Anderson Accelerated PMHSS for Complex-Symmetric Linear Systems

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Complex-valued linear systems

$$(A + iB)x = b. \quad A, B \in \mathbb{R}^{n\times n} \text{ and } x, b \in \mathbb{C}^n \tag{1}$$

Many PDEs

- Electromagnetics
- Waves
- etc.

There are many methods for solving linear systems

- Splitting methods: Jacobi, Gauss-Seidel, ...
- Projection methods
- Krylov subspace methods: CG, GMRES, ...
- Multigrid methods

PMHSS-splitting

Preconditioned modified skew-Hermitian splitting (PMHSS), comes from a family of splitting: alternating direction iteration (ADI).

$$(\alpha V + A)\hat{x}_{k+1/2} = (\alpha V - iB)\hat{x}_k + b \tag{2}$$
$$(\alpha V + B)\hat{x}_{k+1} = (\alpha V + iA)\hat{x}_{k+1/2} - ib. \tag{3}$$

For $V \in \mathbb{R}^{n\times n}$ and $\alpha > 0$, as k increase, $\hat{x}$ tends to the solution of (1). For the choice $\alpha = 1$ and $V = A$ we have:

$$(A + B)\hat{x}_{k+1/2} = \frac{(1+i)}{2}(A - iB)x_k - \frac{(1-i)}{2}b \tag{4}$$

the take away

This iteration is conditionally converging to x independently of $\hat{x}_0$. If the iteration matrix $\Psi = (A + B)^{-1}\frac{(1+i)}{2}(A - iB)$ has a spectrum covered by the unit disk $\rho(\Psi) < 1$.

The fixed-point iteration

$$\Psi = \frac{(1+i)}{2}(A+B)^{-1}(A-iB), \quad c = \frac{(1-i)}{2}(A+B)^{-1}b. \tag{5}$$

Assuming an initial guess $\hat{x}_0 = 0$ (and thus $\hat{x}_1 = c$), repeated application of the update rule gives us the following relation:

$$\hat{x}_{k+1} = \Psi(\ldots(\Psi c + c) + \ldots) + c = (\Psi^k + \ldots + \Psi + I)c. \tag{6}$$

The expression in the parentheses is a geometric sum (of matrices), which has the closed form $(I-\Psi)^{-1}(I-\Psi^k)$. Hence, we have

$$\hat{x}_{k+1} = (I-\Psi)^{-1}(I-\Psi^k)c. \tag{7}$$

When the spectral radius $\rho(\Psi) < 1$ as in, we have that $(I-\Psi)^{-1}(I-\Psi^k) \to (I-\Psi)^{-1}$ as $k \to \infty$. Thus, in the limit, the solution obtained satisfies:

$$(I-\Psi)\hat{x} = c. \tag{8}$$

Solving the inner system in-exactly

The following linear system needs to be solved each iteration.

$$(A + B)\hat{x}_k = \frac{(1+i)}{2}(A - iB)x_k - \frac{(1-i)}{2}b \tag{9}$$

Evaluating the error

$$\begin{aligned} ||e_0(k)|| &= ||x^*_{k+1} - \hat{x}_k|| && (10)\\ &\approx ||\hat{x}_{k+1} - \hat{x}_k|| && (11)\\ &= ||(I - \Psi)^{-1}(\Psi^k - \Psi^{k+1})c|| && (12)\\ &= ||(I - \Psi)^{-1}(I - \Psi)\Psi^k c|| && (13)\\ &\leq ||\Psi^k|| \cdot ||c||. && (14) \end{aligned}$$

The take away

Each outer iteration generates a solution x that is a better approximation for the inner solver.

As a preconditoner

The *iteration matrix* from the splitting has been used with Krylov solvers such as GMRES.

PMHSS preconditioning, where q is the current residual in the iterative method (GMRES in our case).

1: Solve $(A + B)z = q$
2: Set $x = \frac{(1-i)}{2}z$

Applying the preconditioner

Note that the linear system that is solved as the preconditioner is not the same as the one in the fixed-point.

AA-PMHSS

Anderson Acceleration is a method that is used to accelerate fixed-point iterations by recasting it as an optimization problem.

$$x = f(x), \quad g(x) := f(x) - x \tag{15}$$

With the minimization defined as:

$$\text{argmin}_{\alpha_k \in A_k} ||G_k \alpha||_2 \quad A_k = \{\alpha \in \mathbb{C}^k : \sum_i \alpha_i = 1\}, \tag{16}$$

where $G_k = [g_0, ..., g_k]$. Then the current best solution is updated accordingly.

$$x_{k+1} = F_k \alpha_k \quad F_k = [f_0, ..., f_k] \tag{17}$$

A single step in our algorithm

1: Solve : $(A + B)x_{k+1} = \frac{(1+i)}{2}(A - iB)\bar{x}_k + \frac{(1-i)}{2}b$

2: $X_k = [x_1 - x_0, ..., x_{k-1} - x_k]$
$G_k = [g_1 - g_0, ..., g_{k-1} - g_k]$
$g_k = x_{k+1} - \bar{x}_k$

3: Solve : $\text{argmin}_{\alpha_k \in A_k} ||g_k - G_k \alpha||_2, A_k = \{\alpha \in \mathbb{C}^k\}$

4: $\bar{x}_{k+1} = x_k + g_k - (X_k + G_k)\alpha_k$

Anderson Acceleration and GMRES

fixed-point

$$x \in F(x_0, f(x_0), f(f(x_0)), f(f(f(x_0))), \ldots)$$

Krylov

$$x \in K(r_0, Ar_0, A^2 r_0, A^3 r_0, \ldots) \tag{18}$$

AA

$$\text{argmin}_{x \in F(x_0, f)} ||f(x) - x||$$

GMRES

$$\text{argmin}_{x \in K(r_0, A)} ||r(x)||$$

Essentially equivalent

Accelerating the fixed-point iteration defined by $f(x) = Ax + b$ with AA is equivalent to solving $(I - A)x = b$

Spectrum

Assume A is SPD and B is SPSD so that the eigenvalues μ of $A^{-1}B$ are real and non-negative. we have that $(A + B)^{-1}(A + iB) = (I + (i - 1)(I + A^{-1}B)^{-1}(A^{-1}B))$ thus the preconditioned eigenvalues are:

$$\lambda_{\text{PMHSS-GMRES}} = 1 + (i - 1)\frac{\mu}{\mu + 1}. \tag{19}$$

We then have, if $\mu_{\min} \le \mu \le \mu_{\max}$,

$$\frac{1}{1 + \mu_{\max}} \le \mathfrak{Re}(\lambda) \le \frac{1}{1 + \mu_{\min}}, \tag{20}$$

$$\frac{\mu_{\min}}{1 + \mu_{\min}} \le \mathfrak{Im}(\lambda) \le \frac{\mu_{\max}}{1 + \mu_{\max}}. \tag{21}$$

Modelling the AA-PMHSS as GMRES with $(I - \Psi)$ and similar analysis as before, gives us the preconditioned eigenvalues for the AA-PMHSS iteration as

$$\lambda_{\text{AA-PMHSS}} = 1 - \bar{\lambda}_{\text{PMHSS-GMRES}} \tag{22}$$

$$= 1 + (i + 1)\frac{\mu}{\mu + 1}. \tag{23}$$

Conclusions

- This is the same spectrum but mirrored around the real axis.
- The spectrum is discretization independent

Test Systems

Padé approximation

$$\left[\left(L + \frac{3-\sqrt{3}}{h}I\right) + i\left(L + \frac{3+\sqrt{3}}{h}I\right)\right]x = b \tag{24}$$

Inhomogeneous Helmholtz equation or Shifted ω-system

$$\left[L + (\mu + i\omega)I\right]x = b. \tag{25}$$

Here we use the coefficients $\mu = 0$ and $\omega = 0.01$.

Equations of Motion

$$\left[\left(K - \omega^2 M\right) + i\left(\omega C_V + C_H\right)\right]x = b. \tag{26}$$

Where M and K are the inertia- and the stiffness matrices, C_V and C_H are the viscous- and hysteretic dampening matrices.

Time-harmonic Eddy Current simulation

High-order FEM system in three sizes.
With a conditioning parameter ω

$$\begin{bmatrix} \underline{A} & \underline{B}^T \\ \underline{B} & \underline{C} \end{bmatrix} \mathbf{x} = \mathbf{b} \tag{27}$$

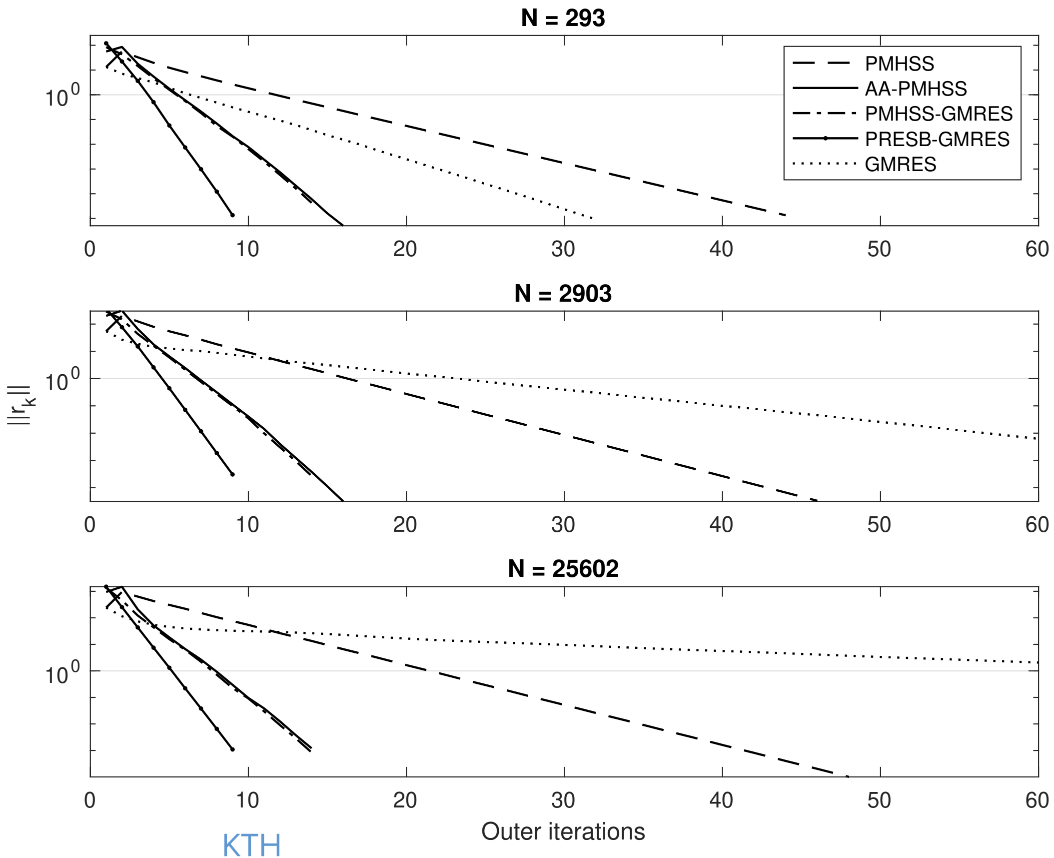
Where $\underline{B}$ is a complex matrix, $\underline{A}$ and $\underline{C}$ are complex-symmetric matrices.

Rate of Convergence

- Unpreconditioned GMRES only converge for the smallest system.
- PMHSS-GMRES and AA-PMHSS converges at essentially the same rate.

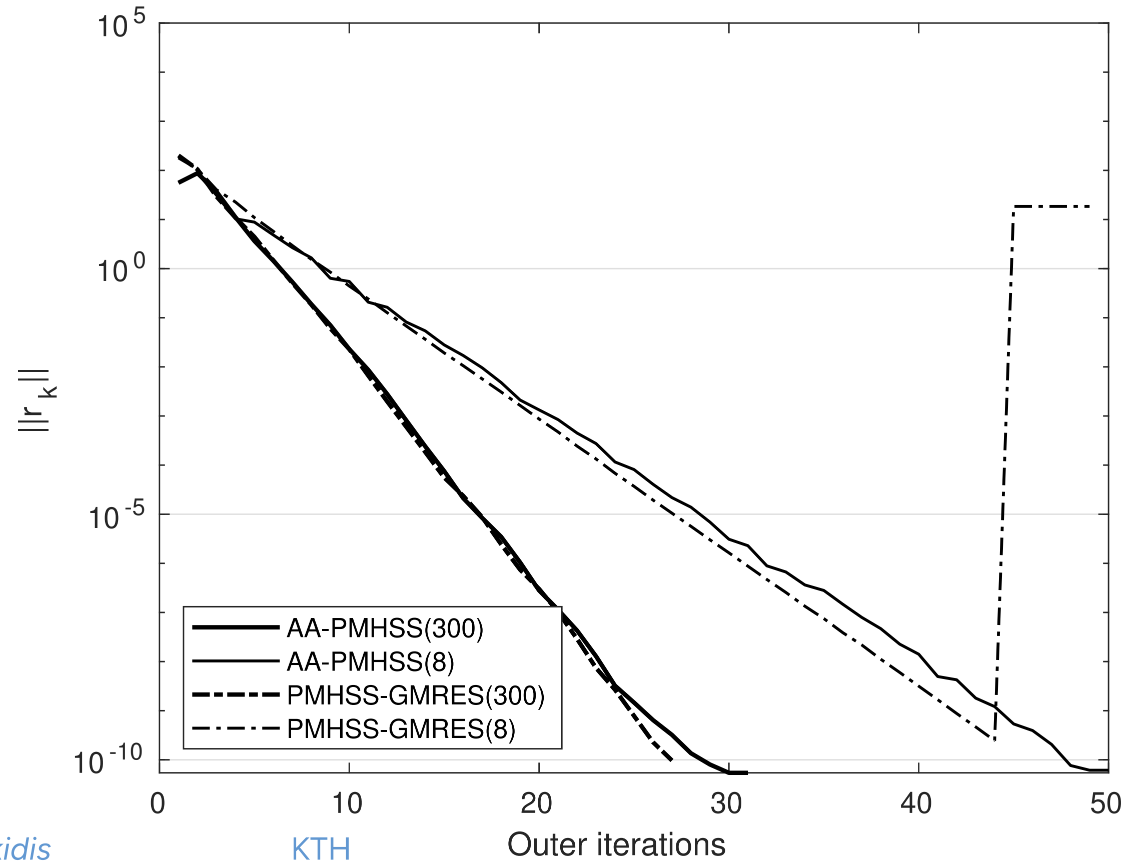
PRESB preconditioner

The PRESB preconditioner needs to solve **two** systems with $(A + B)$ for each GMRES iteration.



Outer iterations

- Number of outer iterations
- PMHSS-GMRES is more prone to break down due to accuracy of inner solver

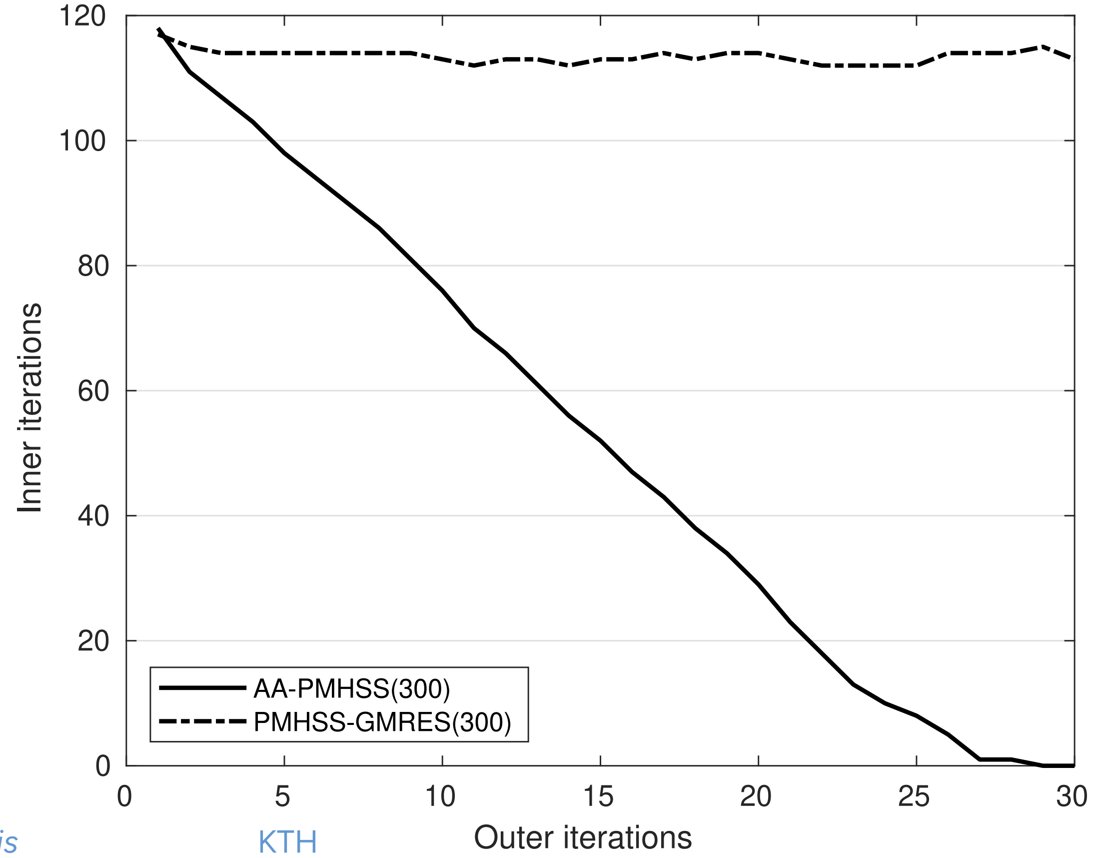


Inner iterations

- Inner/Outer
- 300 iterations was pessimistic
- We see a linear decay in the number of needed inner iterations for AA-PMHSS.

Fewer CG calls

A 1/3 as many CG iterations in total



Results

Method/size	outer iter.	inner iter.	T ± σ [s]	$\|\|r\|\|$	$\|\|x^* - x\|\|$	$\|\|(A+B)^{-1}r\|\|$
			Padé			
PMHSS						
10000	33	4172	0.677228 ± 5.79%	3.44893e-16	6.24067e-15	4.99637e-15
40000	34	6134	2.63969 ± 0.8817%	1.71351e-17	6.20946e-16	4.99868e-16
90000	34	7531	6.13483 ± 0.3547%	4.10001e-18	2.16516e-16	1.74593e-16
GMRES						
10000	133	-	0.638218 ± 1.767%	7.715e-15	6.87689e-14	-
40000	188	-	3.4308 ± 1.579%	9.54629e-16	2.35029e-14	-
90000	227	-	9.44645 ± 2.2%	2.9451e-16	1.0854e-14	-
AA-PMHSS						
10000	10	1300	**0.238979** ± 5.973%	1.11205e-15	6.81956e-16	4.95078e-16
40000	11	1963	**1.00926** ± 1.607%	3.94656e-17	3.33882e-17	2.47074e-17
90000	11	2432	**2.37411** ± 0.4164%	1.31937e-17	1.36944e-17	1.01987e-17
PMHSS-GMRES						
10000	9	2204	0.345996 ± 0.02171%	1.96557e-14	1.37958e-14	1.00285e-14
40000	10	3203	1.36888 ± 0.009568%	5.67274e-16	5.10832e-16	3.77199e-16
90000	10	3995	3.27446 ± 0.01784%	1.92527e-16	1.97563e-16	1.46642e-16
PRESB-GMRES						
10000	8	3464	0.258084 ± 0.008148%	3.35243e-15	4.61427e-15	2.46771e-15
40000	8	5637	1.28754 ± 0.02749%	1.1019e-15	2.12654e-15	1.18669e-15
90000	8	7030	3.05243 ± 0.02684%	3.76795e-16	8.44006e-16	4.7808e-16

Results

Method/size	outer iter.	inner iter.	T ± σ [s]	$\|\|r\|\|$	$\|\|x^* - x\|\|$	$\|\|(A+B)^{-1}r\|\|$
			Shifted-ω system			
PMHSS						
10000	49	6281	1.085 ± 0.2419%	2.58145e-10	7.72275e-11	7.63703e-11
40000	50	7126	3.157 ± 0.2576%	9.04324e-11	2.94851e-11	2.90853e-11
90000	50	7187	6.058 ± 0.6971%	6.02718e-11	1.97633e-11	1.9518e-11
GMRES						
10000	212	-	1.677 ± 3.722%	7.91011e-11	2.32285e-09	-
40000	232	-	5.214 ± 0.508%	3.87483e-11	1.35325e-09	-
90000	233	-	10.05 ± 1.007%	2.6577e-11	9.42004e-10	-
AA-PMHSS						
10000	18	2751	0.5119 ± 5.645%	1.61867e-11	1.2482e-11	1.03118e-11
40000	21	3498	1.783 ± 1.185%	2.50785e-11	2.48957e-11	2.05558e-11
90000	22	3648	3.639 ± 0.7017%	1.28299e-11	1.19634e-11	1.00378e-11
PMHSS-GMRES						
10000	18	4340	0.7649 ± 0.004377%	1.06948e-10	1.1078e-10	8.60833e-11
40000	22	5572	2.461 ± 0.03121%	4.01809e-11	4.64125e-11	3.75068e-11
90000	22	5906	5.013 ± 0.03158%	4.72434e-11	5.3194e-11	4.32722e-11
PRESB-GMRES						
10000	12	5616	**0.4379** ± 0.009439%	5.23277e-11	7.00731e-11	4.42568e-11
40000	12	6793	**1.561** ± 0.02302%	5.95516e-11	7.75276e-11	4.89482e-11
90000	12	6544	**2.866** ± 0.03836%	6.26606e-12	7.18707e-11	4.42628e-11
AA-PMHSS(50)						
10000	21	1049	**0.2244** ± 3.837%	4.67345e-12	4.88027e-11	4.2427e-11
40000	25	1248	**0.8066** ± 1.546%	1.16763e-12	1.0343e-11	8.89348e-12
90000	26	1299	**1.78** ± 1.487%	1.12012e-12	7.91642e-12	6.65226e-12

Results

Method/size	outer iter.	inner iter.	T ± σ [s]	$\|\|r\|\|$	$\|\|x^* - x\|\|$	$\|\|(A+B)^{-1}r\|\|$
			Eq. of Motion			
PMHSS						
10000	49	10358	1.786 ± 1.65%	1.25823e-10	7.30042e-11	7.09021e-11
40000	51	20638	8.945 ± 1.766%	3.13699e-11	3.25443e-11	3.16235e-11
90000	52	30185	24.9 ± 0.1285%	1.45818e-11	2.19632e-11	2.13458e-11
GMRES						
10000	280	-	3.057 ± 0.8814%	7.83319e-11	2.34518e-09	-
40000	548	-	28.78 ± 1.626%	3.97398e-11	4.39533e-09	-
90000	807	-	117.2 ± 1.591%	2.63963e-11	6.403e-09	-
AA-PMHSS						
10000	12	2732	**0.5376** ± 3.711%	4.22335e-13	6.91976e-13	5.76201e-13
40000	12	5369	**2.679** ± 1.429%	5.5309e-12	4.84056e-12	4.36451e-12
90000	12	7855	**7.421** ± 0.6799%	5.67128e-12	4.05111e-12	3.65619e-12
PMHSS-GMRES						
10000	11	4096	0.7076 ± 0.002372%	2.31419e-10	2.14003e-10	1.91861e-10
40000	11	8092	3.542 ± 0.007765%	1.2527e-10	1.82148e-10	1.63178e-10
90000	11	12055	9.983 ± 0.05302%	7.93328e-11	1.53629e-10	1.38611e-10
PRESB-GMRES						
10000	11	8210	0.6628 ± 0.05686%	1.59327e-10	2.3776e-10	1.60705e-10
40000	11	16261	3.716 ± 0.04519%	1.33754e-10	2.88983e-10	2.06747e-10
90000	11	24320	10.34 ± 0.0956%	4.37123e-11	1.14813e-10	8.5615e-11

Results

Method	outer iter.	inner iter.	T ± σ [s]	$\|\|r\|\|$	$\|\|x^* - x\|\|$	$\|\|(A+B)^{-1}r\|\|$
$\omega = 10^4$						
PMHSS						
LU	67	-	25.43 ± 0.592%	2.73197e-09	1.03058e-09	1.02994e-09
CG	67	2491	1.162 ± 2.973%	2.73819e-09	1.03532e-09	1.03377e-09
AA-PMHSS						
LU	22	-	8.733 ± 0.4441%	1.71475e-09	6.70805e-10	5.38084e-10
CG	22	824	0.5365 ± 0.447%	1.93437e-09	7.51107e-10	6.1096e-10
CG(50)	23	765	0.514 ± 0.3678%	9.89885e-10	3.953e-10	3.25222e-10
CG(25)	23	496	0.3881 ± 0.6916%	1.66947e-09	6.44053e-10	5.23233e-10
PMHSS-GMRES						
LU	23	-	9.009 ± 0.03202%	1.00433e-09	3.90251e-10	2.1615e-10
CG	23	1679	0.8161 ± 0.0251%	1.01339e-09	3.9347e-10	3.05682e-10
PRESB-GMRES						
LU	14	-	10.95 ± 0.06775%	1.88122e-09	9.2189e-10	5.98921e-10
CG	14	2262	0.6489 ± 0.01114%	1.8851e-09	9.22169e-10	5.99389e-10
$\omega = 10^{-4}$						
PMHSS						
LU	80	-	30.25 ± 0.6644%	5.62865e-11	1.13009e-09	1.12844e-09
CG	78	12506	5.491 ± 1.285%	2.06198e-10	3.7422e-09	3.79037e-09
AA-PMHSS						
LU	25	-	9.861 ± 0.1814%	3.58754e-10	6.31284e-10	5.02025e-10
CG	26	4061	2.099 ± 0.5552%	5.69164e-10	4.03492e-09	3.88251e-09
CG(50)	32	1489	0.9801 ± 1.043%	5.93055e-10	4.06493e-09	3.82198e-09
CG(25)	43	1012	0.9603 ± 1.684%	2.29485e-10	5.43464e-09	5.05516e-09
PMHSS-GMRES						
LU	23	-	9.572 ± 0.08122%	4.73915e-09	1.18588e-08	6.48492e-09
CG	23	7500	3.33 ± 0.03415%	5.09979e-09	1.35183e-08	1.11445e-08
PRESB-GMRES						
LU	15	-	11.67 ± 0.07115%	3.23933e-09	6.54481e-09	4.27435e-09
CG	15	10184	2.686 ± 0.02967%	4.00906e-09	8.49476e-09	7.52229e-09

Conclusions

- AA-PMHSS converges in a mesh-independently with respect to the number of *outer* iterations under assumptions on A and B. As PMHSS, PMHSS-GMRES, and PRESB-GMRES.
- AA-PMHSS' convergence behavior can be explained by the relationship between AA and GMRES.
- AA-PMHSS has improved the numerical properties of the inner solver compared with previous methods.
- AA-PMHSS is more flexible, as it is possible to tune the inner solver relax the tolerances.

Future Work

- Restarted methods
- Orthogonalization
- General study on splittings
  - PSS splitting for saddle-point problems

Thank you!

Registration and travel support for this presentation was provided by **Professor W. Randolph Franklin**.

and by KTH Jubileumsanslaget.

Please join us at the MS on **Modern Preconditioners and Linear Solvers in Scientific Applications**. In this room tomorrow at 11.

[1] M. I. Andersson, F. Liu, and S. Markidis, *Anderson accelerated pmhss for complex-symmetric linear systems*, in Proceedings of the 2024 SIAM Conference on Parallel Processing for Scientific Computing (PP), SIAM, 2024, pp. 39–52.

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