A block minimum residual norm subspace solver with partial convergence management for sequences of linear systems -IB-BGCRO-DR

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A block minimum residual norm subspace solver with partial convergence management for sequences of linear systems — IB-BGCRO-DR

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Summary

01

Overview

Minimum residual norm block "Krylov" solver: **first two years** of my PhD

- Joint work with
  Luc Giraud (Inria Bordeaux - Sud-Ouest, my PhD supervisor)
  Yan-Fei Jing (UESTC)

- Outcome
  1. SIMAX (SIAM J. Matrix Anal. Appl.) paper, 2022, pp.30
     https://doi.org/10.1137/21M1401127
  2. Research report in HAL-Inria, 2022, pp.60
     https://hal.inria.fr/hal-03146213v3
  3. C++ implementation in *Fabulous*
     https://gitlab.inria.fr/solverstack/fabulous/

02

Scientific background

- Generate **Arnoldi relation** (Arnoldi algorithm):

$$AV_j = V_{j+1}\underline{H}_j, \quad \text{span}(V_{j+1}) = \text{span}(v_1, v_2, \cdots, v_{j+1}) \quad (1)$$

- Generate nested and **orthonormal basis**:

$$V_{j+1}^H V_{j+1} = I_{j+1}$$

$$\mathcal{K}_{j+1}(A, v_1) = \text{span}(r_0, Ar_0, \cdots, A^j r_0) = \text{span}(V_{j+1}) \text{ with } v_1 = \frac{r_0}{\|r_0\|_2},$$

and $\underline{H}_j$ is upper Hessenberg matrix

- Generate **Arnoldi relation** (Arnoldi algorithm):

$$AV_j = V_{j+1}\underline{H}_j, \quad \text{span}(V_{j+1}) = \text{span}(v_1, v_2, \cdots, v_{j+1}) \qquad (1)$$

- Generate nested and **orthonormal basis**:

$$V_{j+1}^H V_{j+1} = I_{j+1}$$

- Solve a small dimensional **least-squares problem** (Minimal Residual approach):

$$x_j = \underset{x \in x_0 + \mathcal{K}_j(A, v_1)}{\text{argmin}} \|b - Ax\|_2 \text{ with } x_j = x_0 + V_j y_j, \text{ thus}$$

$$\underbrace{\|b - Ax_j\|_2}_{x_j \in \mathbb{C}^n} = \left\| V_{j+1}(V_{j+1}^H r_0 - \underline{H}_j y_j) \right\|_2 = \underbrace{\left\| \beta e_1 - \underline{H}_j y_j \right\|_2}_{y_j \in \mathbb{C}^j},$$

where $j \ll n$ and

$$y_j = \underset{y \in \mathbb{C}^j}{\text{argmin}} \left\| \beta e_1 - \underline{H}_j y \right\|_2 \text{ with } \beta = \|r_0\|_2 \qquad (2)$$

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- Generate **block-Arnoldi relation** (Arnoldi algorithm):

$$A\mathscr{V}_j = \mathscr{V}_{j+1}\underline{\mathscr{H}}_j, \quad \text{span}(\mathscr{V}_{j+1}) = \text{span}(V_1, V_2, \cdots, V_{j+1}) \quad (3)$$

- Generate nested and **orthonormal basis**:

$$\mathscr{V}_{j+1}^H \mathscr{V}_{j+1} = I_{n_{j+1}} \text{ with } n_{j+1} = (j+1) \times p,$$

$$\mathcal{K}_{j+1}(A, V_1) = \text{span}(R_0, AR_0, \cdots, A^j R_0) = \text{span}(\mathscr{V}_{j+1}),$$

where p is the number of right-hand sides, and $R_0 = V_1\Lambda_1$;
$\underline{\mathscr{H}}_j$ is upper Hessenberg matrix with $p \times p$ block elements

- Generate **block-Arnoldi relation** (Arnoldi algorithm):

$$A\mathscr{V}_j = \mathscr{V}_{j+1}\underline{\mathscr{H}}_j, \quad \text{span}(\mathscr{V}_{j+1}) = \text{span}(V_1, V_2, \cdots, V_{j+1}) \quad (3)$$

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- Solve a small dimensional **least-squares problem** (Minimal Residual approach):

$$X_j = \underset{X \in X_0 + \mathcal{K}_j(A, V_1)}{\text{argmin}} \|B - AX\|_F \text{ with } X_j = X_0 + \mathscr{V}_j Y_j, \text{ thus}$$

$$\underbrace{\|B - AX_j\|_F}_{X_j \in \mathbb{C}^{n \times p}} = \left\| \mathscr{V}_{j+1}(\mathscr{V}_{j+1}^H R_0 - \underline{\mathscr{H}}_j Y_j) \right\|_F = \underbrace{\left\| \Lambda_j - \underline{\mathscr{H}}_j Y_j \right\|_F}_{Y_j \in \mathbb{C}^{n_j \times p}},$$

where $n_j \ll n$ and

$$Y_j = \underset{Y \in \mathbb{C}^{n_j \times p}}{\text{argmin}} \left\| \Lambda_j - \underline{\mathscr{H}}_j Y \right\|_F \text{ with } \Lambda_j = [\Lambda_1^T, 0_{p \times n_j}]^T \quad (4)$$

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- **Inexact Breakdown (IB) caused by partial convergence or linear combination**

$$A\mathscr{V}_j = \left[\mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \mathscr{F}_j, \tag{5}$$

then $\mathscr{V}_{j+1} = [\mathscr{V}_j, \mathbb{V}_{j+1}]$ where $\mathbb{V}_{j+1} \in \mathbb{C}^{n \times p_{j+1}} (p_{j+1} \leq p)$

> Eq. (5) comes from block-Arnoldi relation in BGMRES: $A\mathscr{V}_j = [\mathscr{V}_j, V_{j+1}]\,\underline{\mathscr{H}_j}$ with $V_{j+1} \in \mathbb{C}^{n \times p}$

> $\mathbb{V}_{j+1}$ corresponds to the components within $[P_{j-1}, \widetilde{W}_j] \in \mathbb{C}^{n \times p}$ that contribute the most to the residual norms

> P_j are the abandoned directions at iteration j that contribute the less to the residuals.

> $\mathscr{F}_j$ is no longer upper Hessenberg as soon as one IB occurs

IB-BGMRES [Robbé and Sadkane, 2006]

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- **Inexact Breakdown (IB) caused by partial convergence or linear combination**

$$A\mathscr{V}_j = \left[\mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \mathscr{F}_j, \tag{5}$$

then $\mathscr{V}_{j+1} = [\mathscr{V}_j, \mathbb{V}_{j+1}]$ where $\mathbb{V}_{j+1} \in \mathbb{C}^{n \times p_{j+1}} (p_{j+1} \leq p)$
IB-BGMRES [Robbé and Sadkane, 2006]

- **The growth of memory and computational requirements**
deflated restarting/subspace recycling strategy for accelerating convergence – BGMRES-DR [Morgan, 2005], IB-BGMRES-DR [Agullo et al., 2014], BGCRO-DR [Parks et al., 2016]

Bibliography (not exhaustive)

- BGMRES-DR: Restarted block-GMRES with deflation of eigenvalues. [R. B. Morgan. *Applied Numerical Mathematics*, 2005, 54:(2), pp. 222-236]
- IB-BGMRES: Exact and inexact breakdowns in the block GMRES method. [M. Robbé and M. Sadkane. *Linear Algebra and its Applications*, 2006, 419:(1), pp. 265-285]
- IB-BGMRES-DR: Block GMRES Method with Inexact Breakdowns and Deflated Restarting. [E. Agullo, L. Giraud and Y.-F. Jing. *SIAM Journal on Matrix Analysis and Applications*, 2014, 35:(4), pp. 1625-1651]
- BGCRO-DR: A block Recycled GMRES method with investigations into aspects of solver performance. [M. L. Parks, K. M. Soodhalter and D. B. Szyld. *arXiv*, 2016]

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03

IB-BGCRO-DR

Motivation: devise **block solver** for **sequences of linear systems** with multiple left and right hand sides: $A^{(\ell)}X^{(\ell)} = B^{(\ell)}, \ell = 1, 2, \ldots$ families

1. **For block method**: Block GMRES method with inexact breakdown and deflated restarting – IB-BGMRES-DR

   > Combine the inexact breakdown mechanism aiming for handling rank deficiency in block iterations and the deflated restarting augmenting with some approximated eigenvectors for accelerating convergence of the next cycles.

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Motivation: devise **block solver** for **sequences of linear systems** with multiple left and right hand sides: $A^{(\ell)}X^{(\ell)} = B^{(\ell)}, \ell = 1, 2, \ldots$ families

1. **For block method**: Block GMRES method with inexact breakdown and deflated restarting – IB-BGMRES-DR

2. **For sequences of linear systems**: A block recycled GMRES method– BGCRO-DR

   > Subspace recycling: accelerate convergence rate of the next cycles as well as the next families to be solved.

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Motivation: devise **block solver** for **sequences of linear systems** with multiple left and right hand sides: $A^{(\ell)}X^{(\ell)} = B^{(\ell)}, \ell = 1, 2, \ldots$ families

1. **For block method**: Block GMRES method with inexact breakdown and deflated restarting – IB-BGMRES-DR

How to combine inexact breakdown mechanism and subspace recycling strategy for solving sequences of linear systems with multiple left and right-hand sides ?

2. **For sequences of linear systems**: A block recycled GMRES method– BGCRO-DR

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- Generate **block-Arnoldi like relation**

$$A[U_k, \mathscr{V}_j] = \left[C_k, \mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \underline{\mathscr{F}}_j = \widehat{\mathscr{V}}_{j+1} \underline{\mathscr{F}}_j, \qquad (6)$$

  - **IB**: $A\mathscr{V}_j = * + \left[\mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \mathscr{F}_j$ from IB-BGMRES
  - **BGCRO-DR**: $AU_k = C_k$, $C_k^H C_k = I_k$ (computed by Harmonic-Ritz, Rayleigh-Ritz or other techniques); and $\underline{\mathscr{F}}_j = \begin{bmatrix} I_k & \mathcal{B}_j \\ 0_{(n_j+p)\times k} & \mathscr{F}_j \end{bmatrix} \in \mathbb{C}^{(k+n_j+p)\times(k+n_j)}$, $\mathcal{B}_j = C_k^H A\mathscr{V}_j \in \mathbb{C}^{k\times n_j}$

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- Generate **block-Arnoldi like relation**

$$A[U_k, \mathscr{V}_j] = \left[C_k, \mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \underline{\mathscr{F}}_j = \widehat{\mathscr{V}}_{j+1} \underline{\mathscr{F}}_j, \qquad (6)$$

- Generate **orthonormal basis**:

$$\widehat{\mathscr{V}}_{j+1}^H \widehat{\mathscr{V}}_{j+1} = I_{(k+n_j+p)} \text{ with } n_j = \sum_{i=1}^{j} p_i$$

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- Generate **block-Arnoldi like relation**

$$A[U_k, \mathscr{V}_j] = \left[C_k, \mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \underline{\mathscr{F}}_j = \widehat{\mathscr{V}}_{j+1} \underline{\mathscr{F}}_j, \qquad (6)$$

- Generate **orthonormal basis**:

$$\widehat{\mathscr{V}}_{j+1}^H \widehat{\mathscr{V}}_{j+1} = I_{(k+n_j+p)} \text{ with } n_j = \sum_{i=1}^{j} p_i$$

- Solve a small dimensional **least-squares problem**:

$$X_j = \underset{X \in X_0 + \text{Range}([U_k, \mathscr{V}_j])}{\text{argmin}} \|B - AX\|_F \text{ with } X_j = X_0 + [U_k, \mathscr{V}_j] Y_j,$$

where $X_j \in \mathbb{C}^{n \times p}$, $Y_j \in \mathbb{C}^{(k+n_j) \times p}$ with $k + n_j \ll n$ and

$$Y_j = \underset{Y \in \mathbb{C}^{(k+n_j) \times p}}{\text{argmin}} \left\|\Lambda_j - \underline{\mathscr{F}}_j Y\right\|_F, \quad \Lambda_j \in \mathbb{C}^{(k+n_j+p) \times p} \qquad (7)$$

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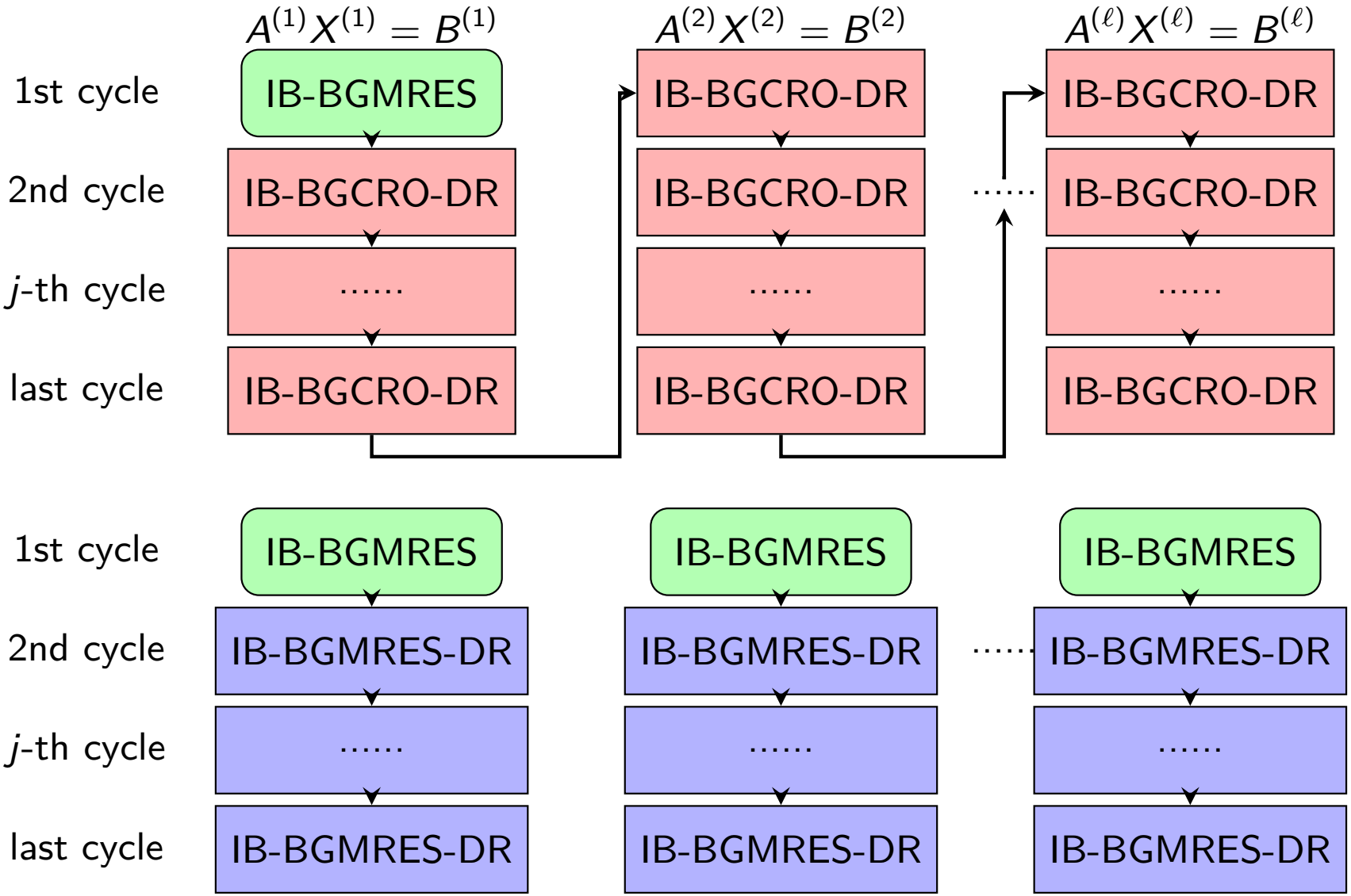
Flowchart of reusing spectral information



Different search space expansion policies can be defined

- Residual based (IB-BGMRES, Robbé-Sadkane, 2006): all the residual norms will be smaller than prescribed threshold
- Backward error on b based (IB-BGMRES-DR, Agullo et al., 2014): all the backward error η_b will be smaller than prescribed threshold

$$\begin{aligned}\eta_b(x_j) &= \min_{\Delta b} \left\{\tau > 0 : \|\Delta b\|_2 \leq \tau \|b\|_2 \text{ and } Ax_j = b + \Delta b\right\} \\ &= \frac{\|Ax_j - b\|_2}{\|b\|_2}\end{aligned}$$

- Backward error on A and b based (IB-BGCRO-DR): all the backward error $\eta_{A,b}$ will be smaller than prescribed threshold

$$\begin{aligned}\eta_{A,b}(x_j) = \min_{\Delta A, \Delta b} &\left\{\tau > 0 : \|\Delta A\|_2 \leq \tau \|A\|_2 \,,\, \|\Delta b\|_2 \leq \tau \|b\|_2 \right. \\ &\left. \text{and } (A + \Delta A)x_j = b + \Delta b\right\} \\ = &\frac{\|Ax_j - b\|_2}{\|A\|_2 \|x_j\|_2 + \|b\|_2}\end{aligned}$$

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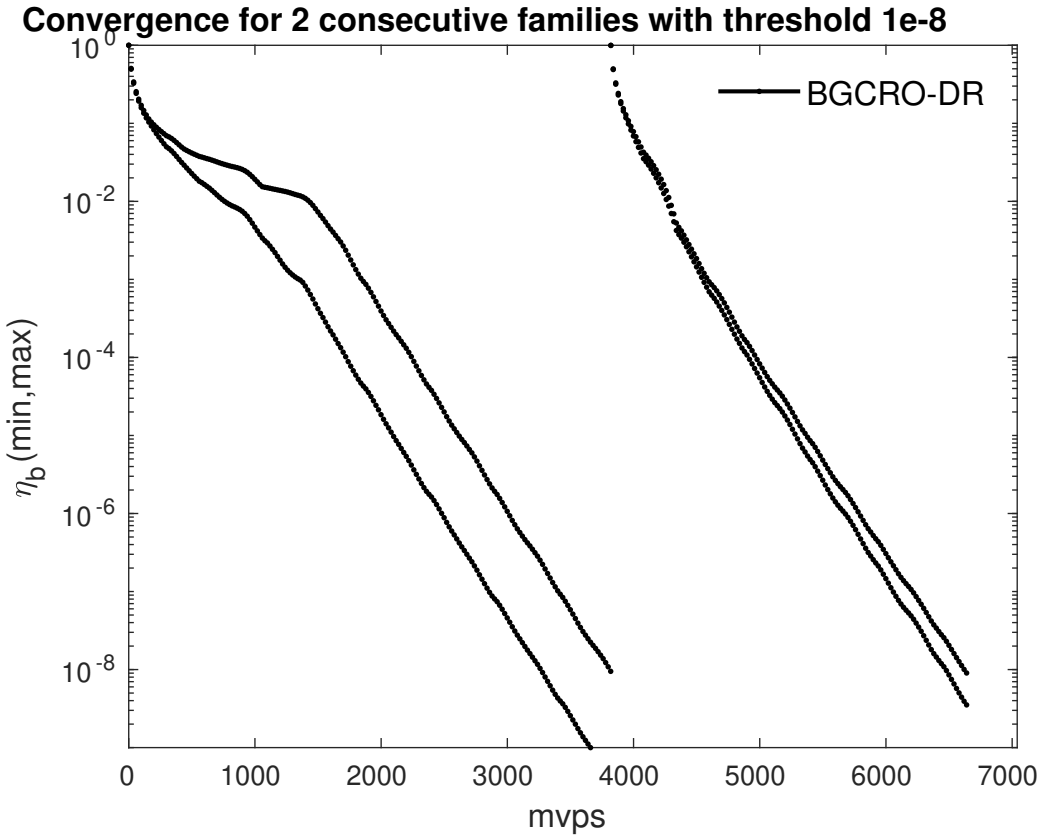
04

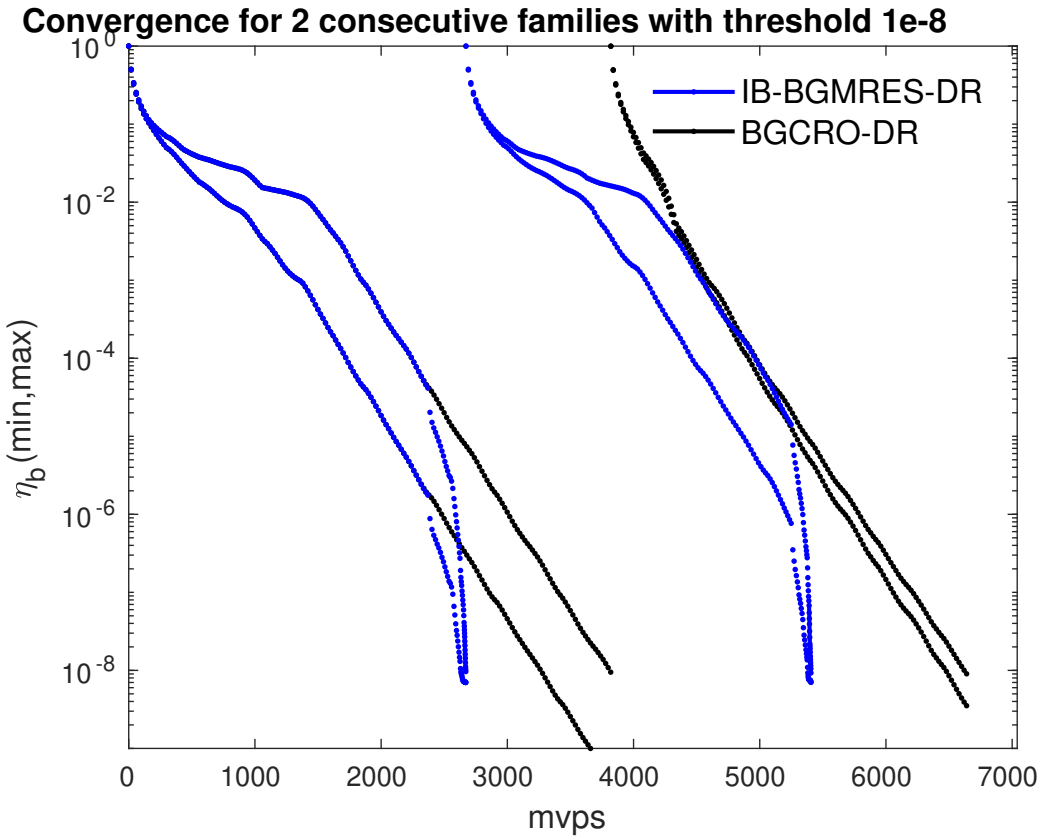
Experimental results

Benefits of IB and DR between the families



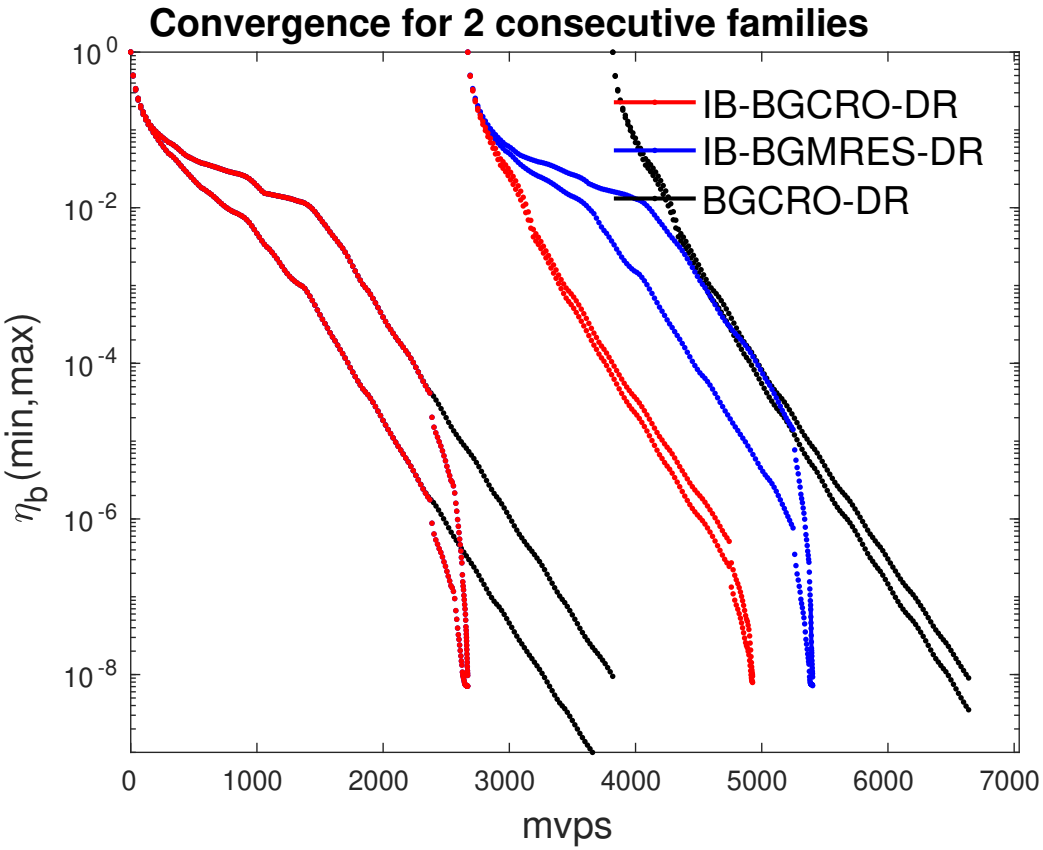
- The solution of the second family benefits from recycled information from the previous family solution

Benefits of IB and DR between the families



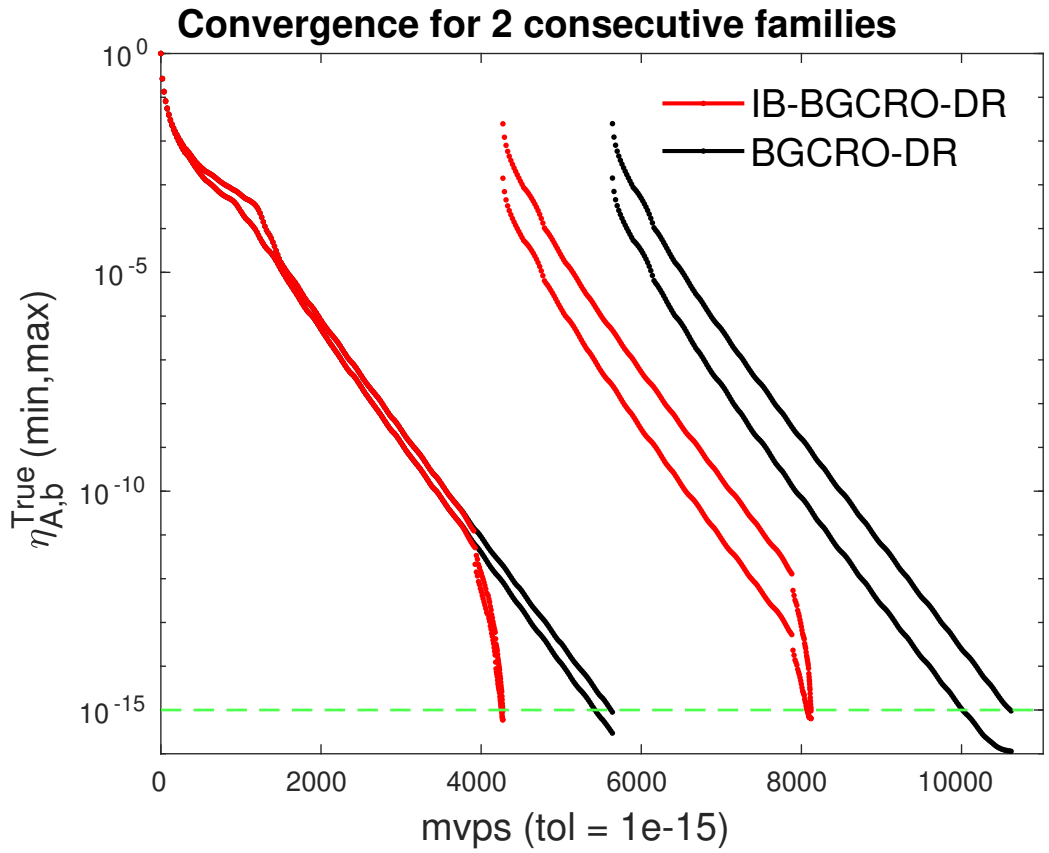
- IB-BGMRES-DR history overlaps BGCRO-DR until the first IB
- IB-BGMRES-DR history is the same for the two families

Benefits of IB and DR between the families



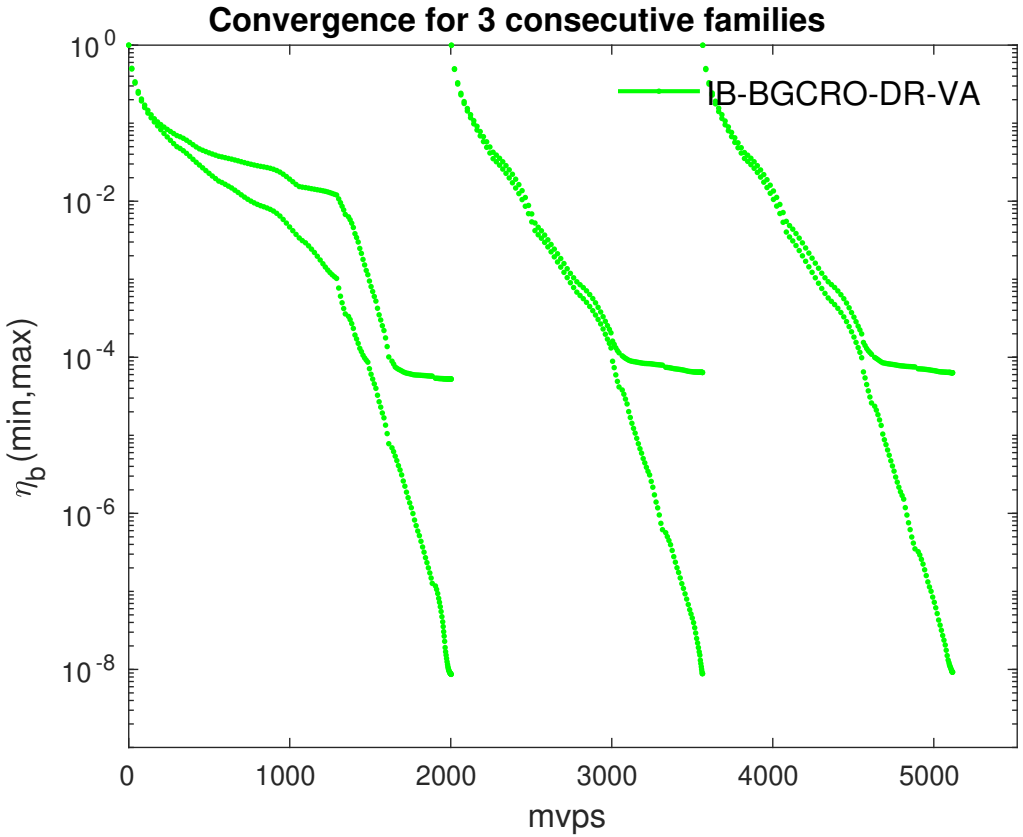
- IB-BGCRO-DR history overlaps IB-BGMRES-DR for the first family
- IB-BGCRO-DR inherits all the good genes of IB, DR and GCRO

The backward error stopping criterion: $\eta_{A,b}$



- IB-BGCRO-DR is able to decrease $\eta_{A,b}$ to a very low value close to the machine epsilon: $\mathcal{O}(10^{-16})$

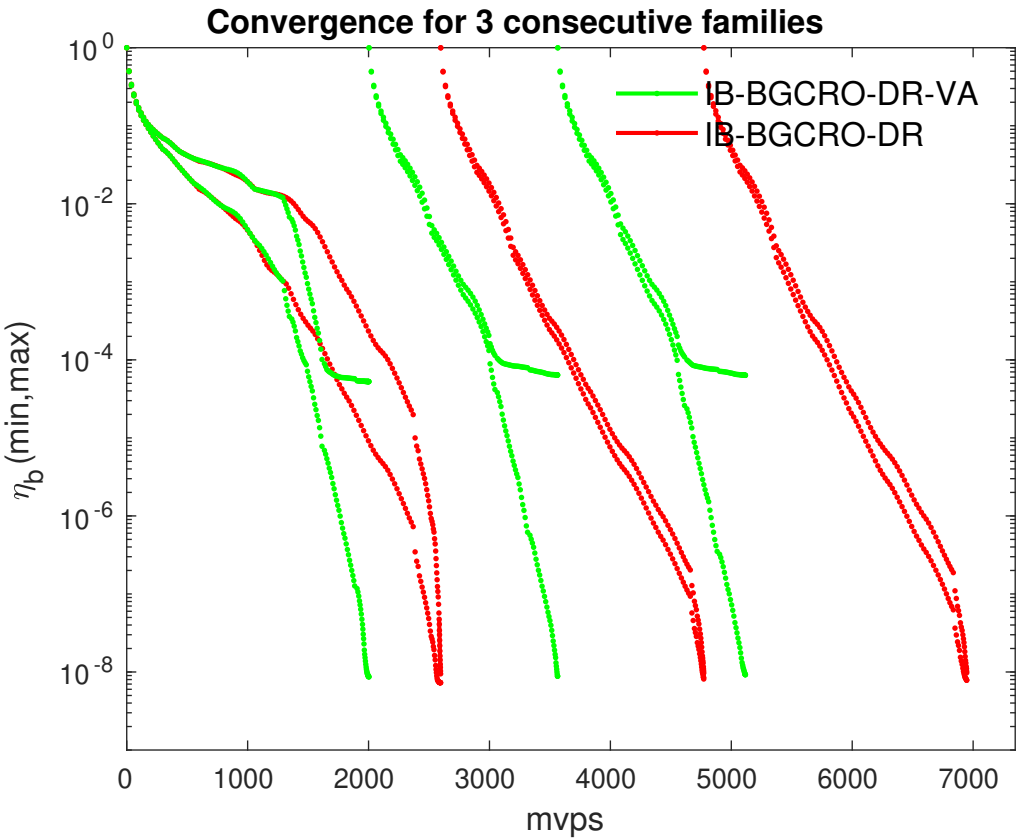
*-VA : individual convergence threshold



Once converged:

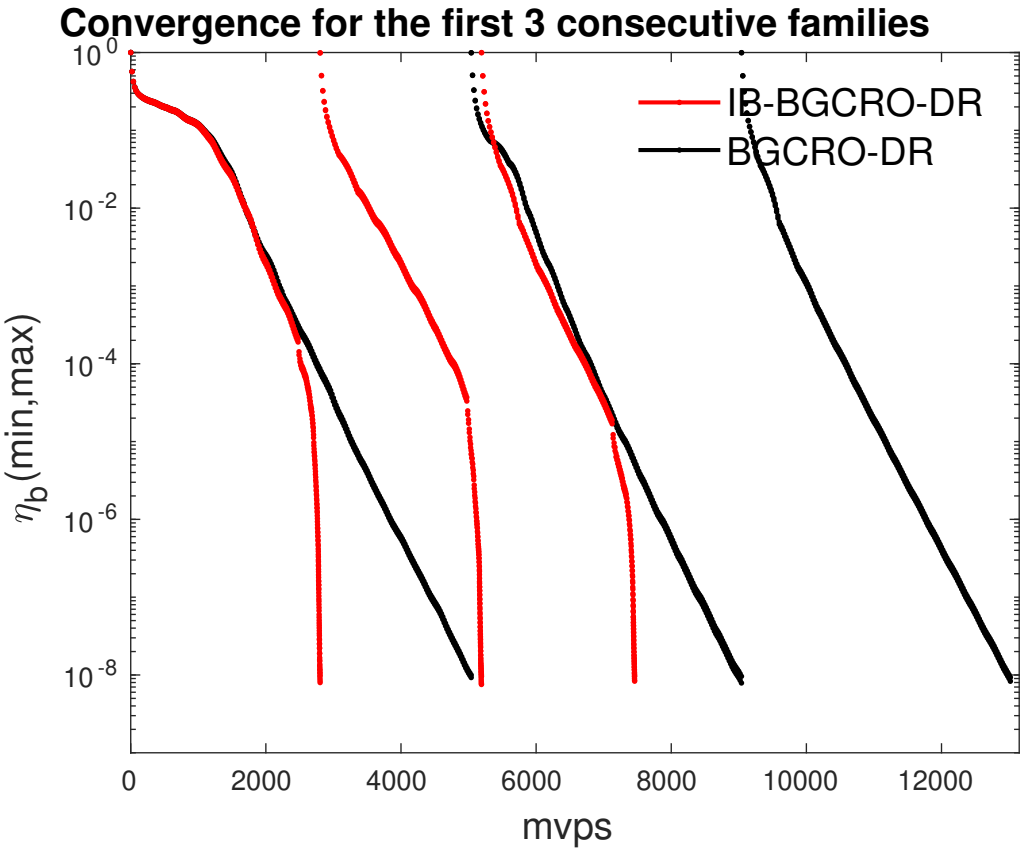
- the ones with largest thresholds do not progress anymore
- computation effort focuses on the ones with smallest thresholds

*-VA : individual convergence threshold



- Significant gains compared to converging all solutions with the most stringent threshold

Test system with slowly varying left-hand sides



- $A^{(\ell)}X^{(\ell)} = B^{(\ell)}$ with $\ell = 1, 2, 3$
- Obvious gains compared to another related block iterative solver

05

Conclusion

IB-BGCRO-DR: **subspace recycling** block GCRO-DR method with **partial convergence** management

- **Subspace recycling** strategies : Harmonic-Ritz, Rayleigh-Ritz or other techniques can be used to define the space to be recycled

IB-BGCRO-DR: **subspace recycling** block GCRO-DR method with **partial convergence** management

- **Subspace recycling** strategies
- **Search space expansion policies** governed by
  - > the partial convergence management (IB-, *-VA and *-CB)
  - > the backward error stopping criterion (η_b and $\eta_{A,b}$)

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IB-BGCRO-DR: **subspace recycling** block GCRO-DR method with **partial convergence** management

- **Subspace recycling** strategies
- **Search space expansion policies** governed by
  - the partial convergence management (IB-, *-VA and *-CB)
  - the backward error stopping criterion (η_b and $\eta_{A,b}$)
- **Flexible preconditioning** (mixed-precision): IB-BFGCRO-DR

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IB-BGCRO-DR: **subspace recycling** block GCRO-DR method with **partial convergence** management

- **Subspace recycling** strategies
- **Search space expansion policies** governed by
  - the partial convergence management (IB-, *-VA and *-CB)
  - the backward error stopping criterion (η_b and $\eta_{A,b}$)
- **Flexible preconditioning** (mixed-precision): IB-BFGCRO-DR
- Remarks on some **computational** and **algorithmic aspects**
  - Partial convergence detecting in the initial residuals $\rightarrow$ address possible initial rank deficiency & reduce computation
  - The MGS re-orthogonalization among $k + p$ columns (between the columns of recycling space and initial block Arnoldi basis) at restart $\rightarrow$ generate a good enough orthonormal basis

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IB-BGCRO-DR: **subspace recycling** block GCRO-DR method with **partial convergence** management

- **Subspace recycling** strategies
- **Search space expansion policies** governed by
  - > the partial convergence management (IB-, *-VA and *-CB)
  - > the backward error stopping criterion (η_b and $\eta_{A,b}$)
- **Flexible preconditioning** (mixed-precision): IB-BFGCRO-DR
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Thanks for your attention. Questions ?

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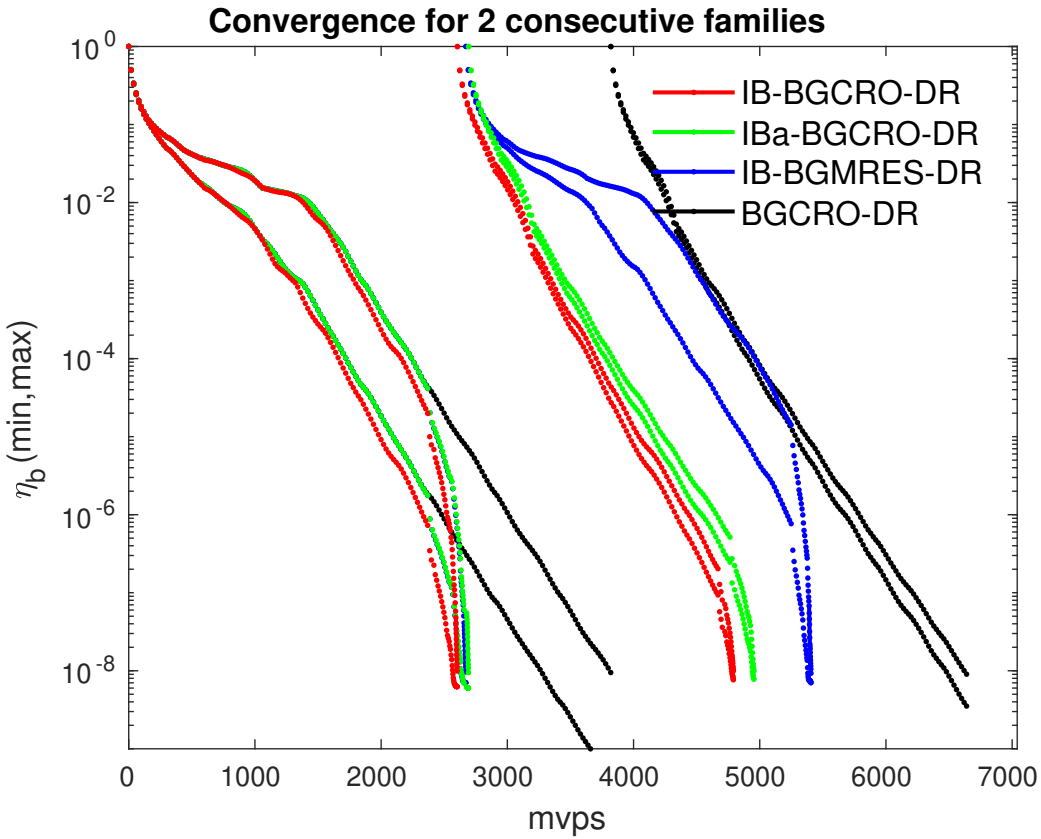
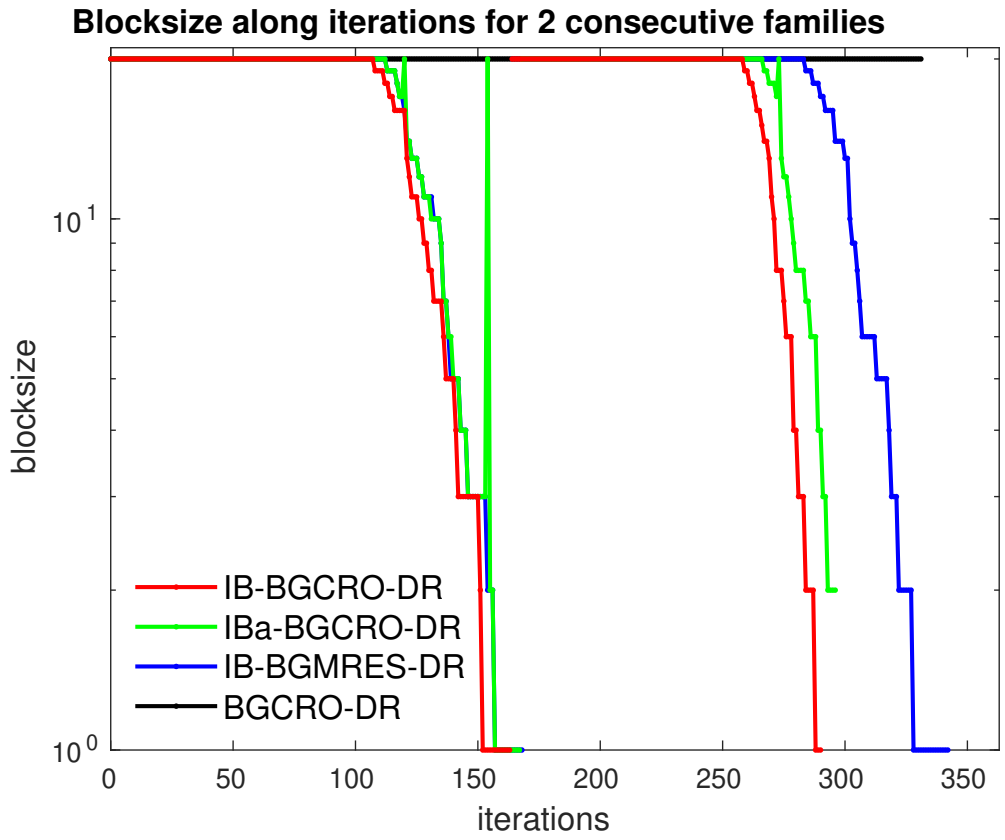
IB detecting in the initial basis or after ?



- Execute IB detecting in the initial basis helps reduce (even though slightly) the consuming mvps

IB detecting in the initial basis or after ?

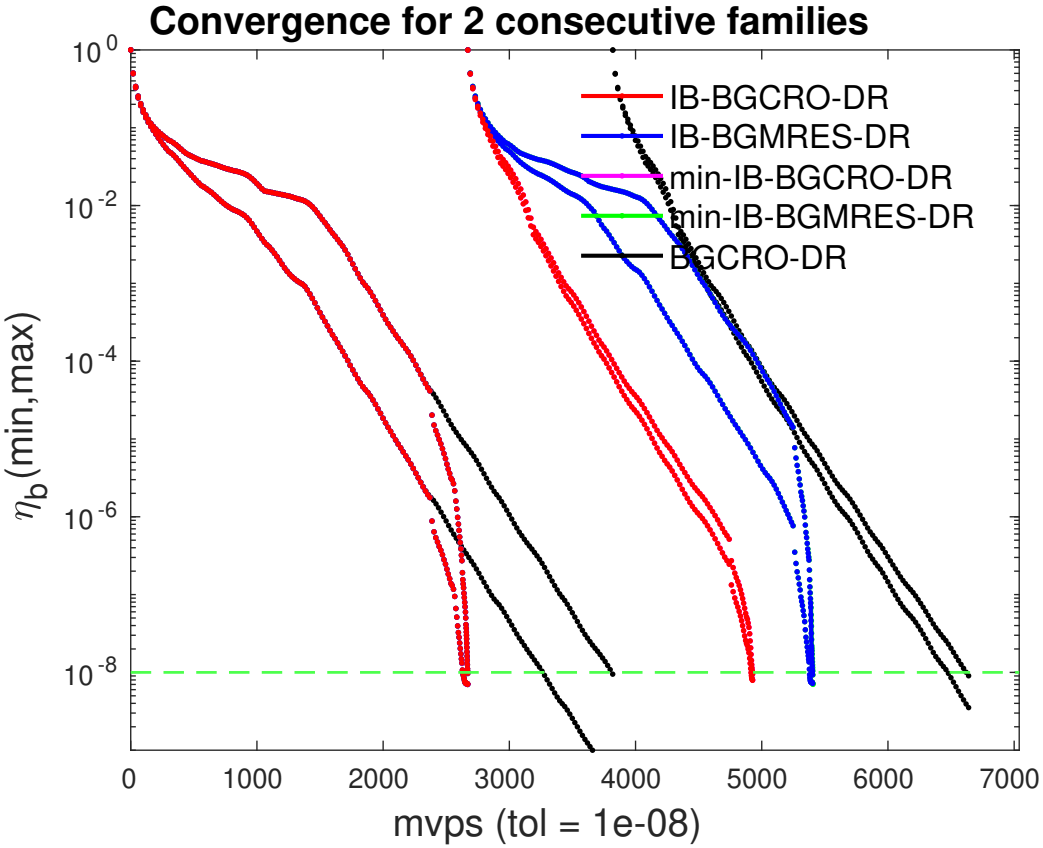


- Such slight gains comes from the benefits of addressing the initial rank deficiency accumulated at restart

Diagonal scaled IB vs min-IB

$\|(B - AX_j)D_\varepsilon\|_2 \leq 1$ **vs** $\|b^{(i)} - Ax_j^{(i)}\|_2 < \|B - AX_j\|_2 \leq \varepsilon \min_{i=1,\ldots,p} \|b^{(i)}\|_2$

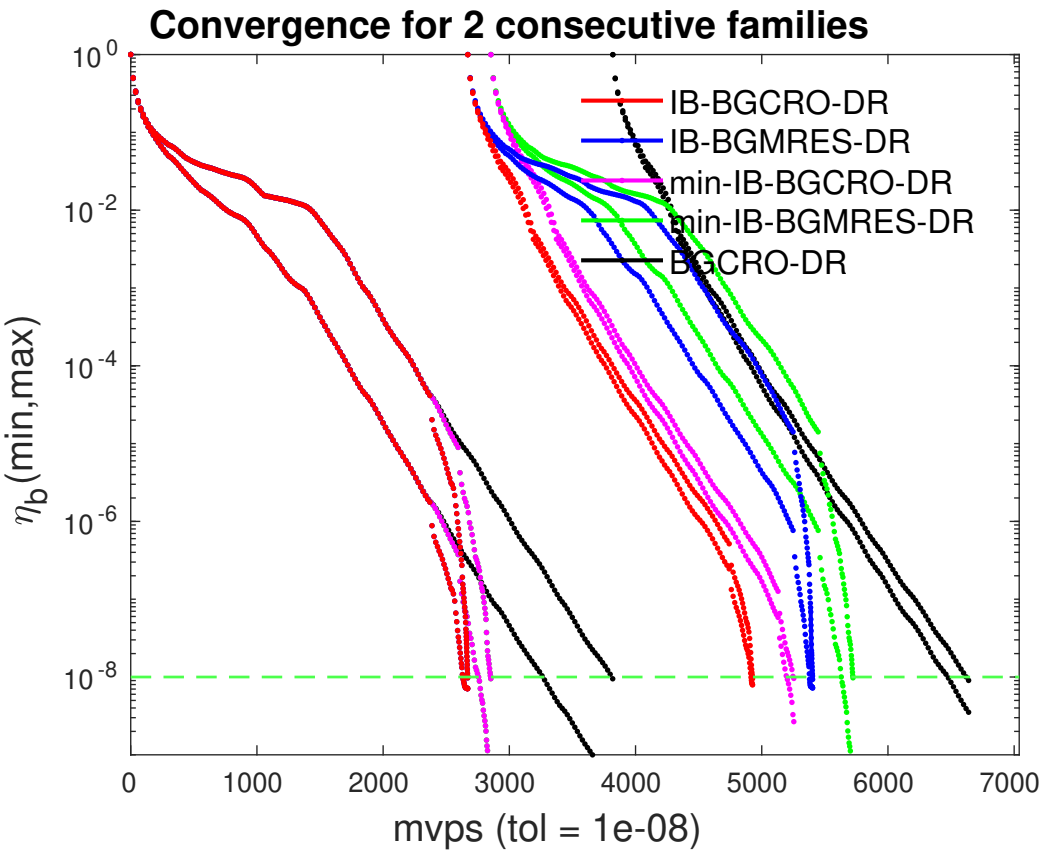
[E. Agullo, L. Giraud and Y.-F. Jing. *SIAM J. Matrix Anal. Appl.*, 2014]



- $D_\varepsilon = \varepsilon^{-1}\mathrm{diag}(\|(b^{(1)})^{-1}\|_2, \ldots, \|(b^{(p)})^{-1}\|_2)$; $B = rand(n, p)$

Diagonal scaled IB vs min-IB

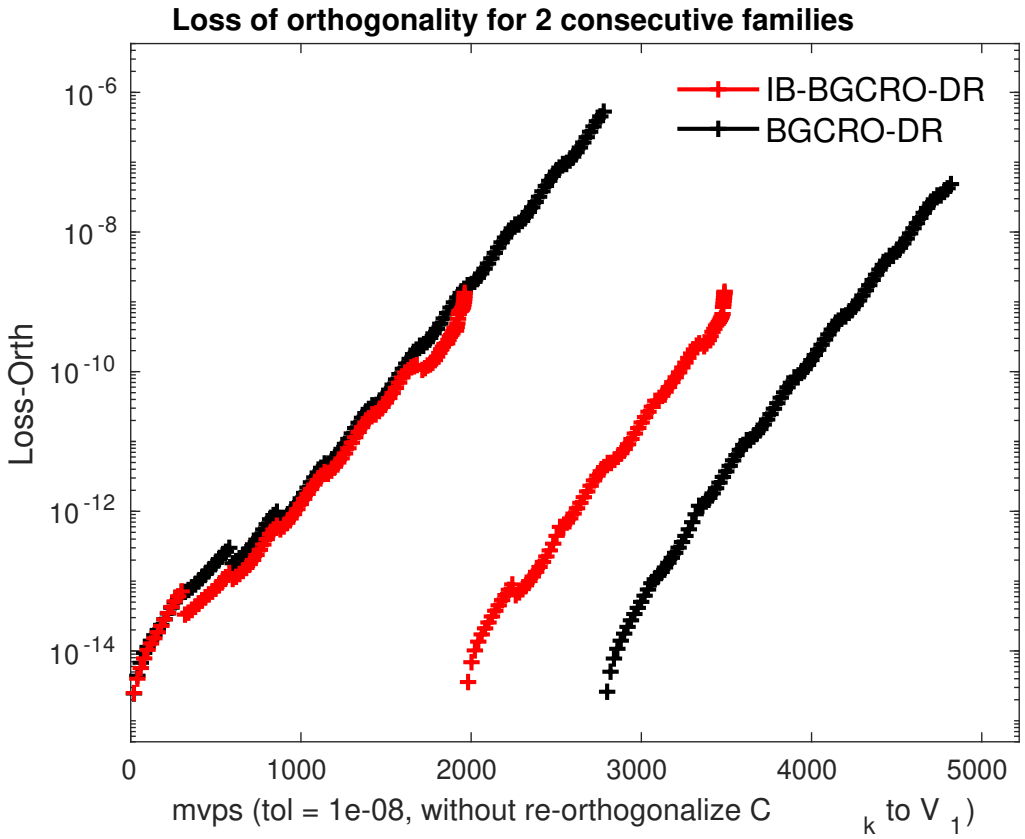
$\|(B - AX_j)D_\varepsilon\|_2 \leq 1$ **vs** $\|b^{(i)} - Ax_j^{(i)}\|_2 < \|B - AX_j\|_2 \leq \varepsilon \min_{i=1,\ldots,p} \|b^{(i)}\|_2$



- $B = rand(n, p)$ and then multiply 20 to the first $\frac{p}{2}$ columns of B

Loss of orthogonality of the Krylov basis

$$\text{Loss-Orth} = \left\| \widehat{\mathcal{V}}_{j+1}^H \widehat{\mathcal{V}}_{j+1} - I_{j+1} \right\|_2$$



- Without re-orthogonalization of C_k to $\mathbb{V}_1$ (or V_1) at restart

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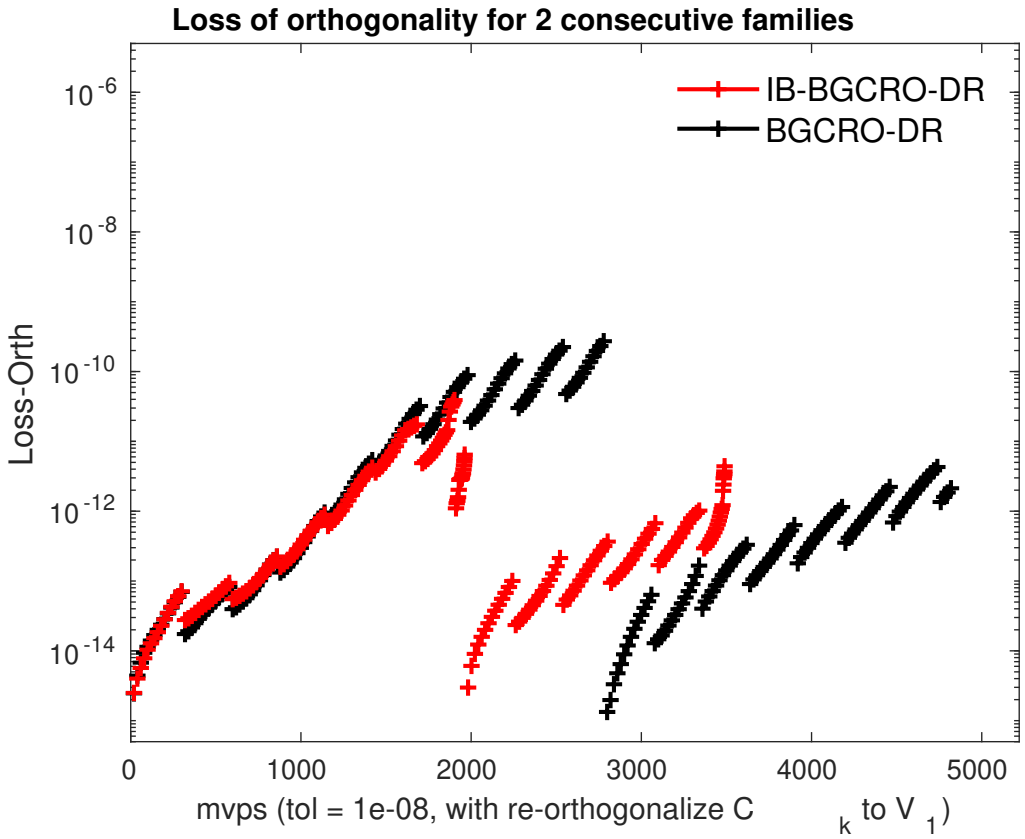
Loss of orthogonality of the Krylov basis

$$\text{Loss-Orth} = \left\| \widehat{\mathcal{V}}_{j+1}^H \widehat{\mathcal{V}}_{j+1} - I_{j+1} \right\|_2$$



- With re-orthogonalization of C_k to $\mathbb{V}_1$ (or V_1) at restart (by $\mathbb{V}_1 = (I - C_k * C_k^H)\mathbb{V}_1$ implemented in column-column way)

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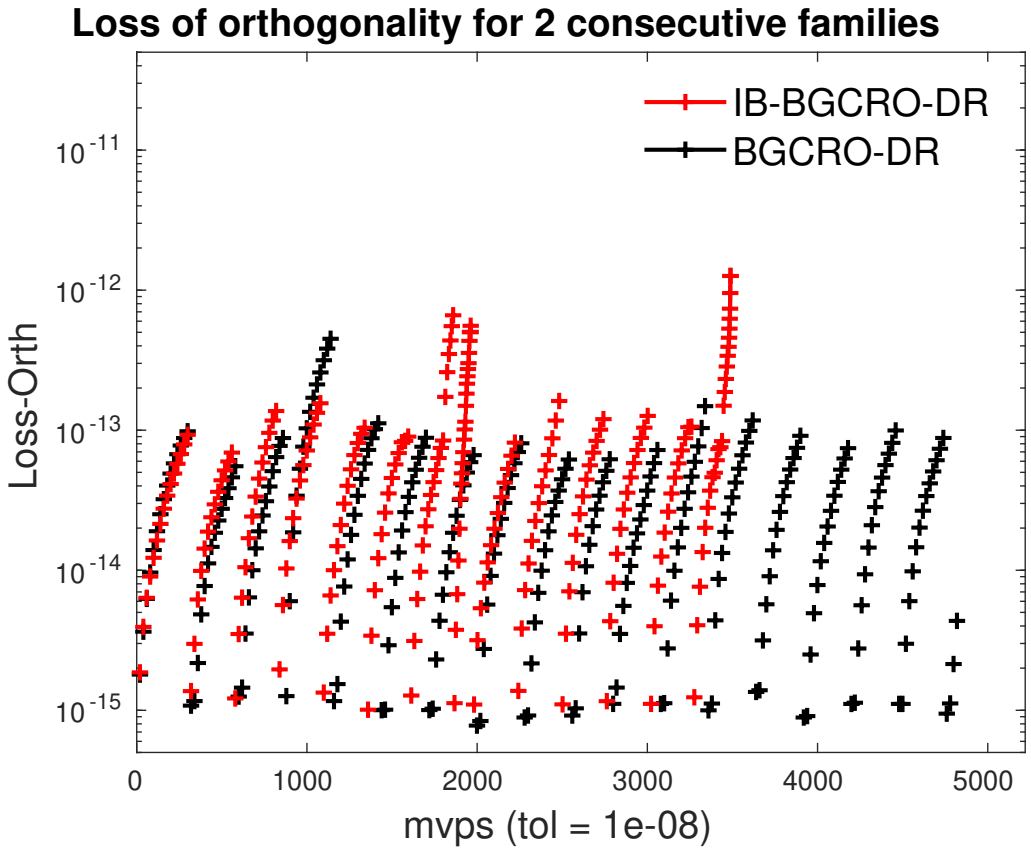
Loss of orthogonality of the Krylov basis

$$\text{Loss-Orth} = \left\| \widehat{\mathcal{V}}_{j+1}^H \widehat{\mathcal{V}}_{j+1} - I_{j+1} \right\|_2$$



- Apply re-orthogonalization to all the columns of $[C_k, [\mathbb{V}_1, P_0]]$ by the modified Gram-Schmidt (MGS) process at restart