Framework for Development of Data-Movement Centric Applications

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Motivation

In recent several years, we have been thinking about numerical algorithms and applications in the *Post Moore Era*. If we design and develop those on the Post-Moore supercomputer systems, we have to consider the following issues:

- High bandwidth in memory and network, Large capacity of memory and cache
- Large and heterogeneous latency due to hierarchy in memory and network
- Utilization of FPGA
- High concurrency with $O(10^3)$ threads on each node

Currently, *memory wall* is the most critical issue for performance of modern HPC systems. Therefore, increasing *compute intensity* is essential for extracting potential performance of such systems efficiently. Although strategies for design and development of numerical algorithms and applications on the Post Moore System are not so different from current ones, we should pay more attention to *data movement intensity*. Therefore, we believe that it is very important and helpful for the convergence of BDA and HPC to think about algorithms and applications in the Post Moore Era.

Numerical Algorithms towards Data Movement Intensity

We need the following libraries and frameworks for efficient development of applications on supercomputers in the Post Moore Era:

- Linear solver library for both of sparse and dense matrices
- Framework for automatic-tuning (AT)
- Framework for application development

Because *implicit schemes* are very feasible for such supercomputers, we need to design and develop efficient and robust implicit solvers for both of sparse and dense matrices.

Generally, parallelization and domain decomposition of FEM and FDM have been done in *space* direction. In order to keep scalability on future supercomputer systems with large number of nodes with hierarchical network, parallelization in *time* direction for time-dependent problems is essential. This type of method is called *parallel-in-space/time (PiST)*, and it can be effective if more than several hundred MPI processes are applied [1]. PiST approach is suitable for supercomputer systems with large latency and with network hierarchy in the Post Moore Era.

Since 2011, we have been developing *ppOpen-HPC* [2]. ppOpen-HPC is an open source infrastructure for development and execution of optimized and reliable simulation code on post-peta-scale (pp) parallel computers based on many-core architectures, and it consists of various types of libraries, which cover general procedures for scientific computation. ppOpen-HPC includes the four components, ppOpen-APPL (application development framework), ppOpen-MATH (math library), ppOpen-AT (automatic-tuning framework), and ppOpen-SYS (system software) (Fig.1).

Automatic tuning (AT) is one of the critical technologies for performance portability of scientific applications on future supercomputer systems in the Post Moore Era. ppOpen-AT is an framework for AT with directive-based special language, and automatically and adaptively generates optimum implementation for efficient memory accesses in the processes of methods for scientific computing in each component of ppOpen-HPC. Although ppOpen-AT provides *compute intensity*, we will develop new strategy for AT towards *data movement intensity* in this study.

Finally, we integrate these libraries (linear solvers (dense and sparse matrices), and AT capabilities into a new framework for application development.

Application Framework

In this study, we develop an extended version ppOpen-HPC (ppOpen-APPL and part of ppOpen-MATH) [2] by *parallel-in-space/time (PiST)* method [1] for supercomputer systems in the Post Moore Era. ppOpen-APPL is a set of libraries covering various types of procedures for five methods (FEM, FDM, FVM, BEM, and DEM), such as parallel I/O of data-sets, assembling of coefficient matrix, linear-solvers with robust and scalable preconditioners, adaptive mesh refinement (AMR), and dynamic load-balancing. ppOpen-MATH is a set of libraries for multigrid, visualization, loose coupling, etc. The following components of the application framework with *parallel-in-space/time (PiST)* method are developed:

- Nonlinear Algorithm
- Adaptive Mesh Refinement (AMR)
- Visualization
- Coupler for Multiphysics

Although the PiST method was originally implemented to linear time-dependent problems, it is also feasible for nonlinear problems [3]. We develop robust and efficient non-linear algorithm by PiST method and apply the developed method to integrated earthquake simulation code by FEM [4] developed by our collaborators.

ppOpen-MATH/MP is a coupling software applicable to the models employing various discretization (Fig.2). It was originally developed for coupled simulation of NICAM (atmospheric model, semi-unstructured FVM) and COCO (ocean model, structured FDM) on K computer [5]. The developed tool has been extended for coupling of general scientific applications developed in the ppOpen-HPC project, and applied to coupled earthquake simulation, where seismic wave propagation (Seism3D on ppOpen-APPL/FDM) and building vibration (FrontISTR+ on ppOpen-APPL/FEM) have been coupled [6]. Performance of the coupled code has been evaluated using 4,560 nodes (72,960 cores) of Fujitsu PRIMEHPC FX10 at the University of Tokyo (Oakleaf-FX). We develop a coupling tool with PiST. Moreover, we develop parallel AMR and visualization tools with PiST. Coupling, AMR and visualization are data-movement centric processes in scientific computing, and implementation of PiST to such processes is very challenging.

Finally, developed methods are validated through real simulations for atmosphere/ocean science, earthquake science, material science, fluid mechanics and structural engineering. Utilization of FPGA to complicated procedures of real applications are also evaluated.

References

[1] Falgout, R.D. et al., Parallel Time Integration with Multigrid, SIAM Journal on Scientific Computing, 2014

[2] Nakajima, K. et al., ppOpen-HPC: Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications on Post-Peta-Scale Supercomputers with Automatic Tuning (AT), Optimization in the Real World - Towards Solving Real-Worlds Optimization Problems, Mathematics for Industry 13, 15-35, Springer, 2015

[3] Falgout, R.D. et al., Parallel Time Integration with Multigrid Reduction for a Compressible Fluid Dynamics Application, LLNL-JRNL-663416, 1-15, 2015

[4] Ichimura, T. et al., Implicit Nonlinear Wave Simulation with 1.08T DOF and 0.270T Unstructured Finite Elements to Enhance Comprehensive Earthquake Simulation, IEEE/ACM Proceedings of SC15, 2015

[5] Arakawa, T. et al., Performance Evaluation and Case Study of a Coupling Software ppOpen-MATH/MP, Procedia Computer Science 29, 924-935, 2014

[6] Matsumoto, M. et al., Multi-scale Coupling Simulation of Seismic Waves and Building Vibrations Using ppOpen-HPC, Procedia Computer Science 51, 1514-1523, 2015

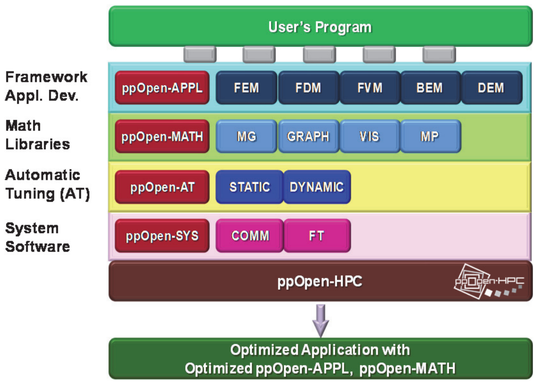

Fig.1 Overview of ppOpen-HPC [2]

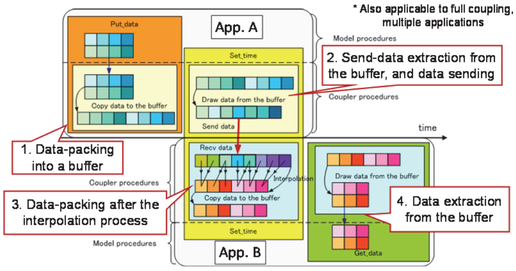

Fig.2 Data Flow in ppOpen-MATH/MP [6]