

Development of Solid Earth Simulation Platform

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In FY.2002, parallel FEM platform based on GeoFEM has been implemented to the Earth Simulator. Each component of the platform, such as parallel I/O, parallel linear solvers and parallel visualization modules were optimized on the Earth Simulator. In FY.2003, parallel iterative solvers with selective-blocking preconditioning, which are suitable for ground motion applications with nonlinearity due to contact boundary conditions, have been ported to the Earth Simulator. Furthermore, parallel visualization modules have been extended to various types of applications and mesh systems. Tools developed in this project have been widely used by many groups in the consortium for solid earth simulation.

Keywords: Parallel Finite Element Method, Solid Earth Analysis Platform, GeoFEM, Parallel Iterative Solver, Parallel Visualization, Selective Blocking

1. Overview of Software

GeoFEM consists of the components 'platform', 'analysis modules' and 'utilities'. Platform includes device-independent I/O interface, iterative equation solvers and visualizers. Analysis modules are linked to platform on memory by device-independent interface such that the copies of data should be avoided as much as possible for large scaled-data and high-speed calculations. To deal with various problems of solid earth, analysis modules plugged-in are elastic, plastic, viscoelastic and contact structural analysis, wave propagation analysis, thermal analysis and incompressible thermal fluid analysis modules. Utilities are for domain partitioning and pre/post viewers.

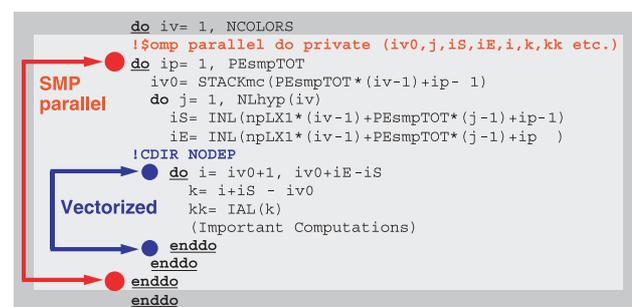
GeoFEM is written in Fortran90 (in C for visualization module). Inter-node parallelization is done by the domain decomposition based SPMD with MPI. For Intra-node parallelization, OpenMP (Pthread for visualization module) is used. Intra-node parallelization and vectorization are done by considering the reordering of the matrices such that the long vector length of the independent operations can be obtained.

2. Optimization of Iterative Solvers and Performance Evaluation

Each subdomain is assigned to one SMP node. In order to achieve efficient parallel/vector computation with unstructured grids, the following 3 issues are critical: 1) Local operation and no global dependency, 2) Continuous memory access, 3) Sufficiently long loops. In order to satisfy these

requirements, sophisticated reordering technique has been integrated with parallel iterative solvers with localized preconditioning. The reordering procedures are summarized as follows: (1) RCM(Reverse Cuthill McKee) reordering on the original local matrix for independent sets. (2) CM(Cyclic Multicolor) reordering to obtain loops whose length is sufficiently long and uniform. (3) DJDS(Descending-order Jagged Diagonal Storage) reordering for efficient vector processing, producing 1D arrays of coefficients with continuous memory access. (4) Cyclic reordering for load-balancing among PEs on an SMP node. (5) Parallel DJDS/CM-RCM reordering is complete.

The typical loop structure of the matrix-vector operations for PDJDS /CM-RCM reordered matrices with vector and OpenMP directives is described as follows:



As shown in Fig.1, simple 3D linear elastic problems up to 2.2×10^9 DOF using 176 SMP nodes (1,408 PEs) have been solved by the localized 3×3 block ICCG(0) with the additive Schwarz domain decomposition and PDJDS/CM-RCM

reordering. In this series of computations, DOF per SMP node is fixed. When using 176 SMP nodes, 3.8 TFLOPS (33.7% to peak) has been attained. The work ratios are more than 95%.

3. Selective Blocking Preconditioning

In ground motion simulations, material, geometric and boundary nonlinearity should be considered. Boundary nonlinearity due to fault-zone contact is the most critical. In GeoFEM, the augmented Lagrange method (ALM) and penalty method are implemented, and a large penalty number λ is introduced for constraint conditions around faults. The nonlinear process is solved iteratively by the Newton-Raphson (NR) method. A large λ can provide an accurate solution and fast nonlinear convergence for the Newton-Raphson method, but the condition number of the coefficient matrices is large. Therefore, many iterations are required for convergence of iterative solvers.

In this project, special method called selective blocking was also developed for contact problems. In the selective blocking method, strongly coupled finite-element nodes in the same contact group coupled through penalty constraints are placed into the same large block (selective block or super node) and all of the nodes involved are reordered according

to this blocking information. Full LU factorization is applied to each selective block, as shown in Figure 2. Thus, local equations for coupled finite-element nodes in contact groups are solved by means of a direct method during preconditioning. SB-BIC(0) (i.e., BIC(0) preconditioning with selective blocking reordering) usually requires a greater number of iterations for convergence compared to BIC(1) and BIC(2), but the overall performance is better because the computation time for each iteration and set-up is much shorter. Because no inter-block fill-in is considered for SB-BIC(0), the memory requirement for this method is usually as small as that in BIC(0) with no fill-in.

Example tests using 10 SMP nodes of the Earth Simulator have been done for the globally refined Southwest Japan model (7,684,072 elements, 7,767,002 nodes, 23,301,006 DOF (Figure 3)) for both of flat MPI and hybrid parallel programming model. Figure 4 shows the results. In the cases with many colors, fewer iterations are required for convergence, but the performance is worse due to the smaller loop length and greater overhead. In the hybrid parallel programming model, performance of 163.4 GFLOPS (25.5% of peak performance) for the Southwest Japan has been obtained. As for the flat MPI, the performance was 190.4 GFLOPS (29.8%) for the Southwest Japan, respectively. These results

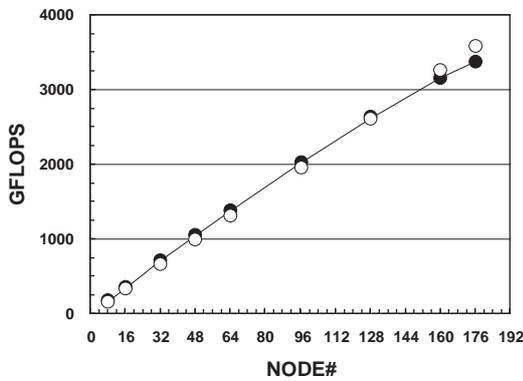


Fig. 1 Problem size and parallel performance (GFLOPS rate) for the 3D linear elastic problem, using up to 176 SMP nodes (Black circle: Flat MPI, White circle: Hybrid)

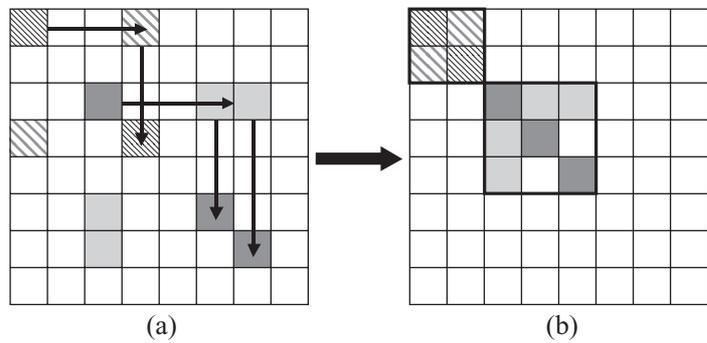


Fig. 2 Procedure of the selective blocking : Strongly coupled elements are put into the same selective block. (a) searching for strongly coupled components and (b) reordering and selective blocking.

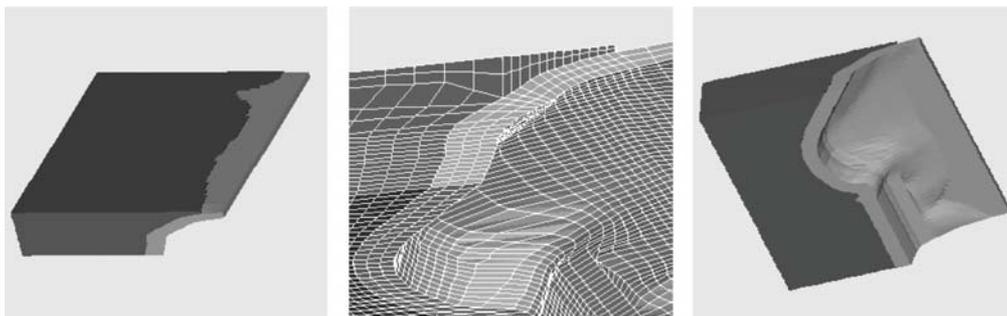


Fig. 3 Description of the Southwest Japan model This model consists of crust (dark gray) and subduction plate (light gray). 997,422 nodes (2,992,266 DOF) and 960,509 tri-linear (1st order) hexahedral elements are included.

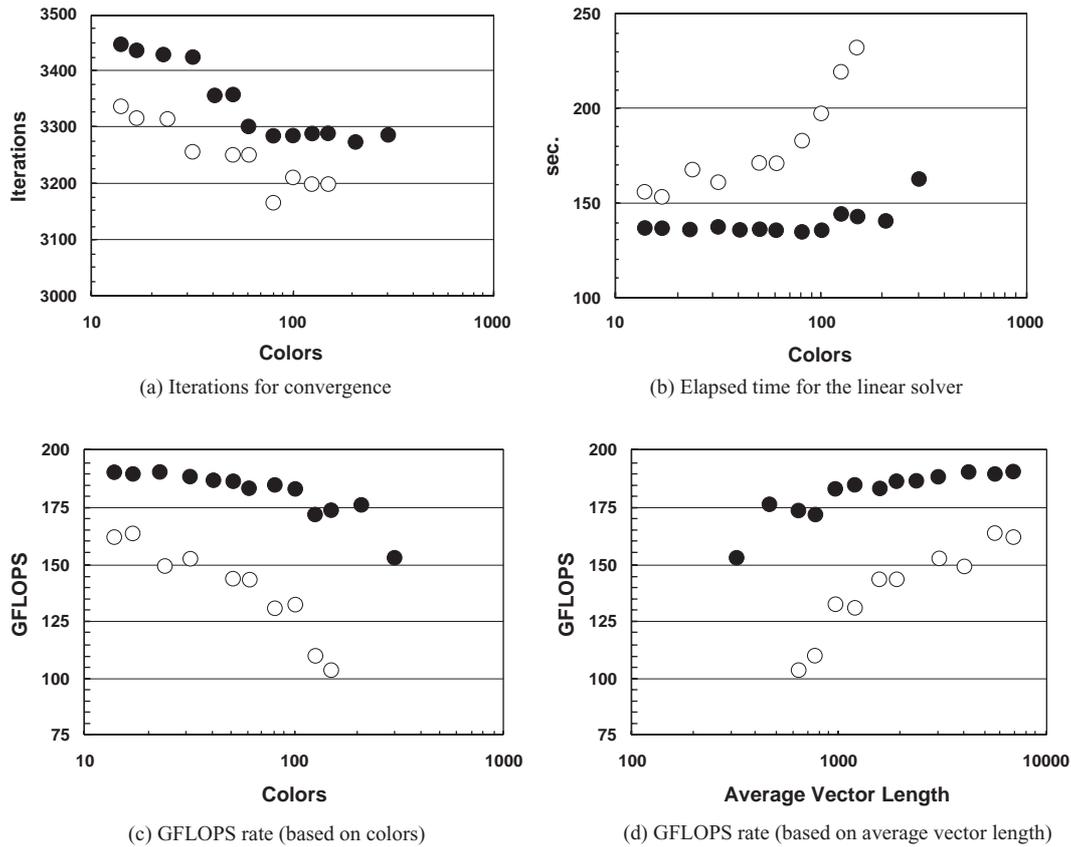


Fig. 4 Performance on 10 SMP node of the Earth Simulator (peak performance = 640 GFLOPS) using SB-BIC(0) CG for the 3D elastic contact problem with MPC condition ($\lambda = 10^6$) in Figure 3 (Southwest Japan model, 23,301,006 DOF). (a) Iterations for convergence, (b) Elapsed time for the linear solver, (c) GFLOPS rate (based on colors) and (d) GFLOPS rate (based on average vector length) (BLACK Circles: Flat MPI, WHITE Circles: Hybrid).

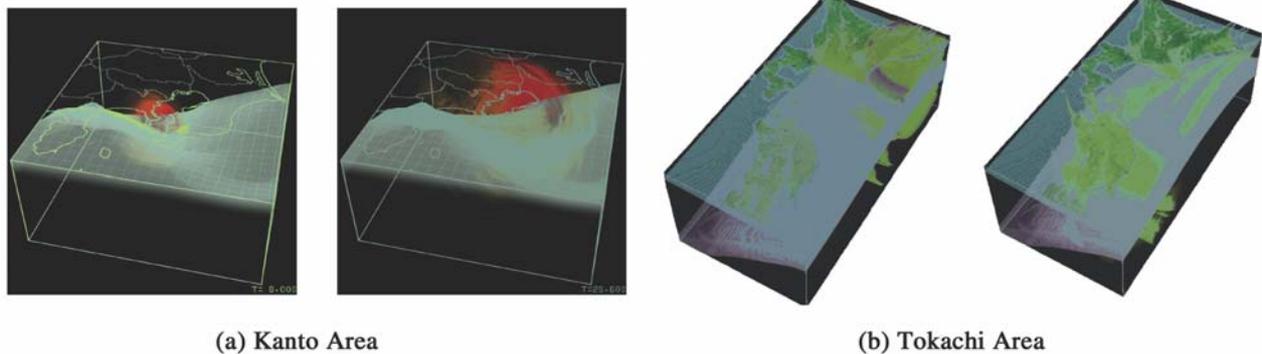


Fig. 5 Results of simulations on seismic wave propagation visualized by the parallel volume rendering modules in GeoFEM (Courtesy of simulation results: Professor Takashi Furumura, ERI/University of Tokyo).

are as excellent as those in Figure 1 by ICCG solvers for simple geometries with homogeneous boundary conditions, which are 196.1 GFLOPS for 30M DOF (30.6% of the peak performance) with hybrid programming model, and 218.9 GFLOPS (34.2%) with flat MPI. Number of iterations for convergence is smaller in hybrid than in flat MPI due to the effect of local preconditioning, but performance based on GFLOPS rate is better in flat MPI. Hybrid parallel program-

ming model is much more sensitive to color number and innermost vector length than flat MPI due to the synchronization overhead.

4. Parallel Visualization for Seismic Wave Propagation

Parallel volume rendering modules in GeoFEM has been extended for mesh systems of hybrid spectral-finite difference applications on seismic wave propagation, developed

by Professor Takashi Furumura, ERI/University of Tokyo. The concurrent visualization with analysis modules on the Earth Simulator has been implemented. Thus, there is no need to save the results generated by analysis modules on the hard disk or transfer huge data by network, which can avoid the limitations of storage capacity for large-scale data. Meanwhile, full use of the Earth Simulator's huge memory

can be made to complete visualization. Moreover, at each time step, multiple visualization methods can be performed to generate visualization results by different visualization methods and different parameters. Figure 5 shows results of simulations on seismic wave propagation visualized by the modules developed in this project.