

# Iterative Methods and Multigrid

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## Part 3: Methods based on the two-sided Lanczos algorithm

### Short Recurrence Methods?

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GMRES optimal in iterations but expensive in time and memory if many iterations required. Main cost is keeping all vectors and complete orthogonalization.

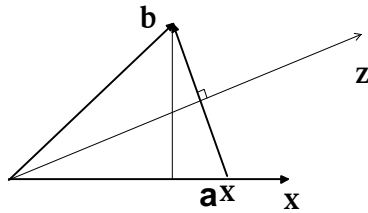
[Can we devise an optimal method with a short recurrence?](#)

No, unless (non-Hermitian) matrix very special.  
(Faber&Manteuffel result)

However, we can construct short recurrence methods that are very good in most cases.

# Oblique Projection

Find approximation to  $\mathbf{b}$  in  $\text{range}(\mathbf{x})$  such that  $\mathbf{b} - \alpha\mathbf{x} \perp \mathbf{z}$



This gives  $\mathbf{z}^H(\mathbf{b} - \alpha\mathbf{x}) = \mathbf{0} \Rightarrow \alpha = \frac{\mathbf{z}^H\mathbf{b}}{\mathbf{z}^H\mathbf{x}}$ .

If  $\mathbf{z}^H\mathbf{x} = \mathbf{0}$  no solution exists.

The quality of the approximation from this oblique projection depends on the angle between the search space,  $\text{range}(\mathbf{x})$ , and the space that defines the projection,  $\text{range}(\mathbf{z})$ .

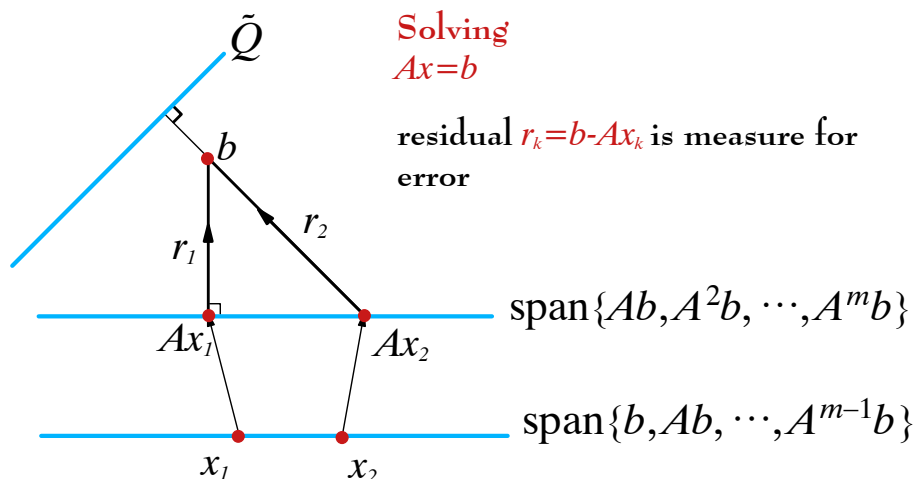
More generally, the quality of an approximation from oblique projection depends on *the angles* between the search space and the space that defines the projection.

Residual from oblique projection may be much larger than optimal.

# Methods based on Oblique Projection

Two types of Krylov subspace methods (general matrices):

1. Orthogonal projection methods: optimal, but expensive (GMRES).
2. Oblique projection methods: cheap, but often converge poorly.
  - a. economize on optimal methods (restart or truncate)
  - b. create different space (BiCG):  $\text{span}\{\tilde{\mathbf{b}}, A^H\tilde{\mathbf{b}}, \dots, (A^H)^{m-1}\tilde{\mathbf{b}}\}$



## Methods based on Oblique Projection

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In multiple dimensions the quality of the approximation from an oblique projection depends on *the canonical or principal angles* between the search space and the space that defines projection.

The residual from an oblique projection may be much larger than the optimal residual.

Result may be very poor if one or more angles near  $\pi/2$ .

Linear system:  $\mathbf{Ax} = \mathbf{b}$ ,

$\mathbf{x} \in \text{range}(\mathbf{V}_m)$  and  $\mathbf{r} = \mathbf{b} - \mathbf{AV}_m\mathbf{y} \perp \text{range}(\tilde{\mathbf{V}}_m)$

$$\tilde{\mathbf{V}}_m^H(\mathbf{b} - \mathbf{AV}_m\mathbf{y}) = \mathbf{0} \quad \Leftrightarrow \quad \tilde{\mathbf{V}}_m^H\mathbf{AV}_m\mathbf{y} = \tilde{\mathbf{V}}_m^H\mathbf{b}$$

Solve  $m \times m$  system (small).

Computation of  $\tilde{\mathbf{V}}_m^H\mathbf{AV}_m\mathbf{y}$ ,  $\tilde{\mathbf{V}}_m$ , and  $\mathbf{V}_m$  using short recurrences requires special choices for  $\tilde{\mathbf{V}}_m$ .

## Biorthogonality

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In order to use a short recurrence we need to make special choices.

Given arbitrary  $\mathbf{v}_1$  and  $\tilde{\mathbf{v}}_1$  we generate two Krylov sequences:

$$\mathbf{v}_i = (\mathbf{A}\mathbf{v}_{i-1} - \sum_{j < i} a_j \mathbf{v}_j) / \|\cdot\| \in \mathbf{K}^i(\mathbf{A}, \mathbf{v}_1)$$

$$\tilde{\mathbf{v}}_i = (\mathbf{A}^H \tilde{\mathbf{v}}_{i-1} - \sum_{j < i} a_j \tilde{\mathbf{v}}_j) / \|\cdot\| \in \mathbf{K}^i(\mathbf{A}^H, \tilde{\mathbf{v}}_1)$$

Neither the vectors  $\mathbf{v}_i$  nor the vectors  $\tilde{\mathbf{v}}_i$  are orthogonal.

However,  $\mathbf{v}_i^H \tilde{\mathbf{v}}_j = \mathbf{0}$  for  $i \neq j$  and  $\mathbf{v}_i^H \tilde{\mathbf{v}}_i \neq \mathbf{0}$  by choice of  $a_i$  and  $\tilde{a}_i$ .

We now have the following orthogonality results (analogous to CG):

$$\mathbf{A}\mathbf{v}_i \perp \tilde{\mathbf{v}}_j \text{ for } j < i - 1 \text{ since } (\mathbf{A}\mathbf{v}_i)^H \tilde{\mathbf{v}}_j = \mathbf{v}_i^H \mathbf{A}^H \tilde{\mathbf{v}}_j = \mathbf{v}_i^H \left( \sum_{k=1}^{j+1} \gamma_k \tilde{\mathbf{v}}_k \right) \text{ and}$$
$$\mathbf{A}^H \tilde{\mathbf{v}}_i \perp \mathbf{v}_j \text{ for } j < i - 1.$$

So we can generate two mutually orthogonal (° biorthogonal) sequences of vectors using short recurrences.

Note that in this case  $\tilde{\mathbf{V}}_i^H \mathbf{A} \mathbf{V}_i$  is tridiagonal.

## BiCG (three-term recurrence)

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Solve  $Ax = b$ ; choose  $x_0 \rightarrow r_0 = b - Ax_0$ ; choose  $\tilde{r}_0$ ;

Iterate:

$$\delta_m = \tilde{r}_m^* r_m, \quad a_m = \tilde{r}_m^* A r_m / \delta_m, \quad \beta_{m-1} = \gamma_{m-1} \frac{\delta_m}{\delta_{m-1}}, \quad \gamma_m = -a_m - \beta_{m-1}.$$

$$\begin{aligned} r_{m+1} &= \gamma_m^{-1} (A r_m - a_m r_m - \beta_{m-1} r_{m-1}); & A R_m &= R_{m+1} \underline{T}_m; \\ \tilde{r}_{m+1} &= \tilde{\gamma}_m^{-1} (A^* \tilde{r}_m - \bar{a}_m \tilde{r}_m - \bar{\beta}_{m-1} \tilde{r}_{m-1}); & A^* \tilde{R}_m &= \tilde{R}_{m+1} \underline{\tilde{T}}_m; \\ x_{m+1} &= -\frac{a_m}{\gamma_m} x_m - \frac{\beta_{m-1}}{\gamma_m} x_{m-1} - \gamma_m^{-1} r_m; \end{aligned}$$

$$\begin{aligned} \tilde{R}_m^* R_m &= \Delta_m = \text{diag}(\delta_0, \delta_1, \dots, \delta_{m-1}); \\ x_{m+1} &= x_0 + R_m y \rightarrow r_{m+1} = r_0 - R_{m+1} \underline{T}_m y; \quad r_{m+1} \perp \tilde{R}_m; \end{aligned}$$

$$\begin{aligned} \tilde{R}_m^* (r_0 - A R_m y) &= 0 \Rightarrow \delta_0 e_1 - \Delta_n T_n y = 0 \Rightarrow y = T_n^{-1} e_1; \\ r_{m+1} &= R_{m+1} (e_1 - \underline{T}_m T_m^{-1} e_1); \end{aligned}$$

## BiCG (coupled two-term recurrence)

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Using again an implicit decomposition of the tridiagonal matrix  $T_k = L_k D_k U_k$  we get a coupled two term recurrence that allows us to discard old vectors.

$x_0 \rightarrow r_0 = b - Ax_0$ ;  $p_0 = r_0$ ; choose  $\tilde{r}_0 : \tilde{r}_0^H r_0 \neq 0$  and  $\tilde{p}_0 = \tilde{r}_0$ .

For  $k = 1, 2, \dots$

$$a_{k-1} = \frac{\tilde{r}_{k-1}^H r_{k-1}}{\tilde{p}_{k-1}^H A p_{k-1}}; \quad x_k = x_{k-1} + a_{k-1} p_{k-1};$$

$$r_k = r_{k-1} - a_{k-1} A p_{k-1}; \quad \tilde{r}_k = \tilde{r}_{k-1} - \bar{a}_{k-1} A^H \tilde{p}_{k-1};$$

$$\beta_{k-1} = \frac{\tilde{r}_k^H r_k}{\tilde{r}_{k-1}^H r_{k-1}};$$

$$p_k = r_k + \beta_{k-1} p_k; \quad \tilde{p}_k = \tilde{r}_k + \bar{\beta}_{k-1} \tilde{p}_k;$$

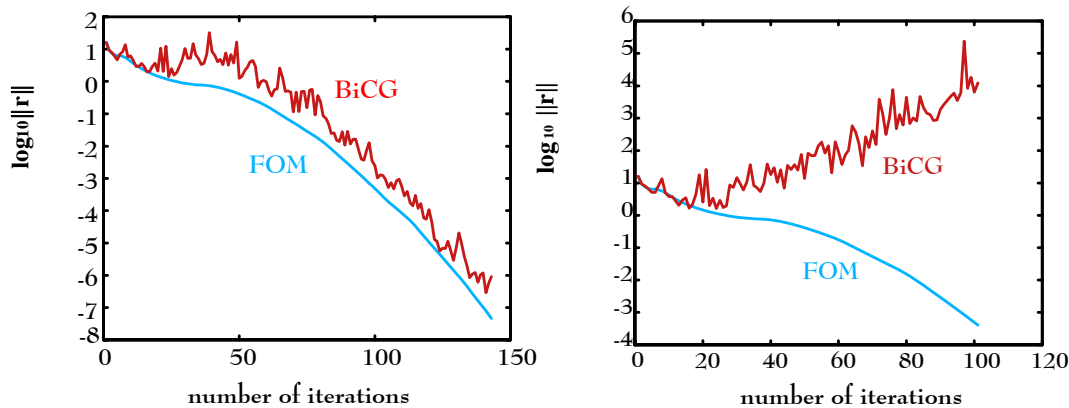
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Drawbacks of BiCG?

# Oops! (two choices of left starting vector)

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Some of the most popular methods today are derived from BiCG:  
CGS, BiCGstab, TFQMR, QMR, ...



## Drawbacks of BiCG

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1. In general, method does not satisfy any (strict) minimization property and hence may converge (very) erratically. (In practice the method often converges surprisingly well -- this is not a drawback--).
2. Two matvec.s per iteration, only one extends search space.
3. Need  $A^H$  which may be more expensive to work with or may not even be available (matrix-free implementations)
4. Breaks down without finding solution:
  - a.  $\tilde{\mathbf{r}}_k = \mathbf{0}$ , which means  $\mathbf{K}^k(A^H, \tilde{\mathbf{r}}_k)$  is invariant
  - b.  $\tilde{\mathbf{r}}_k^H \mathbf{r}_k = \mathbf{0}$ , where  $\tilde{\mathbf{r}}_k \neq \mathbf{0}$  and  $\mathbf{r}_k \neq \mathbf{0}$ .
  - c.  $\mathbf{T}_k$  singular (only for coupled 2-term recurrence)

## QMR

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If BiCG fails because  $\mathbf{T}_k$  is singular, we may solve the system

$\|\mathbf{r}_0\| \mathbf{e}_1 - \mathbf{T}_k^{(k+1) \times k}$  in least squares sense:

$$\mathbf{r}_k = \mathbf{r}_0 - \mathbf{A}\mathbf{V}_k\mathbf{y}_k = \mathbf{V}_{k+1} \left( \|\mathbf{r}_0\| \mathbf{e}_1 - \mathbf{T}_k \mathbf{y}_k \right)$$

Minimize  $\left\| \|\mathbf{r}_0\| \mathbf{e}_1 - \mathbf{T}_k \mathbf{y}_k \right\|_2$  as in GMRES (or MINRES).

Major difference:  $\mathbf{V}_{k+1}$  is not (at all) orthogonal, hence not optimal.

This least squares system always has a solution (removes one breakdown condition).

Compared with GMRES we have  $\left\| \mathbf{r}_k^Q \right\|_2 \leq \kappa(\mathbf{V}_{k+1}) \left\| \mathbf{r}_k^G \right\|_2$ .

Unfortunately there is no bound (in general) for  $\kappa(\mathbf{V}_{k+1})$ .

## CGS

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Cunning Plan (P. Sonneveld): If we only need  $\mathbf{K}(\mathbf{A}^H, \tilde{\mathbf{r}}_0)$  for projection, then all we need are the inner products with the vectors  $\tilde{\mathbf{r}}_i$  and  $\tilde{\mathbf{p}}_i$ .

Since  $\tilde{\mathbf{r}}_i = \tilde{\mathbf{R}}_i(\mathbf{A}^H)\tilde{\mathbf{r}}_0$  we have

$$\tilde{\mathbf{r}}_i^H \mathbf{r}_i = [\tilde{\mathbf{R}}_i(\mathbf{A}^H)\tilde{\mathbf{r}}_0]^H [\mathbf{R}_i(\mathbf{A})\mathbf{r}_0] = \tilde{\mathbf{r}}_0^H \mathbf{R}_i^2(\mathbf{A})\mathbf{r}_0$$

Analogously, the other inner products are products of polynomials in  $\mathbf{A}$ . If we can find (easy) recurrences to represent the products of polynomials times a vector (like  $\mathbf{R}_i^2(\mathbf{A})\mathbf{r}_0$ ), then we only need  $\tilde{\mathbf{r}}_0$  and we can discard the Krylov space generated with  $\mathbf{A}^H$ .

Moreover we now compute approximations from Krylov space  $\mathbf{K}^{2i}(\mathbf{A}, \mathbf{r}_0)$  using  $2 \times i$  matvecs. So, we no longer waste matvecs.

Finally, if  $\mathbf{R}_i(\mathbf{A})\mathbf{r}_0$  small, then *typically*  $\mathbf{R}_i^2(\mathbf{A})\mathbf{r}_0$  much smaller. Unfortunately, when  $\mathbf{R}_i(\mathbf{A})\mathbf{r}_0$  large ...

## CGS

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Since CGS ‘squares the residual’ the residual may be large when  $\mathbf{R}_i(\mathbf{A})\mathbf{r}_0$  not small. In fact, even when  $\mathbf{R}_i(\mathbf{A})\mathbf{r}_0$  small,  $\mathbf{R}_i^2(\mathbf{A})\mathbf{r}_0$  may not be.

This may lead to very irregular (nervous) convergence behavior with large peaks in the residual norm. This may ruin accuracy and sometimes convergence. Nevertheless, for a long time CGS was the method of choice for a large class of problems.

Instead of squaring the polynomial, to avoid large peaks in CGS convergence, we may multiply by another polynomial:

$$\mathbf{r}_k = \mathbf{M}_k(\mathbf{A})\mathbf{R}_k(\mathbf{A})\mathbf{r}_0$$

where,  $\mathbf{M}_k$  is used to improve convergence and avoid peaks.

For example, one-step minimum residual polynomial. This yields the BiCGStab (Stabilized) method. Currently among the most popular Krylov methods with GMRES and TFQMR (QMR squared).

## BiCGSTAB

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To avoid the large oscillations in CGS we try yet another cunning plan.

Take  $\mathbf{r}_k = \mathbf{M}_k(\mathbf{A})\mathbf{R}_k(\mathbf{A})\mathbf{r}_0$  with  $\mathbf{R}_k$  the BiCG residual polynomial and

$\mathbf{M}_k = (1 - \omega_k z) \cdots (1 - \omega_1 z)$  with  $\omega_k$  chosen (in step  $k$ ) to minimize

$$\|\mathbf{r}_k\|_2 = \|(\mathbf{I} - \omega_k \mathbf{A})\mathbf{M}_{k-1}\mathbf{R}_k(\mathbf{A})\mathbf{r}_0\|_2$$

This leads to BiCGSTAB (most cited paper in math in the 1990s - ISI).

Let  $\mathbf{R}_k(\mathbf{A})\mathbf{r}_0$  be the BiCG residual and  $\mathbf{P}_k(\mathbf{A})\mathbf{r}_0$  the BiCG search vector.

We need recurrences for  $\mathbf{r}_k = \mathbf{M}_k(\mathbf{A})\mathbf{R}_k(\mathbf{A})\mathbf{r}_0$  and  $\mathbf{p}_k = \mathbf{M}_k(\mathbf{A})\mathbf{P}_k(\mathbf{A})\mathbf{r}_0$

Using the BiCG recurrence we see that

$$\mathbf{r}_k = (\mathbf{I} - \omega_k \mathbf{A})\mathbf{M}_{k-1}(\mathbf{A})(\mathbf{R}_{k-1}(\mathbf{A}) - a_{k-1}\mathbf{A}\mathbf{P}_{k-1}(\mathbf{A}))\mathbf{r}_0 \rightarrow$$

$$\mathbf{r}_k = (\mathbf{I} - \omega_k \mathbf{A})(\mathbf{r}_{k-1} - a_{k-1}\mathbf{A}\mathbf{p}_{k-1})$$

$$\mathbf{p}_k = \mathbf{M}_k(\mathbf{A})(\mathbf{R}_k(\mathbf{A}) + \beta_k \mathbf{P}_{k-1}(\mathbf{A}))\mathbf{r}_0 \rightarrow$$

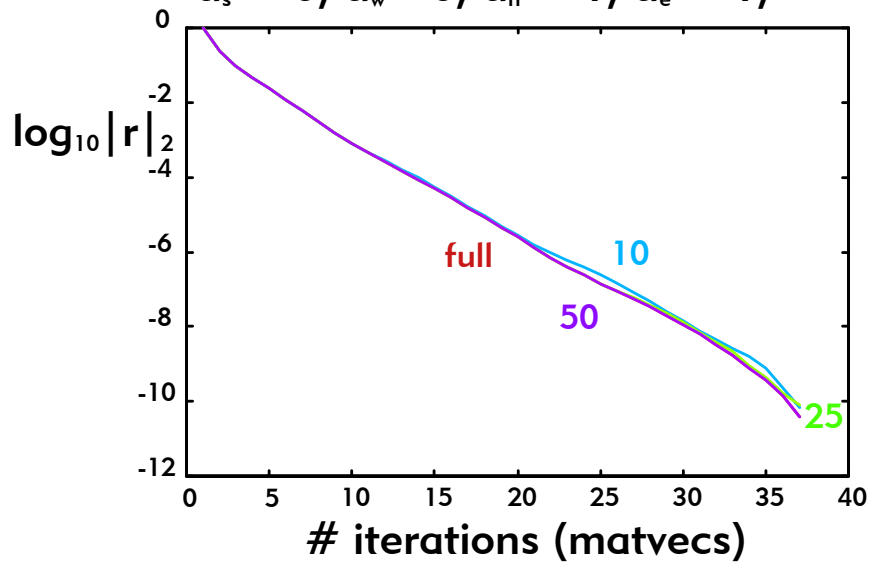
$$\mathbf{p}_k = \mathbf{r}_k - \beta_k(\mathbf{I} - \omega_k \mathbf{A})\mathbf{p}_{k-1}$$

Rewriting the recurrences for  $a_k$  and  $\beta_k$  in terms of new vectors, and deriving a formula for  $\omega_k$  yields the algorithm (see Section 7.13).

## GMRES(m) with $r=s=70$

$p=q=1; r=s=70; h=1/31;$

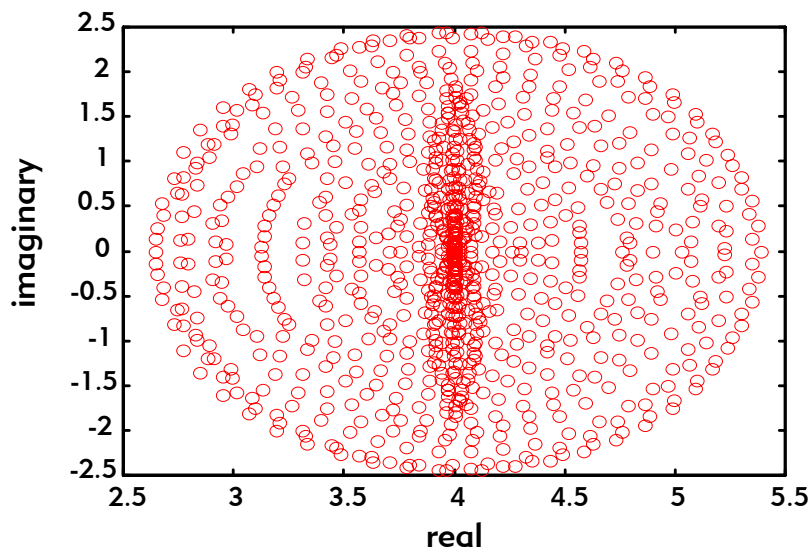
$u_s=0; u_w=0; u_n=1; u_e=1;$



## Eigenvalues

$p=q=1; r=s=70; h=1/31;$

$u_s=0; u_w=0; u_n=1; u_e=1;$

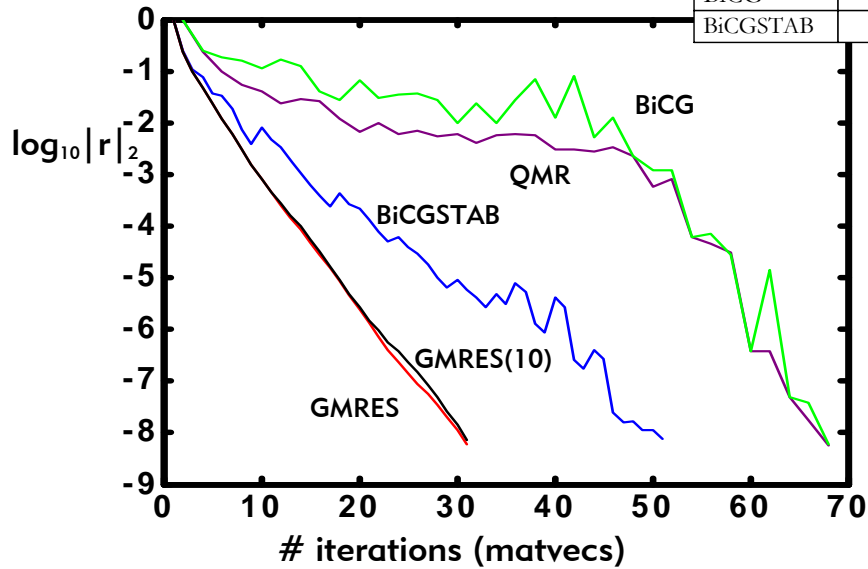




# Comparison

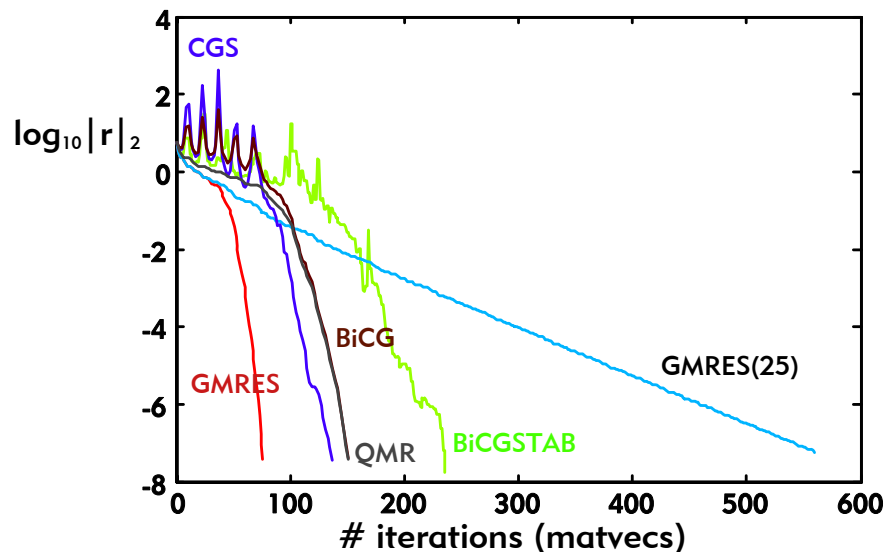
$p=q=1; r=s=70; h=1/31;$   
 $u_s = 0; u_w=0; u_n = 1; u_e = 1;$

	#matvec	time (s)
GMRES	30	3.57
GMRES(10)	40	0.5
QMR	66	0.38
BiCG	66	0.28
BiCGSTAB	50	0.33



# Hermitian Indefinite Problem

$A=\text{diag}(1,2,\dots,25,-1,-2,\dots,-5,31,32,\dots,100)$



# Early iterations

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$$A = \text{diag}(1, 2, \dots, 25, -1, -2, \dots, -5, 31, 32, \dots, 100)$$

