Development of high-performance parallel finite element system for solid earth - GeoFEM Project -

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Abstract

GeoFEM is a parallel finite element analysis system intended for multi-physics/multi-scale problems and is being developed at RIST. Within "Earth Simulator" project, the GeoFEM group will deal with the modeling and simulation of solid earth field phenomena, and the development of large-scale parallel software for the "Earth Simulator". Since there are models which are not completely established in the solid earth field, the simulation must be carried out on a trial and error basis. Therefore, a joint venture with the geoscience modeling research group is crucial for the development of a targeted simulation software system. This project is expected to be a breakthrough in bridging the geoscience and information science fields. When complete, this software system will be able to solve problems in the scale of 100 million degree of freedoms.

Introduction

In order to solve global environmental problems and to take measures against the natural disasters, the Science and Technology Agency aims to predict the global change by global observation, global change process research, and computer simulation. The agency began a five–year project from the fiscal year of 1997 to develop an "Earth Simulator[1]", which enables the forecast of various Earth phenomena through the simulation of "virtual Earth"placed in a supercomputer. The project is considered as one of the top priorities among our national scientific agendas and the research fee available amounts to 40 billion yen in that time span. It is also expected to be a breakthrough in bridging the geoscience and information science fields.

The specific research topics of the project are as follows:

1. Development of "Earth Simulator", a high performance massively parallel processing computer
2. Modeling of atmospheric and oceanic field phenomena and carrying out of high–resolution simulation
3. Modeling and simulation of solid earth field phenomena

4. Development of large–scale parallel software for the "Earth Simulator"

The "Earth Simulator" to be developed in 1 of the above, will be the fastest massively parallel computer in the world with about 40 TFLOPS of peak speed and about 5 TFLOPS of effective speed, which is about 1000 times faster in processing speed than the current supercomputers. In 2 of the above, modeling and processing of high–resolution simulation, including the advancement of the prediction technology of the global warming phenomena through the global coupling of atmosphere and ocean, will be aimed. Through the simulation, the project aims to forecast the regional climatic changes resulting from the influence of the global warming and to establish a one–kilometer–mesh meteorology, which will be able to reproduce the cloud activities and precipitation processes in three dimensions. In the field of geosciences mentioned in 3, the challenge for long–term prediction of the activities of the plate and mantle near the Japanese archipelago through the modeling and calculation of the solid earth analysis, including the dynamics and heat transfer inside the Earth, will be tackled. In case 4 of above, the development and research team will be formed in a way which is believed to accomplish the mission the best and a sophisticated parallel software will be developed on the "Earth Simulator" through the unification of the knowledge of earth science and information science.

The GeoFEM group deals with the topics 3 and 4 of above. Hence, a sophisticated parallel software system to be run on the "Earth Simulator" is to be developed to solve problems involving the solid earth, which will be discussed in the next section. The GeoFEM[2] system is a parallel finite element analysis system intended for multi–physics/multi–scale problems and is being developed at RIST, or Research Institute for Information Science and Technology. Since there are models which are not completely established in the solid earth field, the simulation must be carried out on a trial and error basis. Therefore, a joint venture with the geoscience modeling research group is crucial for the development of a targeted simulation software system. The overview of the GeoFEM will be reviewed in the following passages.

Problems in computational science involving solid earth

(1) Processing of large–scale distributed data

The mesh generation, including domain partitioning, has greater importance than ever before in calculation. It now becomes difficult to maintain a large–scale data as 1 domain data or even save it onto a hard disk because of massiveness. Domain partitioning greatly influences such factors as the amount of communication, load distribution, and convergence of the analysis algorithm. Furthermore, data modeling which can process various data formats such as the geological, CAD, FEM, visualization data, will become necessary.

(2) Massively large–scale parallel computation technology

In the field of engineering, a lot of experience has been gained concerning large–scale computation by the finite element method. However, a large–scale analysis of up to 100 million degree of freedoms in the earth science field is rare even in the field of engineering. Furthermore, a new problem such as developing a system where modeling to visualization must be carried out on the memory of the massively parallel processing computer in an single uninterrupted flow, arises.

(3) Multi–physics/multi–scale

As mentioned in the previous passage, in order to solve problems involving the solid earth, the system is required to include functions to run stress analysis, heat fluid analysis, and the coupled analysis of the two. Moreover, the system needs to take into consideration the vastness of the object to be analyzed, which are spatially, few to several thousand kilometers and seconds to millions of years, time wise. Currently, the problems involving different scales are separated into different problems. However, analysis which considers heat–chemical process at the boundaries of the outer layer behaving as a solid and inner earth behaving as a fluid, and heterogeneity is necessary.

(4) Visualization of large–scale unstructured grid data

Development of real time visualization and high–speed data transfer technology are necessary in appropriately processing huge calculation result. A method where I/O of the large–data are processed at high rate and real time visualization of the computational result are carried out even while it is still computing are the problem. Furthermore, a method for data reduction/extraction and parallel image processing are problems to be solved as well.

Grand design of the GeoFEM

The GeoFEM group is planning to develop the software system in the following 2 phases.

(1) GeoFEM/Tiger (1997–1998)

This phase involves the development of a multi–purpose parallel finite element software which may be applied to various scientific fields as well as becoming the basis for the "Earth Simulator"program to be developed in the next phase. A platform where various solid earth models may be read in a plug–in style, will be developed.

(2) GeoFEM/Snake (1999–2001)

A software system specialized in the simulation of solid earth phenomena through the use of GeoFEM/Tiger will be developed in this phase.

Objectives for GeoFEM/Tiger

(1) Analysis scale

The problems of up to 100 million degree of freedoms is to be solved.

(2) Physical phenomena to solve

The dynamics of the whole earth, which are mantle convection solved as heat–matter transfer phenomena of the viscous fluid will be simulated. Furthermore, the mechanical interaction between the crust and the mantle will be solved by modeling the plate as a shell and taking into consideration the coupling effect of the two. In the Japanese islands scale, the motion of the dislocation, buildup of tectonic stress, deformation of plates will be simulated by modeling them as elastic, viscoelastic and viscous fluid, etc. The simulation in the regional scale will involve solving of the seismic wave propagation.

Specifications for the GeoFEM/Tiger development environment

(1) Hardware environment

"Earth Simulator" will be composed of multi–pipelines connecting several thousand processing elements each with approximately 10 GFLOPS of processing speed. As a whole system, it is believed that approximately 30 TFLOPS of peak processing speed will be achieved. It is also believed that several terabytes of memory capacity will be necessary. However, until this "Earth Simulator" hardware is available, development of the software system will be carried out on the existing hardware platforms. When "Earth Simulator" does become available for use, then the software will be improved for higher level of accuracy.

(2) Software environment

Script language for the simulation software
For the main calculations, fortran90 will be implemented. Control parallelization by the use of MPI as the message passing library will be implemented. However, for visualization and special maintenance of the memory, this may not be the case.

Script language for the documents The design specifications for the source codes will be maintained in LaTeX.

Script for the interface between the subsystems
By providing the specifications for device–independent data transfer method, subsystems will be blocked from one another which will raise the level of independence at the time of the development.

System composition of GeoFEM/Tiger

The system will be composed of the subsystems and integrated environment. Each subsystem is on the assumption that they will be linked in the memory by the device–independent interfaces. The copying of data will be avoided because of the large–scale data and pursuit of high speed calculation.

(1) Partitioning subsystem

Graph partitioning is carried out based on the data from the large-scale complex CAD and mesh generator. The partitioning data, including the neighboring information, will be transferred to the other succeeding subsystems. Partitioning elementa and node wise, and overlapped subdomains will be taken into consideration.

Generally, partition with larger number of edgecuts lead to bad convergence. In GeoFEM, multilevel methods combined with Kernighan-Lin optimization heuristics are developed as a graphical partitioner for the complicated geometries.

(2) Structural analysis subsystem [3], [4]

Static or assumed time dependent algorithms will be used in the cases of linear elastic, viscoelastic, elastoplastic, large deformation, to be able to handle various analysis conditions. Contact analysis will be supported for the modeling of dislocations. Since the stiffness matrix is created locally and transferred to the solver subsystem in a form of a subroutine call, message passing is not apparent within the subsystem.

The structure analysis "sub-system" of GeoFEM deals with lithospheric motion analysis of earth's solidus behavior. Solid earth phenomena to be simulated by the GeoFEM system are the lithospheric plate motions and earthquake wave propagation problems. Large scale and complex nonlinearity must be considered in order to solve such a kind of problems. However, for the first order approximation, these problems may be solved with linear system of equations. Although an explicit method is usually adopted in the computation of the dynamic problems as in the latter, static techniques may be implemented by excluding the time integration scheme. At this stage, the largest problem solved by GeoFEM structure sub-system is with more than 100 million degree of freedoms on 1,000PE Hitachi SR2201 of University of Tokyo, either linear or dynamic problems.

On the other hand, solid earth has very complex dynamics, which have material nonlinearity, geometrical nonlinearity, time dependency and multi-phase dynamics. Furthermore, GeoFEM must also consider not only the continuum, but also discontinuum models as well. The discontinuum model will be implemented for the representation of the faults, which becomes a very complex contact problem.

(3) Thermal flow analysis subsystem

This subsystem will carry a function incompressible viscous flow analysis. Boussinesq approximation will be implemented for the temperature field and coupling. The dependence of physical values in relation to temperature, and heterogeneity of the media will be considered. As is with the structural analysis subsystem, this subsystem also creates stiffness matrix locally and transfers it to the solver subsystem, thus message passing is not apparent within this subsystem as well.

For example, mantle convection is the movement of various kinds of material as a result of higher temperature in the inner part of earth. In addition, various physical factors influence this mantle convection. Therefore, the mantle convection process is governed by sets of very complex nonlinear equations. These equations may be expressed using time, space and temperature dependent rheology or viscoelastic models. The present stage of the flow modeling "sub-system" of GeoFEM is carrying out of coupled heat and viscosity analysis by employing a parallelized FEM code. In the actual computation using the GeoFEM, large-scale numerical simulations of the natural convection flow will be approximated using a double sphere region to represent the inner structure of the earth.

(4) Solver subsystem [5]

In a large-scale scientific computing, linear sparse solver is one of the most time-consuming processes. In GeoFEM, various types of preconditioned iterative methods (CG, BiCGSTAB, GPBiCG, GMRES, TFQMR) are implemented on massively parallel computers. It has been well-known that ILU(0) factorization is a very effective preconditioning method for an iterative solver. But it has also been well-known that this method is globally dependent data-wise and this is not the optimal methodology on parallel computers where locality is of utmost importance. In GeoFEM, "Localized" ILU(0) preconditioning method has been implemented to the various types of iterative solvers. This method provides data locality on each processor and good parallelization effect. Convergence of iterative solvers are largely affected by partition.

(5) Visualization subsystem [6], [7]

Parallel image processing for the large-scale unstructured mesh data, including data reduction and extraction will be carried out in this subsystem. Image processing calculation will be held in a same phase as the analysis for real–time visualization. As one of the image output device, CABIN, a property of the Intelligent Modeling Lab of the University of Tokyo, will be implemented.

The subsystems (1) through (5) will be controlled using shells. Furthermore, different types of data such as the geographical, CAD, FEM and visualization data will be be managed using a data structure model to be developed. An object-oriented system configuration will be made possible by integrating the subsystems in a device independent fashion[8].

Concluding remarks

The overview of GeoFEM, a parallel finite element analysis system intended for the simulation of multi-physics/multi-scale problems involving the solid earth on an "Earth Simulator", was reported. GeoFEM/Tiger is a various objective parallel finite element software which is believed to become the basis in the parallel finite element analysis field by implementing new technologies to such factors as data structures, preconditioning under parallel environments, memory management to maximize the MPP calculations, parallel image processing of unstructured mesh data and object-oriented subsystem configuration.

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