jh210002-NAHI

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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.

● Main Contributors

- 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

● Prediction of execution time by AT in each GPU&CPU implementation in Ozaki Method (**DHPMM_F**)

Execution on the Supercomputer "Flow"(N=2000)

● **Predicted Time [s.] by proposed AT method**

Sparcity \ CPU&GPU Implementation Candidates	1	2	3	4	5	6	7	8	9	11
90	0.195	3.239	0.338	0.308	0.630	2.212	0.334	0.292	0.699	0.377
92	0.244	2.591	0.258	0.239	0.458	1.803	0.259	0.231	0.513	0.471
94	0.195	1.994	0.202	0.187	0.352	1.394	0.204	0.183	0.396	0.376
96	0.244	1.419	0.131	0.127	0.197	1.032	0.137	0.130	0.228	0.470
98	0.196	0.750	0.065	0.066	0.074	0.575	0.074	0.075	0.092	0.376

● **Relative Errors Between Predicted Time and Measured Time**

Maximum relative error 15.9%

Sparcity \ CPU&GPU Implementation Candidates	1	2	3	4	5	6	7	8	9	11
90	-2.9%	-3.7%	0.6%	-9.9%	-11.0%	5.0%	-0.4%	-7.6%	-10.7%	-1.1%
92	-2.6%	-2.1%	2.5%	-9.5%	-6.2%	-6.9%	3.3%	-4.6%	-6.2%	-0.9%
94	-3.6%	-4.0%	2.9%	-10.0%	-6.0%	15.9%	4.8%	-7.3%	-10.2%	-1.0%
96	-2.9%	-3.7%	11.1%	-7.6%	3.3%	11.5%	7.2%	-5.1%	4.1%	-0.9%
98	-3.6%	-1.6%	11.2%	-1.6%	-1.7%	3.8%	1.1%	-3.6%	-0.3%	-0.9%

We made a prototyping for an accuracy assured library for real symmetric eigenproblem with Ogita-Aishima method.

The results indicates that developed library with Ogita-Aishima method establishes speedup to **pdsyevd** routine (double precision) in LAPACK by using iteration.

In addition, the accuracy for the developed library is superior to **pssyevd** routine (single precision) in LAPACK.

● Research Plan

● The Year 3 (FY2021):

1. Topic 1: Establishing high-performance implementation for UNC-HPC libraries based on the Year 2-Topic 1. (CPU and GPU)
2. Topic 2: Developing accuracy assured libraries for real symmetric eigenproblem based on the Year 2-Topic 2. (CPU)
3. Topic 3: Discussing extension to non-linear problems based on The Year 2-Topic 3. (CPU)
4. Topic 4: Prototyping and developing AT based on the Year 2-Topics 1 and 2. (CPU and GPU)

● Evaluation result for an accuracy assured library for real symmetric eigenproblem ($N=2^{14}$)

[Eva. A] Supercomputer "Flow" (Type I Subsystem)

$n=2^{14}$, 4 Nodes	Pdsyevd (Double)	Pssyevd (Single)	Iterations to result of pssyevd by Ogita-Aishima method.		
			0th iter.	1st iter.	2nd iter.
time [s]	5.5e+01	3.2e+01	3.9e+01	4.6e+01	5.3e+01
$\max(\lvert D_i-\tilde{D}_i\rvert/\lvert D_i\rvert)$	8.9e-16	1.9e-06	2.7e-09	2.2e-09	5.9e-12
$\mathrm{median}(\lvert D_i-\tilde{D}_i\rvert/\lvert D_i\rvert)$	0.0e+00	3.1e-07	4.4e-11	3.3e-11	8.7e-16
$\lVert X-\tilde{X}\rVert/\lVert X\rVert$	2.6e-12	2.6e-03	2.5e-03	1.4e-05	5.9e-06

[Eva. B] Oakforest-PACKS

$n=2^{14}$, 64 Nodes	Pdsyevd (Double)	Pssyevd (Single)	Iterations to result of pssyevd by Ogita-Aishima method.		
			0th iter.	1st iter.	2nd iter.
time [s]	7.7e+01	6.5e+01	7.3e+01	8.1e+01	8.8e+01
$\max(\lvert D_i-\tilde{D}_i\rvert/\lvert D_i\rvert)$	8.9e-16	1.2e-06	7.8e-09	7.8e-09	6.5e-13
$\mathrm{median}(\lvert D_i-\tilde{D}_i\rvert/\lvert D_i\rvert)$	0.0e+00	1.7e-07	3.0e-11	2.0e-11	1.5e-16
$\lVert X-\tilde{X}\rVert/\lVert X\rVert$	2.6e-12	2.1e-03	2.0e-03	9.8e-06	3.7e-06