Efficient Developments of Parallel FE Programs Using HPC-MW

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Abstract. Recent computer systems have the hierarchical memory / network configurations. Processor type may be either a scalar or vector architecture. Due to such situation, it has become difficult to develop the simulation programs, which can attain the good effective performance on various systems. HPC-MW[1] is a series of upper-level libraries, which enables the software engineers to efficiently develop the parallel FE simulation codes optimized for various high-end computer environments. Functions supported by HPC-MW are re-ordering, matrix assembling, I/O, equation solvers, visualization, utilities for parallel computing and so on. Parallel iterative solvers inherits from those of the GeoFEM project[2] optimized for the Earth Simulator. Two types of parallel FE programs, i.e. the structural analysis code and the incompressible flow analysis codes have been developed using HPC-MW. Efficiency of the development process as well as the performance of the developed codes is described.

1 Introduction

Various types of HPC (High-Performance Computing) environments, including massively parallel computers and PC clusters, have recently become available. Moreover, advancement of "GRID" technology allows us to access a variety of computer resources very easily. However, in order to make the best use of these resources, we need optimization and tuning for individual hardware.

"HPC-Middleware (HPC-MW)[1]" is an infrastructure for developing optimized and reliable simulation codes making efficient use of procedures in the finite-element method (FEM). The source code developed on a PC with a single processor is easily optimized for various types of parallel computers including vector/scalar processors, SMP cluster architectures, and PC clusters by plugging-in the source code to the HPC-MW installed on the target computer (Fig.1). HPC-MW narrows the gap between compilers and applications. HPC-MW supports various kinds of capabilities required for FEM simulations, such as parallel I/O, parallel visualization, large-scale linear solvers, adaptive mesh refinement, dynamic load-balancing, and coupling for multi-component simulations.

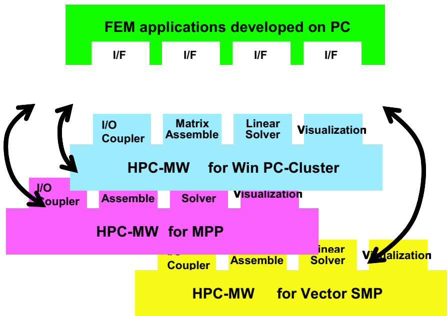

Fig. 1. FE applications developed on HPC-MW

Two types of parallel FE programs, i.e. the structural analysis code and the incompressible flow analysis code have been developed using HPC-MW. Efficiency of the development process as well as the performance of the developed codes is described.

2 Data Structure for the Distributed Memory Parallelization

In order to obtain the high parallel performance for the distributed memory environments, in particular, for the machine with hundreds of computational nodes, the data structure should be thoughtfully designed such that the data locality is sufficiently maintained and that the programming style is kept simple. The data structure of HPC-MW inherits from that of GeoFEM[3][4], which had been developed as one of the parallel FE programs optimized for the Earth Simulator[5]. Figure 2 schematically shows the data structure for the domain decomposition. The communication table, which tells the connection among the subdomains, is included in the mesh data. Thus, the SPMD type parallel program is realized.

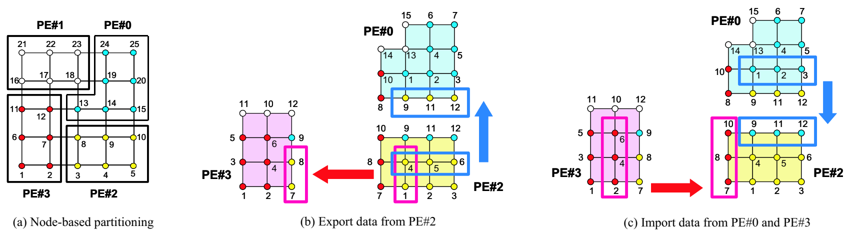

Fig. 2. Data structure for domain decomposition

3 Utilization of HPC-MW

HPC-MW provides dramatic efficiency, portability, and reliability in the development of simulation codes by FEM. For example, the number of steps of the source code is expected to be on the order of thousands, and the duration for parallelizing legacy codes is expected to be order of 2-3 weeks. HPC-MW is a library for scientific simulation but its approach for development is very unique. Scientific simulation methods such as FEM consist of typical and common procedures, such as re-ordering, matrix assembling, I/O, equation solvers, visualization. Conceptual source program utilizing HPC-MW is shown in Figure 3.

```
program sample_main
  use hpcmw
  implicit none
  type (hpcmwST_local_mesh) ::hpcMESH
  type (hpcmwST_matrix    ) ::hpcMAT
  character(len=HPCMW_FILENAME_LEN) :: name_ID

  call hpcmw_init

  call hpcmw_get_mesh(name_ID,hpcMESH)
      ……
      …… (matrix construction, etc)
      ……
  call hpcmw_solve_33 (hpcMESH, hpcMAT)

  call hpcmw_finalize

end program sample_main
```

Fig. 3. Conceptual source program utilizing HPC-MW

4 FE Parallel Applications Utilizing HPC-MW

The structural analysis code and the incompressible flow analysis codes have been developed using HPC-MW. The structural code called "FrontSTR", which will be released to the public through the web site, has functions of static and dynamic linear elastic analysis, eigen value analysis, elastic-plastic analysis and thermal analysis. Size of the source code is over 100,000 lines, and almost 75% of the code is hidden by HPC-MW, which implies that the amount of the application program is dramatically reduced.

Two types of flow analysis codes have been developed[6]. One is based on the fractional step algorithm in which the velocity is explicitly advanced in time, and the pressure Poisson's equation is solved at every time step. The other code, employing the SUPG/PSPG stabilization, solves the coupled equation of the velocity and the pressure at each time step. Both codes, though constructed with quite different solution algorithms, have been efficiently developed. As for the fractional step version, 57% of the code is hidden by HPC-MW. Figure 4 is the speed-up of the cavity flow analysis by the fractional step code.

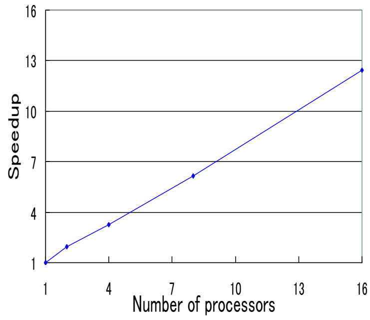

Fig. 4. Speedup of cavity flow computation (125,000 nodes, 2.8GHz Xeon cluster)

5 Concluding Remark

The idea of HPC-MW and its utilization for the development of parallel FE programs are described. Enhancement of HPC-MW is continuously conducted within the RSS21 (Revolutionary Simulation Software) project[7], 2005 - 2007, and its outcome including the source code will be open to the public through the web site.

ACKNOWLEDGEMENTS

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