DIRECT NUMERICAL SIMULATION OF COMPOSITE STRUCTURES

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SUMMARY: Composite materials consist of two or more constituents bonded together. Thus, to understand and predict not the averaged or homogenized behavior but the real behavior of composite structures, full microscopic modeling that can describe the behavior of each constituent is required. Analysis of full microscopic models of composite structures, what we will call Direct Numerical Simulation (DNS) of composite materials, requires huge computing resources. In this work, an efficient parallel direct solver, which can utilized distributed computing resources unlimitedly, is developed as a powerful analysis tool for DNS by using the multifrontal technique. And it is shown that DNS of composite structures is feasible by virtue of the high performance parallel multifrontal solver. DNS of composite materials is performed for some example problems up to about 1.4 million unknows and the usefulness and the feasibility of DNS is verified.

KEYWORDS: fiber-reinforced composites, microstructure, finite element method, direct numerical simulation (DNS), multifrontal solver, parallel computing

INTRODUCTION

Composite materials are more and more widely used in many engineering fields such as aerospace structures that require high strength-to-weight ratios. However, in spite of superior properties of composite materials, there exist difficulties in predicting the behavior of composite structures using numerical simulations, and these difficulties make the application of composite materials somewhat restricted.

Two approaches can be considered in dealing with numerical simulation or numerical stress analysis of composite structures. The one is the macroscopic approach and the other is the microscopic approach. By the macroscopic approach, composite materials are considered as homogenized anisotropic materials and anisotropic constitutive equations are directly used. By using this approach, the global behavior of the whole composite structures can be described and predicted in ‘averaged sense’. However, this approach cannot properly describe the local interactions between the constituents of the composite structures. By the microscopic

approach, composite materials are regarded as mixtures of different isotropic or anisotropic materials and the constituents of composite materials are modeled separately. The unit cell or Representative Volume Element (RVE) method [1, 2] to predict the effective properties of composite materials may be classified as the microscopic approach, but this method is rather another methodology for homogenization since it assumes identical states for all the unit cells. Thus, this method also cannot describe the local behavior of the constituents of the composite materials. For complete description of the behavior of real composite structures, a detail modeling incorporating microscopic structures is necessary. However, full microscopic modeling of the whole composite structures has rarely been done mainly due to limited computing power, and this is one of the major difficulties in numerical simulation for the behavior of composite materials. For example, most of the failure mechanisms of composite materials are initiated from microscopic level and propagated to macroscopic level, thus full microscopic modeling is required. However, due to difficulties in numerical simulation, the prediction of failure still largely depends on experimental data. It is almost impossible to analyze full microscopic models using conventional solution methods since computing resources required are so enormous.

Therefore, in this research, we developed a new efficient solution procedure that enabled us to analyze the full microscopic models of composite structures. Modeling the whole composite structure as it is without any simplification or homogenization will be called Direct Numerical Simulation (DNS) of composite materials. DNS of composite materials is expected to be able to supplement and/or replace many of experiments that are essential to understand and predict the behavior of composite structures. Computing resources (computing time and storage) required to perform the DNS of composite materials can be considerably reduced by using the multifrontal solution technique [3, 4]. But using this technique is not enough for DNS since available computing resources for single machine are limited by hardware technology on CPU, memory, and storage device. What we need for DNS is enormous or almost unlimited computing resources and they are achievable only by the distributed parallel computing technique which can combine numerous distributed computing resources together into single huge computing resource. Thus, the solution procedure must be adapted to distributed parallel computing environment in order to obtain required computing resource for DNS by fully utilizing distributed computing resources. In this research, by parallelizing the multifrontal solver for distributed parallel computing environment, an efficient numerical tools for DNS of composite materials was developed.

MULTIFRONTAL SOLVER

The concept of the multifrontal method was first introduced by Duff *et al*. [5] as a generalization of the frontal method of Irons [6]. The frontal method was originally proposed as a solution procedure for the finite element method and it has earned the reputation of being easy and inexpensive to use. The elimination process of the frontal method is illustrated in Fig. 1.

In their paper, Duff *et al.* [5] used the concept of ‘generalized elements’ to deal with general indefinite sparse matrices. They proposed to combine a few different fronts or generalized elements together to have larger fronts for better choices of pivoting. Geng *et al.* [3] applied the multifrontal solver to finite element analysis by combining the method with the nested dissection ordering14 and showed the efficiency. The elimination process of the multifrontal method applied to finite element procedure is illustrated in Fig. 2.

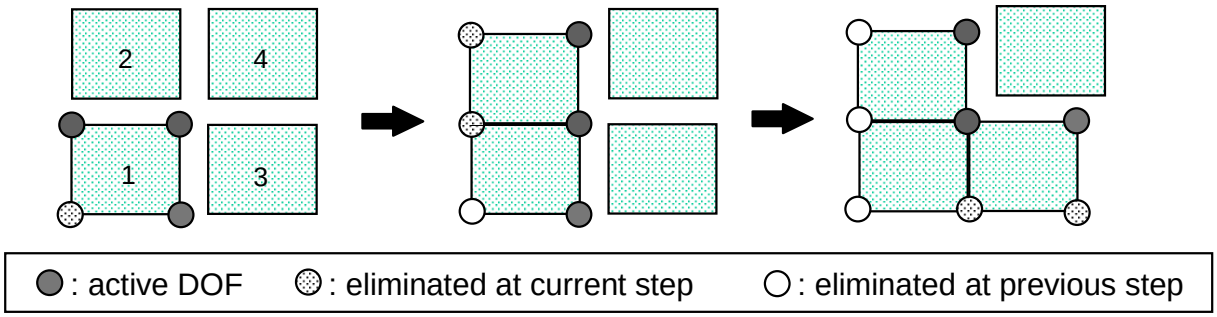


Fig. 1: Elimination process of the frontal method

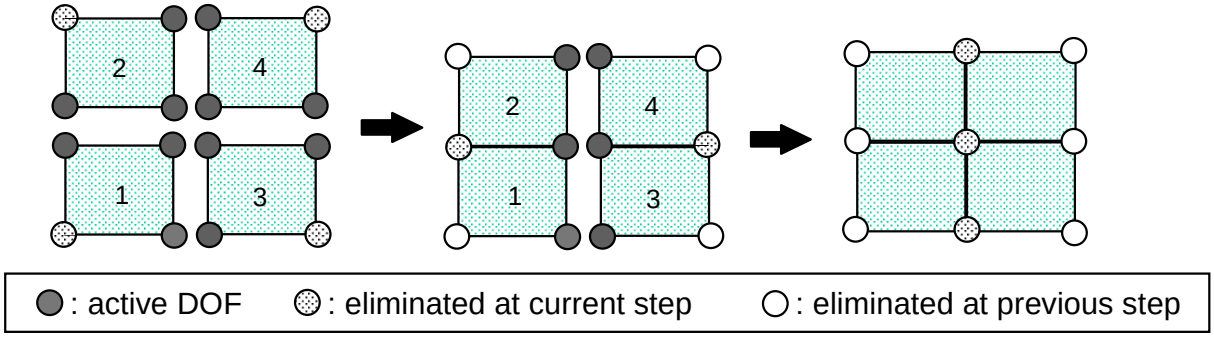


Fig. 2: Elimination process of the frontal method

The difference between the elimination process of the conventional single frontal method and that of the multifrontal method can be understood by comparing Fig. 1 with Fig. 2. By the single frontal method, one front is used and it spreads out on all over the whole domain as fully assembled degrees of freedom (DOFs) are eliminated from the front. By the multifrontal method, a given domain is divided into two subdomains recursively and each subdomain has its own fronts. Then, after the recursive bisection of the given domain is completed, the internal DOFs of each subdomain are eliminated first by the frontal method. Remaining interface DOFs of each subdomain after eliminating internal DOFs become new 'fronts' and they are merged with each other recursively in the reverse order by which the given domain is divided. At each merging stage, fully assembled DOFs are eliminated immediately.

Table 1: The performance of the multifrontal solver vs. the single frontal solver for the 3D composite shell structure with 4 layers

Solution Method	Total Solution Time	Memory Usage	Disk Usage
Single Front	2822 sec	12MB	482MB
Multifront	664 sec	31MB	185MB

In the previous research by the authors [4], the superior performance of the multifrontal solver to the conventional frontal solver was shown and the authors extended the multifrontal solver so as to manipulate irregular meshes successfully by combining the solver with mesh partitioning techniques. Some of the results are listed in Table 1 and Table 2. These results are

the computing time and storage required to perform finite element analysis of the irregular mesh shown in Fig. 3 using the conventional frontal solver and the multifrontal solver. A system which has Pentium Pro 200MHz CPU and 128MB of main memory is used to perform this analysis. The system runs Linux operating system and GNU C/C++ compiler.

Table 2: The performance of the multifrontal solver vs. the single frontal solver for the 3D composite shell structure with 8 layers

Solution Method	Total Solution Time	Memory Usage	Disk Usage
Single Front	16,180 sec	30MB	1,563MB
Metis-WEM	3,063 sec	77MB	520MB

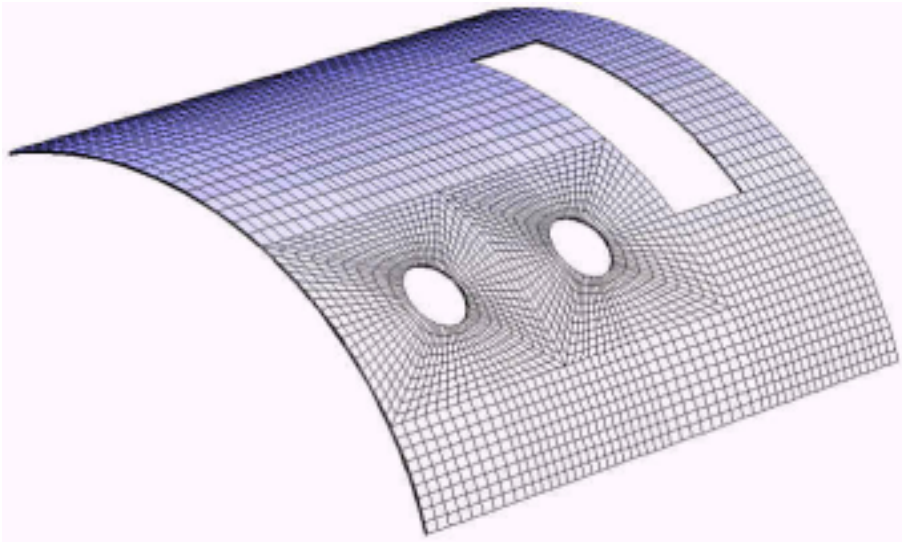


Fig. 3: Finite element mesh of three dimensional composite shell with cutouts

The finite element mesh of the composite shell with cutouts shown in Fig. 3 has 46,680 DOFs and 11,664 elements. This macroscopic finite element model for the composite structure consists of four layers of composite laminates. The computation performance with 2048 fronts is compared with that of the single frontal method with spectral element reordering [7] and shown in Table 1. The performance of the multifrontal solver is more than 4.2 times faster than that of the single frontal method with element reordering and the total storage usage (memory and disk usage) for the multifrontal solver is much less than that for the single frontal solver. In this case, memory and disk usage can be converted each other to fit available system resource size, and what matters is the total storage usage.

The computing results for the finite element model with the same geometry that has eight layers are shown in Table 2. This model has 84,024 DOFs and 23,328 elements. The performance with 4096 fronts is the best and it is also compared with that of the single frontal method in Table 2. The results are similar to the results in Table 1 and the developed multifrontal solver is about 5.3 times faster than the single frontal method in this case.

As shown above, by using the multifrontal solver, computing resources required to solve structural analysis problems can be reduced remarkably and large-scale structural analysis

problems can be solved within tolerable computing time on a machine with affordable core memory. However, DNS of composite materials requires so much computing resources that multiple distributed computing resources must be combined together. In this study, the multifrontal solver is parallelized to utilize distributed computing resources. Parallelization of the multifrontal solver will be discussed in the next section.

PARALLEL MULTIFRONTAL SOLVER

Parallelization of the Multifrontal Solver

The multifrontal solver itself has inherent parallelism. By exploiting the inherent parallelism, distributed parallel computing resources such as massively parallel processors (MPPs) or clusters of workstations or PCs can be fully utilized, and consequently enormous computing resources for DNS of composite materials can be obtained.

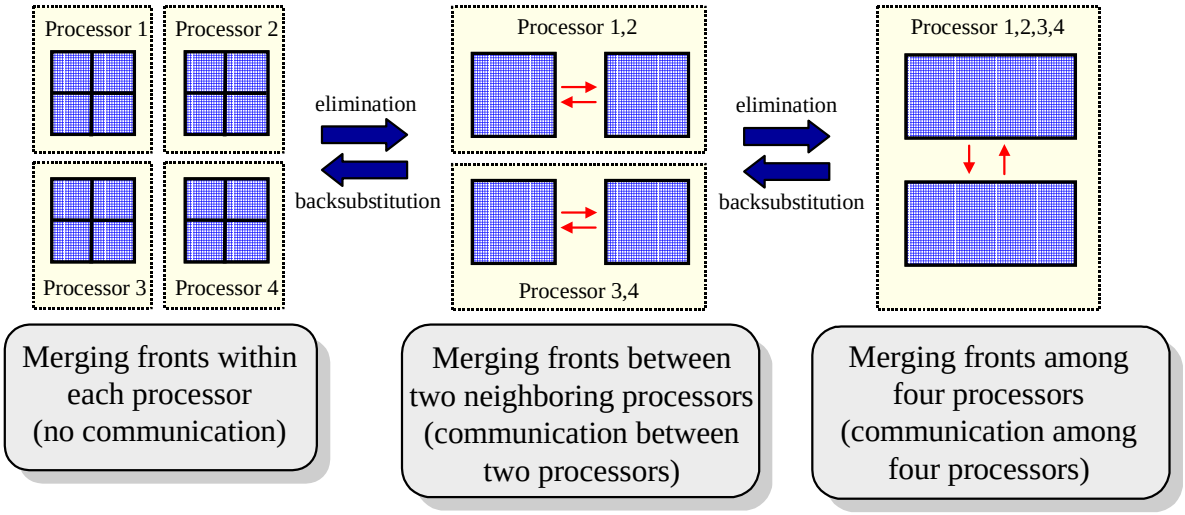


Fig. 4: Parallel implementation of the multifrontal solver using 4 processors

An illustration for parallel implementation of the multifrontal solver is shown in Fig. 4 for four processor case. During the recursive bisection procedure for obtaining front partition, each front is assigned to one processor respectively when the number of the front partition reaches the number of processors to be used. And each front assigned to a processor is further recursively bisected until the optimal number of fronts for the best performance is obtained. Then, front merging in each processor can be performed independently. There is complete parallelism in this procedure. This is the inherent parallelism of the multifrontal solver. After front merging or the elimination of the interior degrees of freedom (DOFs) is completed in each subdomain or processor, the same procedure is performed between two neighboring subdomains or processors and this procedure requires communications between the processors. And then, front merging is performed among four processors, eight processors, and so on. Good parallel performance can be obtained since all communications are localized during these procedures. The performance of the parallel multifrontal solver will be shown in the next section.

Parallel Performance of the Multifrontal Solver

The inherent parallelism of the multifrontal solver makes it possible for the solver to obtain excellent parallel performance compared with other direct solvers. The parallel performance of the parallel multifrontal solver is tested using the IBM SP2 system that has the same hardware configuration as workstation clusters except that it has faster network connection. The first problem to evaluate the performance is a three-dimensional stress analysis problem with 16×16×16 solid elements. The speedup and computing time using up to 16 processors are shown in Fig. 5 and Fig. 6, respectively.

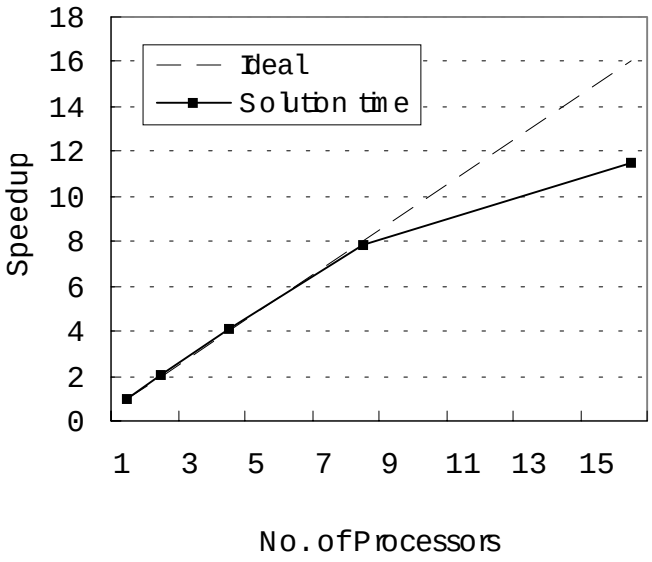


Fig. 5: Speedup for 16×16×16 solid elements

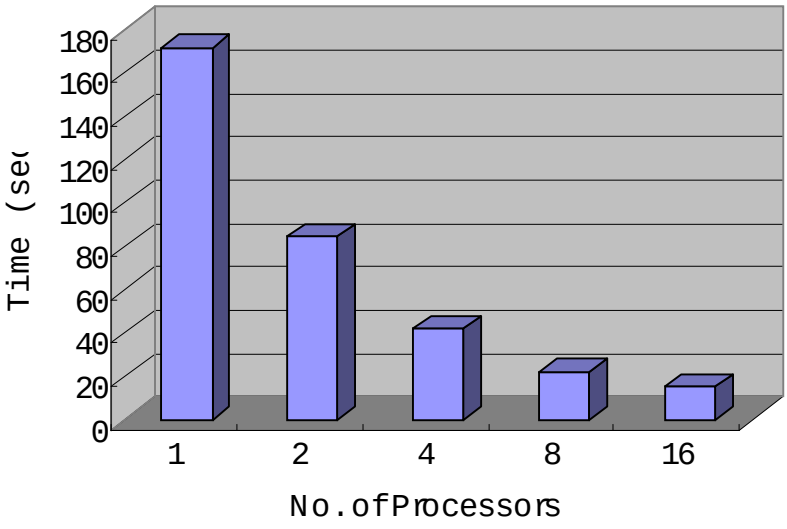


Fig. 6: Computing time for 16×16×16 solid elements

By using 16 processors, the same problem can be solved about 12 times faster than using the serial multifrontal solver. Up to eight processors, the parallel performance is near to ideal speedup. The relatively poor parallel efficiency for 16 processors means that the size of this problem is too small to be solved on 16 processors. A larger problem with 32×32×16 solid elements is tested. The results are presented in Table 3.

Table 3: Speedup for 32×32×16 solid elements

No. of Processors	Elapsed Time (sec)	Speedup
1	2987	1.00
2	1589	1.88
4	774.5	3.86
8	375.0	7.97
16	178.0	16.8
32	103.9	28.8

This problem is too large to fit in the main memory of single machine. Thus, disk space must be used up to eight processors. However, this problem does not need to use disk space at all when more than 16 processors are used. The 'super speedup' in Table 3 seems to be occurred by this reason.

The parallel multifrontal solver developed by the authors shows excellent parallel performance and makes it possible to utilize distributed computing resources. Therefore, it can be used as an ideal analysis tool for DNS of composite materials.

DIRECT NUMERICAL SIMULATION OF COMPOSITE MATERIALS

Modeling of Composite Materials for DNS

In this research, DNS of fiber-reinforced composite materials was performed. A unit cell that contains fiber and matrix is modeled with 20 node solid elements as shown in Fig. 7. This unit cell is repeated to form a finite element mesh for DNS. A typical finite element model for DNS is shown in Fig. 8.

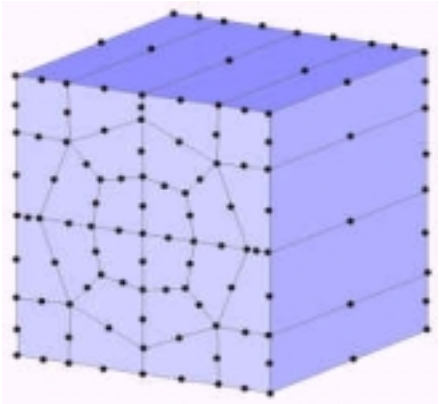


Fig. 7: Finite element mesh for unit cell

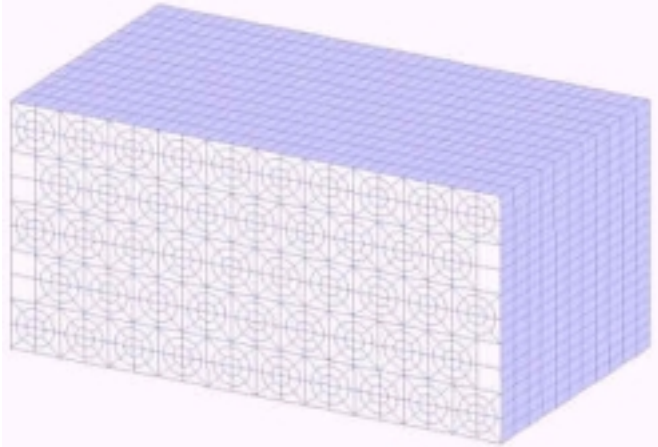
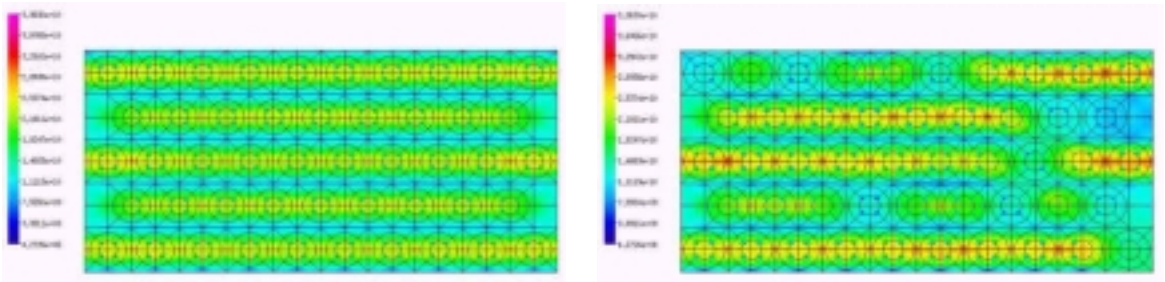


Fig. 8: Typical finite element model for DNS

One of the major advantages of the DNS is that it can deal with irregular fiber distributions. However, modeling real composite structures in detail to microscopic level is very difficult and complicated. Thus, by replacing the material properties of fibers with those of matrices, irregular fiber distributions are simulated in this work.

Example problems for DNS

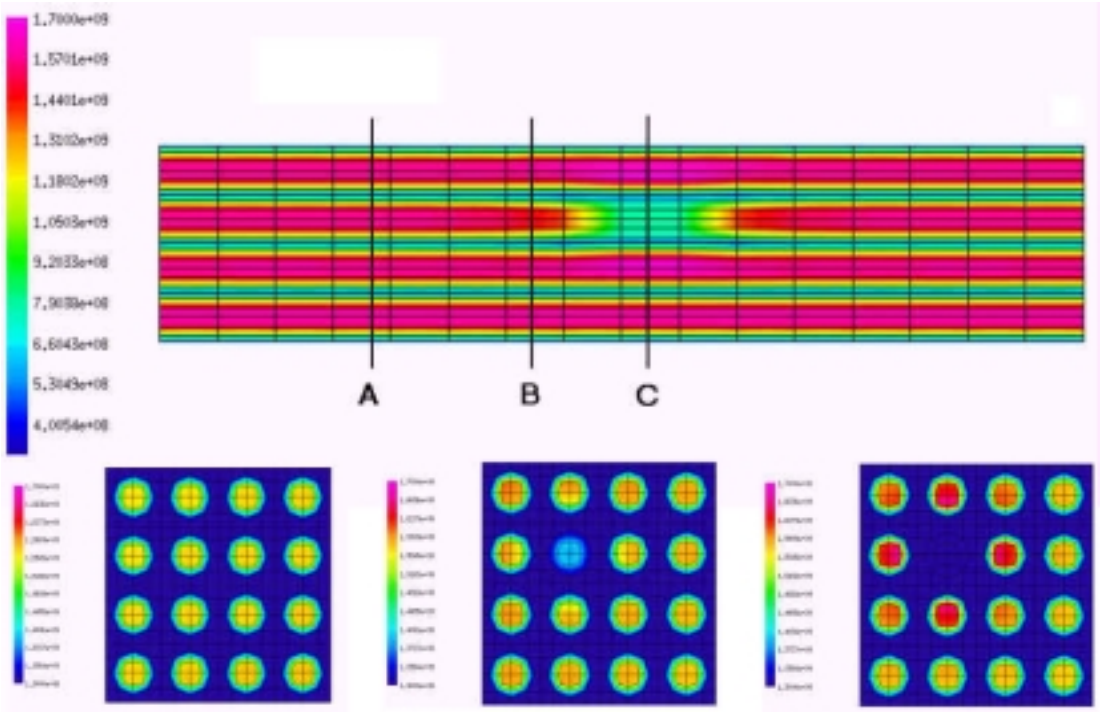
To show the necessity of microscopic models in understanding the failure mechanism, two microscopic models were analyzed and the results were compared. These two models have the same configuration as shown in Fig. 8 with 106,740 degrees of freedom (DOFs) and they are under the same transverse loading condition. The two models also have the same volume fraction. According to the mixture rule, they have the same homogenized properties such as Young's moduli, Poisson's ratios, etc. The only difference is the distribution of fibers and matrices. The results for stress analyses are shown in Fig. 9. The model whose results shown in Fig. 9 (a) has uniform fiber distributions while the model in Fig. 9 (b) has several defects where the material properties of fibers are replaced by those of matrices. But the volume fractions of the whole structures are the same. The distribution of transverse normal stress σ_{22} in front face of each model is plotted in Fig. 9. The distributions are not uniform and the results show the differences in stress distributions between these two models. The maximum of σ_{22} in matrix region of the defect model is 1.2 times larger than that of the uniform model, which shows the importance of full microscopic modeling for failure prediction, in other words, the DNS of composite materials



(a) Uniform fiber distribution *(b) Fiber distribution with defect*

Fig. 9: Normal stress σ_{22} distribution

Next, a composite structure with fiber breakage was analyzed using DNS. One end of the structure is fixed and non-zero displacement is specified on the other end. The stress distributions for this model are shown in Fig. 10. Near the breakage point, fibers around the broken fiber carry more loads as shown in Fig. 10 (c). By using DNS with this model, it is expected to be able to predict the fiber pull out under more complicated load states.



(a) Stress at plane A *(b) Stress at plane B* *(c) Stress at plane C*

Fig. 10: Stress distribution σ_{11} of the fiber breakage model

Finally, a huge-scale composite structure model that had about 1.4 million DOFs was solved using the parallel multifrontal solver. The computing power of 64 processors of a Cray T3E system and the distributed memory of each processor are fully utilized by the multifrontal solver. The usage for computational resources is listed in Table 4. Each processor of the Cray T3E system has 128MB of distributed local memory and they can be combined together to solve one huge-scale DNS problem successfully.

Table 4: Usage for computational resources for DNS

Global DOFs	1,385,859
No. of Elements	98,304
No. of Processors	64
Maximum Memory Usage	6.58 GB
Total CPU Time	191,361 sec
Elapsed Time	6,795 sec

CONCLUSIONS

In this work, an efficient parallel direct solver was developed as a powerful analysis tool for DNS by using the multifrontal technique. And it was shown that the full microscopic modeling of fiber-reinforced composite structures to simulate the behaviors of the composite structures into the microscopic level was feasible by virtue of the high performance parallel multifrontal solver. Direct numerical simulations of composite materials were performed for some example problems and the usefulness and the feasibility of DNS was verified. Further work must be done to solve problems of larger size and to model more realistic composite structures including angle-ply laminates.

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REFERENCES

1. Sun, C. T. and Vaidya, R. S., "Prediction of composite properties from a representative volume element", *Composite Science and Technology*, Vol. 56, 1996, pp. 171-179.

2. Zhang, W. C. and Evans, K. E., "Numerical prediction of mechanical properties of anisotropic composite materials", *Computers and Structures*, Vol. 3, 1988, pp. 413-422.

3. Geng, P., Oden, J. T. and Geijn, R. A. van de, "A parallel multifrontal algorithm and its implementation", *Computer Methods in Applied Mechanics and Engineering*, Vol. 149, No. 1-4, 1997, pp. 289-302.

4. Kim, J. H. and Kim, S. J., "A multifrontal solver combined with graph partitioners", AIAA Journal, In Press, 1999.

5. Duff, I. S. and Reid, J. K., "The multifrontal solution of indefinite sparse symmetric linear equations", *ACM Trans. Math. Software*, Vol. 9, 1973, pp. 302-325.

6. Irons, B. M., "A frontal solution program for finite element analysis", *International Journal for Numerical Methods in Engineering*, Vol. 2, 1970, pp. 5-32.

7. Paulino, G. H., Menezes, I. F. M., Gattass, M. and Mukherjee, S., "Node and element resequencing using the Laplacian of a finite element graph : Part I - General concepts and algorithm", *International Journal for Numerical Methods in Engineering*, Vol. 37, 1994, pp. 1511-1530.