jh190022-NAJ

High performance simulations using FreeFem++ on mixed distributed-plus shared-memory architecture

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Supercomputers used to perform numerical simulations nowadays typically consist of clusters of multi-core processing units nodes. In such a cluster, there are two different kinds of workload distribution: through shared-memory, e.g., using POSIX threads or OpenMP, and through distributed memory, e.g., using MPI (Message Passing Interface). For numerical simulations of physical three-dimensional phenomena described by partial differential equations, it is essential to solve large linear and nonlinear systems usually stored as sparse matrices. A domain specific language, "FreeFem++" has capability to describe various multi-physics problems with variational formulation and to generate sparse linear systems. The aim of this project is to combine the high efficiency of Dissection direct sparse solver inside one node through shared-memory parallelism and the numerical robustness of HPDDM iterative solver over distributed nodes to tackle large-scale FEM problems.

1. Basic Information

(1) Collaborating JHPCN Centers

Cybermedia Center, Osaka University

(2) Research Areas

☒ Very large-scale numerical computation

☐ Very large-scale data processing

☐ Very large capacity network technology

☐ Very large-scale information systems

(3) Roles of Project Members

- Atsushi Suzuki (Cybermedia Center, Osaka University): Implementation of Dissection direct solver in HPDDM with GenEO
- Pierre Jolivet (CNRS, Toulouse Institute of Compter Science Research, France): Improvement of interface of HPDDM to FreeFem++
- Daisuke Furihata (Cybermedia Center, Osaka University): Principal contact of the research

2. Purpose and Significance of Research

Supercomputers used to perform numerical simulations nowadays typically consist of clusters of multi-core processing units nodes. In such a cluster, there are two different kinds of workload distribution: through shared-memory, e.g., using POSIX threads or OpenMP, and through distributed memory, e.g., using MPI. For numerical simulations of physical three-dimensional (3D) phenomena described by partial differential equations (PDE), it is essential to solve large linear and nonlinear systems usually stored as sparse matrices, whose dimensions are within the 10 to 100 million range. In this project, we are focused on the finite element method (FEM), which is, among other methods such as finite differences or finite volumes, a widely used method for discretizing PDEs. One of its advantages is that the FEM may handle irregular 3D geometries used as computing domains. Using a union of arbitrarily refined tetrahedral, one may pick a discretization accuracy according to the smoothness of the solution and the available computational resources. During the past decades F. Hecht et al. at Laboratoire Jacques-Louis Lions (LJLL), Sorbonne

Universite, have been developing a domain specific language, “FreeFem++”. It provides the most important and powerful tools to perform finite element analyses. This is done through a simple description of the weak formulation of a PDE using keywords very close to the actual mathematical formulation. It also provides automatic mesh decomposition for discretization, and operators to access or modify sparse and dense matrices or vectors. Through this language, linear systems from weak formulations with selected finite element space are automatically generated. The user only needs to describe nonlinear iterations and/or time evolution algorithms. Various kind of finite elements are available, e.g., standard piecewise polynomials in a tetrahedron for elasticity and fluid problems, vector-valued finite elements for oil reservoir simulation and semi-conductor problems, where satisfying a conservation principle is important, and edge elements designed specially for electromagnetic problems.

The aim of this project is to combine the high efficiency of direct solver whose name is “Dissection” inside of one node through shared-memory parallelism and the numerical robustness of iterative solver named “HPDDM” over distributed parallelism to tackle large-scale problems.

3. Significance as JHPCN Joint Research Project

There are several software engineering projects to implement numerical linear algebra algorithm to solve linear systems or to solve eigenvalue problems as a general purpose library, but almost of them result in solvers for problems consisting of dense matrices, and are not fit to solve sparse matrices that are obtained from discretization of PDEs. However, this project targets solution of linear sparse matrices generated in FreeFem++. Thanks to FreeFem++ and its ability to describe complex mathematical models, real-world three dimensional computations using a mixed shared- and distributed-memory parallelism will be feasible in different fields such as shape optimization or fluid–structure interaction. These will be directly applicable to various problems in the manufacturing industry.

In Japan, there is the "ADVENTURE" project, started in late 1990 to provide a finite element simulation software with domain decomposition methods. The software consists of several separated packages to perform numerical simulation of specific physical phenomena: heat flow, incompressible flow, elasticity, electromagnetic, where the user sets value of predefined physical parameters to fit physical models. This employs a completely different approach than the one of FreeFem++ with HPDDM, where the finite element matrices are generated from a given weak formulation.

An LU factorization of one million unknowns by multi-frontal methods, e.g., PARDISO, MUMPS, and Dissection, requires about 60GB memory and one million unknowns stays in a kind of sweat spot of the computational complexity with efficient use of cache memory to compensate low factor of byte/FLOP in modern multi-core architectures.

Cybermedia center of Osaka University has been providing vector- and scalar-architecture clusters. Both hardware resources are ideal platforms with multi- and many-core CPU to demonstrate effectiveness and robustness of the combined strategy of direct and iterative solvers enhanced by eigenvalue analysis in complex actual engineering and multi-physics problems that are currently only solvable by a monolithic direct solver.

4. Outline of Research Achievements up to FY2018

This project started in FY 2019.

5. Details of FY2019 Research Achievements

HPDDM provides a unified framework for domain decomposition methods including additive Schwarz methods and iterative substructuring methods. Those methods will be enhanced through GenEO. HPDDM has comparable performance to multigrid methods such as GAMG or BoomerAMG.

For linear system with one million unknowns, direct solvers based on the LU factorization may reach up to 40% of the peak performance of shared-memory architecture. The multi-frontal method and blocked operations lead to the task of dense matrix-matrix products, which is efficient on modern CPU.

A careful combination of Dissection and HPDDM is expected to deliver a high parallel efficiency, which could be applicable to a wide range of problem, easily prototyped through FreeFem++.

There are three steps, depending on the level of sophistication of preconditioner for domain decomposition iteration.

The first step is for the domain decomposition solver with both overlapping/non-overlapping subdomains without preconditioner. This implementation is rather straightforward to follow the existing routines to send and receive sparse matrices data and solutions of dense vector, for other director solvers, PARDISO and MUMPS. The improved interface is accessible through open source repository of HPDDM, https://github.com/hpddm/hpddm

The second step is for a preconditioner in the iterative substructuring method with enhanced coarse space, which is known as the balancing domain decomposition (BDD) method. Construction of coarse space is realized by collecting zero energy mode of the local stiffness matrix. Especially for the linear elasticity problem, the zero energy mode is explicitly written as set of rigid body vectors. Therefore, HPDDM has an interface to receive such vectors through FreeFem++, where user can define rigid body vectors based on geometrical information with finite element meshes. In contrast to HPDDM, ADVENTURE also uses BDD but a regularization parameter is employed to avoid singular matrices, which may perturb the convergence of a preconditioned iterative method when condition numbers are high. HPDDM follows mathematical setting of BDD without modification and archives fast and robust convergence. However difficulty comes for nonlinear elasticity problems. Newton iteration is a common tool to solve nonlinear system, but for finite element approximation to the nonlinear elasticity introduces some perturbation to the zero energy mode by interpolation. Therefore, it is impossible to predict exact eigenvectors corresponding to zero eigenvalue of the stiffness matrix explicitly.

Dissection has implemented a powerful algorithm for rank-deficient problem, which can numerically detect dimension of the kernel space of the large sparse matrix.

In addition to existing routines to pass data on sparse matrix and solution vector between Dissection local solver inside of the node and HPDDM over distributed nodes, dynamic allocation of kernel vectors which depends on characteristics of local matrix can handle automatic generation of the coarse space only by algebraic procedure without physical and/or mathematical knowledge of the finite element matrix.

The third step is for a sophisticated preconditioner named GenEO, which is also developed in LJLL. The main idea of GenEO is an extension of the coarse space consisting of zero eigenvalue to of smaller ones. GenEO utilizes information retrieved by performing concurrent eigenvalue analysis of each local problem. This is realized by different state-of-the-art numerical linear algebra libraries. For additive Schwarz methods with non-verlapping subdomains, the local problems consist of a sparse matrix and the local generalized eigenvalue problems are resolved by ARPACK, where a series of matrix-vector products are performed as part of the Arnoldi process. This process is furthermore preconditioned, and thus it is essential to solve linear systems with a sparse matrix, which requires usage of Dissection within ARPACK. For the iterative substructuring method, GenEO requires a dense eigensolver, as implemented in LAPACK using a tridiagonal-ization process. The generalized eigenvalue problems consist of a local Schur complement with Dirichlet boundary conditions, and a restriction of the global Schur complement. Here, it is necessary to compute all elements of the Schur complement using solutions of the direct solver with sparse right-hand sides (RHS).

6. Progress during FY2019 and Future Prospects

The key ingredient to enhance performance of combined packages “Dissection” and “HPDDM” is developed, which is realized by improvement of sparse multiple RHS solver of Dissection for creation of Schur complement matrix in the GenEO preconditioner. Dissection has better implementation to compute solution of linear system with multiple RHS of dense vectors. This procedure has been extended to sparse vector by analyzing nonzero pattern of the sparsity. Thanks to the binary tree structure of nested-dissection ordering, complexity of forward substitution could be at least half. More precise measurement on performance update will be a future issue.

The other progress is on implementation of FreeFem++ on vector architecture provided as NEC SX-ACE with proprietary C++ compiler. FreeFem++ is written with the standard C++11 features and template library. It was necessary to introduce slight modification of C++ template instantiation by adding explicit declarations. However, it is not possible to implement a useful feature of FreeFem++, dynamic loading facility due to lack of shared library system of SX-ACE operating system.

7. List of Publications and Presentations

(1) International conference Papers (Non-refereed)

[1] "Dissection sparse direct solver and parallel task management", *A. Suzuki*, HPC Asia 2020, Fukuoka, Japan

[2] "An industrial application of a free boundary problem with contact angle and volume constraint", *A. Suzuki*, 11th FreeFEM days, Paris, France

(2) Presentations at domestic conference (Non-refereed)

[3] “Finite element solution of a free boundary problem of the liquid phase with contact angle and volume constraint” *A. Suzuki*, 65th NCTAM, Sapporo, Japan