Convergence acceleration method of large-scale parallel iterative solvers for heterogeneous properties

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Abstract

In large-scale scientific computing, linear sparse solver is one of the most time-consuming process. In GeoFEM, various types of preconditioned iterative method is implemented on massively parallel computers. It has been well-known that ILU(0) factorization is very effective preconditioning method for iterative solver. But it's also well-known that this method requires global data dependency and this is not the optimal way on parallel computers where locality is of utmost importance. In this paper, "Localized" ILU(0) preconditioning method has been implemented to various type of iterative solvers. This method provides data locality on each processor and good parallelization effect. Developed system performance has been also evaluated on workstation cluster with MPI.

Linear Solvers In GeoFEM

In GeoFEM, preconditioned iterative method is implemented on massively parallel computers in order to solve large scale problems with more than 10^8 DOFs. GeoFEM solves both of symmetric and un-symmetric matrices. Therefore CG (Conjugate Gradient) for symmetric matrices and BiCGSTAB (Bi-Conjugate Gradient Stabilized) and GMRES (Generalized Minimal Residual) methods are implemented. GMRES is especially suitable for nonlinear problems.

Message passing type programming model is adopted and the program is written in Fortran 90 with MPI [1]. Whole region is partitioned by node-based manner. Local operation is considered to be very important in order to handle large data easily and to attain good parallelization effect. Local data structure with communication table described in [2] is implemented. Thus data handling and matrix assemble operations are fully localized and global operation occurs only in the solver subsystem (Fig.1). Actually, no global information except partition to partition connectivity is required.

In iterative solvers, preconditioning is very important for convergence. In this paper strong and stable preconditioning method for parallel computing is developed and discussed.

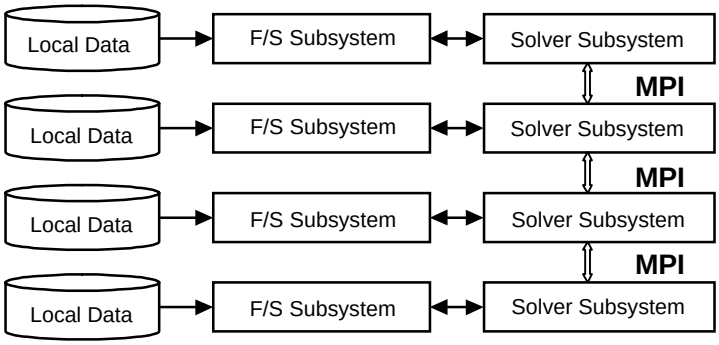

Figure 1: Global/Local Data Operation in GeoFEM

Iterative solvers & preconditioning

Convergence rate of iterative solvers for large-scale linear sparse systems in scientific and engineering computations:

$$Ax = b \quad , \tag{1}$$

strongly depends on the spectral properties of the coefficient matrix A. A preconditioner M transforms the linear system into one with more favorable spectral properties. M transforms (1) into the following equation:

$$A^{'}x = b^{'},\ A^{'} = MA,\ b^{'} = Mb \quad . \tag{2}$$

Equation (2) has same solution as (1), but the spectral properties of the coefficient matrix A'=M-1A may be more favorable and convergence is faster. ILU (Incomplete Lower-Upper) factorization method is a very strong preconditioning method for unsymmetric matrices [3]. Among the ILU preconditioner family, ILU(0) with no fill-in allowed beyond the original non-zero pattern is the most popular.

ILU(0) formulation for 3D 7-point structured finite-difference method is as follows:

ILU Decomposition

$$\begin{aligned} a_i,\ b_i,\ c_i \quad & \textit{lower triangular components} \\ e_i,\ f_i,\ g_i \quad & \textit{upper triangular components} \\ d_i \quad & \textit{diagonal component} \\ d_i^{-1} \quad = \quad & d_i - a_i g_{i-mn} d^{'}_{i-mn} - b_i f_{i-m} d^{'}_{i-mn} - c_i e_{i-1} d^{'}_{i-1} \end{aligned}$$

Back/Forward Substitutions

$$\begin{aligned} y_i &= d^{'}_i\,(r_i - a_i y_{i-mn} - b_i y_{i-m} - c_i y_{i-1}) \qquad i = 1 \sim n \\ z_i &= y_i - d^{'}_i\,(e_i y_{i+1} - f_i y_{i+m} - g_i y_{i+mn}) \qquad i = 1 \sim n \end{aligned}$$

The latter part (back/forward substitution, BFS) is repeated in each iteration. This part requires global data dependency and is not suitable for parallel processing where the locality is of utmost important.

In this paper, Localized ILU(0) preconditioning method suitable for parallel processing is implemented to various type of iterative solvers with domain partition strategies and performance is evaluated for some examples. Developed system performance has been also evaluated on simulated parallel processors by workstation cluster with MPI [1].

Localized ILU(0) preconditioning

Most of preconditioned iterative process are combination of:

- matrix-vector product calculation
- vector-vector inner product calculation
- SAXPY operations and vector scaling
- preconditioning operation

First 3 operations can be relatively easily parallelized [3]. Generally speaking, preconditioning (back/forward substitution, BFS) operation requires almost 50% of the whole calculation if ILU(0) is implemented as preconditioner. Therefore it is very important to get high degree of parallelization in the BFS operation. Higher degree of parallelization in ILU(0) is possible if a different ordering of unknowns are used but such an ordering usually adversely affects the convergence of iterative solvers [3]. In Ref [4], pseudo ILU(0) preconditioner for parallel processors is proposed. This method is not a global method but a local one in each processor or domain. In this method, ILU(0) operation is carried out for each processor by zeroing out the matrix components outside the processor domain. This Localized ILU(0) method provides data locality on each processor and good parallelization effect because there are no inter-processor communications during ILU(0) operation.

But it's not as strong a method as the global preconditioner. Generally, convergence rate goes worse for more processors and domains. At the critical end if processor number is equal to number of DOF, this method is identical with diagonal scaling. Overlapping effect between partitions are also considered in order to keep convergence rate in cases with many partitions and PEs.

Large scale plate motion analysis

Examples

Some example calculations are done on DEC Alpha EWS cluster with 4 CPUs. Fig. 2 shows the convergence history for Poisson equation example by Localized ILU preconditioned BiCGSTAB method with 643 meshes upto 512 partitions. Calculations was done by MPP simulator on single CPU workstation. In 512 PE case, iteration number increases twice as many as single PE case.

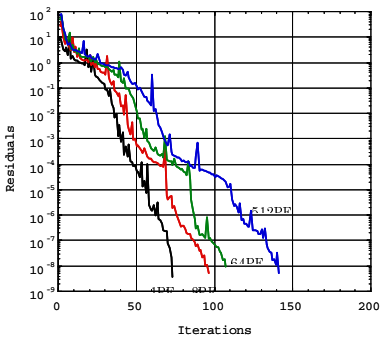

Figure 2: Iteration History for Poisson Eqn's in 64^3 Meshes by Localized ILU–BiCGSTAB Solver with Various Numbers of PEs

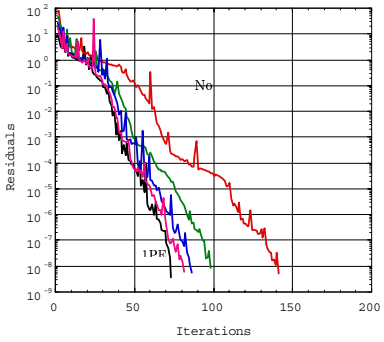

Figure 3: Iteration History for Poisson Eqn's in 64^3 Meshes by Localized ILU–BiCGSTAB Solver with 512 PEs Effect of Overlapping Depth

Fig.3 shows the case with overlapping effect for 512 PEs. In this case, iteration number decreases according to depth of overlapping although additional calculations and communications are required.

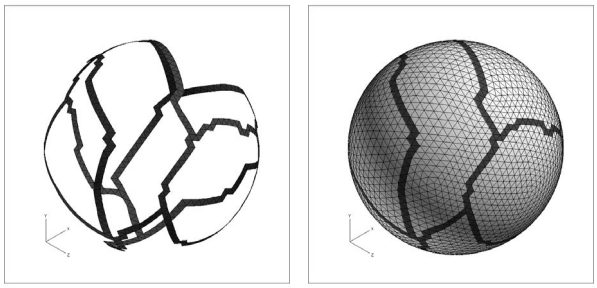

Figure 4: Surface Grid Partition of Geophysical Application Model in 8 Regions

Concluding remarks

Localized ILU/IC preconditioning suitable for parallel computing has been developed and evaluated. This method is efficient and stable even if PE number increases. The method is stabilized by considering overlapping effect in spite of some additional calculations and communications. Further calculations are going to be done for geophysical applications on the model such as in Fig.4. In order to get higher stability and efficiency for preconditioning, the following improvement are required :

- coarse grid smoothing
- effect of fill-in
- ordering

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