Application Specific Computing

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SciDAC Accelerator Simulation Project

SLAC leads the Electromagnetic Systems Simulation (ESS) component that

- Concentrates on developing parallel tools based on unstructured grids for the design, analysis, and optimization of complex electromagnetic components and systems in accelerators.

- Applies these tools to improve existing facilities (PEP-II IR heating, Tevatron lifetime), to design future accelerators (NLC structure), and to advance accelerator science (Dark current).

- Collaborates with SAPP/ISIC partners to target challenging electromagnetic problems that require Large-scale simulations, e.g. modeling small beams in long structures of complex geometry with high accuracy.
ACD Overview - SciDAC

Accelerator Modeling & Simulation
- NLC
- PEP-II
- LCLS
- Klystron
- FNAL
- ANL...

Parallel Code Development
- Accel. Mod.
- Comp. Math.
- Comp. Tech.

- LBNL
- Stanford
- SNL
- UC Davis
- LLNL
- RPI

SBIR (STAR, Inc.) / USPAS / Grad & Undergrad Research
# Contributors/Collaborators

(SciDAC - HENP/OASCR)

<table>
<thead>
<tr>
<th>Accelerator Modeling</th>
<th>Computational Mathematics</th>
<th>Computing Technologies</th>
</tr>
</thead>
<tbody>
<tr>
<td>V. Ivanov, A. Kabel, K. Ko, Z. Li, C. Ng, L. Stingelin (PSI)</td>
<td>Y. Liu, I. Malik, W. Mi, J. Scoville, K. Shah, Y. Sun (Stanford)</td>
<td>N. Folwell, A. Guetz, L. Ge, R. Lee, M. Wolf, G. Schussman (UCD), M. Weiner (Harvey Mudd)</td>
</tr>
</tbody>
</table>

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**SAPP- Stanford, LBNL, UCD; ISICs – TSTT, TOPS**

**LBNL**
- E. Ng, P. Husbands, X. Li, A. Pinar

**UCD**
- K. Ma, G. Schussman

**LLNL**
- D. Brown, K. Chand, B. Henshaw, D. White

**Stanford**
- G. Golub, O. Livne

**SNL**
- P. Knupp, T. Tautges, L. Freitag, K. Devine

**RPI**
- M. Shephard, Y. Luo
Parallel EM Simulation – CS/AM Issues

CAD Model → Meshing → Partitioning → Solvers

Parallel Performance

Refinement → Visualization → Verification

<table>
<thead>
<tr>
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<th>Numerical (MHz)</th>
<th>Meas. (MHz)</th>
<th>Diff. (MHz)</th>
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</table>
Code Development - Omega3P, Tau3P, Tfe3P

**Omega3P** (Parallel finite element eigensolver) –
(1) Improvements to ISIL solver for tackling tightly clustered eigenvalues that include Block algorithm, Deflation techniques, and Thick restart,
(2) AV formulation to accelerate convergence,
(3) ESIL solver (LBNL) as alternative and for verification.

(1) Periodic B.C.,
(2) More efficient filtering schemes,
(3) Complex eigensolver to treat lossy cavities.

**Tau3P** (Parallel time domain solver on modified Yee grid) –
(1) Wakefield version ported to NERSC’s IBM SP2,
(2) Restart capability to enable long wakefield runs,
(3) Lossy dielectrics

**Tfe3P** (New parallel finite element time domain solver) –
(1) Development of efficient linear solvers,
(2) Higher order elements and basis functions.
**Code Development - S3P, Track3P**

**S3P** (New parallel finite element scattering matrix solver) –

1. Benchmarked against known solutions,
2. Implementations on NERSC’s IBM SP2.

1. Higher order elements for improved accuracy,
2. AWE technique to enable quick frequency sweep,
3. Extension to include lossy material

**Track3P** (Particle tracking module) using E & B fields from

**Omega3P** (for standing wave cavities),
**S3P** (for open cavities), or
**Tau3P** (for traveling wave structures)

\[
\frac{d\vec{p}}{dt} = e(\vec{E} + \frac{1}{c}[\vec{v} \times \vec{B}]), \quad \vec{p} = m\gamma\vec{v}, \quad \gamma = \frac{1}{\sqrt{1 - v^2 / c^2}}
\]

**Surface physics** - injection, thermal emission, field emission & secondaries.

Parallelization, Ionization, Collisions…..
Surface Physics - Track3P

**Particle Injection**

\[ I(t) = \frac{I_{\text{max}}}{1 + \left( \frac{v_0}{a} \left( \frac{t - \phi_0}{\omega} - iD_t \right) \right)^2} \]

**Thermal Emission (Child – Langmuir)**

\[ J(r,t) = \frac{4}{9} \varepsilon_0 \sqrt{\frac{2QE^2}{Md}} \]

**Field Emission (Fowler - Nordheim)**

\[ J(r,t) = 1.54 \times 10^8 \left( \frac{-6 + 4.52}{\sqrt{\phi'}} \right) \left( \frac{\beta E}{\phi} \right)^2 e^{\left( \frac{-6.53 \times 10^9 \phi^{1.5}}{\beta E} \right)} \]

**Secondary Emission**

\[ \sigma = \frac{I_{\text{secondary}}}{I_{\text{primary}}} = \delta + \eta + r; \]
\[ \delta - \text{true secondary emission (0-50 eV).} \quad \varepsilon_m \sim 2-4.5 \text{ eV}; \]
\[ \Delta \varepsilon \sim 12-15 \text{ eV}; \]
\[ \eta - \text{non elastic reflection (50 eV-} \varepsilon_{\text{pri}}) \]
\[ r - \text{elastic reflection;} \quad r = 0.05-0.5 \text{ for metals.} \]
Benchmarking 3D trajectories against results from 2D model

G = 50 MV/m

G = 100 MV/m

Particle Tracking – Track3P
Weak/Strong Beam-beam - PlibB

- Directly computes lifetimes in hadron machines, not dynamic apertures
- Does $10^{12}$ beam-beam interactions for typical Tevatron calculation (NERSC)
- Tracking and beam-beam kick engines designed for speed and fed by code generated data based on machine description
- Calculates lifetimes up to 10h for Tevatron with all 72 parasitic crossings
Code Development - PlibB

- Expanded to cover more physics:
  - Full 6-D coupling (linear case)
  - Chromaticity
  - Fast truncated power series tracking engine
  - Noise
- Accelerated BB-Engine
- Collaborated with FNAL to obtain DA map
- Running convergence studies for DA map

Future Plans:
- Integrate w/ existing parallel strong/strong beam-beam-code PaBB
  - To simulate the Tevatron collision case
  - To simulate PEP-II w/inclusion of IP and parasitic crossings
- Combine PaBB with parallel PIC/Tracking modules
  - To simulate ECI and beam-beam effects in PEP-II and future accelerators
Collaborating with FNAL on machine parameters (T. Sen, B. Erdalyi, M. Xiao)

Currently running parameter scan studies for lifetime at Injection Stage (150GeV)

Lifetime estimates track 400,000 particles for 100,000 turns on 256 processors on NERSC’s IBM SP2

Working with FNAL on tool suite to automatically create DA/MAD mappings
H60VG3 (55 cells including power couplers) is being considered as a baseline structure design for the NLC for which detuning and damping are planned to suppress dipole wakefields. Entire structure simulation has begun to calculate long-range wakefields in the detuned structure to be followed by modeling of the final damped, detuned design.
Eigenmodes in H60VG3 – Omega3P

Omega3P is used to find eigenmodes needed for calculating wakefields by mode summation – 1\textsuperscript{st} Dipole Band

Dipole Modes in Structure

Impedance Spectrum

Impedance of the 1\textsuperscript{st} dipole band

Gaussian Detuning

Coupler Loading

Frequency (GHz)
Coupler Loading on Dipole Mode – S3P

Q = 81.4

\( f_0 = 15.717 \text{ GHz} \)

Transmission

Reflection

Transmission

Reflection
Beam Excitation of H60VG3 – Tau3P

**Tau3P** is used to excite wakefields directly by a transit beam and calculate the impedance spectrum covering all bands.

**Beam Transit through Structure**

**1st Band Impedance Spectrum**

Eigenmode Frequencies from Omega3P
Dipole Wakefield in H60VG3

**Omega3P** – Sum of Modes from 1st Band

**Tau3P** – Direct Simulation

![Wakefield Graph](image)

**Wakefield**

- Y-axis: 1e+17 to 1e+12
- X-axis: 0 to 35 (Length in m)

![Transverse Wakefield Graph](image)

- Y-axis: 10^8 to 10^1 (Amplitude)
Trapped Modes in PEP-II IR – Tau3P

Find localized modes in IR complex for beam heating analysis by direct excitation (Tau3P) for comparison with eigenmodes found by Omega3P
Extension to Full IR model (crotch-to-crotch) will confirm Omega3P mode analysis and enable calculations for operation at higher currents.

Trapped mode from Omega3P
30-cell Structure – Tau3P

(J. Wang – ARDA)

- NLC X-band structure showing damage after high power test
- Realistic simulation needed to understand underlying processes

Distributed model on a mesh of half million hexahedral elements for Tau3P simulation of field evolution
Transient Effect - Tau 3P

Power Spectrum

Displacement Diagram

Electric field vs time

Rise time = 10 ns

Disk 1

Disk 15

Disk 29

Rise time = 10 ns
Peak Fields – Tau3P

- When and where Peak Fields occur during the pulse?
- Transient fields up to 20% higher than steady-state value due to dispersive effects

Drive pulse

Electric field vs time

Rise time = 10, 15, 20 ns

Steady-state Surface Electric field amplitude
Modeling High Power Test – Track3P

(C. Adolphson – NLC)

- High power test on a 90 degree square bend provides measured data for benchmarking the secondary emission model in Track3P on a simple geometry

**Using Fields from Tau3P**

Square Bend Used at NLCTA to Transport SLED II Output Power to Structures

- Electric Field
- Magnetic Field
Benchmark Surface Physics – Track3P

X-Ray Energy Spectrum – Good agreement between Track3P and Measurement and simulation indicates high energy X-Ray is due to elastic scattered secondary electrons.
Cyclotron COMET - Omega3P

First ever detailed analysis of an entire cyclotron structure
- L. Stingelin, PSI

„Dee“: RF electrode
„Liner“: outer shell of RF cavity

Magnetic Field

Electric field in acceleration gap

Proton trajectories

Fig. 1. The cyclotron COMET
Effort towards end-to-end modeling of the RFQ has started
CS/AM Collaborations - SAPP, ISICs

- **CAD Model/Mesh Generation** – T. Tautges (SNL/TSTT)

- **Quality metrics to improve meshes** - P. Knupp (SNL/TSTT)

- **Improvements to the Eigensolver** – Y. Sun, G. Golub (Stanford); E. Ng, P. Husbands, X. Li, C. Yang (LBNL/TOPS)

- **Improvement studies for the DSI scheme** - B. Henshaw (LLNL/TSTT)

- **Visualization of multiple data sets** - G. Schussman, K. Ma (UCD/SAPP)

- **Parallel adaptive refinement** - Y. Luo, M. Shephard (RPI/TSTT)

- **Improving parallel performance** - A. Pinar (LBNL/TOPS), K. Devine (SNL)
CAD/Mesh Issues - Tau3P

(T. Tautges – SNL/TSTT)

Fixing CAD model and Optimizing Tau3P
Primary/Dual Mesh

Worst deviation = 41°

Worst deviation < .001°
Mesh Effects on Stability – Tau3P

(P. Knupp – SNL/TSTT)

Stability is measured by the number of time steps before reaching a preset instability threshold (or error bound).
Selected quality metrics are being incorporated into **CUBIT** to aid in generating better meshes for **Tau3P**.
ESIL Solver - Omega3P

(E. Ng, P. Husbands, X. Li, C. Yang – LBNL/SAPP, TOPS)

- Integrated an Exact Shift-Invert Lanczos (ESIL) eigensolver, developed by LBNL, into Omega3P
- Uses SuperLU for complete factorization of sparse matrices and combines with PARPACK to compute interior eigenvalues accurately
- Verifies Omega3P hybrid solver on a 47-cell structure calculation and can provide better efficiency at the expense of increased memory

<table>
<thead>
<tr>
<th>Speed (larger is better)</th>
<th>Omega3P</th>
<th>Omega3P with EISL</th>
<th>Omega3P with AV</th>
</tr>
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<tbody>
<tr>
<td>1.0</td>
<td>2.57</td>
<td>3.41</td>
<td></td>
</tr>
</tbody>
</table>
Stable Algorithm Development – Tau3P

(B. Henshaw – LLNL/TSTT)

The DSI (Discrete Surface Integral) scheme in Tau3P exhibits instabilities for long time integration on non-orthogonal grids that result in non-self-adjoint operator. Explored 3 possible ways to develop a stable algorithm:

(1) **Spatial artificial dissipation** - Initial numerical experiments indicate that a sixth-order dissipation is very effective with very little damping of the energy over long times.

(2) **Dissipative time integration** - Studied the ABS3 (Adams-Bashforth Staggered-Grid Order-3) scheme but found it not suitable even though it improves the convergence properties.

(3) **A symmetric scheme** - developed 2nd-order and fourth-order accurate approximations that are self-adjoint but only for grids that are logically rectangular, not for general unstructured meshes. The fourth-order approximation could be used in the context of overlapping grids to give an accurate and very efficient solver.
Visualizing Mesh/Field/Particle – Track3P

(G. Schussman, K. Ma – UCD/SAPP)

• Simultaneous rendering of field/particle data
• Extremely dense particle trajectories/field lines
• Complex data abstraction to overcome limited display resolution
• Interactive user interface needed to reveal structures
Optimization - Omega3P

(Y. Luo, M. Shephard – RPI/TSTT)

- Developing optimization strategy to obtain higher order accuracy in frequency & wall loss calculations in **most efficient** way
- Optimal use of solver and *h-p* adaptive refinement based on energy gradient error metric

\[
 r_e = \int e \left( \nabla \cdot U \right)^2 dv \\
 U = \frac{\varepsilon}{2} |E|^2 + \frac{\mu}{2} |H|^2
\]

- Integrate with RPI framework to deal with mesh partitioning and load balancing

<table>
<thead>
<tr>
<th>h - mesh size</th>
<th>p – polynomial</th>
<th>E – solver converg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 (Linear)</td>
<td>1 (Lanczos)</td>
</tr>
<tr>
<td>1/2</td>
<td>2 (Quadratic)</td>
<td>2 (Jacobi-Davidson)</td>
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Sandia’s Zoltan library is implemented to access better partitioning schemes for improved parallel performance over existing ParMETIS tool through reduced communication costs.

**Domain Decomposition - Tau3P**

(TOPS: K. Devine/SNL, A. Pinar - LBNL)

<table>
<thead>
<tr>
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<tr>
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<tr>
<td>RCB-3D</td>
<td>5</td>
<td>1965</td>
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8 processor partitioning comparison on Linux cluster
Summary

- Under SciDAC, ACD has developed a powerful suite of numerical tools for solving challenging electromagnetic problems facing existing and planned accelerators,
- These are parallel codes based on unstructured grids that target high accuracy design and system level studies,
- ACD’s multi-disciplinary team approach mirrors the SciDAC concept and has been effective in accessing the computing and computational resources within the DOE,
- With SAPP/ISIC collaborators, ACD is building the high performance computing infrastructure needed to enable very LARGE (Ultra) scale simulations,
- New capability has been applied successfully to a range of applications and its potential to support DOE’s mission is just beginning to be realized.