

THE U.S. DOE GRAND CHALLENGE IN COMPUTATIONAL ACCELERATOR PHYSICS *

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Abstract

Particle accelerators are playing an increasingly important role in basic and applied science, and are enabling new accelerator-driven technologies. But the design of next-generation accelerators, such as linear colliders and high intensity linacs, will require a major advance in numerical modeling capability due to extremely stringent beam control and beam loss requirements, and the presence of highly complex three-dimensional accelerator components. To address this situation, the U.S. Department of Energy has approved a “Grand Challenge” in Computational Accelerator Physics, whose primary goal is to develop a parallel modeling capability that will enable high performance, large scale simulations for the design, optimization, and numerical validation of next-generation accelerators. In this paper we report on the status of the Grand Challenge.

1 INTRODUCTION

Several accelerator projects are planned or under consideration that will have major impacts in basic and applied scientific research. Examples include the Next Linear Collider (NLC), the Large Hadron Collider (LHC), the Spallation Neutron Source (SNS), and fourth-generation light sources. All of these projects will require high-resolution modeling far beyond that which has ever been performed by the accelerator community. Similar modeling will be needed for proposed accelerator-driven technologies, including Accelerator Production of Tritium (APT), Accelerator Transmutation of Waste (ATW), and Accelerator Driven Energy Production (ADEP).

For example, future high average power linear accelerators, such as the APT, will have to operate with extremely low beam loss (~ 0.1 nA/m) to prevent unacceptably high levels of radioactivity. To ensure that this requirement will be met, simulations with on the order of 100 million particles are needed. An equally challenging modeling problem exists in the NLC for which the linac design is dominated by the issue of beam emittance growth due to long-range transverse wakefields. To suppress this effect, a complex 3D accelerating structure, the Damped Detuned

Structure (DDS), has been developed to control the wakefields and it is necessary to verify the effectiveness of the design by numerical simulation. This entails modeling a complete accelerator section that consists of 206 complex three-dimensional cavities requiring hundreds of GBytes of memory. It is evident that these simulations are beyond the desktop computer’s capabilities, and can only be performed on the most advanced high performance computing (HPC) platforms using software and algorithms targeted to parallel and distributed environments.

In 1997 the U.S. Department of Energy initiated a Grand Challenge in Computational Accelerator Physics to support a collaborative effort involving LANL, SLAC, UCLA, and Stanford, together with two HPC centers, the National Energy Research Scientific Computing Center (NERSC) and the Advanced Computing Laboratory (ACL). The primary goal of this project is to develop a new generation of accelerator modeling tools for HPC platforms, and to apply them to large complex problems of importance in future accelerators, including those mentioned above. In this paper we will report the progress-to-date in two main thrust areas: electromagnetics and beam dynamics.

2 ELECTROMAGNETIC MODELING

The development of new electromagnetic tools for the Grand Challenge project originated from advanced accelerator structure research for the NLC. The main thrust of the effort is aimed towards large-scale simulations of realistic 3-D structures. Such a capability can be applied to system-scale analysis such as finding the wakefields in the entire DDS as described in Fig. 1, or to individual component design such as one cell in the DDS Fig. 2, by modeling with an accuracy approaching fabrication tolerance level. The new set of tools incorporates the following features to enable the high-resolution modeling required: (i) the use of unstructured grids to capture realistic geometries, (ii) the development of refinement algorithms to improve accuracy and optimize computing resources, and (iii) the implementation on parallel platforms to take advantage of the latest in HPC resources for large-scale simulations.

Presently, there are two types of solvers being developed for the tool set. The first type is formulated in the frequency domain using linear and quadratic finite elements on an ir-

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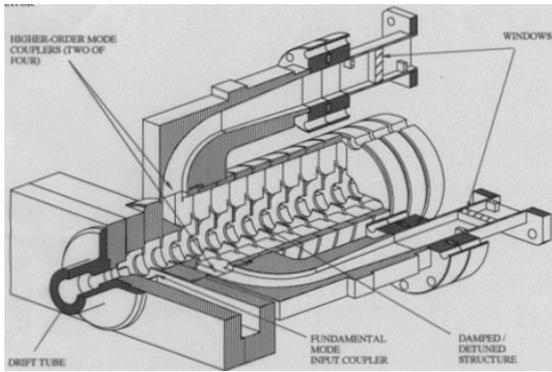


Figure 1: One end of the DDS 206-cell section including the input coupler and HOM load termination.

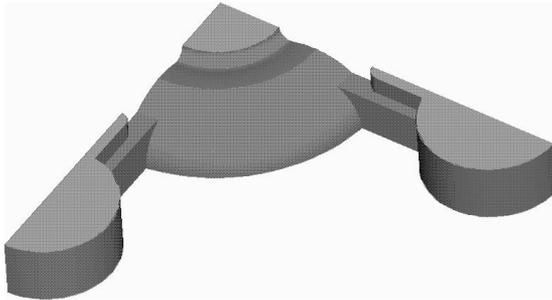


Figure 2: One-eighth of the DDS cell geometry from a solid model.

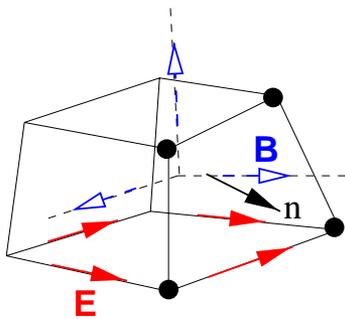


Figure 3: A non-orthogonal cell for the generalized Yee algorithm used in $\tau 3$.

regular grid, and includes eigenmode solvers in two and three dimensions, named $\Omega 2$ and $\Omega 3$ respectively. The parallel versions, $\Omega 2P$ and $\Omega 3P$, use MPI and currently run on the SGI/Cray T3E at NERSC. In the case of $\Omega 3P$, the calculation proceeds in three steps: First, there is the mesh distribution step with a module called DistMesh that uses the parallel library ParMETIS for partitioning unstructured graphs. This is followed by the matrix assembly step which consists of the finite element formulation that provides the mass and stiffness matrices for the generalized eigenvalue problem. The final step is a solution step, with Lanczos or Jacobi-Davidson algorithms, that utilizes the parallel itera-

tive library AZTEC to solve the sparse linear systems.

The other type of solver is a three-dimensional time-domain code, called $\tau 3$, that uses a generalized Yee algorithm on an unstructured grid [1][2], Fig. 3. A leapfrog time advancement scheme with filtering is implemented as well as a broadband termination at the waveguide ports. Therefore it is able to handle pulse transmission for S-parameter evaluations of RF components over a wide frequency range in a single run. Dipole excitation is also possible to calculate external Q's of waveguide-loaded cavities. A parallel version, $\tau 3P$, currently runs on a shared memory machine, like the 4-node Intel Xeon server, using threads while the distributed memory version for the T3E is presently under development. The inclusion of a transiting rigid beam to compute wakefields is planned.

2.1 Examples

We present here some recent results from $\Omega 3P$ and $\tau 3$. First, we report the modeling of a single DDS cell using $\Omega 3P$ on the T3E. Fig. 4 shows the cell geometry partition-

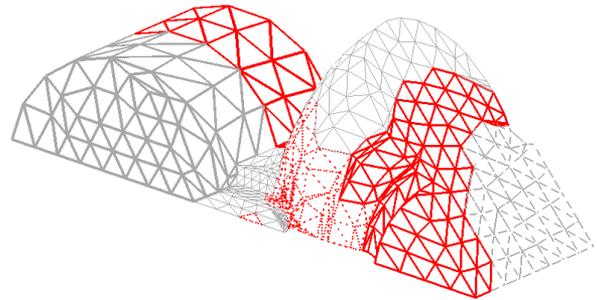


Figure 4: Domain decomposition of the DDS cell.

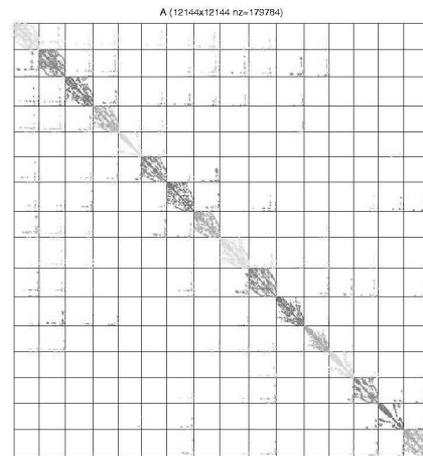


Figure 5: Mass matrix distribution over 16 processors.

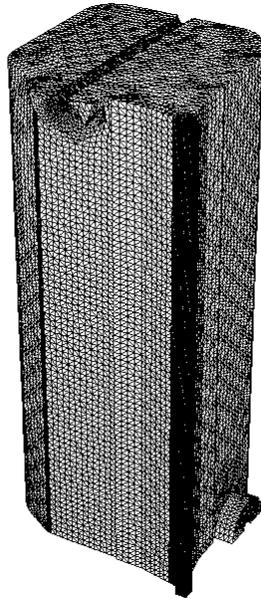


Figure 6: RFQ cavity for the SNS.

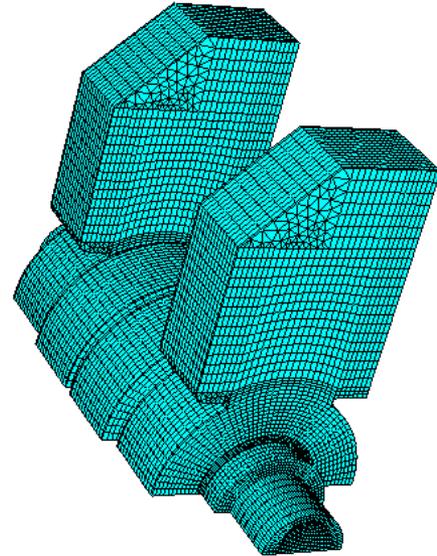


Figure 8: Input power coupler for the NLC linac modeled by $\tau 3$.

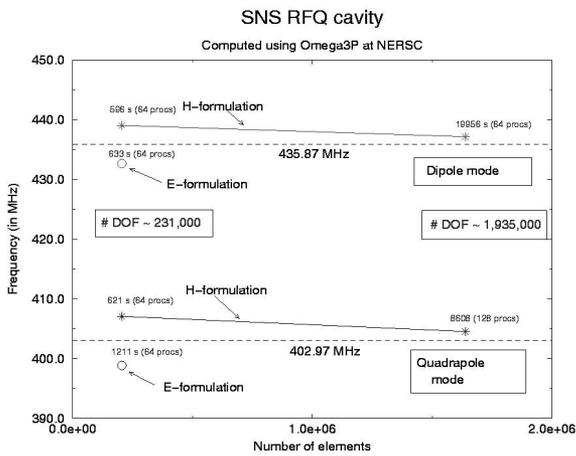


Figure 7: Calculated frequencies and measured data for two modes of the SNS RFQ cavity.

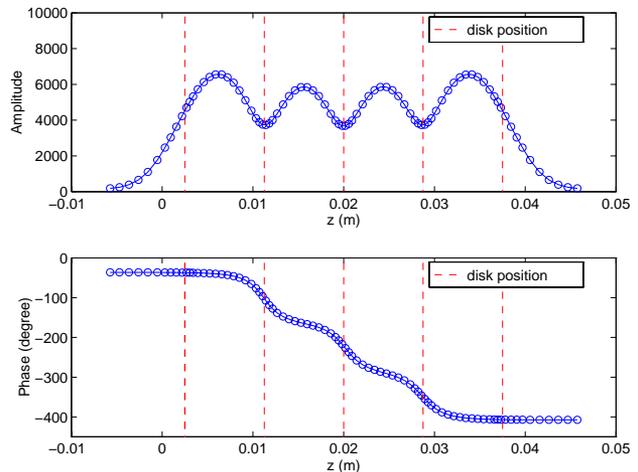


Figure 9: Field amplitude and phase of accelerating field at matched condition.

ing into 8 pieces using DistMesh/ParMETIS. Fig. 5 is the mass matrix distribution over 16 processors. Together they demonstrate the importance of domain decomposition to achieve load balancing. Currently, $\Omega 3P$ is the tool we use to determine the new dimensions for improved versions of the DDS design. Another $\Omega 3P$ result comes from the Spallation Neutron Source project for which we modeled the RFQ cavity as shown in Fig. 6. This cavity is difficult to simulate accurately due to the disparate lengthscales between the focusing vanes, the stabilizing rods, and the cavity proper. Fig. 7 shows the convergence of the calculated frequencies to measured data for the two modes of interest when the resolution is increased to require several million degrees of freedom in the simulation.

The $\tau 3$ capability is demonstrated by the matching and tuning of the input power coupler for the NLC accelerator section. Fig. 8 shows the mesh used in modeling a pair of couplers separated by two regular cells. $\tau 3$ finds the match by either single frequency or pulse excitation. The reflection is determined to be 0.005 at 11.424 GHz. The match is confirmed by the accelerating field amplitude and phase along the beam axis. Fig. 9 indicates the field that is due to a travelling wave with the correct phase advance of 120 degrees per cell from coupler to coupler. The advantage of $\tau 3$ over other commercial packages will be the ability to model much larger problems when the parallel version, $\tau 3P$, is completed.

3 BEAM DYNAMICS SIMULATIONS

Many systems involving intense charged-particle beams can be described by the Vlasov/Poisson equations. There are two main approaches to solving these equations: particle simulation techniques and direct methods.

In the particle simulation approach, the beam distribution function is represented by a number of macroparticles, typically 10's to 100's of millions in a large scale simulation. Often the single particle equations of motion are derived from a Hamiltonian which includes both externally applied fields and a mean field due to the beam's space charge: $H = H_{ext} + H_{sc}$. Such a form is ideally suited to the application of symplectic split-operator methods [3]. These methods provide a powerful framework capable of dealing with the complicated Hamiltonians often encountered in accelerator physics, where the Hamiltonian is usually approximated by a high-order polynomial in the phase space variables. Besides being able to treat Hamiltonians with many terms, the split-operator approach is easily generalized to high-order accuracy in time. A well-known fourth-order algorithm is due to Forest and Ruth [4], and an arbitrary-order scheme was derived by Yoshida [5]. There are also implicit symplectic methods that do not require the Hamiltonian to be split into a sum of exactly solvable pieces [3]. Finally, time-dependent systems are easily treated by "extending the phase space" [4].

Unlike some split-operator treatments that separate the Hamiltonian into terms involving only position and only momentum, our particle simulations separate the Hamiltonian into terms involving the external fields and terms involving the self fields. The external fields are treated using well-established techniques from magnetic optics. One advantage of this approach is that it enables one to take large time steps, since the dynamics due to external fields is usually dominated by a linear map which is easily obtained analytically or numerically. To treat the self fields, we use a 3D Particle-In-Cell (PIC) approach with area weighting. Open boundary conditions are treated using the convolution method of Hockney [6]. We are currently using and evaluating several methods of implementing our parallel particle simulation codes: High Performance Fortran (HPF), C++ with message passing via the POOMA framework [7], and Fortran 90 with message passing [8]. In our HPF codes, charge deposition and field interpolation are parallelized using the method of Ferrell and Bertschinger [9]. In our codes that use explicit message passing, a "particle manager" is used to make the data needed by processors local to the processors prior to charge deposition and field interpolation.

Stochastic corrections to Vlasov/Poisson evolution occur due to particle collisions and noise in external fields. To treat these effects we have modified our PIC codes to include Langevin forces and damping, which corresponds to solving the Fokker-Planck equation for the distribution function. An example is shown in the next section.

3.1 Examples

Fig. 10 shows the horizontal and vertical rms emittances from a 2D Langevin simulation of a beam in a potential that can produce chaotic dynamics. In the absence of damping and diffusion, the motion is governed by the Hamiltonian,

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \alpha x^4 + \beta y^4 + \frac{1}{2}x^2y^2 + q\Psi, \quad (1)$$

where α and β are constants, and where Ψ is scalar potential associated with the beam space charge. Damping and diffusion were turned on at $t = 0$ in the simulation, and the beam approached thermal equilibrium quickly, as is evident from the emittance curves which reach their final values after about 20 units of time. As further evidence that that beam has reached equilibrium, we turned off the damping and diffusion at $t = 100$ and observed little or no change in the emittances.

Though early work in beam halo physics emphasized 1D and 2D models of the transverse beam halo, recent activity has turned to 3D models including longitudinal beam halo. We have developed a parallel PIC code called HALO3D specifically for studying beam halo formation in 3D bunches. Such a code is extremely useful for testing analytical models of halo formation, such as particle-core models. A unique feature of the code is that it has a capability to model a new 3D beam equilibrium distribution, developed by R. Gluckstern and A. Fedotov of the University of Maryland [10]. It also has the ability to include nonlinear rf focusing fields, a feature incorporated in collaboration with J. Barnard and S. Lund of Lawrence Livermore National Laboratory. Based on their CTP ("core test particle") code, Barnard and Lund had predicted that the period-2 parametric resonance widely known to be a major source of beam halo could be detuned by the presence of nonlinear rf fields. This was supported by HALO3D simulations, as shown in Figs. 11 and 12. These figures show a stroboscopic plot in longitudinal phase space of test particles moving in the field of a mismatched beam. The resonance is evident in Fig. 11, which has a linear model of the rf fields. In contrast, the resonance is absent in Fig. 12, which has a nonlinear model of the rf fields.

In addition to HALO3D, we are also developing a new 3D beam dynamics code called IMPACT (Integrated-Map and Particle Accelerator Tracking code). This code has an accurate and efficient treatment of RF accelerating gaps, obtained by numerical integration of the gap transfer map rather than integration of single particle trajectories. The code is especially useful for modeling superconducting proton linacs, where there are only a few types of accelerating cavities. An example input geometry that was used to test the code is shown in Fig. 13. The figure shows the quadrupole gradient in a FODO cell along with the electric field on-axis due to accelerating cavities between the quadrupoles. Finally, we have developed a parallel version of a code called LINAC, developed by K. Crandall, which is the primary code used by the APT project for halo simulations. In addition to parallelizing LINAC, we also added

a 3D space charge capability, as described in the preceding section.

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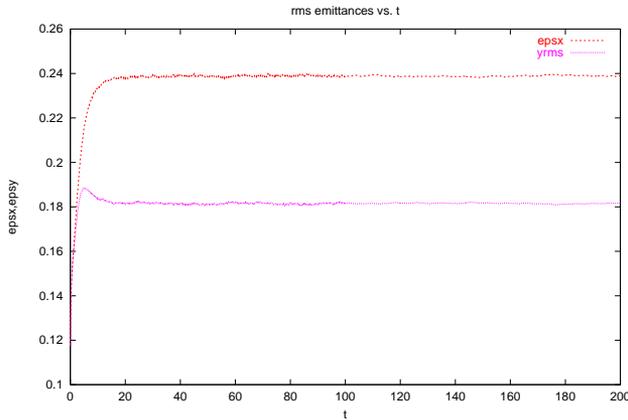


Figure 10: Emittance curves from a 2D Langevin simulation of a beam driven to thermal equilibrium.

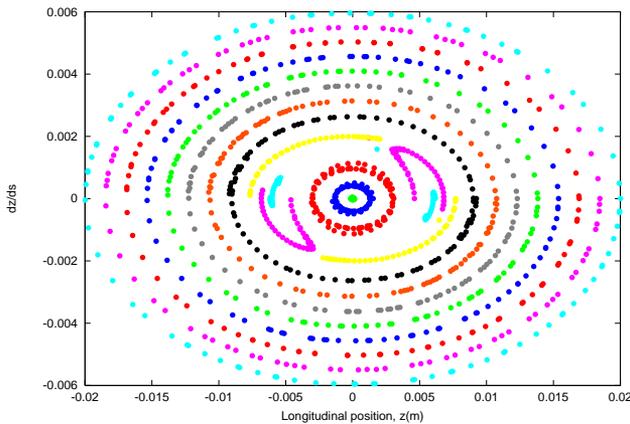


Figure 11: z-pz phase space plot from a HALO3D simulation without rf nonlinearity.

5 REFERENCES

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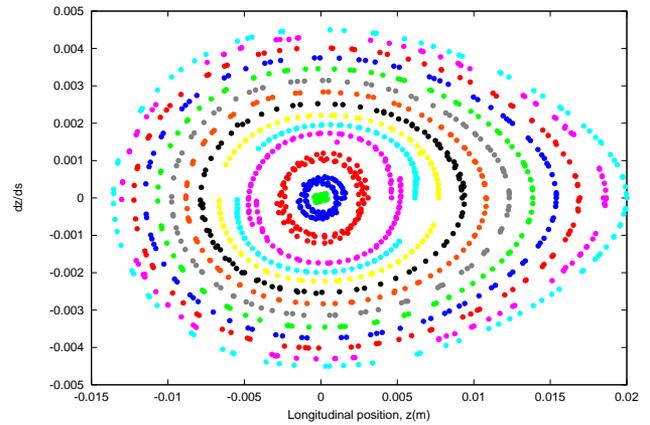


Figure 12: z-pz phase space plot from a HALO3D simulation with rf nonlinearity.

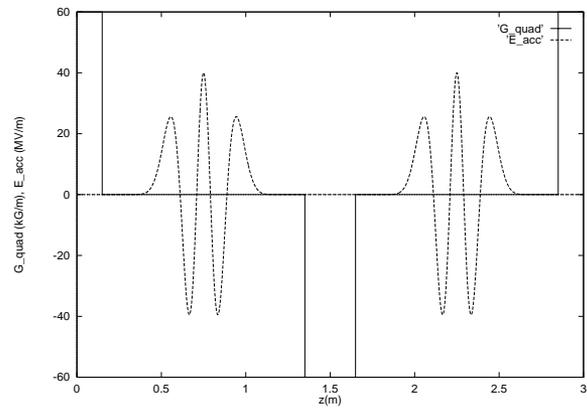


Figure 13: Example cell geometry for IMPACT simulation.

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