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Developing Accuracy Assured High Performance Numerical Libraries for Eigenproblems

● Background

- Eigenproblem is one of essential numerical problems for several numerical simulations. Its accuracy, however, is not well-assured in many conventional numerical computations.
- Basic Linear Algebra Subprograms (BLAS) is a frequently used to perform linear algebra computations. Ensuring the accuracy of the computational results of BLAS operations is a still crucial problem now. Even in solving linear equations using LAPACK is also a typical example, because LAPACK is rich in BLAS operations, especially matrix-matrix multiplication (MMM) operations for solving linear equations.
- We focus on the following three topics:
  (1) Developing an accuracy assured numerical libraries for eigenproblems;
  (2) Development of high-performance implementation and AT technology for the developed accuracy assured numerical libraries;
  (3) Discussing an extension for non-liner problems based on obtained knowledge of accuracy assured algorithms.

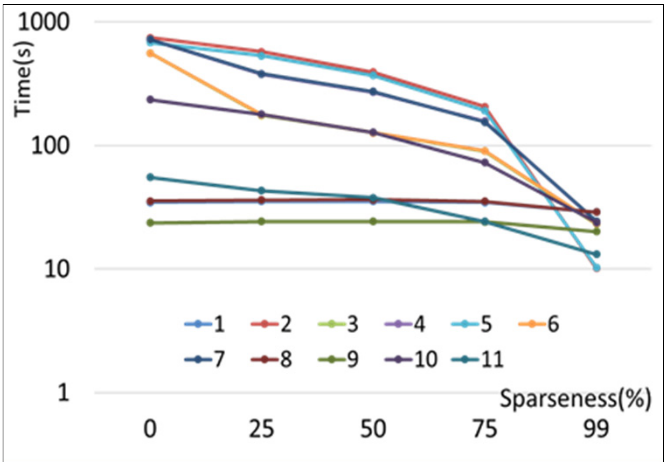
● Members

- Prof. Katagiri: high-performance implementation of Osaki method for recent multicore CPUs, and applying auto-tuning technologies.
- Prof. Hwang: Non-linear algorithms for actual engineering problems.
- Dr. Marques: Algorithms and implementations for eigenproblem.
- Prof. Nakajima: Sparse iterative algorithms for liner equation solvers, such as parallel preconditioners.
- Prof. Ogita: Iterative refinement algorithm to assure accuracy of real symmetric eigenproblem.
- Prof. Ohshima: GPGPU implementations.
- Prof. Ozaki: Accurate MMM algorithm (Ozaki method)
- Prof. Wang: Eigenvalue algorithms for actual engineering problems.

Current Result

● Accurate Matrix-Matrix Multiplication (Ozaki Method) on CPU and GPU

Execution Time in Ozaki method on the Reedbush-H. N=10,000 (U. Tokyo)



We have developed for 11 kinds of implementations for Ozaki method (DHPMM_F) in CPU and GPU. The implementations from No. 1 to No. 7 are CPU implementations. The above figure shows that the best implementation is changed according to the sparseness. This implies that auto-tuning facility is required to select the best implementation with respect to sparseness for input matrix.

Accuracy is assured for 1.5 million dimension problem!

● Research Plan

● The Year 2 (FY2020):

1) Topic 1: Improvement of high-performance implementation for UNC-HPC libraries.
2) Topic 2: Prototyping accuracy assured libraries for real symmetric eigenproblem.
3) Topic 3: Discussing extension to non-linear problems based on The Year 1-Topic 3.
4) Topic 4: Discussing and performance evaluation of auto-tuning for the Topics 1 and 2.

● Accuracy Assured Linear Equation Solver

[Evaluation A] Check real answer of large-scale linear equations for liner solver with residual iteration refinement. Using 1750,000 dimensions (A random matrix) for linear equations. Using 2500 nodes (80,000 cores) of the Fujitsu PRIMEHPC FX100. (Nagoya U.)

(First Step) Residual Norm: 4.019007e-14
(Second Step) Residual Norm: 0.000000e+00

[Evaluation B] Evaluate assured accuracy computation for solving linear equation with a random matrix. Given accuracy is improved by the iterative refinement procedure shown in the [Evaluation A].We set a real answer with (1,1,1,…,1)^T. Using 2500 nodes (80,000 cores) of the Fujitsu PRIMEHPC FX100. (Nagoya U.)

(1 million dimension) Upper bound of error: 1.111484e-16
(1.5 million dimension) Upper bond of error: 1.113360e-16