Performance Evaluation of Verified Computation for Linear Systems on Parallel Computers

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1. Introduction

We are concerned with the computational performance of a numerical algorithm with verification for linear systems

$$Ax = b.$$

The purpose of this research is to investigate the computational efficiency of verified computation for linear systems on parallel computers.

There are a number of numerical algorithms to verify an approximate solution obtained by a numerical algorithm [1, 2]. In the following, we introduce a fundamental theorem to calculate the error bound for an approximate solution.

Theorem Let A be a real $n \times n$ matrix and b be a real n-vector. Let $\tilde{x}$ be an approximate solution of $Ax = b$, x be an exact solution and R be an approximate inverse of A. If

$$\| RA - I \|_\infty < 1$$

for I denoting the $n \times n$ identity matrix, then A is nonsingular and

$$\| x - \tilde{x} \|_\infty \le \frac{\| R(A\tilde{x} - b) \|_\infty}{1 - \| RA - I \|_\infty}.$$

2. Verification algorithm

We assume that A is dense and that an approximate solution of $Ax=b$ is calculated through the LU decomposition of A and backward substitution. In the verification algorithm, an approximate inverse of A is needed, and we therefore calculate it from the LU factors.

Verification algorithm < Computational Cost >

1. Calculate an approximate solution — $\frac{2}{3}n^3 + O(n^2)$
   LU decomposition + backward substitution
2. Verify the approximate solution
   2.1 Check the nonsingularity — $\frac{10}{3}n^3 + O(n^2)$
   Inverse calculation using the LU factors
   Matrix matrix multiplication for RA
   2.2 Calculate the error bound — $O(n^2)$
   Matrix vector multiplication and etc.

< Theoretical Cost > without verification : with verification $\cong$ 1 : 6

How expensive on an actual parallel computer?

3. Evaluation on K computer and FX100

By using the K computer and the FX100 system, we compare the execution time between the computation with verification and that without verification (Fig. 1), and investigate their detail breakdown (Figs. 2 and 3).

ScaLAPACK routines used in numerical experiments

- Calculation of an approximate solution : pdgetrf + pdgetrs
- Calculation of an approximate inverse of A : pdgetri
- Matrix matrix multiplication : pdgemm
- Matrix vector multiplication : pdgemv

Computation without verification : pdgetrf + pdgetrs
Computation with verification : pdgetrf + pdgetri + pdgemm + pdgemv

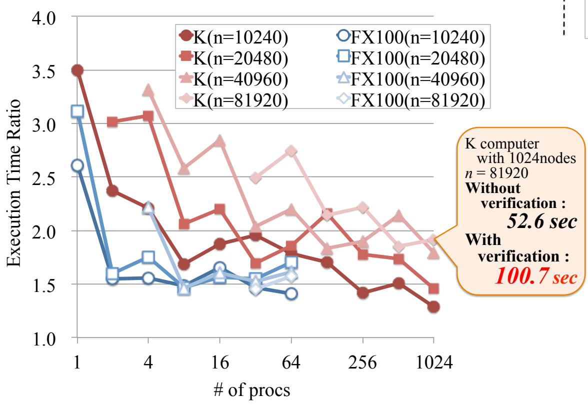

Fig.1: The ratio of execution time: with verification / without verification (K computer & FX100)

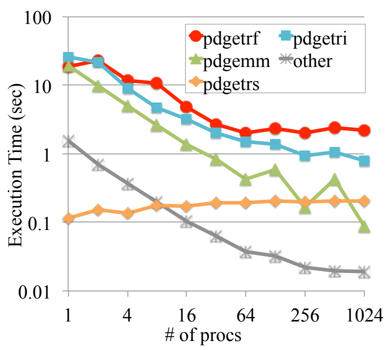

Fig. 2: Breakdown of execution time (K computer, n = 10240)

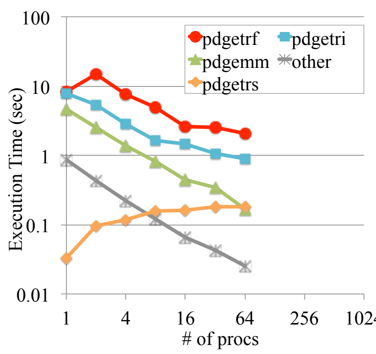

Fig. 3: Breakdown of execution time (FX100, n = 10240)

The relative execution time of the computation with verification to the computation without verification decreases as the number of processes increases. This is because "pdgetri" and "pdgemm" have better scalability than "pdgetrf" on parallel processing. It is also observed that the ratio tends to be smaller on the FX100 system than on the K computer.

Tab. 1: Computed error bounds (K computer, 1024 procs)

Matrix size (n)	Upper error bound
10240	2.20E-05
20480	1.51E-04
40960	1.15E-04
81920	3.12E-03

Note:
1) One node of the K computer has 8 cores. We assigned 1 MPI process per node and 8 threads per process.
2) One node of the FX100 system has 2 Core-Memory-Groups (CMGs), and each CMG consists of 16 computation cores. We assigned 1 MPI process per CMG (i.e. 2 processes per node) and 16 threads per process.
3) The elements of the test matrix A used in the evaluation were random numbers.

4. Conclusion

We presented the results of the performance evaluation of the verified computation for linear systems on the K computer and the FX100 system. The cost of the computation with verification is theoretically 6x that without verification. However, the execution time of the computation with verification was less than 2x that without verification when the number of the processes was sufficiently large. In order to clarify whether the computational cost for the verified computation can be acceptable, additional and detailed investigation is required. (e.g. is the current implementation of pdgetrf in ScaLAPACK optimal?)

Reference:
[1]. S. Oishi and S. M. Rump, Fast Verification of Solutions of Matrix Equations, Numer. Math., vol. 90, no. 4, pp. 755--773, 2002.
[2]. T. Ogita, S.M. Rump, and S. Oishi. Verified solution of linear systems without directed rounding. Technical Report 2005-04, Advanced Research Institute for Science and Engineering, Waseda University, Tokyo, Japan, 2005.

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