jh190015-NAJ

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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

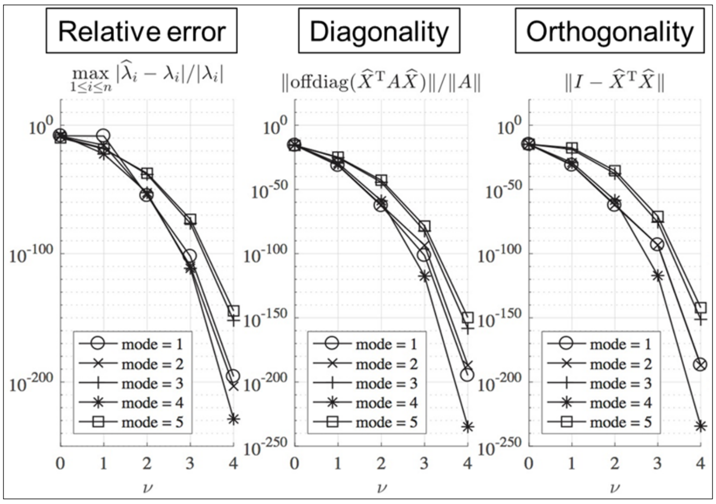
- Prof. Katagiri: high-performance implementation of Osaki method for recent multicore CPUs, and applying auto-tuning technologies.
- Prof. Hwang: Non-linear algorithms for actual engineering problems.
- Dr. Marques: Algorithms and implementations for eigenproblem.
- Prof. Nakajima: Sparse iterative 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.

● Refinement of Approximate Eigenvectors of a Symmetric Matrix

Input: $A = A^{\mathrm{T}} \in \mathbb{R}^{n\times n}$; $\widehat{X} \in \mathbb{R}^{n\times \ell}$
Output: $X' \in \mathbb{R}^{n\times \ell}$; $\widetilde{D} = \mathrm{diag}(\widetilde{\lambda}_i) \in \mathbb{R}^{\ell\times \ell}$; $\widetilde{E} \in \mathbb{R}^{\ell\times \ell}$; $\delta \in \mathbb{R}$

function $[X', \widetilde{D}, \widetilde{E}, \delta] \leftarrow \mathrm{RefSyEv}(A, \widehat{X})$
 $R \leftarrow I - \widehat{X}^{\mathrm{T}}\widehat{X}$
 $S \leftarrow \widehat{X}^{\mathrm{T}} A \widehat{X}$
 $\widetilde{\lambda}_i \leftarrow s_{ii}/(1 - r_{ii})$ for $i = 1, \cdots, \ell$ ▷ Approximate eigenvalues
 $\widetilde{D} \leftarrow \mathrm{diag}(\widetilde{\lambda}_i)$
 $\delta \leftarrow 2(\|S - \widetilde{D}\|_2 + \|A\|_2\|R\|_2)$
 $\widetilde{e}_{ij} \leftarrow \begin{cases} \dfrac{s_{ij} + \widetilde{\lambda}_j r_{ij}}{\widetilde{\lambda}_j - \widetilde{\lambda}_i} & \text{if } |\widetilde{\lambda}_i - \widetilde{\lambda}_j| > \delta \\ r_{ij}/2 & \text{otherwise} \end{cases}$ for $1 \le i, j \le \ell$
 $X' \leftarrow \widehat{X} + \widehat{X}\widetilde{E}$ ▷ Update $\widehat{X}$ by $\widehat{X}(I + \widetilde{E})$.
end function

● Result



We can confirm quadratic convergence!

● Research Plan

● The Year 1 (FY2019):

1) Topic 1: Performance evaluation of high-performance implementations for UNC-HPC libraries between multi-core and many-core CPUs and a GPU.
2) Topic 2: Designing accuracy assured libraries for real symmetric eigenproblem.
3) Topic 3: Discussing extension to non-linear problems.

Current Result

● Accurate Matrix-Matrix Multiplication (Ozaki Method)

Speedups using sparse operations in Ozaki method in the Fujitsu PRIMEHPC FX100. (Nagoya University)