

# Solving large linear systems with multiple right-hand sides

Julien Langou

CERFACS – Toulouse, France.

# Motivations

In electromagnetism design, it is necessary to be able to predict the currents induced by an incident plane wave on a given object.

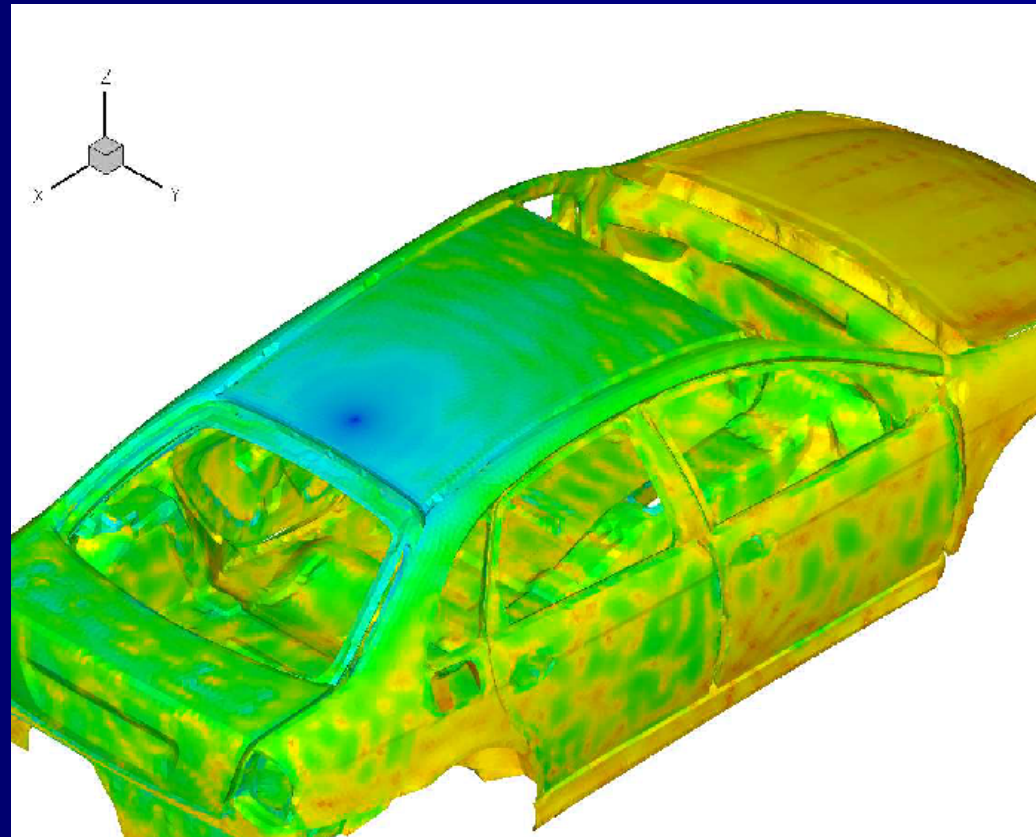
Using the boundary element method on the Maxwell equation, this amounts to solve the linear system

$$\mathbb{Z}x = b$$

where

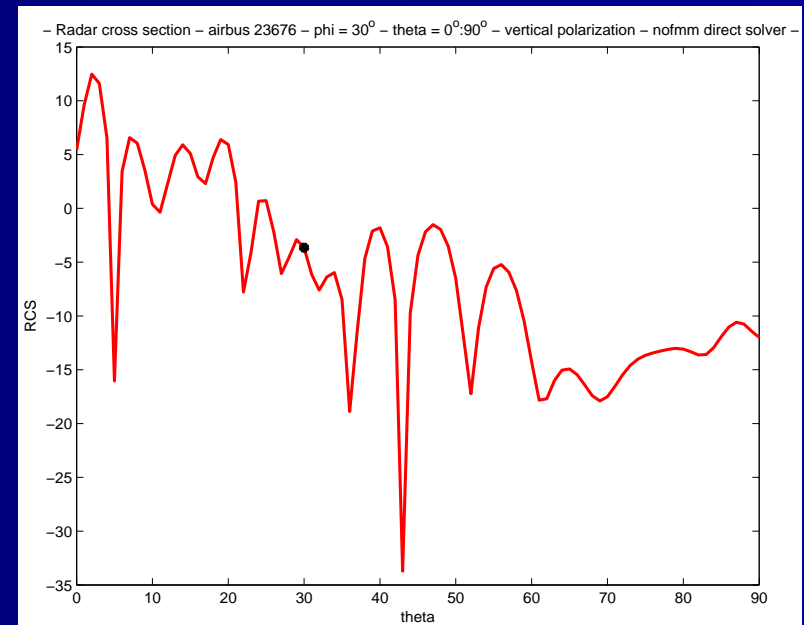
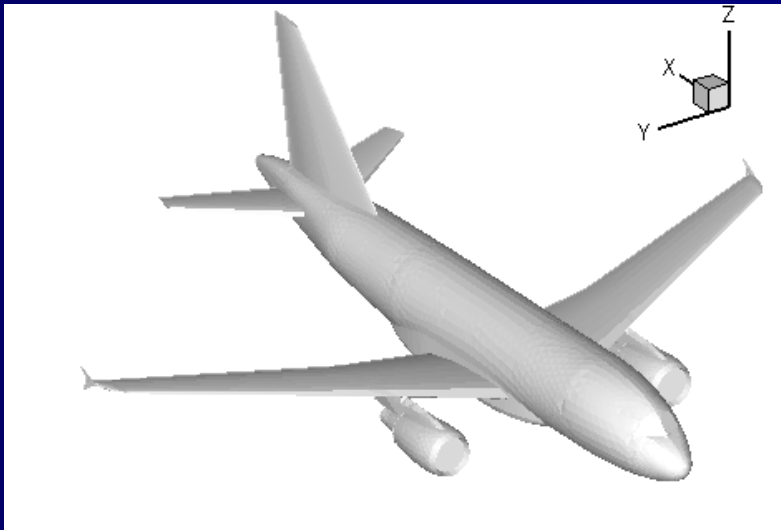
- $\mathbb{Z}$  represents the impedance of the object ( Ohm )
- $b$  represents the incident field ( Volt )
- $x$  represents the current on the object ( Ampere )

# Antenna design



Representation of the electric current due to an antenna on the Citroën C5 car.

# Monostatic radar cross section



Monostatic Radar Cross Section (RCS) for the Airbus 23676.

# Motivation

This class of problem naturally leads to

$$\mathcal{Z}(x_1, x_2, \dots, x_p) = (b_1, b_2, \dots, b_p),$$

that is to say

**solve a linear system with multiple right-hand sides.**

# Outline

- Study of the Gram–Schmidt algorithm and its variants
- Implementation of iterative methods
- The electromagnetism applications

# Study of the Gram–Schmidt algorithm and its variants

# The GMRES method

The GMRES method (Saad & Schultz '86) gives, at each step  $n$ , the approximate solution  $x_n$  that solves the least-squares problem

$$\min_{x \in \mathcal{K}_n(\mathbb{Z}, b)} \|b - \mathbb{Z}x\|_2$$

where  $\mathcal{K}_n(\mathbb{Z}, b)$  is the Krylov space

$$\mathcal{K}_n(\mathbb{Z}, b) = \text{Span}(b, \mathbb{Z}b, \mathbb{Z}^2b, \dots, \mathbb{Z}^{n-1}b).$$



# Link with QR-factorization

$$\begin{array}{ccc} (b, \mathbb{Z}V_n) & = & V_{n+1} \quad (e_1\beta, H_{n+1,n}) \\ \downarrow & & \downarrow \quad \quad \downarrow \\ A & = & Q \quad \quad R \end{array}$$

To summarize the GMRES methods needs

- a matrix–vector product operation (and also a preconditioner operation)
- an orthogonalization scheme

# Gram–Schmidt algorithm

Starting from  $\mathbf{A} = (\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{R}^{m \times n}$  with full rank, the Gram–Schmidt algorithm computes  $\mathbf{Q}$  and  $\mathbf{R}$  so as

- $\mathbf{A} = \mathbf{QR}$
- $\mathbf{Q} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}_n$
- $\mathbf{R} \in \mathbb{R}^{n \times n}$ ,  $\mathbf{R}$  is upper triangular with positive elements on the diagonal

# Gram–Schmidt algorithm



Jörgen P. Gram



Erhard Schmidt

```
for  $j = 1, n$  do  
     $\mathbf{w} = \mathbf{a}_j$   
     $\mathbf{w} = (\mathbf{I} - \mathbf{Q}_{j-1}\mathbf{Q}_{j-1}^T)\mathbf{a}_j$   
     $\mathbf{q}_j = \mathbf{w} / \|\mathbf{w}\|_2$   
end for
```

# Outline of the first part

- When modified Gram-Schmidt generates a well conditioned set of vectors
- Reorthogonalization issues: twice is enough
- Reorthogonalization issues: about selective reorthogonalization criterion
- Reorthogonalization issues: a–posteriori reorthogonalization algorithm in the modified Gram–Schmidt algorithm

# Classical/Modified

## Classical Gram–Schmidt (CGS)

```
for  $j = 1, n$  do  
     $\mathbf{w} = (\mathbf{I} - \mathbf{Q}_{j-1}\mathbf{Q}_{j-1}^T)\mathbf{a}_j$   
     $\mathbf{q}_j = \mathbf{w}/\|\mathbf{w}\|_2$   
end for
```

## Modified Gram–Schmidt (MGS)

```
for  $j = 1, n$  do  
     $\mathbf{w} = (\mathbf{I} - \mathbf{q}_{j-1}\mathbf{q}_{j-1}^T) \dots (\mathbf{I} - \mathbf{q}_1\mathbf{q}_1^T)\mathbf{a}_j$   
     $\mathbf{q}_j = \mathbf{w}/\|\mathbf{w}\|_2$   
end for
```

# An experimental fact

Let take  $A$  is the 12-by-12 Hilbert matrix with elements  $1/(i + j - 1)$

$$A = \text{hilb}(12) = \begin{pmatrix} 1 & 1/2 & 1/3 & \dots & 1/12 \\ & 1/3 & 1/4 & \dots & 1/13 \\ & & 1/5 & \dots & 1/14 \\ & & & \ddots & \vdots \\ & & & & 1/23 \end{pmatrix}.$$

It is an example of a ill-conditioned matrix, we have  $\kappa(A) = 1.68e + 16$ .

$$\|I_n - Q^T Q\|_2 = 0.302364$$

$\Rightarrow Q$  is far from being orthogonal.

# Round-off errors

Computation in floating-point arithmetic implies in general round-off error.

Standard exists to control these errors, we work here with the IEEE 754 standard

$$\text{fl}(x \text{ op } y) = (x \text{ op } y)(1 + \delta) \quad |\delta| < u$$

# Björck ('67)

$A \in \mathbb{R}^{m \times n}$  with full rank  $n \leq m$ , with singular values :

$\sigma_1 \geq \dots \geq \sigma_n > 0$ ,  $\kappa(A) = \sigma_1/\sigma_n$ ,

MGS computes  $\bar{Q}$  so as  $\|I_n - Q^T Q\|_2 = 0 \rightarrow$

$$\|I_n - \bar{Q}^T \bar{Q}\|_2 \leq \bar{c}_2 \kappa(A) u$$

where  $\bar{c}_2 = 1.5n^{\frac{3}{2}}$  and  $u$  is the unit round-off. These results hold

under the assumptions :

$$\bar{c}_2 u \kappa(\mathbf{A}) < 1.$$



# An experimental fact

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$$\|I_n - Q^T Q\|_2 = 0.302364$$

$\Rightarrow Q$  is far from being orthogonal.

However,

$$\kappa(Q) = 1.3$$

$\Rightarrow Q$  is **well conditioned**.

# Giraud Langou ('02) – IMAJNA

Let us define  $U$  the polar factor of  $\bar{Q}$  ( $U^T U = I_n$ ) then Schönemann ('66), Higham ('94) showed

$$\|\bar{Q} - U\|_2 \leq \|I - \bar{Q}^T \bar{Q}\|_2.$$

Björck ('67) showed that

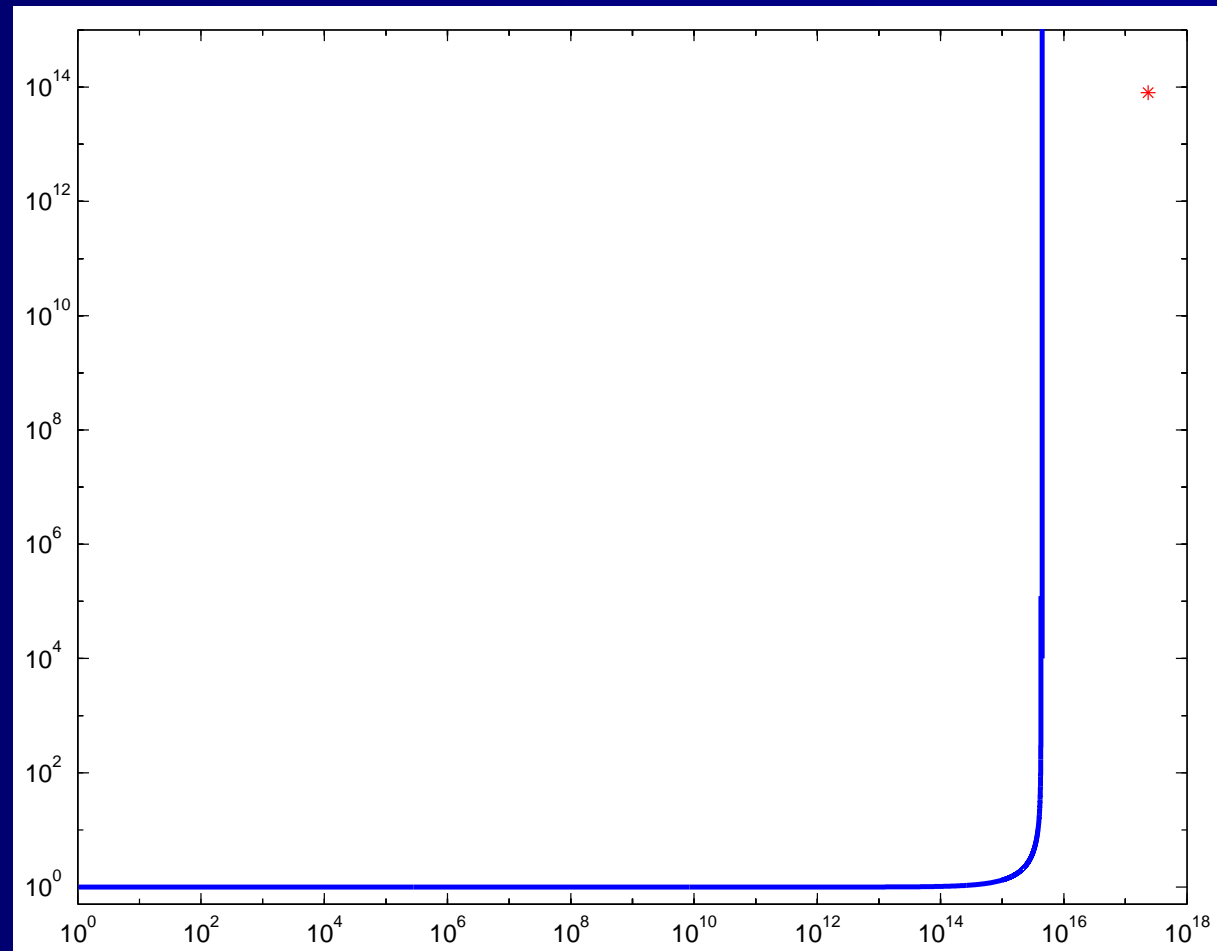
$$\|I - \bar{Q}^T \bar{Q}\|_2 \leq \bar{c}_2 \kappa(A) u.$$

This implies that

$$\kappa(\bar{Q}) \leq \frac{1 + \bar{c}_2 \kappa(A) u}{1 - \bar{c}_2 \kappa(A) u}.$$

# Giraud Langou ('02) – IMAJNA

$$\frac{1 + \bar{c}_2 u \kappa(\mathbf{A})}{1 - \bar{c}_2 u \kappa(\mathbf{A})}$$



$\kappa(A)$

# Two MGS loops

$$\begin{array}{ccccc} A & \xrightarrow{\text{MGS}} & \bar{Q}_1 & \xrightarrow{\text{MGS}} & \bar{Q}_2 \\ \bar{c}_2 u \kappa(A) \leq 0.1 & & \kappa(\bar{Q}_1) \leq 1.3 & & \|I_n - \bar{Q}_2^T \bar{Q}_2\|_2 \leq \bar{c}_2 \kappa(\bar{Q}_1) u \end{array}$$

$$cu\kappa(A) \leq 0.1 \longrightarrow \|I_n - \bar{Q}_2^T \bar{Q}_2\|_2 \leq 40.52 \cdot u \cdot n^{\frac{3}{2}}.$$

# TMGS / MGS2

$$Q^{(0)} = A$$

**for**  $r = 1, 2$  **do**

**for**  $j = 1, n$  **do**

$$w = q_j^{(r-1)}$$

**for**  $i = 1, j - 1$  **do**

$$r_{ij}^{(r)} = q_i^{(r)T} w$$

$$w = w - q_i^{(r)} r_{ij}^{(r)}$$

**end for**

$$r_{jj}^{(r)} = \|w\|_2$$

$$q_j^{(r)} = w / r_{jj}^{(r)}$$

**end for**

**end for**

$$Q = Q^{(2)}$$

$$R = R^{(2)} R^{(1)}$$

**for**  $j = 1, n$  **do**

$$w = a_j$$

**for**  $r = 1, 2$  **do**

**for**  $i = 1, j - 1$  **do**

$$r_{ij}^{(r)} = q_i^{T} w$$

$$w = w - q_i r_{ij}^{(r)}$$

**end for**

**end for**

$$r_{jj}^{(2)} = \|w\|_2$$

$$q_j = w / r_{jj}^{(2)}$$

**end for**

$$R = R^{(2)} + R^{(1)}$$

# MG S2( $K$ ), $K = 1, \infty$

**for**  $j = 1, n$  **do**

$$\mathbf{w} = \mathbf{a}_j$$

**for**  $r = 1, 2$  **do**

**for**  $i = 1, j - 1$  **do**

$$r_{ij}^{(r)} = \mathbf{q}_i^T \mathbf{w}$$

$$\mathbf{w} = \mathbf{w} - \mathbf{q}_i r_{ij}^{(r)}$$

**end for**

**if**  $\frac{\|\mathbf{a}_j\|_2}{\|\mathbf{w}\|_2} \leq K$  **then** reorthogonalize **endif**

**end for**

$$r_{jj}^{(2)} = \|\mathbf{w}\|_2$$

$$\mathbf{q}_j = \mathbf{w} / r_{jj}^{(r)}$$

**end for**

$$\mathbf{R} = \mathbf{R}^{(2)} + \mathbf{R}^{(1)}$$

# Giraud Langou Rozložník ('01)

twice is enough for CGS2 (and MGS2 as well) if  $A$  is not too ill conditioned

Sketch of the proof

For all  $j$ , we have

$$\frac{\|\mathbf{a}_j\|_2}{\|\mathbf{w}\|_2} \leq 1.1\kappa(A).$$

and then by induction on  $\|I - \bar{Q}_j^T \bar{Q}_j\|_2$ .

# Giraud and Langou ('03) – SISC

A rather commonly used criterion (Rutishauser ('67), Gander ('77), Ruhe('83), Hoffmann ('89), Dax ('00))

$$\frac{\|a_j\|_2}{\|w\|_2} \leq \sqrt{2} \Leftrightarrow \frac{\sqrt{\sum_{i=1}^{j-1} r_{ij}^2}}{r_{jj}} \leq 1 \Rightarrow \text{no proof exists ...}$$

Giraud–Langou ('03)

$$\frac{\sum_{i=1}^{j-1} |r_{ij}|}{r_{jj}} \leq 1$$

Abdelmaleck ('72) & Kielbasiński ('74)

$$\frac{\sqrt{\sum_{i=1}^{j-1} r_{ij}^2}}{\sqrt{j-1} \cdot r_{jj}} \leq 1$$

Daniel, Gragg, Kaufman and Stewart ('76)

$$\frac{\|a_j\|_2}{\|w\|_2} + \omega \frac{\|Q_{j-1}^T a_j\|_2}{\|w\|_2} \leq \sqrt{2} \text{ where } \omega \sim \|I - Q_{j-1}^T Q_{j-1}\|_2.$$



# Giraud Langou ('03) – SISC

$(K)$	$K = 1.40$	$K = 1.30$	$K = 1.17$	$K = 1.05$
matrix $B$	$B(400, 0.97)$	$B(500, 0.82)$	$B(1000, 0.50)$	$B(2500, 0.30)$
$\kappa(B)$	$3.4 \cdot 10^{15}$	$8.6 \cdot 10^{14}$	$1.8 \cdot 10^{13}$	$5.9 \cdot 10^{12}$
MGS2( $K$ )	$7.2 \cdot 10^{-1}$	$1.1 \cdot 10^0$	$1.0 \cdot 10^{-2}$	$7.6 \cdot 10^{-3}$
MGS2	$1.5 \cdot 10^{-14}$	$1.9 \cdot 10^{-14}$	$3.5 \cdot 10^{-14}$	$8.0 \cdot 10^{-14}$
CGS2( $K$ )	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$
CGS2	$1.2 \cdot 10^{-14}$	$1.5 \cdot 10^{-14}$	$2.8 \cdot 10^{-14}$	$6.0 \cdot 10^{-14}$

$$\|I_n - Q^T Q\|_2$$

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<b>CGS2</b> ( $K$ )	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$
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<b>CGS2(<math>K</math>)</b>	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$	$1.6 \cdot 10^0$
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$$\|I_n - Q^T Q\|_2$$

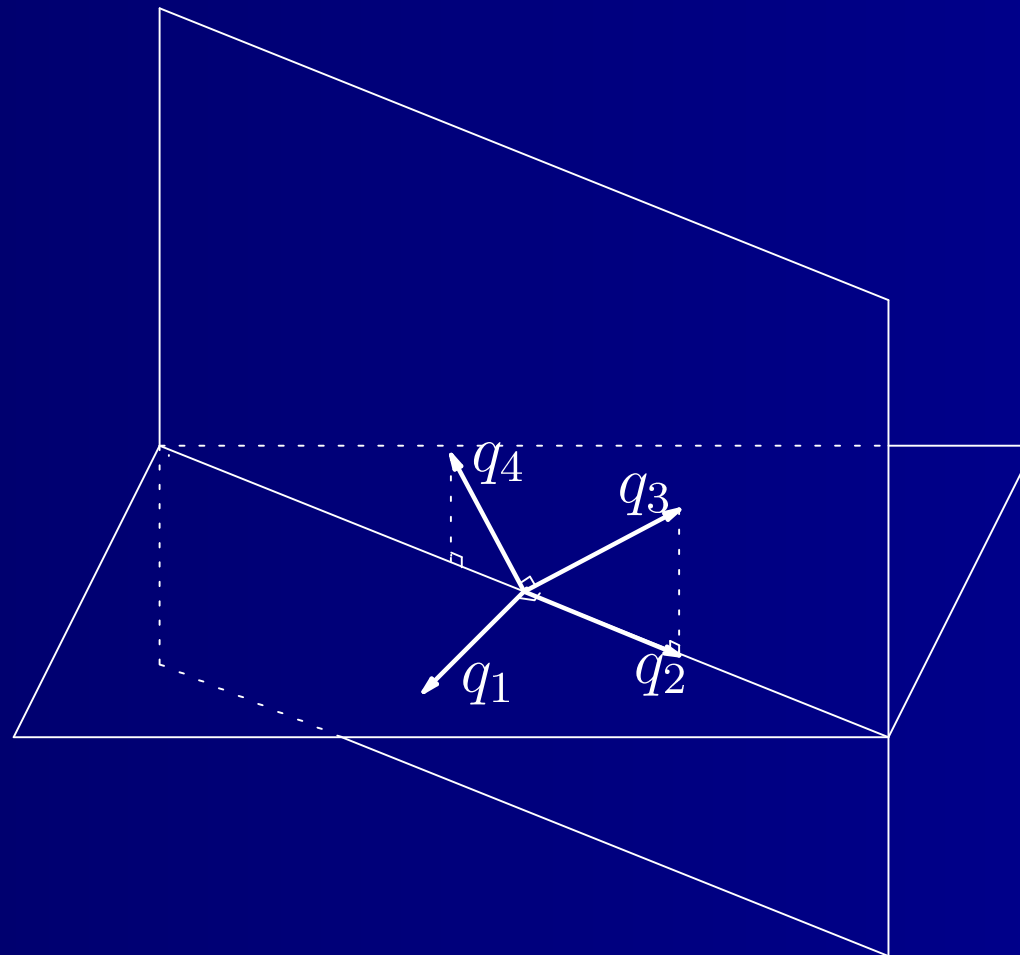
# Blindy MGS

$$A = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

*gives*

$$Q = \begin{pmatrix} 1 & 0 & 1/2 & -1/2 \\ 0 & 1 & 1/2 & -1/2 \\ 0 & 0 & \sqrt{2}/2 & \sqrt{2}/2 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{2}/2 \\ 0 & 0 & 0 & \sqrt{2}/2 \end{pmatrix}$$

# Blindy MGS



$(q_1, q_2, q_3, q_4)$  given by blindy MGS on  $A$ .

# Giraud Gratton Langou ('03)

Singular values study.

$$F = \tilde{Q} - \hat{Q}$$

under the assumption  $cu\kappa < 1$ , for all  $i = 1, \dots, n$ ,

$$\sigma_i(F) \leq 2cu \frac{\|A\|_2}{\sigma_{n-i+1}(A)}.$$

E.g.

$$\sigma_1(F) \leq 2cu \frac{\|A\|_2}{\sigma_n(A)}$$

$$\sigma_2(F) \leq 2cu \frac{\|A\|_2}{\sigma_{n-1}(A)}$$

# Proof

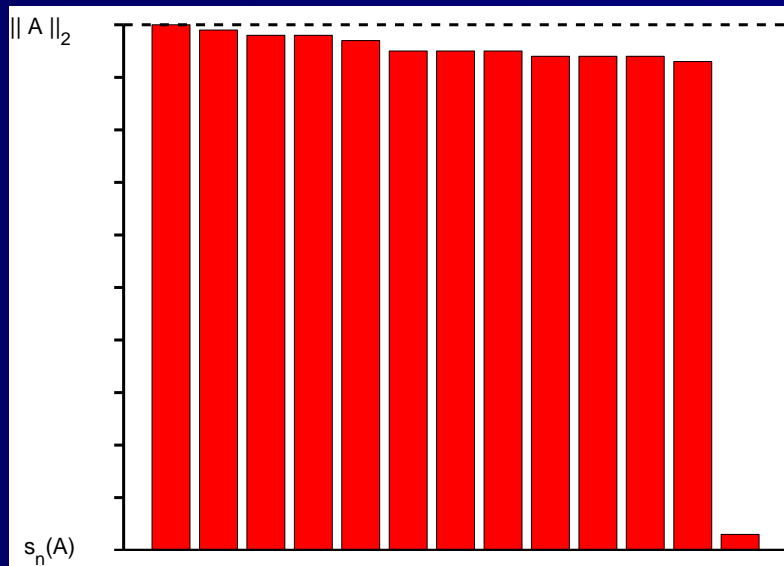
Follow **Björck and Paige ('92)** and instead of doing

$$\|AB\|_2 \leq \|A\|_2 \|B\|_2,$$

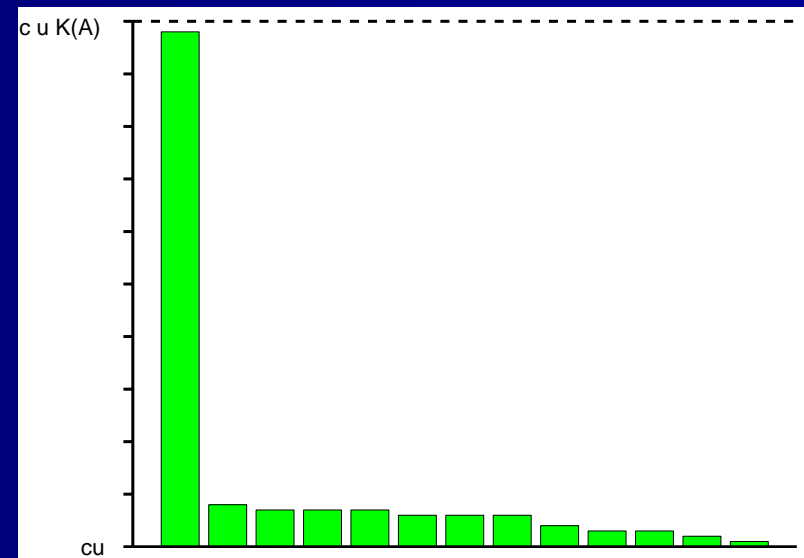
do

$$\sigma_i(AB) \leq \sigma_i(A) \|B\|_2, \quad i = 1, \dots, n.$$

# Interpretation in term of rank.



Singular values of  $A$



Singular values of  $F$



# How to find $F$ ? - the rank-1 case

- Run MGS to have  $Q$  and  $R$ .
- Form  $T$  and find its singular value decomposition such that  $T = u_T \sigma_T w_T^T$ .
- Compute  $c = \sigma + \sigma^2(w_T^T u_T)$  and  $s = \sqrt{1 - c^2}$ .
- Form  $F$  :

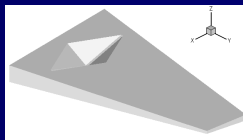
$$F = \left( \left( Q \left( w_T(1 - s^{-1}) + u_T(1 - s^{-1} - c) \right) \right) w_T^T \right).$$

**This algorithm needs  $8mn$  flops!** For comparison, we recall that a complete reorthogonalization loop costs  $2mn^2$  flops.

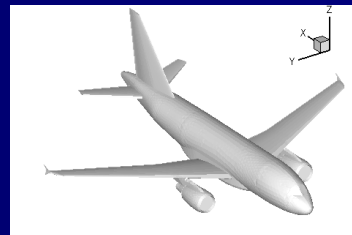
# Application to iterative methods

	$m$	# iter	$\kappa$	$\kappa_2$
Cetaf	5391	31	$9.7 \cdot 10^{14}$	27
Airbus	23676	104	$3.6 \cdot 10^{14}$	14
Sphere	40368	59	$3.9 \cdot 10^{14}$	6.4
Almond	104973	71	$5.1 \cdot 10^{14}$	5.9

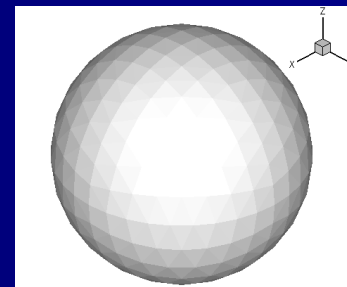
Characteristics of  $A = (b, \mathbb{Z}V_{n-1})$



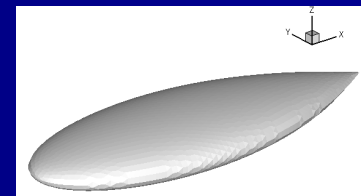
(a) cetaf



(b) airbus



(c) sphere



(d) almond

# Application to iterative methods

	MGS	MGS2( $\sqrt{2}$ )	a-posteriori reorth.
Cetaf	$2.8 \cdot 10^{-17}$	$1.8 \cdot 10^{-16}$	$2.9 \cdot 10^{-16}$
Airbus	$4.0 \cdot 10^{-17}$	$2.7 \cdot 10^{-16}$	$4.4 \cdot 10^{-16}$
Sphere	$5.8 \cdot 10^{-17}$	$1.6 \cdot 10^{-16}$	$2.7 \cdot 10^{-16}$
Almond	$3.9 \cdot 10^{-17}$	$3.9 \cdot 10^{-16}$	$2.2 \cdot 10^{-16}$

Residual errors –  $\|A - QR\|_2 / \|A\|_2$

# Application to iterative methods

	MGs	MGs2( $\sqrt{2}$ )	a-posteriori reorth.
Cetaf	$1.6 \cdot 10^{-02}$	$2.8 \cdot 10^{-16}$	$2.4 \cdot 10^{-15}$
Airbus	$1.8 \cdot 10^{-02}$	$3.7 \cdot 10^{-16}$	$1.6 \cdot 10^{-15}$
Sphere	$3.9 \cdot 10^{-02}$	$3.0 \cdot 10^{-16}$	$7.8 \cdot 10^{-16}$
Almond	$4.1 \cdot 10^{-02}$	$2.8 \cdot 10^{-16}$	$7.9 \cdot 10^{-16}$

Orthogonality –  $\|I_n - \bar{Q}^T \bar{Q}\|$

# Summary

- MGS generates a well conditioned set of vectors
- twice is enough
- a new selective reorthogonalization criterion has been exhibited
- counter example matrices for the  $K$ -criterion are given
- a new a-posteriori reorthogonalization schemes is provided

# Future work

- the singular case has not been treated (RRQR, SVD,...)
- currently, we are interested in CGS
- as well as the study of Gram–Schmidt algorithm with non Euclidean scalar product

# Implementation of iterative methods

# The electromagnetism applications



# Motivations

- Boundary element method in the Maxwell equations that leads to complex, dense and huge linear systems to solve,
  - $\mathbb{Z}J = F(\varphi)$ , where  $\varphi = 0^\circ : 1^\circ : 180^\circ$ ,
  - $\mathbb{Z}$  is accessed via matrix–vector products using the fast multipole method, a Krylov solver is used,
  - Previous work:
    - Frobenius norm minimizer preconditioner,
    - flexible GMRES solver (inner GMRES preconditioner),
    - spectral low rank update preconditioner,
- ⇒ still problematic to have a *complete* monostatic radar cross section.

# Outline of the third part

- I.* techniques to improve one right-hand side solvers for multiple right-hand sides problem,
- II.* seed-GMRES algorithm: two cases, two problems and two remedies,
- III.* linear dependencies of the right-hand sides in the electromagnetism context.

# Collaborators

This presentation uses results and codes provided by **Guillaume Alléon** **EADS**, **Guillaume Sylvand** (**INRIA(Sophia–Antipolis)–CERMICS**), **Bruno Carpentieri** and **Émeric Martin**.

**Iain S. Duff** (**CERFACS–RAL**) and **Luc Giraud** (**CERFACS**) supervise the work at CERFACS.

**Francis Collino** is also working with us.

# The single right–hand side solver

1. increase the amount of work in the preconditioner in order to increase its efficiency. In our case, for example, we can
  - 1.a. increase the density of the Frobenius norm minimizer preconditioner (**Bruno**)
  - 1.b. add a spectral low rank update that shifts the smallest eigenvalue close to one (**Émeric**)

# The single right–hand side solver

1. increase the amount of work in the preconditioner in order to increase its efficiency
2. find an initial approximate solution for the current system  $\ell$  from the previous systems solved
  - 2.a. An obvious strategy is to take

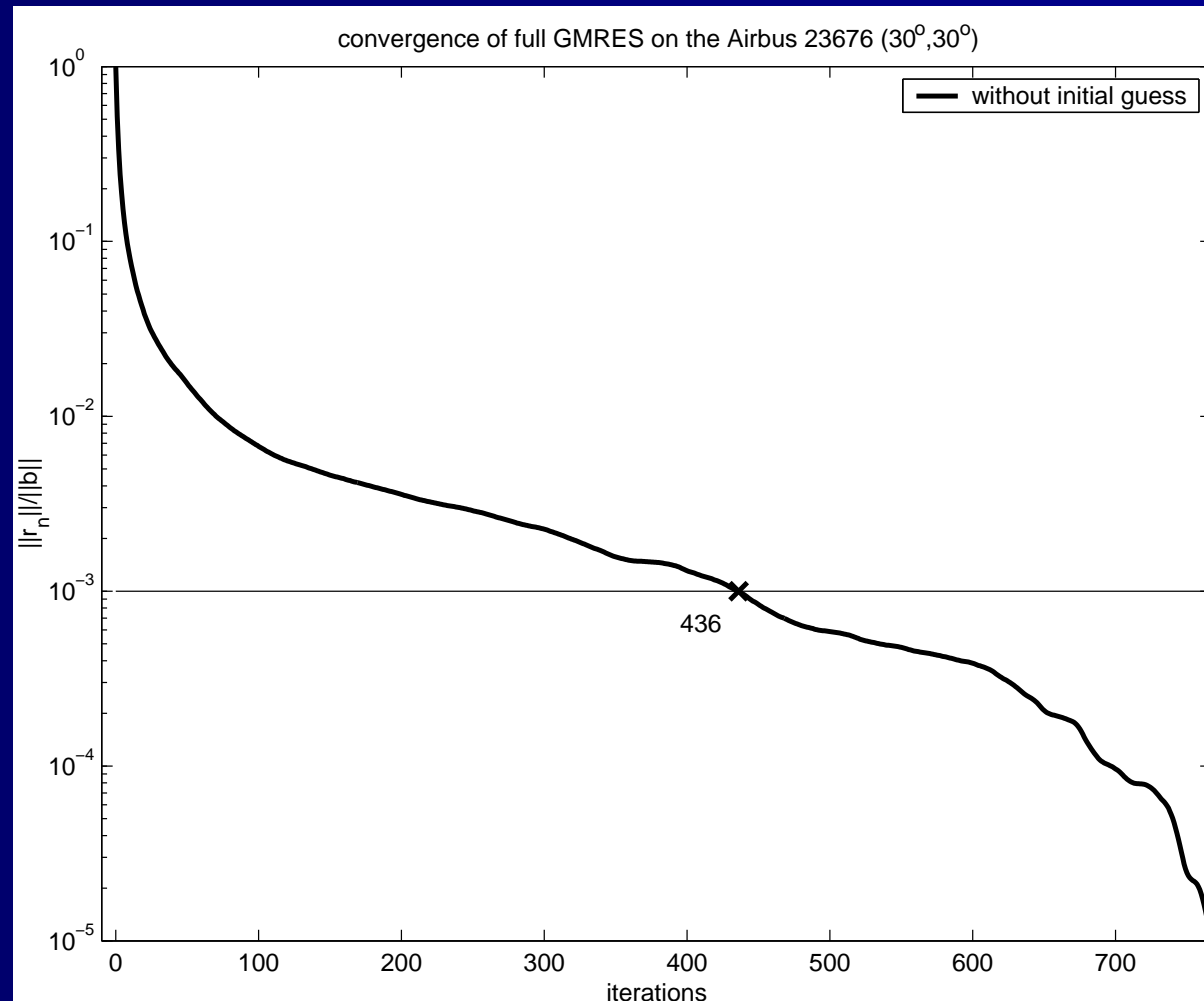
$$J^{(0)}(\varphi_\ell) = J(\varphi_{\ell-1})$$

- 2.b. Another strategy is to solve the least squares problem

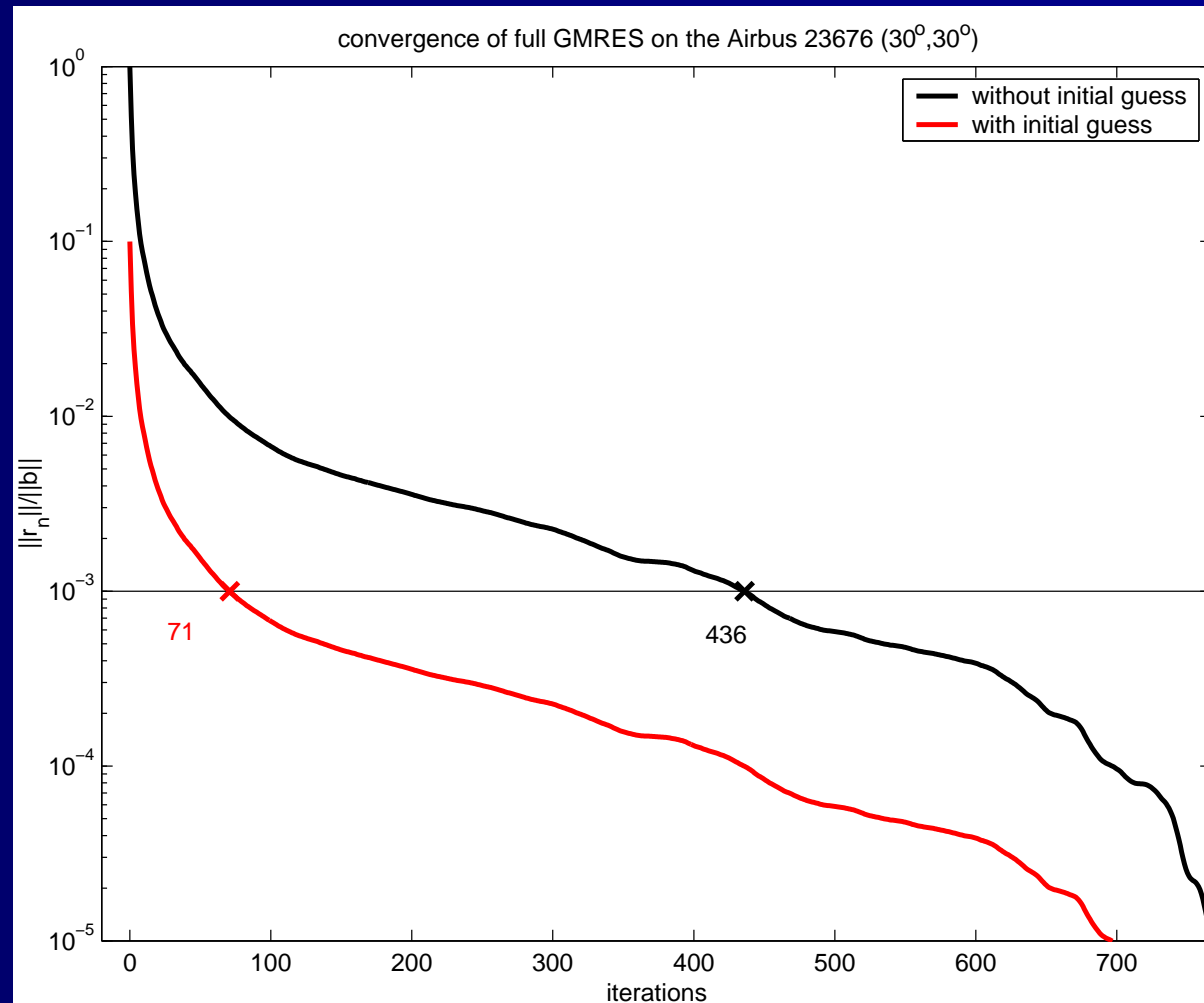
$$\min_{y \in \mathbb{R}^{\ell-1}} \left\| F(\varphi_\ell) - \sum_{j=0}^{\ell-1} F(\varphi_j) y_j \right\|_2$$

then take the initial guess  $J^{(0)}(\varphi_\ell) = \sum_{j=0}^{\ell-1} J(\varphi_j) y_j$

# The single right-hand side solver



# The single right-hand side solver



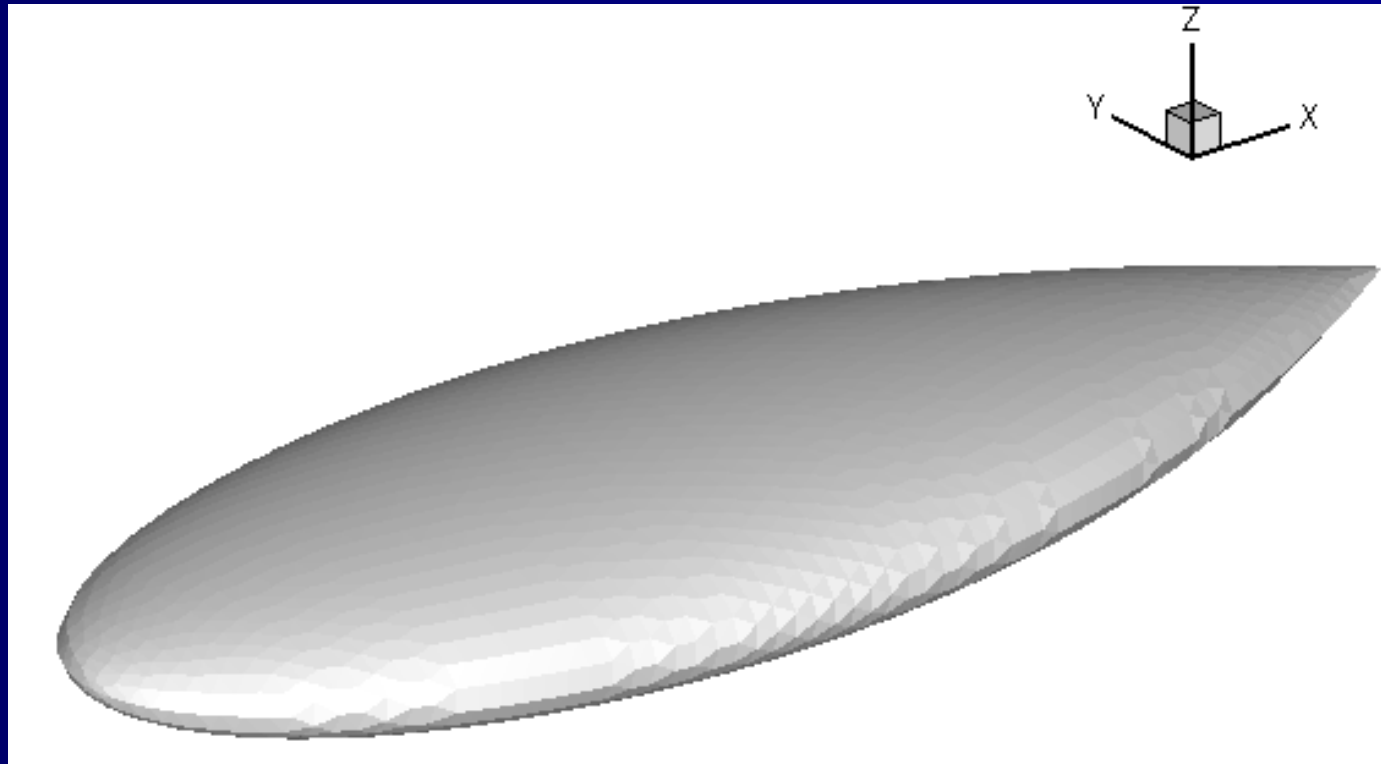
# The single right–hand side solver

1. increase the amount of work in the preconditioner in order to increase its efficiency
2. find an initial approximate solution for the current system  $\ell$  from the previous systems solved
3. gathered multiple GMRES iterations



# The almond case

A first test case: the almond 104793  $\theta = 0^\circ : 0.5^\circ : 180^\circ$  and CFIE formulation (JINA 2002)



# The almond case

	# iterations	elapse time (s)
seed-GMRES	1185	
GMRES with initial guess strategy 2	1791	

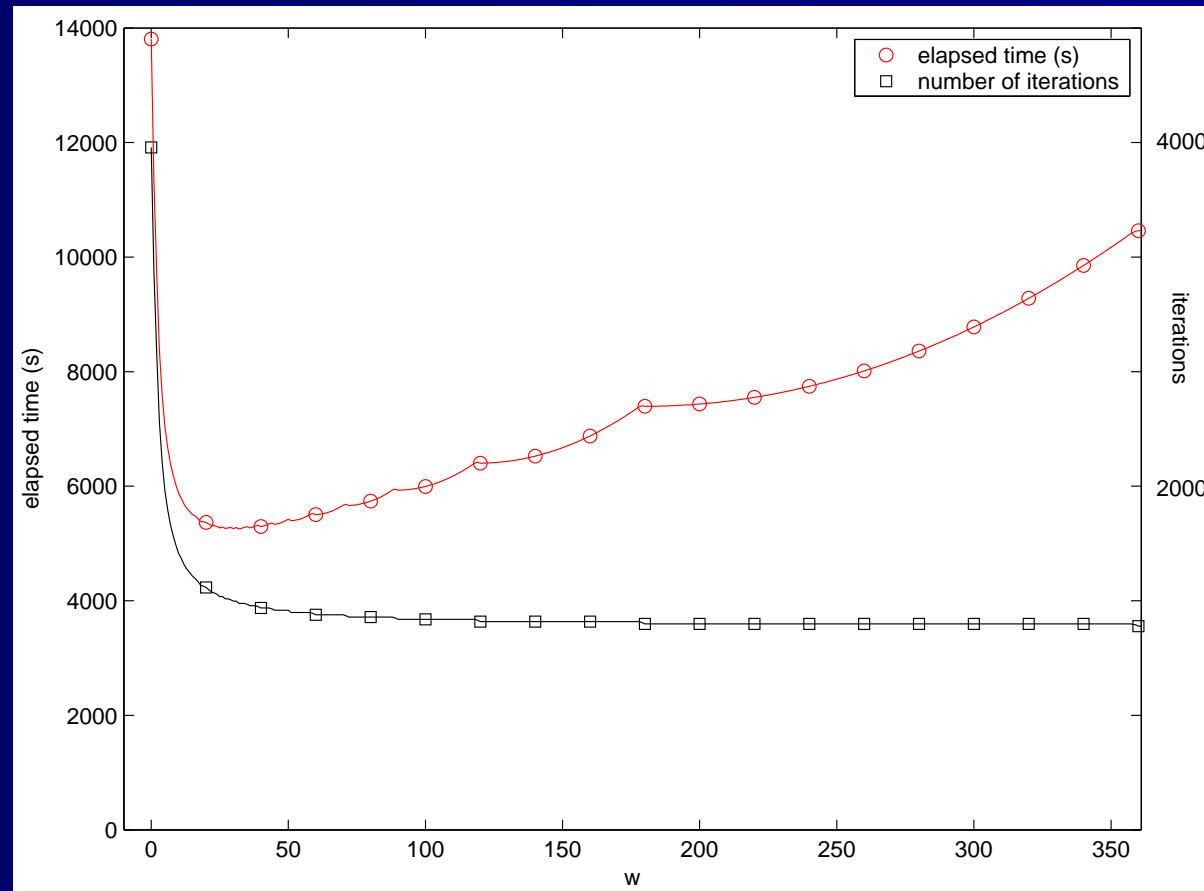
# iterations and elapsed time (s) on 8 processors  
(Compaq-CERFACS).

# The almond case

	# iterations	elapse time (s)
seed-GMRES	1185	10460
GMRES with initial guess strategy 2	1791	6202

# iterations and elapsed time (s) on 8 processors  
(Compaq-CERFACS).

# The almond case



Elapsed time and number iterations versus the size of the restart  $w$  for restart seed-GMRES.

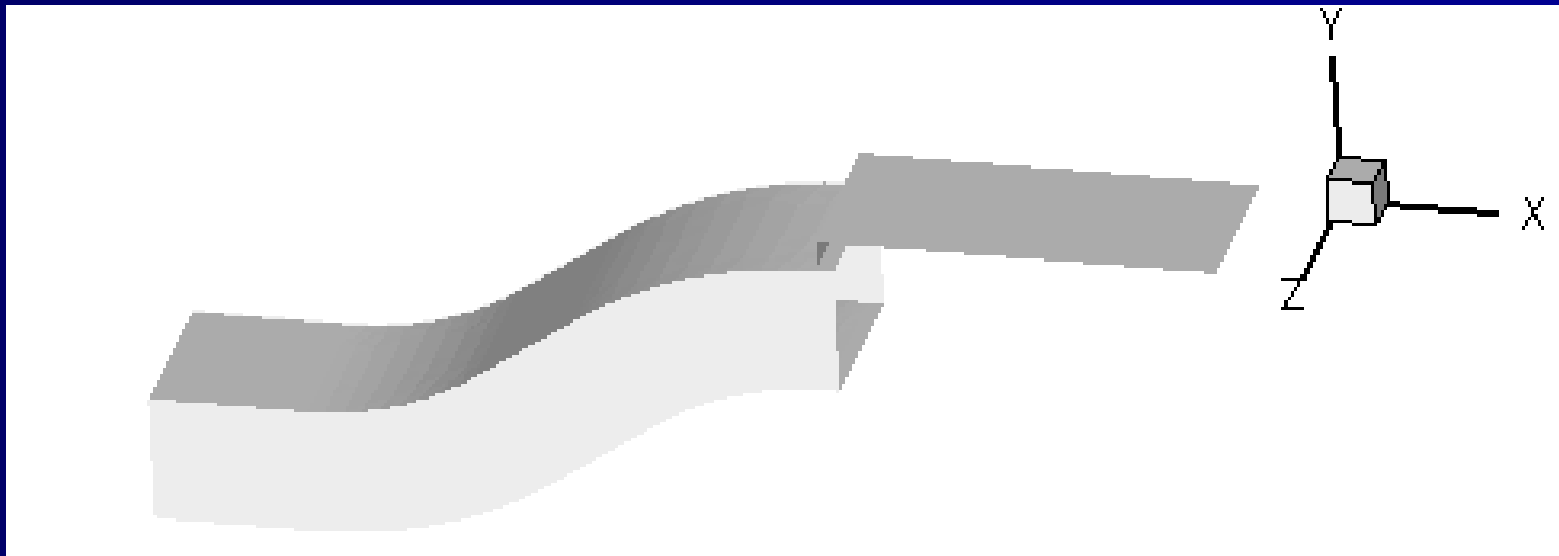
# The almond case

	# iterations	elapse time (s)
seed-GMRES	1185	10460
GMRES with initial guess strategy 2	1791	6202
seed-GMRES ( $w = 33$ )	1318	5300

# iterations and elapsed time (s) on 8 processors  
(Compaq-CERFACS).

# The cobra case

A second test case: the cobra 60695  $\theta = 0^\circ : 0.5^\circ : 180^\circ$  and EFIE formulation



# The cobra case

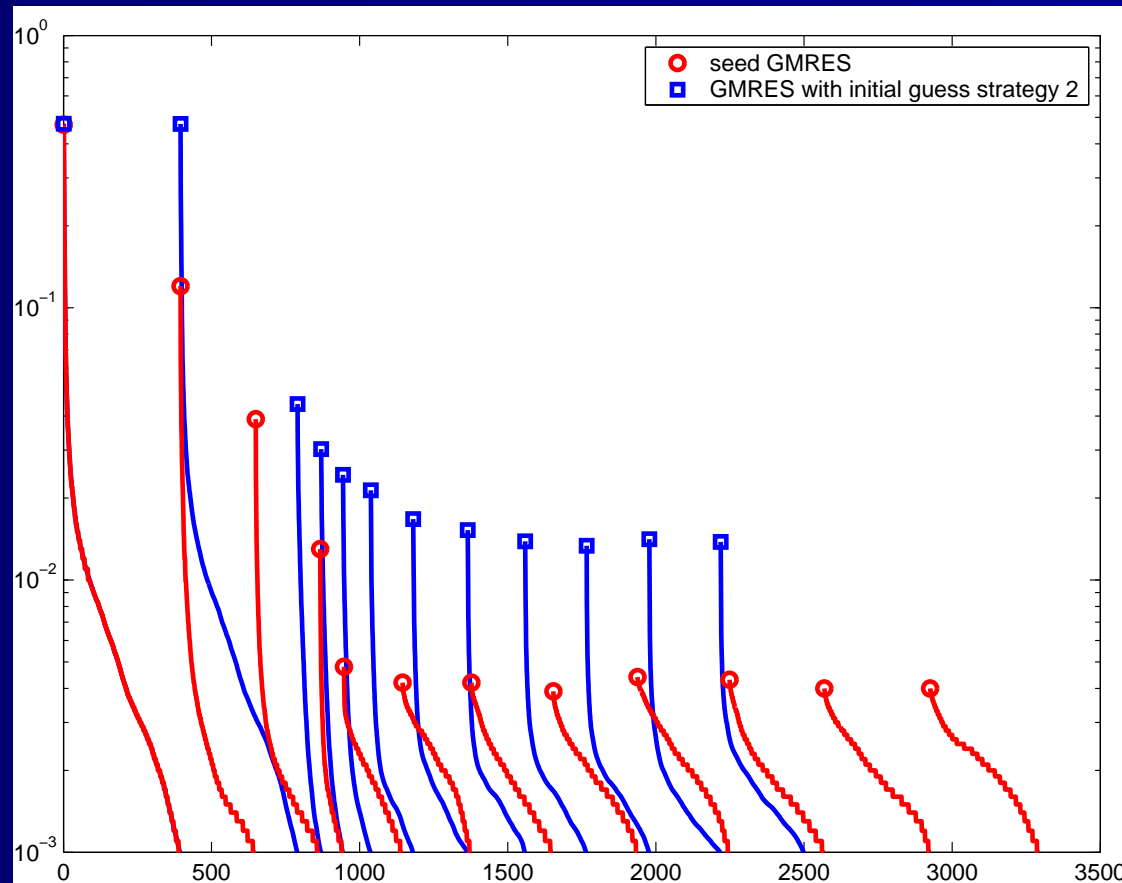
$(\theta, \varphi)$	default guess	strat. 2		seed-GMRES	
	# iter	# iter	$\ r_0\ _2/\ F\ _2$	# iter	$\ r_0\ _2/\ b\ _2$
(0.0,0.0)			1.000		1.000
(0.5,0.0)			1.000		0.230
(1.0,0.0)			0.071		0.074
(1.5,0.0)			0.048		0.024
(2.0,0.0)			0.039		0.007
(2.5,0.0)			0.037		0.004
(3.0,0.0)			0.028		0.004
(3.5,0.0)			0.028		0.004
(4.0,0.0)			0.024		0.004
(4.5,0.0)			0.022		0.004
(5.0,0.0)			0.027		0.004
(5.5,0.0)			0.022		0.004

# The cobra case

$(\theta, \varphi)$	default guess	strat. 2		seed-GMRES	
	# iter	# iter	$\ r_0\ _2/\ F\ _2$	# iter	$\ r_0\ _2/\ b\ _2$
(0.0,0.0)	338	338	1.000	338	1.000
(0.5,0.0)	339	339	1.000	190	0.230
(1.0,0.0)	340	63	0.071	210	0.074
(1.5,0.0)	341	56	0.048	130	0.024
(2.0,0.0)	341	81	0.039	197	0.007
(2.5,0.0)	341	116	0.037	215	0.004
(3.0,0.0)	342	139	0.028	237	0.004
(3.5,0.0)	342	151	0.028	226	0.004
(4.0,0.0)	343	159	0.024	254	0.004
(4.5,0.0)	344	180	0.022	258	0.004
(5.0,0.0)	345	179	0.027	265	0.004
(5.5,0.0)	346	192	0.022	299	0.004



# The cobra case



Comparison between the seed-GMRES method and the GMRES method with initial guess strategy 2.

# The cobra case

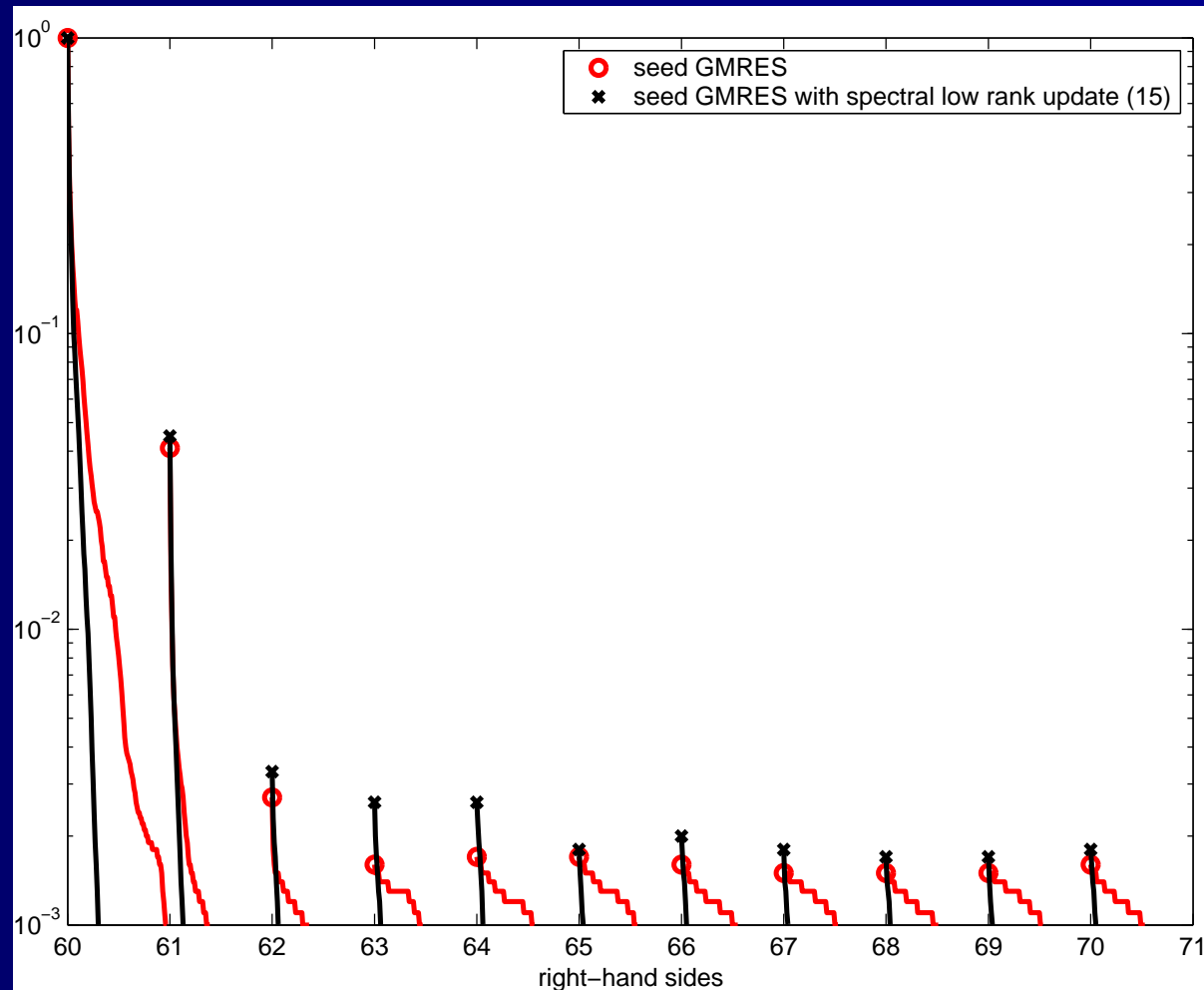
Seed moral in *le Cid*

Ô rage ! Ô désespoir ! Ô vieillesse ennemie !  
N'ai-je donc tant tant vécu que pour cette infamie ?  
Ô Anger! Ô despair! Ô enemy of age! Should I have lived so much for such infamy?

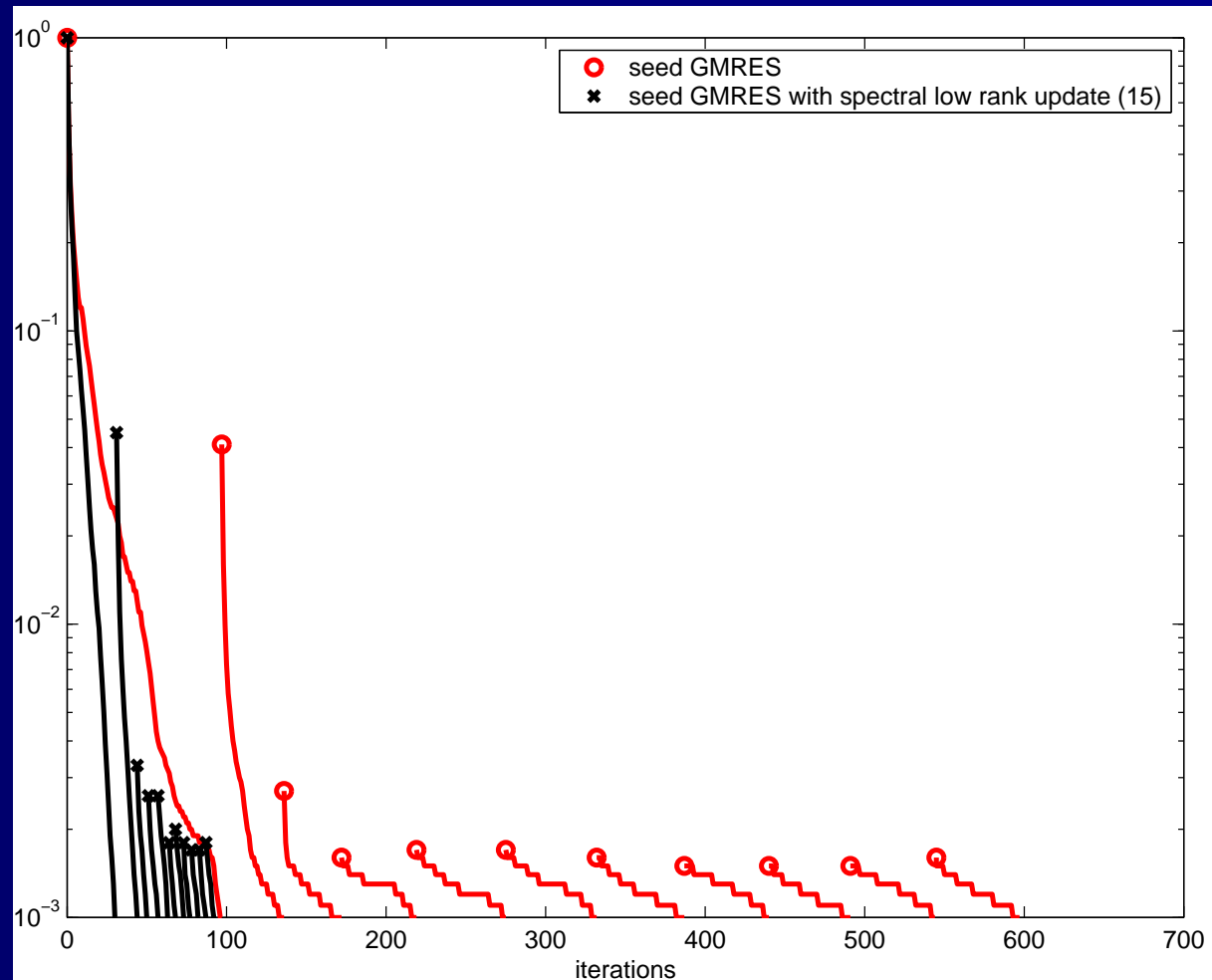


Corneille (1682), *Le Cid*.

# Seed GMRES + Spectral LRU



# Seed GMRES + Spectral LRU



# Seed GMRES + Spectral LRU

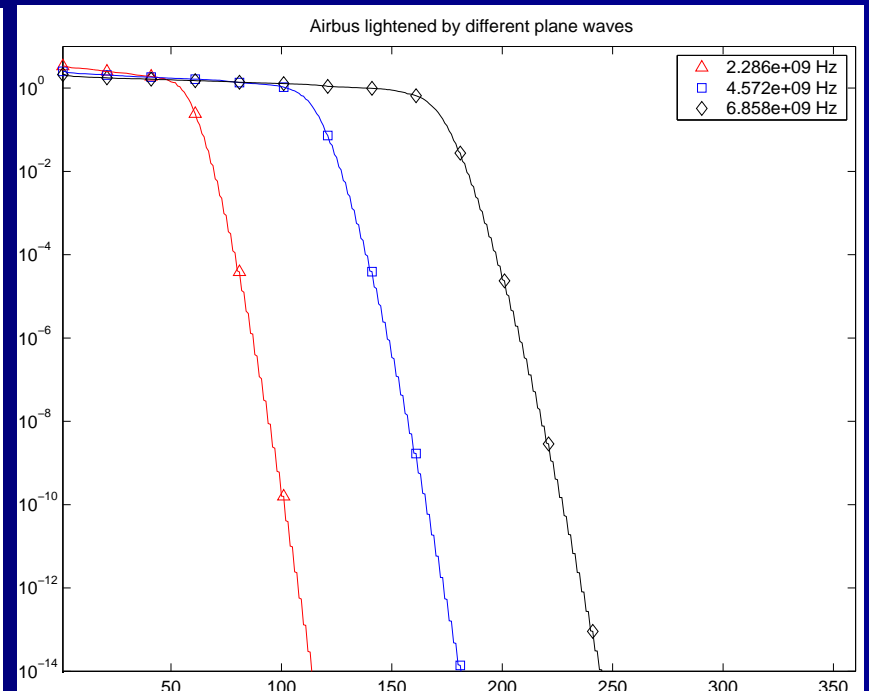
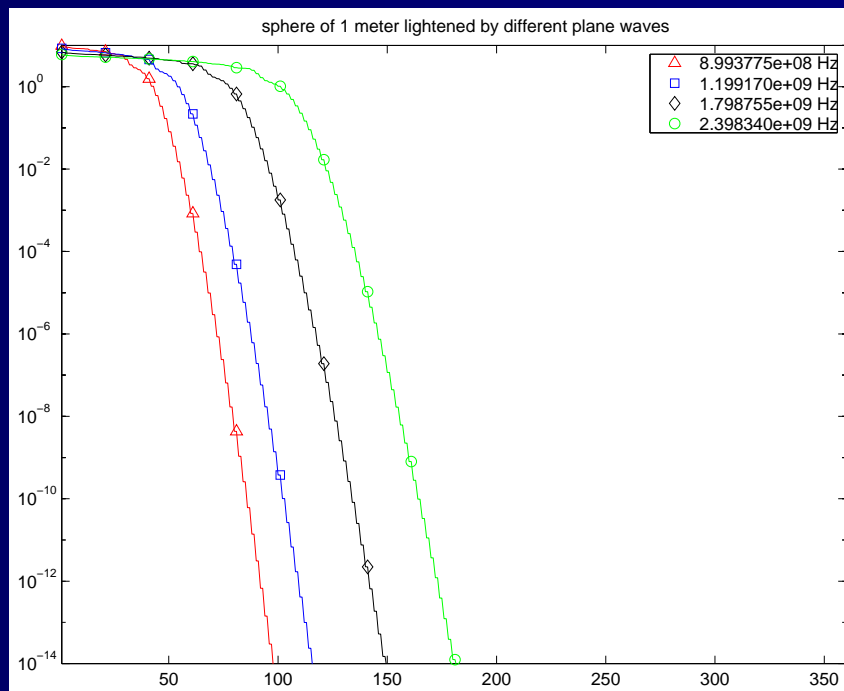
in a race starting close from the arrival  
and running fast ensures to finish first!

# Seed GMRES + Spectral LRU

in a race starting close from the arrival  
and running fast ensures to finish first!

Luc Giraud ( my thesis advisor).

# Linear dependencies RHS



Singular values distribution of  $[F(0^\circ), \dots, F(360^\circ)]$ .

# $p$ , the size in wavelengths

	dof	$F$	$\lambda$	$p$
cetaf	5391	3.0 GHz	10.0 cm	6
sphere	40368	0.9 GHz	33.3 cm	6
sphere	71148	1.2 GHz	25.0 cm	8
sphere	161472	1.8 GHz	16.7 cm	12
sphere	288300	2.4 GHz	12.5 cm	16
Airbus	23676	2.3 GHz	13.0 cm	14
Airbus	94704	4.6 GHz	6.5 cm	29
Airbus	213084	6.9 GHz	4.3 cm	44
cobra	3823	1.0 GHz	30.0 cm	2
cobra	60695	10.0 GHz	3.0 cm	24
almond	8112	0.7 GHz	42.8 cm	6
almond	104793	2.6 GHz	11.5 cm	22



# Harmonic spheric decomposition

$$M = 2(\pi p + C_\varepsilon \log(\pi p + \pi)) + 1,$$

where  $C_\varepsilon$  is such that the errors done by representing the right-hand sides in the basis of the spherical harmonic is  $10^{-C_\varepsilon}$ .

This is joint work with **Francis Collino**.

# Comparison of $M$ and $q$

	dof	$F$	$\lambda$	$p$	$M$	$q$
cetaf	5391	3.0 GHz	10.0 cm	6		
sphere	40368	0.9 GHz	33.3 cm	6		
sphere	71148	1.2 GHz	25.0 cm	8		
sphere	161472	1.8 GHz	16.7 cm	12		
sphere	288300	2.4 GHz	12.5 cm	16		
Airbus	23676	2.3 GHz	13.0 cm	14		
Airbus	94704	4.6 GHz	6.5 cm	29		
Airbus	213084	6.9 GHz	4.3 cm	44		
cobra	3823	1.0 GHz	30.0 cm	2		
cobra	60695	10.0 GHz	3.0 cm	24		
almond	8112	0.7 GHz	42.8 cm	6		
almond	104793	2.6 GHz	11.5 cm	22		

We take  $C_\varepsilon = 4$  and compute  $M$ , we compare with  $q$ , the number of singular values greater than  $10^{-4}$ .

# Comparison of $M$ and $q$

	dof	$F$	$\lambda$	$p$	$M$	$q$
cetaf	5391	3.0 GHz	10.0 cm	6		
sphere	40368	0.9 GHz	33.3 cm	6	63	60
sphere	71148	1.2 GHz	25.0 cm	8	78	76
sphere	161472	1.8 GHz	16.7 cm	12	106	104
sphere	288300	2.4 GHz	12.5 cm	16	133	130
Airbus	23676	2.3 GHz	13.0 cm	14		
Airbus	94704	4.6 GHz	6.5 cm	29		
Airbus	213084	6.9 GHz	4.3 cm	44		
cobra	3823	1.0 GHz	30.0 cm	2		
cobra	60695	10.0 GHz	3.0 cm	24		
scriptsize almond	8112	0.7 GHz	42.8 cm	6		
almond	104793	2.6 GHz	11.5 cm	22		

We take  $C_\varepsilon = 4$  and compute  $M$ , we compare with  $q$ , the number of singular values greater than  $10^{-4}$ .

# Comparison of $M$ and $q$

	dof	$F$	$\lambda$	$p$	$M$	$q$
cetaf	5391	3.0 GHz	10.0 cm	6	63	24
sphere	40368	0.9 GHz	33.3 cm	6	63	60
sphere	71148	1.2 GHz	25.0 cm	8	78	76
sphere	161472	1.8 GHz	16.7 cm	12	106	104
sphere	288300	2.4 GHz	12.5 cm	16	133	130
Airbus	23676	2.3 GHz	13.0 cm	14	120	80
Airbus	94704	4.6 GHz	6.5 cm	29	220	139
Airbus	213084	6.9 GHz	4.3 cm	44	317	198
cobra	3823	1.0 GHz	30.0 cm	2	32	17
cobra	60695	10.0 GHz	3.0 cm	24	186	68
almond	8112	0.7 GHz	42.8 cm	6	63	26
almond	104793	2.6 GHz	11.5 cm	22	133	67

We take  $C_\varepsilon = 4$  and compute  $M$ , we compare with  $q$ , the number of singular values greater than  $10^{-4}$ .

# Linear dependency of RHS

To solve the  $p$  systems

$$\mathbb{Z}J = F,$$

since we can write

$$F = US + E \quad \text{with} \quad \|E\|_2 = \sigma_{q+1},$$

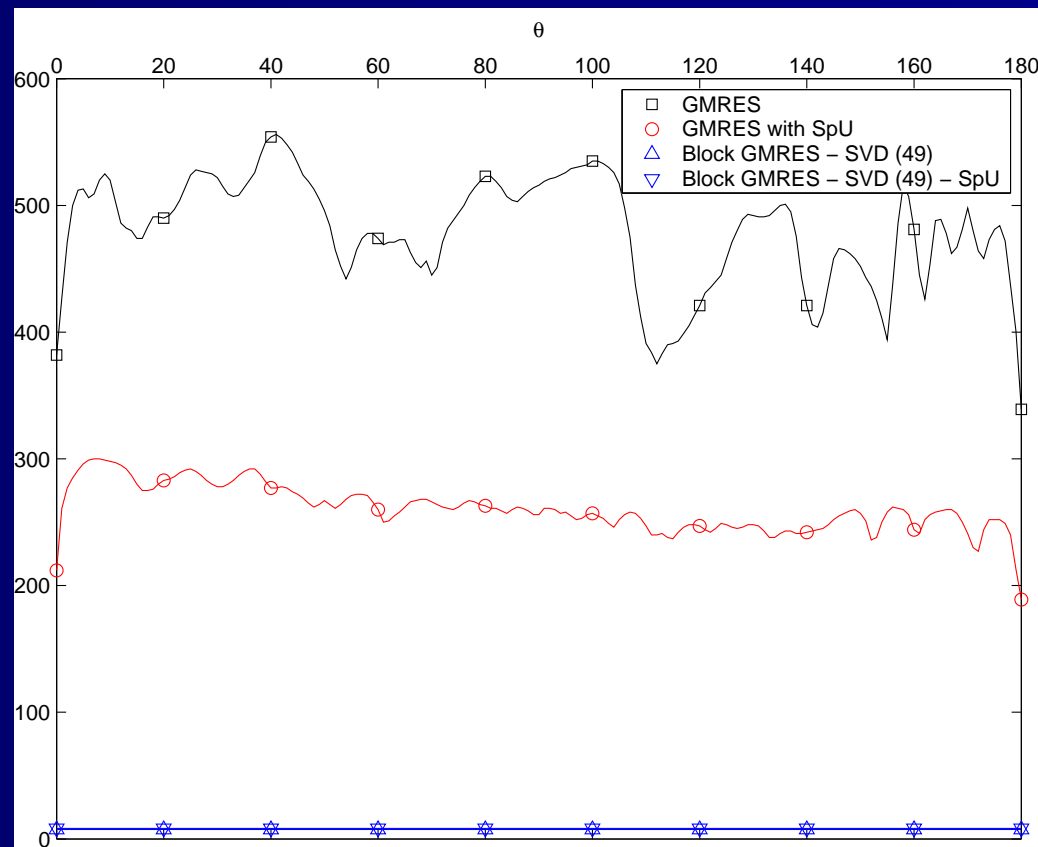
1. we solve the system with the  $q$  right-hand sides  $U$

$$\mathbb{Z}X = U$$

and then update the solutions with  $J = XS$ .

2. with block-GMRES algorithm, we minimize the right-hand sides  $F$  on the block-Krylov space constructed with  $U$ .

# On the Airbus 23676



For each right-hand sides we plot the number of iterations (matrix-vector product) required to converge. The test example is the Airbus 23676  $\theta = 0^\circ : 1^\circ : 180^\circ$ .

# Results

	DOF	# RHS	# SVD	# it	avr. # it SVD	avr. # it classic
coated cone sphere	77604	181	15	285	1.5	20
almond	104793	361	63	532	1.4	10
cobra LRU(15)	60695	91	35	1712	18.8	185
Airbus (5e-2)	94704	181	70	1430	7.9	130

# Summary

- adapting one right hand–side solver to the multiple right–hand sides case is worthy to be considered
- seed–GMRES algorithm may greatly be improved by restart or spectral low rank update
- linear dependencies of the right–hand sides is systematic in the electromagnetism context
- SVD preprocessing and use with the block–GMRES algorithm is the best method at that moment

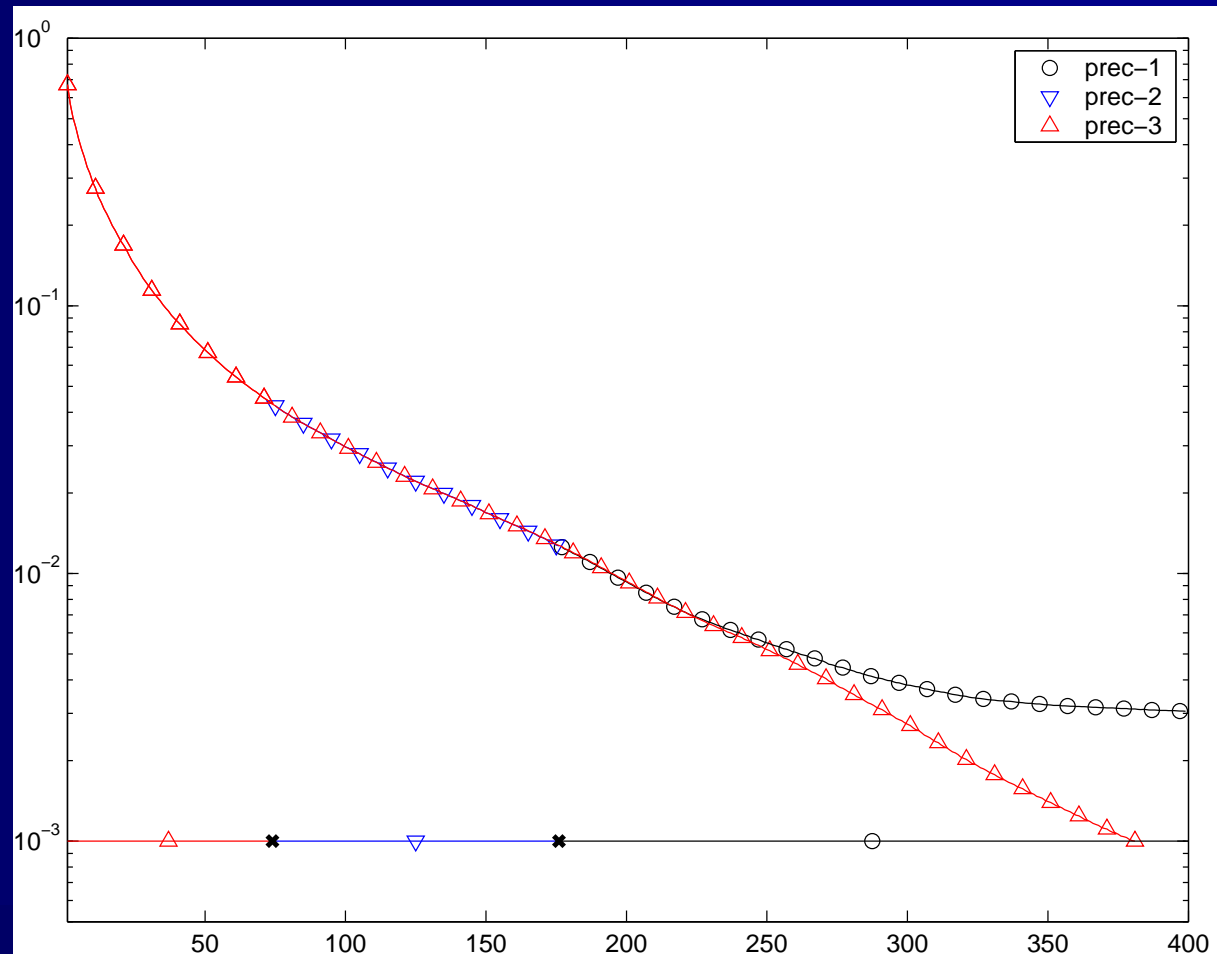


# Prospectives (1) – block/seed

- set the vectors **in-core** to gain in the orthogonalization process
- restart in block-GMRES has the same catastrophic effect (in our case) than restart in GMRES and prevents from convergence on hard cases, block-GMRES with restart and spectral low rank update is therefore tested on big test cases where full block-GMRES is not affordable anymore. Also we are thinking on how implementing **block-GMRES-DR** algorithm in the code since GMRES-DR works fine.

# Prospectives (2) – relax

Relaxing the accuracy of the matrix–vector product operation during the convergence of GMRES – Bouras, Frayssé and Giraud ('00) strategy



# Jury

Guillaume Alléon	Director of project, EADS-CCR
Åke Björck	Professor, Linköping University
Iain S. Duff	Project leader CERFACS et RAL
Luc Giraud	Senior researcher, CERFACS
Gene H. Golub	Professor, Stanford University
Gérard Meurant	Research director, CEA
Chris C. Paige	Professor, McGill University
Yousef Saad	Professor, University of Minnesota

# Study of the Gram–Schmidt algorithm and its variants

# Classical/Modified

## Classical Gram-Schmidt (CGS)

```
for  $j = 1, n$  do
   $\mathbf{w} = \mathbf{a}_j$ 
  for  $i = 1, j - 1$  do
     $r_{ij} = \mathbf{q}_i^T \mathbf{a}_j$ 
     $\mathbf{w} = \mathbf{w} - \mathbf{q}_i r_{ij}$ 
  end for
   $r_{jj} = \|\mathbf{w}\|_2$ 
   $\mathbf{q}_j = \mathbf{w} / r_{jj}$ 
end for
```

## Modified Gram-Schmidt (MGS)

```
for  $j = 1, n$  do
   $\mathbf{w} = \mathbf{a}_j$ 
  for  $i = 1, j - 1$  do
     $r_{ij} = \mathbf{q}_i^T \mathbf{w}$ 
     $\mathbf{w} = \mathbf{w} - \mathbf{q}_i r_{ij}$ 
  end for
   $r_{jj} = \|\mathbf{w}\|_2$ 
   $\mathbf{q}_j = \mathbf{w} / r_{jj}$ 
end for
```

# The Arnoldi algorithm

The Arnoldi method provides, at each step  $n$ , an orthonormal basis  $V_{n+1}$  for the Krylov space  $\mathcal{K}_n(\mathbb{Z}, b)$  that verifies

$$(b, \mathbb{Z}V_n) = V_{n+1}(e_1\beta, H_{n+1,n}).$$

So

find  $x_n \in \mathcal{K}_n(\mathbb{Z}, b)$  that minimizes  $\|b - \mathbb{Z}x\|_2$   
 $\Leftrightarrow$  find  $y_n \in \mathbb{R}^n$  that minimizes  $\|e_1\beta - H_{n+1,n}y\|_2$   
and set  $x_n = V_n y_n$ .

# Björck ('67)

$A \in \mathbb{R}^{m \times n}$  with full rank  $n \leq m$ , with singular values :  
 $\sigma_1 \geq \dots \geq \sigma_n > 0$ ,  $\kappa(A) = \sigma_1/\sigma_n$ ,  
MGS computes  $\bar{R}$  so as

$$A = QR \rightarrow$$

$$A + \bar{E} = \bar{Q}\bar{R}, \quad \|\bar{E}\|_2 \leq \bar{c}_1 u \|A\|_2$$

$$\|I_n - Q^T Q\|_2 = 0 \rightarrow$$

$$\|I_n - \bar{Q}^T \bar{Q}\|_2 \leq \bar{c}_2 \kappa(A) u$$

where  $\bar{c}_i$  are constants depending on  $m$ ,  $n$  and the details of the arithmetic, and  $u$  is the unit round-off.

# Björck ('67)

$$\bar{c}_1 = 1.5n^{\frac{3}{2}} \quad \text{and} \quad \bar{c}_2 = 31.6863n^{\frac{3}{2}}.$$

These results hold under the assumptions :

$$2.12 \cdot (m + 1) \cdot u < 0.01 \quad \text{and} \quad \bar{c}_2 u \kappa(\mathbf{A}) < 1.$$



# Gram–Schmidt algorithm

```
for  $j = 1, n$  do  
   $\mathbf{w} = \mathbf{a}_j$   
  for  $i = 1, j - 1$  do  
     $r_{ij} = \mathbf{q}_i^T \mathbf{a}_j$   
     $\mathbf{w} = \mathbf{w} - \mathbf{q}_i r_{ij}$   
  end for  
   $r_{jj} = \|\mathbf{w}\|_2$   
   $\mathbf{q}_j = \mathbf{w} / r_{jj}$   
end for
```

cost:  $2mn^2$  flops

# Unitary transformations



GRAM



SCHMIDT

VS



GIVENS



HOUSEHOLDER

# Householder & Givens

**Idea :** find a series of unitary matrix  $(Q_i)_{i=1,\dots,n}$  such that for all  $i = 1, \dots, n$ , the  $i$ -th first columns of

$$Q_i \dots Q_1 A = A_i$$

are upper triangular.

**Choice :** typically we use

Givens rotations:  $Q_i = \begin{pmatrix} \cos & -\sin \\ \sin & \cos \end{pmatrix}$ ,

Householder reflections:  $Q_i = I_m - 2z_i z_i^T$  where  $\|z_i\|_2 = 1$ .

**Cost :**  $2mn^2 - n^3/3$  for  $R$ ,  $2 \times (2mn^2 - n^3/3)$  for  $R$  and  $Q$ .

# Advantages & drawbacks

## Advantages :

- possibility to exploit the structure of  $A$  (e.g.  $A$  Hessenberg  $\longrightarrow$  Givens rotations)
- if only the  $R$  factor is needed then the number of flops is less than Gram–Schmidt algorithm
- the  $Q$  factor has columns orthonormal up to machine precision (Wilkinson, '63)

## Drawbacks :

- to obtain  $Q$  doubles the cost of the method
- the fact that unitary transformations implies a  $Q$  factor with orthonormal columns highly depends on the dot product used

# Björck and Paige ('92)

$A \in \mathbb{R}^{m \times n}$  with full rank  $n \leq m$ , with singular values :  $\sigma_1 \geq \dots \geq \sigma_n > 0$ ,  $\kappa(A) = \sigma_1/\sigma_n$ , MGS computes  $\bar{R}$  such that

$$A + \hat{E} = \hat{Q}\bar{R}, \quad \hat{Q}^T \hat{Q} = I_n \quad \text{and} \quad \|\hat{E}\|_2 \leq cu\|A\|_2,$$

where  $c = 18.53n^{\frac{3}{2}}$  and  $u$  is the unit round-off. This results holds under the assumptions  $2.12 \cdot (m + 1) \cdot u < 0.01$  and  $cuk\kappa(\mathbf{A}) < 1$ .

# Daniel and al. ('76)

Let take  $Q \in \mathbb{R}^{m \times n}$  such that

$$\|I_n - Q^T Q\|_2 = 10^{-3} \quad (\text{e.g.})$$

and  $w^{(0)} \in \mathbb{R}^m$ , we consider the serie of vectors  $(w^{(i)})$

$$w^{(i)} = (I_n - QQ^T)w^{(i-1)}.$$

Then Daniel and al. showed that

$$\|Q^T w^{(i)}\|_2 / \|w^{(i)}\|_2 \leq \xi_i,$$

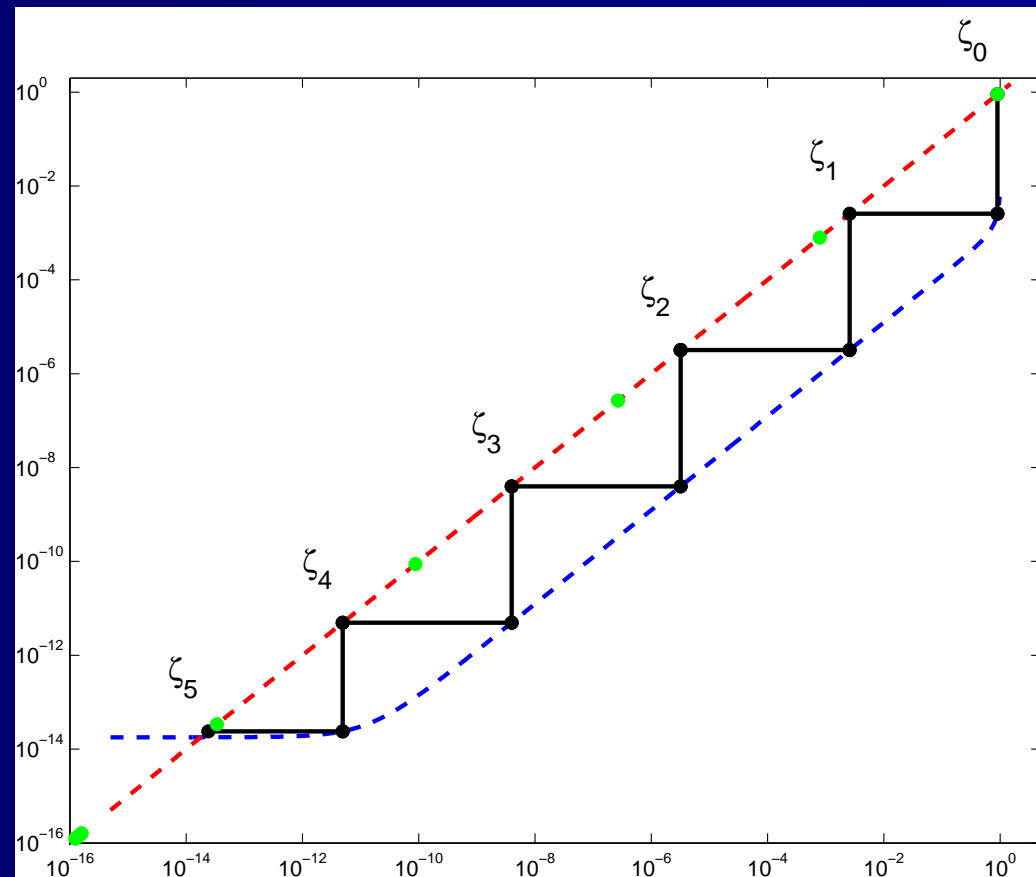
where  $\xi_i$  is defined via

$$\xi_0 = \|Q^T w^{(0)}\|_2 / \|w^{(0)}\|_2 = 10^0 \quad (\text{e.g.})$$

$$\xi_i = \varphi(\xi_{i-1}), \quad i = 1, \dots$$

# Giraud, Langou and Rozložník ('0

$$\|I - Q^T Q\|_2 = 10^{-3}, \quad \xi_0 = \|Q^T w^{(0)}\|_2 / \|w^{(0)}\|_2 = 10^0$$



- $\|Q^T w^{(i)}\|_2 / \|w^{(i)}\|_2$ , -  $y = \varphi(x)$ , -  $y = x$ , •  $\xi_i$

# How to find $F$ ?

$$\begin{aligned} F &= Q - \hat{Q}, \\ &= P_{21}(I - T) - \hat{Q}, \\ &= U_2(S - I)W^T - P_{21}T, \\ &\sim U_{2k}(S_k - I)W_k^T - P_{21}(U_{Tk}\Sigma_{Tk}W_{Tk}^T). \end{aligned}$$

We have expressed  $F$  as a sum of to low rank matrix of rank  $k$ . The choice of  $k$  is a compromise between **accuracy** and **efficiency**.



# 2D case

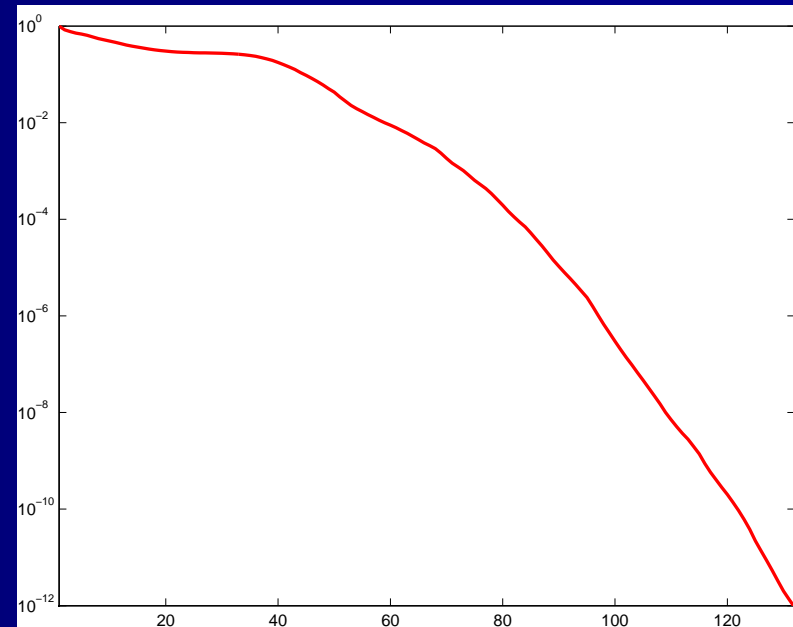


GOLDORAK ( $n = 715$  ,  $\kappa(A) = 546$ ).

# 2D case

We run full GMRES with MGS without preconditionner and a right-hand side corresponding to an incident wave at  $0^\circ$ .  
The tolerance is fixed to  $10^{-12}$ .

$$- \|r_m\|_2 / \|b\|_2$$



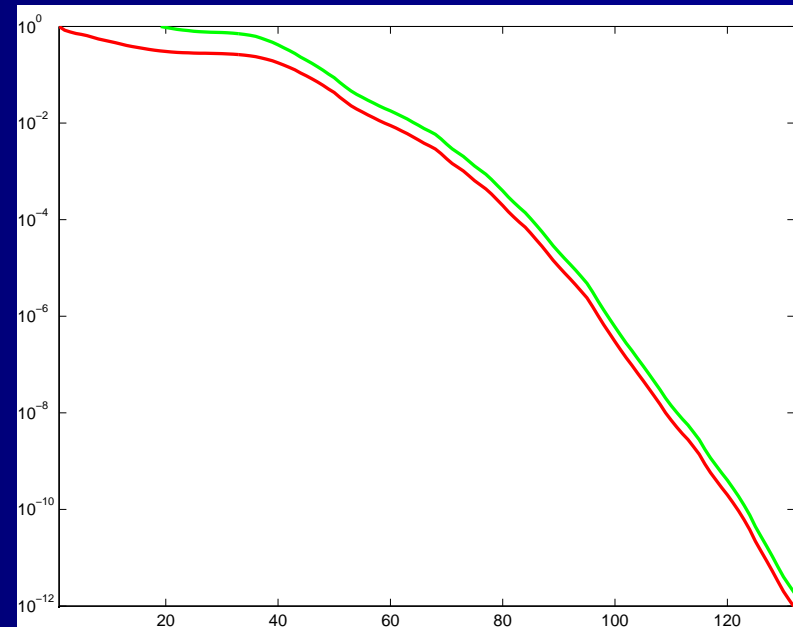
# 2D example

From Greenbaum, Rozložník and Strakoš ('97) we know that

$$\|r_m\|_2 \sim \sigma_{\min}(v_0, AV_m)$$

-  $\|r_m\|_2 / \|b\|_2$

-  $\sigma_{\min}(v_0, AV_m) / \sigma_{\min}(A)$



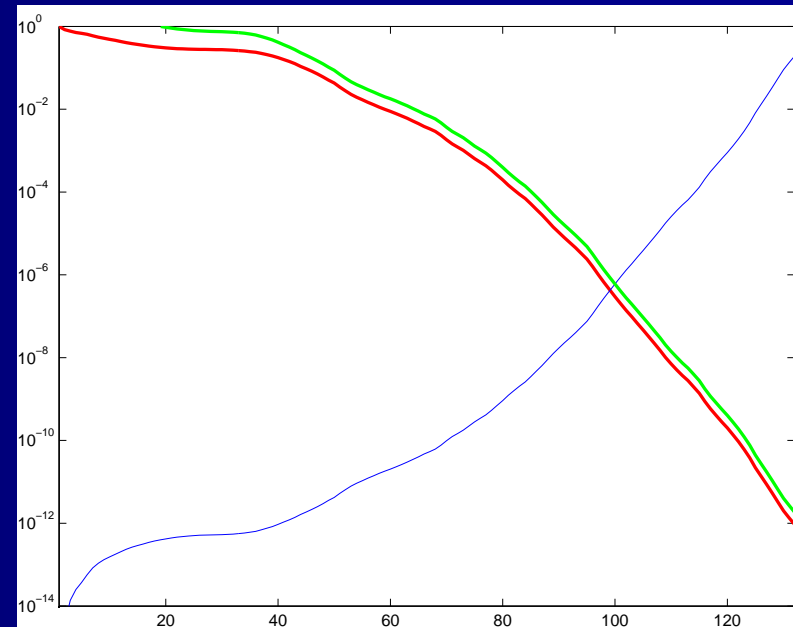
# 2D example

so from Björck (1967) we can check that the loss of orthogonality is proportionnal to  $1/\|r_m\|_2$ .

$$- \|r_m\|_2 / \|b\|_2$$

$$- \sigma_{\min}(v_0, AV_m) / \sigma_{\min}(A)$$

$$- \|I - V_m^T V_m\|_2$$



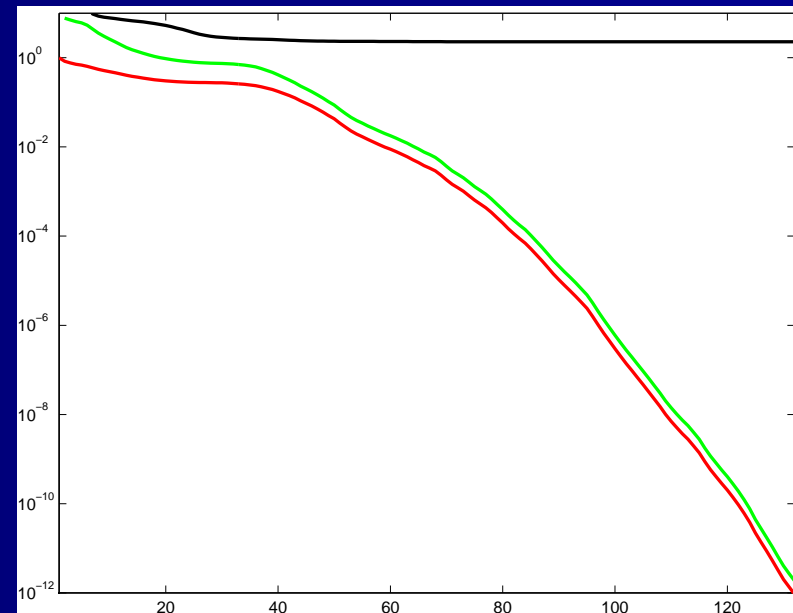
# 2D example

As  $AV_m = V_m \bar{H}_m$ ,  $V_m$  and  $A$  are well-conditioned, we deduced that the second smallest singular value of  $(v_0, AV_m)$  is reasonably big.

$$- \|r_m\|_2 / \|b\|_2$$

$$- \sigma_{m+1}(v_0, AV_m) / \sigma_{\min}(A)$$

$$- \frac{\sigma_m(v_0, AV_m)}{\sigma_{\min}(A)}$$



# LLS problems with multiple RHS

with MGS

$$\begin{pmatrix} v_1^T b^{(i)} \\ v_2^T (I_m - v_1 v_1^T) b^{(i)} \\ \vdots \\ v_n^T (I_m - v_{n-1} v_{n-1}^T) \cdots (I_m - v_1 v_1^T) b^{(i)} \end{pmatrix}$$

when using an orthonormal basis  $Q$

$$\begin{pmatrix} q_1^T b^{(i)} \\ q_2^T b^{(i)} \\ \vdots \\ q_n^T b^{(i)} \end{pmatrix}$$

# Application to iterative methods

	MGS2( $\sqrt{2}$ )	MGS2(2)	MGS2( $\sqrt{5}$ )
Cetaf	$2.8 \cdot 10^{-16}$ ( $\nu = 2.00$ )	$6.3 \cdot 10^{-16}$ ( $\nu = 1.90$ )	$1.2 \cdot 10^{-15}$ ( $\nu = 1.87$ )
Airbus	$3.7 \cdot 10^{-16}$ ( $\nu = 2.00$ )	$3.9 \cdot 10^{-03}$ ( $\nu = 1.02$ )	$8.8 \cdot 10^{-03}$ ( $\nu = 1.01$ )
Sphere	$3.0 \cdot 10^{-16}$ ( $\nu = 2.00$ )	$7.5 \cdot 10^{-15}$ ( $\nu = 1.52$ )	$4.9 \cdot 10^{-04}$ ( $\nu = 1.07$ )
Almond	$2.8 \cdot 10^{-16}$ ( $\nu = 2.00$ )	$1.7 \cdot 10^{-03}$ ( $\nu = 1.06$ )	$5.2 \cdot 10^{-03}$ ( $\nu = 1.03$ )

$$\|I_n - \bar{Q}^T \bar{Q}\| .$$

# Implementation of iterative methods



# Outline

- GMRES–DR
- seed–GMRES
- block–GMRES

# GMRES-DR

$$V_{k+1}^{\text{new}} \longleftarrow V_{n+1}P_{k+1},$$

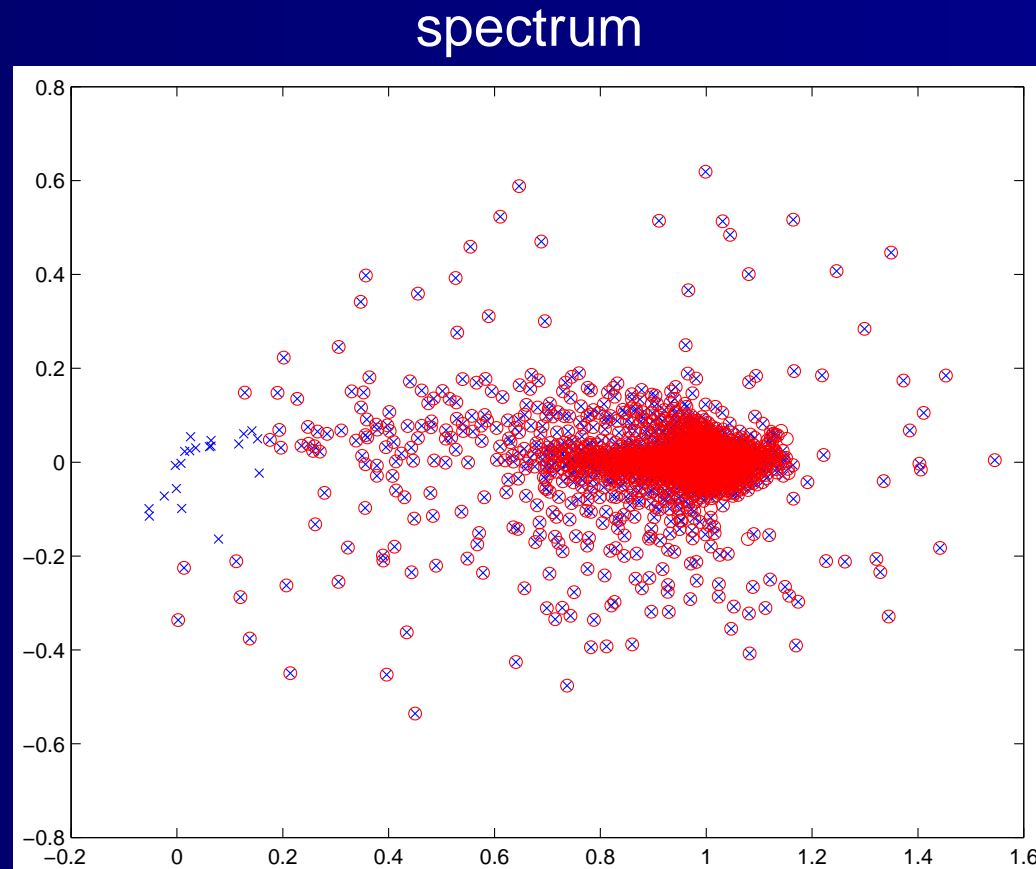
need  $n + k + 2$  vectors of size  $m$ . whereas if we first perform the LU decomposition of  $P_{k+1}$  and then do

$$V_{k+1}^{\text{new}} \longleftarrow (V_{n+1}L)U$$

; we only need  $n + 1$  vectors.

# The electromagnetism applications

# One right-hand side solvers



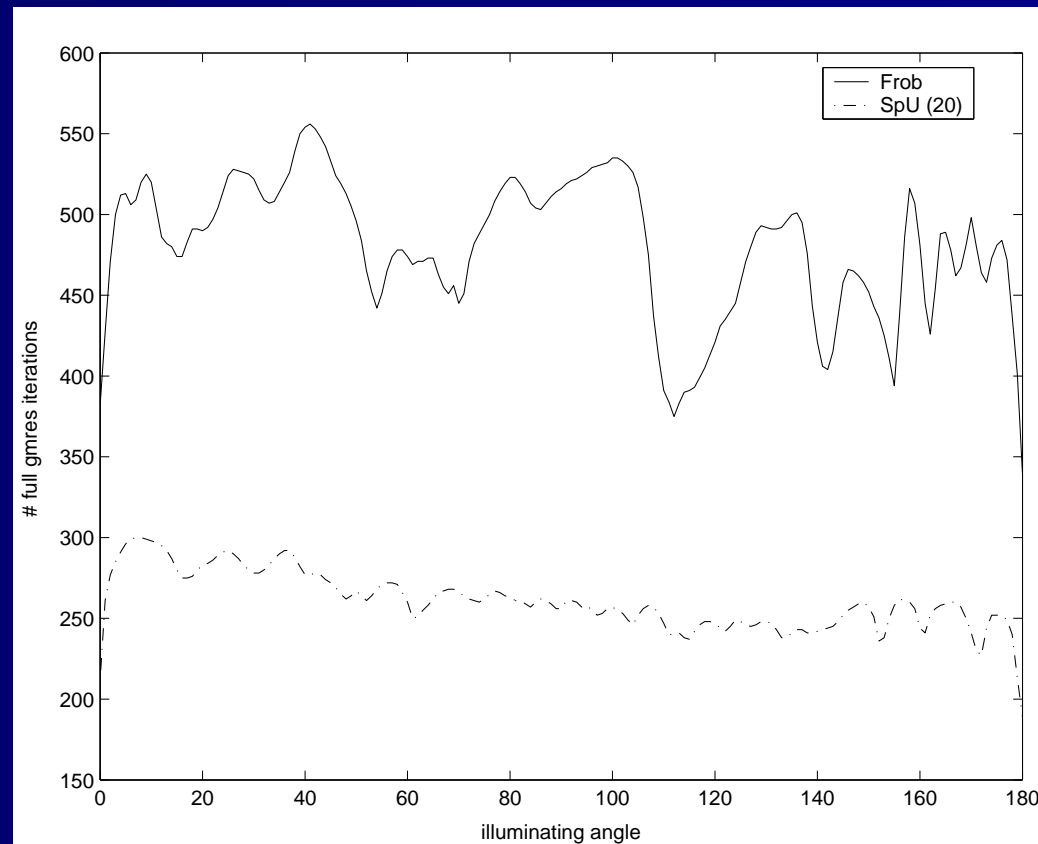
- × Cetaf preconditioned with “default” Frobenius norm minimizer preconditioner
- Cetaf preconditioned with “default” Frobenius norm min-

# One right-hand side solvers

	assembly			application			# procs
	FMM	Frob	SLRU	FMM	Frob	SLRU	
cetaf 5391	9.6	631.8	3.7 (20)	0.25	0.11	0.02 (20)	4
Airbus 23676	114.8	184.8	36.7 (20)	1.86	0.29	0.03 (20)	4
cobra 60695	33.3	120.2	30.6 (15)	1.93	0.22	0.03 (15)	8
almond104793	53.1	345.8	182.8 (60)	2.92	0.41	0.10 (60)	8
almond104793	53.1	345.8	59.3 (20)	2.92	0.41	0.05 (20)	8

Time of assembly and application of the FMM (prec-3), the Frobenius preconditioner and the spectral update (the number of shifted eigenvalues is given in bracket).

# One right-hand side solvers



Airbus 23676

# Gathered multiple GMRES

	unitary FMM (s)	unitary Precond (s)	# FMM &Precond	total
gathered GMRES (10)	0.7	0.05	180	205.1
GMRES with zero as initial guess	1.8	0.27	177	401.4

(a) Airbus 23676.

	unitary FMM (s)	unitary Precond (s)	# FMM &Precond	total
GMRES gathered (19)	1.6	0.13	931	2340.8
GMRES with strategy 2 for the initial guess	7.1	0.42	856	7703.2

(b) coated cone sphere 77604.

# The seed GMRES algorithm (1)

We first run GMRES to solve the linear system  $\mathbb{Z}J(\varphi_0) = F(\varphi_0)$ . This amounts to solving the linear least squares problem

$$\min_{J \in \mathcal{K}_0} \|F(\varphi_0) - \mathbb{Z}J\|_2,$$

where  $\mathcal{K}_0$  is the Krylov space of size  $n$  built with an Arnoldi process on  $\mathbb{Z}$  using the starting vector  $F(\varphi_0)$ .

In most applications, the computational burden lies in the matrix–vector products and the scalar products required to solve this linear least squares problem.

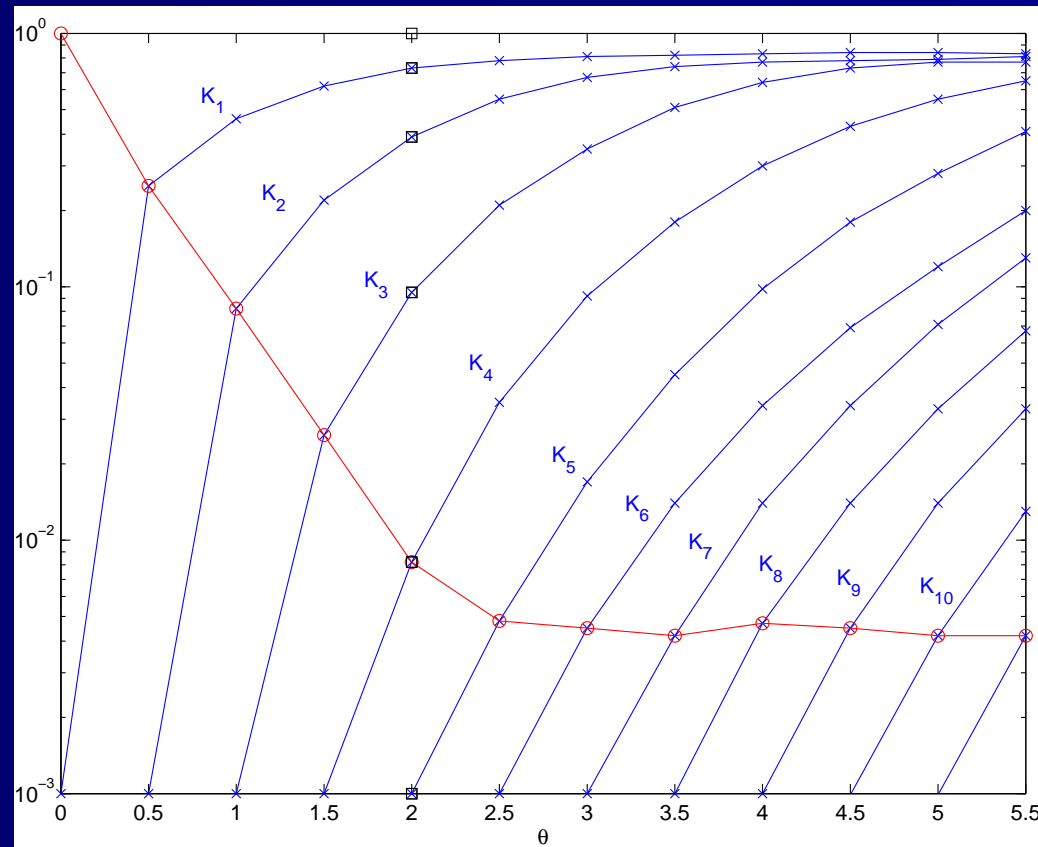
In seed–GMRES, the subsequent right–hand sides benefit from this work. An effective initial guess  $J^{(0)}(\varphi_\ell) = V_n^{(0)} y^{(\ell)}$  for the system  $\ell$  is obtained by solving the same linear least squares problem but with another right–hand side, namely

$$\min_{J \in \mathcal{K}_0} \|F(\varphi_\ell) - \mathbb{Z}J\|_2.$$

The additional cost is  $n$  dot products and  $2n$  zaxpy operations per right–hand sides.



# The seed GMRES algorithm (2)



Norm of the residuals after each minimization on the Krylov spaces. The test example is the cobra 60695,  $\theta = 0^\circ : 0.5^\circ : 5.5^\circ$ .

# The almond case

Starting the seed-GMRES method from the right-hand side  $F(\theta = 0^\circ)$ , we obtain the following sequence for the number of iterations for the first 15 right-hand sides:

$\theta$	$0^\circ$	$0.5^\circ$	$1^\circ$	$1.5^\circ$	$2^\circ$	$2.5^\circ$	$3^\circ$	$3.5^\circ$	$4^\circ$	$4.5^\circ$	$5^\circ$	$5.5^\circ$	$6^\circ$
# iter	11	7	5	3	3	3	3	2	3	3	2	3	2

# The almond case

Starting the seed-GMRES method from the right-hand side  $F(\theta = 0^\circ)$ , we obtain the following sequence for the number of iterations for the first 15 right-hand sides:

$\theta$	$0^\circ$	$0.5^\circ$	$1^\circ$	$1.5^\circ$	$2^\circ$	$2.5^\circ$	$3^\circ$	$3.5^\circ$	$4^\circ$	$4.5^\circ$	$5^\circ$	$5.5^\circ$
# iter	11	7	5	3	3	3	3	2	3	3	2	3

We define the **transient phase** by the sequence 11, 7 and 5; the **stationnary phase** is the remaining where the number of iterations does not change much. It is well defined by a plateau at a value equal to the average number of iterations for the right-hand sides solved in this stationnary phase. Finally we obtain the following model law:

$\theta$	$0^\circ$	$0.5^\circ$	$1^\circ$	$1.5^\circ$	$2^\circ$	$2.5^\circ$	$3^\circ$	$3.5^\circ$	$4^\circ$	$4.5^\circ$	$5^\circ$	$5.5^\circ$
# iter	11	7	5	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67

This law describes the number of iterations of the seed-GMRES method on 15 right-hand sides starting from  $F(\theta = 0^\circ)$ . We assume that this behaviour holds for any starting right-hand side  $F(\theta)$ .

# Kernel operations

	zaxpy	zdscal	zcopy	zdot	precond	FMM	# proc.
Airbus 23676	0.0027	0.0026	0.0019	0.0024	0.27	1.83	4
Airbus 94704	0.0066	0.0063	0.0046	0.0051	0.80	4.61	8
Airbus 213084	0.0148	0.0142	0.0105	0.0106	1.78	11.13	8
sphere 40368	0.0044	0.0042	0.0030	0.0036	0.29	2.16	4
sphere 71148	0.0079	0.0059	0.0079	0.0061	0.54	3.84	4
sphere 161472	0.0131	0.0129	0.0093	0.0098	0.61	4.63	8
sphere 288300	0.0202	0.0194	0.0143	0.0140	1.09	8.25	8
cetaf 5391	0.0010	0.0001	0.0001	0.0013	0.13	0.25	4
cobra 60695	0.0045	0.0003	0.0004	0.0040	0.22	1.93	8
almond 104793	0.0082	0.0006	0.0007	0.0064	0.41	2.92	8

Elsapsed time for each basic operation needed by the iterative solvers.

# Kernel operations

	100 zaxpy	100 zdscal	100 zcopy	100 zdot	precond	FMM	# proc.
Airbus 23676	14.75	14.21	10.38	13.11	14.75	100	4
Airbus 94704	14.32	13.67	9.98	11.06	17.35	100	8
Airbus 213084	13.30	12.76	9.43	9.52	15.99	100	8
sphere 40368	20.37	19.44	13.89	16.67	13.42	100	4
sphere 71148	20.57	15.36	20.57	15.89	14.06	100	4
sphere 161472	28.29	27.86	20.09	21.17	13.17	100	8
sphere 288300	24.48	23.52	17.33	16.97	13.21	100	8
cetaf 5391	40.80	2.40	2.40	50.80	52.00	100	4
cobra 60695	23.47	1.66	2.18	20.89	11.40	100	8
almond 104793	28.05	1.89	2.47	21.99	14.04	100	8

Percentage of time required by 100 calls to each basic operations with respect to one call to the FMM

# The cobra case

$(\theta, \varphi)$	default guess	strat. 2		seed-GMRES	
	# iter	# iter	$\ r_0\ _2/\ F\ _2$	# iter	$\ r_0\ _2/\ b\ _2$
# iterations	4102		2005		2819
elapsed time (s)	15565.6		6765.6		9863.7

# The cobra case

rien ne sert de courir, il faut partir à point



Jean de la Fontaine.

# Special feature RHS

The  $j$ -st entry of the right-hand side  $F(\varphi)$  corresponding to a plane wave coming from the direction  $\varphi$  and wave number  $k$  on the object  $\Gamma$  is

$$F_j(\varphi) = \int_{\Gamma} e^{ikx \cdot \hat{u}_r(\varphi)} \hat{z} \cdot \vec{\Psi}_j(x) ds(x)$$



# Seed-GMRES $\neq$ SVD preprocess.

## Linear dependency of RHS Lötstedt and Nilsson

('02) use initial guess strategy 2.b. :  
solve the least squares problem

$$\min_{y \in \mathbb{R}^{\ell-1}} \|F(\varphi_\ell) - \sum_{j=0}^{\ell-1} F(\varphi_j) y_j\|_2,$$

then take the initial guess  $J^{(0)}(\varphi_\ell) = \sum_{j=0}^{\ell-1} J(\varphi_j) y_j$ .

## Seed GMRES

$$\min_{x \in \mathcal{K}_1} \|F(\varphi_\ell) - \mathbb{Z}x\|_2$$

# Control of the error

# SVD	# it	$\ E\ $	# verif
15	—	2.285445132223185E-003	
16	299	9.430404985428857E-004	603
17	303	3.785604066482061E-004	243
18	316	1.416418780336473E-004	196
19	322	5.349504623890520E-005	184
20	334	1.892546027913748E-005	182
21	341	6.750489170848254E-006	181
22	350	2.264388221336797E-006	181

# Cost of the SVD preprocessing

Size of the problem	Elapsed time SVD	Elapsed time GMRES	# procs
40368	1063	214	4
71148	1903	388	4
161472	2992	550	8
288300	4923	1649	8

Elapsed time to compute the SVD for 360 right-hand sides the sphere. For comparison, we give the average elapsed time for the solution of one right-hand side using full GMRES (assembly of the preconditioner phase not included). The backward error is set to  $10^{-2}$  for the GMRES solve.

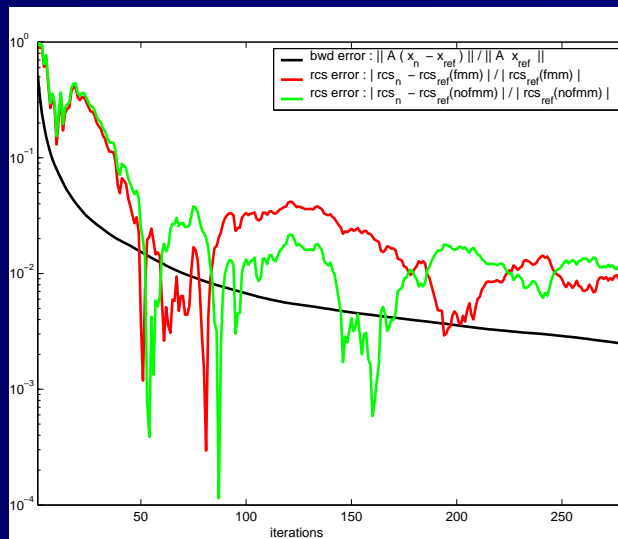
# On the coated-cone-sphere

	# iterations	elapsed time (s)
GMRES with second strategy initial guess	3797	29726
seed-GMRES	784	10328
seed-GMRES SVD(16)	632	10930
block-GMRES SVD(19)	329	8894

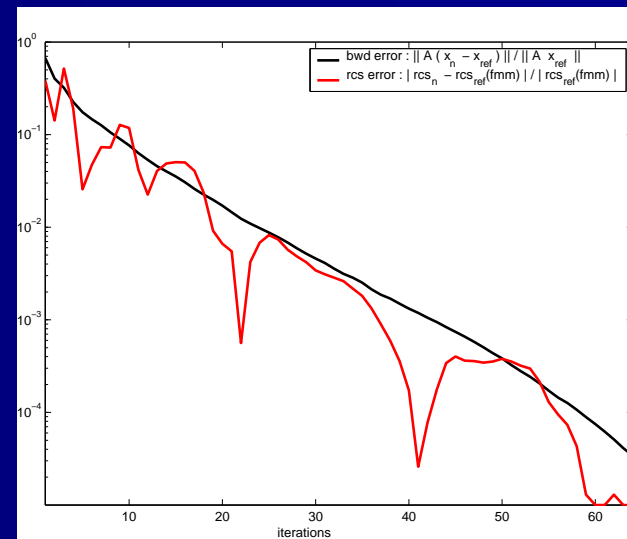
Four competitive methods on the coated cone sphere,  
 $\theta = 0^\circ : 1^\circ : 180^\circ$ .

# Prospectives (3/4)

Toward an adapted stopping criterion

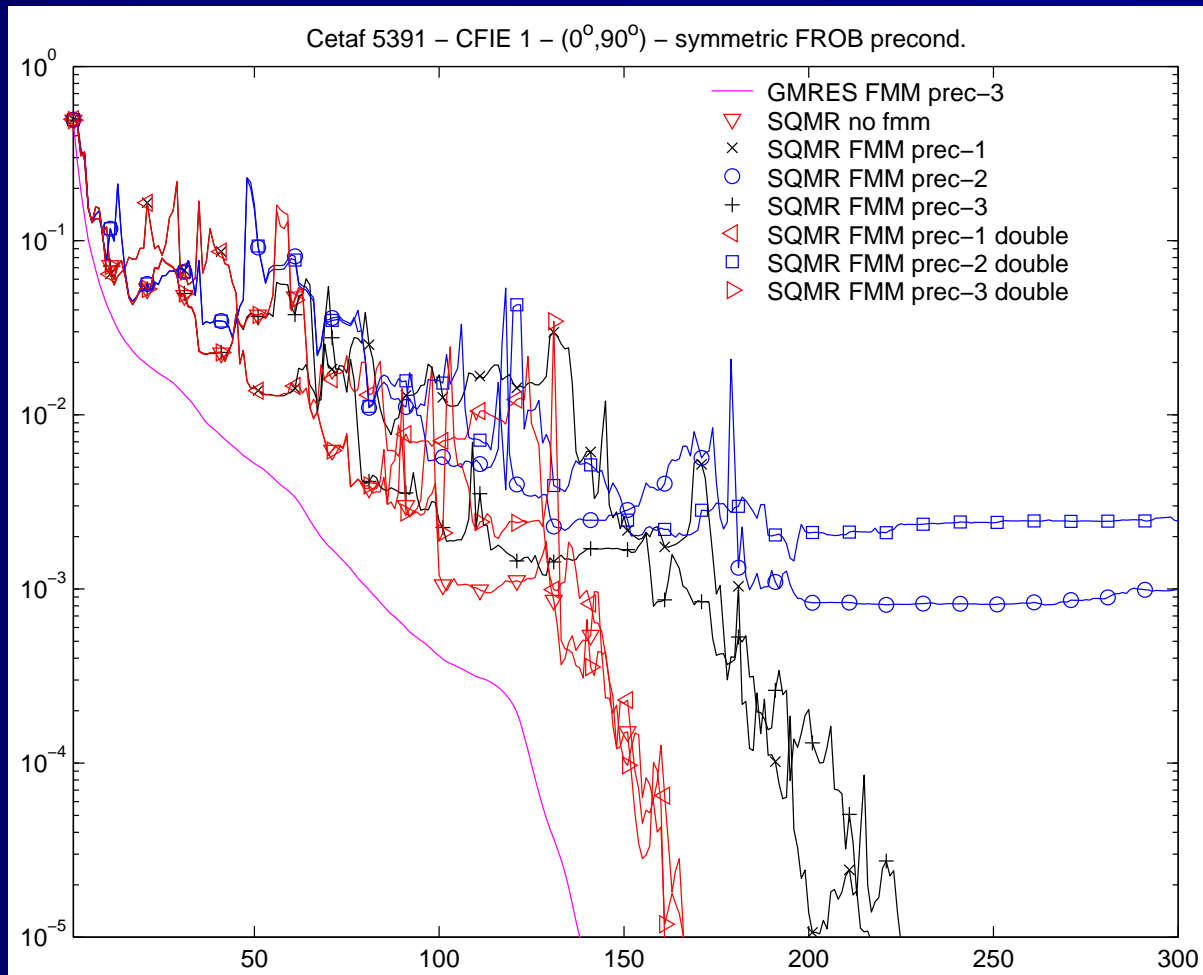


Airbus 23676

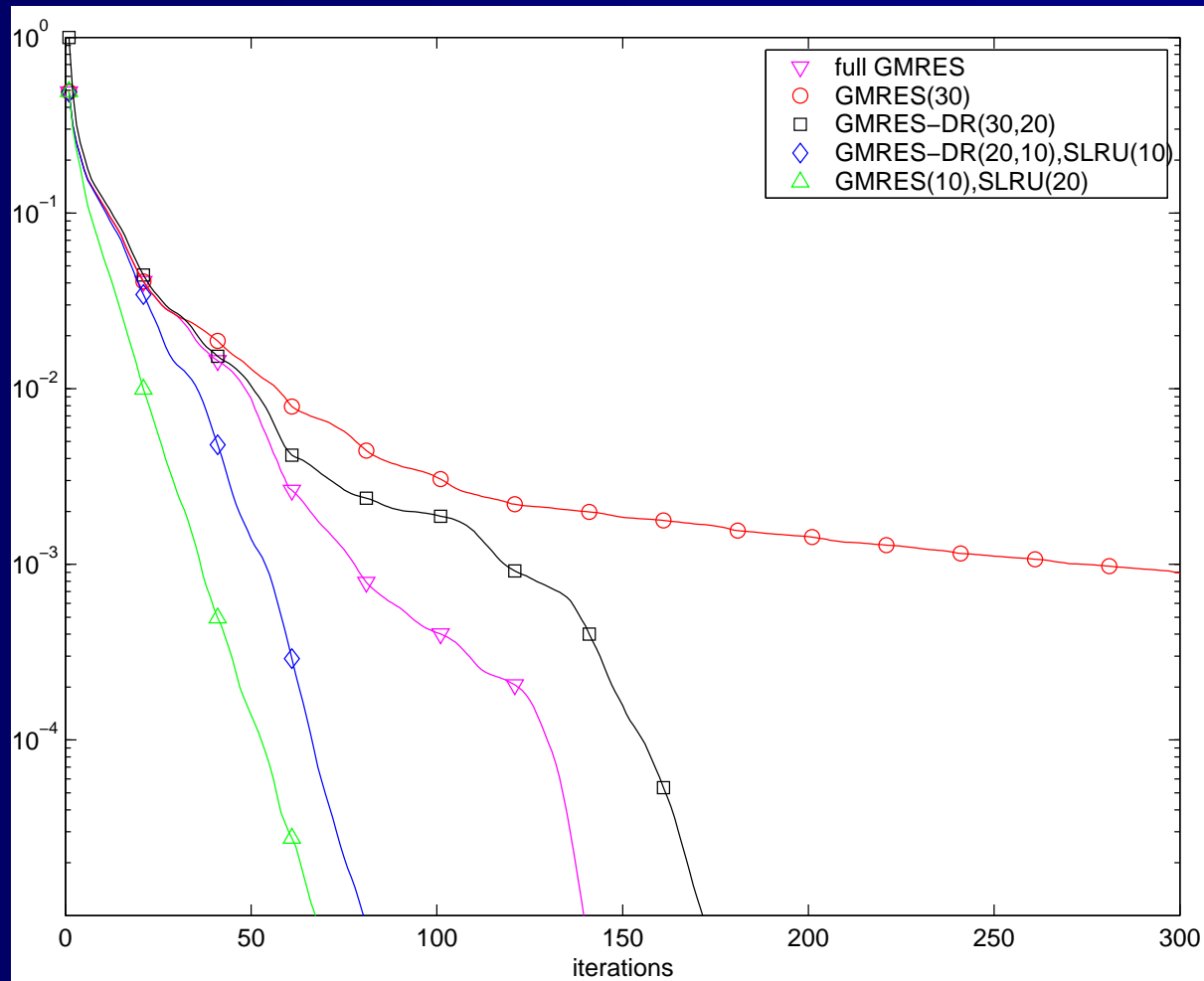


coated cone 77604

# Prospectives (4/4)



# GMRES-DR



# GMRES-DR

