High Performance Computing in Parallel Electromagnetics Simulation Code suite ACE3P

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***Abstract*—A comprehensive set of parallel finite-element codes suite ACE3P (Advanced Computational Electromagnetics 3D Parallel) is developed by SLAC for multi-physics modeling of particle accelerators running on massively parallel computer platforms for high fidelity and high accuracy simulation. ACE3P enables rapid virtual prototyping of accelerator and RF component design, optimization and analysis. Advanced modeling capabilities have been facilitated by implementations of novel algorithms for numerical solvers. Code performance on state-of-the-art high performance computing (HPC) platforms for large-scale RF modeling in accelerator applications will be presented in this paper. All the simulations have been performed on the supercomputers at National Energy Research Computer Center (NERSC).**

Keywords—Finite element method, high performance parallel computing, hybrid MPI+OpenMP, multi-physics modeling, particle accelerator

I. INTRODUCTION

High energy accelerators are complex multi-million dollar scientific instruments. Successful design and operation of an accelerator has to satisfy RF, thermal, mechanical and beam requirements. Through the support of Department of Energy (DOE), SLAC has developed a comprehensive set of conformal, higher-order, parallel finite element electromagnetics modelling code suite ACE3P (Advanced Computational Electromagnetics 3D Parallel) for accelerator cavity and structure design including integrated multi-physics effects in electromagnetic, thermal, and mechanical characteristics with two unique features: (1) Based on higher order curved finite elements for high-fidelity modelling and improved solution accuracy; (2). Implemented on massively parallel computers for increased memory and speed. The codes are capable of using massively parallel supercomputers for modelling large accelerator structures with higher accuracy and speed.

II. ACE3P MODULES

The electromagnetics codes in ACE3P solves Maxwell equations in the frequency and time domains using unstructured grids with elements represented by Nedelec basis functions. Together with the conventional nodal finite element methods used in solving thermal and mechanical equations, ACE3P has six multi-physics parallel simulation modules to address different physics aspects of accelerator applications [1-7], and the modules are (1) Omega3P, an electromagnetic eigensolver for finding resonator modes and their damping in RF cavities; (2) S3P, a frequency-domain solver for calculating scattering parameters of RF components; (3) TEM3P, a multi-physics code in frequency domain for calculating integrated electromagnetic, thermal and mechanical effects; (4) Track3P, a particle tracking code for calculating dark current and multipacting in the presence of external fields; (5) T3P, a time-domain solver for calculating transient responses of driven systems and for wakefields due to charged particle beams; and (6) Pic3P, a particle-in-cell code for self-consistent simulation of particle and RF field interactions in space-charge dominated devices.

In a typical accelerator cavity simulation, the electromagnetic modules discretize the vacuum region inside the accelerator cavity, while the thermal and mechanical solvers are formulated in the frequency domain for the computational volume of the cavity walls and their surroundings. Relevant physical data are transferred at the interface of the two computational domains for integrated multi-physics simulation.

Several direct and iterative linear solvers have been implemented in ACE3P for the solution of a linear system of equations arising from the finite element formulations [5]. The eigensolver Omega3P can solve linear and quadratic eigenproblems for cavities with and without energy loss. Recently, in collaboration with applied mathematicians, a nonlinear eigensolver based on the CORK algorithm has been added to determine resonant mode external quality factor for cavities equipped with external waveguides [6].

III. PARALLELIZATION STRATEGY AND SOFTWARE DESIGN

ACE3P code suite is written in C++ and uses MPI for inter process communication. It takes a tetrahedral mesh in NetCDF format as input for the geometry of a cavity. The parallelization in ACE3P with the exception of Track3P is done using domain decomposition, where the mesh is partitioned into P subdomains

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using ParMetis and Zoltan, where P is the number of the MPI tasks. The mesh region at each subdomain boundary is replicated for data communication with adjacent subdomains. The hierarchical basis functions are employed for representing the electric field. The edge, face and volume degrees of freedom are located and the matrices assembled in parallel for each subdomain. Due to the nature of the resulting linear system, direct solvers are used in the frequency domain for fast solution convergence, and iterative solvers in the time domain for its parallel scalability for large-scale problems.

The particle tracking module Track3P is essentially embarrassingly parallel. Each compute node owns the whole finite element mesh and the associated external fields while particles are uniformly distributed among the compute cores, and thus no communication between the cores is required. High computational efficiency is achieved if the mesh and fields can fit into the shared memory of each processor. For large problems, the total size of the mesh and fields exceeds the shared memory of each processor, and therefore some processors are left idle by reducing the number of MPI tasks within a compute node. To improve the computational performance on state-of-the-art computing facilities with multi cores at NERSC, a hybrid MPI+OpenMP parallel programing model has been implemented for the particle tracking algorithms in Track3P.

IV. HPC PERFORMANCE STUDY

The use of HPC enables the solution of large-scale problem at the system level which is not readily achieved on desktop computers. The strong scalability of Omega3P solver running on supercomputers has been presented in [5]. Fig. 1 shows an Omega3P calculation using the nonlinear eigensolver to calculate the damping factors of resonant modes in a structure coupled with waveguides with different mode cutoff frequencies. Using second order basis functions, we obtained a discretized problem with 20 million degrees of freedom (DOFs). The computation was completed within 10 wall clock minutes on the NERSC Edison computer employing 960 processors for 16 trapped modes. Fig. 2 shows a TEM3P calculation for the lowest longitudinal mechanical modes profiles in PIP-II 650 MHz cryomodule (CM) consisting of six superconducting RF (SRF) cavities. The problem was solved using 10 nodes, 320 processors on Cori at NERSC and took less than 1 minute per mode calculation. For SRF cavity thermal simulations, thermal conductivity, surface resistance, and Kapitza conductance are temperature dependent. Due to the strong nonlinearity, care must be taken in the solution of nonlinear thermal equation. TEM3P uses Newton method for solving the nonlinear thermal equation, which needs robust implementation for strongly nonlinear problems. We use an inexact Newton method for solving the nonlinear equations, each of which requires the solution of a system of linear equations. The resulting linear equations are solved using the iterative preconditioned Krylov space methods, such as GMRES.

Fig. 1. Electric field amplitude profile for the highest external Q mode in the 3rd dipole passband in an ideal LCLS-II cryomodule.

Hybrid MPI+OpenMP programing performance study has been carried out on the NERSC Edison supercomputer for a Track3P simulation on dark current simulation in a chain of 8 LCLS-II SRF cavities. 4 times speedup has been achieved for one tracking cycle compared with pure MPI implementation.

Fig. 3 shows the strong scalability of T3P running on the NERSC Cori. The test problem was solving electromagnetic wave propagation in human body. The computer model has 2.5M tetrahedral elements. As a comparison, the perfect linear scalability is also plotted as the black line. It is evident that T3P scales very well for this problem up to 10k processors. In the case using 4096 processors, each processor on average has less than 650 tetrahedral elements.

Fig. 2. The longitudinal cavity mechanical mode displacement profile at longitudinal plane in PIP-II 650 MHz SRF CM.

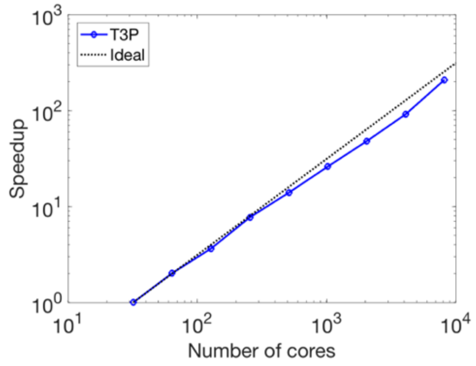

Fig. 3. Strong parallel scaling of T3P on NERSC Cori.

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