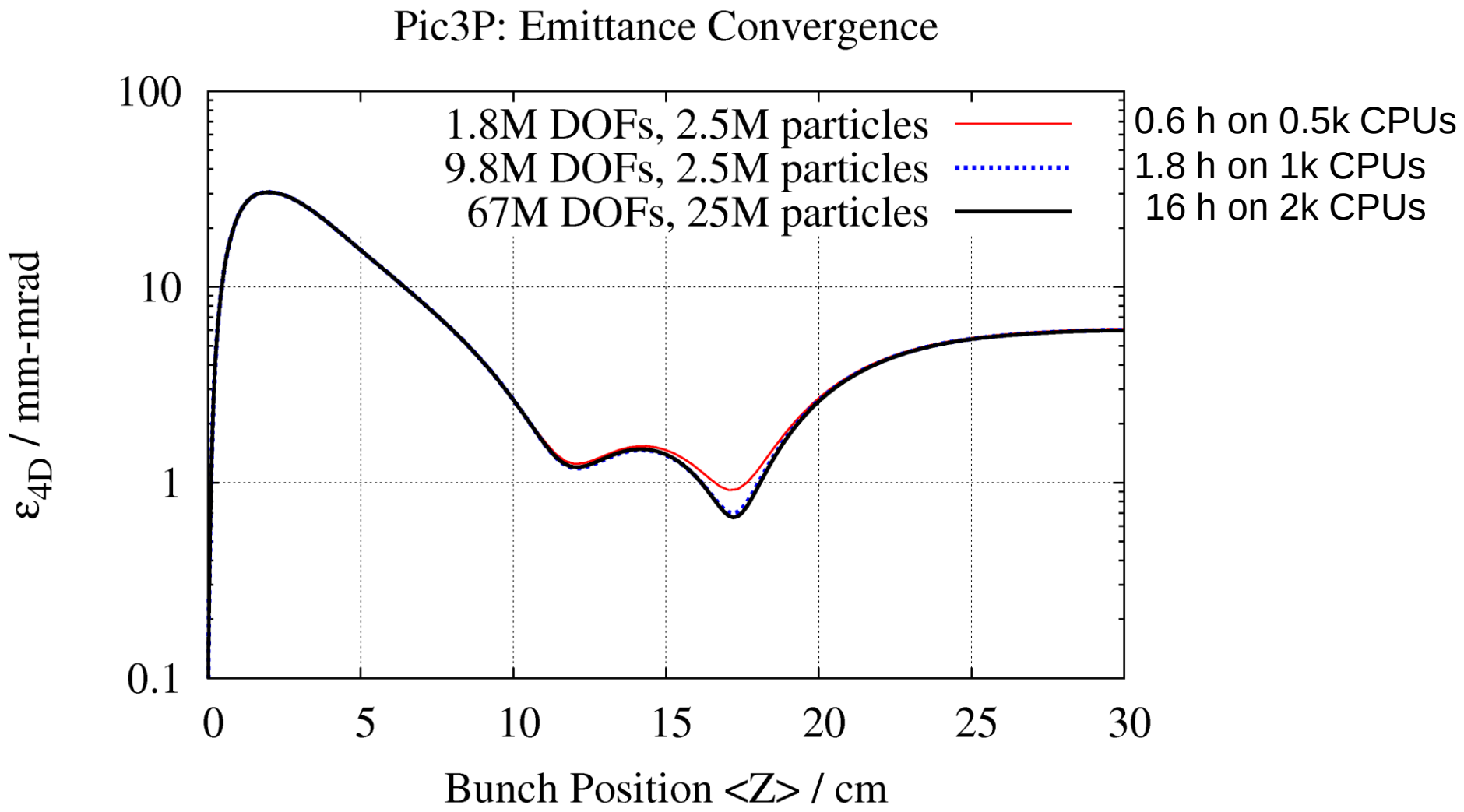


Cut-view of unstructured mesh near cathode



Self-fields during bunch transit

BNL SRF Gun Emittance Convergence



Pic3P - Summary

- **Pic3P** was designed for accurate self-consistent simulations of beam-cavity interactions in space-charge dominated regimes
- **Pic3P** has been thoroughly validated
- Many features are still under development, so

please contact Arno Candel

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if you are interested in using Pic3P.