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

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Our project aims to develop a crack propagation analysis system that can deal with arbitrary shaped cracks in three-dimensional solids. The system is consisting of mesh generation software for crack propagation, a large-scale finite element analysis program and a fracture mechanics module. The fracture mechanics module is based on Virtual Crack Closure-Integral Method (VCCM) for the quadratic tetrahedral finite element to evaluate the stress intensity factors. The rate and direction of crack propagation are predicted by using appropriate formulae based on the stress intensity factors, and new shape of linked-up crack is generated when some propagated cracks get closer. Combined with ADVENTURE system, a large-scale fully automatic fracture analysis can be performed on Earth Simulator 2.

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

1. Introduction

To realize sustainable society in the 21 century, structural integrity assessments for gradually aging social infrastructures are increasingly gaining their importance. Fracture mechanics simulation will be one of the key numerical methodologies for the structural integrity assessments. However, three-dimensional crack analyses for realistic highly complex structures have not widely been used so far, because of many obstacles such as 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] [3]. A general-purpose structural analysis solver, ADVENTURE Solid, is one of the solver modules of the ADVENTURE system. On the other hand, the authors have been developing a fracture mechanics analysis system that can deal with arbitrary shaped cracks in three-dimensional structures. The system consists of mesh generation software, a finite element analysis program and a fracture mechanics module. In our system, a Virtual Crack Closure-Integral Method (VCCM) for the quadratic tetrahedral finite elements [4] is adopted to evaluate the stress intensity factors. This system can perform the three-dimensional fracture analyses. Fatigue and SCC (stress corrosion cracking) crack propagation analyses with more than one cracks of arbitrary complicated shapes and orientations. The rate and direction of crack propagation are predicted by using appropriate formulae based on the stress intensity factors.

In this year, we developed new mesh generation module to generate new crack face that integrated 2 closest cracks, and compare performances between the Earth Simulator 2 and the K computer.

2. Overview of VCCM

VCCM for the quadratic tetrahedral elements that is proposed by Okada et al. [4] is adopted for the computations of the stress intensity factors. In this section, a very brief summary of the VCCM is presented. The readers are referred to Okada et al. [4] for the full details of the VCCM. In the VCCM, the energy release rate is expressed by energy which is required to virtually close a finite element face which is adjacent to the crack front. the is able to evaluate the energy release rate G_I from nodal displacement and reaction force nearby crack front calculated by structural analysis.

$$G_{I}(S_{1}) = \frac{2\delta W_{I}(S_{1})}{3S_{1}}$$
(1)

$$G_I(S_2) = \frac{2\delta \overline{W}_I(S_2)}{S_2} \tag{2}$$

where G_I is the mode I energy release rate, S_1 and S_2 are the areas of element faces whose vertex node and edge are on the crack front, respectively. S_1 and S_2 are illustrated in Figs. 1 (a) and (b). $\partial \overline{W}_I(S_1)$ and $\partial \overline{W}_I(S_2)$ are the energies that are required to virtually close the faces S_1 and S_2 . $\partial \overline{W}_I(S_1)$ and $\partial \overline{W}_I(S_2)$ can be computed by using the nodal crack opening displacements \overline{W}_{COD}^I and the nodal forces \overline{P}_Z^I arising from the cohesive stress on the element faces at the ligament side. \overline{W}_{COD}^I and \overline{P}_Z^I are schematically presented in Fig. 1. The energies $\partial \overline{W}_I(S_1)$ and $\partial \overline{W}_I$ (S_2) are expressed by:

$$\delta \overline{W}_{I}(S_{1}) = \frac{1}{2} \sum_{I=1}^{5} \overline{P}_{Z}^{I}(S_{1}) \overline{w}_{COD}^{I}(S_{1})$$
(3)

$$\delta \overline{W}_{I}(S_{2}) = \frac{1}{2} \sum_{I=1}^{3} \overline{P}_{Z}^{I}(S_{2}) \overline{w}_{COD}^{I}(S_{2})$$
(4)

The stress intensity factor is computed from the energy release rate. The stress intensity factor K_I is expressed, by: $K_I = \sqrt{E'G_I}$ (5)

where
$$E' = E$$
 or $E' = E/(1-v^2)$ for the plane stress or the plane

where E' = E or E' = E/(1-v) for the plane stress or the plane strain conditions. E and v are the Young's modulus and the Poisson's ratio, respectively.



3. Mesh Generation with Coalesced Crack

In crack propagation analysis with multiple cracks, if 2 propagated cracks get closer, these cracks link up and new coalesced crack shape is created. We developed new crack coalescence method [5]. Coalescence conditions are defined by plastic zones along crack fronts (Fig. 2). When plastic zones are overlapped, "coalescence point" can define by crossing points of plastic zone fronts (Fig. 3). The shape of new coalesced crack is created using these coalescence points. Figure 4 shows a sample case of coalescence has planar shapes, but new crack after coalescence has complex shape.



Fig. 2 Plastic zones along crack fronts.



Fig. 3 Crossing plastic zone fronts and Coalesce point.



Fig. 4 Sample case of 2 crack coalescence.

4. Performance Test on ES2 and K-computer

To estimate performance of next-generation HPC, Authors demonstrated static elastic stress analysis using a building model with 70M nodes (210M degrees of freedom) on the ES2 and K Computer. Analysis configurations and test results are shown as Table. 1.

	5		
Model	ES2	K Computer	K Computer
# nodes	64	512	1,024
# subdomains	18K	25K	33K
Solver type	BDD-DIAG	BDD	BDD-DIAG
CG tolerance	10-6	10-7	10-3
Data storage type	Skyline	Skyline	CSR
# iterations	776	885	147
Time [s]	2829	827	64.4
Memory [TB]	2.64	2.95	0.72
FLOPS/PEAK	1.2TF / 2.4%	8.9TF / 13.6%	-
[%]			

Table 1 Analysis conditions and test results

5. Conclusions

In 5 years of this project, we accomplished to develop an analysis system which can perform large scale fracture analyses on ES2. The quadratic tetrahedral finite element is adopted so that we can make use of automatic mesh generation methodologies.

We are planning to adopt results of this project to next generation HPC. Porting the ADVENTURE system to K Computer is proceeding in "Filed 4 of HPCI Strategic Programs for Innovative Research (SPIRE)" [6] and we are developing a numerical library based on hierarchical domain decomposition for post petascale simulation In JST CREST "Development of System Software Technology for post-Peta Scale High Performance Computing" project [7].

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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

プロジェクト責任者

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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、昨年度までの成果を基に、き裂進展解析に必要な要素技術の高精度化として、領域積分法に基づく、ロバストかつ精度の良い三次元J積分手法の提案およびプログラムの実装を行った。モデル作成技術に関しても、数百から数千のき裂を含んだモデルの亀裂進展解析を見据えて、複数き裂の進展に伴うき裂の結合に対応したメッシュ生成技術を開発するとともに、き裂パラメータ計算の精度向上のため、メッシュ細分割の際に亀裂前縁の節点位置を最適化し、き裂形状を正確に再現できるように改良した。

また、次世代 HPC 環境への対応を進めるため、ES2 と京コンピュータの性能比較を行った。同一の大規模複雑形状の 2.1 億自由度モデルを使って解析を行い、解析時間、反復法における反復回数、メモリ使用量を比較した。

 $\pm - 7 - 1$; fracture mechanics, crack propagation analysis, finite element method, domain decomposition method, aging structure