Verified Solutions of Large Sparse Linear Systems Arising from 3D Poisson Equation

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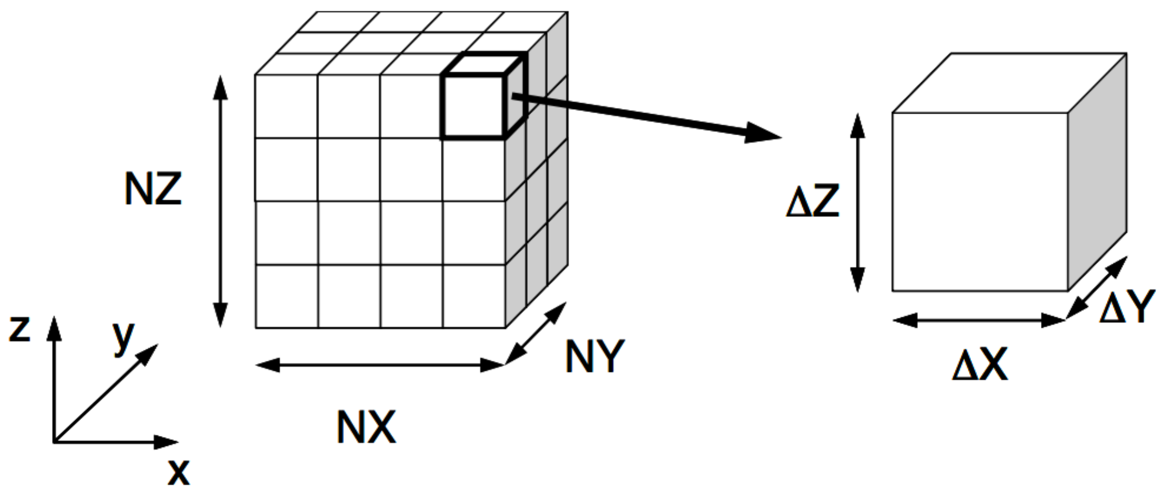
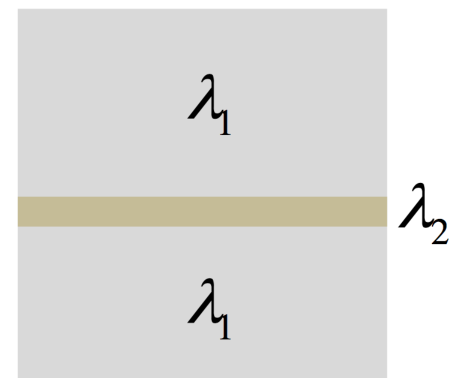
Outline

- Develop verified solutions of linear systems discretized from 3D Poisson equation

→ Frequently used for benchmarking in HPC





$$-\nabla \cdot (\lambda \nabla \phi) = f, \quad f(x,y,z) = x + y + z$$

(Dirichlet boundary condition)

λ : thermal conductivity

$$\frac{\lambda_1}{\lambda_2} \sim \mathrm{cond}$$

λ_2 is considered as thermal insulation.

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What we focus on

PDE (3D Poisson equation)

↓ Discretization by FDM, FEM, etc.

- Discretization error
- Rounding error

Linear system $Ax = b$

↓ Iterative solver, such as CG, GMRES, etc.

- Truncation error
- Rounding error

Approximate solution

In this talk, we consider this part. (Linear system $Ax = b$ → Approximate solution)

Condition

- 7-point FDM mesh
- Discretized by finite volume method

↓

- Matrices have M-property. $(A^{-1} \geq O)$
- We can apply fast verification methods [1,2] for linear systems with M-matrices.

[1] T. Ogita, S. Oishi, Y. Ushiro: Fast verification of solutions for sparse monotone matrix equations, Computing, Supplement **15** (2001), 175-187.

[2] A. Minamihata, K. Sekine, T. Ogita, S. M. Rump, S. Oishi: Improved error bounds for linear systems with H-matrices, Nonlinear Theory and Its Applications, IEICE, **6:3** (2015), 377-382.

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Verification algorithm (1)

1. Solve a discretized linear system $Ax = b$.
   - $\hat{x}$: a computed solution
2. Solve a linear system $Ay = e$ where all elements of e are 1's.
   - $\hat{y}$: a computed solution
3. Verify M-property of A using $\hat{y}$. $(\hat{y} > 0 \;\Rightarrow\; A\hat{y} > 0)$
4. Compute an error bound using

$$\|x - \hat{x}\|_\infty \leq \frac{\|\hat{y}\|_\infty \|b - A\hat{x}\|_\infty}{1 - \|e - A\hat{y}\|_\infty}$$

if $\|e - A\hat{y}\|_\infty < 1$.

$$\|A^{-1}\|_\infty \leq \frac{\|\hat{y}\|_\infty}{1 - \|e - A\hat{y}\|_\infty}$$

Numerical results (1)

- Computer: Reedbush-U (1 node)
  - Intel Xeon E5-2695v4 (2.1GHz, 18 cores) x 2 sockets
  - 1.21 TFLOP/s per socket
  - 256 GiB (153.6GB/s)
- Solver: ICCG with CM-RCM, MC(20)
- Stopping criteria:
  - For $Ax = b$, $\frac{\|b - A\hat{x}\|_2}{\|b\|_2} < 10^{-12}$
  - For $Ay = e$, $\|e - A\hat{y}\|_\infty < 10^{-2}$
- FP64 (double precision), OpenMP (36 threads)

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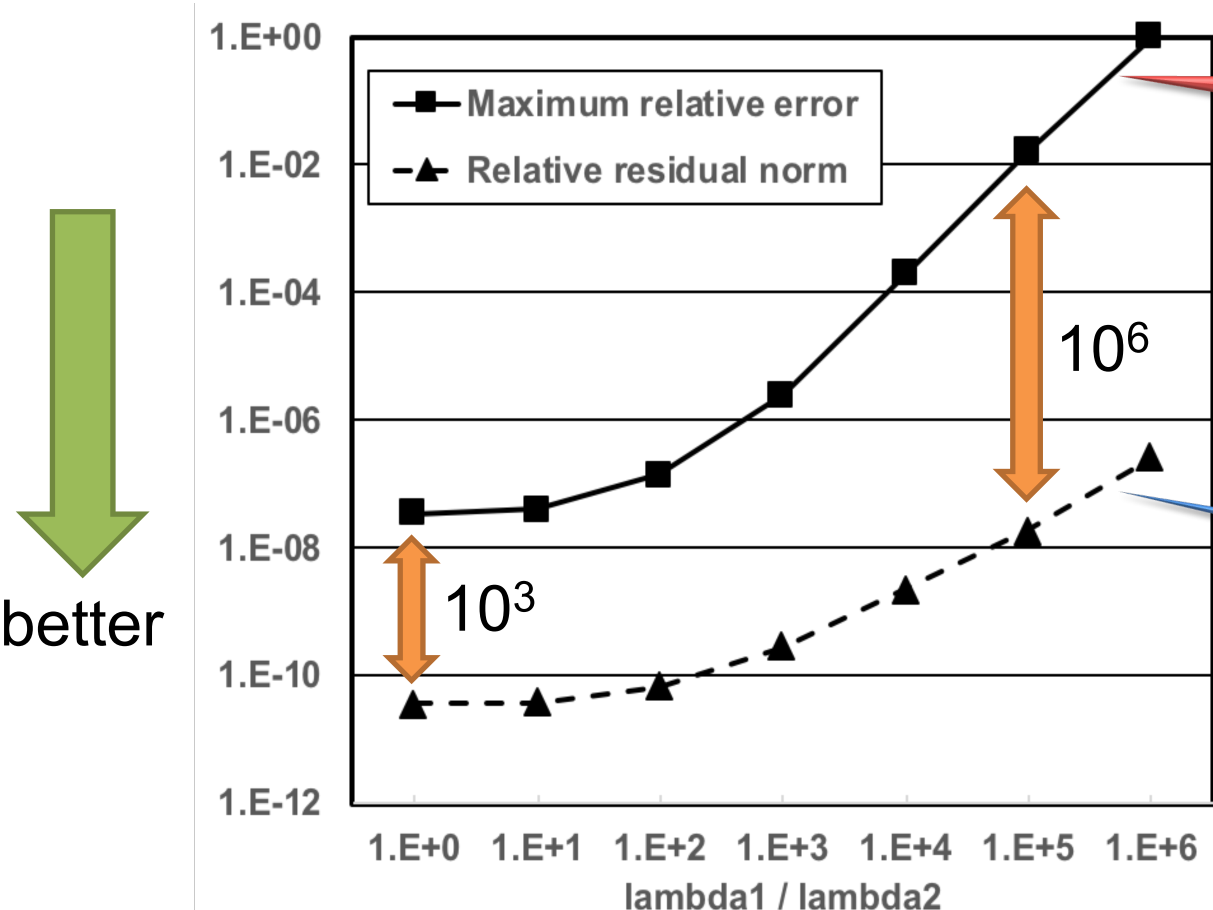
Result (1-1): $\lambda_1 = \lambda_2 = 1.0$ NX=NY=NZ=128 (n = 2,097,152)

- Upper bounds of maximum relative error and relative residual norm:
  - $\max_{1 \le i \le n} \left| \frac{x_i - \hat{x}_i}{x_i} \right| \le 3.38 \times 10^{-8}$
  - $\frac{\|b - A\hat{x}\|_2}{\|b\|_2} < 3.66 \times 10^{-11}$
- Computing time

	Approximation (Solve $Ax = b$)	Verification (Solve $Ay = e$)
Elapsed time (sec.)	3.75	1.60
#iterations for ICCG	415	176

Result (1-2): NX=NY=NZ=128

Vary $\lambda_1/\lambda_2 \sim \mathrm{cond}$ between 1 and 10^6



Error bound

$$\max_{1 \le i \le n} \left| \frac{x_i - \hat{x}_i}{x_i} \right|$$

Residual norm

$$\frac{\|b - A\hat{x}\|_2}{\|b\|_2}$$

It is difficult to estimate the error of a computed solution only from residual norm!

Improved error bound

- To reduce the overestimation, we replace

$$\|x - \hat{x}\|_\infty \le \frac{\|\hat{y}\|_\infty \|b - A\hat{x}\|_\infty}{1 - \|e - A\hat{y}\|_\infty}$$

by

$$\|x - \hat{x}\|_\infty \le \|\hat{z}\|_\infty + \frac{\|\hat{y}\|_\infty \|b - A(\hat{x} + \hat{z})\|_\infty}{1 - \|e - A\hat{y}\|_\infty}.$$

$$x - \hat{x} = A^{-1}(b - A\hat{x}) = \hat{z} + A^{-1}(b - A(\hat{x} + \hat{z}))$$

- The correction term $\hat{z}$ is obtained by solving a linear system $Az = r$ with $r = b - A\hat{x}$.

[3] T. Ogita, S. Oishi, Y. Ushiro: Fast inclusion and residual iteration for solutions of matrix equations, Computing, Supplement **16** (2002), 171-184.

Verification algorithm (2)

1. Solve a discretized linear system $Ax = b$.
2. Solve a linear system $Ay = e$.
3. Verify M-property of A using $\hat{y}$. ($\hat{y} > 0 \;\Rightarrow\; A\hat{y} > 0$)
4. Compute $r = b - A\hat{x}$ with an error bound.
   - $\hat{r}$: a computed residual, e_r: an error bound of $\hat{r}$
5. Solve a linear system $Az = \hat{r}$.
6. Compute an error bound using

$$\|x - \hat{x}\|_\infty \le \|\hat{z}\|_\infty + \frac{\|\hat{y}\|_\infty(\|\hat{r} - A\hat{z}\|_\infty + \|e_r\|_\infty)}{1 - \|e - A\hat{y}\|_\infty}.$$

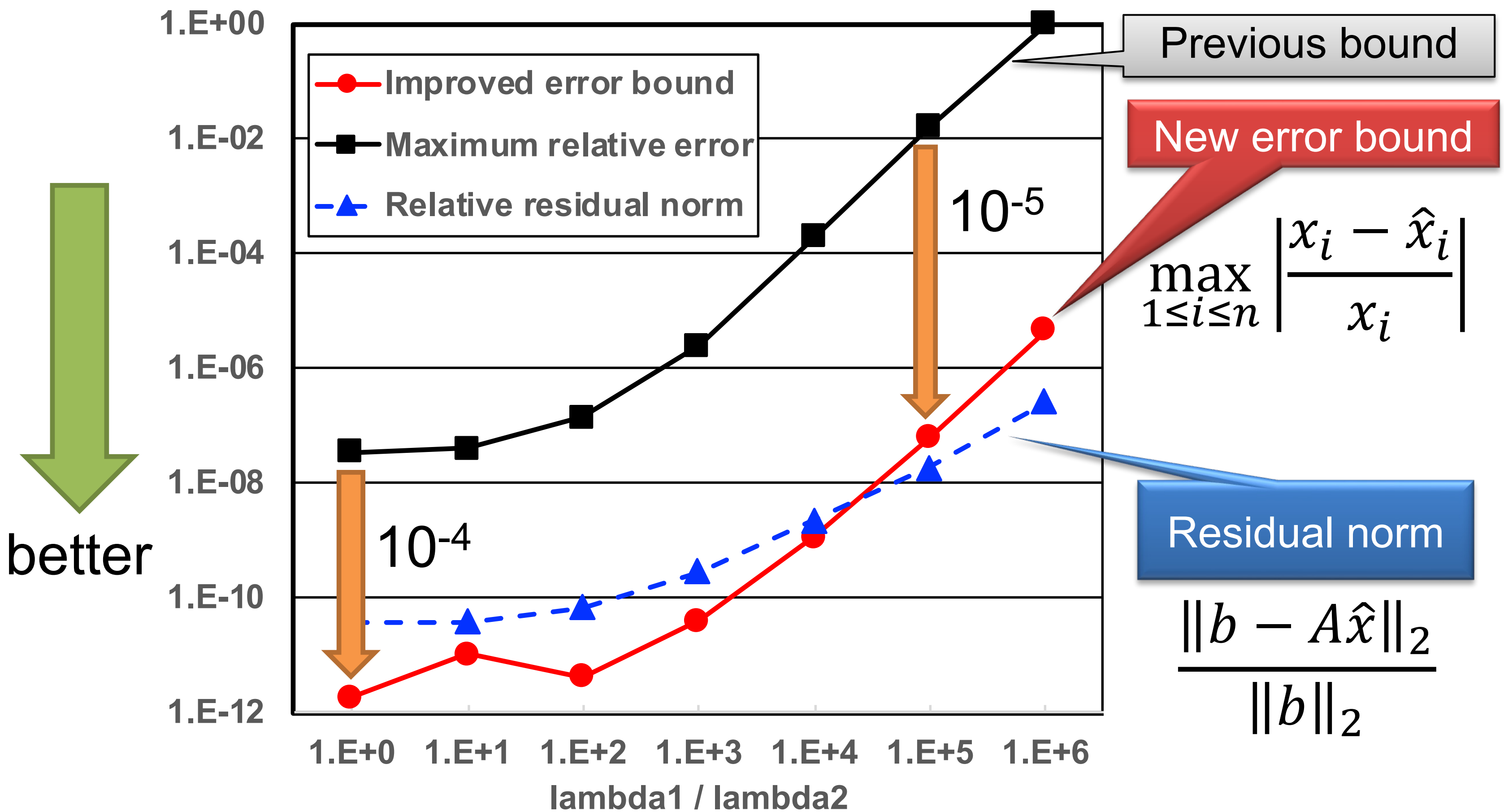
[4] T. Ogita, S. M. Rump, S. Oishi: Accurate sum and dot product, SIAM Journal on Scientific Computing, **26:6** (2005), 1955-1988.

Numerical results (2)

- Computer: Reedbush-U (1 node)
  - Intel Xeon E5-2695v4 (2.1GHz, 18 cores) x 2 sockets
  - 1.21 TFLOP/s per socket, 256 GiB (153.6GB/s)
- Solver: ICCG with CM-RCM, MC(20)
- Stopping criteria:
  - For $Ax = b$, $\frac{\|b - A\hat{x}\|_2}{\|b\|_2} < 10^{-12}$
  - For $Ay = e$, $\|e - A\hat{y}\|_\infty < 10^{-2}$
  - For $Az = \hat{r}$, $\frac{\|\hat{r} - A\hat{z}\|_2}{\|\hat{r}\|_2} < 10^{-9}$
- FP64 (double precision), OpenMP (36 threads)

Result (2-1): NX=NY=NZ=128

Vary $\lambda_1/\lambda_2 \sim \mathrm{cond}$ between 1 and 10^6



Computed error bounds are significantly improved!

Result (2-2): Computing time

- Elapsed time (sec.) and #iterations for ICCG

NX=NY=NZ=128 (n = 2,097,152)	Approximation (Solve $Ax = b$)	Verification (Solve $Ay = e$ and $Az = \hat{r}$)
$\lambda_1/\lambda_2 = 1$	3.75 (415)	4.47 (493 = 176 + 317)
$\lambda_1/\lambda_2 = 10^6$	6.83 (686)	7.85 (777 = 328 + 449)

NX=NY=NZ=256 (n = 16,777,216)	Approximation (Solve $Ax = b$)	Verification (Solve $Ay = e$ and $Az = \hat{r}$)
$\lambda_1/\lambda_2 = 1$	76.64 (903)	80.89 (964 = 387 + 577)
$\lambda_1/\lambda_2 = 10^6$	110.15 (1377)	120.07 (1504 = 639 + 865)

Future work

1) Accelerate verification process:
   - Apply mixed-precision approach
   - Optimization with double right-hand side
2) Consider the discretization error
3) Develop efficient verification algorithms for other matrix classes:
   - For example, positive definite matrices