# Condition Number Estimation in a Solution Process of a Large and Sparse Linear System

Yuya Kudo[1], Yuki Satake[1], Takeshi Fukaya[1], Takeshi Iwashita[2]
1: Hokkaido University 2: Kyoto University

## 1. INTRODUCTION

### ◆ Solving a system of linear equations

▶ We consider solving a system of linear equations (SLE).

$$A\boldsymbol{x} = \boldsymbol{b}$$

- $A$ : large sparse coefficient matrix ($N \times N$)
- $\boldsymbol{x}$ : solution vector
- $\boldsymbol{b}$ : right-hand side vector

▶ This equation often appears in a wide variety of applications.
E.g) Thermal dynamics, Electrodynamics,…

▶ The iterative methods are typically used to solve the linear system.

**The iterative method**

▶ A defined procedure is repeated to update an approximate solution.
▶ It is important to know when to stop the repetition.
→ Judge convergence based on the residual vector $\boldsymbol{r}$ ($:= A\boldsymbol{x} - \boldsymbol{b}$).
It is common to stop iterations when $\frac{\|\boldsymbol{r}\|_2}{\|\boldsymbol{b}\|_2} \leq \varepsilon$.

Here, $\frac{\|\boldsymbol{r}\|_2}{\|\boldsymbol{b}\|_2}$ is the relative residual norm, $\varepsilon$ is defined threshold.

### ◆ Background

It is important to estimate the error of an approximate solution $\tilde{\boldsymbol{x}}$.
The error vector is calculated as $\boldsymbol{e} = \boldsymbol{x}^* - \tilde{\boldsymbol{x}}$ ($\boldsymbol{x}^*$: the exact solution).
**Problem** It is difficult to calculate the relative error norm.
(There is no information on the exact solution.)

Indirectly assess the indicator using the following inequality. :

$$\frac{\|\boldsymbol{e}\|_2}{\|\boldsymbol{x}^*\|_2} \leq \kappa_2(A)\frac{\|\boldsymbol{r}\|_2}{\|\boldsymbol{b}\|_2}, \quad \kappa_2(A) = \|A\|_2\left\|A^{-1}\right\|_2$$

Here, $\kappa_2(A)$ is called the (2-norm) condition number of $A$.
$\kappa_2(A)$ is important for evaluating the accuracy of the solution.

## 2. RESEARCH SUMMARY

### ◆ Problem setting

- $A$ is a large sparse symmetric positive-definite matrix.
→ $\kappa_2(A)$ is given by $\kappa_2(A) = \lambda_{\max}/\lambda_{\min}$
($\lambda_{\max}$ : largest eigenvalue of $A$, $\lambda_{\min}$ : smallest eigenvalue of $A$)
- Calculating $\kappa_2(A)$ while solving a SLE.
- We use a (parallel) ICCG solver.

### ◆ Research assignment and content

▶ Estimating the smallest eigenvalue can be challenging.
→ We consider two eigenvalue solvers for large-scale matrix.
- Lanczos method
- Error vector sampling (ES) method [1]

▶ The additional cost of computing $\kappa_2(A)$ may be high.
→ Combine identical calculations for greater efficiency.

**Research Purpose**
To evaluate two methods for estimating the condition number.

**Research contents**
▶ Evaluate the accuracy of the condition number $\kappa_2(A)$.
▶ Discuss computational cost when running alongside with the ICCG.

## 3. METHOD

**Eigenvalue Problem**

$$A\boldsymbol{v} = \lambda\boldsymbol{v}$$

**Calculate the condition number**

$$\kappa_2(A) = \frac{\lambda_{\max}}{\lambda_{\min}}$$

**Apply the Rayleigh-Ritz method.**
Set a subspace and calculate approximate eigenvalues of $A$.
▶ Lanczos method : Krylov subspace → Obtain $\lambda_{\max}$ and $\lambda_{\min}$.
▶ ES method : Space spanned by the error vector → Obtain $\lambda_{\min}$.
**Note** The maximum eigenvalue is obtained by the power method.

## 4. COMPUTATIONAL COST

SpMV needs to be calculated for each method.
(SpMV is sparse matrix-vector multiplication.)

**ICCG method** Compute SpMV for the search direction vector.
**Lanczos method** Compute SpMV for a subspace configuration.
**ES method** Compute SpMV for the power method.

Compute of SpMV $A\boldsymbol{w}_1$, $A\boldsymbol{w}_2$ for any vectors $\boldsymbol{w}_1$, $\boldsymbol{w}_2$.

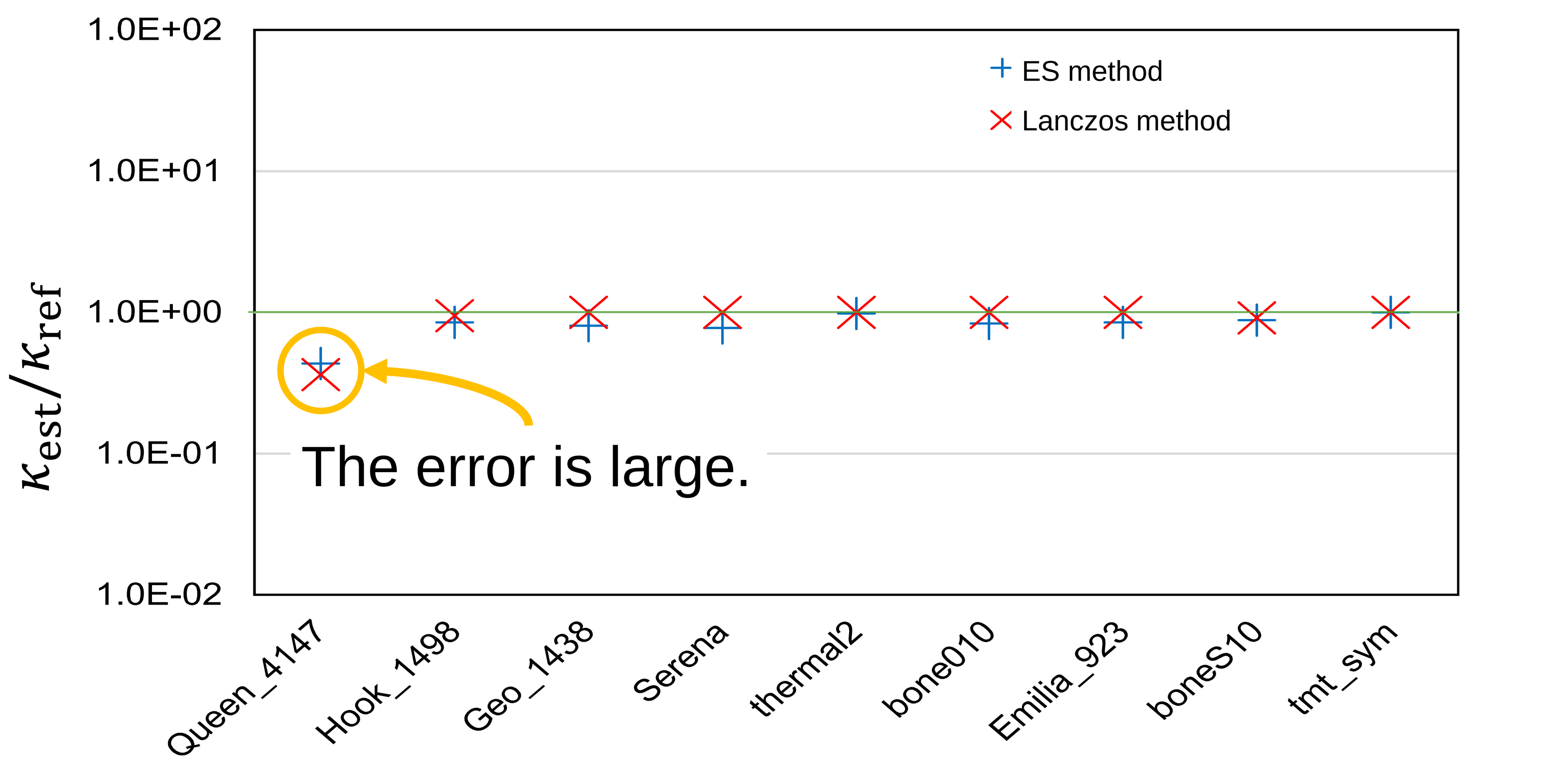
Using blocking for $A[\boldsymbol{w}_1, \boldsymbol{w}_2]$ can make the computation more efficient.

## 5. NUMERICAL RESULTS

▶ We use 9 different test matrices with over 500,000 dimensions.
▶ We use the Localized IC preconditioning for parallelization of ICCG.
▶ We use one node of the Grand Chariot at Hokkaido University.
(Intel Xeon Gold 6148 (2.4 GHz, 20-Core) x2 and 384GB memory)
▶ Compiler : Intel icc (2022.3.1) and mkl (2022.0.2, with -mkl=parallel)
▶ Runs on 40 threads.

### ◆ Accuracy

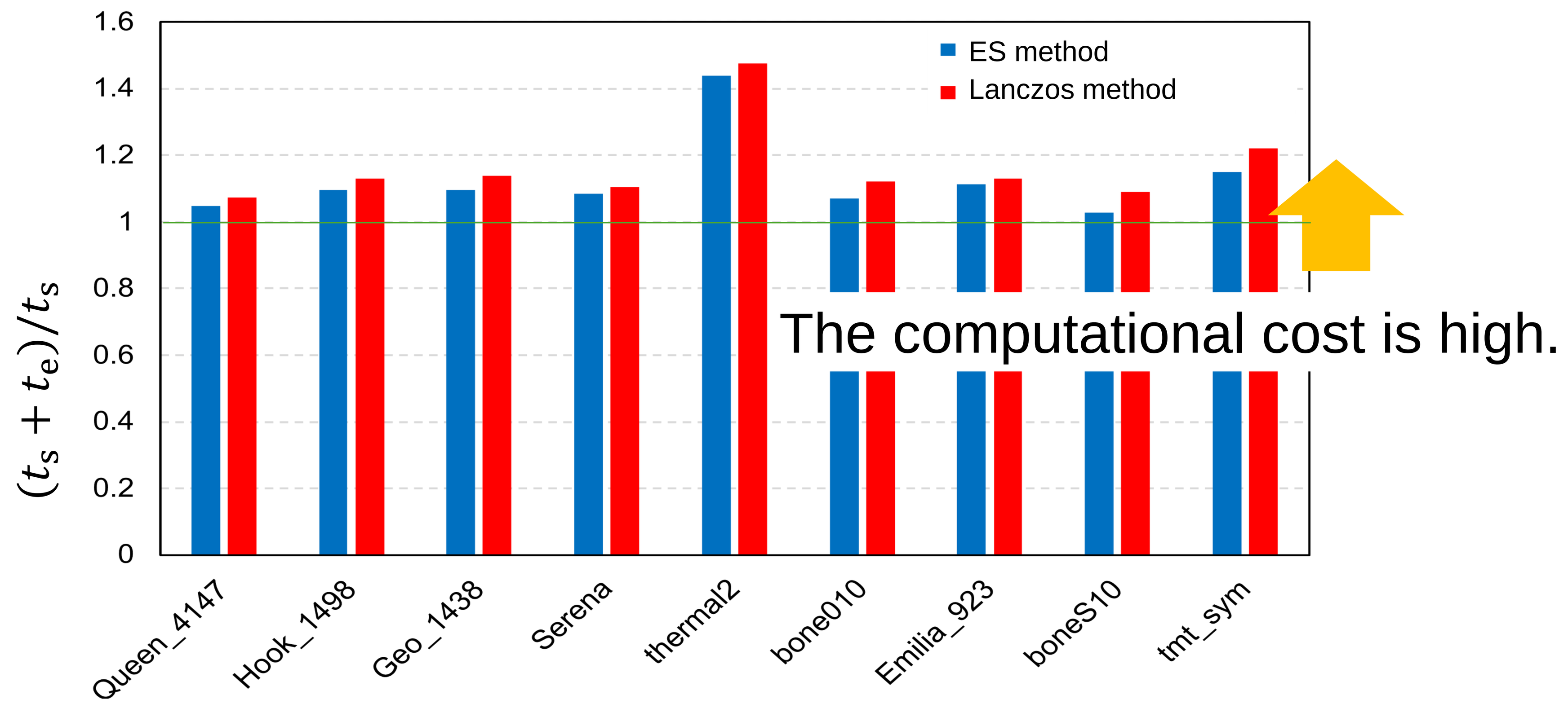
Two methods are comparable in terms of the accuracy.




$\kappa_{\text{ref}}$ : reference value, $\kappa_{\text{est}}$ : estimated value
($\kappa_{\text{ref}}$ is calculated by the power method and inverse iteration method)

### ◆ Execution time

Both methods could estimate $\kappa_2(A)$ in 10-20% of the solution time.
(Excluding thermal2)




$t_s$ : time for solution process
$t_e$ : additional time for the condition number estimation

## 6. CONCLUSION

**Conclusion**
▶ We examined two condition number estimation methods.
▶ Both methods can be used for the condition number estimation.

**Future work**
▶ We consider non-symmetric matrices.

## REFERENCE

[1] Takeshi Iwashita, Kota Ikehara, Takeshi Fukaya, and Takeshi Mifune. 2023. Convergence acceleration of preconditioned conjugate gradient solver based on error vector sampling for a sequence of linear systems. NLAA (2023), e2512