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
  Higher-order (p=1…6) Whitney basis functions:
  \[
  \mathbf{E}(\mathbf{x}, t) = \sum_i e_i(t) \cdot \mathbf{N}_i(\mathbf{x})
  \]
  ![LCLS RF Gun](image)

- **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

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

RMS Bunch Radius vs Z

\( \sigma_r / \text{mm} \)

\( r=1 \text{ mm} \)
10 ps
\( \text{no solenoid} \)

MAFIA
Pic2P
PARMELA

1.5 nC
1 nC
0.5 nC
10^{-6} \text{ nC}

Z / cm
Normalized Transverse RMS Emittance vs Z

$r=1$ mm
10 ps
no solenoid

PARMELA: No retardation

MAFIA
Pic2P
PARMELA

Z / cm

$\varepsilon_x$ / mm-mrad

1.5 nC
1 nC
0.5 nC
$10^{-6}$ nC
LCLS RF Gun Phasespace (1.5 nC)
Pic2P - Performance

Normalized Transverse RMS Emittance vs Z

Parallel Speedup

Pic2P 100k DOFs, 10 minutes!

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

RF gun + drift with focusing solenoid  
Z=60 cm

only scattered fields shown
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)