

Parallel and Vector Performances of GeoFEM and Its Extensions to a Solid Earth Simulator

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Abstract

GeoFEM is parallel FE software challenging for wide range of solid earth problems as well as various practical issues in engineering and sciences. Linear equation solver, one of the key technologies of GeoFEM, has been successfully parallelized and vectorized to make the best use of GS40, which will be available in March, 2002. Also, some solid earth applications have been explored such as stress accumulation on a fault surface, earthquake wave propagation, dynamics of outer core, etc. Recent advances of GeoFEM include extension of framework to other grid systems than FEM, coupler to manipulate interactions among modules and/or grids, enrichment of parallel visualization functions.

Introduction

Solid earth is a coupled system of various complicated phenomena extending over a wide range of spectrum of space and time. To simulate this, there needs large-scale parallel technologies, combining the sophisticated models of solid earth processes and the large amount of observation data. The Science and Technology Agency, Japan, has begun an Earth Simulator project from the fiscal year of 1997, which tries to forecast various earth phenomena through the simulation of virtual earth placed in a supercomputer. GeoFEM challenges for long-term prediction of the activities of the plate and mantle near the Japanese islands through the modeling and calculation of the solid earth problems, including the dynamics and heat transfer inside the earth. GeoFEM is planned to develop the system in the following two phases:

Phase I GeoGEM/Tiger (1997-1998) : Multi-purpose parallel finite element software, which may be applied to various fields in engineering and sciences as well as becoming the basis for the solid earth simulator to be developed in Phase II. The objective here is to develop a high performance computational platform that can incorporate various models (various computer codes) of solid earth in a plug-in manner.

Phase II GeoFEM/Snake (1999-2001) : A software system optimized for GS40 and specialized for the simulation of solid earth phenomena such as mantle-core convection, buildup of tectonic stress, deformation of plates and seismic wave propagation.

In the following sections, computational strategies employed in GeoFEM and its parallel/vector performances are described. Also, depicted are recent computational results, ranging from engineering to solid earth fields.

Development Environment and Software Systems

Hardware environment

Platforms used for developing Tiger include Alpha cluster, Linux PC cluster and SR2201. Portability to SR8000, SX4, T3E, ORIGIN2000 and VPP5000 has been confirmed. Snake will tackle with transition to development environment with GS40 architecture in mind.

Software systems

GeoFEM consists of two portions, i.e. 'platform' and 'subsystems'. Platform covers parallel I/O, generic data input and communications among subsystems. Linear equation solvers [1] are also included in platform and are used via subroutine-call from subsystems. Subsystems are static linear, dynamics linear, static elasto-plastic, quasi-static contact, transient thermal, thermal fluid and visualization. Subsystems are linked 'on memory' by device-independent interface supported by platform. This is to avoid copying of data as much as possible for considering large scaled-data and high-speed calculations. Also, by specifying device-independent data transfer method as interface script between subsystems, subsystems are not directory connected to each other, enhancing the level of independence in development phase. And this leads to plug-in type of system establishment. For the main calculations, Fortran 90 is implemented and MPI is used for the message-passing library.

Parallel and Vector Performances

Scalar parallel performance on SR2201 / 1,000PEs

One of the targets of GeoFEM/Tiger was to deal with a problem of up to 100 million degrees of freedom, that is a necessary scale for the earth to be analyzed "as a whole". Both static elastic analysis [2] and dynamic elastic analysis [3] with the targeted 100 million degrees of freedom have been realized for simple shape (cube) and boundary conditions. The computer used for these problems is SR2201 at the University of Tokyo. For parallel processing, the region is partitioned into 1,000 regions and 1,000 processors are used.

For the static elastic analysis, localized ILU(0)-CG solver is used. Based on the (estimated) elapsed time using 1 PE, speed-up 612 (Efficiency 61.2 %) is attained. The work-ratio is kept to be over 96 %, which implies that the communications among PEs are efficiently performed. Efficiency of 61.2 % is due to the increase of CG iterations because the effect of preconditioning is deteriorated after domain partitioning. For the dynamic elastic analysis, there is no need to use equation solvers since an explicit scheme is employed here for the time integration. Thus, both work ratio and efficiency are measured to be over 98%.

Here, we should note that, in the above examples, the computational speed of each PE has reached only 3% of its peak speed. From the measurement on T3E, similar value, i.e. 3% of the peak speed has been obtained. To improve the single PE performance, vectorization is indispensable, which will be described in the next section.

Vector performance on SX4 / 1PE

Since an element PE of GS40 is a vector processor, vector performance is another important requirement. Computational scheme using the unstructured grid like FEM is generally less efficient in vectorization compared to the structured grid methods like FDM. Though indirect reference is inherently inevitable in the unstructured grid, by incorporating sophisticated ordering and memory array, vector performance to a considerable extent would be obtained. RCM and cyclic multicolor ordering with descending jagged diagonal storage [4] has been applied to GeoFEM's

ICCG solver. An elastic problem of 210,000 dof is solved by using 1PE of NEC SX-4 at JAERI/CCSE at the speed of 970 Mflops, which corresponds to 49 % of peak performance (2Gflops).

Vector/parallel performance on SR2201 / 216PEs and speed estimation for GS40

Considering that GS40 consists of 640 distributed nodes and that each node has 8 vector processors sharing a memory, next issue to investigate towards the optimization for GS40 is to attain good intra-node vector/parallel performance with keeping inter-node parallel efficiency.

As a preliminary test for this goal, vectorized GeoFEM described before is implemented to SR2201, and static linear elastic problems of a cube are solved. With keeping dof per PE to be 1.0×10^5 , various sizes of problems are solved by using various numbers of PEs. In the largest case, 216 PEs are used for solving 23 million dof problem. The computational speed measured is 13.9 Gflops, which corresponds to 21 % of peak performance of 216 PEs (64.8GFlops), while the work ratio is 94 %. We recall that the computational speed of the scalar version has reached only 3 % of the peak. This result implies that the vectorization is also effective in the pseudo-vector architecture of SR2201, and that both intra-node vector (1PE/node in this case) and the inter-node parallel efficiency are maintained.

An intra-node vector/parallel performance should be investigated on SMP architectures like SX4. The intra-node parallel may be conducted either using MPI or taking advantage of the microtasking (or OpenMP). Here, it is noted that if MPI is chosen for the intra-node parallel, then we need no modifications about the source code anymore, since both intra-node and inter-node parallelisms are based on the same idea. Whichever of the intra-node strategies is chosen, if assuming the intra-node parallel efficiency be around 80%, our current estimation of the computational speed of GeoFEM's solver on GS40 will be better than 10 Tflops.

An Example to Engineering Practical Problem

A full model of tube sheet, which is an experimental component in the nuclear engineering field, is carried out by the transient thermal subsystem. Three FE models, which have 54,084, 540,590 and 1,053,906 nodes, are built to model the tube sheet. The largest mesh is shown in Fig.1 (left). SR2201 up to 64 PEs is used. In the transient thermal analysis, 60 steps are advanced in time dynamically varying the time increment. Figure 2 shows the speed-up where the elapsed time of using 1PE was estimated. As the number of PEs increases, the speed-up is gradually deteriorated because of decrease of granularity. Thermal stress and deformations are also computed for this model by using the elasto-plastic subsystem as depicted in Fig.1 (right).

Solid Earth Applications and Frame Extensions

Three plate collision problem

Figure 3 shows 'three plate collision problem' (1,183,038 degrees of freedom) near the Japanese islands [5], solved by the quasi-static contact subsystem. Three plates collision is modeled in the region of 1,020km x 840km x 600km near the Japanese Islands, giving consideration to gravity and contacts at faults. The Newton-Raphson method is used for processing of non-linearity and the Augmented Lagrangian method is used for the constraint conditions of contact. It takes 9,140 seconds for computation with 32 PEs of SR2201.

Outer core problem

Three-dimensional, time-dependent thermal convection of the outer core is computed by the thermal fluid subsystem. Governing equations are incompressibility constraint, momentum conservation and energy conservation, assuming Boussinesq approximation, self gravity and Coriolis

force. FE model and results are shown in Fig. 4. Computational results have been successfully compared with those obtained by a spectral method.

Frame extensions

In collaboration with solid earth researchers, various modules are being developed in such fields as earthquake cycle, faulting and propagation, mantle/core dynamics, seismic wave propagation, GPS data assimilation etc. Along with these developments, GeoFEM platform is being extended to other grid systems than FEM, that is, BEM, Spectral Methods and Particle Methods. Couplers, which manipulate the interactions among modules and/or grids, are also under development. Figure 5 typically shows a framework for coupled regional tectonic process around Japan islands.

Concluding Remarks

Parallel/vector performances of GeoFEM and its applications to engineering and solid earth fields have been described. To attain the final goal of this project, i.e. accurate solid earth simulation using GS40, there will need further developments in various aspects. Linear solvers in the Snake phase are focusing on the following two procedures to obtain more stable convergence. One is new preconditioning methods with deflation. The other is multigrid or multilevel method for global smoothing. Various solid earth problems will be also investigated.

References

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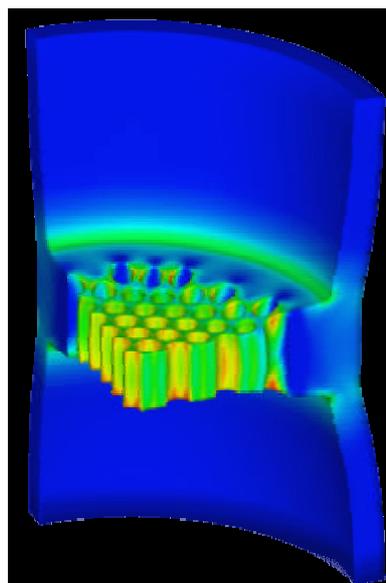
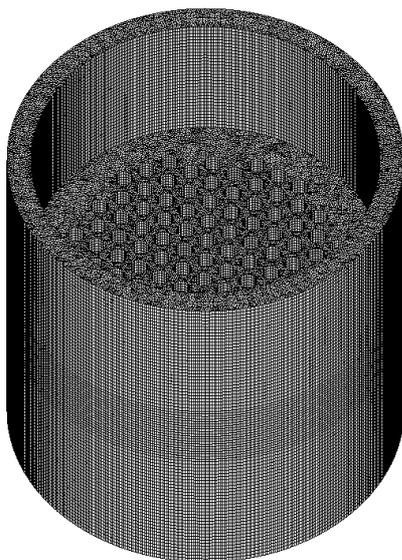


Figure 1 Tube sheet

FE mesh (left)
1,053,906 nodes
949,512 elements

Thermal stress deformations (right)

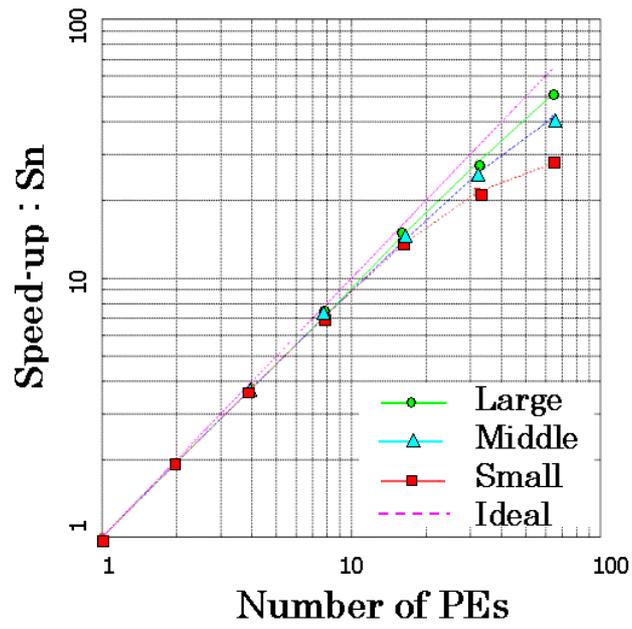


Figure 2 Speed-up of tube sheet analysis (transient thermal analysis)

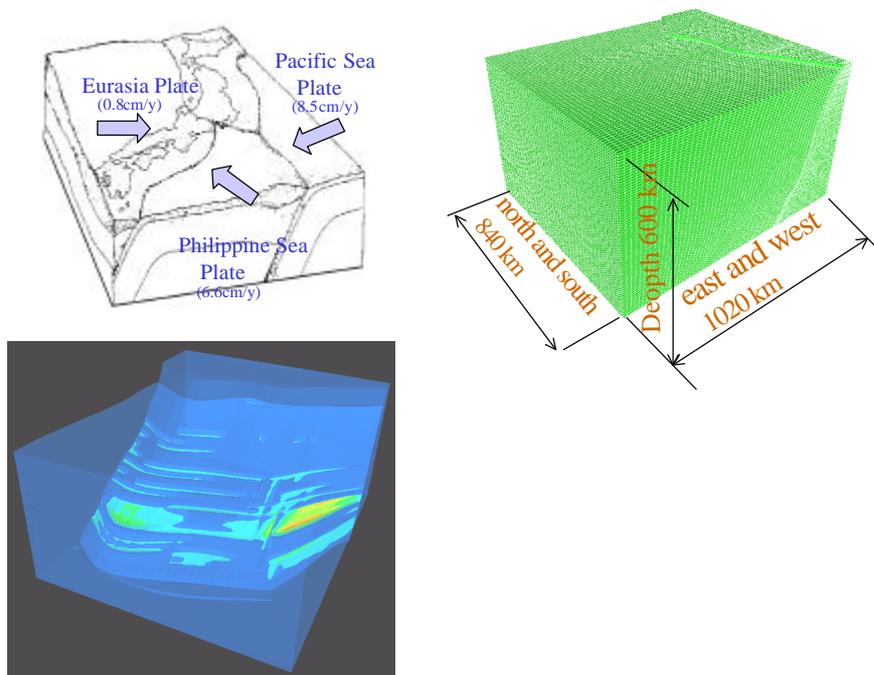


Figure 3 Three plates collision problem

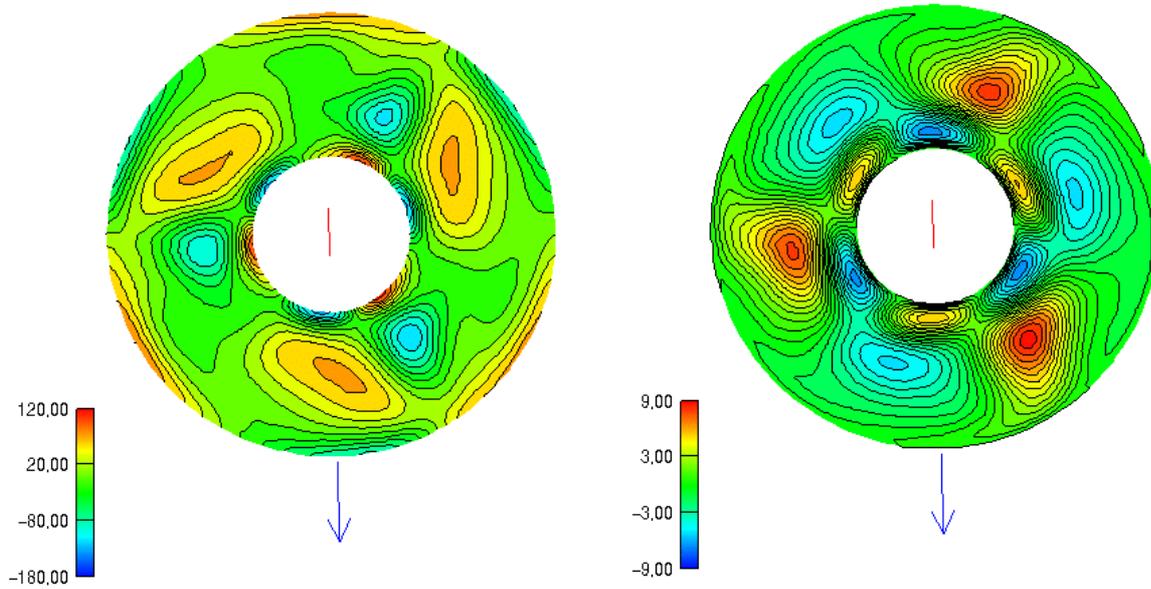


Figure 4 Z-component of vorticity (left) and velocity (right) on a cross section of $z=0.35$ at a quasi-steady state

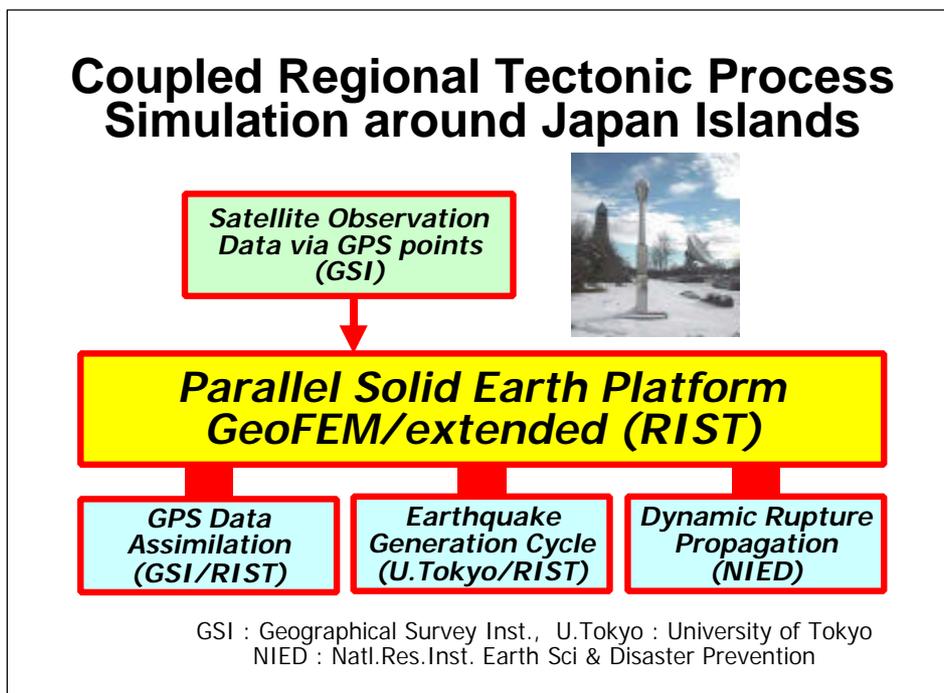


Figure 5 Framework for coupled regional tectonic process simulation around Japan islands