

# Krylov Subspace Methods for Linear Systems and Matrix Equations

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# Projection methods for large-scale problems

Given the system of  $n$  equations

$$\mathcal{F}(x) = 0 \quad x \in \mathbb{R}^n$$

- Construct approximation space  $\mathcal{K}_m$  ( $m = \dim(\mathcal{K}_m)$ )
- Find  $\tilde{x} \in \mathcal{K}_m$  such that  $\tilde{x} \approx x$
- ★ **Projection** onto a much smaller space  $m \ll n$



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★ **Projection** onto a much smaller space  $m \ll n$

Approximation process:

**residual:**  $r := \mathcal{F}(\tilde{x})$

Construct (left) space  $\mathcal{L}_m$  of dimension  $m$  and impose

$$r \perp \mathcal{L}_m$$



# Challenges

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General idea:

Construct sequence of approximation spaces  $\mathcal{K}_m \subset \mathcal{K}_{m+1}$  such that

$$\tilde{x}_m \in \mathcal{K}_m \quad \text{and} \quad \tilde{x}_m \rightarrow x \quad \text{as} \quad m \rightarrow \infty$$

(in some sense)

Analogously,  $\mathcal{L}_m \subset \mathcal{L}_{m+1}$



# More specific problems

$$\mathcal{F}(x) = 0$$

$$A \in \mathbb{R}^{n \times n}$$

•  $Ax - b = 0$        $(\varphi_k(A)x - b = 0)$  where  $\varphi_k$  polynomial of degree  $k$



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- $AX + XA^T + Q = 0$
- Evaluation of Transfer and other matrix functions



# Choosing $\mathcal{L}_m$

Focus on linear system:

$$Ax = b, \quad A \text{ nonsing.}$$

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★  $\mathcal{L}_m = \mathcal{K}_m$  If  $A$  symmetric positive definite,

$$r_m = b - Ax_m \perp \mathcal{L}_m \quad \Leftrightarrow \quad \|x - x_m\|_A = \min_{\tilde{x} \in \mathcal{K}_m} !$$



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★  $\mathcal{L}_m = A\mathcal{K}_m$

$$r_m = b - Ax_m \perp \mathcal{L}_m \quad \Leftrightarrow \quad \|r_m\|_2 = \min_{\tilde{x} \in \mathcal{K}_m} !$$



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★  $\mathcal{L}_m = AK_m$

$$r_m = b - Ax_m \perp \mathcal{L}_m \Leftrightarrow \|r_m\|_2 = \min_{\tilde{x} \in \mathcal{K}_m} !$$

“Optimal” properties hold for any choice of  $\mathcal{K}_m$  Eiermann & Ernst A.N. '01

Typically:  $\mathcal{L}_m = \mathcal{K}_m \Rightarrow$  FOM, CG  $\quad \mathcal{L}_m = AK_m \Rightarrow$  GMRES, MINRES



# Relaxing optimality in $\mathcal{L}_m$ . Truncation

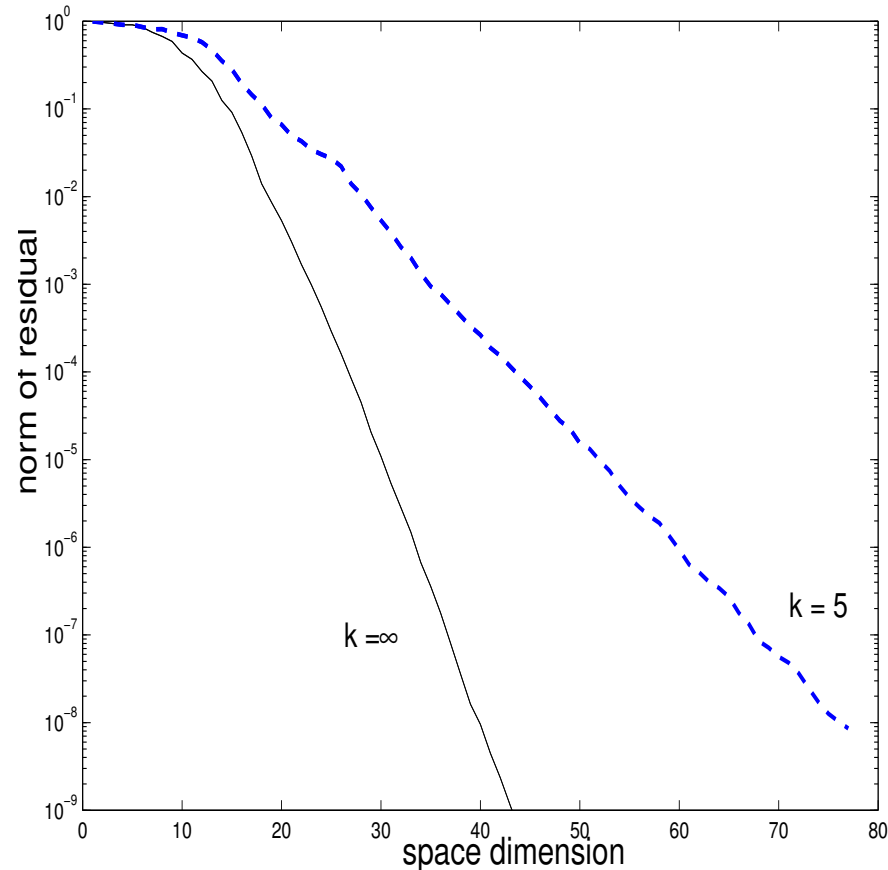
Example:  $A$  is non-normal, but “nice”       $\mathcal{L}_m = AK_m$



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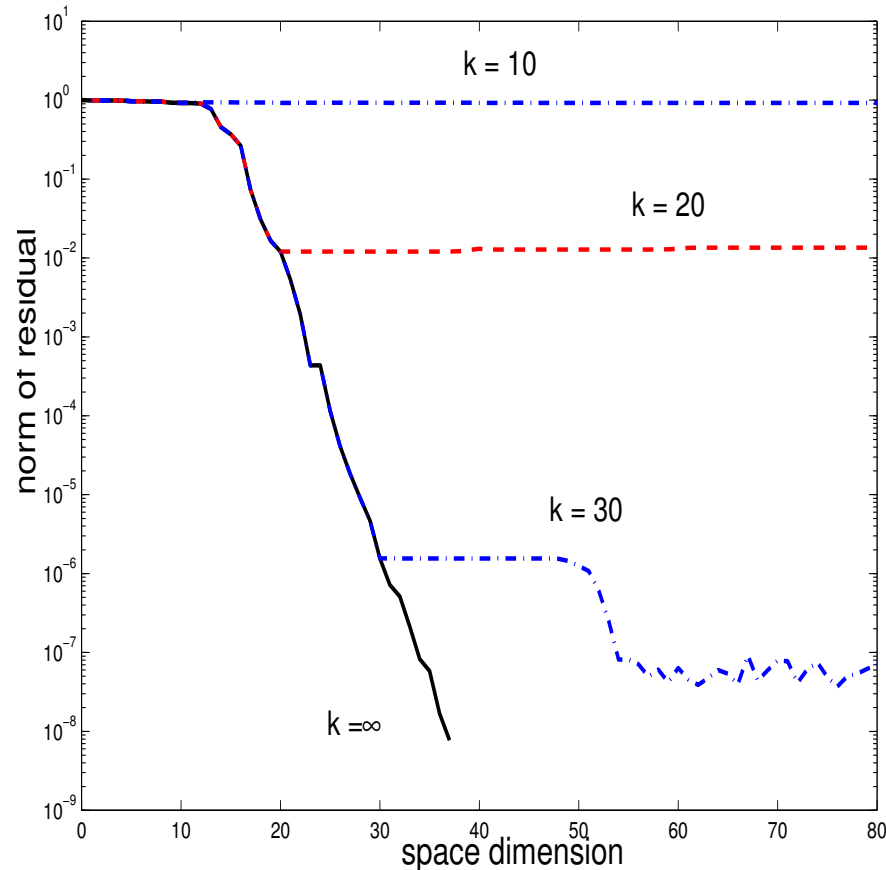
(- -):  $r \perp_{loc} \mathcal{L}_m$

$k$  gives “locality”



# Relaxing optimality in $\mathcal{L}_m$ . Truncation

Example:  $A$  is non-normal, more “nasty”       $\mathcal{L}_m = A\mathcal{K}_m$



(-):  $r \perp \mathcal{L}_m$

(- -):  $r \perp_{loc} \mathcal{L}_m$

Simoncini & Szyld, Num.Math.'05



# Choosing $\mathcal{K}_m$

The “classical” approach

$$\mathcal{K}_m := \mathcal{K}_m(A, v) = \text{span}\{v, Av, \dots, A^{m-1}v\}$$

(e.g.,  $v = b$  in linear systems)

$$\tilde{x} \in \mathcal{K}_m, \quad \tilde{x} = p_{m-1}(A)v$$



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Nice Properties:

- For  $m$  sufficiently large,  $\mathcal{K}_m(A, v)$  invariant for  $A$
- Convergence (analysis) in terms of spectral properties of  $A$
- Variants of “basic” methods by acting on polynomial  $p_{m-1}$



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This choice of  $\mathcal{K}_m$  is good, but no longer *sufficiently good*



# Getting greedy

$$\mathcal{K}_m = \mathcal{K}_{m-k}(A, v) \cup \mathcal{S}_k \quad \text{New question: } \mathcal{S}_k?$$



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- ★ Faster approximation when spectral a-priori knowledge is available (even for  $A$  Hermitian)



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★ Faster approximation when spectral a-priori knowledge is available (even for  $A$  Hermitian)

★ Main motivating problem:

Large  $m$  may be required for accurate approximation  $x_m$



Computational/Memory costs increase **nonlinearly** with  $m$   
( $A$  non-normal)



# Intermezzo. Restarting procedure

Computational/Memory costs increase **nonlinearly** with  $m$   
( $A$  non-normal)

Restarting procedure:  $x_0$  initial approx,  $r_0 = b - Ax_0$

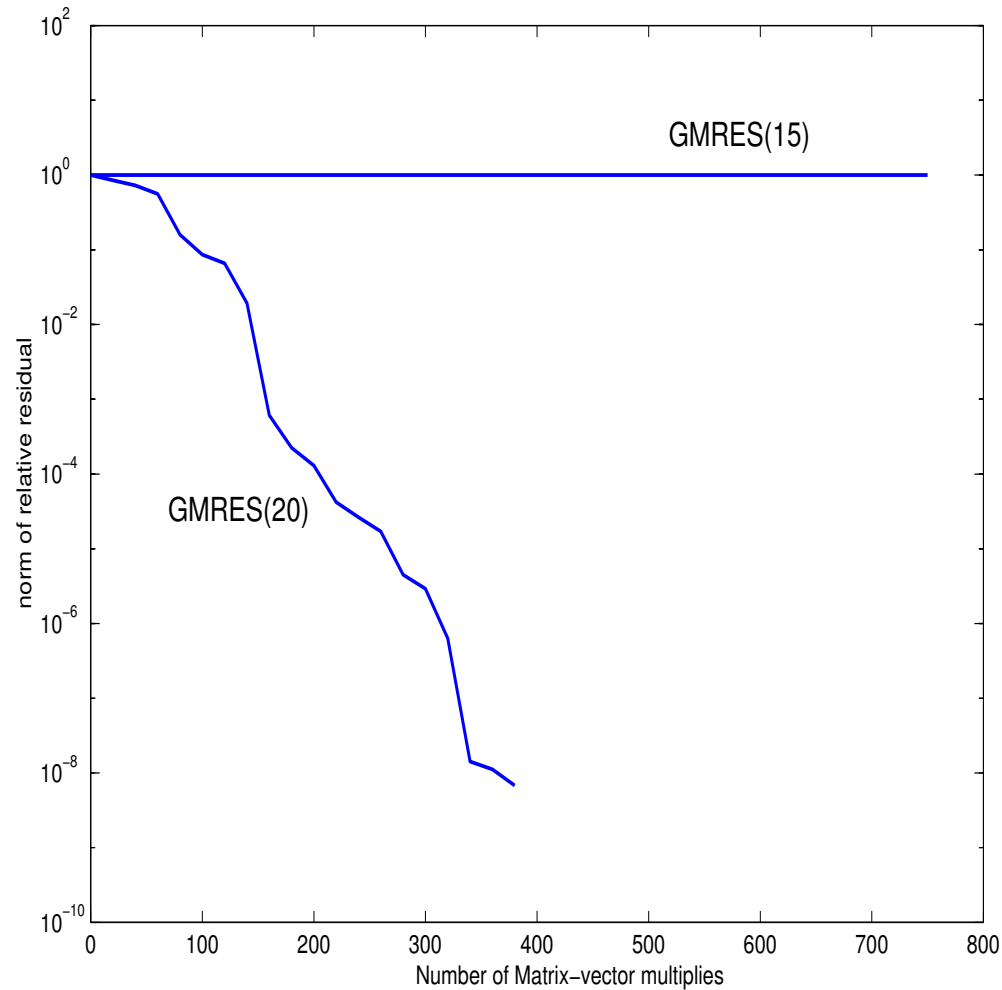
$$\begin{array}{ccc} \mathcal{K}_m(A, r_0) & \rightarrow & x_m^{(1)}, r_m^{(1)} \\ \mathcal{K}_m(A, r_m^{(1)}) & \rightarrow & x_m^{(2)}, r_m^{(2)} \\ & \vdots & \vdots \end{array}$$

**Warning:** Larger  $m$  not always implies faster convergence  
(Embree, Ernst, ...)



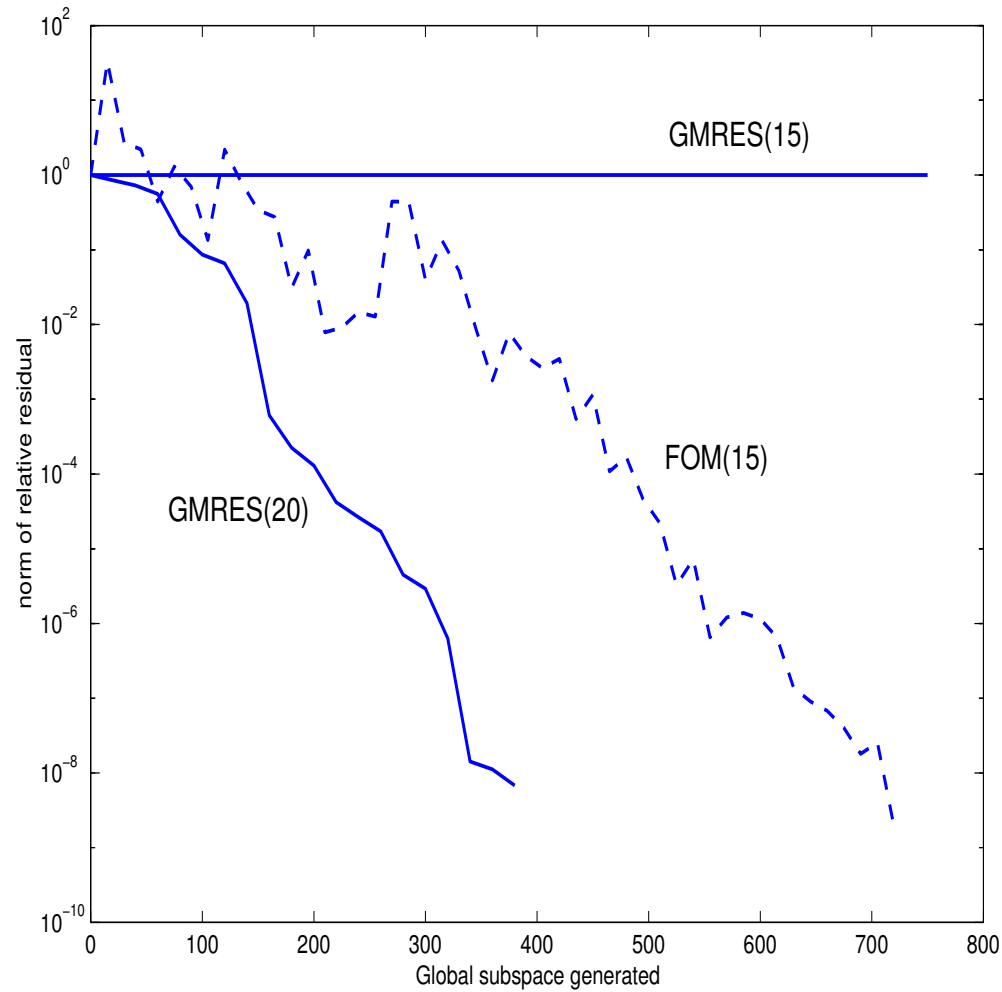
# Restarted Methods

Convergence strongly depends on choice of  $m$  ...



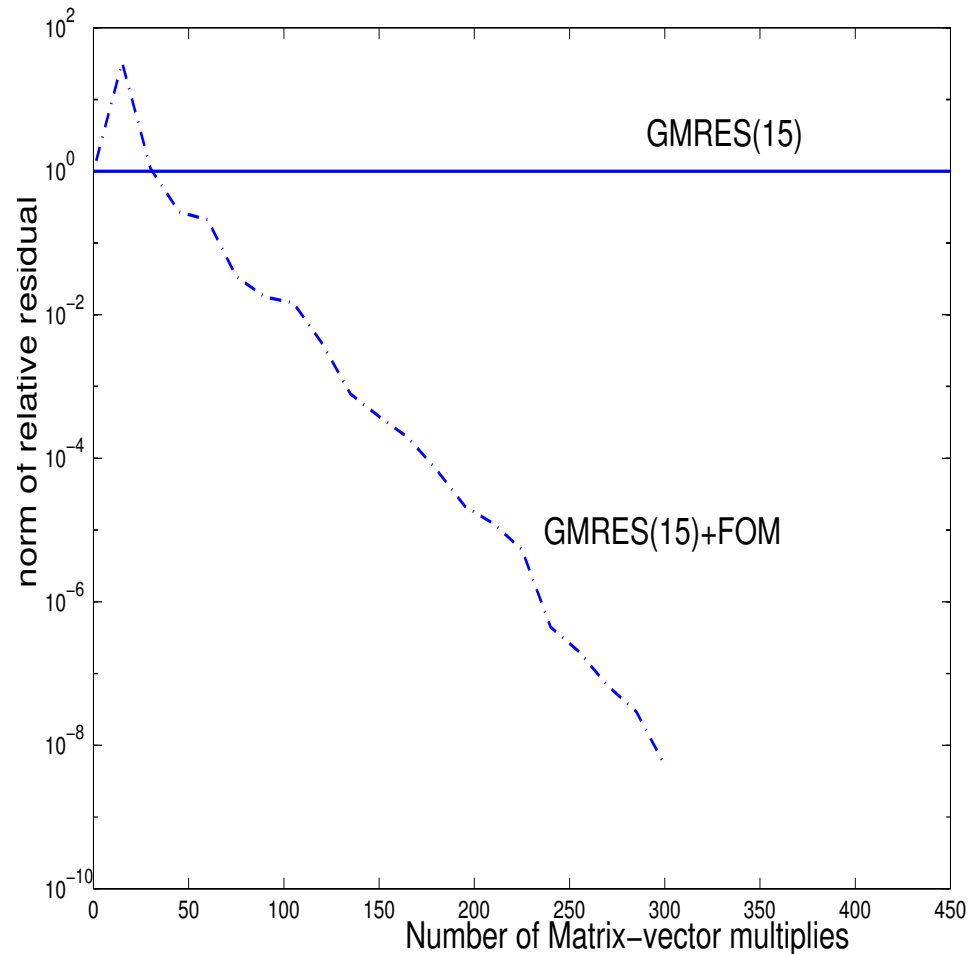
# Restarted Methods

Convergence strongly depends on choice of  $m$  ... true?



# Restarted Methods

Switch to FOM residual vector only at the very first restart



Pictures from Simoncini, SIMAX 2000.

Intermezzo ends.



# Augmented projection spaces

$$\mathcal{K}_m = \mathcal{K}_{m-k}(A, v) \cup \mathcal{S}_k$$

- $\mathcal{S}_k$  from spectral information of  $A$

$$\mathcal{K}_{m-k}(A, v) \cup \mathcal{S}_k = \text{span}\{v, Av, \dots, A^{m-k-1}v, y_1, y_2, \dots, y_k\}$$

$y_1, \dots, y_k$  approximate eigenvectors of  $A$  associated to cluster

(Baglama, Calvetti, Erhel, Morgan, Nabben, Reichel, Saad, Sorensen, Vuik ...)



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- $\mathcal{S}_k$  **important** space from previous restarts

Ranking based on “error” or “effectiveness” of the past spaces

(De Sturler, Baker, Jessup, Manteuffel, ...)



# Augmented method. Spectral Information available.

Structural Dynamics problem:  $(\mathcal{A}\mathcal{B}^{-1} + \sigma I)x = b$

$\mathcal{A}, \mathcal{B}$  complex sym.  $n = 86,000$ . Solve for  $\sigma$  in a wide interval

Note: at each iteration solve system with matrix  $\mathcal{B}$

$\mathcal{B} = \mathcal{B}(\kappa)$   $\kappa$  related to artificial stiff springs at ground boundaries

$\mathcal{B}$  numerically singular as  $\kappa \rightarrow 0$



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	Fill-in p=5		Fill-in p=15	
	E. Time [s]	# its (outer/ avg. inner)	E. Time [s]	# its (outer/ avg. inner)
$\kappa = 0$ <b>ACG</b>	14066	296/38	12790	281/33
$\kappa = 100$	14072	117/120	13739	121/102
$\kappa = 1000$	8694	88/96	8724	89/83

$\kappa = 1000$  unrealistic

Perotti & Simoncini, '02

ACG: Augmented CG, Saad & Yeung & Ehrel & Guyomarc'h, 2000

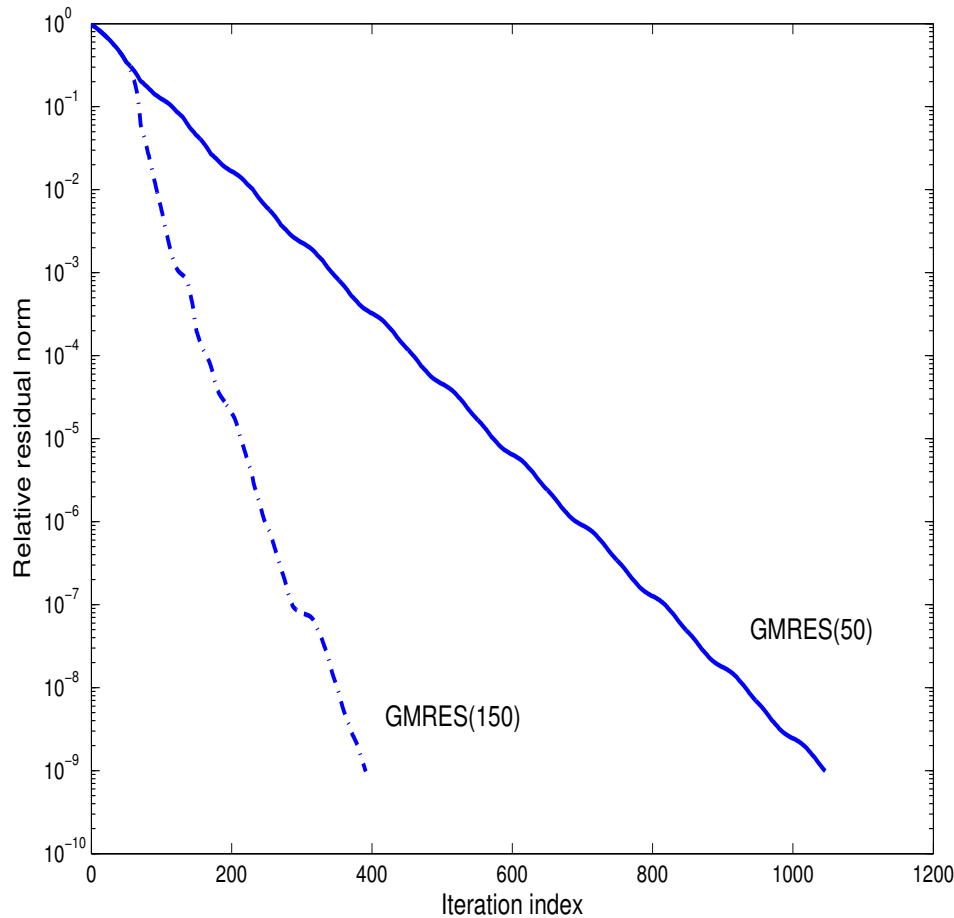


# Example of Augmented method. Error Space

Tricky way to enhance approximation space

$$A \quad \text{from } L(u) = -1000\Delta u + 2e^{4(x^2+y^2)}u_x - 2e^{4(x^2+y^2)}u_y$$

$$n = 40\,000$$

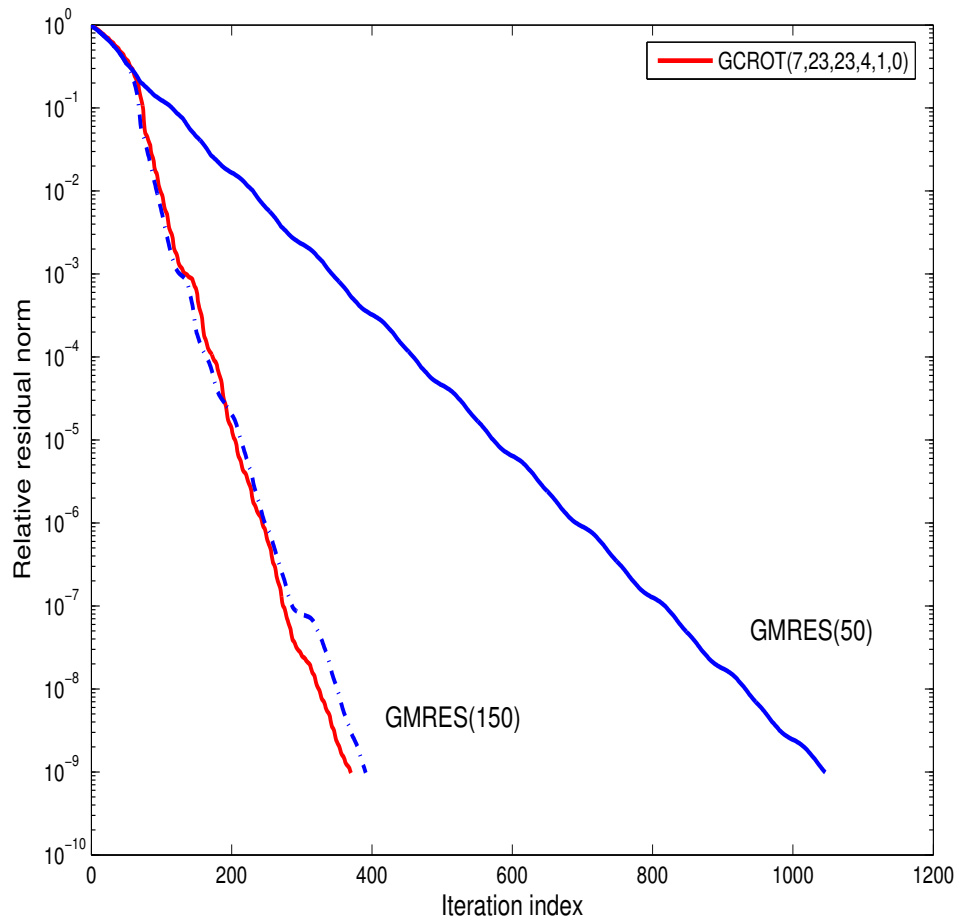


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Code: courtesy of Oliver Ernst

see also Baker, Jessup, Manteuffel '05



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# Changing $\mathcal{K}_m$

Modify  $\mathcal{K}_m$  instead of augmenting it!

- Increase flexibility
- Cope with “involved” operators
- ...



# Changing $\mathcal{K}_m$ . Flexible methods

Original problem

$$AP^{-1}x = b \quad P \text{ preconditioner}$$

$$\mathcal{K}_m(AP^{-1}, b) = \text{span}\{b, AP^{-1}b, \dots, (AP^{-1})^{m-1}b\}$$

at each iteration  $i$ :  $z_i = P^{-1}v_i$



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Flexible variant:

Saad, '93

$$\text{Iteration } i: \quad z_i = P^{-1}v_i \quad \Rightarrow \quad z_i = P_i^{-1}v_i$$

$$\tilde{\mathcal{K}}_m \in \text{span}\{b, z_1, z_2, \dots, z_{m-1}\} \neq \mathcal{K}_m(AP^{-1}, b)$$



# Flexible methods. An example

Flexible method may be used as a Truncated/Augmented method.

$$z = P^{-1}v \quad \Leftrightarrow \quad z \approx A^{-1}v$$

$$\text{span}\{b, z_1, z_2, \dots, z_{m-1}\}$$



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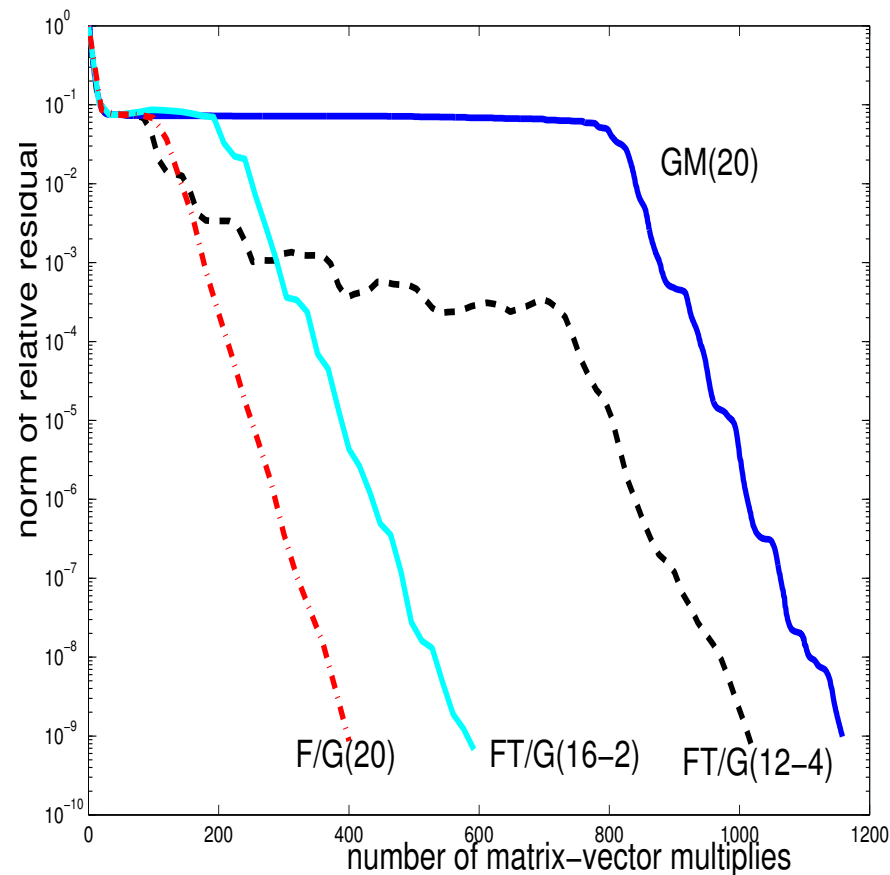
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$A$  from  $L(u) = -\Delta u + 1000xu_x$

$$n = 900$$



Simoncini & Szyld, SINUM '03

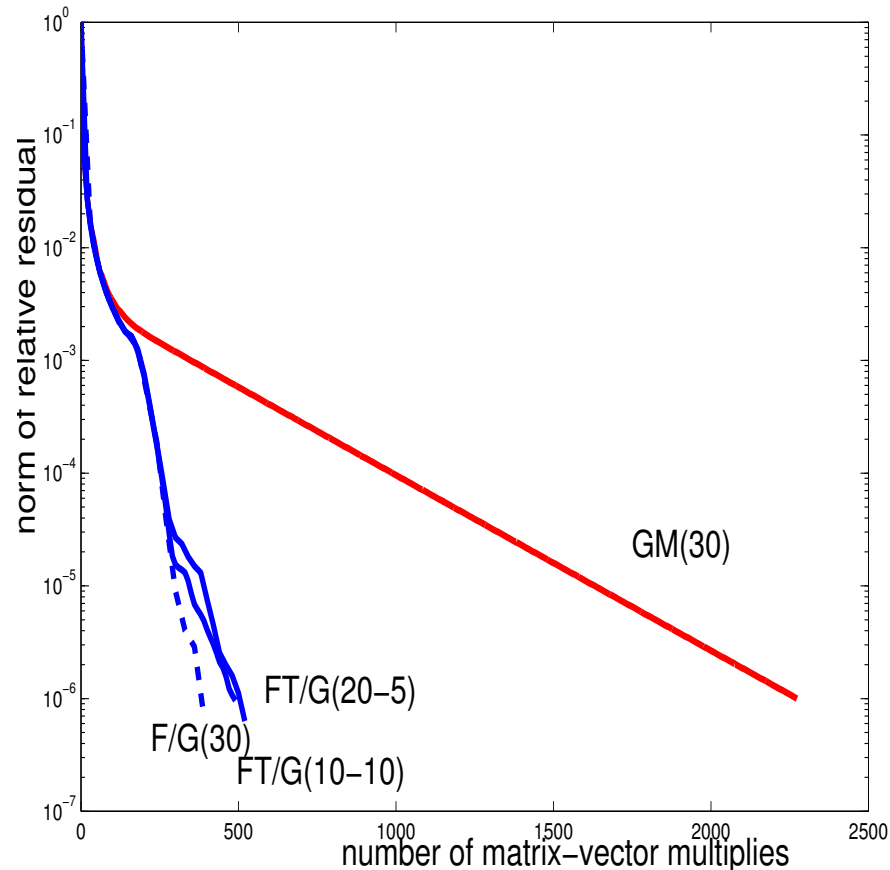


# Flexible methods. A second example

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$$A \quad \text{from } L(u) = -1000\Delta u + 2e^{4(x^2+y^2)}u_x - 2e^{4(x^2+y^2)}u_y \quad n = 40\,000$$



Simoncini & Szyld, SINUM '03



# Changing $\mathcal{K}_m$ . Inexact methods.

Original problem

$$Ax = b \quad A \quad \text{Possibly not available exactly}$$

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Inexact (relaxed) variant:

$$\text{Iteration } i: \quad z_i = Av_i \quad \Rightarrow \quad z_i = Av_i + f_i$$

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♣ “Worse” than for Flexible methods:

$$r_m = b - Ax_m \quad \text{not available!}$$

Available:  $\tilde{r}_m$  computable residual



# Inexact Methods. An example

if  $\|f_i\| = O\left(\frac{\varepsilon}{\|\tilde{r}_{i-1}\|}\right) \quad \forall i \quad \Rightarrow \quad \|b - Ax_m\| \leq \varepsilon$  for  $m$  large enough



# Inexact Methods. An example

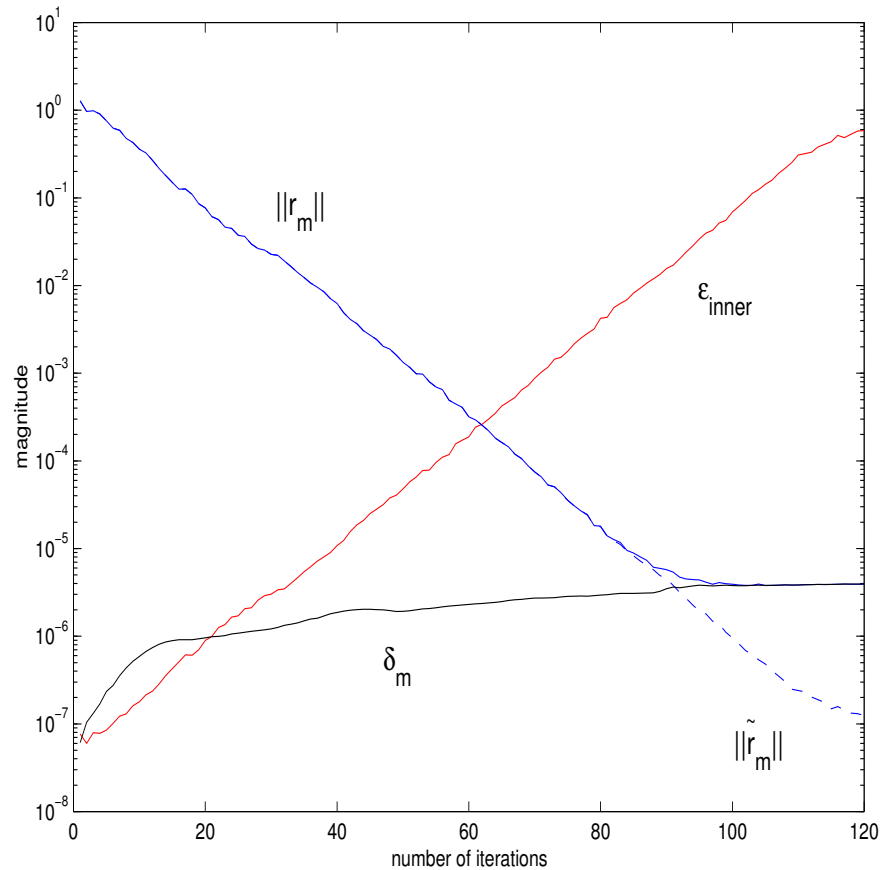
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$$\underbrace{B^T S^{-1} B}_A x = b$$

At each it.  $i$  solve:

$$Sw_i = Bv_i$$

$$\|Sw_i - Bv_i\| \leq \epsilon_{\text{inner}}(\|f_i\|)$$



$$\delta_m = \|r_m - \tilde{r}_m\|$$

Simoncini & Szyld, SISC '03



# A different application. The Lyapunov equation

$$AX + XA^T + Q = 0$$

with  $A$  dissipative,  $Q = BB^T$  of low rank  $X \approx \tilde{X}$  low rank



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• Standard Krylov approach:  $\tilde{X} \in \mathcal{K}_m(A, B)$  and

$$R = A\tilde{X} + \tilde{X}A^T + Q \perp \mathcal{L}_m = \mathcal{K}_m(A, B)$$

$\tilde{X} = V_m Y_m V_m^T$  for some  $Y_m$   $\text{Range}(V_m) = \mathcal{K}_m(A, B)$  Saad, '90



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● New “Enhanced” approach:  $\tilde{X} \in \mathcal{K}_k(A, B) \cup \mathcal{K}_k(A^{-1}, B)$  and

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★ Very competitive w.r.to Cyclic ADI method

Simoncini, tr. 2006



# An example. Time-invariant linear system

$$\mathbf{x}' = \mathbf{x}_{xx} + \mathbf{x}_{yy} + \mathbf{x}_{zz} - 10x\mathbf{x}_x - 1000y\mathbf{x}_y - 10z\mathbf{x}_z + \mathbf{b}(x, y)\mathbf{u}(t)$$

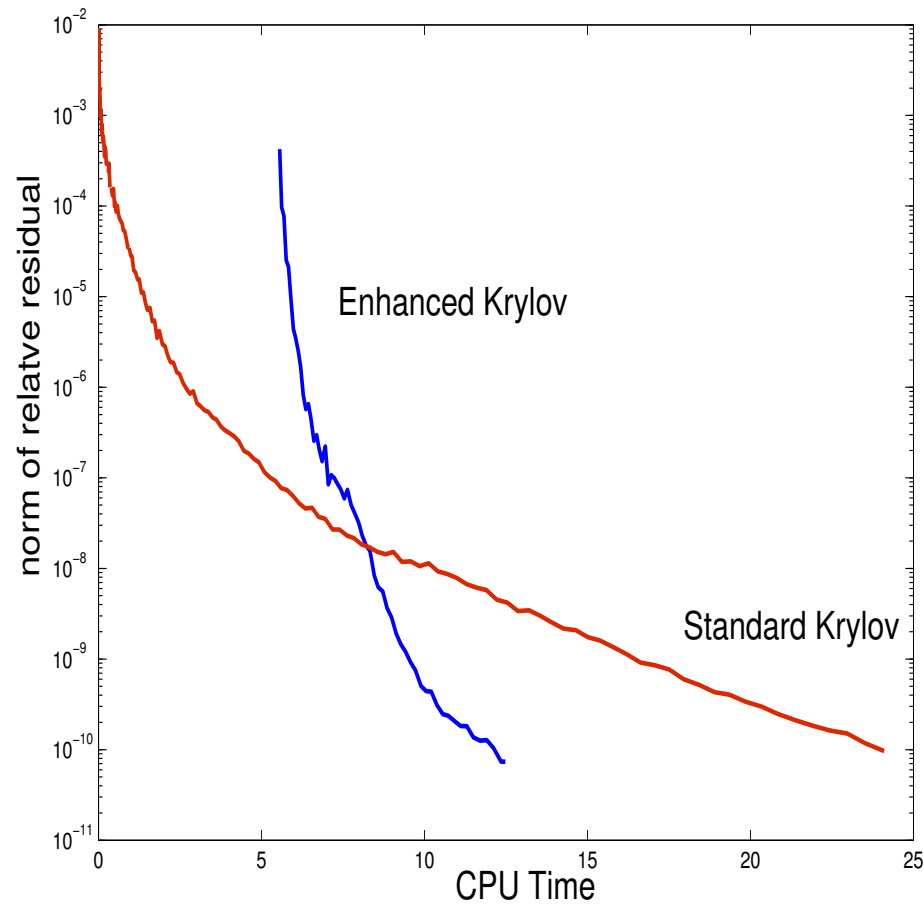
A matrix  $18^3 \times 18^3$



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approximation space dim.: 146 (Standard Krylov)

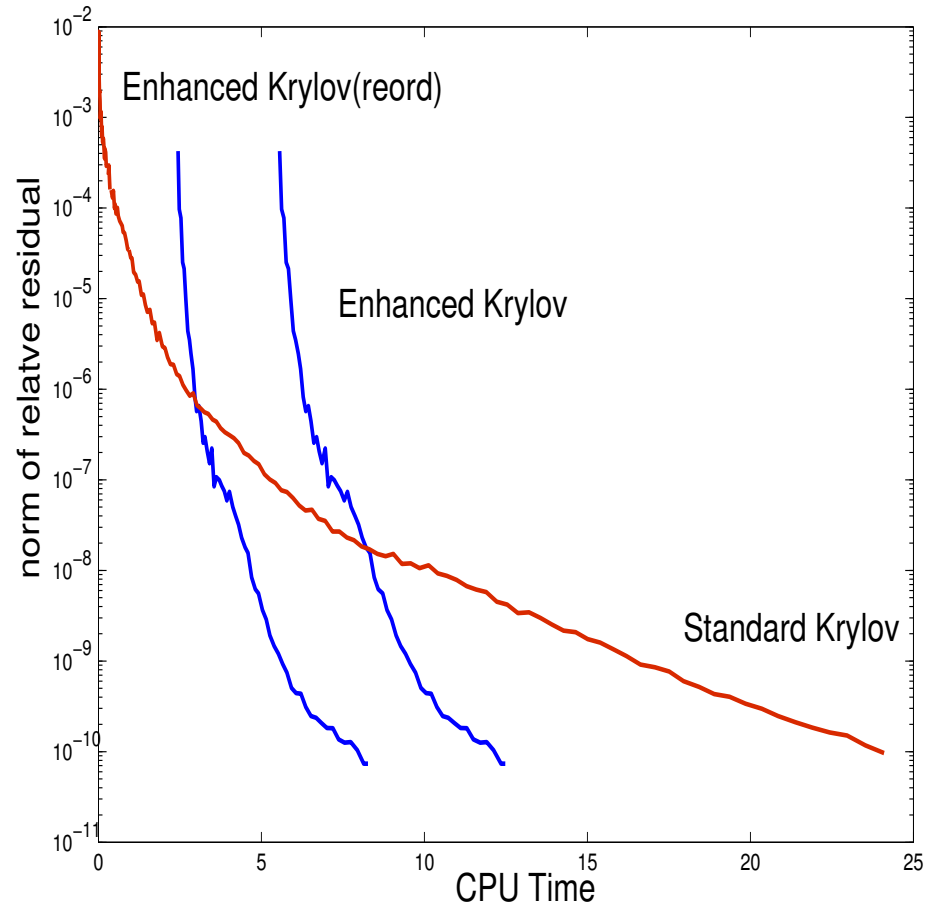
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$A$  matrix  $18^3 \times 18^3$



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112 (Enhanced Krylov)



# Conclusions and Pointers

- Projection is a versatile tool

Lots of room for improvements on hard problems



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- Survey

*“Recent computational developments in Krylov Subspace Methods for linear systems”*

with Daniel Szyld, Temple University

To appear in J. Numerical Linear Algebra w/Appl. (352 refs)

This and other papers at

<http://www.dm.unibo.it/~simoncin>



# Structural Dynamics Problem

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{C}\dot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{f}(t) \quad n \text{ d.o.f.}$$

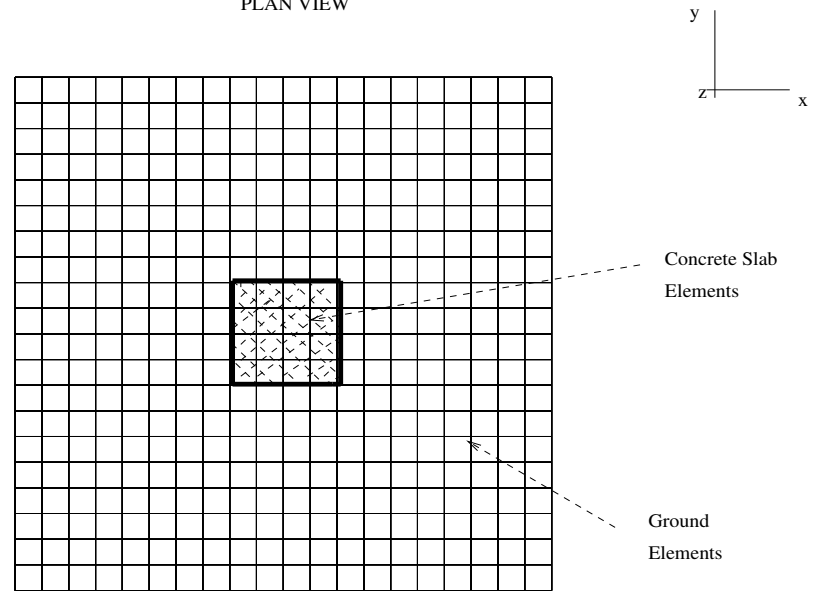
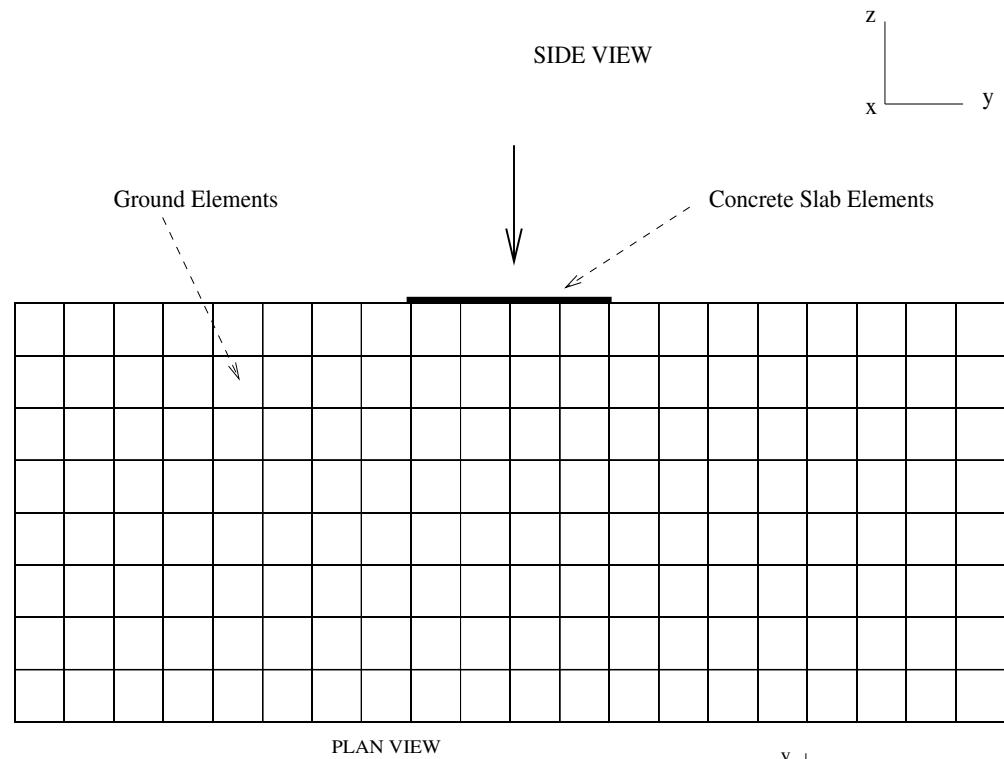
- Linearization under small deformations
- Direct frequency analysis for damping modeling  
(as opposed to modal or time analysis)
  - ★ ideal for mechanical properties depending on frequency
    - influence of deformation velocity on materials
    - presence of hysteretic damping, ...

In the frequency domain: ( $\bar{\mathbf{a}} = -(2\pi f)^2 \bar{\mathbf{q}}(f)$ ):

$$\left( \frac{1}{-(2\pi f)^2} \mathbf{K}_* + \frac{1}{i(2\pi f)} \mathbf{C}_V + \mathbf{M} \right) \bar{\mathbf{a}} = \mathbf{b}$$

$$\mathbf{C} = \mathbf{C}_V + \frac{1}{2\pi f} \mathbf{C}_H, \quad \Rightarrow \quad \mathbf{K}_* := \mathbf{K} + i\mathbf{C}_H$$





# Model Problem: 3D Soil-Structure interaction

★ viscous damping at the boundary  $\Rightarrow \mathbf{K}_*$  singular

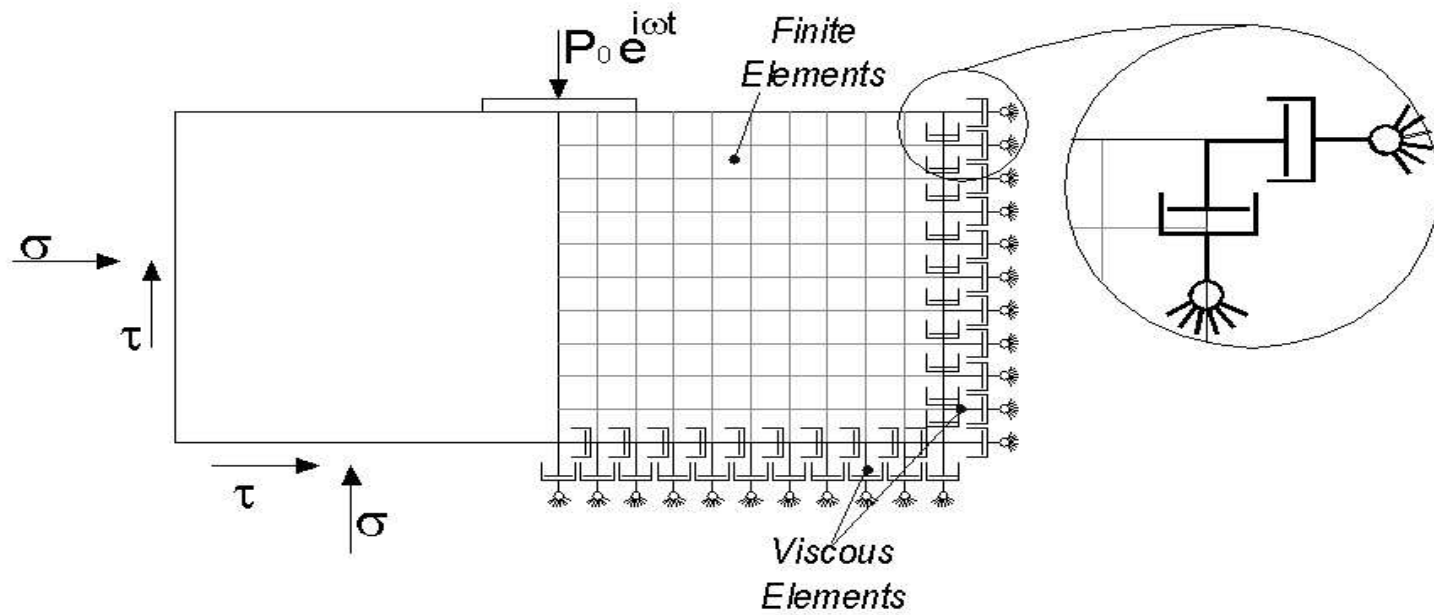
$\Rightarrow$  FE discretization,  $\mathbf{K}_*$  almost singular

**Algebraic Linearization:**  $(\sigma^2 \mathbf{K}_* + \sigma i \mathbf{C}_V - \mathbf{M}) \mathbf{x} = \mathbf{b}$ ,  $\mathbf{x} = \mathbf{x}(\sigma)$   
equivalent to

$$\left( \underbrace{\begin{bmatrix} i\mathbf{C}_V & -\mathbf{M} \\ -\mathbf{M} & 0 \end{bmatrix}}_A + \sigma \underbrace{\begin{bmatrix} \mathbf{K}_* & 0 \\ 0 & \mathbf{M} \end{bmatrix}}_B \right) \begin{bmatrix} \mathbf{y} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix}$$

with  $\mathbf{y} = \sigma \mathbf{x}$





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