Parallel Mesh Partitioning at SLAC

Michael M. Wolf









- DOE laboratory managed by Stanford University
- Established 1962
- Located at Stanford University in Menlo Park, CA
- "Mission is to design, construct and operate state-of-the-art electron accelerators and related experimental facilities for use in high-energy physics and synchrotron radiation research."
- 3 kilometers long (e-gun to start of rings)
- 3 Nobel Prize Winners
- Home of the first U.S. Website







Courtesy Stanford Linear Accelerator Center











Stanford e+e- Linear Collider (SLC)





Advanced Computations Department





ACD Organization/Collaborators

Advanced Computations Department

| Accelerator Modeling | Computational Mathematics Computing Techno | |
|--|---|--|
| V. Ivanov, A. Kabel, K. Ko, Z. Li, C. Ng, L. Stingelin (PSI) | Y. Liu, I. Malik, W. Mi, J. Scoville, K. Shah, Y. Sun (Stanford) | N. Folwell, L. Ge, A. Guetz, R. Lee, M. Wolf |
| | Collaborators | |
| LBNI (SCG) | Stanford (SCCM) | Sandia |
| E. Na, P. Husbands, | G. Golub, | P. Knupp, T. Tautges, |
| S. Li, A. Pinar | O. Livne, | L. Freitag, K. Devine |
| UCD (VGRG) | LLNL (CASC) | RPI (SCOREC) |
| K. Ma, G. Schussman | D. Brown, K. Chand, B. Henshaw | M. Shephard, Y. Luo |





- Accurate modeling essential for modern accelerator design.
- Uncertainty in design greatly increases cost
- Accurate computer models reduce design costs and design cycle
- Need for accurate cavity design tools
- ACD develops these simulation codes
 - E&M field, resonant frequency, particle tracking simulations
 - Conformal meshes (Unstructured grid)
 - Parallel processing
- Codes: Omega3P, Tau3P, Track3P, S3P, Phi3P





Challenges in E&M Modeling of Accelerators

- Ø Accurate geometry is important due to tight tolerance
 - needs unstructured grid to conform to curved surfaces
- Ø Large, complex electromagnetic structures
 - large matrices after discretization (100's of millions of DOF), needs parallel computing for both problem storage and reduction of simulation time
- Small beam size ~ delta function excitation in time & space
 - Time domain needs to resolve beam size leading to huge number of grid points, long run time & numerical stability issues
 - Frequency domain wide, dense spectrum to solve for thousands of modes to high accuracy





Motivation for New EM Capability

Modeling RDDS Cell with standard accelerator code MAFIA using Structured Grid on Desktops demonstrates the need for MORE ACCURATE EM codes





Typical ACD problems





Heating in PEP-II Interaction Region





FULL-SCALE OMEGA3P MODEL FROM CROTCH TO CROTCH

Beam heating in the beamline complex near the IR limited the PEP-II from operating at high currents. Omega3P analysis helped in redesigning the IR for the upgrade.





Next Linear Collider (NLC)



| | SLC | NLC |
|---------------------|---------------|----------------|
| Center of Mass | 100 GeV | 500 GeV |
| Bunches per pulse | 1 | 95 |
| Operating Frequency | (S) 2.856 GHz | (X) 11.424 GHz |
| Number of Cavities | 80,000 | 2 million |
| Post-Tuning | yes | No |







The NLC Accelerating Structure

206-Cell Round Damped Detuned Structure RDDS



- Ø Needs accelerating frequency calculated to 0.01% accuracy to maintain structure efficiency
- Ø Optimized design could save \$100 million in machine cost





NLC Structure Design Requirements



Ø <u>RDDS Cell</u> : Design to 0.01% accuracy in accelerating frequency,

Ø <u>RDDS Section</u> : Model damping/detuning of dipole wakefields.





Particle Tracking in 5 Cell RDDS (Tau3P/Track3P)







Cyclotron COMET (Omega3P)

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







Where we want to go





End-to-end NLC Structure Simulation

(J. Wang, C. Adolphsen – SLAC)

- NLC X-band structure showing damage in the structure cells after high power test
- Theoretical understanding of underlying processes lacking so realistic simulation is needed





End-to-end NLC Klystron Simulation

Field and particle data estimated to be TB size

PPM Focused Klystron









Tau3P Parallel Time-Domain 3D Field Solver





Follows evolution of E and H fields on primary/dual meshes (hexahedral, tetrahedral and pentahedral elements) using leap-frog scheme in time (DSI scheme)

$$\oint E \bullet ds = -\iint \frac{\partial B}{\partial t} \bullet dA$$



$$\oint H \bullet ds^* = \iint \frac{\partial D}{\partial t} \bullet dA^* + \iint j \bullet dA^*$$







Discrete Surface Integral Method

- Electric fields on primary grid
- Magnetic fields on dual grid
- Primary and dual grids non-orthogonal
- Dual grid constructed by joining centers of primary cells
- Electric and magnetic fields advanced in time using the leapfrog algorithm
- Reduces to conventional finite difference time domain method (FDTD) for non-orthogonal grids
- Conforms to complicated geometry by appropriate choice of element types

Ref: N. K. Madsen, J. Comp. Phys., **119**, 34 (1995)



Tau3P Applications





Time Domain Design & Analysis (Tau3P)





Output Coupler loading on HOM modes at the RDDS output end





Wakefield Calculation (Tau3P)

- Response of a 23-cell X-Band Standing Wave Structure w/ Input Coupler & Tapered Cells to a transit beam in Tau3P.
- Direct wakefield simulation of exact structure to verify approximate results from circuit model.







Determining Peak Fields (Tau3P)

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



Steady-state Surface Electric field amplitude





15-Cell H90VG5 Model

- Peak field appears near the middle of the structure
- About 25% overshoot in peak field due to the narrower bandwidth







Electric Fields (Tau3P)







Tau3P Matrices





Discrete Surface Intergral Formulation

$$\oint E \bullet ds = -\iint \frac{\partial B}{\partial t} \bullet dA$$

$$\oint H \bullet ds^* = \iint \frac{\partial D}{\partial t} \bullet dA^* + \iint j \bullet dA^*$$



- The DSI formulation yields:
 - efield += a*AH*hfield
 - hfield += \u03b8*AE*efield
 - efield, hfield are vectors of field projections along edges/dual-edges
 - AH, AE are matrices
 - α , β are constants proportional to dt





Tau3P Implementation



Example of Distributed Mesh







Tau3P Matrix Properties



Typical Distributed Matrix

- Very Sparse Matrices
 - 4-20 nonzeros per row
- 2 Coupled Matrices (AH,AE)
- Nonsymmetric (Rectangular)



Tau3P Performance Problems





Load Balancing Issues in Tau3P

- Load balancing problem inTau3P Modeling of NLC I nput Coupler.
 - Unstructured meshes lead to matrices for which nonzero entries are not evenly distributed.
 - Complicates work assignment and load balancing in a parallel setting.
 - Tau3P originally used ParMETIS to partition the domain to minimize communication.



NZ Distribution over 14 cpu's



Parallel Speedup







Parallel Performance of Tau3P

- 257K hexahedrons
- 11.4 million non-zeroes









Communication in Tau3P (ParMetis Partitioning)





Communication in Tau3P (ParMetis Partitioning)







Improved Mesh Partitioning Schemes





Luxury in Tau3P Mesh Partitioning

- Long simulation times
 - Tens of thousands of CPU hours
- Long time spent in time stepping
 Millions of time steps
- Problem initialization short
- Static (not dynamic) mesh partitioning
- Willing to pay HI GH price upfront for increased performance of solver





Zoltan Overview

- Developed at Sandia National Laboratory (NM)
- Collection of Data Management Services for Parallel, Unstructured, Adaptive, and Dynamic Applications
- Supports Several Load Balancing Methods:
 - Graph Partitioning Algorithms
 - ParMETIS
 - Jostle
 - Geometric Partitioning Algorithms (1D/2D/3D)
 - Recursive Coordinate Bisection (RCB)
 - Recursive Inertial Bisection (RIB)
 - Hilbert Space-Filing Curve (HSFC)
 - Octree Partitioning (various traversal schemes including HSFC)
 - Refinement Tree Based Partitioning (mesh refinement)
- Supports Dynamic Load Balancing/Data Migration





Zoltan Partitioning Methods





ParMETIS (Graph)







Recursive Coordinate Bisection (Geometric)







Recursive Inertial Bisection (Geometric)













Hilbert Space Filling Curve (Geometric)







Tau3P Partitioning Results





RDDS (5 cell w/ couplers) ParMETIS Partition







RDDS (5 cell w/ couplers) RCB-1D(z) Partition







RDDS (5 cell w/ couplers) RCB-3D Partition







RDDS (5 cell w/ couplers) RIB-3D Partition







RDDS (5 cell w/ couplers) HSFC-3D Partition







5 Cell RDDS (8 processors) Partitioning

| | Tau3P Runtime | Max Adj. Procs | Sum Adj. Procs | Max Bound. Objs | Sum Bound. Objs |
|------------|------------------|-------------------|-------------------|--------------------|--------------------|
| ParMETIS | 288.5 s | 3 | 14 | 585 | 2909 |
| RCB-1D (z) | 218.5 s | 2 | 14 | 3128 | 14363 |
| RCB-3D | 343.0 s | 5 | 26 | 1965 | 11961 |
| RIB-3D | 282.4 s | 3 | 18 | 1570 | 7927 |
| HSFC-3D | 387.3 s | 5 | 32 | 2030 | 9038 |

2.0 ns runtime IBM SP3 (NERSC)





5 Cell RDDS (32 processors) Partitioning

| | Tau3P Runtime | Max Adj. Procs | Sum Adj. Procs | Max Bound. Objs | Sum Bound. Objs |
|------------|------------------|-------------------|-------------------|--------------------|--------------------|
| ParMETIS | 165.5 s | 8 | 134 | 731 | 16405 |
| RCB-1D (z) | 67.7 s | 3 | 66 | 2683 | 63510 |
| RCB-3D | 373.2 s | 10 | 208 | 1404 | 24321 |
| RIB-3D | 266.8 s | 8 | 162 | 808 | 20156 |
| HSFC-3D | 272.2 s | 10 | 202 | 1279 | 26684 |

2.0 ns runtime IBM SP3 (NERSC)





H60VG3 ("real" structure)



55 cells (w/ coupler) 1,122,445 elements





H60VG3 RDDS Partitioning (w/o port grouping)

| # of Procs | ParMETIS Max Adj. Procs | ParMETIS Speedup | ParMETIS Runtime | RCB-1D Runtime | RCB-1D Speedup | RCB-1D Max Adj. Procs |
|---------------|-------------------------------|---------------------|---------------------|-------------------|-------------------|-----------------------------|
| 8 | 2 | 8/8 | 3930.7 s | 3898.6 s | 8/8 | 2 |
| 16 | 3 | 11.6/16 | 2703.3 s | 2458.5 s | 12.7/16 | 2 |
| 32 | 4 | 21.6/32 | 1455.0 s | 1236.6 s | 25.2/32 | 2 |
| 64 | 4 | 42.7/64 | 736.6 s | 627.2 s | 49.7/64 | 2 |
| 128 | 10 | 48.9/128 | 643.0 s | 265.1 s | 117.6/128 | 2 |
| 256 | 11 | 87.3/256 | 360.0 s | 129.2 s | 241.4/256 | 2 |
| 512 | 14 | 107.7/512 | 292.1 s | 92.3 s | 337.9/512 | 4 |
| 1024 | 16 | 96.0/1024 | 327.5 s | 99.0 s | 315.0/1024 | 8 |

1.0 ns runtime IBM SP3 (NERSC)





RCB Scalability Leveling Off







RCB Scalability Leveling Off







Coupler Port Grouping Complication







Coupler Port Grouping Complication

TARES ELEVA Mean pict Meani Kiann 181 2.a.io 191 2.a.io 191 8. 8 Time 8. 8.88 Mesn pict Mesh: Mesh H: H.S.Lu 2yt e: 0 Time: 0.022 Mesh plot Mesh: resh DB: M.S.To 7777 15. e: K Time: 0.000 TTT: Ctt) CH1 Ctr. Hi. Mosh plot Mesh: mesh 13. Takino System B 1 y Het In 1900 C II (((())) ((fff)) <u>السینین</u> -1 Meisn r Heit Meisne Mesn [[بر]] ل Ds: E.c.To Dys e: R Time: C.000 Mesh plot Mesh: wesh DB: 7.silo Dyt e: 8 Lime: KiNNN



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H60VG3 RDDS Partitioning (w/ coupler port grouping)

| # of Procs | ParMETIS Max Adj. Procs | ParMETIS Speedup | ParMETIS Runtime | RCB-1D Runtime | RCB-1D Speedup | RCB-1D Max Adj. Procs |
|---------------|-------------------------------|---------------------|---------------------|-------------------|-------------------|-----------------------------|
| 8 | 2 | 8/8 | 3856.2 s | 3826.5 s | 8/8 | 2 |
| 16 | 3 | 7.2/16 | 4257.0 s | 2405.4 s | 12.7/16 | 2 |
| 32 | 3 | 14.3/32 | 2158.3 s | 1820.7 s | 16.8/32 | 2 |
| 64 | 7 | 31.0/64 | 995.1 s | 889.3 s | 34.4/64 | 3 |
| 128 | 7 | 47.5/128 | 649.6 s | 599.0 s | 51.1/128 | 6 |
| 256 | 9 | 69.7/256 | 442.9 s | 516.5 s | 59.3/256 | 11 |
| 512 | 12 | 70.4/256 | 438.1 s | 531.1 s | 57.6/512 | 21 |

1.0 ns runtime IBM SP3 (NERSC)





Constrained Mesh Partitioning





| Method | Max Adj. Procs |
|------------|----------------|
| HSFC-3D | 14 |
| ParMETIS | 8 |
| RCB-1D-z | 14 |
| RCB-2D-xy | 5 |
| RCB-2D-xz | 14 |
| RCB-2D-yz | 6 |
| RCB-3D | 8 |
| RI B-2D-xy | 6 |
| RI B-2D-xz | 14 |
| RIB-2D-yz | 5 |
| RIB-3D | 7 |



| Method | Max Adj. Procs |
|------------|----------------|
| HSFC-3D | 17 |
| ParMETIS | 14 |
| RCB-1D-z | 29 |
| RCB-2D-xy | 7 |
| RCB-2D-xz | 29 |
| RCB-2D-yz | 7 |
| RCB-3D | 11 |
| RI B-2D-xy | 7 |
| RI B-2D-xz | 29 |
| RIB-2D-yz | 6 |
| RIB-3D | 12 |



Future Work I Would Have Done

- Stitching Multiple Partitions Together
- Competition
- Onion Partition growing
- Dynamic Partitioning for Track3P





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