Krylov Subspace Methods

for Linear Systems and Matrix Equations

V. Simoncini

Dipartimento di Matematica

Università di Bologna

valeria@dm.unibo.it

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

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Projection methods for large-scale problems

Given the system of n equations

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

- Construct approximation space $\mathcal{K}_m$ $\qquad (m = \dim(\mathcal{K}_m)\ )$

- Find $\widetilde{x} \in \mathcal{K}_m$ such that $\quad \widetilde{x} \approx x$

$\star$ Projection onto a much smaller space $\qquad m \ll n$

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Approximation process:

$$\text{residual:} \qquad r := \mathcal{F}(\widetilde{x})$$

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

$$\widetilde{x}_m \in \mathcal{K}_m \qquad \text{and} \quad \widetilde{x}_m \to x \qquad \text{as} \quad m \to \infty$$

(in some sense)

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

More specific problems

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

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

- $Ax - b = 0$ $\quad (\varphi_k(A)x - b = 0)$ where φ_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:

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

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

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

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"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 $\quad$ $\mathcal{L}_m = A\mathcal{K}_m$ $\Rightarrow$ GMRES, MINRES

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

Example: A is non-normal, but "nice" $\mathcal{L}_m = A\mathcal{K}_m$

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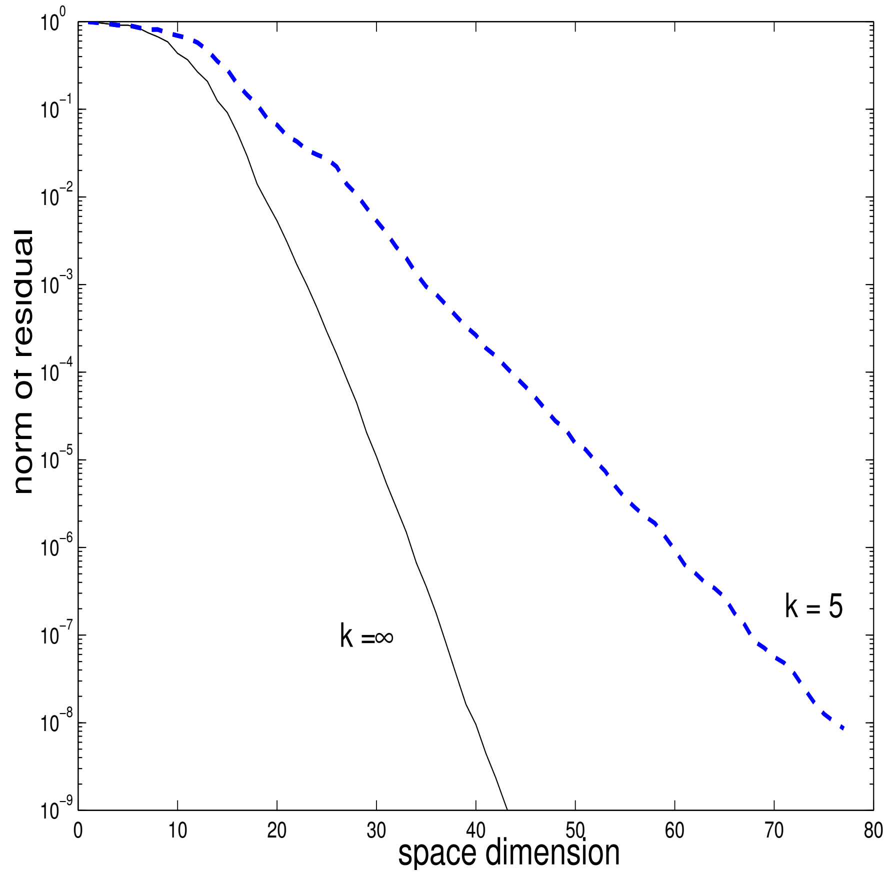

(-): $r \perp \mathcal{L}_m$ $\qquad$ (- -): $r \perp_{loc} \mathcal{L}_m$ $\qquad$ k gives “locality”

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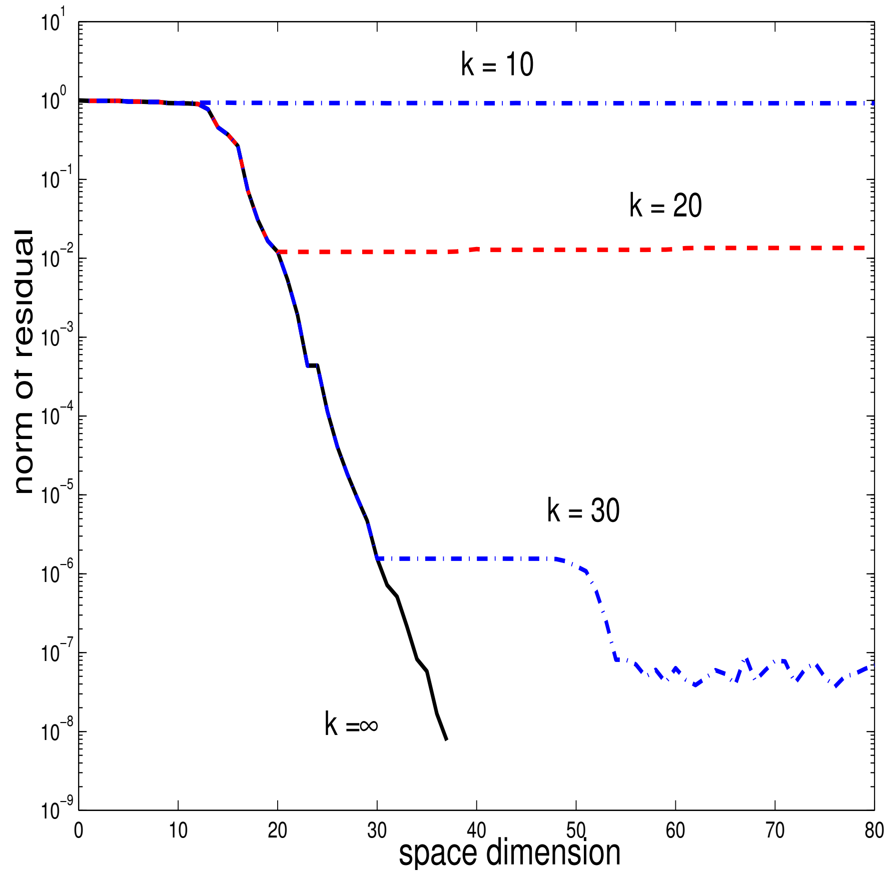
Relaxing optimality in $\mathcal{L}_m$. Truncation

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



(-): $r \perp \mathcal{L}_m$ $\qquad$ (- -): $r \perp_{loc} \mathcal{L}_m$ $\qquad$ Simoncini &Szyld, Num.Math.'05

Choosing $\mathcal{K}_m$

The "classical" approach

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

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

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

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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

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

  $$\Downarrow$$

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

Intermezzo. Restarting procedure

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

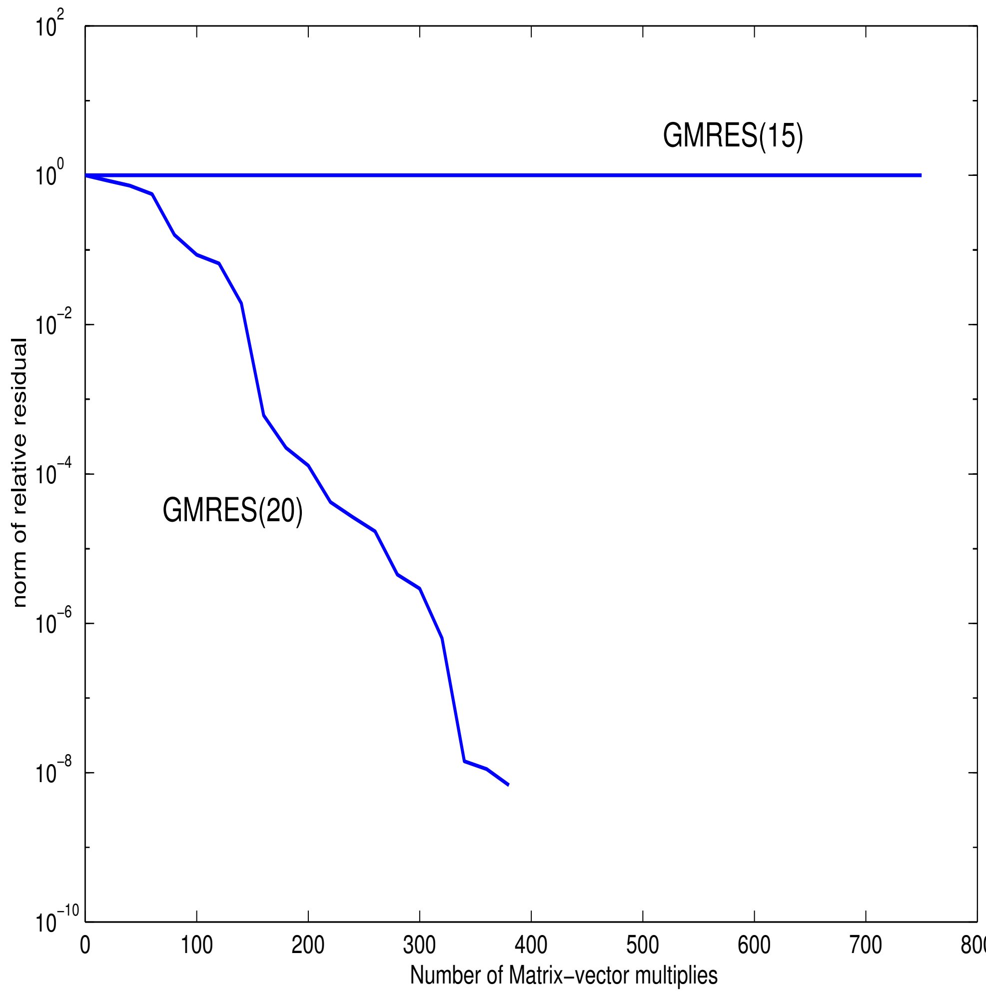
Restarting procedure: x_0 initial approx, $r_0 = b - Ax_0$

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

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

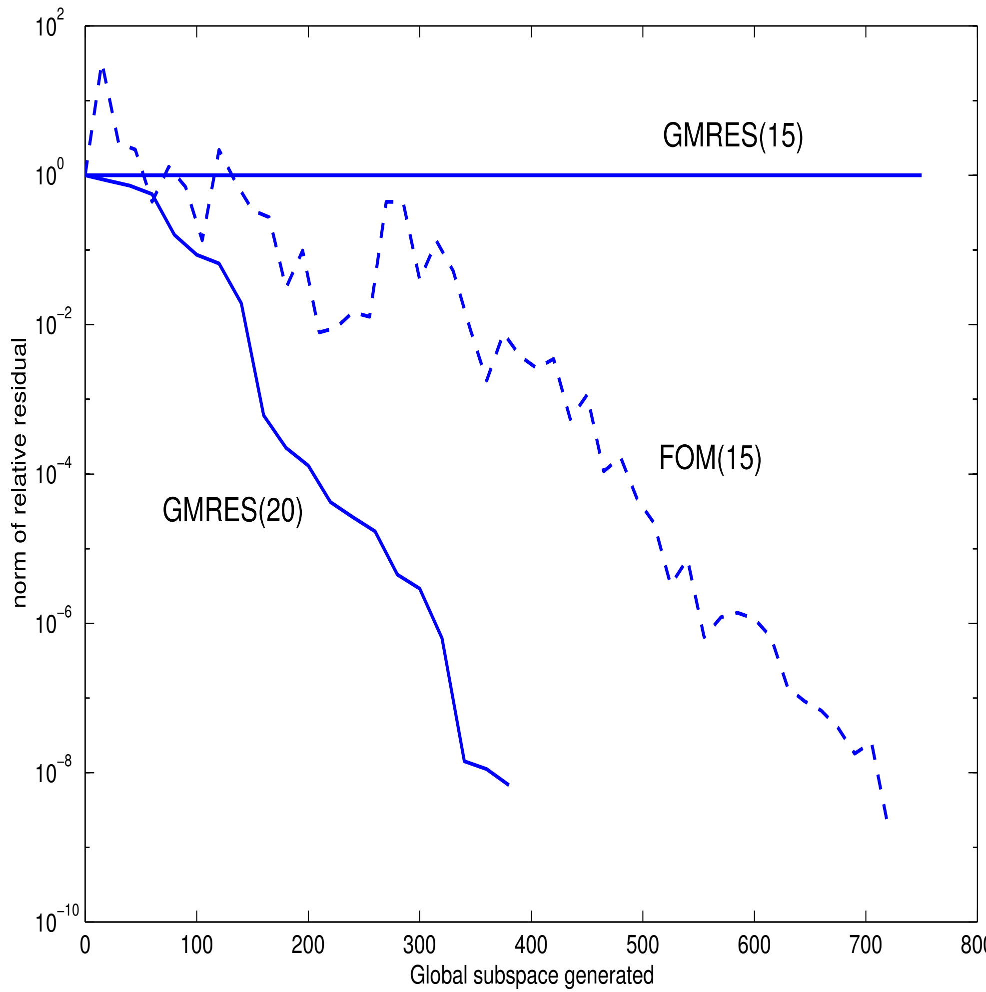
Restarted Methods

Convergence strongly depends on choice of m ...



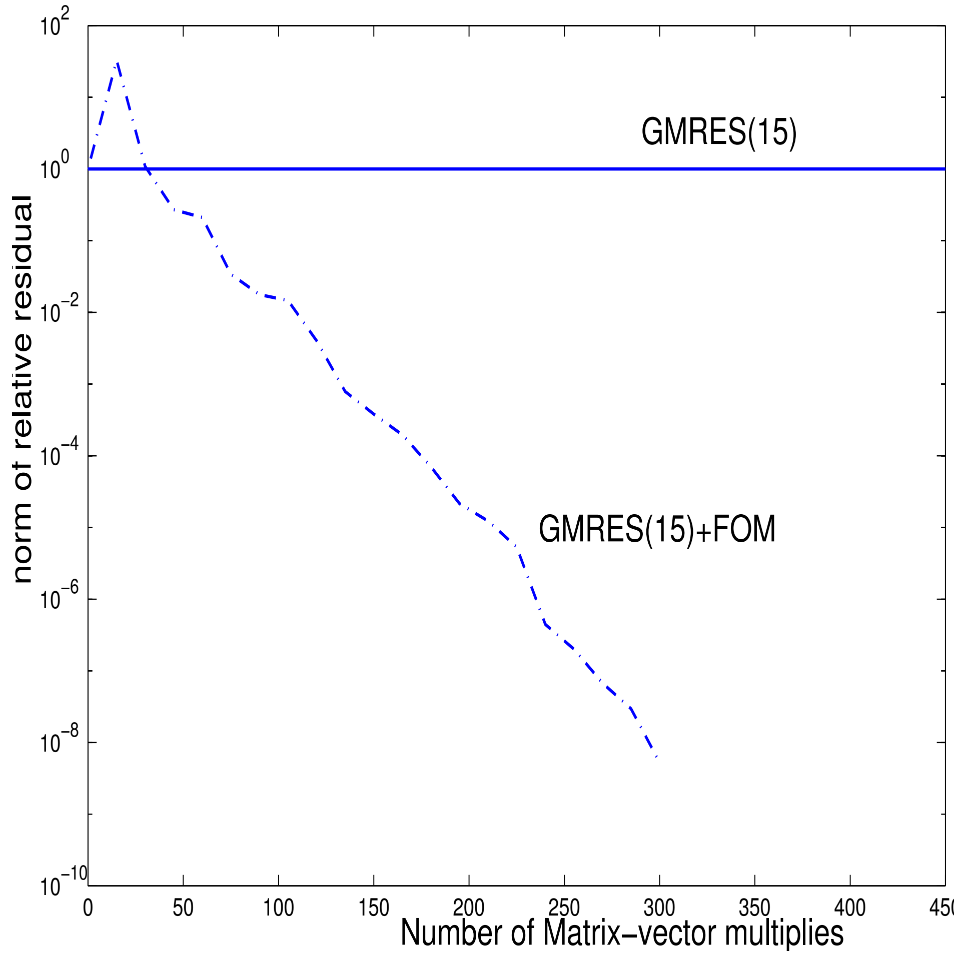
Restarted Methods

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

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

$y_1, \ldots, y_k$ 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 σ in a wide interval

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

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

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

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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)
$\kappa = 0$ ACG	14066	296/38	12790	281/33
$\kappa = 100$	14072	117/120	13739	121/102
$\kappa = 1000$	8694	88/96	8724	89/83

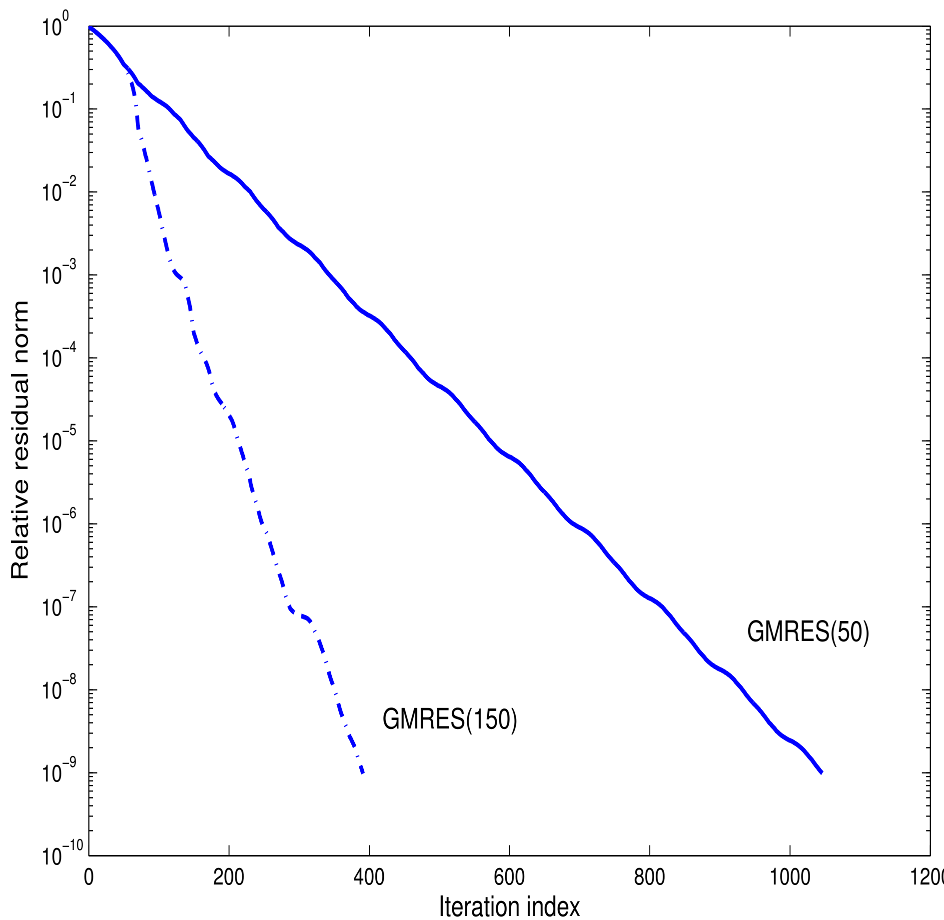
$\kappa = 1000$ unrealistic Perotti & Simoncini, '02

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

Example of Augmented method. Error Space

Tricky way to enhance approximation space

A 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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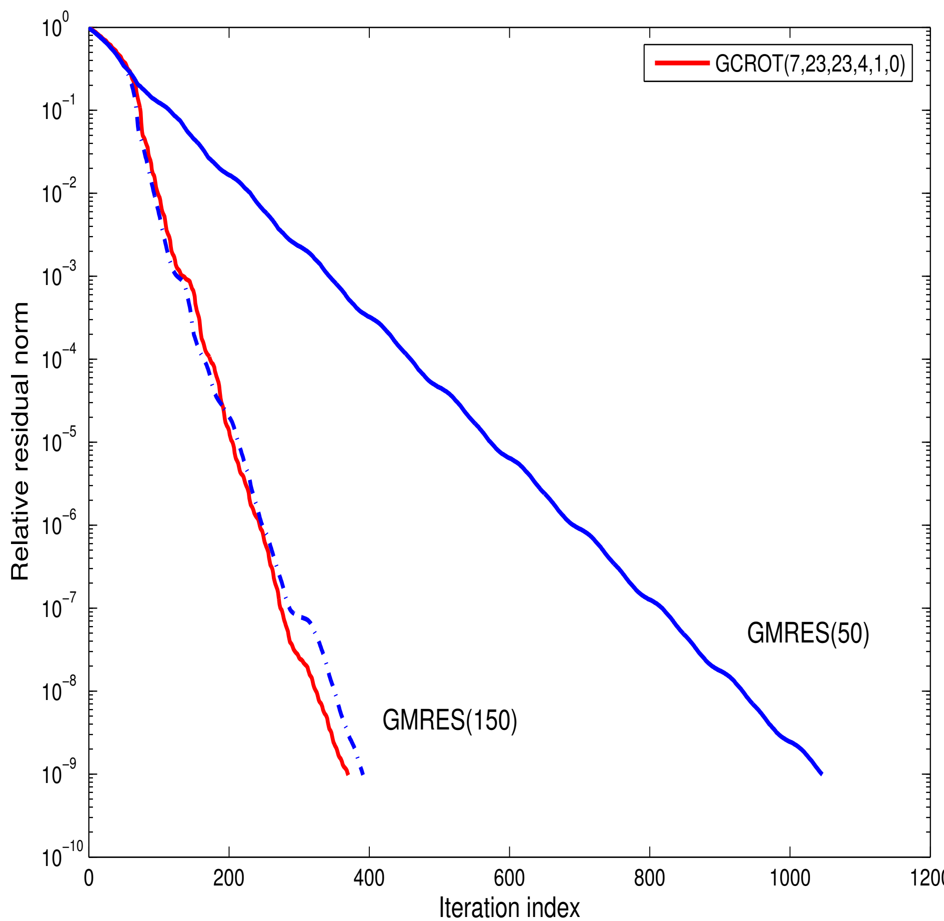

Code: courtesy of Oliver Ernst

see also Baker, Jessup, Manteuffel '05

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

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

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

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

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Flexible variant: Saad, '93

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

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

Flexible methods. An example

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

$z = P^{-1}v \quad \Leftrightarrow z \approx A^{-1}v$ span$\{b, z_1, z_2, \ldots, z_{m-1}\}$

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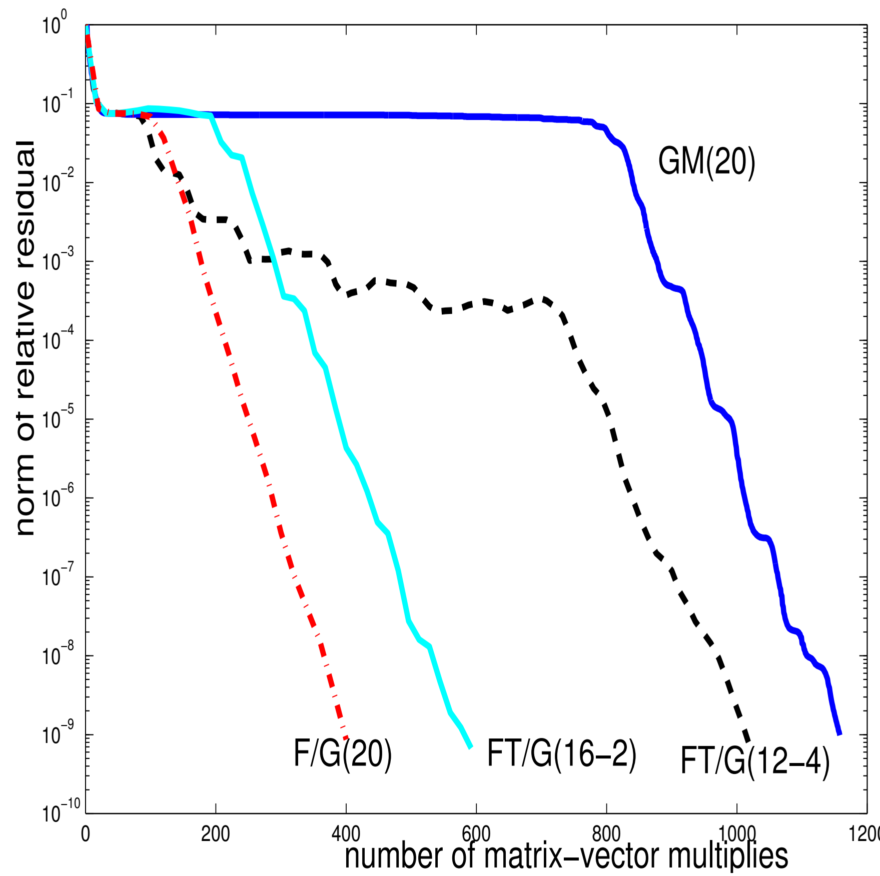
A from $L(u) = -\Delta u + 1000xu_x$ $n = 900$



Simoncini & Szyld, SINUM '03

Flexible methods. A second example

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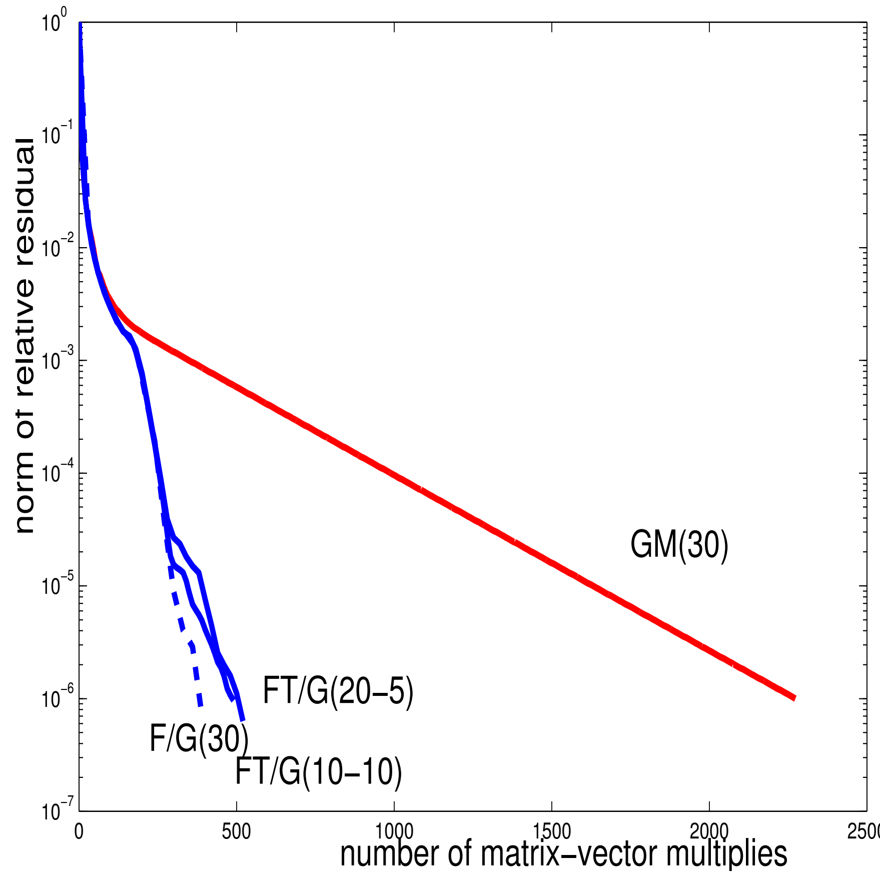

Simoncini & Szyld, SINUM ’03

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

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

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Inexact (relaxed) variant:

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

$$\widetilde{x}_m \in \text{span}\{b, z_1, z_2, \ldots, z_{m-1}\} \neq \mathcal{K}_m(A, b)$$

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♣ “Worse” than for Flexible methods:

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

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

Inexact Methods. An example

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

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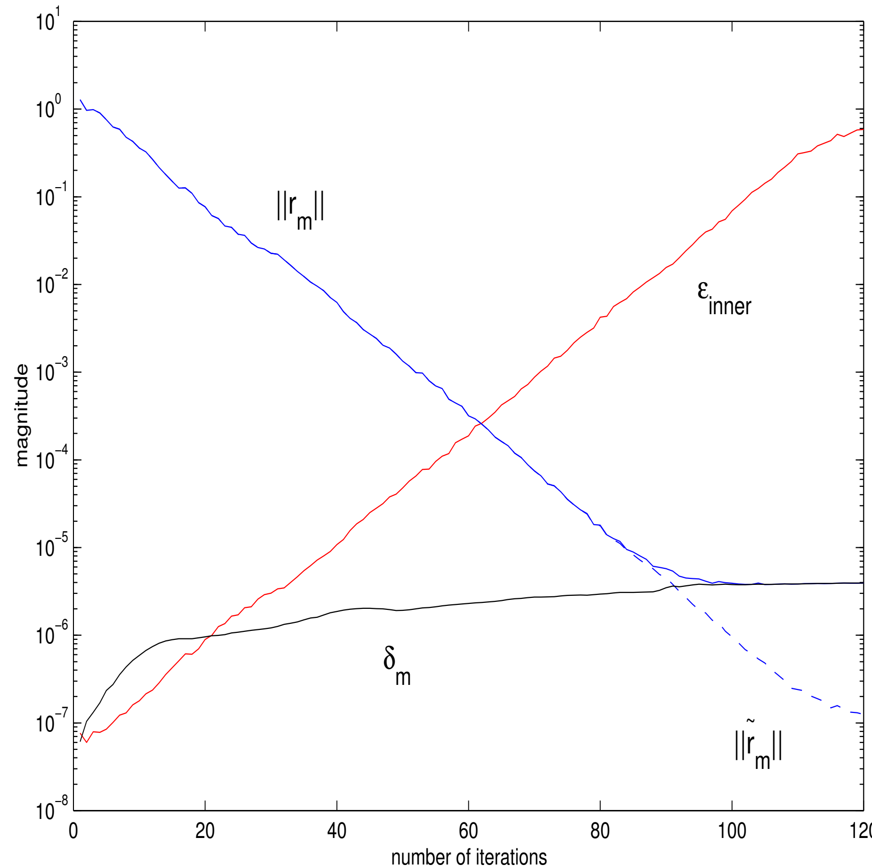
$$\underbrace{B^T S^{-1} B}_{A} x = b$$

At each it. i solve:

$$S w_i = B v_i$$

$$\|S w_i - B v_i\| \le \epsilon_{\text{inner}}(\|f_i\|)$$

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



Simoncini & Szyld, SISC '03

A different application. The Lyapunov equation

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

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- Standard Krylov approach: $\quad \widetilde{X} \in \mathcal{K}_m(A, B)$ and

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

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

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- New "Enhanced" approach: $\quad \widetilde{X} \in \mathcal{K}_k(A, B) \cup \mathcal{K}_k(A^{-1}, B)$ 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 $\quad 18^3 \times 18^3$

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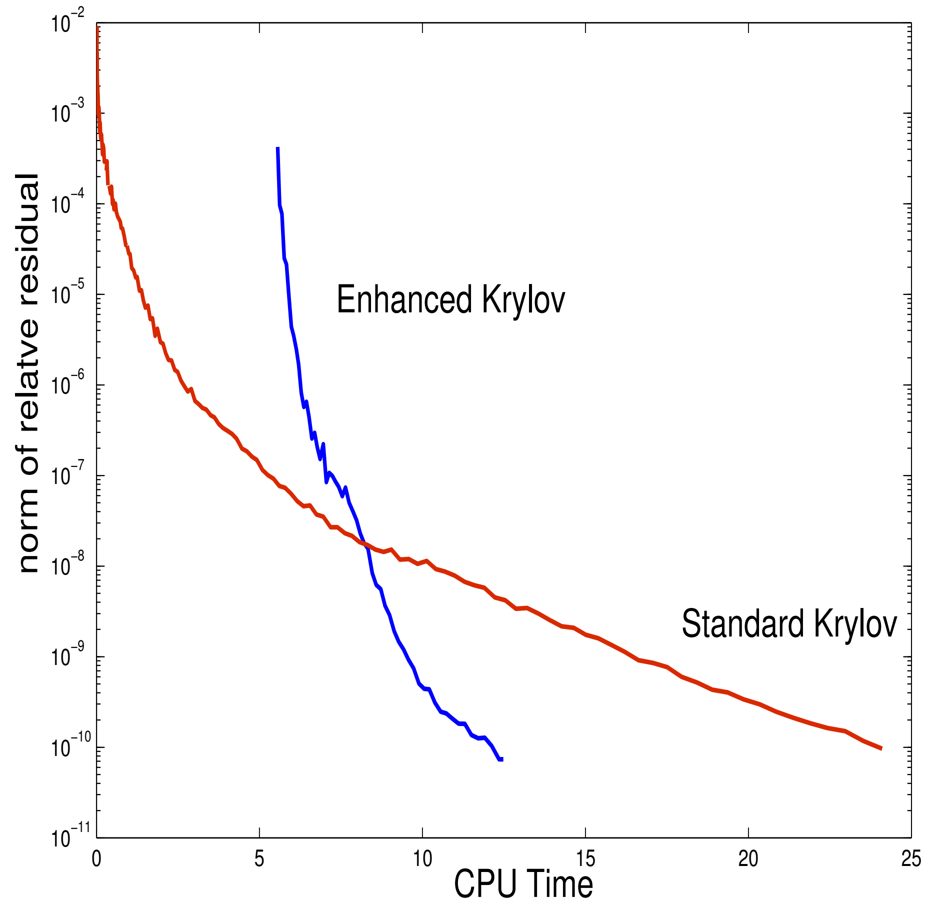

approximation space dim.: 146 (Standard Krylov) 112 (Enhanced Krylov)

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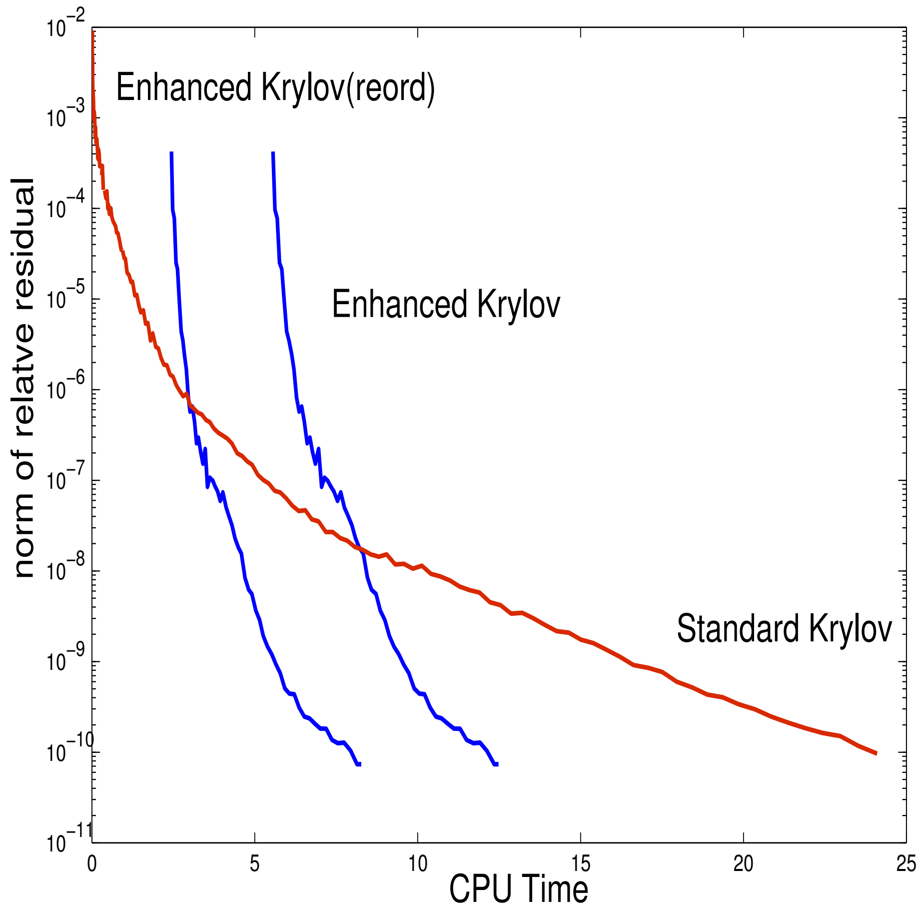

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Conclusions and Pointers

- 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

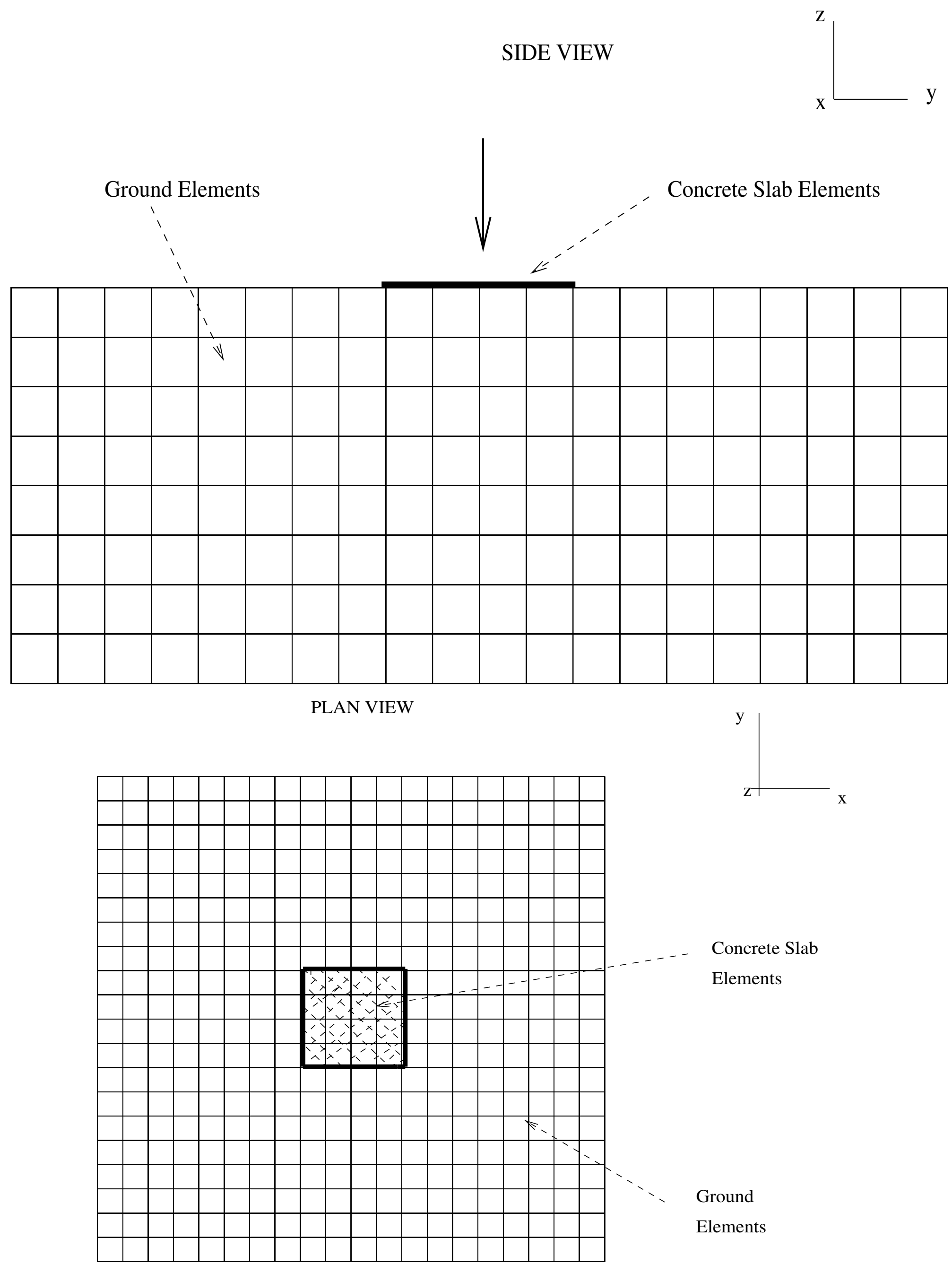
$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{C}\dot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{f}(t) \qquad n \text{ d.o.f.}$$

- 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: ($\overline{\mathbf{a}} = -(2\pi f)^2 \overline{\mathbf{q}}(f)$):

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

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


SIDE VIEW
z
x
y
Ground Elements
Concrete Slab Elements
PLAN VIEW
y
z
x
Concrete Slab
Elements
Ground
Elements

Model Problem: 3D Soil-Structure interaction

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

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

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

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

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

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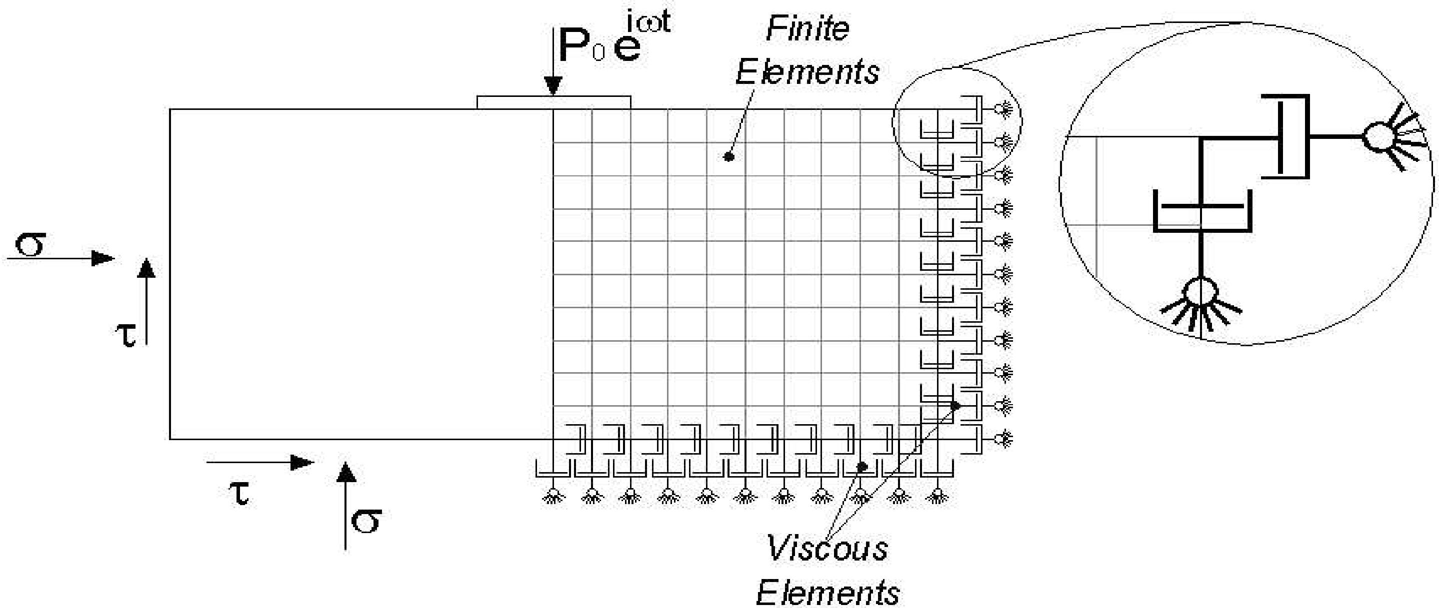
$P_0 e^{i\omega t}$
Finite
Elements
σ
τ
τ
σ
Viscous
Elements