Development of Solid Earth Simulation Platform

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In this project, GeoFEM, a parallel FEM platform for solid earth simulation, has been ported to the Earth Simulator and optimized. Various types of special procedures for solid earth simulations have been developed and added to the GeoFEM platform. Feasibility of GeoFEM for various types of applications has been also evaluated on the Earth Simulator. In FY.2005, we developed robust and efficient iterative linear solvers for ill-conditioned problems with abrupt change of mesh size and a library for Fast Multipole Method (FMM). For ill-conditioned problems with abrupt change of mesh size, RCM (Reverse Cuthill-Mckee) ordering provides faster and robust convergence than multicolor ordering. Moreover, procedures of GeoFEM for elastic solid mechanics have been evaluated through stress analysis of trabecular bones.

Keywords: GeoFEM, iterative solvers, preconditioning, ordering, Fast Multipole Method

1. Preconditioned Iterative Solvers on the Earth Simulator with Ordering for Ill-conditioned Problems with Abrupt Change of Mesh Size

In order to achieve minimal parallelization overhead in symmetric multiprocessor (SMP) cluster, multi-level *hybrid* programming model with MPI and OpenMP, and *flat MPI* approach have been widely employed [1]. Efficiency depends on hardware performance (CPU speed, communication bandwidth, memory bandwidth, and their balance), features of applications, and problem size [2].

In the previous work [1], author developed an efficient parallel iterative solver for finite-element applications on the Earth Simulator (ES) [3]. The method employs three-level hybrid parallel programming model consisting of MPI, OpenMP and vectorization. Multicolor-based reordering methods have been applied in order to achieve optimum performance, in the ILU/IC type method. Developed method attained 3.8 TFLOPS with 176 SMP nodes of ES, corresponding to more than 33% of the peak performance (11.3 TFLOPS).

While the three-level hybrid and flat MPI parallel programming models offer similar performance, the hybrid programming model outperforms flat MPI in the problems with large numbers of SMP nodes [1].

Convergence of the iterative solvers using multicolor-type reordering method can be improved by increasing the number of colors because of fewer incompatible local graphs [1]. But this reduces the number of elements in each color, which means shorter innermost loops for vectorization.

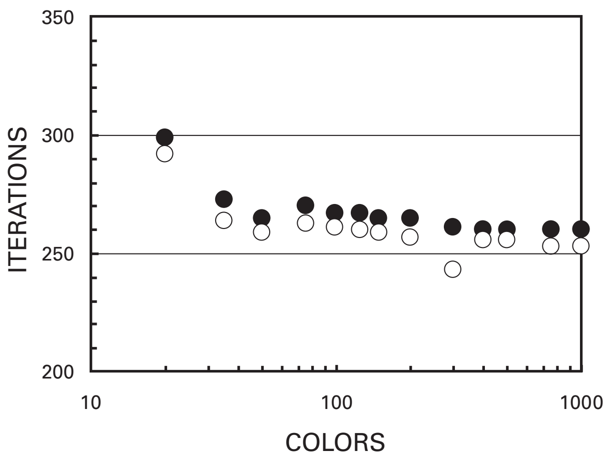


Fig. 1 Effect of color number in multicolor reordering. Iteration number for convergence ($\varepsilon = 1.0^{-8}$) on 3D linear elastic problem in a cube [1] (Problem size = 3,000,000 DOF (3×100^3) using 1 SMP node (8 PE's). (BLACK Circles: Flat MPI, WHITE Circles: Hybrid).

Figure 1 shows the effect of color number on convergence of ICCG solvers with multicolor reordering for linear elastic problem on a cube [1]. Iteration number for convergence decreases as color number increases in both of flat MPI and hybrid parallel programming models. Hybrid programming model requires slightly smaller number of iterations for convergence.

Figure 2 shows effect of color number on performance of the Earth Simulator. In both of flat MPI and hybrid, GFLOPS rate decreases as color number increases. Therefore, elapsed

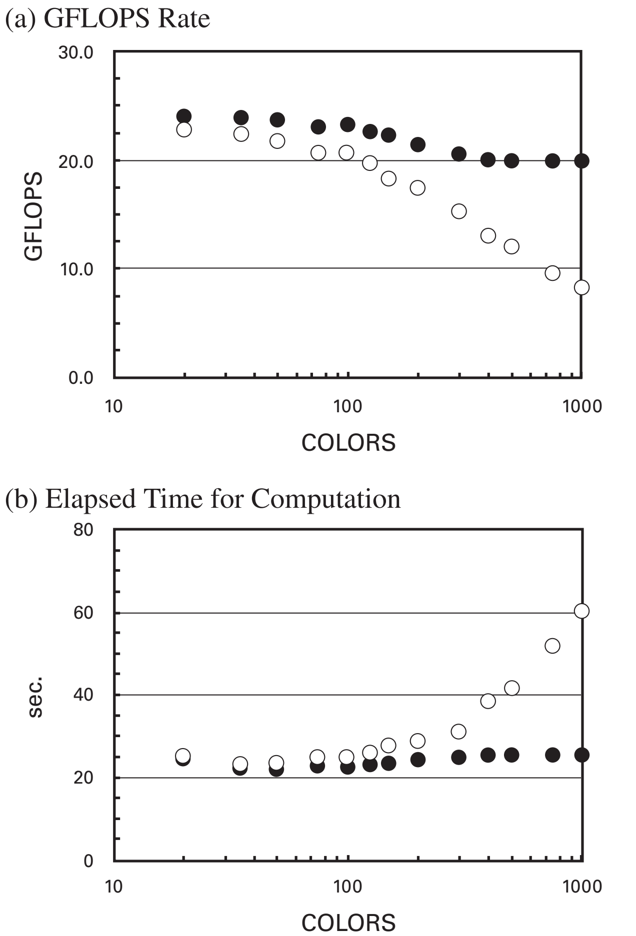


Fig. 2 Effect of color number in multicolor reordering on the Earth Simulator with 1 SMP node (8 PE's). 3D linear elastic problem in a cube [1] (Problem size = 3,000,000 DOF (3 × 100^3). (a) GFLOPS rate, (b) Elapsed Time for Computation. (BLACK Circles: Flat MPI, WHITE Circles: Hybrid).

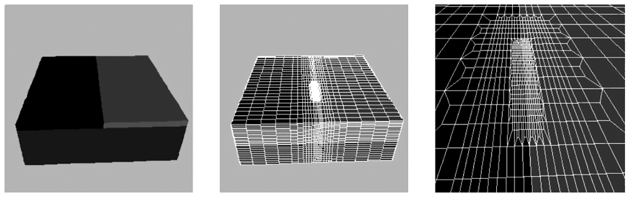


Fig. 3 Meshes with adaptive local refinement for stress accumulation simulations at fault boundaries.

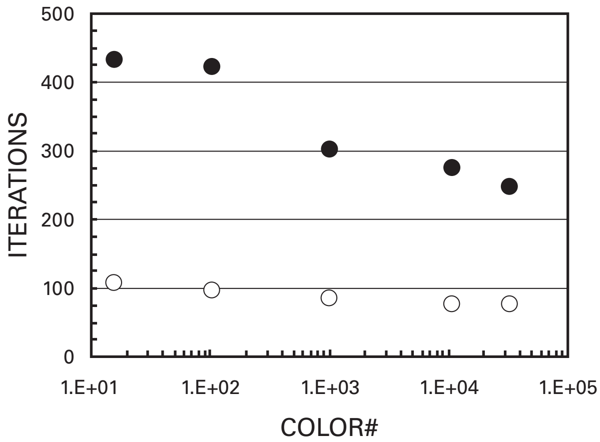


Fig. 4 Effect of color number on iterations for convergence of 3D linear elastic problem in a cube [1] (Problem size = 98,304 DOF (3 × 32^3). (BLACK Circles: Irregular Mesh (Max. Ratio of Neighboring Mesh Size is 33, WHITE Circles: Uniform Mesh).

time for computation is longer for 1,000 color cases, although iteration number decreases, as shown in Fig. 2. This feature is much more significant in hybrid than in Flat MPI. Size of vector register in the Earth Simulator is 256 [3]. In this case with 100^3 finite-element nodes on 8 PE's, average innermost loop-length is 256 for the case with 488 colors. But, Fig. 2 shows that the performance of hybrid programming model decreases when the color number is about 100. This is mainly because of synchronization overhead of OpenMP.

In visco-elastic FEM simulations for stress accumulation at plate boundaries using split-node models [4, 5], adaptive mesh refinement (AMR) is applied to the area with large slip conditions for accurate solutions, as shown in Fig. 3. Abrupt change of local mesh size provides slow convergence of iterative solvers due to large condition number.

Fig. 4 shows effect of color numbers on iterations for convergence of 3D linear elastic problems in a cube [1] with multicolor reordering, where maximum ratio of neighboring mesh length is 33. Cube includes 32^3 nodes and problem has been solved on a single processor of the Earth Simulator.

In this type of problems, many colors are usually required for convergence. Therefore, vector performance is reduced due to smaller loop length. Sometimes, as many number of color as FEM node number is required for convergence in reasonable number of iterations. In such situations, vector performance is significantly reduced.

RCM (Reverse-Cuthill Mckee) reordering has been introduced in place of multicolor reordering. RCM method is a typical level set reordering method. In Cuthill-Mckee reordering, the elements of a level set are traversed from the nodes of the lowest degree to those of the highest degree according to dependency relationships, where the degree refers to the number of nodes connected to each node. In RCM, permutation arrays obtained in Cuthill-Mckee reordering are reversed. RCM results in much less fill-in for Gaussian elimination and is suitable for iterative methods with IC or ILU preconditioning. Usually, RCM provides fewer incompatible nodes [1] than multicoloring, therefore convergence of the method with RCM ordering is faster. But, numbers of the elements in each level set is irregular, as shown in Fig. 5 (a). Remedy is RCM with cyclic-multicoloring (CM) proposed in [1], but CM-RCM provides slower convergence than original RCM. In this study, original RCM has been applied.

Fig. 6 shows convergence of multicolor (MC) and RCM reordering for 3D linear elastic problems in a cube, where maximum ratio of neighboring mesh length is 33. Fast convergence has been attained with RCM. Fig. 7 shows effect of

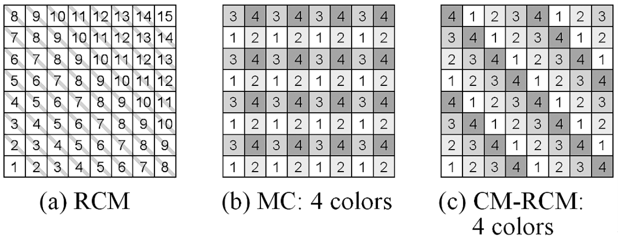


Fig. 5 Example of hyperplane/RCM, multicoloring and CM-RCM reordering for 2D geometry [1].

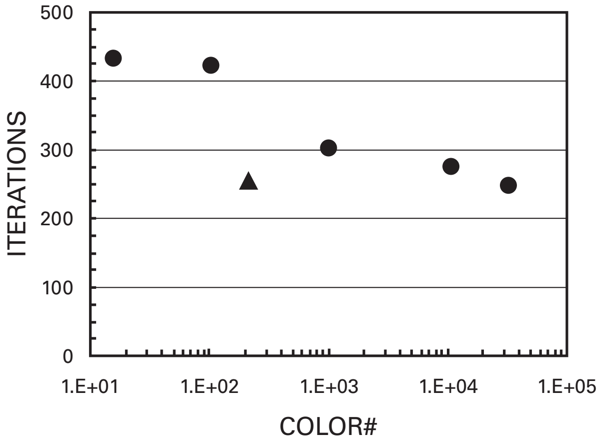


Fig. 6 Effect of color number on iterations for convergence of 3D linear elastic problem in a cube [1] with abrupt change of mesh size, where maximum ratio of neighboring mesh size is 33. (Problem size = 98,304 DOF (3 × 32^3). (BLACK Circles: Multicolor (MC) reordering, BLACK Triangle: RCM reordering).

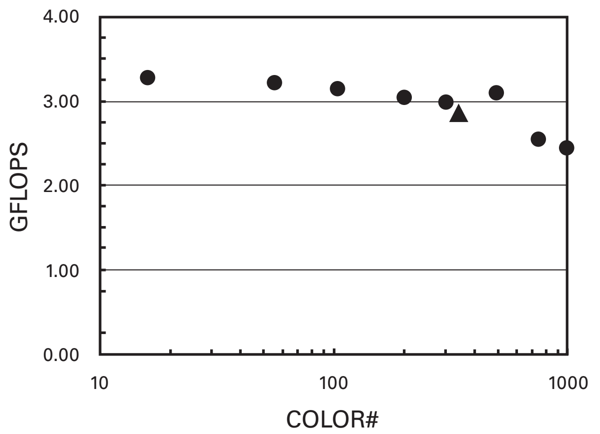


Fig. 7 Effect of color number on performance of 3D linear elastic problem in a cube [1] with abrupt change of mesh size, where maximum ratio of neighboring mesh size is 33. (Problem size = 98,304 DOF (3 × 32^3). (BLACK Circles: Multicolor (MC) reordering, BLACK Triangle: RCM reordering).

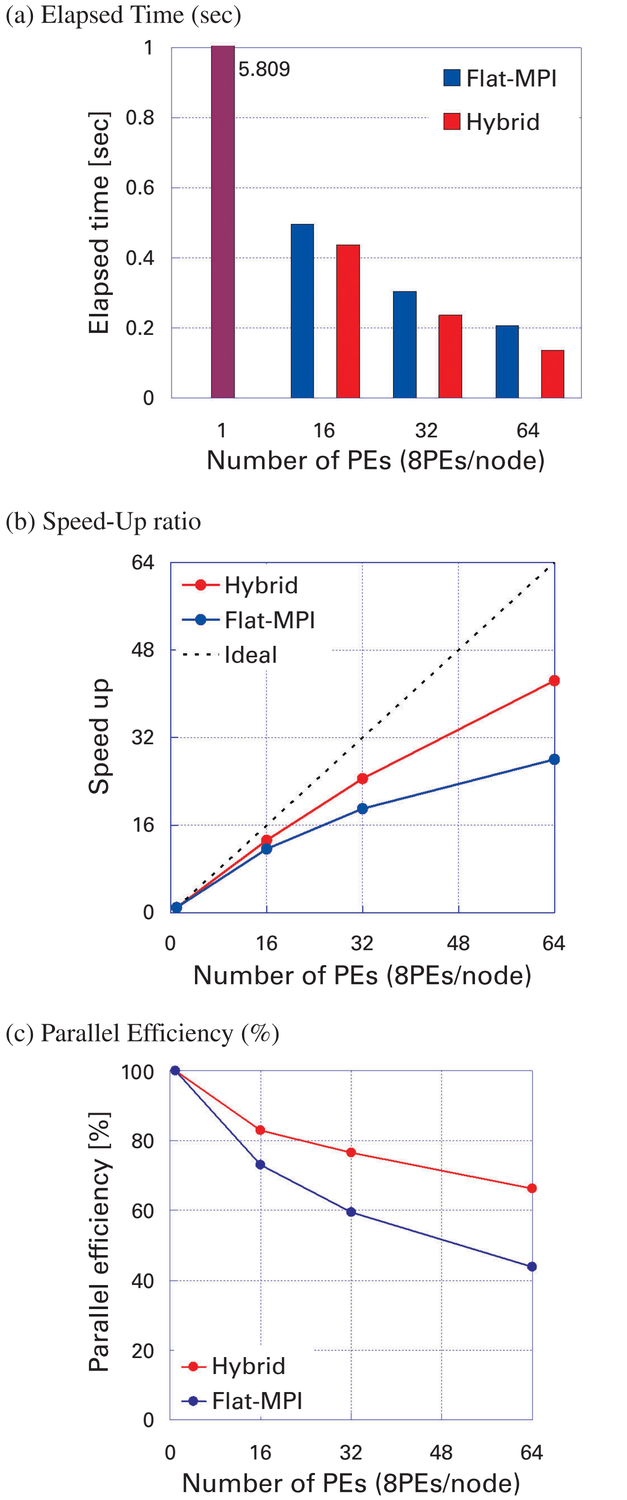
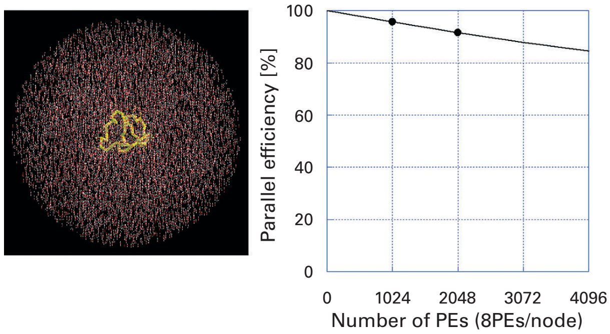


Fig. 8 Comparison of Flat MPI and Hybrid programming model for replica-exchange simulations with FMM.

colors on performance. Performance of RCM is competitive with MC with close number of colors. Effect of irregular number of elements in each level-set seems small in single PE (and flat MPI) cases.

2. Library for Fast Multipole Method (FMM)

In FEM, effect of only neighboring elements is considered, therefore coefficient matrices are usually sparse and size of storage is O(N), where N is number of unknown. On the contrast, boundary element method (BEM) and certain category of methods for molecular dynamics (MD) require global information for accurate computation. In these cases, coefficient matrices are usually dense. O(N^2) storage is required. Fast Multipole Method (FMM) [6] is remedy for reducing O(N^2) storage to O(NlogN) or O(N). There are many approaches, but common idea is to cluster the effects



(a) Initial Structure (b) Parallel Efficiency

Fig. 9 Performance of Large-scale Simulations (Hybrid Parallel Programming Model)

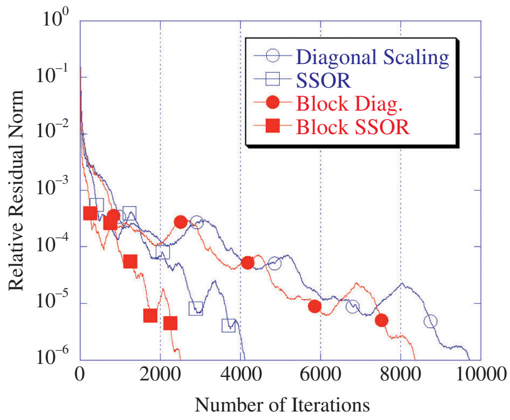
of elements in far field [6]. In this study, FMM library based on Anderson's method has been developed and applied to protein folding simulation code based on replica-exchange method [6].

Fig. 8 shows comparison between *flat MPI* and *hybrid* parallel programming model for replica-exchange simulations with FMM. *Hybrid* parallel programming model provides much better performance than flat MPI. Fig. 9 shows performance of large-scale protein folding simulations in water using hybrid parallel programming model. 117,649 atom's with 512 replica's are considered with 2,048 PE's of the Earth Simulator. Parallel efficiency was 91.56%, vector operation ratio was 99.07% and total performance was 3.9 TFLOPS (24% of peak).

3. Stress Analysis of Trabecular Bone using GeoFEM

Finally, static stress analysis has been conducted by static linear application of GeoFEM [7]. Trabecular bone has very complicated structure, as shown in Fig.10. Arrangement of molecules in crystal is heterogeneous. If heterogeneity is considered, coefficient matrices are ill-conditioned even for elastic problems, therefore convergence of iterative solver is slower. Fig.11 shows effect of heterogeneity on convergence of linear elastic problems for trabecular bone in Fig.10 with 200,000 elements. Various types of preconditioning methods provided by GeoFEM have been tested. Generally, block-type preconditioning methods, such as block diagonal and block SSOR, provide faster convergence. This feature is significant in heterogeneous cases. Finally, Fig.12 shows displacement distribution of 3D static linear analysis of quail's leg model with 5.2 × 10^7 elements (> 10^8 DOF). It took 12 hours until convergence using 10 SMP nodes of the Earth Simulator.

(a) Homogeneous



(b) Heterogeneous

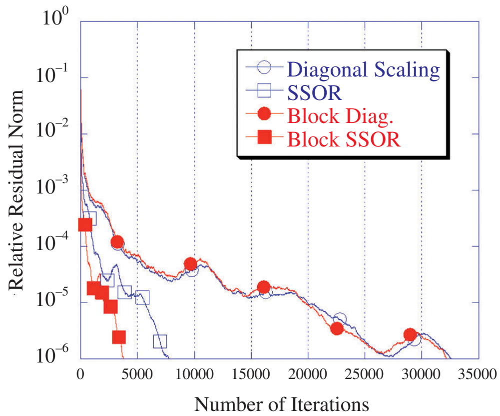


Fig.11 Convergence history of 3D linear elastic stress analysis on trabecular bone model in Fig. 5 with 200,0000 elements [7].

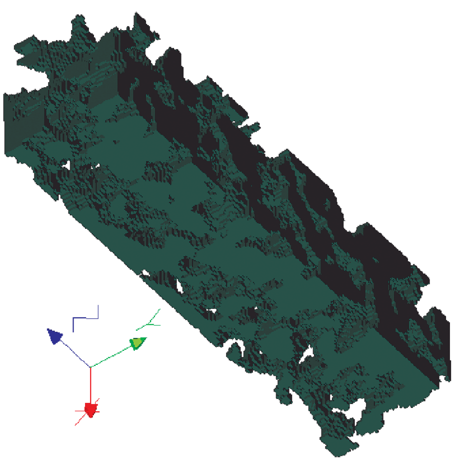


Fig.10 Structure of trabecular bone [7].

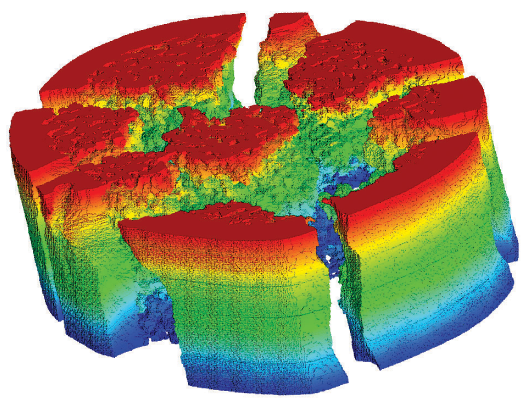


Fig.12 Displacement distribution of 3D static linear analysis of quail's leg model with 5.2 × 10^7 elements (> 10^8 DOF). It took 12 hours until convergence using 10 SMP nodes of the Earth Simulator.

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固体地球シミュレーションプラットフォームの開発

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(1) 悪条件問題向け高速反復法ライブラリの整備

有限要素法、差分法などにおいて、メッシュサイズが局所的に急激に変化する場合、係数マトリクスの条件数が大きくなるため、反復法の収束回数が増加する。本年度研究では、局所細分化を含む断層の三次元粘弾性解析問題を対象として、高速に安定な収束解が得られる手法を整備した。従来は、高いベクトル性能、並列性を得るためにマルチカラーオーダリング(MC法)による並び替えを実施していた。MC法では特に悪条件問題においては収束回数を減少させるために色数を増加させる必要があるが、ループ長が小さくなるために性能が低下する。本年度研究では、Reverse Cuthill Mckee (RCM) 法を適用することによって、色数を増加させることなく安定な収束解を効率的に得ることができた。

(2) 高速多重極展開法(Fast Multipole Method, FMM)ライブラリの開発と適用

高速多重極展開法(Fast Multipole Method, FMM)はN体問題において、遠方の影響をクラスタリングすることによって、精度を損なうことなく記憶容量を削減する方法であり、大規模シミュレーションに有効である。本年度研究では、Anderson法によるライブラリを開発し、レプリカ交換法によるタンパク質構造解析に適用した。「地球シミュレータ」の256ノード(2,048プロセッサ)を使用して、117,649原子、512レプリカにより、水球中のタンパク質折り畳みシミュレーションを実施し、並列化効率91.56%、ベクトル化率99.07%、実効性能3.9 TFLOPS (ピークの24%)を達成した。

(3) 海綿骨大規模応力解析

「GeoFEM」の弾性静解析モジュールを、複雑な構造を有する海綿骨の応力解析に適用した。結晶配向性による異方性を考慮した場合は、係数行列の条件が悪化し、収束までの反復回数が増加する。「GeoFEM」が提供する様々な前処理手法のうち、ブロック化した手法は他の手法と比較して安定性に優れている。ウズラ大腿骨の応力解析を、実物から画像処理によって生成した解析モデル(約52百万ボクセル、1億自由度以上)に対して実施した。「地球シミュレータ」10ノード(80プロセッサ)を使用して、収束までに約12時間を要した。

キーワード:GeoFEM, 並列反復解法, 前処理, オーダリング, 高速多重極展開法