Combining the augmented Lagrangian preconditioner with the SIMPLE Schur complement approximation

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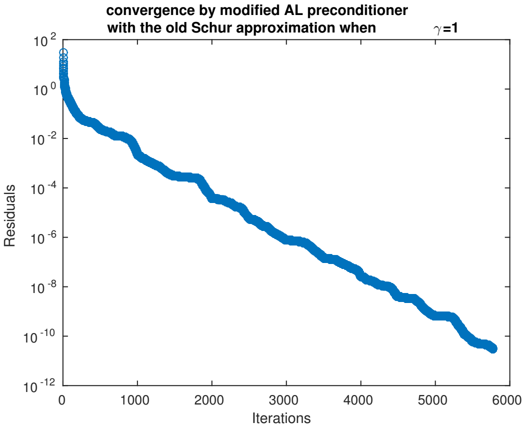
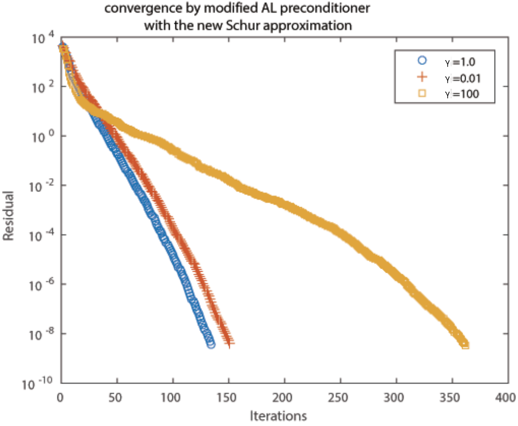
The convergence rate of modified AL



The convergence rate of modified AL, new version



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1. Motivation

Lid driven cavity $\Rightarrow$ Container ship

FEM	$\Rightarrow$	FVM
LBB satisfied	$\Rightarrow$	Stabilized
Reynolds $= 10^2$ (laminar)	$\Rightarrow$	Reynolds $= 10^8$ (turbulent)
Aspect ratio 1	$\Rightarrow$	Aspect ratio 10^4
Square	$\Rightarrow$	Complex geometry (Ship hull)

2. Incompressible Navier-Stokes equations

$$
\begin{aligned}
\int_S \rho \mathbf{u}\mathbf{u}\cdot\mathbf{n}\, dS + \int_S p\mathbf{n}\, dS - \int_S \mu_{\text{eff}}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot\mathbf{n}\, dS = \int_\Omega \rho\mathbf{b}\, d\Omega,\\
\int_S \mathbf{u}\cdot\mathbf{n}\, dS = 0
\end{aligned}
\tag{1}
$$

- $\mathbf{u}$: the velocity, p: the pressure, ρ: the constant density.
- $\mu_{\text{eff}} = \mu + \mu_{\text{t}}$
  effective viscosity is the sum of the constant dynamic viscosity μ and the variable turbulent eddy viscosity μ_{t}
- $\Omega \in \mathcal{R}^{2 \text{ or } 3}$ is a bounded domain with a surface S

$$\mathbf{u} = \mathbf{g} \text{ on } S_D, \quad \mu\frac{\partial\mathbf{u}}{\partial\mathbf{n}} - \mathbf{n}p = 0 \text{ on } S_N$$

Linear system

$$\begin{bmatrix} Q & G \\ D & C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ g \end{bmatrix} \text{ with } \mathcal{A} := \begin{bmatrix} Q & G \\ D & C \end{bmatrix}.$$

- Q: the diagonal blocks Q_{ii} correspond to the convection-diffusion operator.
- D, G: the divergence and gradient matrices.
  $D_\alpha = G_\alpha$ on structured and unstructured grids.
  Only on structured grids $D_\alpha = -D_\alpha^T \Rightarrow D = -G^T$ as in FEM.
- C: stabilization matrix arising from the pressure-weighted interpolation (PWI) methods.
  $C = D\text{diag}^{-1}(Q)G - \text{diag}^{-1}(Q_{ii})L_p$ (L_p: Laplacian matrix)
- $\mathcal{A}$: sparse and non-symmetric.

3. Block structured preconditioners

The block $\mathcal{LDU}$ decomposition of $\mathcal{A}$ is

$$\mathcal{A} = \mathcal{LDU} = \begin{bmatrix} Q & G \\ D & C \end{bmatrix} = \begin{bmatrix} I & O \\ DQ^{-1} & I \end{bmatrix} \begin{bmatrix} Q & O \\ O & S \end{bmatrix} \begin{bmatrix} I & Q^{-1}G \\ O & I \end{bmatrix},$$

$S = C - DQ^{-1}G$ is the Schur-complement matrix.

Block structured preconditioners $\mathcal{P}_L$ and $\mathcal{P}_U$

$$\mathcal{P}_L = \mathcal{LD} = \begin{bmatrix} Q & O \\ D & \widetilde{S} \end{bmatrix}, \quad \mathcal{P}_U = \mathcal{DU} = \begin{bmatrix} Q & G \\ O & \widetilde{S} \end{bmatrix},$$

- solve the velocity subsystem with Q,
- solve the pressure subsystem with $\widetilde{S} \approx S$.

How to find a spectrally equivalent and cheap approximation of S.

Block structured preconditioners

- PCD
  Silvester, Elman, Kay, Wathen 2001, Elman, Tuminaro 2009
- LSC
  Elman, Howle, Shadid, Shuttleworth, Tuminaro 2006
- SIMPLE
  Patankar, Spalding 1972, Vuik, Saghir, and Boerstoel 2000, Klaij and C. Vuik 2013
- Augmented Lagrangian
  Benzi and Olshanskii 2006, Benzi, Olshanskii, and Wang 2011
- Overview
  Elman, Silvester, and Wathen 2005, 2014, Benzi, Golub, and Liesen 2005

4. The augmented Lagrangian preconditioner

System $\begin{bmatrix} Q & G \\ D & C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ g \end{bmatrix}$ is transformed into

$$\begin{bmatrix} Q_\gamma & G_\gamma \\ D & C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f}_\gamma \\ g \end{bmatrix} \quad \text{with} \quad \mathcal{A}_\gamma := \begin{bmatrix} Q_\gamma & G_\gamma \\ D & C \end{bmatrix}$$

- $Q_\gamma = Q - \gamma G W^{-1} D$, $G_\gamma = G - \gamma G W^{-1} C$, $\mathbf{f}_\gamma = \mathbf{f} - \gamma G W^{-1} g$.
- $\gamma > 0$ and W are scalar and nonsingular matrix parameters.
- the Schur complement of $\mathcal{A}_\gamma$ is $S_\gamma = C - D Q_\gamma^{-1} G_\gamma$.

Ideal AL preconditioner is based on the block $\mathcal{DU}$ decomposition of $\mathcal{A}_\gamma$

$$\mathcal{P}_{IAL} = \begin{bmatrix} Q_\gamma & G_\gamma \\ O & \widetilde{S}_\gamma \end{bmatrix},$$

where $\widetilde{S}_\gamma$ denotes the approximation of S_γ.

The modified AL preconditioner

$$Q_\gamma = \begin{bmatrix} Q_1 - \gamma G_1 W^{-1} D_1 & -\gamma G_1 W^{-1} D_2 \\ -\gamma G_2 W^{-1} D_1 & Q_1 - \gamma G_2 W^{-1} D_2 \end{bmatrix} \text{(coupling of } G_i D_j (i \neq j))$$

$$\widetilde{Q}_\gamma = \begin{bmatrix} Q_1 - \gamma G_1 W^{-1} D_1 & O \\ -\gamma G_2 W^{-1} D_1 & Q_1 - \gamma G_2 W^{-1} D_2 \end{bmatrix} \text{(no coupling of } G_i D_j (i \neq j)$$

Replacing Q_γ by its block lower-triangular part $\widetilde{Q}_\gamma$ and substituting $\widetilde{Q}_\gamma$ into $\mathcal{P}_{IAL}$ gives the modified AL preconditioner $\mathcal{P}_{MAL}$:

$$\mathcal{P}_{MAL} = \begin{bmatrix} \widetilde{Q}_\gamma & G_\gamma \\ O & \widetilde{S}_\gamma \end{bmatrix}.$$

The new Schur approximation in the AL preconditioner

The novel approximation is based on:

Lemma

Assuming that all the relevant matrices are invertible, then the inverse of S_γ is given by

$$S_\gamma^{-1} = S^{-1}(I - \gamma C W^{-1}) + \gamma W^{-1},$$

where $S = C - DQ^{-1}G$ denotes the Schur complement of the original system with $\mathcal{A}$.

Proof: see [1]

[1] X. He, C. Vuik and C. Klaij. Block preconditioners for the incompressible Navier-Stokes equations discretized by a finite volume method. *Journal of Numerical Mathematics*, published online DOI: 2016.

The new Schur approximation in the AL preconditioner

Old option 1: $W_1 = \gamma C + M_p$ and $\widetilde{S}_{\gamma \text{ old}} = C + \gamma^{-1} M_p$.

Choosing $W_1 = \gamma C + M_p$ and substituting W_1 into
$S_\gamma^{-1} = S^{-1}(I - \gamma C W^{-1}) + \gamma W^{-1}$, leads to

$$S_\gamma^{-1} = (\gamma^{-1} S^{-1} M_p + I)(C + \gamma^{-1} M_p)^{-1}.$$

For large values of γ such that $\| \gamma^{-1} S^{-1} M_p \| \ll 1$ we can approximate S_γ by

$$\widetilde{S}_{\gamma \text{ old}} = C + \gamma^{-1} M_p.$$

Comment:

- $W_1 = \gamma C + M_p$ is not a practical option since its inverse is needed in the AL transformation.

The new Schur approximation in the AL preconditioner

Old option 2: $W = M_p$ and $\widetilde{S}_{\gamma \text{ old}} = C + \gamma^{-1} M_p$.
Comments:

- The approximation $\widetilde{S}_{\gamma \text{ old}}$ is obtained if and only if $W_1 = \gamma C + M_p$ and large values of γ are chosen.
- However, $W = M_p$ is close to $W_1 = \gamma C + M_p$ only when γ is small.
- it is contradictory to tune the value of γ so that W and $\widetilde{S}_{\gamma \text{ old}}$ could be simultaneously obtained.

[1] M. Benzi, M.A. Olshanskii, Z. Wang. Modified augmented Lagrangian preconditioners for the incompressible Navier-Stokes equations. *Int. J. Numer. Meth. Fluids.*, 66:486-508, 2011.
[1] X. He, C. Vuik and C. Klaij. Block preconditioners for the incompressible Navier-Stokes equations discretized by a finite volume method. *Journal of Numerical Mathematics*, 2016.

The new Schur approximation in the AL preconditioner

New option: $W = M_p$ and $\widetilde{S}_{\gamma\ \text{new}}^{-1} = \widetilde{S}_{SIMPLE}^{-1}(I - \gamma C M_p^{-1}) + \gamma M_p^{-1}$.

Comments:

- Since M_p is a diagonal matrix with density multiplied with cell volumes in FVM, it is trivial to obtain its inverse.
- The complexity of applying $\widetilde{S}_{\gamma\ \text{new}}$ is focused on solving the system with $\widetilde{S}_{SIMPLE}$.

Comparison between the AL and SIMPLE preconditioners

Implementation costs of the two Schur complement approximations in the AL preconditioner and SIMPLE preconditioner

- Regarding the AL preconditioner, it is difficult to analytically compare the complexity of solving the sub-systems with $\widetilde{S}_{\gamma \text{ new}}$ and $\widetilde{S}_{\gamma \text{ old}}$.
- Numerical experiments show that the number of Krylov subspace iterations preconditioned by the AL preconditioner with $\widetilde{S}_{\gamma \text{ new}}$ is much less than $\widetilde{S}_{\gamma \text{ old}}$. This makes the new Schur complement approximation more efficient and attractive.
- The complexity of solving the sub-systems with Q_γ ($\widetilde{Q}_\gamma$) and $\widetilde{S}_{\gamma \text{ new}}$ in the AL preconditioner is higher than Q and $\widetilde{S}_\gamma$ in the SIMPLE preconditioner, respectively.
- A reduced number of Krylov subspace iterations could pay off the more complexity at each Krylov iteration and makes the AL preconditioner with the new Schur complement approximation gain over the SIMPLE preconditioner.

5. Numerical experiments

Fully turbulent flows are considered ($Re = 10^7$) on block-structured grids.

The grids are refined near the leading and trailing edge of the plate and spread out in the wake of the plate.

Near the middle of the plate, the cells have an aspect ratio $1 : 104$.

All experiments are carried out based on the blocks Q, G, D and C obtained at the 30th nonlinear iteration with 80×40 structured grids.

These blocks are generated by MARIN's CFD software package ReFRESCO and imported to Matlab.

The spectrum of the new Schur approximation $\widetilde{S}_{\gamma \text{ new}}$

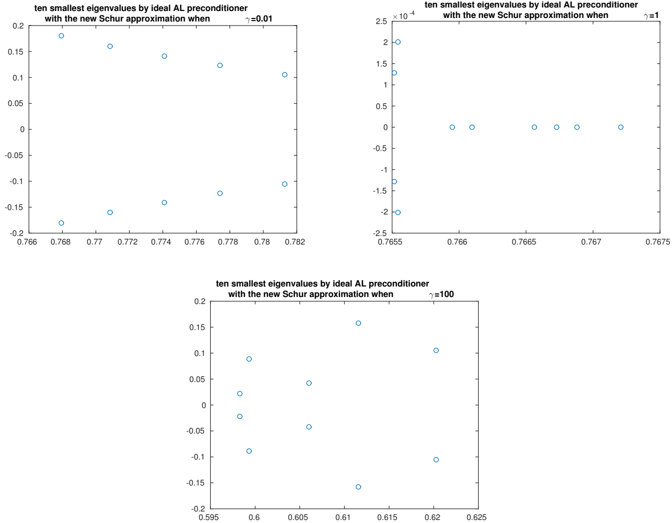
The following figures present ten smallest and largest eigenvalues of $\mathcal{P}_{IAL}^{-1}\mathcal{A}_\gamma$ and $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with the new Schur approximation $\widetilde{S}_{\gamma \text{ new}}$.

We can see:

- the smallest eigenvalues are far away from zero and the spectrum of eigenvalues is clustered. Such a distribution of eigenvalues is favourable for Krylov subspace solvers and a fast convergence rate can be expected.
- The value of γ could effect the distribution of eigenvalues. For relative small values, e.g. $\gamma = 0.01$ and $\gamma = 1.0$ the effect is moderate.
- It appears that the optimal value of γ, which leads to the most clustered eigenvalues, is the same for both the *ideal* and modified AL preconditioners, i.e., $\gamma_{\text{opt}} = 1.0$.

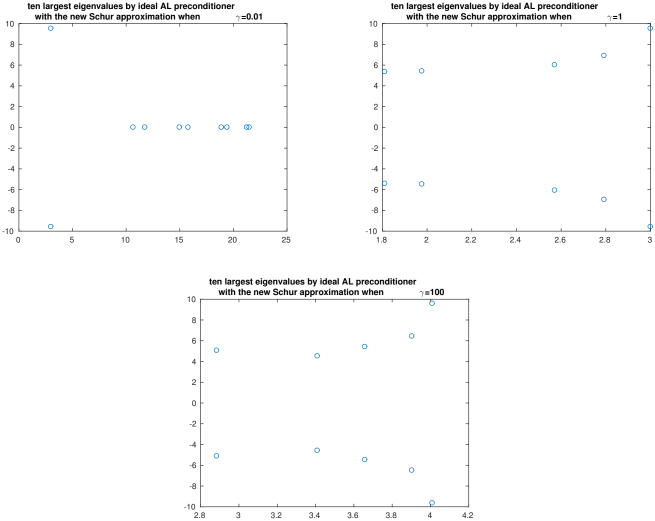
$\mathcal{P}_{IAL}$ with $\widetilde{S}_\gamma$ new

Figure : Ten smallest eigenvalues of $\mathcal{P}_{IAL}^{-1}\mathcal{A}_\gamma$ with $\widetilde{S}_\gamma$ new and different values of γ.



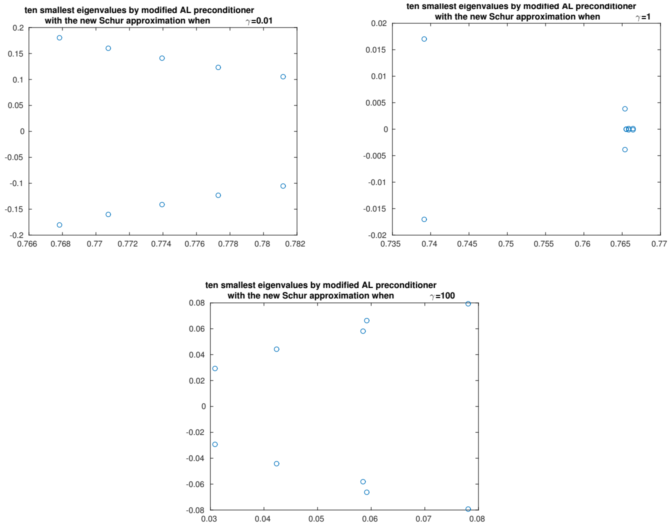
$\mathcal{P}_{IAL}$ with $\widetilde{S}_{\gamma}$ new

Figure : Ten largest eigenvalues of $\mathcal{P}_{IAL}^{-1}\mathcal{A}_{\gamma}$ with $\widetilde{S}_{\gamma}$ new and different values of γ.



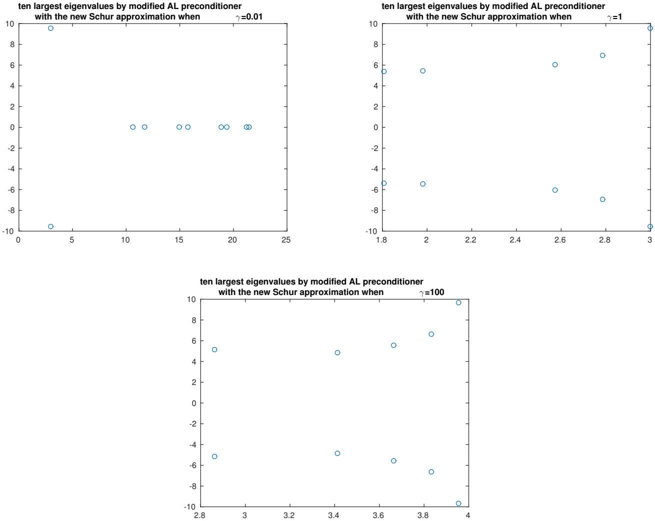
$\mathcal{P}_{MAL}$ with $\widetilde{S}_\gamma$ new

Figure : Ten smallest eigenvalues of $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with $\widetilde{S}_\gamma$ new and different values of γ.



$\mathcal{P}_{MAL}$ with $\widetilde{S}_\gamma$ new

Figure : Ten largest eigenvalues of $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with $\widetilde{S}_\gamma$ new and different values of γ.



The convergence rate with the new Schur approximation $\widetilde{S}_{\gamma \text{ new}}$

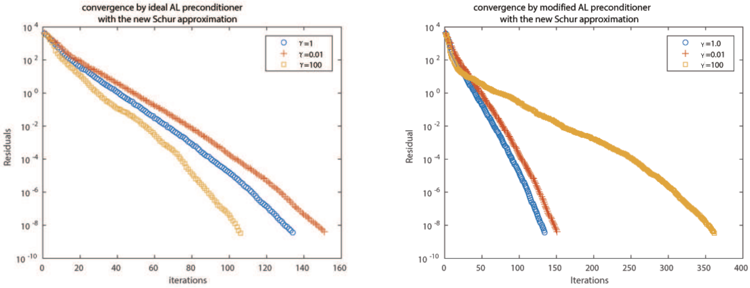
The following figure presents the convergence rate of the Krylov subspace solver preconditioned by the *ideal* and modified AL preconditioners with the new Schur approximation $\widetilde{S}_{\gamma \text{ new}}$.

We can see:

- This conforms the prediction that the new Schur approximation $\widetilde{S}_{\gamma \text{ new}}$ produces the favourable feature for the Krylov subspace solvers.
- The convergence rate varies with different values of γ and $\gamma_{\text{opt}} = 1.0$ results in the fastest convergence. This again confirms the prediction regarding the effect of values of the parameter γ.

The convergence rate with the new Schur approximation $\widetilde{S}_{\gamma_{\text{new}}}$

Figure : The convergence of GMRES (no restart) preconditioned by the *ideal* and modified AL preconditioner with $\widetilde{S}_{\gamma\ \text{new}}$. The involved sub-systems are solved directly.



The eigenvalues of the old Schur approximation $\widetilde{S}_{\gamma \text{ old}}$

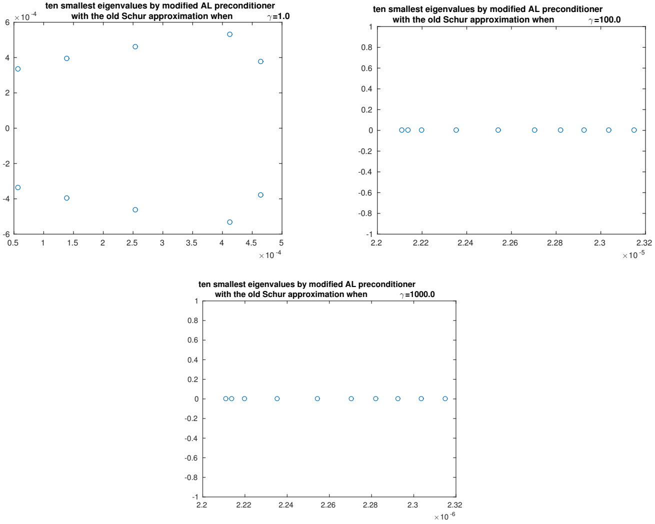
The following figures present ten smallest and largest eigenvalues of $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with the old Schur approximation $\widetilde{S}_{\gamma \text{ old}}$.

We can see:

- The smallest eigenvalues are quite close to zero for all the tested values of γ, which degrades the efficiency of the Krylov subspace solver.

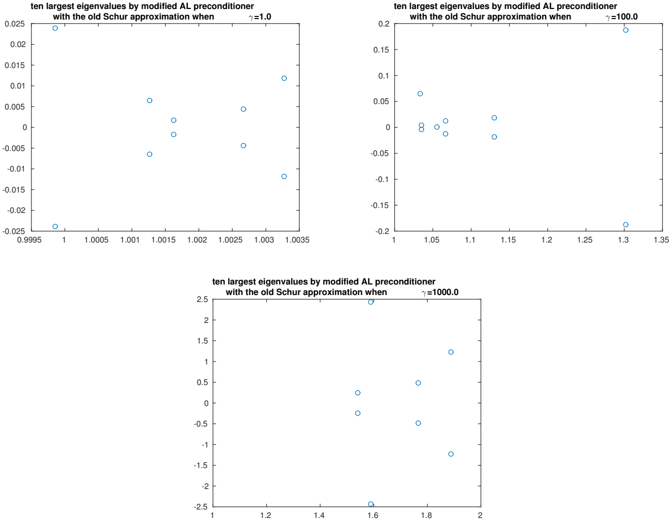
$\mathcal{P}_{MAL}$ with $\widetilde{S}_\gamma$ old

Figure : Ten smallest eigenvalues of $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with $\widetilde{S}_\gamma$ old and different values of γ.



$\mathcal{P}_{MAL}$ with $\widetilde{S}_{\gamma \text{ old}}$

Figure : Ten largest eigenvalues of $\mathcal{P}_{MAL}^{-1}\mathcal{A}_\gamma$ with $\widetilde{S}_{\gamma \text{ old}}$ and different values of γ.



The convergence rate with the old Schur approximation $\widetilde{S}_{\gamma\ \mathrm{old}}$

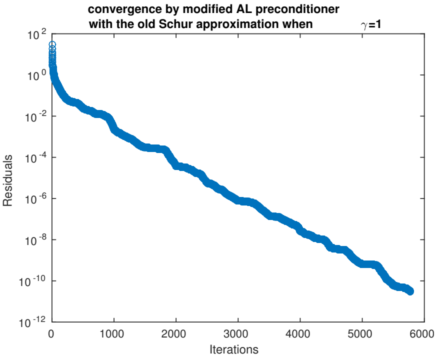
The following figure presents the convergence rate of the Krylov subspace solver preconditioned by the modified AL preconditioner with the old Schur approximation $\widetilde{S}_{\gamma\ \mathrm{old}}$.

We can see:

- The old Schur approximation leads to a very slow convergence.
- The new Schur approximation can significantly improve the performance of the AL preconditioner in the turbulent case.

The convergence rate with the old Schur approximation $\widetilde{S}_{\gamma \text{ old}}$

Figure : The convergence of GMRES (no restart) preconditioned by the modified AL preconditioner with $\widetilde{S}_{\gamma \text{ old}}$. The involved sub-systems are solved directly.



Comparison between the augmented Lagrangian and SIMPLE preconditioner

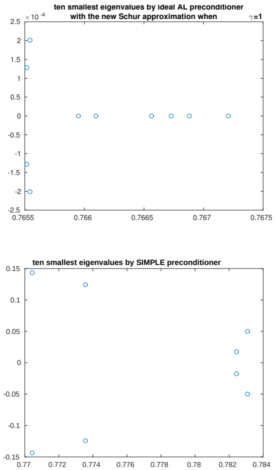
As follows the spectrum of eigenvalues by using the SIMPLE preconditioner is given and compared to the *ideal* AL preconditioner with the new Schur complement approximation $\widetilde{S}_{\gamma \text{ new}}$.

We can see:

- The smallest eigenvalues are nearly the same by using these two preconditioner.
- The SIMPLE preconditioner leads to a bigger ratio between the largest and smallest magnitude of eigenvalues, which means that the spectrum of eigenvalues is less clustered compared to the AL preconditioner.

Comparison between the augmented Lagrangian and SIMPLE preconditioner

Figure : Ten smallest and largest eigenvalues of $\mathcal{P}_{IAL}^{-1}\mathcal{A}_\gamma$ (top) with $\widetilde{S}_{\gamma \text{ new}}$ ($\gamma_{opt} = 1.0$) and of $\mathcal{P}_{SIMPLE}^{-1}\mathcal{A}$ (down).



Comparison between the augmented Lagrangian and SIMPLE preconditioner

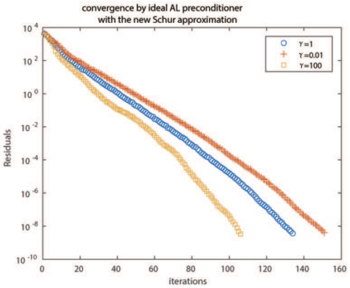
As follows the convergence rate by using the SIMPLE preconditioner is given and compared to the *ideal* AL preconditioner with the new Schur complement approximation $\widetilde{S}_{\gamma \text{ new}}$.

We can see:

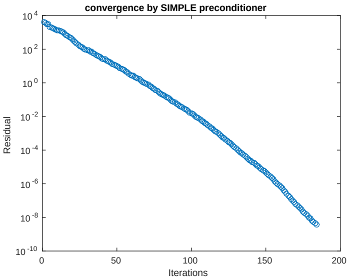
- The number of Krylov subspace iterations by applying the *ideal* AL preconditioner with $\widetilde{S}_{\gamma \text{ new}}$ and $\gamma_{\text{opt}} = 1.0$ is around 140 and is about 180 by employing the SIMPLE preconditioner.
- A faster convergence rate of the Krylov subspace solver is obtained by applying the AL preconditioner.
- Taking into account the more complexity at each Krylov iteration, it seems that the gain of the AL preconditioner in terms of the number of iterations is not sufficient to take an advantage over the SIMPLE preconditioner on this benchmark.

Comparison between the augmented Lagrangian and SIMPLE preconditioner

Figure : The convergence of GMRES (no restart) preconditioned by the *ideal* AL preconditioner with the new Schur approximation $\widetilde{S}_{\gamma\ \mathrm{new}}$ and the SIMPLE preconditioner. The involved sub-systems are solved directly.



(a) ideal AL preconditioner



(b) SIMPLE preconditioner

6. Conclusions

- the proposed new Schur approximation makes the AL preconditioner applicable in the turbulent cases with variable viscosity.
- The convergence and the spectrum of the ideal and modified AL preconditioner with the new Schur approximation are close for γ values around 1.
- In all experiments it appears that the choice $\gamma = 1$ is optimal.
- The convergence and efficiency of the modified AL preconditioner with the new Schur approximation and the SIMPLE preconditioner are comparable.

7. References

1. C. Vuik, A. Saghir, and G.P. Boerstoel
   The Krylov accelerated SIMPLE(R) method for flow problems in industrial furnaces
   International Journal for Numerical methods in fluids, 33 pp. 1027-1040, 2000
2. M. ur Rehman, T. Geenen, C. Vuik, G. Segal, and S.P. MacLachlan
   On iterative methods for the incompressible Stokes problem
   Int. J. Num. Meth. in Fluids, 65, pp. 1180-1200, 2011
3. C.M. Klaij and C. Vuik
   SIMPLE-type preconditioners for cell-centered, colocated finite volume discretization of incompressible Reynolds-averaged Navier-Stokes equations
   International Journal for Numerical Methods in Fluids, 71, pp. 830-849, 2013
4. X. He, C. Vuik, and C. Klaij
   Block preconditioners for the incompressible Navier-Stokes equations discretized by a finite volume method
   Journal of Numerical Mathematics, 25(2), pp. 89-105, 2017
5. X. He, C. Vuik, and C. Klaij
   Combining the augmented Lagrangian preconditioner with the SIMPLE Schur complement approximation
   TUD Report 17-06, 2017