Numerical Libraries and Software Framework for Application Programs in the Post Peta Era

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- Most of supercomputers have cluster configuration.
  - Computational node & High-speed data network
- In a next generation high-end system, the computational node is expected to involve accelerators or many core processors.
  - A number of nodes, A number of cores, Accelerators
- Under this circumstance, how can we support application programmers?
  - To get high performance, following aspects should be considered
    - SIMD vectorization, Multi-threading, Communication optimization (reduced, avoided), Deep memory hierarchy

My opinion for numerical libraries and software framework

1) High performance multi-threaded computational kernel programs (for single node)
   - Linear solvers, eigenvalue solvers, matrix factorization etc.
   - Used for components of large-scale application programs
   - Used in various (lab-level) applications on PCs
- Large benefits to various numerical simulations including Big Data analyses

2) Support for large-scale simulations run on multiple nodes

- Focus on a specific analysis domain or a specific numerical method.
- Complete simulation package or software framework
  - By adding a couple of user subroutines and/or modifying the framework program, users develop their simulation program with minimum programming cost.

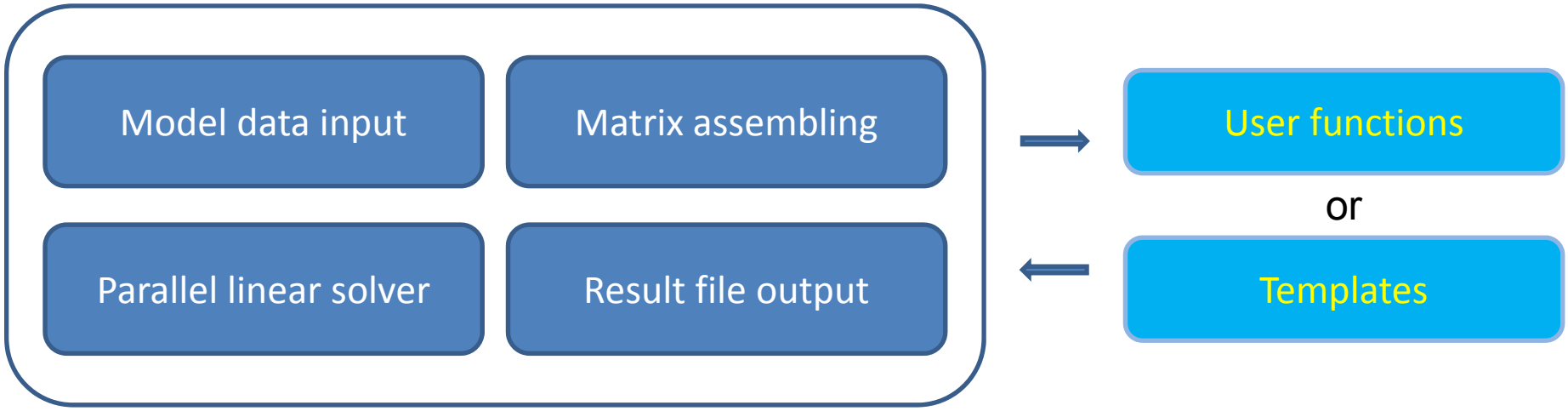
Software framework for parallel BEM analyses

A part of JST CREST project (leader: K. Nakajima@Univ. Tokyo)

http://ppopenhpc.cc.u-tokyo.ac.jp/ppopenhpc/

↳ Software can be downloaded.

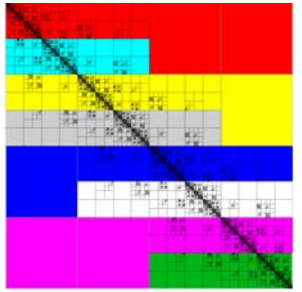
BEM-BB framework



A user obtains a BEM simulation code run on a distributed memory parallel computer by using the framework with user functions or templates, which describe the integral operations and boundary condition setting.

To accelerate the analysis we have developed a new H-matrix library (HacapK) which can be used with the framework.

The H-matrix library is based on hybrid parallel programming model, it can be utilized as a multi-threaded library for various simulations.



Distributed H-matrix

Multi-threaded linear solver

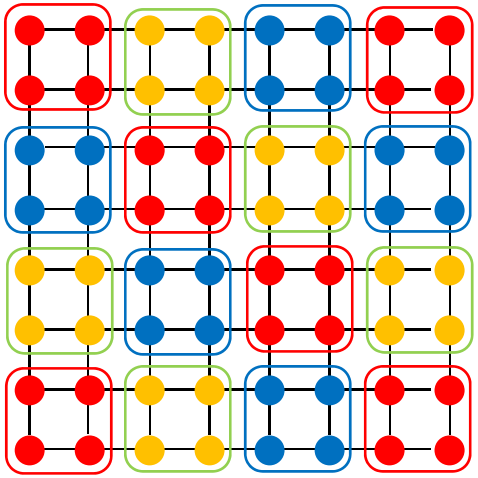
My colleagues and I have studied parallelization of sparse triangular solvers, mainly in a context of parallel ICCG solver.

A sparse triangular solver is also involved in Gauss-Seidel method and SOR method.

We proposed block multi-color ordering for high performance multi-threading of a sparse triangular solver.

T. Iwashita et al., "Comparison Criteria for Parallel Orderings in ILU Preconditioning", SIAM J. SC, 26 (2005), pp. 1234-1260.

T. Iwashita et al., "Algebraic block multi-color ordering method for parallel multi-threaded sparse triangular solver in ICCG method", IPDPS 2012.



Block multi-color ordering

When compared with the additive Schwarz type parallelization method, the proposed technique is advantageous on a many-core processor. Our technique was used for high performance HPCG benchmark implementation on a Xeon Phi coprocessor (Park et al., SC14).