4^{th} Hoscar workshop
September 2014, Gramado, Brazil

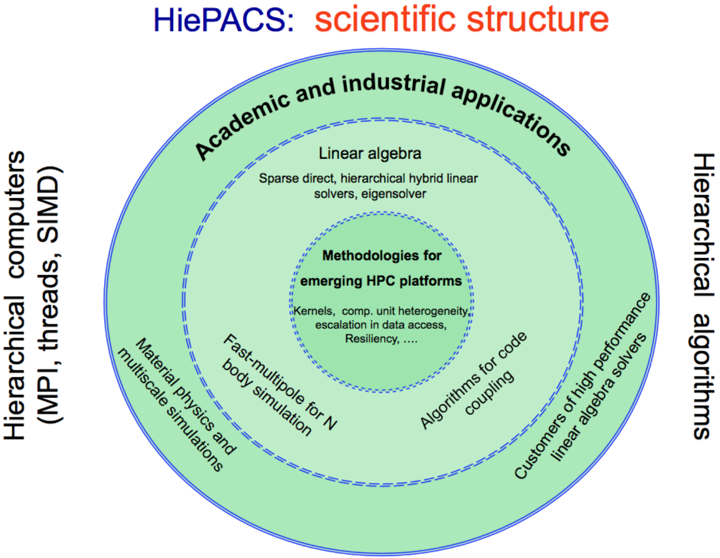
Some Progresses on Krylov Linear Solvers for Multiple Right-Hand Sides

HiePACS

HiePACS Inria Project
Joint Inria-CERFACS lab
INRIA Bordeaux Sud-Ouest

Forewords

HiePACS objectives: Contribute to the design of effective tools for frontier simulations arising from challenging research and industrial multi-scale applications towards exascale computing



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Current collaborations witin Associated teams: MORSE (UTK, ICL, UCL, Kaust), FASTLA (LNBL, Stanford), IPL C2S@Exa and industrial partners

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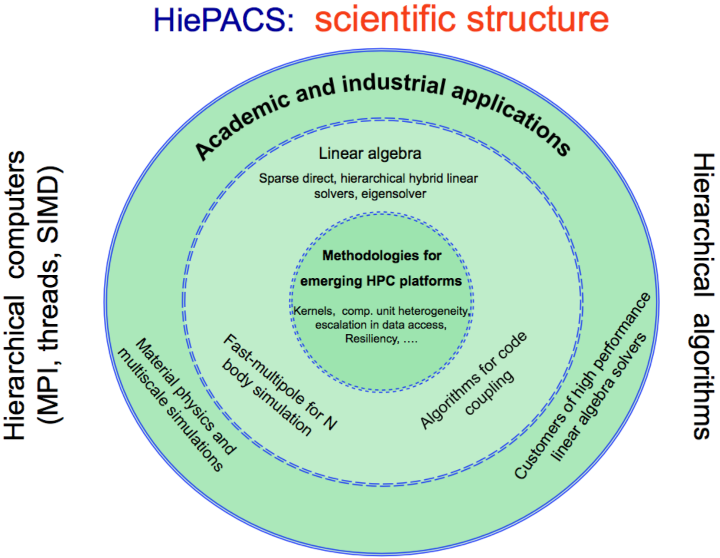

Objectives

Solve

$$AX = B$$

$A \in \mathbb{C}^{n \times n}$, $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}] \in \mathbb{C}^{n \times p}$ $(p \ll n)$, $X \in \mathbb{C}^{n \times p}$

1. Manage properly numerical rank deficiency in block Arnoldi [M. Robbé and M. Sadkane, LAA, 2006]
2. Implement a subspace augmentation at restart [R. Morgan, APNUM, 2005]

Outline

Background

Block GMRES

Numerical experiments

Extension to sequence of multiple right-hand side solves

Concluding remarks

Some basic ingredients in classical GMRES - $Ax = b$

$$x_\ell = \underset{z \in \mathcal{K}_\ell(b,A)}{\operatorname{argmin}} \|b - Az\|_2$$

with $\mathcal{K}_\ell(b, A) = \text{span}(b, Ab, ..., A^{\ell-1}b)$:

1. Construction of an orthonormal basis of the Krylov space
2. Minimiun norm solution

Computational facts

1. Happy breakdown
2. Simple restarting mechanism

Construction of the orthonormal basis

Arnoldi with modified Gram-Schmidt orthogonalization

1: $\beta = \|b\|$ set $v_1 = b/\beta$
2: **for** $j = 1, 2, \ldots, m$ **do**
3: Compute $w_j = Av_j$
4: **for** $i = 1, 2, \ldots, j$ **do**
5: $h_{i,j} = v_i^H w_j$
6: $w_j = w_j - v_i h_{i,j}$
7: **end for**
8: $w_j = v_{j+1} h_{j+1,j}$
9: **end for**

Key equalities :

$$AV_j = V_j H_j + [0_{n\times(j-1)}, w_j] = V_{j+1} \underline{H}_j$$

$$\text{with } V_j^H V_j = I_j \text{ and } V_{j+1}^H V_{j+1} = I_{j+1} \text{ where } V_j = [v_1, ..., v_j]$$

Minimun norm solution

- What we want

$$x_\ell = \underset{z \in \mathcal{K}_\ell(b,A)}{\operatorname{argmin}} \|b - Az\|_2 \quad x_\ell = V_\ell y_\ell$$

Minimun norm solution

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$$x_\ell = \underset{z \in \mathcal{K}_\ell(b,A)}{\operatorname{argmin}} \|b - Az\|_2 \quad x_\ell = V_\ell y_\ell$$

- Key equality

$$\begin{aligned} \|b - Ax_\ell\| = & \quad \|b - AV_\ell y_\ell\| = \|b - V_{\ell+1}\underline{H}_\ell y_\ell\| \\ = & \quad \|V_{\ell+1}(\beta e_1 - \underline{H}_\ell y_\ell)\| = \|\beta e_1 - \underline{H}_\ell y_\ell\| \end{aligned}$$

Minimun norm solution

- What we want

$$x_\ell = \underset{z \in \mathcal{K}_\ell(b,A)}{\text{argmin}} \|b - Az\|_2 \quad x_\ell = V_\ell y_\ell$$

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- Key features that make it works
  1. Arnoldi equality $AV_j = V_{j+1}\underline{H}_j$
  2. Orthonormal basis $V_{j+1}^H V_{j+1} = I_{j+1}$
  3. Right-hand side in search space $b \in \text{span}(V_{j+1})$

Happy breakdown

This situation occcurs when $w_j = 0$ in Arnoldi, meaning the algorithm cannot extend the space

$$AV_j = V_j H_j + [0_{n\times(j-1)}, w_j] = V_j H_j$$

Consequences

- Happy breakdown: the solution $x \in \text{span}(V_j)$
- b can be expressed as a linear combination of j eigenvectors
  Remark: all eigenvectors are not revealed at the same speed in the Krylov space (argument will come back later)

Basic restart mechanism

- Computation per iteration and storage increase linearly with iteration
- Restart mechanism when maximum search space dimension m is attained
- Set $x_0 = x_m$, solve

$$Ae = r_0$$

using GMRES where $r_0 = b - Ax_0$ so that $x_j \in x_0 + \mathcal{K}_j(r_0, A)$
Remark: all eigen-information captured in the Krylov space is lost at restart

Outline

Some key ingredients for block GMRES - $AX = B$

$$X_\ell = \underset{Z \in \mathcal{K}_\ell(V_1, A)}{\operatorname{argmin}} \|B - AZ\|_F$$

with $\mathcal{K}_\ell(V_1, A) = \text{span}(V_1, AV_1, ..., A^{\ell-1}V_1)$:

1. Construction of an orthonormal basis of the Krylov space, where $B = V_1\Lambda_1$ is the reduced QR factorisation of B
2. Minimiun norm solution

Computational challenges

1. Numerical deficiency in W_j - inexact breakdown [Robbé, Sadkane]
2. More sophisticated restarting mechanism [R. Morgan]

Construction of the orthonormal basis

Arnoldi with modified Gram-Schmidt orthogonalization

```
Choose a unitary matrix V_1 of size n × p
for j = 1, 2, ..., m do
    Compute W_j = A V_j
    for i = 1, 2, ..., j do
        H_{i,j} = V_i^H W_j
        W_j = W_j − V_i H_{i,j}
    end for
    W_j = V_{j+1} H_{j+1,j} (reduced QR−factorization)
end for
```

$$A\mathscr{V}_j = \mathscr{V}_j \mathscr{H}_j + [0_{n \times n_{j-1}}, \quad W_j] = \mathscr{V}_{j+1} \underline{\mathscr{H}}_j$$

with $\mathscr{V}_{j+1}^H \mathscr{V}_{j+1} = I_{n_{j+1}}$ where $\mathscr{V}_{j+1} = [V_1, \ldots, V_{j+1}]$

Minimun norm solution

$$\|B - AX_j\|_F = \min_{Y \in \mathbb{C}^{n_j \times p}} \left\| \mathscr{V}_{j+1} \left(\Lambda_j - \underline{\mathscr{H}}_j Y \right) \right\|_F = \min_{Y \in \mathbb{C}^{n_j \times p}} \left\| \Lambda_j - \underline{\mathscr{H}}_j Y \right\|_F$$

because $\mathscr{V}_{j+1}$ forms an orthonormal basis and

$$\Lambda_j = \begin{bmatrix} \Lambda_1 \\ 0 \end{bmatrix} \in \mathbb{C}^{n_{j+1} \times p}$$

Remark: we minimize the Frobenius norm of the block that translates in 2-norm for the individual column residual

Numerical rank deficiency in W_j

- For reasons to be made clear later but related to stopping criterion we decompose

$$W_j = V_{j+1} H_{j+1,j} + Q_j$$

with $(Q_j \perp V_{j+1}) \perp \mathscr{V}_j$.
We still have

$$A\mathscr{V}_j = \mathscr{V}_j \mathscr{H}_j + [\mathcal{Q}_{j-1}, \quad W_j],$$

where $\mathcal{Q}_{j-1} = [Q_1, \ldots, Q_{j-1}] \in \mathbb{C}^{n \times n_{j-1}}$ accounts for all the abandoned directions.

- To characterize a minimum norm solution in $\mathscr{V}_j$ we need to have an orthonormal basis of $[\mathscr{V}_j, \mathcal{Q}_{j-1}, \quad W_j]$ so that

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

Shortcut for deriving the extended Arnoldi equalitiy I

[M. Robbé and M. Sadkane, LAA, 2006]

$$A\mathscr{V}_j = \mathscr{V}_j\mathscr{H}_j + [\mathcal{Q}_{j-1}, \quad W_j]$$

- $\tilde{\mathcal{Q}}_{j-1} = (I - \mathscr{V}_j {\mathscr{V}_j}^H)\mathcal{Q}_{j-1}$, $\mathscr{L}_j = \mathscr{H}_j + {\mathscr{V}_j}^H \left[\mathcal{Q}_{j-1}, 0_{p_j}\right]$ (~~Hessenberg~~)
- $\mathcal{Q}_{j-1}$ is low rank so is $\tilde{\mathcal{Q}}_{j-1} = P_{j-1}G_{j-1}$
  $$\begin{cases} P_{j-1} \in \mathbb{C}^{n\times \tilde{q}_{j-1}} \text{ has orthonormal columns with } {\mathscr{V}_j}^H P_{j-1} = 0, \\ G_{j-1} \in \mathbb{C}^{\tilde{q}_{j-1}\times n_{j-1}} \text{ is of full rank.} \end{cases}$$
- W_j orthogonalized against P_{j-1} with $W_j - P_{j-1}C_j$ where $C_j = P_{j-1}^H W_j$
- $\tilde{W}_j D_j = \text{QR}\left(W_j - P_{j-1}C_j\right)$.
- $[\mathscr{V}_j, P_{j-1}, \tilde{W}_j]$ form an orthonormal basis of $[\mathscr{V}_j, \mathcal{Q}_{j-1}, W_j]$.

Shortcut for deriving the generalized Arnoldi equalitiy II

[M. Robbé and M. Sadkane, LAA, 2006]

- Extended Arnoldi equality

$$
\begin{aligned}
A\mathscr{V}_j &= \mathscr{V}_j\mathscr{L}_j + \left[P_{j-1}G_{j-1}, \left[P_{j-1}, \tilde{W}_j\right]\left[\begin{array}{c} C_j \\ D_j \end{array}\right]\right] \\
&= \left[\mathscr{V}_j, P_{j-1}, \tilde{W}_j\right]\left[\begin{array}{cc} \multicolumn{2}{c}{\mathscr{L}_j} \\ G_{j-1} & C_j \\ 0 & D_j \end{array}\right] \\
&= \left[\mathscr{V}_j, [P_{j-1}, \tilde{W}_j]\right]\mathscr{F}_j
\end{aligned}
$$

- Least-squares problem reads

$$
Y_j = \underset{Y\in\mathbb{C}^{n_j\times p}}{\operatorname{argmin}} \left\|\Lambda_j - \mathscr{F}_j Y\right\|_F, \text{with } \Lambda_j = \left[\begin{array}{c} \Lambda_1 \\ 0 \\ 0 \end{array}\right]
$$

Numerical rank deficiency in $\tilde{W}_j$ vs convergence

- Based on SVD of least-squared residual

$$\Lambda_j - \mathscr{F}_j Y_j = \mathbb{U}_1 \Sigma_1 \mathbb{V}_1^H + \mathbb{U}_2 \Sigma_2 \mathbb{V}_2^H$$

- Decompose

$$\mathbb{U}_1 = \begin{pmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{pmatrix} \text{ in accordance with } \left[\mathscr{V}_j, [P_{j-1}, \tilde{W}_j]\right]$$

- Consider $[\mathbb{W}_1, \mathbb{W}_2]$ so that Range$(\mathbb{W}_1) =$ Range$(\mathbb{U}_1^{(2)})$.
- Define and update

$$V_{j+1} = \left[P_{j-1}, \tilde{W}_j\right] \mathbb{W}_1$$

$$P_j = \left[P_{j-1}, \tilde{W}_j\right] \mathbb{W}_2$$

$$G_j = \mathbb{W}_2^H \begin{bmatrix} G_{j-1} & C_j \\ 0 & D_j \end{bmatrix}$$

Rank deficiency threshold vs stopping criterion

Assuming p inexact breakdowns

$$||B - AX_s||_2 \leq \epsilon^{(R)}.$$

$$\frac{||b^{(i)} - Ax_s^{(i)}||_2}{||b^{(i)}||_2} \leq \frac{||B - AX_s||_2}{||b^{(i)}||_2} \leq \frac{||B - AX_s||_2}{\min\limits_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2} \leq \frac{\epsilon^{(R)}}{\min\limits_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2}$$

It follows that the choice

$$\epsilon^{(R)} = \varepsilon \times \min_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2$$

ensures convergence below the threshold ϵ for individual $b^{(i)}$ if same accuracy required for all the righ-hand sides

A few definitions

Definition

Harmonic Ritz pair. Consider a subspace $\mathcal{U}$ of $\mathbb{C}^n$. Given a matrix $B \in \mathbb{C}^{n\times n}$, $\lambda \in \mathbb{C}$ and $y \in \mathcal{U}$, (λ, y) is a harmonic Ritz pair of A with respect to $\mathcal{U}$ if and only if

$$Ay - \lambda\, y \perp A\mathcal{U}$$

The vector y is a harmonic Ritz vector associated with the harmonic Ritz value λ.

Lemma

The harmonic Ritz pairs $(\tilde{\theta}_i, \tilde{g}_i)$ associated with $\mathcal{U} = \mathrm{span}(\mathscr{V}_m)$ satisfy the following property

$$\mathscr{F}_m^H \left(\mathscr{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0_p \end{bmatrix} \right) = 0, \ \ (i = 1, \dots, n_m),$$

$\tilde{g}_i \in \mathbb{C}^{n_m}$, and $\mathscr{V}_m \tilde{g}_i$ are the harmonic Ritz vectors associated with the corresponding harmonic Ritz values $\tilde{\theta}_i$.

An interesting fact for augmentation at restart

Lemma

Assume that $\mathscr{L}_m$ is of full rank after performing a first cycle of IB-BGMRES, then the column vectors $\left(\mathscr{F}_m\tilde{\mathbf{g}}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix}\right) \in \mathbb{C}^{n_m+p}$ $(i = 1, \ldots, n_m)$ *are all contained in the subspace spanned by the least-squares residuals* $R_{LS_m} = (\Lambda_m - \mathscr{F}_m Y_m) \in \mathbb{C}^{(n_m+p)\times p}$*, i.e.,* $\exists \alpha_i \in \mathbb{C}^p$ *so that*

$$\mathscr{F}_m\tilde{\mathbf{g}}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} = R_{LS_m}\alpha_i.$$

Proposition

The harmonic residual vectors are all linear combinations of the residual vectors from the minimum residual solutions of the linear equation problem after performing a first cycle of the IB-BGMRES.

An interesting fact for augmentation at restart

Lemma

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Proposition

The harmonic residual vectors are all linear combinations of the residual vectors from the minimum residual solutions of the linear equation problem after performing a first cycle of the IB-BGMRES.

Some harmonic vectors can be kept in the search space at restart with the residual vector that must be in the space

Restarting mechanism I

Let $\tilde{G} = [\tilde{g}_1, \ldots, \tilde{g}_k] \in \mathbb{C}^{n_m \times k}$ and form $\underline{G} = \begin{bmatrix} \tilde{G} & R_{LS_m} \\ 0_{p\times k} & \end{bmatrix}$ We denote $\underline{G} = Q_{\underline{G}} R_{\underline{G}}$ the reduced $QR-$factorization of $\underline{G}$,

$$Q_{\underline{G}} = \begin{bmatrix} \Gamma_1 & \Gamma_2 \\ 0_{p\times k} & \end{bmatrix} \in \mathbb{C}^{(n_m+p)\times(k+p)},$$
$$R_{\underline{G}} = \begin{bmatrix} \Theta_1 & \Theta_2 \\ 0_{p\times k} & \end{bmatrix} \in \mathbb{C}^{(k+p)\times(k+p)},$$

so that

$$\tilde{G} = \Gamma_1 \Theta_1,$$
$$R_{LS_m} = Q_{\underline{G}} \Theta_2.$$

Restarting mechanism II

Extended Arnoldi relation

$$A\mathscr{V}_1^{\text{new}} = \left[\mathscr{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}\right] \mathscr{F}_1^{\text{new}} \quad A\mathscr{V}_1^{\text{new}} = \mathscr{V}_2^{\text{new}} \underline{\mathscr{L}}_1^{\text{new}} + \tilde{\mathcal{Q}}_1^{\text{new}},$$

with

$$\left[\mathscr{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}\right] = \left[\mathscr{V}_m, [P_{m-1}, \tilde{W}_m]\right] Q_{\underline{G}}, \quad R_0 = \left[\mathscr{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}\right] \Lambda_1^{\text{new}} \text{ with } \Lambda_1^{\text{new}} = \Theta_2,$$

$$\mathscr{L}_1^{\text{new}} = \Gamma_1^H \mathscr{L}_m \Gamma_1, \quad \mathbb{H}_1^{\text{new}} = \Gamma_2^H \mathscr{F}_m \Gamma_1, \quad \mathscr{F}_1^{\text{new}} = \begin{bmatrix} \mathscr{L}_1^{\text{new}} \\ \mathbb{H}_1^{\text{new}} \end{bmatrix},$$

$$V_2^{\text{new}} = [P_0, \tilde{W}_1]^{\text{new}} \mathbb{W}_1^{\text{new}}, \ P_1^{\text{new}} = [P_0, \tilde{W}_1]^{\text{new}} \mathbb{W}_2^{\text{new}}, \ \mathscr{L}_{2,:}^{\text{new}} = \mathbb{W}_1^{\text{new}\,H} \mathbb{H}_1^{\text{new}}, \ G_1^{\text{new}} = \mathbb{W}_2^{\text{new}\,H} \mathbb{H}_1^{\text{new}},$$

$$\mathscr{V}_2^{\text{new}} = \left[\mathscr{V}_1^{\text{new}}, V_2^{\text{new}}\right], \ \underline{\mathscr{L}}_1^{\text{new}} = \begin{bmatrix} \mathscr{L}_1^{\text{new}} \\ \mathscr{L}_{2,:}^{\text{new}} \end{bmatrix}, \ \tilde{\mathcal{Q}}_1^{\text{new}} = P_1^{\text{new}} G_1^{\text{new}},$$

where $\text{Range}(\mathbb{W}_1^{\text{new}}) = \text{Range}(\mathbb{U}_1^{\text{new}(2)})$ with $\mathbb{U}_1^{\text{new}} = \begin{bmatrix} \mathbb{U}_1^{\text{new}(1)} \\ \mathbb{U}_1^{\text{new}(2)} \end{bmatrix}$ and $\left[\mathbb{W}_1^{\text{new}}, \quad \mathbb{W}_2^{\text{new}}\right]$ is unitary with

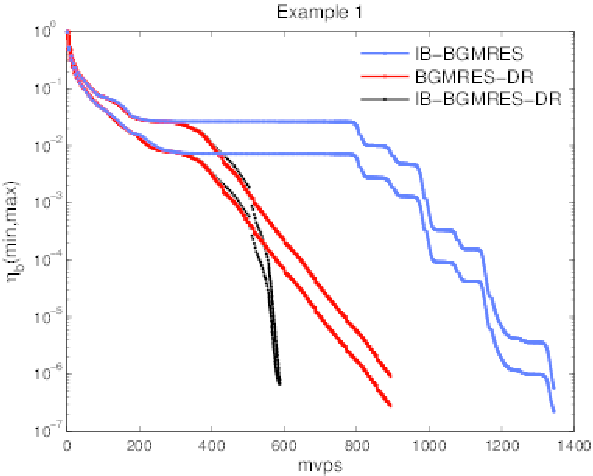
$$\Lambda_1^{\text{new}} - \mathscr{F}_1^{\text{new}} Y_1^{\text{new}} = \mathbb{U}_1^{\text{new}} \Sigma_1^{\text{new}} \mathbb{V}_1^{\text{new}\,H} + \mathbb{U}_2^{\text{new}} \Sigma_2^{\text{new}} \mathbb{V}_2^{\text{new}\,H}, \text{ with SVD trheshold } \epsilon^{(R)}$$

the SVD to detect inexact breakdown in the restarting block residual where

$$Y_1^{\text{new}} = \underset{Y \in \mathbb{C}^{n_1 \times p}}{\operatorname{argmin}} \left\| \Lambda_1^{\text{new}} - \mathscr{F}_1^{\text{new}} Y \right\|_F.$$

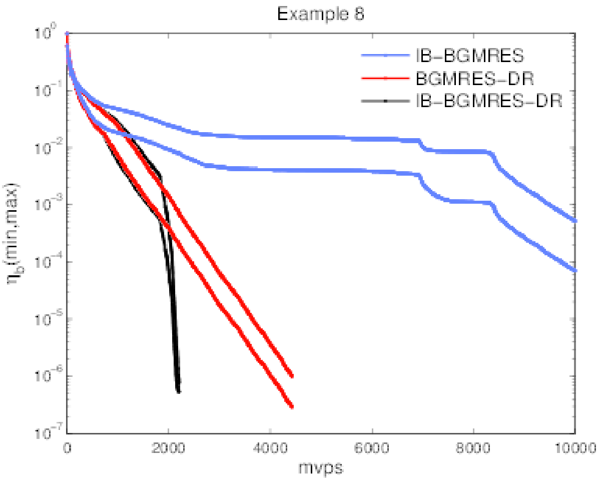
Outline

Comparative covergence rate



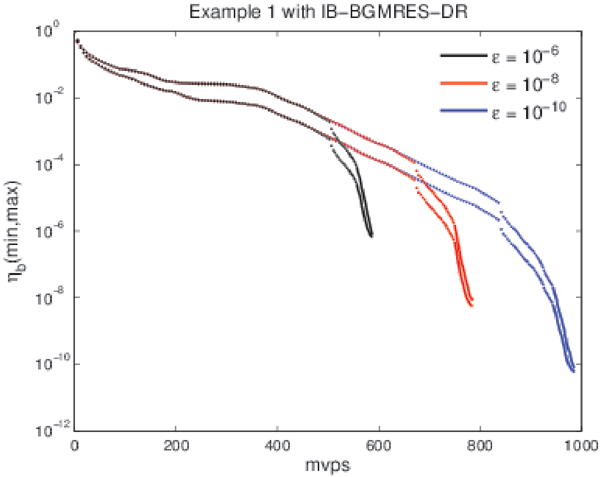
IB-BGMRES [M. Robbé and M. Sadkane, LAA, 2006], BGMRES-DR [R. Morgan, APNUM, 2005]

Comparative covergence rate



IB-BGMRES [M. Robbé and M. Sadkane, LAA, 2006], BGMRES-DR [R. Morgan, APNUM, 2005]

Inexact breakdown vs targeted accuracy



Comparisons with cousins and parents

Iso-memory comparison for basis storage

Example	GMRES	GMRES-DR	IB-BGMRES	BGMRES-DR	IB-BGMRES-DR
1	2536	1077	1344	892	**588**
2	1069	856	788	667	**538**
3	378	378	372	341	**335**
4	**412**	**412**	446	447	440
5	845	694	617	474	**386**
6	464	464	357	294	**248**
7	3154	**2003**	3291	3090	2104
8	10643	3110	-	4426	**2202**

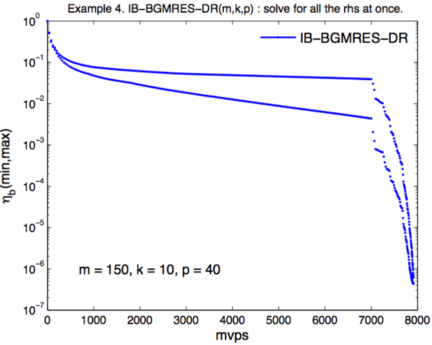
Table: Number of *mvps* for regular GMRES, GMRES-DR, IB-BGMRES, BGMRES-DR and IB-BGMRES-DR with $\varepsilon = 10^{-6}$.

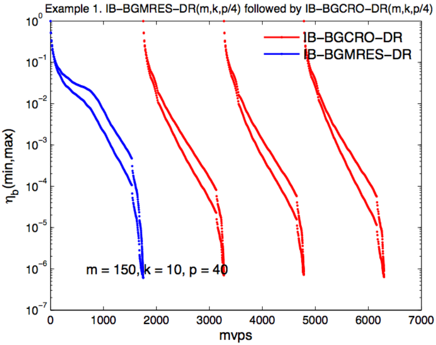
Outline

A priori space augmentation

- IB-BGMRES-DR effective for one block of right-hand sides
- Combine IB-BGMRES-DR with Parks et all [Park et all, SISC, 2006] recycling appraoch
  Split the search space in two orthogonal spaces.
  - multiple right-hand sides
  - multiple left-hand sides (different frequencies ?)

Benefit of the recycling mechanism: flexibility





isomemory experiments

Outline

Concluding remarks

- The new algorithm IB-BGMRES-DR inheritis the positive genes of its parents IB-BGMRES [M. Robbé and M. Sadkane, LAA, 2006] and BGMRES-DR [R. Morgan, APNUM, 2005]
- Flexible variant can be designed to accomodate resiliency or mixed precision calculation
- Task based implementation should be carried out soon

Obrigado for your attention

Questions ?

https://team.inria.fr/hiepacs/