Development of the Next-generation Computational Solid Mechanics Simulator for a Virtual Demonstration Test

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We have been developing an advanced general-purpose computational mechanics system, named ADVENTURE, which is designed to be able to analyze a three-dimensional (3D) finite element model of arbitrary shape with a 10-100 million degrees of freedom (DOF) mesh. Module-based architecture of the system with standardized I/O format and libraries are developed and employed to attain flexibility, portability, extensibility and maintainability of the whole system. Domain-decomposition-based parallel algorithms are also implemented in pre-processes (domain decomposition), main processes (system ma-trix assembling and solutions) and post-processes (visualization), respectively. The hierarchical domain decomposition method with a pre-conditioned iterative solver (HDDM) is adopted in the main processes as one of the major solution techniques. The main processes is successfully applied for complex models analysis over millions DOF with effective performance on Hitachi SR8000/MPP consisting of 1,024 processing elements (PE). This report describes some key technologies employed in the system, and shows some results including elastic stress analysis of a precise 3D model of a nuclear reactor vessel with a 100 million DOF mesh on Earth Simulator (1,024PEs).

Keywords: CAE System, Parallel Finite Element Analysis, Hierarchical Domain Decomposition Method, Balancing Domain Decomposition

1. ADVENTURE system

The ADVENTURE system[1] has employed a hierarchical domain decomposition based massively parallel algorithm as one of the major solution algorithms in order to efficiently handle a huge-scale finite element model with 10-100 million DOF. We have been developing several kinds of main processes for implicit elastic-plastic analysis, rigid-plastic analysis, impact-contact analysis, thermal conductive analy-sis, thermal-fluid analysis and electromagnetic analy-sis. Especially, the implicit elastic-plastic analysis module, named ADVENTURE_Solid, is improved to apply to massively parallel processors (MPP) with over 1,000 PEs and successfully to analyze a simplified pressure vessel model with 100 million DOF mesh[2]. The ADVENTURE_Solid module is applied and tuning for the Earth Simulator.

2. HDDM

In domain decomposition methods (DDM), an analysis model, i.e., a finite element mesh with boundary conditions and material properties, is subdivided into a number of subdomains. We proposed a hierarchical technique to implement the DDM on MPP[3]. This technique was named the HDDM.

In this method, a group of PEs are subdivided into three sub-groups: one Grand Parent PE (Grand Parent), several Parent PEs (Parent/Parents) and many Child PEs (Child/Children). For implicitly solving the linear algebraic equations derived from FEM, a simple substructure-based conjugate gradient (CG) method (the primal substructuring method) is adopted. It was reported that the convergence property of this method is not so good compared with the dual substructuring methods such as the finite element tearing interconnection (FETI), especially when solving ill-conditioned problems such as large-scale thin structures with less constrains[4]. To solve this problem, we employed a pre-conditioner named balancing domain decomposition (BDD) into the HDDM[5,6].

Fig.1 shows the schematic data flow among the three groups of PEs. An analysis model is also subdivided into several "parts" whose number is the same as the number of Parents, and then each part is subdivided into a number of subdomains. Fig.2 shows an example of hierarchically decomposed mesh for ABWR (Advanced Boiled Water Reactor) model. Each Parent stores in its memory a set of the part data, i.e., a number of sets of subdomain data. Each subdomain data includes coordinates of nodes, connectivities of elements, material properties and
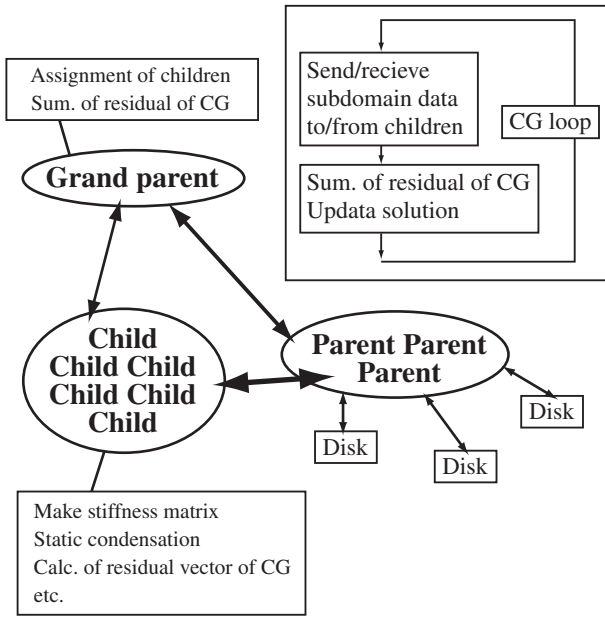
Fig. 1 Flow of HDDM for elastic-plastic analysis.

Fig. 2 Parts of ABWR model.

information on subdomain interfaces. In nonlinear analysis of solid, stresses and displacements are stored in the Parents as well. As a result, large-scale analysis data can be easily handled by increasing the number of Parents.

The design concept of the HDDM architecture is suited to a shared memory architecture as well as distributed memory. On the Earth Simulator which is structured as SMP clusters, the HDDM is expected a good performance, e.g., arrange one Parent and seven Children in one node consisting of eight processing units. However, in this architecture, it is necessary to communicate Parent with Child. To assign all processors as Parent, i.e., all PEs stores a set of part data and analyze of subdomains in own part, it can reduce communications and expect high parallel efficiency.

3. Tuning for ES and numerical results

In DDM for an analysis of solid, there are three main works as follows: (1) the LDL factorization of subdomain's coefficient matrices (SKY_Decomposite), (2) the forward elimination and the back substitution of linear equations (SKY_MkSolution), and (3) the matrices multiplication by a vector (skysl1_addmultvec). We vectorized these functions selectivity. Table 1 shows the results of FTRACE, floating operations per seconds (FLOPS), vector operation ratios (V.OP RATIO) and average of vector length (AVER. V.LEN) in the original codes applied to a model with about 23,000 DOF. As the original codes are programmed for the scalar processor, V. OP RATIO stays on low level and AVER. V.LEN are short because the choice of the number of subdomain is also for scalar processor.

We improved the codes as following policy: to be simplified for easy compiling, to be accessed an array continuity in the most inner loop, and to be unrolled the outer loop by 3 times because each node has 3 DOF in our target problems. And for AVER. V.LEN, we can get a good loop size by decreasing the number of subdomains. Table 2 shows the results of FTRACE

Table 1 FTRACE in the original codes

function name	MFLOPS	V.OP RATIO	AVER. V.LEN
skysll_addmultvec	657.0	93.59	26.3
SKY_MkSollution	775.5	93.66	134.0
SKY_Decomposite	457.6	91.45	123.0

Table 2 FTRACE in the improved codes for the vector processor

function name	MFLOPS	V.OP RATIO	AVER. V.LEN
skysll_addmultvec	3,189.2	**98.55**	202.9
SKY_MkSollution	2,247.3	**98.07**	199.2
SKY_Decomposite	2,041.2	**98.68**	203.2

Table 3 Performances of 100 million model with 64 nodes and 128 nodes

	Time	Memory	FLOPS	V.OP RATIO
64 nodes (512PEs)	1,742.9 sec	608GB	**1.08 T**	**98.1 %**
128 nodes (1,024PEs)	959.6 sec	605GB	**1.90 T**	**98.0 %**

in the improved codes for the same problem. It shows good performances as the over 25% performance to peak FLOPS and the over 98% performance to vectorization.

This system is applied to a simplified pressure vessel model with 100 million DOF mesh using 64 nodes (512PEs) and 128 nodes (1,024PEs). As boundary conditions, bottom plane is fixed and body force by the gravity is taken. Table 3 shows the performances with 512 and 1,024 PEs. The present system with BDD pre-conditioner is successfully to analyze with good performances in FLOPS and vectorization, and the parallel efficiency shows 99.978 % in 128 nodes. It is impossible to solve such a large model with usual general linear solvers.

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次世代固体力学のためのバーチャル実証試験

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　既に多くの超並列計算機やPCクラスタ上において実績を示している、1億自由度級の大規模メッシュを用いた人工物、自然物の丸ごと詳細解析を可能とする汎用計算力学システムADVENTUREを地球シミュレータに導入し、数億自由度規模の有限要素メッシュを用いた非定常非線形解析を実用時間で可能とする技術の確立を目指す。本システムでは、超大規模解析における優れた実行性能、拡張性・保守性・開放性に重点を置き、モジュール型システム・アーキテクチャを採用しており、各モジュールは独立したプログラムとして単独でも、また標準化されたI/Oを介して他のモジュールと協調しても稼動する。主要並列ソルバーの1つとしてBDD前処理付きCG法を用いた階層型領域分割法（HDDM）を開発し、様々な並列分散環境下への高効率での適用を可能としている。ベクトル型プロセッサを備えた地球シミュレータでの最適化を行い、1億自由度規模の非構造メッシュを用いた簡易原子炉圧力容器モデルの静応力解析に成功し、1,024プロセッサで実行性能23.75%（1.90TFLOPS）、並列化率99.978%を示した。

キーワード：CAEシステム、並列有限要素解析、階層型領域分割法、バランシング前処理