Development of the Next-generation Computational Fracture Mechanics Simulator for Constructing Safe and Sustainable Society

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The authors have been developing a crack propagation analysis system that can deal with arbitrary shaped cracks in three-dimensional solids. The system is consisting of mesh generation software, a large-scale finite element analysis program and a fracture mechanics module. To evaluate the stress intensity factors, a Virtual Crack Closure-Integral Method (VCCM) for the second-order tetrahedral finite element is adopted and is included in the fracture mechanics module. The rate and direction of crack propagation are predicted by using appropriate formulae based on the stress intensity factors. Combined with ADVENTURE system, a large-scale fully automatic fracture analysis can be performed on ES2.

Keywords: fracture mechanics, crack propagation analysis, finite element method, domain decomposition method, aging structure

1. Introduction

For the realization of sustainable society in the 21 century, assessment of gradually aging social infrastructure is becoming important. Fracture analysis has been one of the key numerical simulation for such problems. However, a three dimensional crack analysis of a real world, highly complicated structure has not been widely used yet, because of many obstacles including the lack of computational power.

The authors have been developing an open-source CAE system, ADVENTURE [1]. It is based on the hierarchical domain decomposition method (HDDM) with the balancing domain decomposition (BDD) pre-conditioner [2]. A general-purpose structural analysis solver, ADVENTURE Solid is one of the solver modules of the ADVENTURE system. It runs on The Earth Simulator (ES1) with a large scale model hundreds of millions of degrees of freedom [3, 4]. It can achieve vectorization ration 98%, parallel performance 70% (256 nodes) and 25% of the peak performance using an unstructured grid.

On the other hand, we have also been developing a system to support a three dimensional fracture analysis, especially a fatigue or SCC propagation analysis with many cracks of arbitrary complicated shape and orientation. To integrate the large scale structural analysis code with this fully automatic fracture analysis capability, a direct fracture simulation of a highly complicated realistic aging structure with explicit modeling of cracks.

In this year, we conducted mainly two tasks, porting of automatic fracture analysis system on ES2 and performance tuning of ADVENTURE Solid for ES2.

2. Development of automatic fracture analysis system based on VCCM

Most of the fracture analyses have been performed by using the hexahedral finite elements. It takes an enormous amount of manual labor to generate a finite element model for a complex shaped three-dimensional structure with hexahedral finite elements. Thus, methodologies such as element free Galerkin method (EFGM), s-Version finite element method (s-FEM) and eXtended finite element method (x-FEM) were proposed to obviate the processes of mesh generation and were applied to the fracture mechanics problems.

Recently, Okada et al. [5, 6] have developed a virtual crack closure-integral method (VCCM) for tetrahedral finite elements. Based on the VCCM, an analysis system to perform crack propagation analysis system is being developed by present authors. The system is consisting of automatic mesh generation software, a large-scale finite element analysis program and a fracture mechanics module to evaluate the stress intensity factors by using VCCM. When crack propagation analysis is performed, the rate and direction of crack propagation need to be predicted by using appropriate formulae based on the stress intensity factors. Mesh generation software that is a part of ADVENTURE project [1] is extended so that models with cracks can automatically be created. The cracks are regarded as local features in the three-dimensional analysis model ("local model"). They are inserted in an existing finite element model ("global model") without any cracks. Thus, the geometry representation of the structure is unchanged even though the shapes and the sizes of the cracks change as they grow. The crack models are represented by a number of nodal points and they are inserted in the global model. Hence, Delaunay triangulation technique is appropriately applied to generate the finite element mesh with the tetrahedral elements.

The crack propagation analysis system is consisting of parts/modules/programs for 1) model and crack geometry definition, 2) automatic finite element mesh generation with the second order tetrahedral finite elements, 3) finite element analysis using a parallel PC cluster, 4) evaluation for the stress intensity factors by using the virtual crack closure-integral method (VCCM) and 5) predictions for the direction and rate of crack propagation when the crack propagation analysis is performed, as depicted in Fig. 1.

First, the global model that has geometry information of the problem as whole is generated. This is called "base mesh". Only nodal point information of the base mesh is used to generate the crack model. The crack is inserted in the dense mesh region.

Second, the local model for the crack is generated. The procedures of generating the crack model are (1) defining the geometry of crack, (2) assigning the locations of nodal points in the plane of crack so that the model requirements for the VCCM computation is satisfied and (3) staking all the nodal points for the crack in the vertical direction. Nodal points are inserted in the base mesh and a finite element model consisting of second-order tetrahedral finite elements is generated by using the Delaunay triangulation technique. Points with blue and red colors are those on the crack face and those at the crack front.

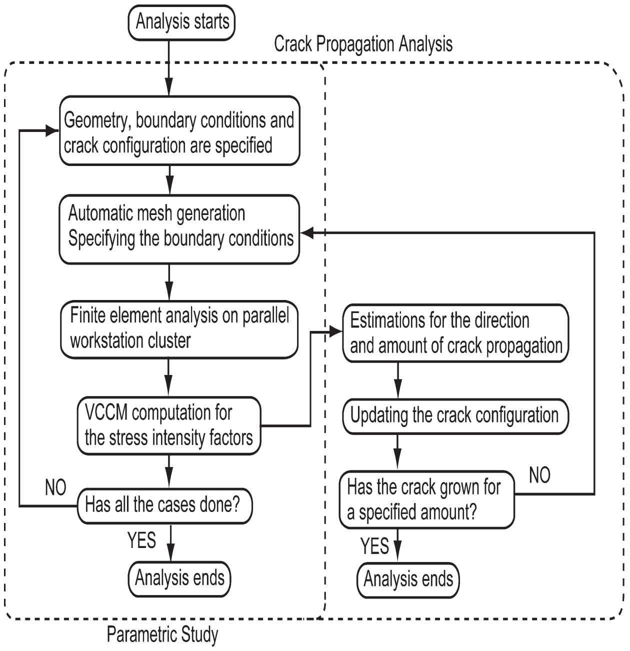

Fig. 1 Crack propagation system (programs and modules).

As an example, a fatigue crack in a circular bar subject to torsion is considered. The stress intensity factors are evaluated along the crack front. The kink angle and the rate of crack propagation are computed.

Finite element mesh for the initial state is shown in Fig. 2. It has a total of about 690,000 nodes and 500,000 elements and the numbers increase as the crack grows. The total numbers of nodes and elements after 15 steps of crack propagation were about 1,120,000 and 800,000, respectively. The growth of crack is shown in Fig. 3.

3. Performance Optimization of ADVENTURE Solid

As a programming style on a vector-type supercomputer such as ES1, ES2 and NEC SX-series, the length of an inner-most loop should be long enough to achieve high performance. On ES1, ADVENTURE Solid had an enough vector loop length to obtain roughly 30 - 40% of peak performance. However, on the new supercomputer, ES2, the vector loop length to obtain good enough vector performance on the current ADVENTURE Solid code has increased. As a result, peak performance ratio dropped to 4 – 5% with the current code. We planned a major revision of ADVENTURE Solid, so that it can regain a good enough vector length on ES2. To investigate the design detail, first we studied performance characteristics of ES2 in the context of the finite element method and the domain decomposition method.

ADVENTURE Solid is based on the hierarchical domain decomposition method (HDDM). In HDDM, a whole analysis domain is subdivided into many small subdomains. The parallelization of ADVENTURE Solid code is primarily based on subdomain-wise FEM calculation. On the FE analysis of each subdomain, a linear system of the subdomain stiffness matrix is solved. A skyline solver is employed for the solution of the relatively small system. In the current version of ADVENTURE Solid, this subdomain-wise skyline solver is identified as a hot spot. The inner-most loop of the hot spot is the double loop in forward and back substitution of the skyline solver. Its loop length, which means the band width of the skyline matrix, is not so large. It is usually about several hundreds.

To increase the vector loop length at the hot spot of ADVENTURE Solid, we tried an approach to move the loop over subdomains, which was located at outer-most, into the inner-most place. Then, the load balance issues among subdomain FEM calculation become important. In case of a large scale model, there can be tens of thousand of subdomains in total. Per processor, the number of subdomains is about 500 - 1000. Through the performance study on ES2, this number was found to be enough to achieve high vector performance.

If the inner-most loop is driven by the number of

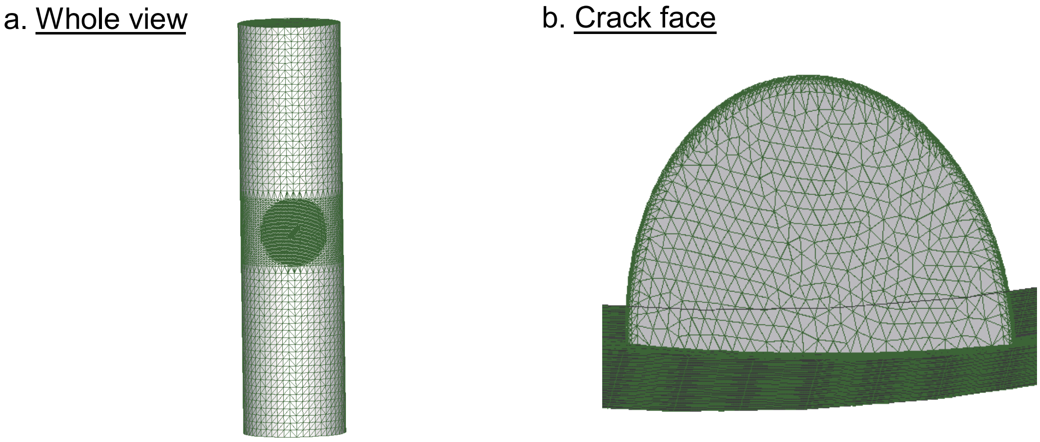

Fig. 2 Finite element mesh for the initial state.

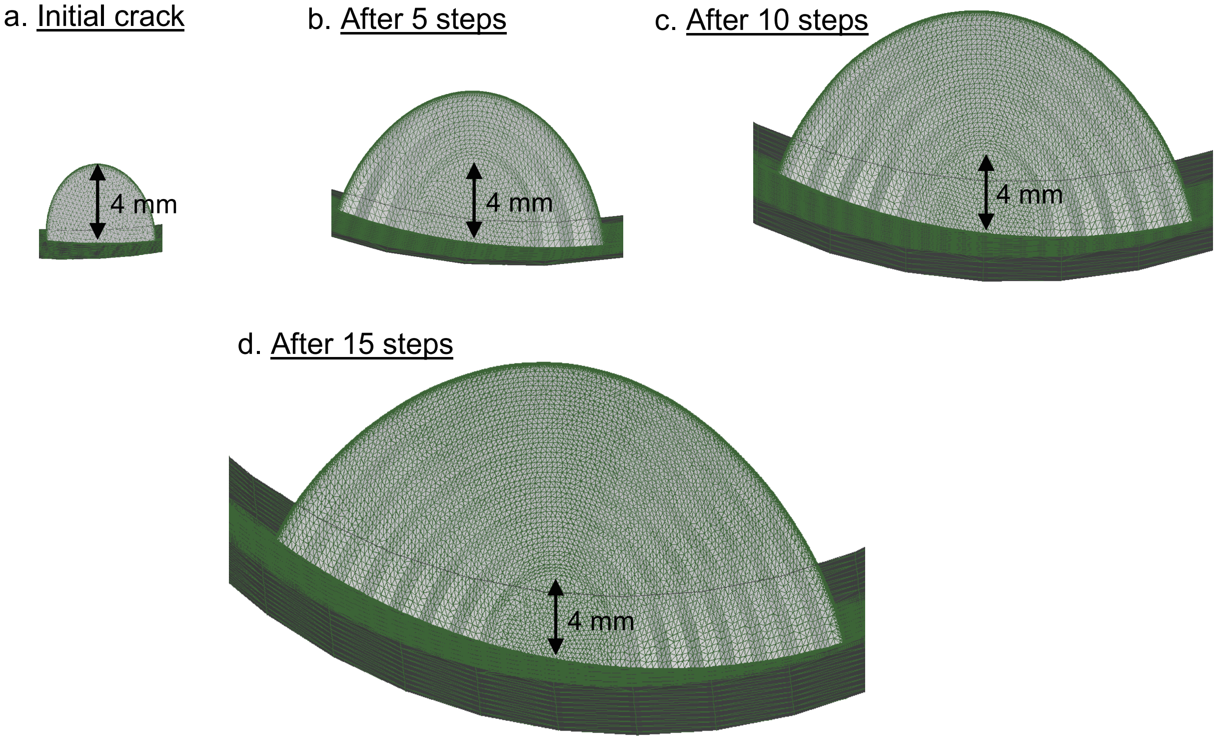

Fig. 3 Evolutions of crack face of the problem of circular bar subject to torsion.

subdomains, computational loads among subdomains should be evenly distributed. Although the domain decomposition process with METIS produces the relatively flat distribution of subdomain size, there are still some differences in mesh subdivision.

There can be two ways to implement this strategy on HDDM. One is to keep the skyline solver and just insert the subdomain-wise loop inside the skyline solver. In this case, load inbalance may be much larger, because the difference of the skyline band width among subdomains may be bigger than the mesh size itself. The other approach is based on explicit evaluation of the local Schur complement of DDM for each subdomain. In this case, the local Schur complement matrix is a symmetric dense square matrix. Although the computational cost increase slightly compared with the skyline approach, the latter approach is much simpler and it can obtain better vector performance. In this work, we have chosen the latter, local Schur complement approach.

According to the performance measurement on ES2 of a prototype code, which is a hot-spot of ADVENTURE Solid, about 37 G flops is achieved using single processor. It is near 40% of the peak performance per single processor, 104 G flops. In detail, the hot spot code is basically a matrix vector product for each subdomain. The matrix is a local Schur complement. It is dense and symmetric. The two outer loops are unrolled in 5 by 5. Also, because the matrix is symmetric, the code is tuned to reduce memory access. With the vector length over 500, near optimum performance has already been achieved. If it is 200, the performance number dropped 20%.

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安全・安心な持続可能社会のための次世代計算破壊力学シミュレータの開発

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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や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をもちいて、実用大規模構造材料・機器の直接破壊シミュレータをES2上で開発し、低炭素社会構築のカギを握る小型高圧水素貯蔵タンクの超精密破壊解析や、安全・安心社会の基盤である経年化した社会的インフラストラクチャーの超精密破壊解析を通して本技術の確立を目指すことにより、21世紀の持続可能社会の構築に寄与することを目的としている。

今年度は保有システムを統合した三次元き裂進展解析システムの構築並びにES2への移植を行うことを目指し、試験片レベル（～100万節点）の三次元完全自動疲労き裂進展解析を行うためのプログラム群を整備し、完全自動疲労き裂進展解析を可能とした。なお、複数き裂問題の試行にも成功した。また、四面体有限要素用三次元J積分プログラムについて、領域積分法に基づく四面体有限要素のための実装方法の検討とそのプログラム実装を行い、マップドメッシュモデルでは六面体要素による結果と同等であることを確認した。さらに、並列有限要素法アルゴリズムのES2向け改良による線形問題計算の高速化のためのアルゴリズムにより、単一プロセッサにおいてピーク性能比約30%を達成した。本システムを用いて、16ノード上でのき裂入り1,700万自由度規模簡易モデルの応力解析を実現した。

キーワード: fracture mechanics, crack propagation analysis, finite element method, domain decomposition method, aging structure