ADVENTURE : AN OPEN SOURCE CAE SOFTWARE SYSTEM FOR LARGE SCALE ANALYSIS AND DESIGN IN PARALLEL AND GRID ENVIRONMENT

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Abstract. The ADVENTURE project started as one of the research projects in the "Computational Science & Engineering" field selected for the "Research for the Future" Program sponsored by the Japan Society for the Promotion of Science during 1997-2002. Since March 2002, the project has continued as an independent project. In the project we have been developing an advanced general-purpose computational mechanics system, named ADVENTURE, running in various kinds of parallel and distributed environment. The system was designed to analyze a three-dimensional finite element model of arbitrary shape with 10-100 million DOFs mesh, and additionally to enable parametric and non-parametric shape optimization. The first version of the system has been released from the project website as open source software since March, 2002. About 1,400 registered users in academia and industries have downloaded about 8,400 modules and been using them, while one company has developed and released its commercial version named ADVentureCluster.

The ADVENTURE system has been successfully implemented in various types of parallel and distributed environments including PC clusters, massively parallel processors such as Hitachi SR8000/MPP and the Earth Simulator, and Grid environments such as ITBL (IT-based Laboratory). The system has also been successfully applied to solve various real world problems such as response of full scale nuclear pressure vessel model and thermoelastic deformation of full scale electric mounting board of mobile PC.
1 INTRODUCTION

Various general-purpose computational mechanics systems have been developed in the last three decades to quantitatively evaluate mechanical / physical phenomena such as deformation of solid, heat transfer, fluid flow and electromagnetics. Nowadays such systems are regarded as infrastructural tools for the present industrialized society. The existing systems, however, can not be used effectively with massively parallel processors (MPPs) with the order of 100-10,000 processing elements (PEs), which are about to dominate the high-performance computing market in this century, as they were developed for single-processor computers. Neither can the current systems be used in heterogeneous parallel and distributed environments such as the Grid.

The ADVENTURE project [1,2] initiated as one of the research projects in the "Computational Science & Engineering" field selected for the "Research for the Future (RFTF)" Program sponsored by the Japan Society for the Promotion of Science (JSPS) [3] during 1997-2002. Since March 2002, the project has continued as an open source software development project. In the project we have been developing an advanced general-purpose computational mechanics system, named ADVENTURE, running in various kinds of parallel and distributed environments. The system was designed to analyze a three-dimensional finite element model of arbitrary shape with 10-100 million DOF mesh, and additionally to enable parametric and non-parametric shape optimization. The first version of the ADVENTURE system has been released from the project website [1] as open source software since March 2002. About 1,400 registered users in academia and industries have downloaded about 8,400 modules, and used them, while one private company has developed and released its commercial version named ADVentureCluster [4,5].

This paper describes latest development of the ADVENTURE system and some industrial applications.

2 OVERVIEW OF THE SYSTEM

2.1 Module-based Architecture

The ADVENTURE system consists of pre-, main- and post-processing modules and design modules that can be used in various kinds of parallel and distributed environments [1, 2]. The system employs a hierarchical domain decomposition method (HDDM) [6-8] based massively parallel algorithm as one of major solution algorithms in order to efficiently handle a large-scale finite element model over 10-100 million DOFs. The system employs module-based architecture and consists of 19 modules as shown in Figure 1. The pre-process modules include the Adve_CAD, the ADVENTURE_TriPatch, the ADVENTURE_TetMesh, the ADVENTURE_BcTool and the ADVENTURE_Metis. The ADVENTURE_CAD is a polygon-based CAD modeler which outputs a collection of triangular surface patches. The ADV_TriPatch is a surface patch generator which converts geometry model data into a collection of triangular surface patches. The ADV_TetMesh is a tetrahedral mesh generator [9]. The ADV_BcTool is an attachment tool of boundary conditions and material properties onto a mesh. The ADV_Metis is a domain decomposer of a finite element model. The kernels of the ADV_Metis are a graph partitioning tool METIS and its parallel version ParMETIS developed in the University of Minnesota [10,11]. The main process modules, i.e. solvers include an implicit elastic-plastic analysis module named ADVENTURE_Solid [7,8,12] which enables large-deformation and implicit dynamic
analyses, a thermal conductive analysis module named ADVENTURE_Thermal, a thermal-fluid analysis module named ADVENTURE_Fluid, a magnetic analysis module named ADVENTURE_Magnetic [13], an explicit impact analysis module named ADVENTURE_Impact, and a rigid plastic analysis module named ADVENTURE_Forge. The post process module named ADVENTURE_Visual is for parallel visualization of analysis results [14]. Common functions related to finite elements are programmed as class libraries named libFEM. Figure 2 shows one of typical large scale meshes, and Figure 3 shows its part decomposition.

2.2 Parallel Algorithms Implemented in ADVENTURE_Solid

A part of the key technology of the ADVENTURE_Solid is the HDDM, which enables parallel finite element calculations on various kinds of parallel and distributed environments [2,7,8,12]. Basically in the HDDM, force equivalence and continuity conditions among subdomains are satisfied through iterative calculations such as the Conjugate Gradient (CG) method. It is indispensable to reduce the number of iterations by adopting some appropriate preconditioning technique especially for solving large-scale ill-conditioned problems. The Balancing Domain Decomposition (BDD) based Neumann-Neumann (N-N) algorithm [15,16] is employed for this purpose. There are several researches on parallelization of the BDD and also the FETI (Finite Element Tearing and Interconnecting) [17-21]. However, most problems solved there are still medium scale such as sub-millions to one million DOFs. The DOFs of the coarse space problem in the BDD formulation is directly related to the number of subdomains, so that it is indispensable to parallelize the solution.
process of the coarse space problem as well when solving large-scale problems. The Salinas system [22], which employs the FETI-DP method [23], is succeeded in solving large-scale problems such as over 100 million DOF mesh of optical shutter model [22]. The BDD is employed together with an incomplete parallel direct method and the HDDM in the ADV_Solid [24].

2.3 Generalized I/O

As a part of the ADVENTURE system, we have developed a generalized I/O named the ADVENTURE_IO [25]. In general, characteristics of I/O data for large scale computational mechanics analyses are summarized as follows:

(1) data size is very huge,
(2) the data must be dealt with in various types of parallel and distributed environments,
(3) the number of data files tends to increase, and
(4) most of the data are of domain-decomposition type.

To efficiently handle such data with characteristics (1) to (3), we have developed "Media Independent Document" as a container of the data. To efficiently deal with domain-decomposition type data for various kinds of mechanics analyses, related to characteristic (4), we have also developed a generalized I/O format.

The Media Independent Document (simply called the Document here) can exist anywhere in a parallel and distributed environment, that is, memory or files on hard disks of computers connected through a network. The Document consists of the following two portions: the "Property" portion and the "Mass Data" portion. Stored in the Property portion are control data, the number of items stored in the Mass Data portion, labels and units of the data. The format of the Property portion is rather simple, i.e. key=value, where the value can be randomly accessed using the key. The Mass Data portion stores a huge amount of data such as nodal constraints, and connectivity of elements and analysis results in a binary format. These data can be accessed by several functions prepared in I/O libraries. The byte order of the binary data is unified to Little Endian. Different endian types among different operating systems are taken care of by the I/O libraries.

Various kinds of input data are required to pass through the domain decomposer, i.e. the ADV_Metis. To avoid complex specification for the domain decomposer, depending on different main modules, the model data other than the mesh are generalized in the following. The data used in a finite element analysis consist of a mesh, i.e. nodes and elements, and the data attached onto the mesh such as initial conditions, boundary conditions, material properties and analysis results. The latter data are attached to either nodes or elements. They can be abstracted in terms of the following eight general data types.

\[
\text{fega\_type} = (\text{All})?(\text{Node}|\text{Element})(\text{Variable}|\text{Constant})
\]

For example, "NodeVariable" type means that some different sets of data in the same format are attached onto several nodes. The eight kinds of generalized data types are called FEGA (Finite Element Generic Attributes). The FEGA is similar to the UCD (Unstructured Cell Data) format of the commercial visualization software, AVS. The ADV_Metis can process any kinds of finite element model data once they are specified with the FEGA.
2.4 Shape Optimization

Owing to the generalized I/O format and libraries, all the modules of the ADVENTURE system are easily integrated in several ways. Optimization calculations are easily performed by combining ADVENTURE's pre-, main- and post modules with Optimization modules. In the project, we have developed two kinds of design optimization modules. One is a module for parametric optimization, named the ADVENTURE_opt. The module implements various optimization algorithms including mathematical programming, gradient-based methods, simulated annealing, genetic / evolutionary algorithms. Users of the ADVENTURE system can easily employ their own optimization algorithms as well, replacing the ADV_opt.

The other is the non-parametric shape optimization module based on the traction method [26], which assures the smoothness of boundaries during shape varying processes. With this module, one can solve volume minimization problems of linear elastic continua under constraint on mean compliances with respect to given external forces.

3 COMPUTING ENVIRONMENTS FOR ADVENTURE

Taking the ADV_Solid as a typical example, we describe computing environments for the ADVENTURE system. The ADV_Solid has shown excellent performance not only on PC clusters consisting of scalar processors, but also on MPPs such as Hitachi SR8000/MPP consisting of 1,024 pseudo-vector processors without changing its code. As the results, the ADVENTURE system has been successfully implemented in the ITBL (IT-Based Laboratory) environment [27], which is one of Japanese National Grid Computing Projects [28]. The ADV_Solid has recently been implemented onto the Earth Simulator (ES) [29] with minor improvement of some functions for vector-type processors [24]. The ES is a massively parallel vector computer system of distributed memory type, and consists of 640 processing nodes (PNs) connected by 640 x 640 single-stage crossbar switches. Each PN has a SMP system with 8 vector-type processing elements (PEs), a 16GB main memory system, a remote access control unit (RCU), and an I/O processor. Peak performance of each PE is 8 GFLOPS. The ES as a whole consists of 5,120 PEs with 10 TB main memory, and thus its theoretical peak performance is 40 TFLOPS. The ADV_Solid is written in C, and has approximately 35,000 lines. The message communication between PNs and that between PEs are both supported by only MPI, i.e. Flat MPI style.

4 INDUSTRIAL APPLICATIONS

4.1 Elastostatic Analysis of ABWR Vessel Model with 35 Million DOFs on SR8000/MPP

This section first describes an elastostatic stress analysis for a precise model of an advanced boiling water reactor (ABWR) vessel with a 35 million DOFs unstructured mesh as shown in Figure 2. Figure 3 shows a part decomposition of the mesh. Size of fine elements placed in nozzle corners and internal pump junctions is about 2mm, while that of average elements is about 10mm. As boundary conditions, the bottom surface of its skirt portion is fixed, and a static gravitational force is applied to the vessel in the horizontal direction, imitating a seismic loading condition. Such a complex shaped and large-scale thin structure with less constraint often results in an ill-conditioned system matrix. In such a case, most iterative solution methods fail in attaining convergence.
However the ADV_Solid successfully overcomes this problem owing to the employment of the BDD-based preconditioner. The calculation is performed on Hitachi SR8000/MPP consisting of 1,024PEs whose theoretical peak performance is 1.8TFLOPS. In the analysis, the calculation is successfully converged with about 1,400 iterations in about 20 minutes. As this model is divided into about 30,000 subdomains, the number of DOFs of the coarse space becomes about 180,000. This coarse space problem is solved in only 30 seconds with the incomplete factorization based parallel direct method.

Figure 4(a) shows calculated stress distribution and enlarged deformation of the ABWR vessel subjected to the quasi-static seismic loading. Its calculation time is 1.5 hours. Figure 4(b) also shows the calculated stress distribution of the ABWR vessel subjected to hydrostatic internal pressure, imitating a hydrostatic pressure test. The calculation time is 1 hours. By solving a whole reactor vessel with a sufficiently large scale finite element mesh, various local stress concentration regions can be clearly indicated, and even stress values concentrated in local regions can be precisely evaluated, without employing other approximate methods such as zooming.

4.2 Elastostatic Analysis of Pressure Vessel Model with 100 Million DOF on the ES

The ADV_Solid is implemented on the ES consisting of 256 nodes, i.e. 2,048 PEs with 4TB of main memory, whose theoretical peak performance is 16 TFLOPS. The second problem is an elastostatic stress analysis of a simplified pressure vessel model with 100 million DOFs unstructured mesh. As a boundary condition, the bottom surface of the vessel is fixed, and a static gravitational force is applied to the vessel in the horizontal direction, being similar to the previous problem.

This problem is also successfully solved with the calculation speed of 5.1TFLOPS, which is 31.8% of the peak performance of the ES with 256 PNs [24]. The calculation time is only 8.5 minutes. The calculation time of the same problem by Hitachi SR8000/MPP with 1,024 PEs is 2.6 hours. Parallel ratio over 99.9% is achieved, and then parallel efficiency exceeds 80% not only for computation time per iteration but also for total computation time.
4.3 Thermal Stress Analysis of Electric Mounting Board of PC

The ADVENTURE_Thermal and the ADVENTURE_Solid are used to perform thermal stress analysis of an electric mounting board of mobile PC. Figure 5 shows its FE model with 6.4 million DOFs. Figure 6 shows its thermal stress distributions. Without any zooming technique, overall as well as local stress distributions are calculated precisely. It takes 30 minutes using a PC cluster with 24 Itanium2.

5 CONCLUSIONS

We have been developing an advanced general-purpose finite element analysis system, named ADVENTURE, which is designed to analyze a model of arbitrary shape with a 10-100 million DOF mesh. The first version of the ADVENTURE system has been released from the project website as open source software. The ADVENTURE system has been successfully implemented on a single PC, PC clusters, and massively parallel processors such as Hitachi SR8000/MPP and the Earth Simulator, and Grid environments. Some industrial applications clearly show practical performances of the ADVENTURE system. All the information on the ADVENTURE system is available on the project website [1].
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