Technical Report of
ADVENTURE Project
ADV-99-1 (1999)

OVERVIEW OF ADVENTURE PROJECT

- Development of Computational Mechanics System for Large Scale Analysis and Design -

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1 BACKGROUND & OBJECTIVES

Most critical issues in the 21st century include understanding of global scale phenomena towards appropriate actions for global environmental problems, risk reduction caused by natural disasters as well as accidents of complex large systems, and the production of novel artifacts for welfare. In order for any of these issues, it is strongly required to predict behaviors of natural things or artifacts accurately, and design, control and operate them appropriately based on the prediction.

Various general-purpose computational mehanics systems have been developed in the last three decades to quantitatively evaluate natural phenomena such as deformation of solids, 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 with massively parallel processors with the order of 100-10,000 PEs, which are expected to dominate the high-performance computing market in the 21st century, as they were developed for single-processor computers, which took leadership an age ago. Neither the current systems can be used in heterogeneous parallel and distributed computing environments. Owing to the fact, they can deal with only medium scale problems with millions degrees of freedom (DOFs) at most.

In the ADVENTURE project, we will develop an advanced general-purpose computational mechanics sytem which can analyze a model of arbitrary shape with 10 to 100 millions DOFs within 1 hour to 1 day using the world's fastest computer with 30-100 TelaFLOPS in 2002, and which additionally enables optimal and satisfactory design.

To efficiently deal with such an ultra-large scale model, massively parallel algorithms are embedded in the pre-, main as well as post-processes. Neural networks, fuzzy set theory, genetic algorithms and virtual reality then enable ideal user-friendliness. In addition, an object-oriented design and programming method is employed such that new theories and algorithms can be easily implemented for a variety of heterogeneous parallel and distributed environments. This allows us to improve the prediction of behaviors of natural things and artifacts by two to three orders and to further design and operate them.

2 OVERVIEW OF JSPS RFTF PROJECT

The ADVENTURE project is one of the following seven research subprojects in the "Computational Science and Engineering (CS&E)" field selected for the "Research for the Future (RFTF) Program" sponsored by The Japan Society for the Promotion of Science (JSPS).

- Computational Science and Engineering for Global Scale Flow Systems
  - (Models and Numerical Algorithms)
  - (Large-scale Numerical Simulation)
- Development of Next-generation Massively Parallel Computers
  - (Massively Parallel Computers for Continuous Physical Systems)
  - (Massively Parallel Computer for Particle-based Simulations)
- Material Science Simulation for Future Electronics
- Development of Computational Mechanics Systems for Large Scale Analysis & Design (ADVENTURE Project)
- Development of Simulation Algorithms for the First-principles Prediction of Three-dimensional Structures of Proteins

These projects starded in August, 1997, and are scheduled to finish in March, 2002.

As the world prepares to cross the threshold into the 21st century, JSPS has launched a new, farsighted program entited "Research for the Future (RFTF)". This program, which started in 1996, is funded through capital investment made by the Japanese government to promote and expand the frontiers of scientific research.

It is very important in the fields of science and engineering to recognize, comprehend, predict and design the complicated nonlinear behavior of natual and artificial systems with very high degrees of freedom. To commence these studies with the fundamental and governing rules as known in simpler and smaller scales, it is indispensable to make a series of large scale computing. It is therefore an urgent need to develop a software basis that lays emphasis on the research and development of the architecture and algorithm corresponding to the problems. This project does aim at more advanced R & D based on the distinguished results achieved in Japan.

The computational science and engineering (CS&E) means a scientific measure to delve into a wide variety of scientific and engineering phenomena in space using high-speed computers. In reality, many researches are being made with computational approaches in almost all the domains of science and engineering. Here we will set the following critical issues considered to represent CS&E.

(1) The computational speed is to be increased by one to two orders in coming five years over the present highest speed teraflops class computers. They shall be used for general purpose too.
(2) Development of a software for large scale engineering design that enables to incorporate readily new findings.
(3) Development of an application of effective algorithm to such massive problems as global scale, material and proteins analyses that cannot be solved by any experimental approaches.

3 PROJECT OVERVIEW

The ADVENTURE system is being developed mainly based on the achievements by the research members listed in Table 1.

Various massively parallel algorithms are developed and implemented in pre-processes (mesh generation and hierarchical domain decomposition), main processes (system matrix assembling and solutions) and post-processes (error evaluation and visualization). The hierarchical domain decomposition method with an iterative solver, which realizes excellent parallel performance over 90 % owing to a dynamic work load balancing feature [Yagawa et al., 1993 ; Yagawa and Shioya, 1993], is adopted in the main processes. Softcomputing technologies such as neural networks, fuzzy set theory, genetic algorithms, virtual reality are effectively utilized to achieve ultimate user-friendliness. Object-oriented design and programming approaches for system integration are utilized to realize excellent portability, extensibility and maintainability, so that new theories and algorithms will be easily implemented, and the system will operate in various heterogeneous computing environments.

The planned schedule during 1998FY-2001FY are summarized as follows.

- During 1998FY-1999FY, the prototype systems and modules are developed for pre-, main and post-processes which can solve elastostatic stress problems with arbitrary shape using a 10 million DOF model, and nonlinear or time transient stress problems using an one-million DOF model.
- During 2000FY-2001FY, the prototype systems and modules above will be integrated into one system. The sizes of target problems will increase by one order, i.e. 100 million DOFs for elastostatic problems, and 10 million DOFs for nonlinear or time transient problems.
- In 2002FY, the system will be tested and its development is scheduled to be completed, and its user's manual will be prepared.

4 SYSTEM OVERVIEW

Figure 1 shows a conceptual image of the ADVENTURE system operating in a heterogeneous parallel and distributed computing environment. Its main features are summarized below.

4.1 Preprocesses

Geometry models with specific boundary conditions and material properties are automatically imported to mesh generation modules. Tetrahedral / hexahedral meshes of 100 million DOFs are generated fully automatically. As for the tetrahedral meshes, the fuzzy knowledge processing is utilized to well control node density distribution over an analysis domain with arbitrary shape, the bucketing method is used to generate nodes which meet the specified node density distribution, and the Delaunay method is used to generate tetrahedral elements [Yagawa, Yoshimura et al., 1992 ; Yagawa, Yoshimura et al., 1993]. Computation speed for both the bucketing and Delaunay methods is proportional to the number of nodes. Massively parallel algorithms are developed and implemented for the node and element generation to efficiently deal with large scale meshes of 100 million DOFs with respect to computation speed as well as memory requirement. In the hexahedral mesh generation, we adopt the Intelligent Local Approach (ILA) which imitates human expert's mesh generation techniques by using the fuzzy knowledge processing and the object-oriented approach [Yoshimura, Wada and Yagawa, in Print]. A new hierarchical domain decomposer is developed based on METIS and ParMETIS, both of which are graph partitioning software developed in the University of Minnesota [Karypis and Kumar, 1997], in order to convert a large scale FE mesh of 100 million DOFs into a hierarchical domain decomposition data structure which is compatible to the hierarchical domain decomposition method (HDDM) described subsequently. Massively parallel algorithms are also implemented in the present domain decomposer.

4.2 Main processes

The hierarchical domain decomposition method with an iterative solver is mainly employed [Yagawa et al., 1993 ; Yagawa and Shioya, 1993]. An excellent feature of dynamic load balancing on massively parallel processors with hundreds to thousands processing elements (PEs) is attained by the client-server model combined with a hierarchical domain decomposition data structure. Here all PEs are assigned to one grand father PE, several father PEs, and many child PEs. An elastostatic stress analysis using a model of arbitrary shape with 10 to 100 millions DOFs will be solved within 1 hour to 1 day using the world's fastest computer with 30-100 TelaFLOPS in 2002. One million to 10 million DOF models will be applied for nonlinear or time transient stress analyses, i.e. elastic-plastic, large deformation, vibration, impact, and contact problems.

4.3 Post processes

10 million DOF problems require 300-600MBytes to store the mesh, and their analysis results require 3 to 10 times more memory. The results of time transient analyses require several hundreds to thousands times more memory. 100 million DOF problems require 3-6GBytes to store the mesh. Massively parallel algorithms are thus indispensable in the post process of such ultra large scale problems to attain sufficient computation speed as well as memory storage. In the present project, we adopt the virtural reality system CABIN, which is built in the Intelligent Modeling Laboratory (IML) of the University of Tokyo [Yagawa et al., 1996]. We also develop an internet-based interface for the ADVENTURE system, with which a user can easily access to the system from remote PCs in the world.

4.4 Developing and operating environment

In the ADVENTURE project, C and C++ are fundamental programming languages to build the pre-, main and post-processing modules. MPI is utilized for communication among processors. PVM is partially used during the developing stage. Operating system employed is Unix or Linux. OpenGL and VRML are adopted to deal with graphical data. GUI is developed for Windows NT. These developing and operating environments are selected so as to realize portability among various heterogeneous parallel and distributed computing environments. The ADVENTURE system can also utilize worldwide computer resources connected among others through the Internet (Shioya, Yagawa and Takubo, 1997).

The project will also develop the ADVENTURE framework as a general platform for any pre-, main-, post- and design-modules to run in a heterogeneous distributed and parallel environment. With this framework, one can easily perform various types of coupled analyses and optimization analyses.

This report summarizes main results obtained during April 1, 1998 - March 31, 1999.

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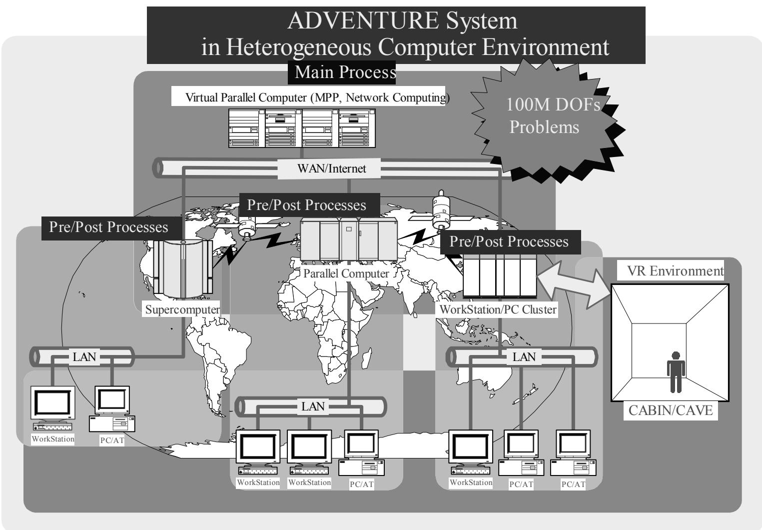

Figure 1 Conceptual Image of ADVENTURE System

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