A parameter tuning technique of a weighted Jacobi-type preconditioner and its application to supernova simulations

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Introduction

- Today's targets

>> Target algorithms

-- We consider ***preconditioning techniques*** for Krylov subspace methods to solve very large, but sparse, linear systems:

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

where *A* is assumed to be nonsymmetric and nonsingular.

>> Target situation

-- The algorithms are used for recent large scale simulations

-> ***high parallel efficiency*** is recognized as extremely important more than high speed and/or high accuracy

Introduction

- Today's targets
  - >> Target preconditioner
    - -- Iterative-type preconditioner based on ***Jacobi iteration***, which has high parallel efficiency

- Today's goals
  - >> ***Introduce a weighted Jacobi-type iteration*** as an improvement of the Jacobi iteration
  - >> ***Propose a parameter tuning technique*** for the weighted Jacobi-type iteration used for preconditioners
  - >> ***Evaluate the performance*** of the parameter tuning technique on the supernova simulation




Outline

- Introduction

- Weighted Jacobi-type iteration used for preconditioners
  >> Krylov subspace methods and preconditioners
  >> Weighted Jacobi-type iteration

- Parameter tuning technique

- Numerical experiments and results

- Conclusions



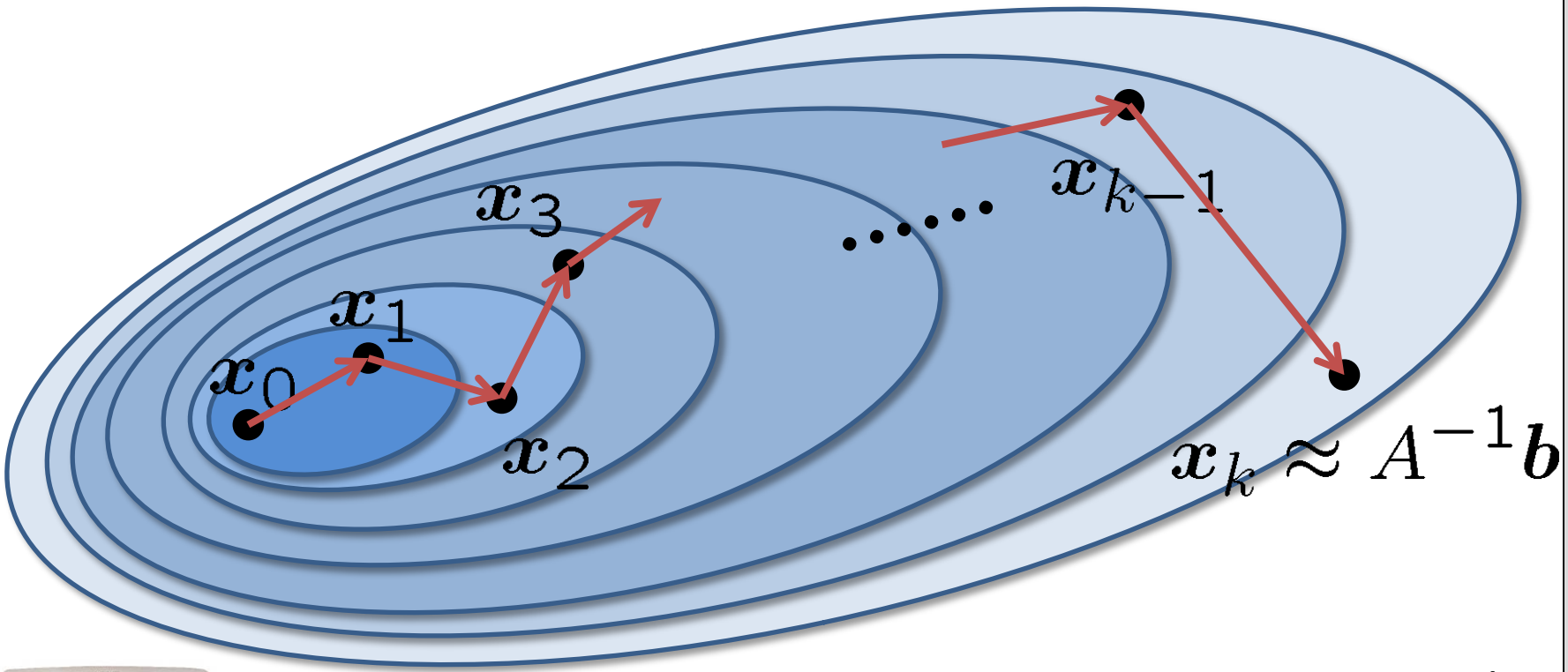

Krylov subspace methods

- Krylov subspace method

  >> Basic ideal:

  -- Projection-type iterative method based on the Krylov subspace

  >> Rough sketch (initial guess: $\boldsymbol{x}_0 \in \mathbb{R}^n$)



Preconditioners

- Preconditioners for Krylov subspace methods

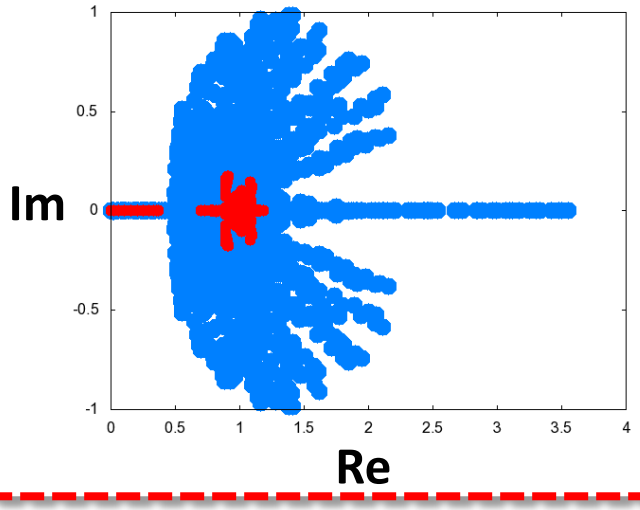
>> Convergence of Krylov subspace methods

Convergence rate depend on ***eigenvalues distribution***

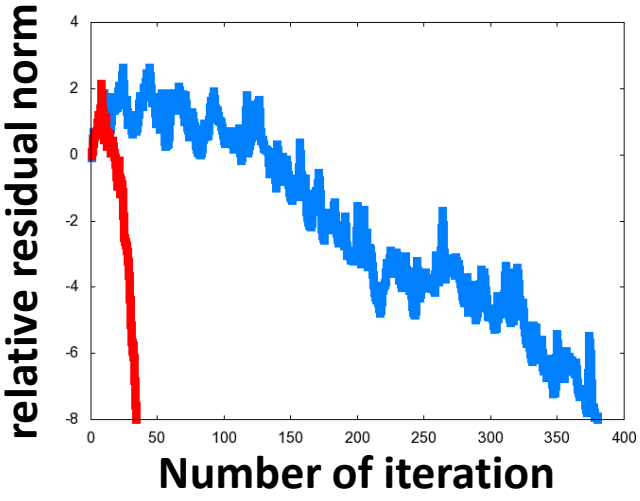
>> Preconditioners (in order to improve convergence rate)

$$Ax = b \quad \Leftrightarrow \quad AK^{-1}y = b, \quad x = K^{-1}y$$

Distribution of eigenvalues



Convergence history



Preconditioners

- How to apply preconditioners

Krylov method

$$A\,x = b$$

$$x_0 \Rightarrow x_1 \Rightarrow x_2 \Rightarrow \cdots \Rightarrow x_{k-1} \Rightarrow x_k$$

Computation of 1 iter. (*MatVec* + DOTs, AXPYs)

Preconditioned Krylov method

$$A\,K^{-1}\,y = b, \quad x = K^{-1}\,y$$

$$\Diamond\, y_0 \Rightarrow y_1 \Rightarrow \cdots \Rightarrow y_k, \Diamond$$

Pre-processing — Computation of 1 iter. — Post-processing

(*MatVec* + *Solve K's system* + DOTs, AXPYs)

Preconditioners

- Classification of preconditioners

>> Direct-type preconditioners

-- Construct K or K^{-1} by direct method such that $K \approx A$ and $Kw = v$ can be solved efficiently

-- In each iteration, systems $Kw = v$ is solved

Good point: small iteration cost

Bad point: large pre-processing cost, large memory

>> Iterative-type preconditioners

-- Do not construct K or K^{-1}

-- In each iteration, instead of solving $Kw = v$ $(K \approx A)$, solve roughly $Aw = v$ by some iterative method

Good point: small memory, small or no pre-processing cost

--> Efficient for recent large scale simulations

Bad point: have many parameters

Weighted Jacobi-type iteration

- Stationary iterative methods

  >> Recurrence formula ($A = M - N$)

$$\boldsymbol{x}_{k+1} = M^{-1}N\boldsymbol{x}_k + M^{-1}\boldsymbol{b}$$

  >> Convergence rate

$$\rho(G) := \rho(M^{-1}N) := \max_i \left|\lambda_i(M^{-1}N)\right|$$

$$A = -A_L - A_D - A_U$$

- Standard stationary iterative methods

	Convergence	Iteration costs	Parallelization
Jacobi	Bad	Good	Good
Gauss-Seidel	Good	Good	Bad
SOR	Bad -- Excellent	Good	Bad

Weighted Jacobi-type iteration

- **Weighted** Jacobi iteration

  >> Basic ideal:

Weighted Jacobi iteration transforms the Jacobi's recurrence formula:

$$\boldsymbol{x}_{k+1} = A_D^{-1}(A_L + A_U)\boldsymbol{x}_k + A_D^{-1}\boldsymbol{b}$$

into

$$\begin{aligned} \boldsymbol{x}_{k+1} &= \omega\left(A_D^{-1}(A_L + A_U)\boldsymbol{x}_k + A_D^{-1}\boldsymbol{b}\right) + (1-\omega)\boldsymbol{x}_k \\ &= \boldsymbol{x}_k + \omega A_D^{-1}(\boldsymbol{b} - A\boldsymbol{x}_k) \end{aligned}$$

by using a ***weight parameter*** $\omega \in \mathbb{R}$ in order to improve the convergence rate of Jacobi iteration.

Weighted Jacobi-type iteration

- Weighted Jacobi-**type** iteration

  >> Basic ideal:

Weighted Jacobi-type iteration transforms the recurrence formula of the weighted Jacobi iteration:

$$\boldsymbol{x}_{k+1} = \omega A_D^{-1}(\boldsymbol{b} - A\boldsymbol{x}_k)$$

into

$$\boldsymbol{x}_{k+1} = \omega D^{-1}(\boldsymbol{b} - A\boldsymbol{x}_k)$$

by using some nonsingular ***scaling diagonal matrix*** D in order to improve the convergence rate without loss of its parallel efficiency.

Optimal ω and D are different with respect to each problems
--> PARAMETER TUNING TECHNIQUE IS STRONGLY REQUIRED !!

Outline

- Introduction
- Weighted Jacobi-type iteration used for preconditioners
- Parameter tuning technique
  - >> Convergence analysis
  - >> Proposal for parameter tuning technique
- Numerical experiments and results
- Conclusions




Convergence analysis

- Convergence of the weighted Jacobi-type iteration

Weighted Jacobi-type iteration can also be recognized as the stationary iterative method with the initial matrix partition:

$$A = M_\omega - N_\omega, \qquad \begin{aligned} M_\omega &= D/\omega, \\ N_\omega &= M_\omega - A \end{aligned}$$

and its convergence rate can be estimated by

$$\rho(G_\omega) := \rho(M_\omega^{-1} N_\omega) = \rho(I - \omega D^{-1} A)$$

We analyze

$$\omega^* := \arg\min_{\omega \in \mathbb{R}} \rho(G_\omega), \qquad \rho(G_{\omega^*}) := \min_{\omega \in \mathbb{R}} \rho(G_\omega)$$

Convergence analysis

- Convergence theorem of weighted Jacobi-type method

Theorem: Optimal weight parameter

Let $C(\gamma, \rho)$ ***be the inner region of the circle with center*** $\gamma \in \mathbb{R}$ ***and radius*** $\rho \in \mathbb{R}$ ***on the complex plane, and let*** $\gamma^*, \rho^* \in \mathbb{R}$ ***be defined by***

$$\gamma^*, \rho^* := \arg\min_{\gamma,\rho} \left|\frac{\rho}{\gamma}\right|,$$

$$s.t. \quad \lambda_i(D^{-1}A) \in C(\gamma, \rho), \quad i = 1, 2, \ldots, n.$$

Then we have

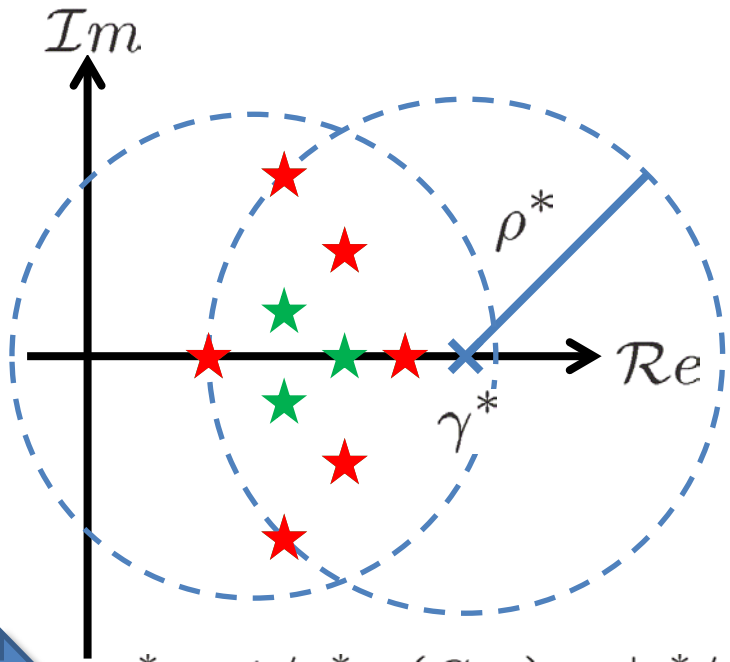
$$\omega^* := \arg\min_{\omega\in\mathbb{R}} \rho(G_\omega) = \frac{1}{\gamma^*}, \quad \rho(G_{\omega^*}) := \min_{\omega\in\mathbb{R}} \rho(G_\omega) = \left|\frac{\rho^*}{\gamma^*}\right|$$

Convergence analysis

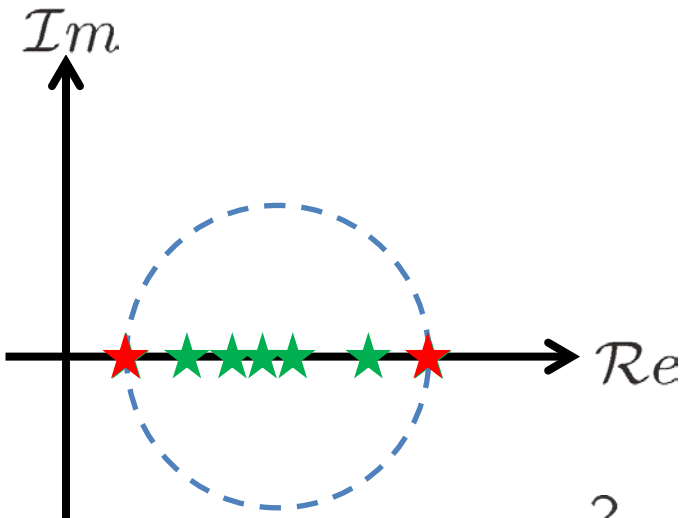
- Convergence theorem of weighted Jacobi-type method

Remark: Eigenvalue distribution and Optimal parameter

Distribution of $\lambda_i(D^{-1}A)$



$\omega^* = 1/\gamma^*, \rho(G_{\omega^*}) = |\rho^*/\gamma^*|$



$$\omega^* = \frac{2}{\lambda_{\max} + \lambda_{\min}}$$

$$\rho(G_{\omega^*}) = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$

Weight parameter can be optimized by ***extreme eigenvalues***

Parameter tuning technique

- Parameter tuning technique

  >> Basic ideal: ***Offline tuning***

  -- ***ω*** and ***D*** are tuned before the algorithm runs.

Input

Initial guess x_0

Choice of diagonal matrices $D_i, i = 1, \ldots, s$

Parameter tuning

1: For *i* = 1, 2, …

2: Optimize $\tilde{\omega}_i$ and get $\rho(G_{\tilde{\omega}_i})$ from approx. extreme eigenvalues $\lambda(D_i^{-1}A)$

3: End For

4: Select the best pair $(\tilde{\omega}_i, D_i)$ s.t. $\min \rho(G_{\tilde{\omega}_i})$

Preconditioned Krylov

Run weighted Jacobi-type preconditined Krylov subspace method with tuned pair $\tilde{\omega}$, D

Parameter tuning technique

- Algorithm of parameter tuning technique
  - >> Approx. eigenvalues are computed by ***the Arnoldi method***
  - >> Iteration of Arnoldi method is stopped by ***relative error of ω***

Parameter tuning

1: For i = 1, 2, …, s
2: For l = 1, 2, …, l_{max}
3: Operate lth step of the Arnoldi method and get l approx. extreme eigenvalues
4: Compute $\tilde{\omega}_l$ and $\rho(G_{\tilde{\omega}_l})$ from computed eigenvalues
5: IF $|\tilde{\omega}_l - \tilde{\omega}_{l-1}/\tilde{\omega}_l| \leq \epsilon$ then exit
6: End For
7: Set $\tilde{\omega}_i = \tilde{\omega}_l, \rho(G_{\tilde{\omega}_i}) = \rho(G_{\tilde{\omega}_l})$
8: End For
9: Select the best pair $(\tilde{\omega}_i, D_i)$ s.t. $\min \rho(G_{\tilde{\omega}_i})$

Outline

- Introduction
- Weighted Jacobi-type iteration used for preconditioners
- Parameter tuning technique
- Numerical experiments and results
  - >> Evaluation of the quality of the parameter tuning
  - >> Evaluation of the performance of the preconditioner
  - >> Evaluation of the performance for real application
- Conclusions




Numerical experiments I

- Purpose: Evaluation of quality of parameter tuning for ω

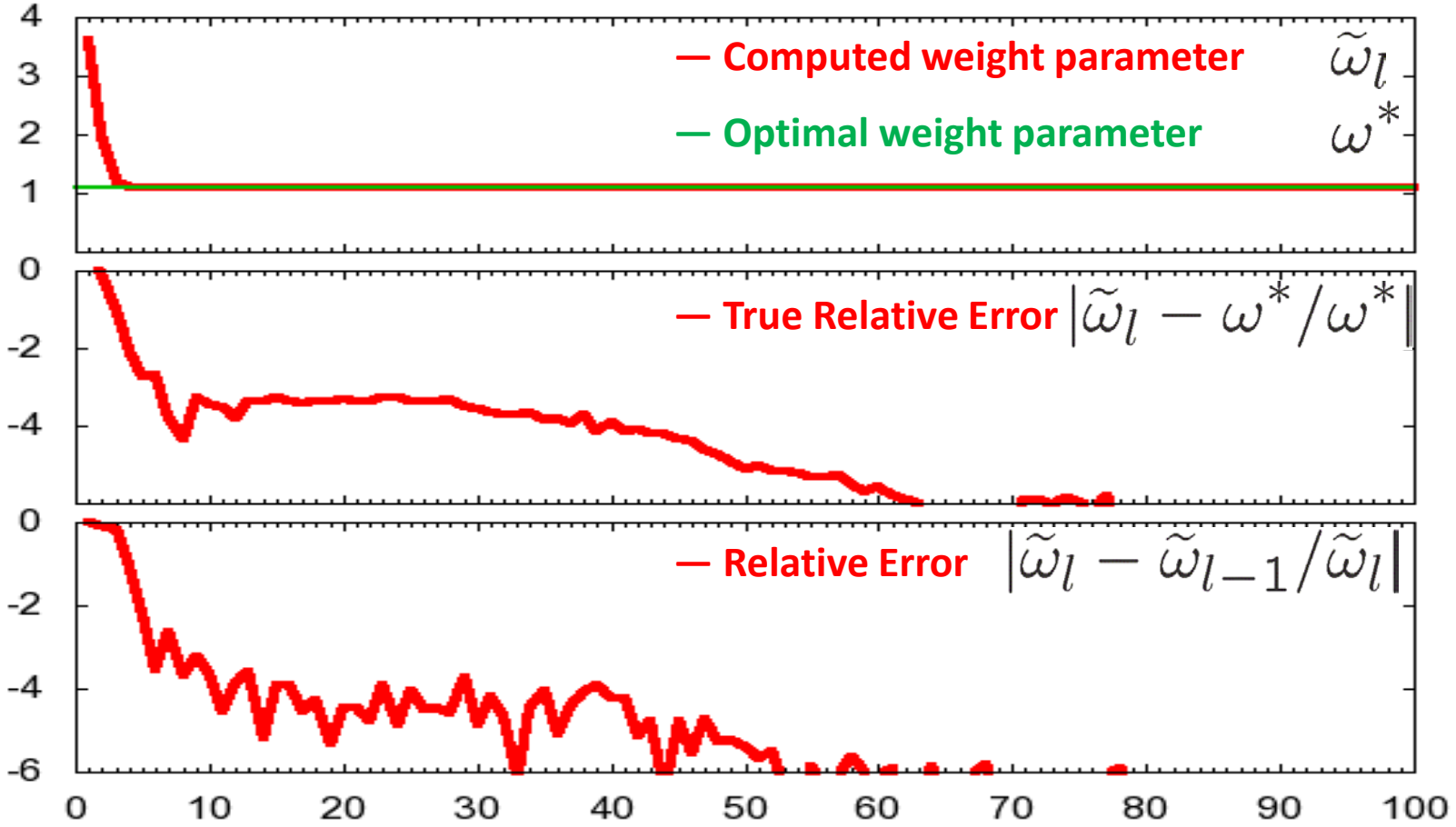
- Test matrices

>> CAVITY05	n = 1182	Fluid dynamics
>> FLOWMETER5	n = 9669	Model reduction
>> RAEFSKY2	n = 3242	Fluid dynamics
>> SHERMAN5	n = 3312	Fluid dynamics

- Experimental condition
  - >> OS: CentOS, CPU: Intel Xeon X5550 (2.67GHz), Memory: 48GB
  - >> Compiler: GNU Fortran ver.4.1.2, Compile option: -O3

Numerical results I

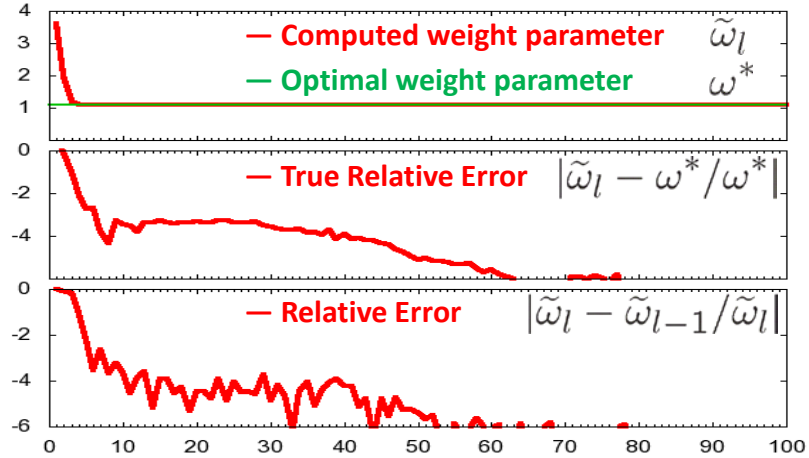
- Convergence history of ω
  - >> CAVITY05



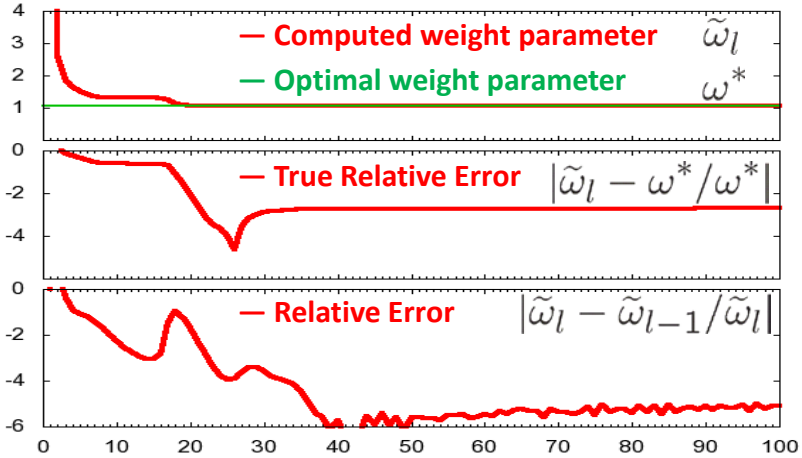
Numerical results I

- Convergence history of ω

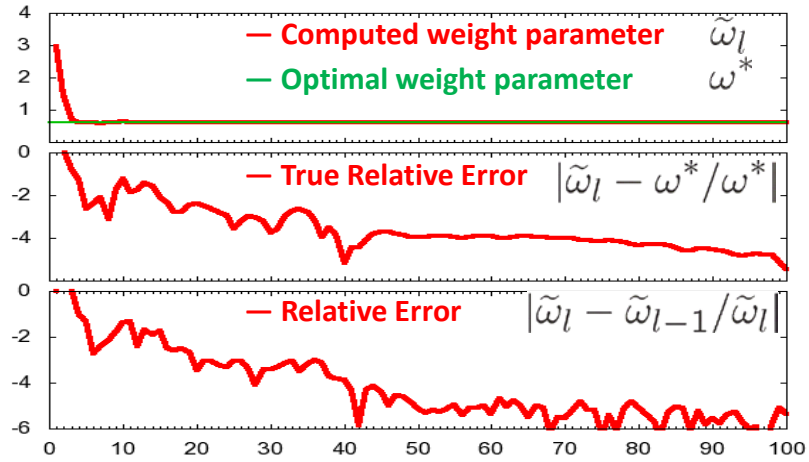
>> CAVITY05



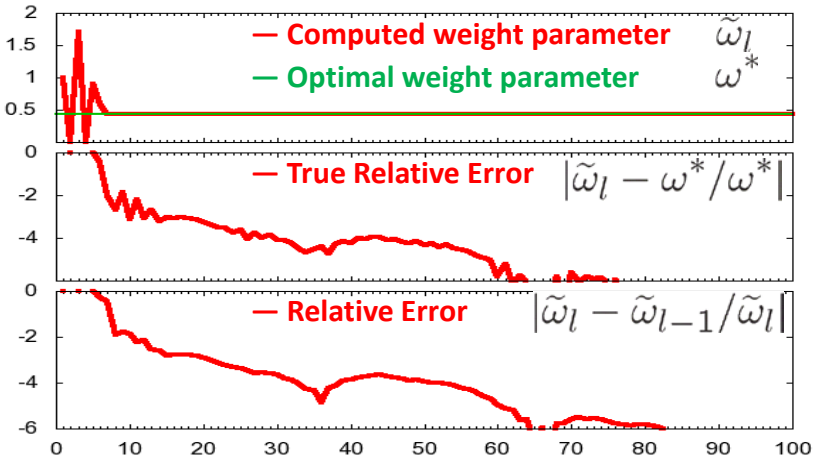
>> FLOWMETER5



>> RAEFSKY2



>> SHERMAN5



Numerical experiments II

- Purpose: Evaluation of performance of preconditioner

- Comparison
  - >> with the tuned parameters
  - >> with the default parameters (same as Jacobi iteration)

- Test matrices (in addition to matrices used in experiments I)

>> AF23560	n = 23560	Fluid dynamics
>> CHIPCOOL0	n = 20082	Model reduction
>> EPB2	n = 25228	Thermal problem
>> FEM_3D_THERMAL2	n = 147900	Thermal problem
>> POISSON3DA	n = 13514	Fluid dynamics
>> POISSON3DB	n = 85623	Fluid dynamics
>> XENON1	n = 48600	Materials problem
>> XENON2	n = 157464	Materials problem

Numerical experiments II

- Other settings
  - >> $\boldsymbol{b} = [1, 1, \ldots, 1]^{\mathsf{T}}, \boldsymbol{x}_0 = [0, 0, \ldots, 0]^{\mathsf{T}}$
  - >> Krylov subspace method: full-GMRES method
  - >> Stopping criterion for Krylov method: $\|\boldsymbol{r}_k\|_2 / \|\boldsymbol{r}_0\|_2 \leq 10^{-10}$
  - >> Stopping criterion for Arnoldi method: $|\widetilde{\omega}_l - \widetilde{\omega}_{l-1} / \widetilde{\omega}_l| \leq 10^{-4}$
  - >> Number of weighted Jacobi-type iteration: 20
  - >> Choice of scaling diagonal matrices:

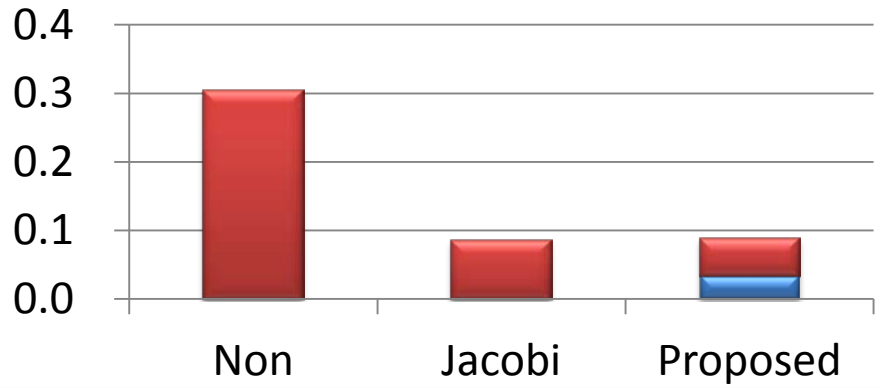
$$
\begin{aligned}
D_1 &: d_i = a_{i,i}, \\
D_2 &: d_i = 1, \\
D_3 &: d_i = \sum_{j=1}^{n} |a_{i,j}|, \\
D_4 &: d_i = \sqrt{\sum_{j=1}^{n} a_{i,j}^2}, \\
D_5 &: d_i = \max_j |a_{i,j}|, \\
D_6 &: \min_D \|D^{-1}A - I\|_F,
\end{aligned}
$$

Numerical results II

: Krylov iteration
: tuning

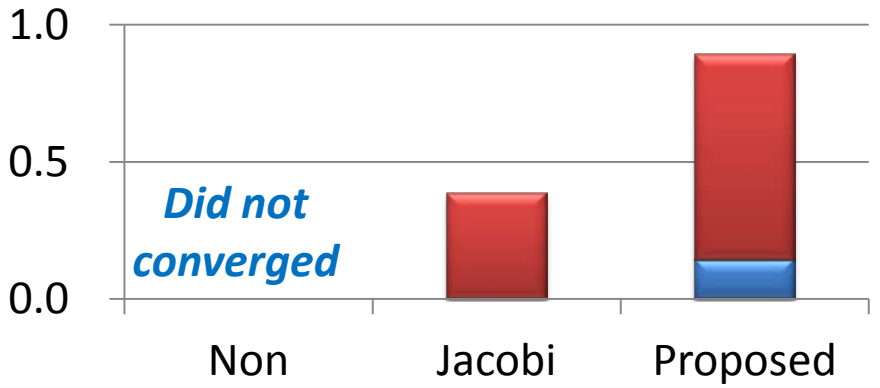
of iteration and Computation time [sec.]

>> CAVITY05



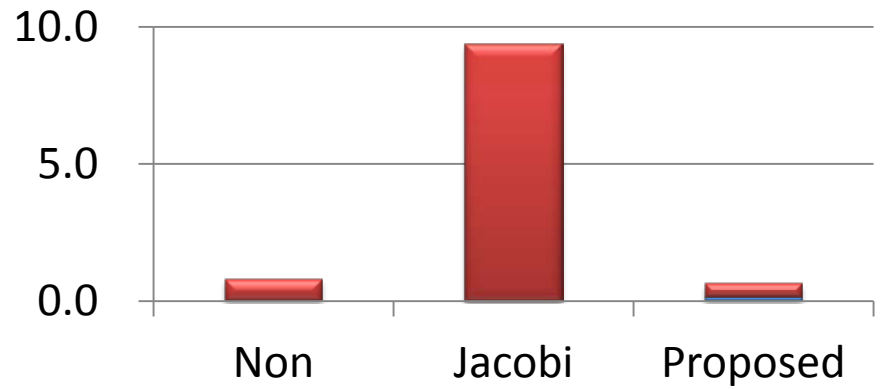
ITER	471	64	42

>> FLOWMETER5



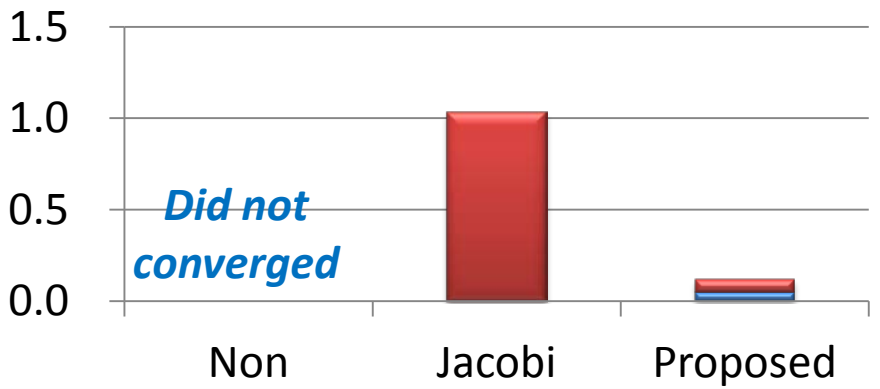
ITER	--	82	140

>> RAEFSKY2



ITER	389	750	50

>> SHERMAN5



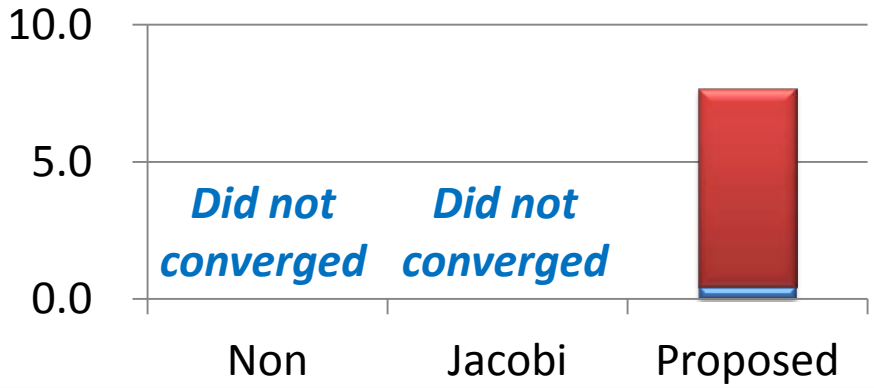
ITER	--	363	47

Numerical results II

: Krylov iteration
: tuning

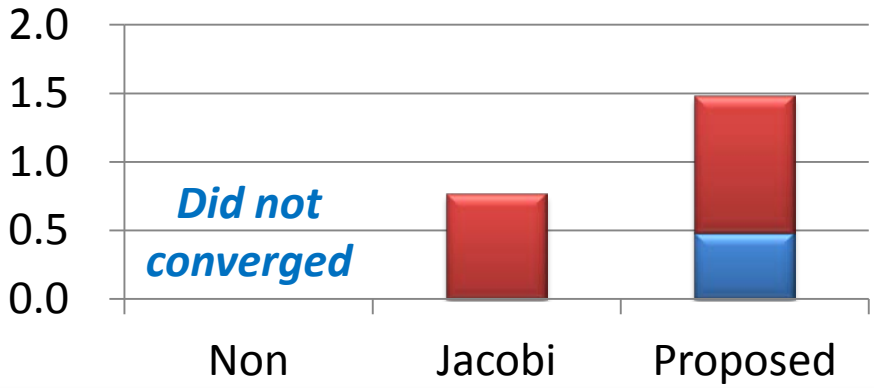
of iteration and Computation time [sec.]

>> AF23560



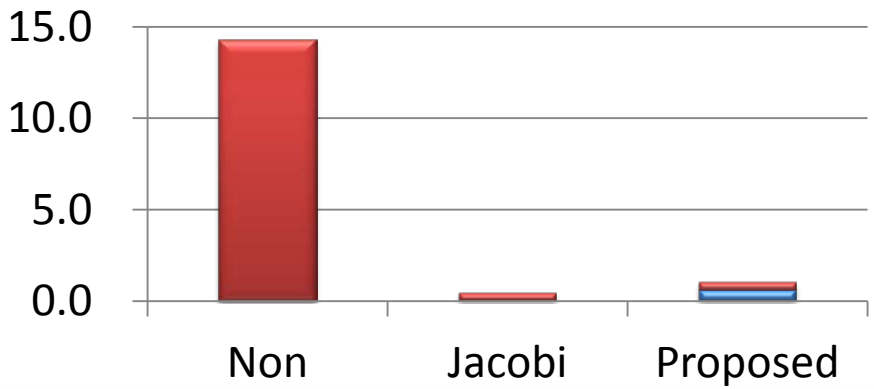
	Non	Jacobi	Proposed
ITER	--	--	259

>> CHIPCOOL0



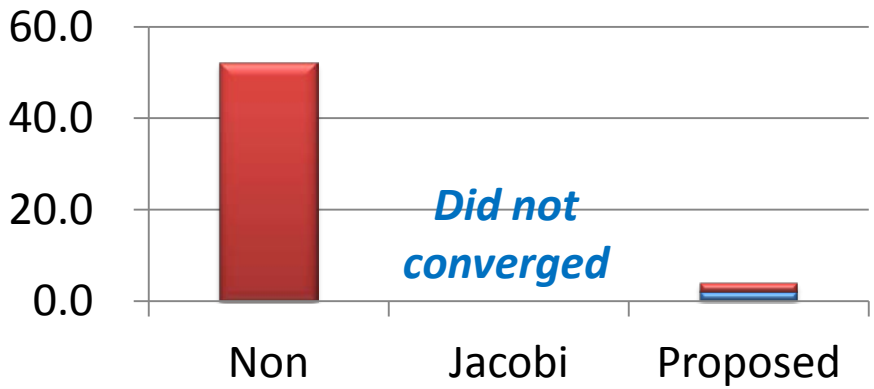
	Non	Jacobi	Proposed
ITER	--	49	63

>> EPB2



	Non	Jacobi	Proposed
ITER	650	39	36

>> FEM_3D_THERMAL2



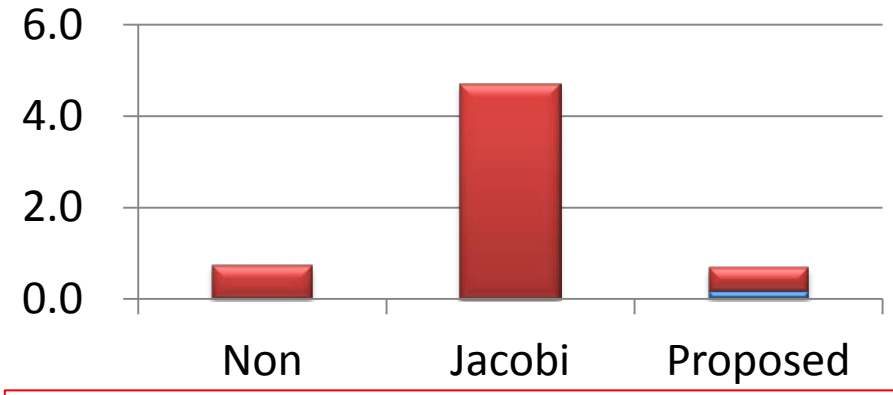
	Non	Jacobi	Proposed
ITER	492	--	11

Numerical results II

: Krylov iteration
: tuning

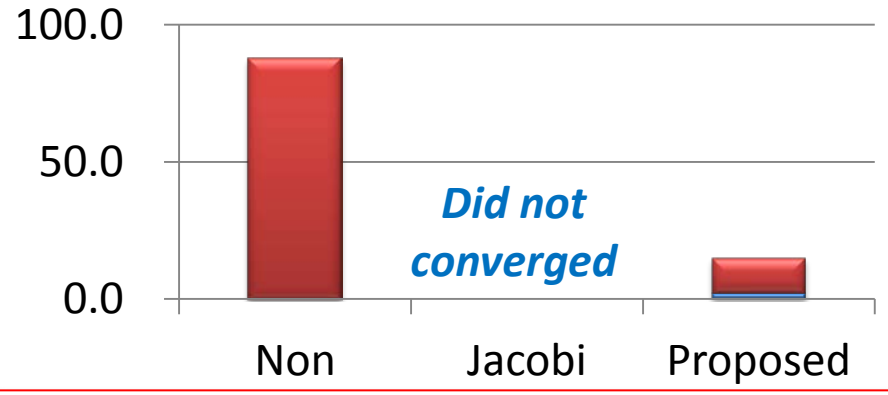
of iteration and Computation time [sec.]

>> POISSON3DA



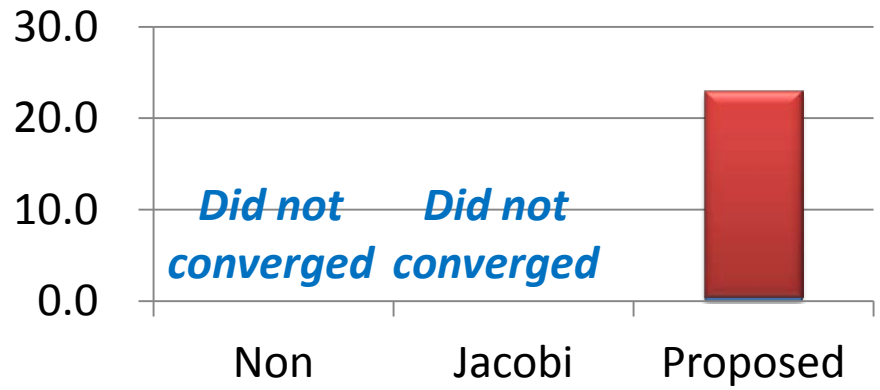
	Non	Jacobi	Proposed
ITER	184	293	31

>> POISSON3DB



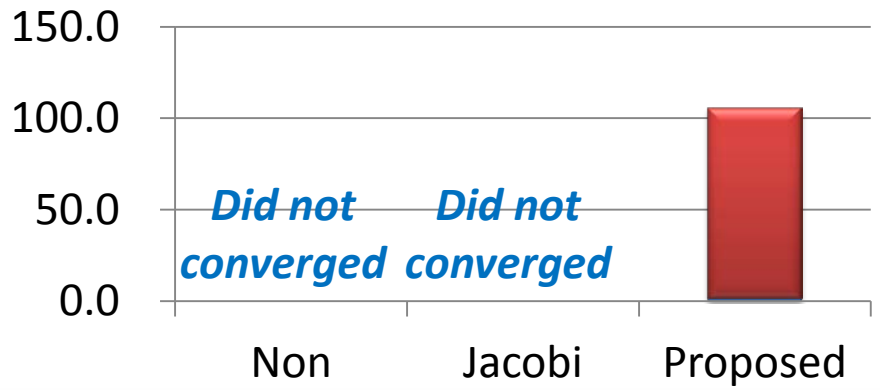
	Non	Jacobi	Proposed
ITER	848	--	66

>> XENON1



	Non	Jacobi	Proposed
ITER	--	--	284

>> FEM_3D_THERMAL2



	Non	Jacobi	Proposed
ITER	--	--	383

Numerical experiments III

- Purpose: Evaluation of performance for real application

- Target simulation
  - >> 3D supernova simulation
    - -- Time evolution : Implicit method
      - → It is required to solve ***very large, but sparse, linear systems***
        (n ≃ 16 million, Nnz ≃ 1.28 billion, Nnz/n ≃ 80)
    - -- Required time evolution : t = 1 [sec.]
      - → Larger time step (Δt) is required ($\Delta t \approx 10^{-5}$ [sec.])
    - -- ***Larger Δt leads to more ill-conditioned systems***

- Compared with
  - >> Jacobi preconditioner
  - >> Diagonal scaling

Numerical experiments III

- Other settings
  - >> Krylov subspace methods: Bi-CGSTAB
  - >> Iteration for preconditioner : 20
  - >> Cutoff parameter : 0.01
  - >> Diagonal matrix :

$$D_1 \ : \ d_i = a_{i,i},$$

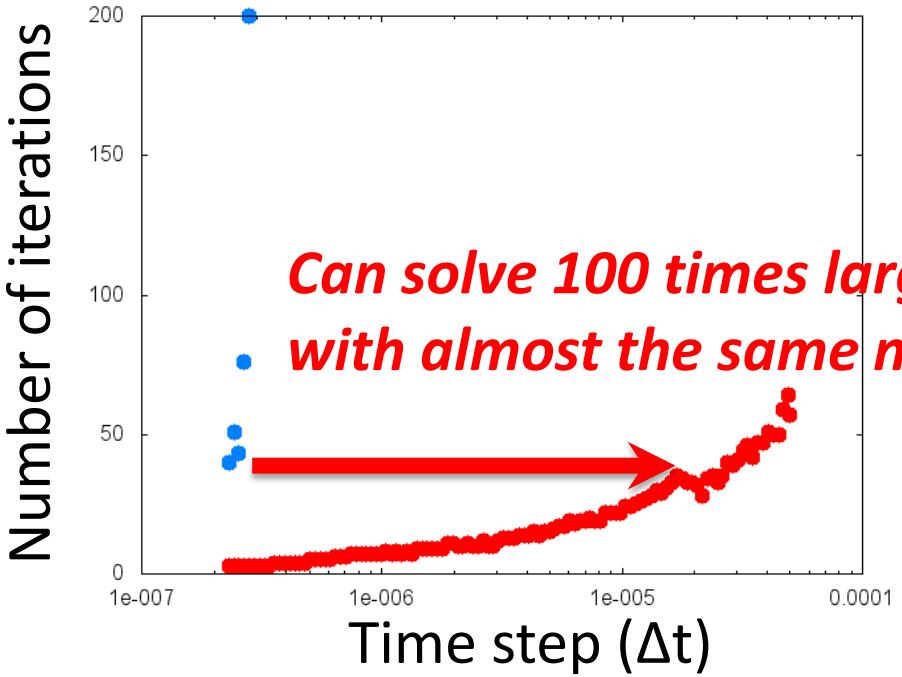
$$D_2 \ : \ d_i = \sum_{j=1}^{n} |a_{i,j}|,$$

$$D_3 \ : \ d_i = \sqrt{\sum_{j=1}^{n} a_{i,j}^2}$$

- Experimental condition
  - >> KEK SR16000/M1
    - -- 1 node 32 cores (logical 64 cores)

Numerical results III

- Numerical results
  - >> Time step (Δt) v.s. number of iterations
    - -- Bi-CGSTAB with ***Diagonal scaling*** / ***Proposed preconditioner***



  - >> Computation time
    - -- ***Diagonal scaling***: 0.3 [sec.] / iter
    - -- ***Proposed***: 3.0 [sec.] / iter (parameter tuning: 9.0 [sec.])

Outline

- Introduction
- Weighted Jacobi-type iteration used for preconditioners
- Auto-tuning technique
- Numerical experiments and results
- Conclusions




Conclusion

- Conclusion

  >> In this presentation, we have

  -- introduced ***a weighted Jacobi-type iteration***

  -- proposed ***a parameter tuning technique***

  >> From our numerical experiments, we have leaned that our tuning technique well played for solving linear systems.

- Further investigation

  >> Further improvement of the parameter tuning technique

  -- Evaluate the parallel efficiency

  -- Apply to other application, and evaluate its efficiency