Implementation of GMRES with Preconditioning in Python

John Tran

University of New Mexico

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Problem

Convection-diffusion problem

$$-au''(x) + bu'(x) = 0, \quad 0 < x < 1$$
$$u(0) = 0, u(1) = 1$$

Right-hand side of differential is 0

Dirichlet boundary conditions

Discretization

Difference equation for u' (backward)

$$u' = \frac{u_i - u_{i-1}}{h} \qquad \text{backward difference}$$

$$u'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

$$-a\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}\right) + b\left(\frac{u_i - u_{i-1}}{h}\right) = 0$$

Forming Tri-diagonal Matrix A

$$-u_{i+1} + (2+c)u_i - (1+c)u_{i-1} = 0$$

where the Péclet number $R = b/a$ and $c = Rh$

Let $m = 5$ (visualization)

$$A_{backward} = \frac{a}{h^2}\begin{bmatrix} 2+c & -1 & & & \\ -(1+c) & 2+c & -1 & & \\ & -(1+c) & 2+c & -1 & \\ & & -(1+c) & 2+c & -1 \\ & & & -(1+c) & 2+c \end{bmatrix}$$

$$y = \frac{a}{h^2}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\gamma \end{bmatrix} = \frac{a}{h^2}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \qquad \gamma = -1 \text{ for backward}$$

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Objective

$x \in x_0 + \mathcal{K}_m$ – a linear combination of basis vectors in $\mathcal{K}_m$

$$x = x_0 + V_m y$$

With results from Arnoldi iteration
Skip Arnoldi iteration (psuedocode)

$$\min_y \|b - A(x_0 + V_m y)\|_2 = \min_y \left\| \beta e_1 - \bar{H}_m y \right\|_2$$

GMRES Plane Rotations

Introduce plane rotation matrix

Reduce Hessenberg matrix (upper triangular)

Progressive manner

Residual at each iteration

$$\Omega_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & s_i & & & \\ & & & -s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}$$

GMRES Plane Rotations Example

Let $m = 3$ (visualization)

$$\bar{H}_3 = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ & h_{22} & h_{23} \\ & & h_{33} \\ & & h_{43} \end{bmatrix}, \qquad \bar{g}_3 = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ 0 \end{bmatrix}$$

$$\bar{R}_3 = \begin{bmatrix} h_{11} & h_{12} & h_{13}* \\ & h_{22} & h_{23}* \\ & & h_{33}* \\ & & 0 \end{bmatrix}, \qquad \bar{g}_3 = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ c_6\gamma_3 \\ -s_6\gamma_3 \end{bmatrix}$$

$$\min_y \left\| \beta e_1 - \bar{H}_m y \right\|_2 = \min_y \left\| \bar{g}_m - \bar{R}_m y \right\|_2$$

Preconditioner (Left)

Preconditioners:

- Jacobi (JA)
- Gauss-Seidel (GS)
- Symmetric Gauss-Seidel (SGS), $\omega = 1$ in SSOR

$$
\begin{aligned}
M^{-1}Ax &= M^{-1}y \\
M_{JA} &= D \\
M_{GS} &= D + L \\
M_{SGS} &= (D + L)D^{-1}(D + U) \\
&= \hat{L}\hat{U} \\
\hat{L} &= (D + L)D^{-1} = I - LD^{-1} \\
\hat{U} &= D + U
\end{aligned}
$$

SGS - forward and backward solve (approximate LU factorization)

Pseudocode

Terminate early (threshold)

Algorithm GMRES (plane rotations) with preconditioning

1: Choose an initial guess x_0
2: Compute $r_0 = M^{-1}(b - Ax_0), \beta = \|r_0\|_2, v_1 = r_0/\beta$
3: **for** j $= 1, 2, \ldots, m$ **do**
4:     START Arnoldi iteration step
5:     Compute $w_j = M^{-1}(Av_j)$
6:     **for** $i = 1, 2, \ldots, j$ **do**
7:         $h_{ij} = (w_j, v_i)$
8:         $w_j = w_j - h_{ij}v_i$
9:     **end for**
10:     $h_{j+1,j} = \|w_j\|_2$
11:     **if** $h_{j+1,j} == 0$ **then** ▷ encountered with ***preconditioning***
12:         Set $m = j$ and goto 22
13:     **end if**
14:     $v_{j+1} = w_j / h_{j+1,j}$
15:     END Arnoldi iteration step
16:     START plane rotation step
17:     Apply rotation matrix to rows $i, i+1$ of h along columns $1, 2, \ldots j$
18:     Update $\bar{g}_m$ on indices $i, i+1$ of $\bar{g}_m$ according to equations given by [1]
19:     If the norm of the residual $|\gamma_{m+1}|$ is less than some threshold, goto 22
20:     END plane rotation step
21: **end for**
22: Define the $(m+1) \times m$ Hessenberg matrix $\bar{H}_m = \{h_{ij}\}$ for $1 \leq i \leq m+1, 1 \leq j \leq m$
23: With plane rotations, let $\bar{R}_m = \bar{H}_m$ where $\bar{R}_m$ is the upper triangular form of $\bar{H}_m$ and removing the zero'd row as an $(m+1) \times m$ matrix
24: Compute y_m the minimizer of $\left\|\bar{g}_m - \bar{R}_m y\right\|_2$
25: Compute $x_m = x_0 + V_m y_m$

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Methods to Compare

Residual and Runtime plots

- LU factorization (using the built-in `scipy.sparse.linalg.splu`)
- Conjugate Gradient (CG) (***added to slides***)
- Preconditioned CG (***added to slides***)
- GMRES
- Preconditioned GMRES

Basic Parameters

Sparse format

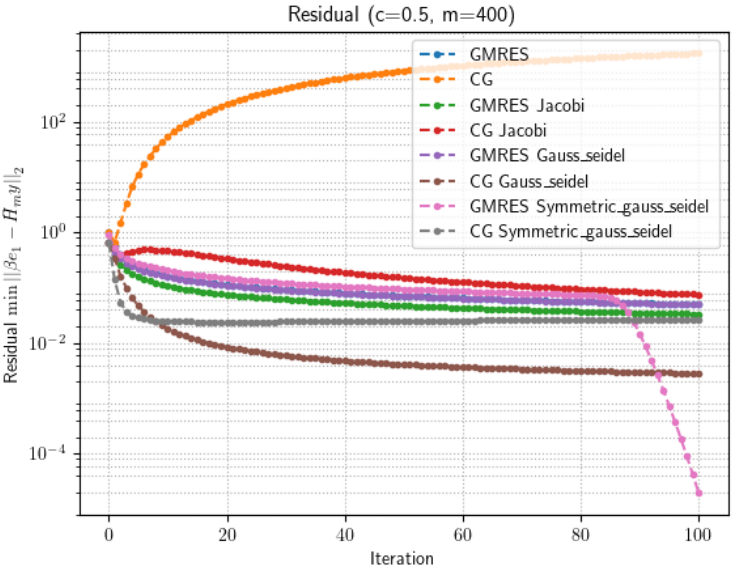
$m = \{400, 800, 1600, 3200, 6400, 12800\}$

$c = \{0.5, 1, 10, 100, 1000\}$

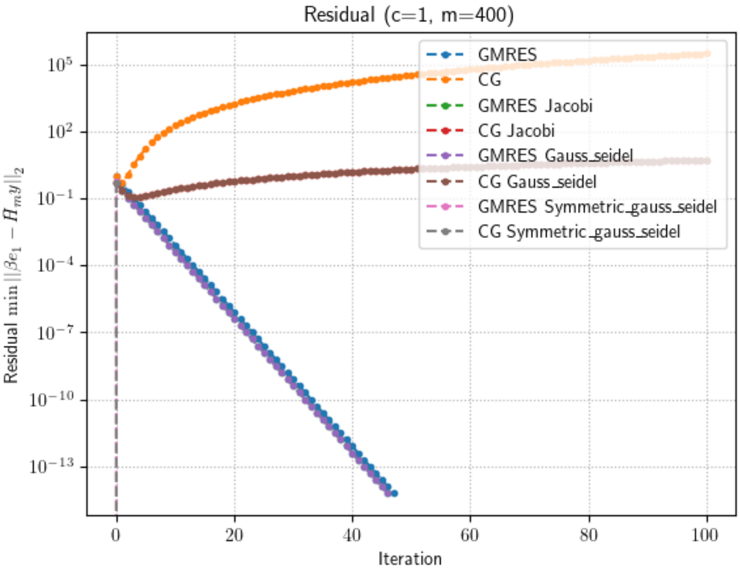
max iterations: 100

tolerance: `1e-14`

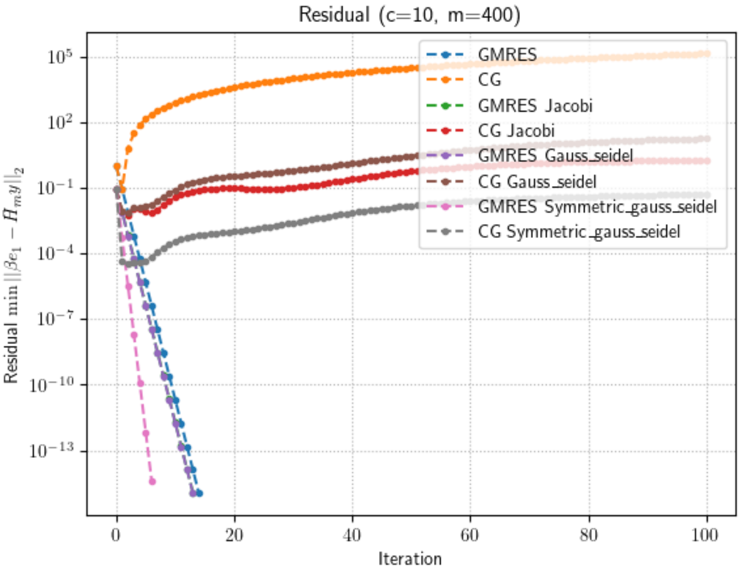
Residual Plots I



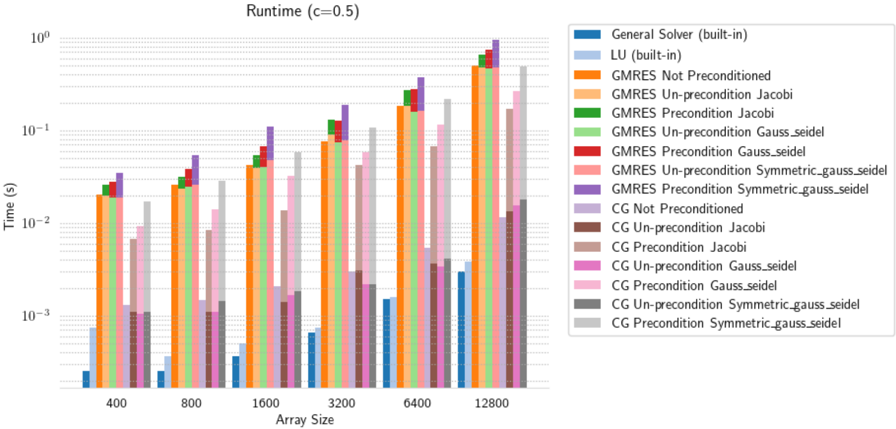
Residual Plots II



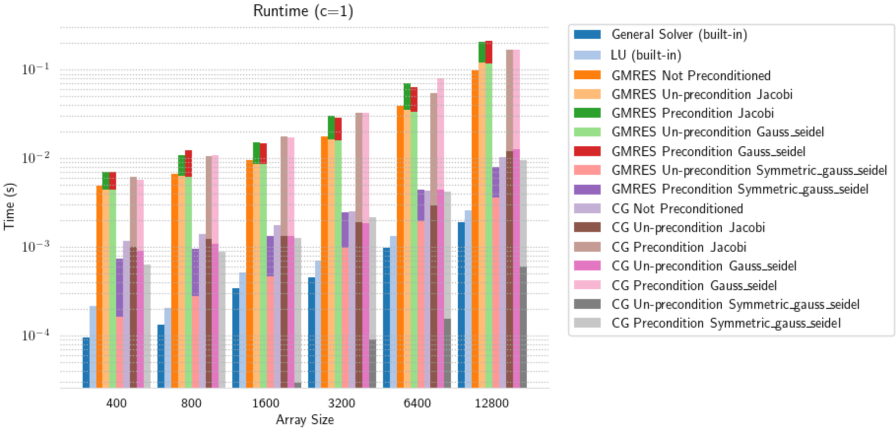
Residual Plots III



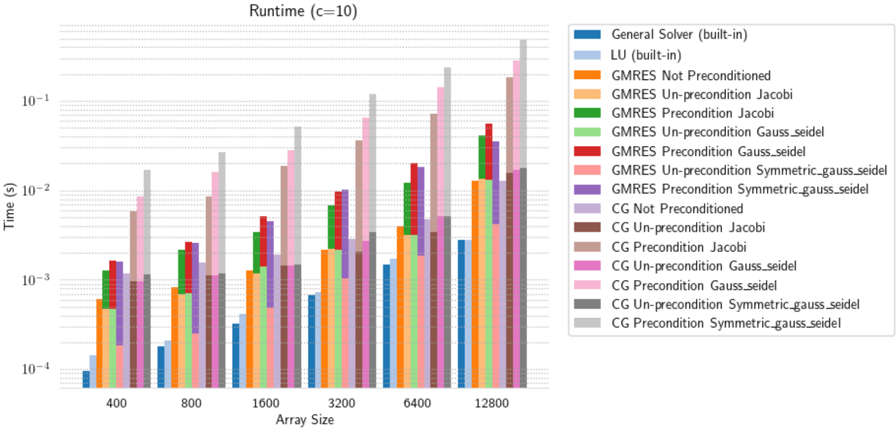
Runtime Plots I



Runtime Plots II



Runtime Plots III



Code Output

```
m: 400
c: 1

LU error: 0.0

precondition: None

GMRES
num iterations: 47
norm error: 4.586533664590355e-15
errors list: [1.0, 0.4472135954999579, 0.21821789023
total runtime (true): 7.700920104980469e-05
total runtime: 0.004621028900146484
precondition time: 0.0001976490020751953
non-precondition time: 0.004423379898071289

Conjugate Gradient
num iterations: 100
norm error: 286.5959730253588
errors list: [1.0, 0.5, 1.2222222222222222, 3.3650519
total runtime (true): 7.700920104980469e-05
total runtime: 0.001104116439819336
precondition time: 0.0003116130828857422
non-precondition time: 0.0007925033569335938
```

```
precondition: PreconditionEnum.JACOBI

GMRES
num iterations: 46
norm error: 9.173067288213951e-15
errors list: [0.5, 0.22360679774997896, 0.1091089451
total runtime (true): 7.700920104980469e-05
total runtime: 0.006892681121826172
precondition time: 0.002471923828125
non-precondition time: 0.004420757293701172

Conjugate Gradient
num iterations: 100
norm error: 1.2487480063507874
errors list: [0.5, 0.25, 0.140625, 0.114067925347222
total runtime (true): 7.700920104980469e-05
total runtime: 0.0067291259765625
precondition time: 0.005760908126831055
non-precondition time: 0.0009682178497314453
```

```
precondition: PreconditionEnum.GAUSS_SEIDEL

GMRES
num iterations: 46
norm error: 9.173067288213951e-15
errors list: [0.5, 0.22360679774997896, 0.1091089451
total runtime (true): 7.700920104980469e-05
total runtime: 0.006891965866088867
precondition time: 0.0025691986083984375
non-precondition time: 0.00432276725769043

Conjugate Gradient
num iterations: 100
norm error: 1.2487480063507874
errors list: [0.5, 0.25, 0.140625, 0.114067925347222
total runtime (true): 7.700920104980469e-05
total runtime: 0.0060389041900634766
precondition time: 0.0050983428955078125
non-precondition time: 0.0009405612945556641
```

```
precondition: PreconditionEnum.SYMMETRIC_GAUSS_SEIDEL

GMRES
ENCOUNTER EXACT SOLUTION
num iterations: 1
norm error: 0.0
errors list: [0.5773502691896257, 0]
total runtime (true): 7.700920104980469e-05
total runtime: 0.0007860660552978516
precondition time: 0.0006048679351806641
non-precondition time: 0.0001811981201171875

Conjugate Gradient
num iterations: 1
norm error: 0.0
errors list: [0.5, 0.0]
total runtime (true): 7.700920104980469e-05
total runtime: 0.0006761550903320312
precondition time: 0.0006520748138427734
non-precondition time: 2.4080276489257812e-05
```

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References I

[1] Y. Saad, *Iterative Methods for Sparse Linear Systems*, Second. Society for Industrial and Applied Mathematics, 2003. DOI: 10.1137/1.9780898718003. [Online]. Available: https://epubs.siam.org/doi/abs/10.1137/1.9780898718003.

[2] Wikipedia contributors, "Generalized minimal residual method — Wikipedia, the free encyclopedia," (2022), [Online]. Available: https://en.wikipedia.org/w/index.php?title=Generalized_minimal_residual_method&oldid=1126405909.

[3] Wikipedia contributors, "Preconditioner — Wikipedia, the free encyclopedia," (2023), [Online]. Available: https://en.wikipedia.org/w/index.php?title=Preconditioner&oldid=1141155872.

[4] G. Fasshauer, "Preconditioning," (2006), [Online]. Available: http://www.math.iit.edu/~fass/477577_Chapter_16.pdf.

References II

[5] A. J. Wathen, "Preconditioning," *Acta Numerica*, vol. 24, pp. 329–376, 2015, Found online copy here at the provided url. DOI: 10.1017/S0962492915000021. [Online]. Available: http://people.maths.ox.ac.uk/wathen/preconditioning.pdf.

[6] J. Verschelde, "Krylov and Preconditioned GMRES," (Oct. 2022), [Online]. Available: http://homepages.math.uic.edu/~jan/mcs471/krylov.pdf.

[7] R. J. LeVeque, *Finite Difference Methods for Ordinary and Partial Differential Equations*. Society for Industrial and Applied Mathematics, 2007. DOI: 10.1137/1.9780898717839. [Online]. Available: https://epubs.siam.org/doi/abs/10.1137/1.9780898717839.

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Questions?