### Advances in Parallel Electromagnetic Codes for Accelerator Science and Development

### Kwok Ko Speaker: Arno Candel

Advanced Computations Group SLAC Sept. 17, 2010

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## Advanced Computations at SLAC & Collaborations

### SLAC Team

#### **Accelerator Physicists:**

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#### **Computational Scientists:**

Lixin Ge, Rich Lee, Vineet Rawat, Greg Schussman

### **Accelerator Collaborators**

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### **Computational Science Collaborators**

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# 3D Electromagnetic Codes for Accelerators

- MAFIA (CST) FD, http://www.cst.com
- Microwave studio (CST) FD, http://www.cst.com
- HFSS (Ansoft) FEM, http://www.ansoft.com
- ANSYS (Ansys, Inc.) FEM, http://www.ansys.com
- GdfidL FDTD, parallel, http://www.gdfidl.de

ACE3P (SLAC) - FEM, massively parallel (>10k CPUs)
 https://slacportal.slac.stanford.edu/sites/ard\_public/bpd/acd/Pages/Default.aspx





# Motivation to Design the ILC Cavity

### International Linear Collider Cavity



### Modeling challenges include:

- **Complexity** <u>HOM coupler</u> (fine features) versus cavity
  - **Problem size** <u>multi-cavity</u> structure (e.g. cryomodule)
- 0
- Speed
- Accuracy <u>10s of kHz mode separation out of GHz</u>
  - <u>Fast</u> turn around time to impact design





## Parallel EM Code Development at SLAC

**DOE's High Performance Computing Initiatives and SLAC support** 

- 1998–2001 HPC Accelerator Grand Challenge
- 2001-07 Scientific Discovery through Advanced Computation (SciDAC-1) -Accelerator Science and Technology (AST)
- 2007-12 Scientific Discovery through Advanced Computation (SciDAC-2) -Community Petascale Project for Accelerator Science and Simulation (ComPASS)

### PhD Research:

**1998** - Xiaowei Zhan, <u>Parallel electromagnetic field solvers using finite element methods with</u> <u>adaptive refinement and their application to wakefield computation of axisymmetric</u> <u>accelerator structure</u>, Stanford University.

**2003** - Yong Sun, <u>The filter algorithm for solving large-scale eigenproblems from accelerator</u> <u>simulations</u>, Stanford University.

**2009** - Sheng Chen, <u>Adaptive error estimators for electromagnetic field solvers</u>, Stanford University.





# Parallel Higher-order Finite-Element Method

### **Strength of Approach – Accuracy and Scalability**

- Conformal (tetrahedral) mesh with quadratic surface
- Higher-order elements (p = 1-6)
- Parallel processing (memory & speedup)







# Accelerator Modeling with EM Code Suite ACE3P

**Meshing** - **CUBIT** for building CAD models and generating finite-element meshes. <u>http://cubit.sandia.gov</u>.

### **Modeling and Simulation** – SLAC's suite of <u>conformal, higher-order, C++/MPI</u> <u>based parallel finite-element electromagnetic codes</u>

https://slacportal.slac.stanford.edu/sites/ard\_public/bpd/acd/Pages/Default.aspx

ACE3P ( <u>A</u> dvanced <u>C</u> omputational <u>E</u> lectromagnetics <u>3P</u> )					
Frequency Domain:	Omega3P – Eigensolver (damping)				
	S3P	– S-Parameter			
<u>Time Domain</u> :	T3P	<ul> <li>Wakefields and Transients</li> </ul>			
Particle Tracking:	Track3P	<ul> <li>Multipacting and Dark Current</li> </ul>			
EM Particle-in-cell:	Pic3P	<ul> <li>RF gun (self-consistent)</li> </ul>			

**Postprocessing** - **ParaView** to visualize unstructured meshes & particle/field data. <u>http://www.paraview.org/</u>.

Goal is the Virtual Prototyping of accelerator structures





## **ACE3P** Capabilities

### • Omega3P can be used to

- optimize <u>RF parameters</u>
- reduce peak surface fields,
- calculate HOM damping,
- find trapped modes & their heating effects,
- design dielectric & ferrite dampers, and others
- **S3P** calculates the transmission (S parameters) in open structures
- **T3P** uses a driving bunch to
  - evaluate the broadband impedance, trapped modes and signal sensitivity,
  - compute the wakefields of short bunches with a moving window,
  - simulate the beam transit in large 3D complex structures
- Track3P studies multipacting in cavities & couplers by identifying MP barriers, MP sites and the type of MP trajectories.
- **Pic3P** calculates the beam emittance in RF gun designs.





# Benchmarks of ACE3P with Measurements







### Omega3P - NLC Cell Design

### Code validated in 3D NLC Cell design in 2001

- Omega3P was used to determine the accelerator dimensions for the JLC/NLC X-Band structures with accuracy orders of magnitude better than machining tolerance,
- The structure cells were high precision machined,
- Microwave QC verified cavity frequency accuracy to 0.01% relative error (1MHz out of 11 GHz) as required for beam stability.







### Omega3P - LCLS RF Gun Cavity

### Provided dimensions for LCLS RF gun cavity to meet design requirements:

- Reduce pulse heating by rounding of the z-coupling iris
- Minimize dipole and quadrupole fields via a racetrack dual-feed coupler design

### Code validated by Measurement

RF parameter	Design	Measured	
fπ (GHz)	2.855987	2.855999	
Qo	13960	14062	
β	2.1	2.03	
Mode Sep. ∆f (MHz)	15	15.17	
Field balance	1	1	







### **S3P** - S-Parameters for LCLS Injector Components

### LCLS injector accelerator structure dual-feed coupler components



LCLS RF Gun Dual-window assembly









# Track3P - Ichiro Cavity Multipacting

### ICHIRIO cavity experienced

- Low achievable field gradient
- Long RF processing time



- > Hard barrier at <u>29.4 MV/m</u> field gradient with MP in the beampipe step
- First predicted by Track3P simulation

ICHIRO #0	Track3P MP simulation		
X-ray Barriers (MV/m)	Gradient (MV/m)	Impact Energy (eV)	
11-29.3 12-18	12	300-400 (6 <sup>th</sup> order)	
13, 14, 14-18, 13-27	14	200-500 (5 <sup>th</sup> order)	
(17, 18)	17	300-500 (3 <sup>rd</sup> order)	
20.8	21.2	300-900 (3 <sup>rd</sup> order)	
28.7, 29.0, 29.3, <mark>29.4</mark>	29.4	600-1000 (3 <sup>rd</sup> order)	

MP Trajectory @ 29.4 MV/m







Large-scale Accelerator Simulation requires Computational Science and High Performance Computing







## Computational Science R&D under SciDAC



#### Mesh correction



#### Adaptive mesh refinement





#### 400 350 300 250





Number of processors



# HPC Resources for Accelerator Modeling

DOE Computing Resources @ LBNL and ORNL to meet SciDAC, Accelerator projects as well as the CW10 user community needs:

#### **Computers** -

NERSC at LBNL - Franklin Cray XT4, 38642 compute cores, 77 TBytes memory, 355 Tflops

NCCS at ORNL - Jaguar Cray XT5, 224,256 compute cores, 300 TBytes memory, 2331 TFlops 600 TBytes disk space



### Allocations -

- NERSC Advanced Modeling for Particle Accelerators 1M CPU hours, renewable
   SciDAC ComPASS Project 1.6M CPU hours, renewable (shared)
   Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators - 300K CPU hours, renewable (shared) each year
- NCCS Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling - **12M CPU hours** in FY10



ACE3P's advances focus on solving challenging problems in Accelerator Science and Development







# **Omega3P** - Towards System Scale Modeling





SciDAC

# T3P - Beam Transit in ILC Cryomodule





Visualization by Greg Schussman



# T3P - Short Bunch Wakefields in ERL



### T3P - Short Bunch Wakefields in ERL





Visualization by Greg Schussman



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### T3P - CLIC Two-Beam Accelerator



## T3P - CLIC PETS Bunch Transit

### <u>Dissipation of transverse wakefields in</u> <u>dielectric loads: eps=13, tan(d)=0.2</u>



Impedance  $Re(Z_T)$  [Ohm/mm/structure]

Transverse Wake [V/pC/mm/structure]

### T3P - CLIC TDA24 Bunch Transit



## T3P - RF Power Transfer in Coupled Structure







# Track3P - Multipacting in SNS Cavity/HOM Coupler



### SNS Cavity

Both Experiment and Simulation show same MP band:
 11 MV/m ~ 15MV/m

### **SNS Coupler**

- SNS SCRF cavity experienced rf heating at HOM coupler
- 3D simulations showed MP barriers close to measurements















# Track3P - Multipacting in SNS Cavity/HOM Coupler



Visualization by Greg Schussman







## Pic3P - LCLS RF Gun



Temporal evolution of electron bunch and scattered self-fields Racetrack cavity design: Almost 2D drive mode. Cylindrical bunch allows benchmarking of 3D code Pic3P against 2D codes Pic2P and MAFIA

Pic3P LCLS RF Gun Emittance Convergence



Unprecedented Accuracy due to <u>Higher-Order</u> Particle-Field Coupling and <u>Conformal</u> Boundaries





### Pic3P - SLAC/LLNL X-Band Gun

#### **3D Emittance Calculations for Bunch with Offset**

- f=11.424 GHz, 200 MV/m peak Ez on cathode
- Solenoid Bz\_max = 0.5658 T at Z=6.3 cm
- Beer can (r=0.5 mm, 2 ps flat top, 0.4 ps rise time), 250 pC
- Bunch injected 30 degrees after zero-crossing





### 4D Emittance vs <Z>





<u>Solving the CEBAF BBU</u> - Joint Efforts from Accelerator Physics + Experiment + Computational Science + Computing







# **CEBAF BBU - Solving the Inverse Problem**

#### High Q modes Deformed 1.E+09 ideal 1.E+08 cav5-meas 1.E+07 1.E+06 X Ø 1.E+05 Ideal CEBAF 12-GeV upgrade – 1.E+04 Deformed 1.E+03 Beam breakup (BBU) observed at beam currents 1.E+02 well below design threshold 2180 2030 2080 2130

- Used measured RF parameters such as f, Q<sub>ext</sub>, 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

### Omega3P

F (MHz)





In collaboration with TJNAF – R. Rimmer, H. Wang



# Optimizing the Choke Mode Cavity Performance

The procedure based on nonlinear iterations with Newton type algorithms that solves the Jlab **inverse problem** can be used to **optimize** the performance of the choke mode cavity in reducing the wakefield effects of higher-order dipole modes





# ACE3P User Community - CW10 Code Workshop

SLAC NATIONAL ACCELERATOR LABORATORY

#### CW10 @ SLAC

#### CW10 ACCELERATOR CODE WORKSHOP

#### Home SLAC ACCESS Agenda All visitors must have a valid photo ID to enter the Laboratory. The SLAC Attendees Main Gate is open 24 hours a day, 7 Software days a week. Workshop Materials MAPS AND DIRECTIONS SLAC Computer Accounts CLIC PETS Structure » More Information Accelerator Code Workshop (CW10) at SLAC for the SLAC GUEST HOUSE ACE3P (Advanced Computational Electromagnetics 3P) Code Suite organized by the Advanced Computations Group (ACG) » More Information September 20-22, 2010 Date — Time — See agenda Place — SLAC National Accelerator Laboratory Menlo Park, California Contact — ACD-CW10@slac.stanford.edu 650-926-2864 650-926-4603 (FAX)

SLAC National Accelerator Laboratory, Menlo Park, CA Operated by Stanford University for the U.S. Dept. of Energy

#### (http://www-conf.slac.stanford.edu/CW10/default.asp)





# CW10 Attendees & Agenda

#### CW10 @ SLAC

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CW10 ACCELERATOR CO	DE WORKSHOP	SLAC NATIONAL AC	AC NATIONAL ACCELERATOR LABORATORY		
Home	A 44 3				
lgenda	Attendees				
Attendees	Institution	Name	Email		
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#### CW10 @ SLAC

Home

Agend

Attend

Softw

Works

SLAC

NERS

ACCELERATOR CODE WORKSHOP		SLAC NATIONAL ACCELERATOR LABORATORY					
a		Agenda					
ees		All sessions are 1 hr 45 min					
are							
hop Materials		9/22 Monday	9/23 Tuesday	9/24 Wednesday			
Computer Accounts				Parallel Sessions			
C Computer Accounts	8 30-10 15	Intro/CUBIT	Track3P	Pic3P			
e computer Accounts	0.00 10.10	Introveobili	TRONO	Applications			
	10.15-10.30	break	break	break			
	10 20 12 15	ACE2D/Dara\/iow	P/ParaView Track3P	TEM3P			
	10.50-12.15	ACCOPTENT		Applications			
	12.15-1.30	lunch	lunch	CW10 Ends			
	1.30-3.15	Omega3P/S3P	ТЗР				
	3.15-3.30	break	break				
	3.30-5.15	Omega3p/S3P	ТЗР				

#### SLACS SLAC National Accelerator Laboratory, Menlo Park, CA Operated by Stanford University for the U.S. Dept. of Energy





- Parallel finite-element (FE) electromagnetics (EM) method demonstrates its strengths in high-fidelity, high-accuracy modeling for accelerator design, optimization and analysis.
- ACE3P code suite, developed under DOE SciDAC and SLAC support, has been benchmarked and used in a wide range of applications in Accelerator Science and Development.
- Advanced capabilities in ACE3P's modules Omega3P, S3P, T3P, Track3P, and Pic3P have enabled challenging problems to be solved that benefit accelerators worldwide.
- Computational science and high performance computing are essential to tackling real world problems through simulation.
- The ACE3P User Community is formed to share this resource and experience and we welcome the opportunity to collaborate on projects of common interest.



