Preconditioned GMRES method applied to aerodynamics optimization problem

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elsAASO-2017 - AS-5.1 Evaluation of preconditioners for GMRES in adjoint equation

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3. Improved GMRES
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- Euler equations related to aerodynamics problems.
- Residual form

$$\mathcal{R}(\boldsymbol{W}, \boldsymbol{X}) = 0, \tag{1}$$

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

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

  where α is the vector of design variables.
- Adjoint equation

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

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

Generalized Minimum Residual method

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

$$A \quad x = \quad b$$
$$\frac{\partial \mathcal{R}}{\partial \boldsymbol{W}}^T \lambda = -\frac{\partial \mathcal{J}}{\partial \boldsymbol{W}}^T.$$

Method: GMRES (Krylov subspace iteration):

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

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

- 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 $\dfrac{\partial \mathcal{R}}{\partial W}^{\text{app}}$ 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.
- 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(ϵ).
- with dual threshold: ILUT(k,ϵ).
- 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

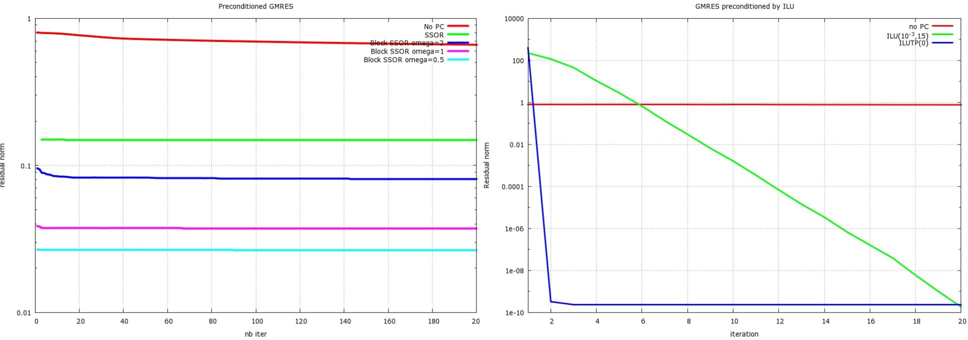

Figure: Flow over Naca0012 profile.
Left: SSOR and block SSOR preconditioning.
Right: ILUT and ILUTP preconditioning.

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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 $j = 1, ..., m$ **do**
    Compute $z_j := \boldsymbol{M_j^{-1}} v_j$
    Compute $w := Az_j$
    for $i = 1, ..., j$ **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 $\boldsymbol{Z_m := [M_1^{-1} v_1, ..., M_m^{-1} v_m]}$,
Compute $x_m = x_0 + \boldsymbol{Z_m} y_m$, where $y_m = \text{argmin}_y ||\beta e_1 - \bar{H}_m y||$
If satisfied stop, else set $x_0 \leftarrow x_m$ and goto 1.

Preconditioned GMRES convergence

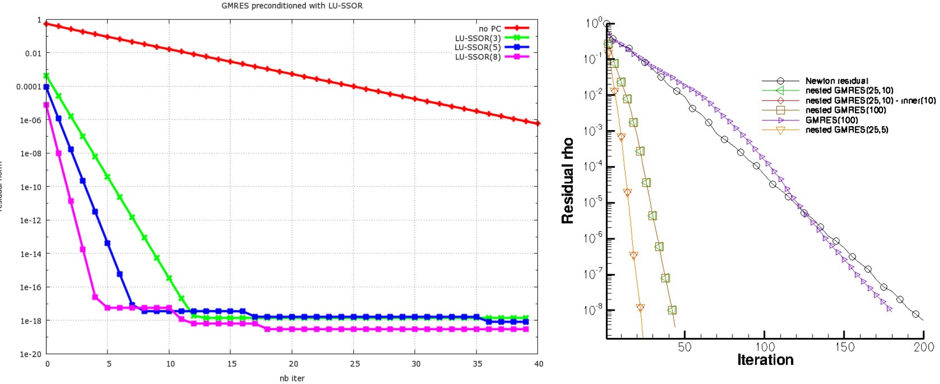

Figure: **Left:** LU-SSOR on advection-diffusion. **Right:** Nested GMRES on flow over the NACA0012 profile.

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 $e_h = P(e_{2h})$.

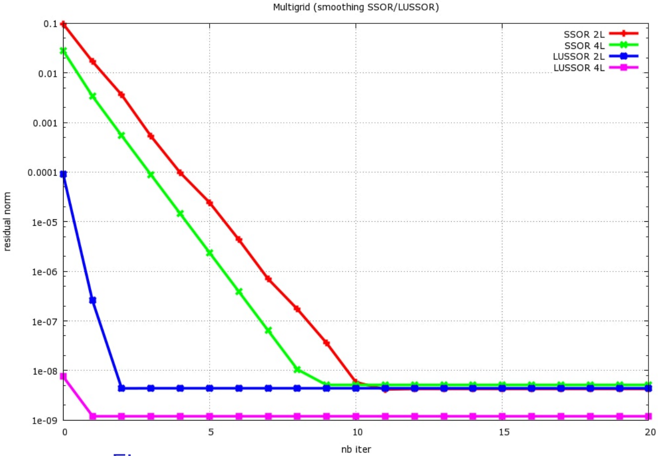

Figure: Multigrid V-cycle (advection-diffusion).

Application

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

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Deflation: restarted GMRES(m,k)

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

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

- 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

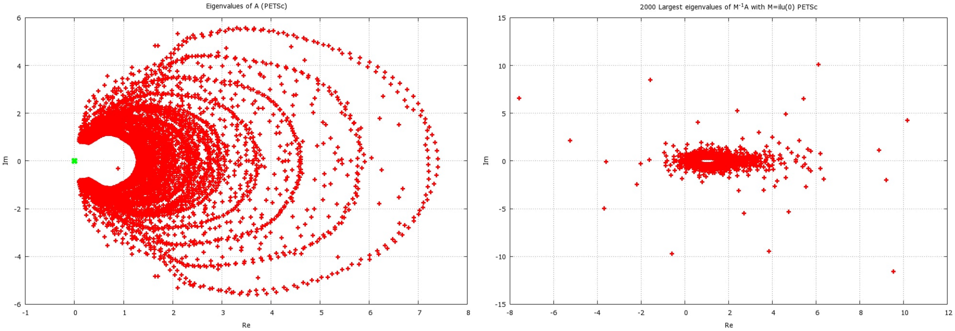

Figure: Flow over the NACA0012 profile. **Left:** Spectra of A. **Right:** Spectra of $M^{-1}A$.

Analytical Jacobian[1]

- $\dfrac{\partial F}{\partial \boldsymbol{W}} = (A, B, C)$ with F the flux vector.
- $A := \dfrac{\partial f}{\partial \boldsymbol{W}}$, $B := \dfrac{\partial g}{\partial \boldsymbol{W}}$, $C := \dfrac{\partial h}{\partial \boldsymbol{W}}$ 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.
- $\dfrac{\partial R}{\partial \boldsymbol{W}} = \dfrac{\partial F}{\partial \boldsymbol{W}} \cdot \boldsymbol{N} = AN_x + BN_y + CN_z$.

Analytical inverse of the Jacobian

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

[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.