Research on Accuracy Assurance and Auto-tuning

Takahiro Katagiri (Information Technology Center, Nagoya University, E-mail: katagiri@cc.nagoya-u.ac.jp)
Takeshi Ogita (Tokyo Woman's Christian University, E-mail: ogita@lab.twcu.ac.jp)
Katsuhisa Ozaki (Shibaura Intitule of Technology, E-mail:ozaki@sic.shibaura-it.ac.jp)

Verified Numerical Computations for Linear Systems

Introduction

The target problem is to solve a large-scale linear system

$$Ax = b,\ A \in R^{n\times n},\ x, b \in R^n,$$

where A is a dense matrix.
We produce an approximate solution and its error bound using a super computer.

Verification Methods

R: an approximate inverse of A
$\tilde{x}$: an approximate solution of $Ax = b$
I: the identity matrix
If $\|RA - I\| < 1$ is satisfied, then

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

We adopt the maximum norm for the above inequalities.
Ref. S. Oishi, S. M. Rump: Fast verification of solutions of matrix equations, Numer. Math., 90:4 (2002), pp. 755-773.

Experimental Settings

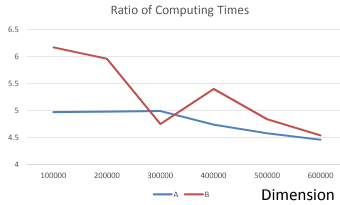
- FUJITSU Supercomputer PRIMEHPC FX100 in Nagoya University
  - Total Nodes: 2,880
  - Cores per node: 32
  - Peak per node: 1.126TFLOPS (Binary64)
  - Memory per node : 32GB
- Set A as a random matrix.
- Set b such that $x \approx (1,1,\dots,1)^T$.

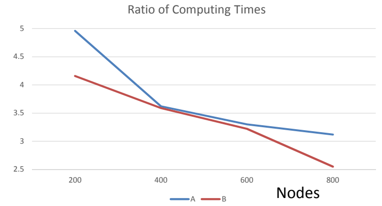
Results

Error Bounds:

Dim.	$1*10^5$	$2*10^5$	$3*10^5$	$4*10^5$	$5*10^5$
E-bound	3.38e-07	8.01e-06	3.29e-06	1.52e-05	6.35e-06

Computing Times:





Method A: #MPI procs. == #nodes
Method B: #MPI procs. == 2*#nodes
Ratio: Time for approximate solutions (PDGESV in ScaLAPCK) is normalized to 1.
Theoretical Ratio (of operations) is 9.

The actual ratio of computing time is much less than 9!

Large-scale Problem:

- Up to 1,750,000 dimensional problem, we have produced an approximate solution and its error bound using 2,500 nodes on FX100.

Dynamic Selection of Preconditioners by Deep Learning

Introduction

Selection of preconditioners for sparse iterative solver is one of crucial issues for many numerical simulations. It is difficult to select the best preconditioners without expert knowledge. In this research, we are developing an auto-tuning (AT) method for the selection by using deep leaning (DL). To adapt DL for the selection, we utilize feature image for input sparse matrices.

Proposed Method

Our method is based on conventional AT approach with DL by Yamada, et. al, in 2018. In this method, color image for the input sparse matrix is used. In our example, the best preconditioners is dynamically changed according to time step on an application. Hence dynamic selection of preconditioners is required.

To solve the above new requirement, we propose an approach for the color images for learning phase. In the application, elements of right-hand-side vector for liner equations, are dynamically changed. To utilize this feature, we make a new image by dividing each pixel by the element by row.

Experimental Settings

- **FFVC (FrontFlow/violet Cartesian)**: A simulator for three dimensional Unsteady incompressible heat flow with cartesian mesh is used.
  *According to a simulation parameter, number of iterations for linear equation solver is dramatically increase. → Need of dynamic preconditioner selection.
- **Xabclib** is used for sparse iterative solver (Restart GMRES method).
- **Tensorflow 2.2.0** is used for DL tool.

Result

The Best Preconditioner

- Accelerating Time (a simulation parameter for FFVC) is set to 0.3.
- 6 Kinds of preconditioners (None, Jacobi, SSOR, ILU0D, ILU0,and ILUT) on Xabclib are checked.
- Time step on simulation: 0 [s] to 800 [s].

The best preconditioner	Number of the best preconditioner
JACOBI	1959
ILU0	140

Estimation Accuracy by the Proposal AT Method

		prediction	
		JACOBI	ILU0
real	JACOBI	1938	21
	ILU0	5	135

This research is a study of FY2020 master thesis by Ryoto Yamamoto in Graduate School of Informatics, Nagoya University.