GP-CMRH: An inner product free iterative method for block two-by-two nonsymmetric linear systems

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Outline

1. Iterative Krylov methods for large linear systems
2. GMRES and CMRH
3. Block two-by-two nonsymmetric linear systems
4. GPMR
5. GP-CMRH
6. Concluding remarks

Linear systems and iterative Krylov methods

- Linear systems of equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \qquad \mathbf{A} \in \mathbb{R}^{m\times m}, \qquad \mathbf{b} \in \mathbb{R}^{m}$$

- Iterative Krylov methods

CG, MINRES, GMRES, Bi-CG, QMR, Bi-CGSTAB ...

- Some research hotspots

(1) new preconditioning techniques (e.g., operator learning, NN, sketching)

(2) randomization techniques (e.g., rGMRES, sGMRES)

(3) inexact or mixed-precision computations

(4) inner-product free (orthogonalization-free) algorithms (e.g., CMRH)

The Arnoldi process and GMRES

- Krylov subspaces: Let $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$,

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \operatorname{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\}.$$

- The Arnoldi process generates an orthonormal basis

$$\mathbf{V}_k = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_k \end{bmatrix}$$

  via the modified Gram–Schmidt (MGS) orthogonalization process. We have the QR factorization

$$\begin{bmatrix} \mathbf{r}_0 & \mathbf{A}\mathbf{V}_k \end{bmatrix} = \mathbf{V}_{k+1} \begin{bmatrix} \|\mathbf{r}_0\|\mathbf{e}_1 & \mathbf{H}_{k+1,k} \end{bmatrix}.$$

- The generalized minimal residual (GMRES) method:

$$\mathbf{x}_k := \underset{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|.$$

The Hessenberg process and CMRH

- The Hessenberg process generates a linearly independent basis for $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$

$$\mathbf{L}_k = \begin{bmatrix} \boldsymbol{\ell}_1 & \boldsymbol{\ell}_2 & \cdots & \boldsymbol{\ell}_k \end{bmatrix}.$$

  We have the "LU factorization"

$$\begin{bmatrix} \mathbf{r}_0 & \mathbf{A}\mathbf{L}_k \end{bmatrix} = \mathbf{L}_{k+1} \begin{bmatrix} \mathbf{e}_1^\top \mathbf{r}_0 \mathbf{e}_1 & \widetilde{\mathbf{H}}_{k+1,k} \end{bmatrix}.$$

  Sometimes, pivoting is necessary. Usually, it is "better" than the Krylov basis.
- The changing minimal residual Hessenberg (CMRH) method:

$$\mathbf{x}_k := \underset{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{L}_{k+1}^\dagger (\mathbf{b} - \mathbf{A}\mathbf{x})\|.$$

- CMRH is inner-product-free, less expensive and requires slightly less storage than GMRES.

H. Sadok. *CMRH: A new method for solving nonsymmetric linear systems based on the Hessenberg reduction algorithm*. Numer. Algorithms, 20(4):303–321, 1999.

Block two-by-two linear systems

- Block two-by-two linear systems of the form

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{B} & \mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}, \quad \mathbf{M} \in \mathbb{R}^{m \times m}, \quad \mathbf{N} \in \mathbb{R}^{n \times n}.$$

- Monolithic methods: solving the system as a whole.
  For example: GMRES, Bi-CG, QMR, Bi-CGSTAB ...
  Segregated methods: exploiting the block structure, but not in preconditioning.
  For example: LSQR, LSMR; GPMR, GPBiLQ, GPQMR ...

- We consider a special case: $\mathbf{A} \neq \mathbf{B}^\top$, $\lambda \in \mathbb{R}$, $\mu \in \mathbb{R}$,

$$\begin{bmatrix} \lambda\mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}.$$

A. Montoison and D. Orban. *GPMR: An iterative method for unsymmetric partitioned linear systems*. SIMAX, Vol. 44, No. 1 (2023)

Simultaneous orthogonal Hessenberg reduction for $(\mathbf{A}, \mathbf{B})$

- Simultaneous orthogonal Hessenberg reduction

$$\mathbf{A}\mathbf{U}_k = \mathbf{V}_{k+1}\mathbf{H}_{k+1,k}, \quad \mathbf{B}\mathbf{V}_k = \mathbf{U}_{k+1}\mathbf{F}_{k+1,k},$$

$$\mathbf{V}_{k+1}^\top \mathbf{V}_{k+1} = \mathbf{U}_{k+1}^\top \mathbf{U}_{k+1} = \mathbf{I}_{k+1},$$

where

$$\mathbf{H}_{k+1,k} = \begin{bmatrix} h_{11} & \cdots & h_{1k} \\ h_{21} & \ddots & \vdots \\ & \ddots & h_{kk} \\ & & h_{k+1,k} \end{bmatrix}, \qquad \mathbf{F}_{k+1,k} = \begin{bmatrix} f_{11} & \cdots & f_{1k} \\ f_{21} & \ddots & \vdots \\ & \ddots & f_{kk} \\ & & f_{k+1,k} \end{bmatrix}.$$

Simultaneous orthogonal Hessenberg reduction for $(\mathbf{A}, \mathbf{B})$

Algorithm 1: Simultaneous orthogonal Hessenberg reduction

Require: $\mathbf{A}$, $\mathbf{B}$, $\mathbf{b}$, $\mathbf{c}$, all nonzero

$\beta \mathbf{v}_1 := \mathbf{b}$, $\gamma \mathbf{u}_1 := \mathbf{c}$ $\qquad$ $\beta > 0, \gamma > 0$ so that $\|\mathbf{v}_1\| = \|\mathbf{u}_1\| = 1$

for $k = 1, 2, \cdots$ **do**

    for $i = 1, 2, \cdots, k$ **do**

        $h_{ik} = \mathbf{v}_i^\top \mathbf{A} \mathbf{u}_k$

        $f_{ik} = \mathbf{u}_i^\top \mathbf{B} \mathbf{v}_k$

    end for

    $h_{k+1,k} \mathbf{v}_{k+1} = \mathbf{A} \mathbf{u}_k - \sum_{i=1}^{k} h_{ik} \mathbf{v}_i$ $\qquad$ $h_{k+1,k} > 0$ so that $\|\mathbf{v}_{k+1}\| = 1$

    $f_{k+1,k} \mathbf{u}_{k+1} = \mathbf{B} \mathbf{v}_k - \sum_{i=1}^{k} f_{ik} \mathbf{u}_i$ $\qquad$ $f_{k+1,k} > 0$ so that $\|\mathbf{u}_{k+1}\| = 1$

end for

GPMR

- The kth GPMR iterate is

$$\begin{bmatrix} \mathbf{x}_k \\ \mathbf{y}_k \end{bmatrix} = \underset{\mathbf{x} \in \text{range}(\mathbf{V}_k),\ \mathbf{y} \in \text{range}(\mathbf{U}_k)}{\text{argmin}} \left\| \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix} - \begin{bmatrix} \lambda \mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \right\|.$$

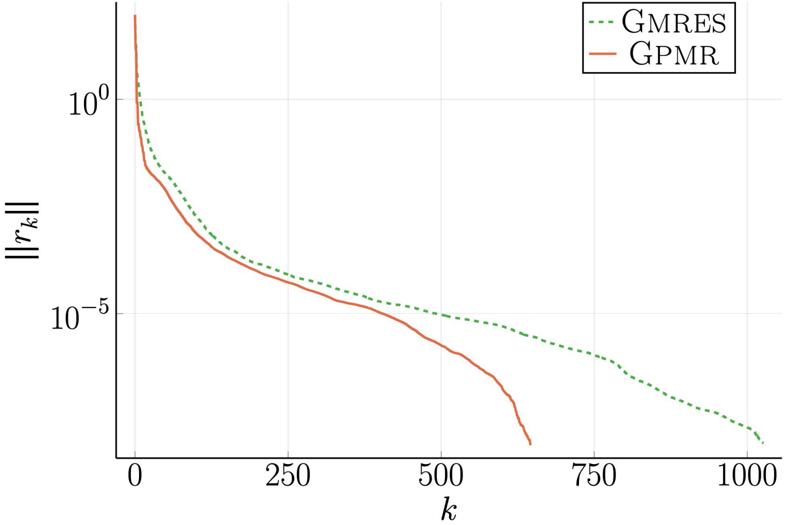
- Equivalent to Block-GMRES:

$$\begin{bmatrix} \lambda \mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x}^1 & \mathbf{x}^2 \\ \mathbf{y}^1 & \mathbf{y}^2 \end{bmatrix} = \begin{bmatrix} \mathbf{b} & \mathbf{0} \\ \mathbf{0} & \mathbf{c} \end{bmatrix}.$$

- GPMR terminates significantly earlier than GMRES on a residual-based stopping criterion with an improvement up to 50% in terms of number of iterations.

A. Montoison and D. Orban. *GPMR: An iterative method for unsymmetric partitioned linear systems*. SIMAX, Vol. 44, No. 1 (2023)

Example: $\mathbf{A} =$ `well1850`, $\mathbf{B} =$ `illc1850`, $\lambda = 1$, $\mu = 0$



Simultaneous Hessenberg reduction for (A, B)

- Simultaneous Hessenberg reduction

$$\mathbf{A}\mathbf{L}_k = \mathbf{D}_{k+1}\widetilde{\mathbf{H}}_{k+1,k}, \quad \mathbf{B}\mathbf{D}_k = \mathbf{L}_{k+1}\widetilde{\mathbf{F}}_{k+1,k},$$

where

$$\widetilde{\mathbf{H}}_{k+1,k} = \begin{bmatrix} \widetilde{h}_{11} & \cdots & \widetilde{h}_{1k} \\ \widetilde{h}_{21} & \ddots & \vdots \\ & \ddots & \widetilde{h}_{kk} \\ & & \widetilde{h}_{k+1,k} \end{bmatrix}, \qquad \widetilde{\mathbf{F}}_{k+1,k} = \begin{bmatrix} \widetilde{f}_{11} & \cdots & \widetilde{f}_{1k} \\ \widetilde{f}_{21} & \ddots & \vdots \\ & \ddots & \widetilde{f}_{kk} \\ & & \widetilde{f}_{k+1,k} \end{bmatrix}.$$

We have

$$\mathrm{range}(\mathbf{D}_k) = \mathrm{range}(\mathbf{V}_k), \quad \mathrm{range}(\mathbf{L}_k) = \mathrm{range}(\mathbf{U}_k).$$

Simultaneous Hessenberg reduction for (A, B)

Algorithm 2: Simultaneous Hessenberg reduction with pivoting

Require: $\mathbf{A}$, $\mathbf{B}$, $\mathbf{b}$, $\mathbf{c}$, all nonzero, $\mathbf{p} = \begin{bmatrix} 1 & 2 & \cdots & m \end{bmatrix}$, $\mathbf{q} = \begin{bmatrix} 1 & 2 & \cdots & n \end{bmatrix}$

Determine i_0 and j_0 such that $|b_{i_0}| = \max\limits_{1 \le i \le m} |\mathbf{e}_i^\top \mathbf{b}|$ and $|c_{j_0}| = \max\limits_{1 \le j \le n} |\mathbf{e}_j^\top \mathbf{c}|$

$\beta = b_{i_0}$, $\mathbf{d}_1 = \mathbf{b}/\beta$, $\gamma = c_{j_0},$, $\boldsymbol{\ell}_1 = \mathbf{c}/\gamma$, $\mathbf{p}(1) \leftrightharpoons \mathbf{p}(i_0)$, $\mathbf{q}(1) \leftrightharpoons \mathbf{q}(j_0)$

for $k = 1, 2, \ldots$ **do**

    $\mathbf{d} = \mathbf{A}\boldsymbol{\ell}_k$, $\boldsymbol{\ell} = \mathbf{B}\mathbf{d}_k$

    for $i = 1, 2, \cdots, k$ **do**

        $h_{i,k} = \mathbf{d}(\mathbf{p}(i))$, $f_{i,k} = \boldsymbol{\ell}(\mathbf{q}(i))$, $\mathbf{d} = \mathbf{d} - h_{i,k}\mathbf{d}_i$, $\boldsymbol{\ell} = \boldsymbol{\ell} - f_{i,k}\boldsymbol{\ell}_i$

    end for

    Determine i_0, j_0 such that $|d_{i_0}| = \max\limits_{k+1 \le i \le m} |\mathbf{d}(\mathbf{p}(i))|$ and $|\ell_{j_0}| = \max\limits_{k+1 \le j \le n} |\boldsymbol{\ell}(\mathbf{q}(j))|$

    $h_{k+1,k} = d_{i_0}$, $\mathbf{d}_{k+1} = \mathbf{d}/h_{k+1,k}$, $f_{k+1,k} = \ell_{j_0}$, $\boldsymbol{\ell}_{k+1} = \boldsymbol{\ell}/f_{k+1,k}$
    $\mathbf{p}(k+1) \leftrightharpoons \mathbf{p}(i_0)$, $\mathbf{q}(k+1) \leftrightharpoons \mathbf{q}(j_0)$

end for

GP-CMRH

- The kth GP-CMRH iterate is

$$\begin{bmatrix} \mathbf{x}_k \\ \mathbf{y}_k \end{bmatrix} = \underset{\mathbf{x}\in\text{range}(\mathbf{D}_k),\ \mathbf{y}\in\text{range}(\mathbf{L}_k)}{\text{argmin}} \left\| \begin{bmatrix} \mathbf{D}_{k+1} & \\ & \mathbf{L}_{k+1} \end{bmatrix}^{\dagger} \left(\begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix} - \begin{bmatrix} \lambda\mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \right) \right\|.$$

Theorem

Let $\mathbf{r}_k^{\text{GP-CMRH}}$ *and* $\mathbf{r}_k^{\text{GPMR}}$ *be the* k*th residuals of* GP-CMRH *and* GPMR, *respectively. Let* $\mathbf{W}_{k+1} = \begin{bmatrix} \mathbf{D}_{k+1} & \\ & \mathbf{L}_{k+1} \end{bmatrix}$. *Then,*

$$\|\mathbf{r}_k^{\text{GPMR}}\| \leq \|\mathbf{r}_k^{\text{GP-CMRH}}\| \leq \kappa(\mathbf{W}_{k+1})\|\mathbf{r}_k^{\text{GPMR}}\|,$$

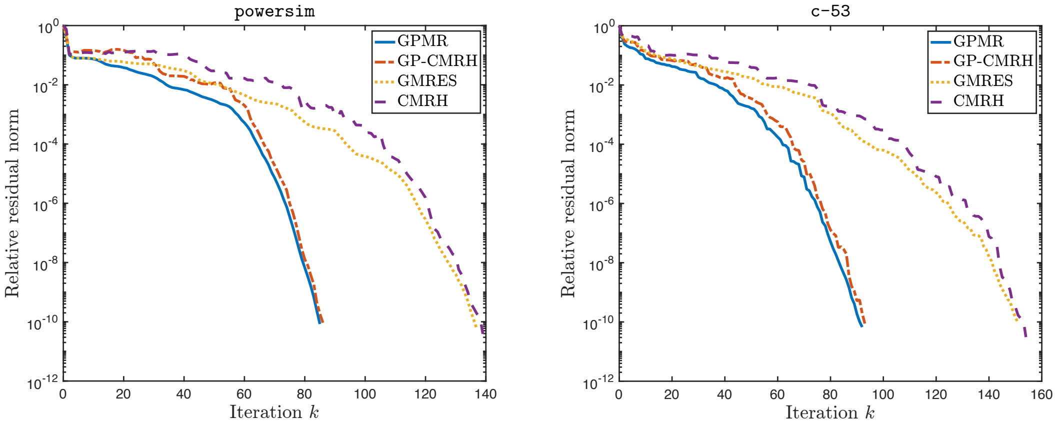
where $\kappa(\mathbf{W}_{k+1}) = \|\mathbf{W}_{k+1}\|\|\mathbf{W}_{k+1}^{\dagger}\|$ *is the condition number of* $\mathbf{W}_{k+1}$.

Numerical experiments

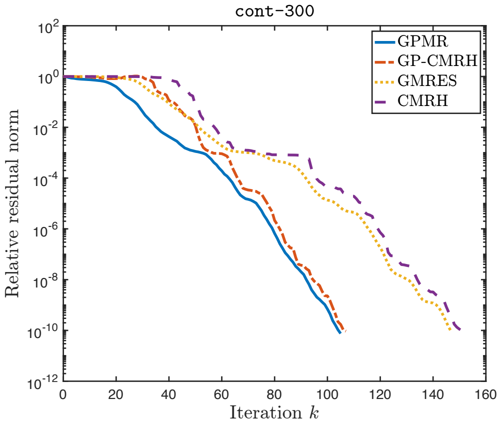
Table 1: Numbers of iterations (Iter), runtimes (Time), and relative residual norms (Rel) of GPMR, GP-CMRH, GMRES, and CMRH on twenty-two matrices from the SuitSparse Matrix Collection. "Nnz" denotes the number of nonzero elements in each sparse matrix. Bold-faced values in the runtime column highlight the shortest time taken among the four methods.

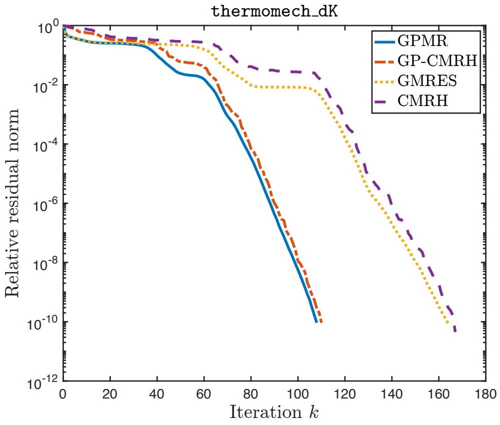
Name	Size	Nnz	GPMR			GP-CMRH			GMRES			CMRH		
			Iter	Time	Rel	Iter	Time	Rel	Iter	Time	Rel	Iter	Time	Rel
`bcsstk17`	10974	428650	121	0.39	3.66e-11	121	**0.28**	8.51e-11	213	1.57	8.17e-11	216	0.72	8.64e-11
`bcsstk25`	15439	252241	62	0.18	5.54e-11	63	**0.15**	8.63e-11	100	0.47	8.13e-11	116	0.37	8.41e-11
`powersim`	15838	64424	85	0.26	8.40e-11	86	**0.20**	9.28e-11	137	1.17	5.64e-11	139	0.42	3.91e-11
`raefsky3`	21200	1488768	37	**0.68**	9.56e-11	40	0.69	8.86e-11	63	1.24	8.59e-11	67	1.15	9.28e-11
`sme3Db`	29067	2081063	65	2.42	6.60e-11	66	**2.23**	7.30e-11	97	4.65	6.30e-11	98	3.27	9.40e-11
`c-53`	30235	355139	92	1.38	6.73e-11	93	**1.21**	8.85e-11	151	3.29	9.34e-11	154	2.17	3.08e-11
`sme3Dc`	42930	3148656	97	5.72	6.12e-11	98	**5.36**	7.67e-11	161	11.05	7.39e-11	163	8.75	6.85e-11
`bcsstk39`	46772	2060662	205	5.72	7.54e-11	209	**3.25**	7.33e-11	381	23.32	9.73e-11	392	5.39	9.50e-11
`rma10`	46835	2329092	41	1.43	6.39e-11	42	**1.33**	6.34e-11	49	1.69	7.02e-11	51	1.53	5.08e-11
`copter2`	55476	759952	211	19.86	7.38e-11	214	**16.11**	9.18e-11	367	50.06	7.04e-11	371	27.06	6.81e-11
`Goodwin_071`	56021	1797934	70	2.77	8.93e-11	72	**2.39**	7.56e-11	88	4.24	8.20e-11	91	2.94	9.34e-11
`water_tank`	60740	2035281	324	46.00	8.07e-11	338	**35.09**	7.20e-11	430	75.59	9.73e-11	464	51.15	8.34e-11
`venkat50`	62424	1717777	34	1.06	5.23e-11	35	**0.97**	6.24e-11	46	1.66	7.99e-11	48	1.29	4.17e-11
`poisson3Db`	85623	2374949	50	**7.57**	6.94e-11	51	7.64	8.84e-11	57	8.76	6.66e-11	59	9.00	5.97e-11
`ifiss_mat`	96307	3599932	33	**2.27**	8.76e-11	35	2.32	3.38e-11	42	3.03	7.08e-11	43	2.73	9.70e-11
`hcircuit`	105676	513072	46	0.80	9.69e-11	46	**0.38**	7.84e-11	58	1.44	4.99e-11	58	0.49	8.66e-11
`PR02R`	161070	8185136	61	**25.13**	8.31e-11	64	26.39	5.15e-11	100	42.66	8.91e-11	105	46.23	4.92e-11
`cont-300`	180895	988195	105	24.34	7.55e-11	107	**21.57**	9.34e-11	147	39.66	8.68e-11	151	32.55	9.49e-11
`thermomech_dK`	204316	2846228	108	14.06	9.26e-11	110	**8.59**	9.20e-11	164	27.30	8.81e-11	167	13.53	4.48e-11
`pwtk`	217918	11524432	190	28.61	8.36e-11	197	**13.83**	8.64e-11	283	56.32	9.94e-11	292	21.83	7.55e-11
`Raj1`	263743	1300261	361	103.21	9.79e-11	398	**80.74**	9.87e-11	532	239.82	9.91e-11	567	89.36	9.71e-11
`nxp1`	414604	2655880	105	25.39	9.94e-11	109	**19.29**	7.62e-11	125	32.31	8.04e-11	129	24.67	8.35e-11

Numerical experiments



Numerical experiments





Concluding remarks

- We propose an inner product free iterative method called GP-CMRH for solving block two-by-two nonsymmetric linear systems.
- GP-CMRH relies on a new simultaneous Hessenberg process that reduces two rectangular matrices to upper Hessenberg form simultaneously, without employing inner products.
- GP-CMRH requires less computational cost per iteration and may be more suitable for high performance computing and low or mixed precision arithmetic due to its inner product free property.
- Our numerical experiments demonstrate that GP-CMRH and GPMR exhibit comparable convergence behavior (with GP-CMRH requiring slightly more iterations), yet GP-CMRH consumes less computational time in most cases.
- GP-CMRH significantly outperforms GMRES and CMRH in terms of number of iterations and runtime efficiency.

Future work

- Develop acceleration techniques that can fully leverage the underlying structure of linear systems.
- Intelligent iterative methods for block two-by-two linear systems?

  Haifeng Zou, Xiaowen Xu, Chen-Song Zhang.

  A survey on intelligent iterative methods for solving sparse linear algebraic equations.

  arXiv:2310.06630 (2023)

The manuscript and slides

- Kui Du and Jia-Jun Fan

  GP-CMRH: An inner product free iterative method for block two-by-two nonsymmetric linear systems.

  arXiv:2509.11272, 2025.

- The slides are available at https://kuidu.github.io/talk.html

Thanks!