Large Scale Finite-Element Electromagnetic Simulations for Projects across DOE Accelerator Complex

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ComPASS All-Hands Meeting
UCLA, December 2-3, 2008

Work supported by DOE ASCR, BES & HEP Divisions under contract DE-AC02-76SF00515
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Massively Parallel Computing in Electromagnetics

- Develop **Parallel** codes in *Electromagnetics*
- Perform research in *Computational Science* by collaborating with **SciDAC** Centers for Enabling Technologies & Institutes
- Focus on **Large-scale simulations** using computers at **NERSC** and **NCCS** (with 1 INCITE and 3 allocation awards)

> solve the most challenging problems in *accelerator design, optimization and analysis* via **High Performance Computing** for the **DOE-SC complex** working on

**HEP** - High Gradient, Laser Acceleration, Muon Collider, ILC, Project X, LARP
**NP** - CEBAF12 GeV Upgrade  
**BES** – LCLS
Higher-order Finite-Element Method

- Tetrahedral conformal mesh with quadratic surface
- Higher-order Finite Elements ($p = 1-6$)
- Parallel processing (large memory & speedup)

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

LL end cell with input coupler only

Error ~ 20 kHz (1.3 GHz)

67000 quad elements (<1 min on 16 CPU, 6 GB)
Parallel Electromagnetics Codes

Suite of scalable Finite-Element Electromagnetics codes to model Large, Complex structures with high accuracy:

**Frequency Domain:** Omega3P – eigensolver (mode damping, non-linear)
  S3P – S-parameter

**Time Domain:** T3P – transients & wakefields
  Pic3P – self-consistent particle-in-cell (PIC)

**Particle Tracking:** Track3P – dark current and multipacting
  Gun3P – space-charge beam optics

**Multi-Physics:** TEM3P – EM-thermal-mechanical

**Visualization:** V3D – meshes, fields and particles

Developed under Grand Challenge and SciDAC1 (2001-2006) in black;
Under development for ComPASS (2007-2011) in red
Development of **Omega3P**

**Goal:** High Fidelity simulation -> CAD drawing -> hardware fabrication  
- from single 2D cavity to a cryomodule of eight 3D ILC cavities  
An increase of $10^5$ in problem size with $10^{-5}$ accuracy over a decade
Activities for Code Development

- **Omega3P**
  - Implement domain specific scalable solvers
  - Develop shape optimization algorithms

- **T3P**
  - Implement Napolı wakefield integration method
  - Improve moving h/p adaptive refined moving window for beam excitation

- **Track3P**
  - Develop surface physics models and parallel particle tracking algorithms for dark current simulation

- **TEM3P**
  - Develop new capabilities for thermal and mechanical solvers for realistic design and analysis of accelerator cavities

- **Pic3P**
  - Implement realistic 3D emission models and moving window for rf gun simulation
**Pic2P** - Finite Element 2D EM PIC Code

LCLS RF Gun has been designed to be cylindrically symmetric in beam region 2.856 GHz, 120 MV/m, \( \pi \)-mode

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- **Cylindrical Bunch (2D)**
  - \( r = 1 \) mm
  - \( Q = 1 \) nC
  - no solenoid

**Pic2P** – Parallel Finite Element 2D EM PIC Code from 1\textsuperscript{st} principles, accurately includes effects of space charge, retardation, and wakefields
PIC Codes at Space Charge Limit

- **MAFIA** and **Pic2P** results agree
- **PARMELA** results* differ at higher space-charge regime

* courtesy Cecile Limborg
Evolution of electron bunch and scattered self-fields

Evolution of transverse phase space, starting from SLAC measured data

Pic3P - LCLS RF Gun Emittance

3D emittance calculations with Pic3P include space-charge, wakefields and retardation effects from first principles. Parallel processing and conformal higher-order finite elements allow unprecedented modeling accuracy.

In collaboration with LCLS
Advancing Multi-physics Simulation Tool

CAD model

TEM3P for design and optimization

Electromagnetics

LCLS
RF Gun

Thermal

Mechanical

Engineering prototype

In collaboration with LCLS
Tem3P – Cooling of CEBAF HOM waveguide

Cold-warm transition for Nb waveguide extension at HOM coupler

- **Simulation goal**
  - Determine design to satisfy cooling requirements including RF and thermal effects

- **Tem3P code development**
  - Implement thermal shell elements for thin layers
  - Develop nonlinear solver for temperature-dependent material properties
  - Implement boundary condition for He convection cooling

In collaboration with TJNAF
Activities for Accelerator Simulation

**High Energy Physics**

- **ILC/Project X** – Wakefield and HOM effects in cryomodule with cavity imperfection; low-emittance rf gun
- **LHC/LARP** – Design and optimization of crab cavity; Wakefield effects in collimator
- **High-Gradient R&D** – Optimization of choke cavities for HOM damping; CLIC PETS and HDX accelerator structure
- **Muon Collider** – Multipacting & dark current studies for muon cooling cavity
- **Laser Acceleration** – Coupler design for optical fiber

**Nuclear Physics**

- **CEBAF 12-GeV Upgrade** – EM, thermal and mechanical analysis of SRF cavity coupler

**Basic Energy Sciences**

- **LCLS RF Gun** – 3D self-consistent PIC simulation
Physics Goal: Calculate wakefield effects in the 3-cryomodule RF unit (26 cavities) with realistic 3D dimensions and misalignments.

The LARGEST problem for time-domain analysis:
- 80 million-element mesh, ~500 million DOFs, 4096 CPUs (Jaguar), 4 seconds per time-step.

For frequency domain:
- 3 million-element mesh, ~20 million DOFs, 1024 CPUs (Seaborg), 300 GB memory, 1 hour per mode.
**T3P** - 1\textsuperscript{st} ever Beam Transit in Cryomodule

ILC cryomodule of 8 superconducting RF cavities

Expanded views of input and HOM couplers

Fields in beam frame moving at speed of light
Trapped Modes in ILC Cryomodule

- **Trapped modes in 3rd dipole band**
  - Modes above cutoff frequency are coupled throughout 8 cavities
  - Modes are generally x/y-tilted & twisted due to 3D end-group geometry
  - Both tilted and twisted modes cause *x-y coupling in the beam*

- **Trapped mode in beampipe between 2 cavities**
  - TM-like mode at 2.948 GHz, higher than 2.943 GHz TM cutoff
  - R/Q = 0.392 Ω, Q = 6320
  - Mode power = 0.5 mW (averaged)
  - *(not a concern for heating in this case)*
Supporting the LHC

**LHC Collimator (Upgrade)**
Impedance and beam heating effects are important for the design.
(Omega3P and T3P)

**LHC Crab Cavity (Upgrade)**
The crab cavities rotate the beams at the IP to produce head-on collisions, improving luminosity. Design for strong damping of SOM/LOM/HOM is needed.
(Omega3P)

Baseline Design of crab cavity for LHC upgrade
Advancing High Gradient R&D

HOM damping & Multipacting studies are needed for High Gradient Structures

CLIC – Hybrid Damped Structure (HDX)

CLIC - Power Extraction & Transfer Structure (PETS)

Slotted-Disk Structure

Choke-Mode Structure

In collaboration with CERN
**Track3P - Multipacting in SRF Cavities**

**ILC Linac TTF-III cavity coupler**
- Simulated MP bands in coaxial waveguide agreed with measurements

**SNS SRF cavity HOM coupler**
- RF heating observed at HOM coupler
- 3D simulations showed MP barriers close to measurements
Advancing Muon Cooling Cavity Design

Particle tracking to study multipacting or dark current damage

2 types of resonant trajectories:

• Between upper and lower irises
• Between upper and lower cavity walls

Slight MP activities observed above 6 MV/m

2 types of resonant trajectories:

• One-point impacts at upper wall
• Two-point impacts at beampipe

MP activities observed above 1.6 MV/m

w/ 2T transverse B field

w/ 2T B field at 10 degree

SEY > 1 for copper

Impact energy of resonant particles vs. field level

In collaboration with BNL and LBNL
Advancing Laser Acceleration

Develop a conceptual design for power coupling into optical fiber

**Model of a fiber slab**

**Defect Mode**

*Omega3P* used to determine defect mode properties

**Coupler**

*S3P* used to determine coupling of power to defect mode
Tests show 3 abnormally high Q modes in #5 of the high-gradient cavities.

Beam-breakup (BBU) threshold current is significantly below design value.

Issues could not be resolved experimentally.

SLAC scientists have made great progress in finding a solution by treating it as an inverse problem.

CEBAF BBU - Solving the Inverse Problem

**CEBAF 12-GeV upgrade** –

- Beam breakup (BBU) observed at beam currents well below design threshold.
- Used measured RF parameters such as $f$, $Q_{\text{ext}}$, and field profile as inputs

- **Solutions to the inverse problem** identified the main cause of the BBU instability: **Cavity is 8 mm shorter** – predicted and confirmed later from measurements

- The fields of the **3 abnormally high Q modes** are shifted away from the coupler

- Showed that experimental diagnosis, advanced computing and applied math worked together to solve a real world problem as intended by SciDAC

In collaboration with TJNAF
SLAC FEM EM simulation tools have had significant impacts on a broad range of DOE accelerator projects in HEP, NP and BES

Parallel EM codes have been tackling the most computationally challenging problems in accelerator design, optimization and analysis

R&D in computational science via SciDAC (and the coming Exascale) is vital to the success of accelerators

Large payback from collaboration of accelerator modeling and computational science such as JLab BBU analysis

See following talk on AM/CS efforts on supporting FEM EM