

Preconditioned GMRES method applied to aerodynamics optimization problem

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March 16 2018

Onera report RT 24/26403 ELSA/DAAA December 2017
elsAASO-2017 - AS-5.1 Evaluation of preconditioners for GMRES in adjoint equation

- 1 Problem statement
- 2 Preconditioning
- 3 Improved GMRES
- 4 Conclusion & perspectives

Plan

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- Euler equations related to aerodynamics problems.
- Residual form

$$\mathcal{R}(\mathbf{W}, \mathbf{X}) = 0, \quad (1)$$

- ▶ \mathcal{R} the flux balance residual related to the fluid dynamics equations,
- ▶ $\mathbf{W} \in \mathbb{R}^N$ is the conservative variables,
- ▶ $\mathbf{X} \in \mathbb{R}^N$ is the mesh coordinates vector.
- Optimization problem: minimize the objective function \mathcal{J} under (1).
- Linearizing around the steady-state equilibrium yields

$$\frac{\partial \mathcal{R}}{\partial \mathbf{W}} \frac{d\mathbf{W}}{d\alpha} = - \frac{\partial \mathcal{R}}{\partial \mathbf{X}} \frac{d\mathbf{X}}{d\alpha}.$$

where α is the vector of design variables.

- Adjoint equation

$$\frac{\partial \mathcal{R}}{\partial \mathbf{W}}^T \lambda = - \frac{\partial \mathcal{J}}{\partial \mathbf{W}}^T.$$

- Numerical resolution:
 - ▶ implicit backward Euler with LU-SSOR algorithm.
 - ▶ GMRES method.

Generalized Minimum Residual method

Problem: solve $Ax = b$ with $A \in \mathbb{C}^{n \times n}$, $b \in \mathbb{C}^n$.

$$A x = b$$

$$\frac{\partial \mathcal{R}}{\partial \mathbf{W}} \lambda = -\frac{\partial \mathcal{J}}{\partial \mathbf{W}}.$$

Method: GMRES (Krylov subspace iteration):

- Krylov subspace associated to A and $r_0 = b - Ax_0$

$$K_m(A, r_0) = \text{span}\{r_0, Ar_0, \dots, A^{m-1}r_0\}.$$

- Approximate solution $x_m \in x_0 + K_m(A, r_0)$.
- Residual norm $\|r_m\| = \|b - Ax_m\|$ minimized over $x_0 + K_m(A, r_0)$.

Goal

improve the GMRES convergence rate

How to improve convergence

- ILU variants.
- Flexible-GMRES \Rightarrow iterative preconditioner:
 - ▶ GMRES.
 - ▶ Multigrid.
- Deflation of eigenvalues.

State of art

- Scaling.
- Approximate $\frac{\partial \mathcal{R}^{\text{app}}}{\partial W}$ order 1.
- LU-SSOR + Multigrid.

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Preconditioning

Left-preconditioning: $M^{-1}Ax = M^{-1}b$, with M the 'preconditioner'.

Right-preconditioning: system $Ax = b$ written as

$$\begin{aligned}AM^{-1}y &= b, \\ y &= Mx.\end{aligned}$$

Effective preconditioning:

- M easy to inverse.
- Ideally AM^{-1} close to the identity matrix.
- $\text{spec}(AM^{-1})$ compressed around 1, well clustered, away from 0.

Various preconditioners:

- Jacobi preconditioner: diagonal of A , i.e. $M_J = \text{diag}(A)$.
- SSOR preconditioner: if $A = L + D + U$, then $M_\omega = (D + \omega L)D^{-1}(D + \omega U)$, with $\omega = 1$ typical.

Incomplete LU factorization (ILU)

- $M = L_{in}U_{in}$ where L_{in} and U_{in} are approximations of L and U of the LU factorization of A , pattern based on lower and upper pattern of A .

ILU variants

- with no fill: $ILU(0)$, with level-of-fill: $ILU(p)$.
 - with threshold: $ILUT$, with drop tolerance: $ILUT(\epsilon)$.
 - with dual threshold: $ILUT(k, \epsilon)$.
 - with pivoting: $ILUP$.
-
- Zero/small pivots \Rightarrow instability ($\|(LU)^{-1}\|$ large).
 - Forward/backward substitutions \Rightarrow rounding errors.
 - A ill-conditioned $\Rightarrow L$ and U more ill-conditioned.

Preconditioned GMRES convergence

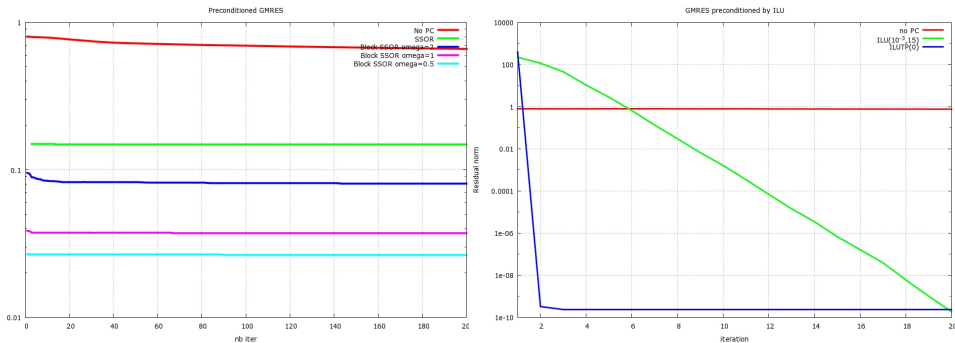


Figure: Flow over Naca0012 profile.

Left: SSOR and block SSOR preconditioning.

Right: ILUT and ILUTP preconditioning.

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Flexible GMRES

- Preconditioner M_j varies at every step j .
- Iterative method as a preconditioner: SSOR, GMRES(inner-outer) ...
- Precondition the inner GMRES: LU-SSOR, Multigrid...

Algorithm 1: Flexible GMRES

Compute $r_0 = b - Ax_0$, $\beta = \|r_0\|$ and $v_1 = r_0/\beta$.

for $j = 1, \dots, m$ **do**

 Compute $z_j := M_j^{-1} v_j$

 Compute $w := Az_j$

for $i = 1, \dots, j$ **do**

$h_{i,j} := (w, v_i)$

$w := w - h_{i,j} v_i$

 Compute $h_{j+1,j} = \|w\|$ and $v_{j+1} = w/h_{j+1,j}$.

Define $Z_m := [M_1^{-1} v_1, \dots, M_m^{-1} v_m]$,

Compute $x_m = x_0 + Z_m y_m$, where $y_m = \operatorname{argmin}_y \|\beta e_1 - \tilde{H}_m y\|$

If satisfied stop, else set $x_0 \leftarrow x_m$ and goto 1.

Preconditioned GMRES convergence

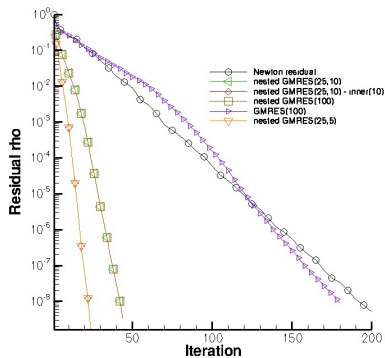
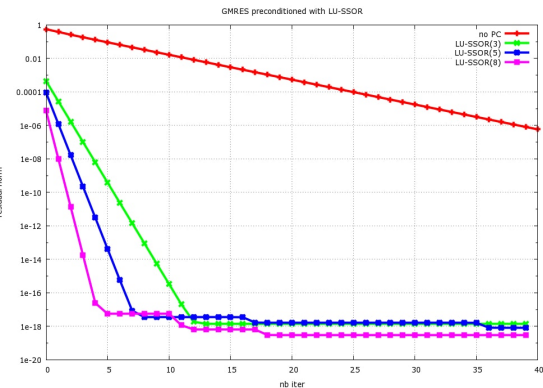


Figure: Left: LU-SSOR on advection-diffusion. Right: Nested GMRES on flow over the NACA0012 profile.

Multi-grid method

Algorithm (V-cycle):

- Smoothing: iterate $Ax = b$ on $\Omega_h \Rightarrow x_h$,
- $r_h = Ax_h - b_h$,
- solve $Ae = r$ on $\Omega_{2h} \Rightarrow e_{2h}$,
- correct $x_h = x - e_h$.
- Post-smoothing.

Transfer operators:

- restriction $R : \Omega_h \rightarrow \Omega_{2h}$ (weighting injection),
- prolongation $P : \Omega_{2h} \rightarrow \Omega_h$, $P = 4R^T$ (interpolation),
- $A_{2h} = RA_hP$,
- $r_{2h} = R(r_h)$ and $e_h = P(e_{2h})$.

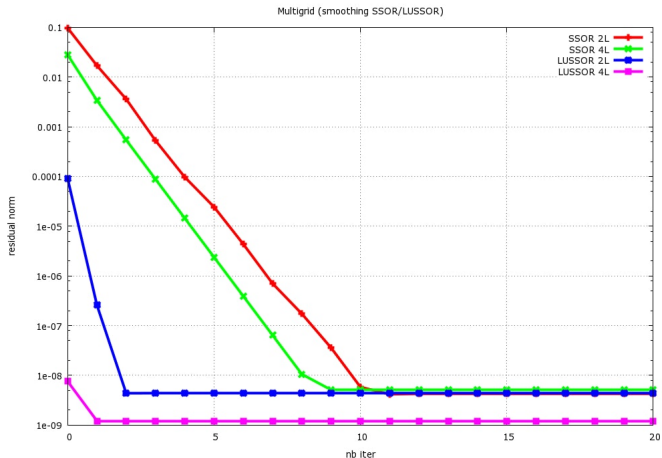


Figure: Multigrid V-cycle (advection-diffusion).

Application

- preconditioner of GMRES.
- preconditioner of LU-SSOR in GMRES.

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Deflation: restarted GMRES(m, k)

- k vectors u_1, \dots, u_k retained from GMRES(m).
- Augment the subspace with k vectors:

$$\text{span}\{r_0, Ar_0, \dots, A^{m-k-1}r_0, u_1, \dots, u_k\}.$$

- Eigenvectors of A , Ritz-vectors (eigenvectors of H)...
- \Rightarrow corresponding eigenvalues deflated from the spectrum.

Deflated eigenvalues:

- k eigenvectors corresponding to k smallest eigenvalues.
- Interior Rayleigh–Ritz (Shift and invert operator):
eigenvalues shifted to the exterior of the spectrum.
 \Rightarrow Interior Arnoldi method: eigenpairs (u_j, λ_j) , $1 \leq j \leq k$, solutions of

$$(H_m + |h_{m+1,m}|^2 H_m^{-T} e_m e_m^T) u_j - \lambda_j u_j = 0.$$

- Clustered eigenvalues.

Spectral analysis

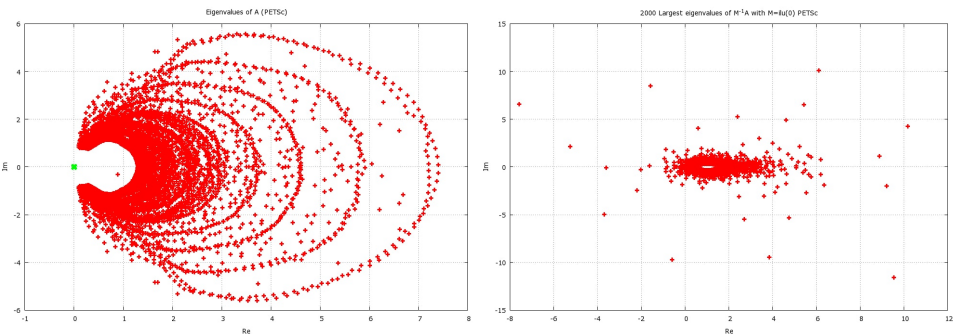


Figure: Flow over the NACA0012 profile. **Left:** Spectra of A . **Right:** Spectra of $M^{-1}A$.

Analytical Jacobian^[1]

- $\frac{\partial F}{\partial \mathbf{W}} = (A, B, C)$ with F the flux vector.
- $A := \frac{\partial f}{\partial \mathbf{W}}$, $B := \frac{\partial g}{\partial \mathbf{W}}$, $C := \frac{\partial h}{\partial \mathbf{W}}$ with f, g, h the flux components.
- Diagonalization:
 $A = P_1 D_1 P_1^{-1}$, $B = P_2 D_2 P_2^{-1}$ and $C = P_3 D_3 P_3^{-1}$, with D_i diagonal.
 \Rightarrow block diagonal matrix.
- $\frac{\partial R}{\partial \mathbf{W}} = \frac{\partial F}{\partial \mathbf{W}} \cdot \mathbf{N} = AN_x + BN_y + CN_z$.

Analytical inverse of the Jacobian

$$\frac{\partial R}{\partial \mathbf{W}}^{-1} \approx (AN_x + BN_y + CN_z)^{-1}$$

[1] C. Hirsch, *Numerical Computation of internal and external flows Vol. 2*, Wiley (1990).

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Conclusion & perspectives

Conclusions:

- ILU effective but sensitive with parameters and instable.
- Flexible GMRES more promising:
 - ▶ nested GMRES.
 - ▶ GMRES preconditioned by multigrid with LU-SSOR.
- Jacobi as scaling...

Perspectives:

- Block ILU more stable.
- From spectral analysis to deflation.
- Multigrid:
 - ▶ vary operators R and P ,
 - ▶ vary cycle V , W ...
- Block LU-SSOR.

Thanks for your attention.