On parametrized linear systems, moments, eigenvalues, gradients, and Krylov methods

Karl Meerbergen

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WSC Spring Meeting — Antwerp

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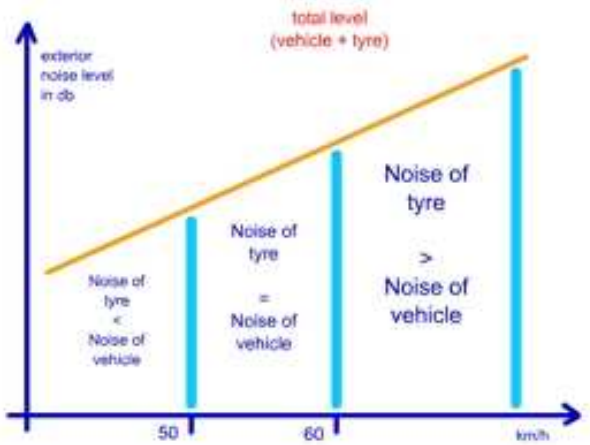
Outline

1. Motivation
2. Overview of methods
   - Modal truncation
   - Vector-Padé approximation
   - Frequency sweeping
   - Input/output MOR
3. Lanczos method
4. Nonlinear frequency dependence
5. Multiple right-hand sides
6. Gradients
7. Conclusions

Examples of vibrating systems

- Car tyres





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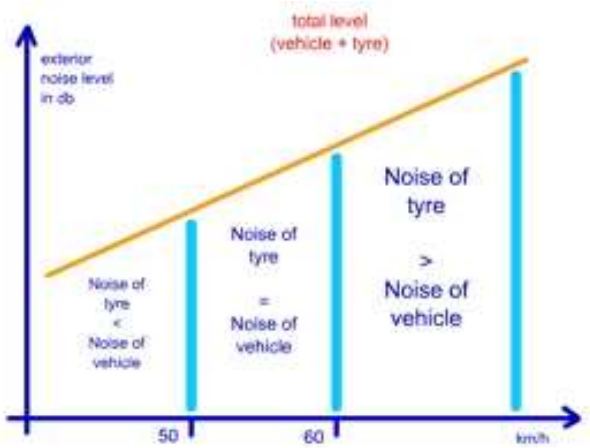




- Windscreens



  - Structural damping
  - Choice of connection (glue) to the car

Examples of vibrating systems

- Planes





Examples of vibrating systems

- Planes



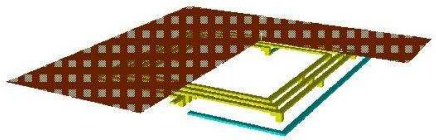


- Bridge vibrating under footsteps and Thames wind



Examples of vibrating systems

- Maxwell-equation – electrical circuits



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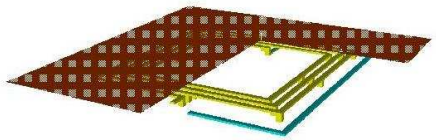


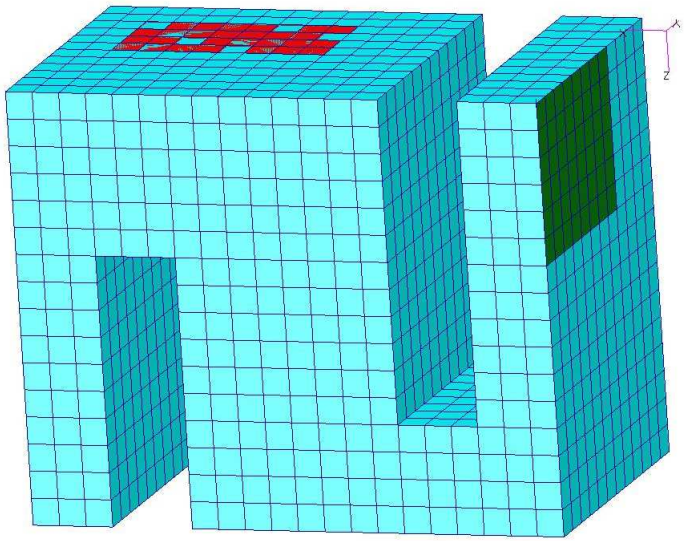
- micro-gyroscope for navigation systems

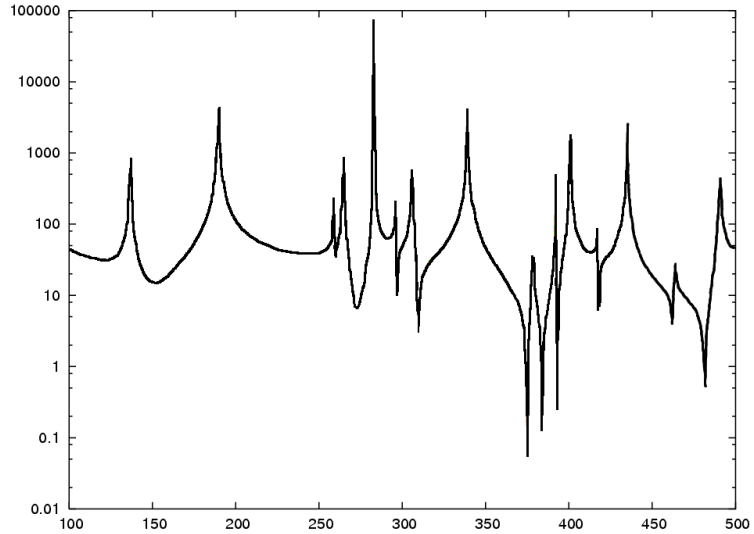


Fourier analysis of finite element model

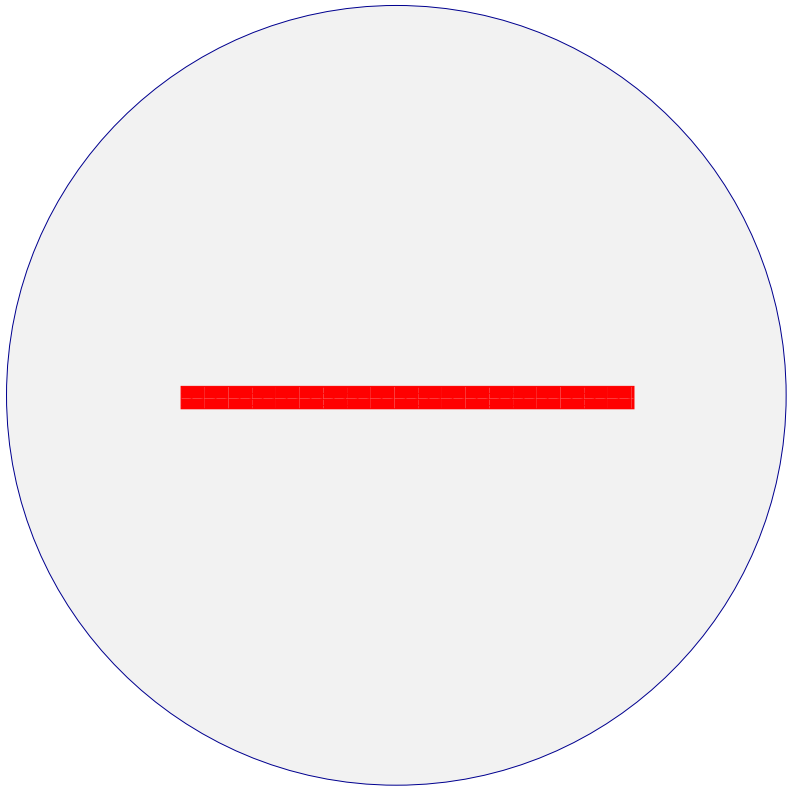
- $$(K + i\omega C - \omega^2 M)\tilde{x} = \tilde{f}$$

  f and x : vectors of length n
  K, C and M : $n \times n$ sparse matrices. In real applications n varies from 10^3 to over 10^6.
- $\tilde{x}$ is called the frequency response function.
- Compute x for $\omega = \omega_1, \ldots, \omega_p \in \Omega = [\omega_{\min}, \omega_{\max}]$.





Acoustic industrial applications : vibro-acoustics



- vibrating structure (modelized by structural modes)
- acoustic domain (finite elements)
- acoustic radiation towards infinity (infinite elements)
- structure is modelized by 'modes' (eigen functions)

Traditional frequency response computation

1. For $\omega = \omega_1, \ldots, \omega_p$
   1.1. Solve the linear system $(K + i\omega C - \omega^2 M)x = f$ for x

- For each frequency, a large system of algebraic equations needs to be solved.
  This requires a linear solver for a large sparse matrix.
  - For a direct solver (based on LU factorization):
  - a sparse matrix factorization $LU = K - \omega^2 M + i\omega C$ (expensive)
  - and a backward solve $LUx = f$ (relatively cheap).

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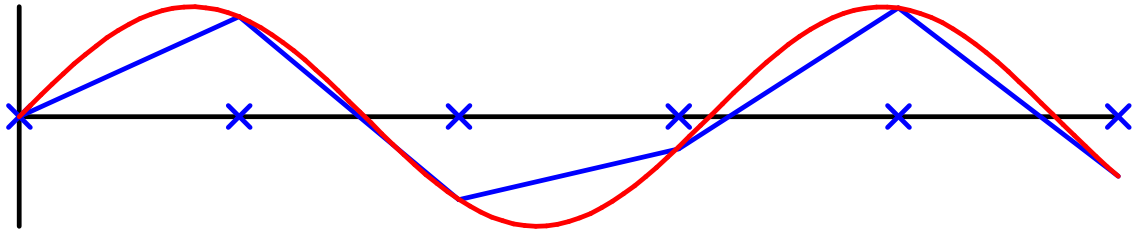
The goal is to reduce the number of matrix factorizations.

Linear system solvers

- Discretization error depends on largest frequency: larger frequency means finer mesh



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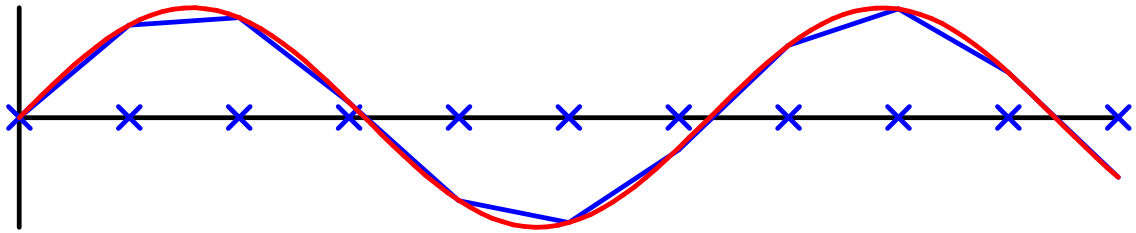


- Direct linear system solver: up to 1M dofs: no problem
  For a complex valued system of 3D volume discretization with 100,000 dofs, direct method solution time is of the order of 10 seconds.
- Iterative linear system solver
  - The last ten years effective preconditioners for the Helmholtz equation have been developed. [Erlangga, Vuik & Oosterlee, 2004, 2006], [van Gijzen, Erlangga, Vuik, 2007], [M. & 2008], [Vanroose & co]
  - Iterative methods can be seen as 'validation' of model
- AMLS [Bennighof]: automated level substructuring

Overview of methods

Consider

$$(K - \omega^2 M)x = f$$

with

- K and M large sparse, real symmetric matrices
- M positive definite
- f independent of ω: typically point loads

Three basic methods:

- Modal truncation
- Padé approximation
- Mixed direct iterative procedure (fast frequency sweeping)

Modal truncation

- Consider the eigendecomposition

$$Ku_j = \lambda_j M u_j$$

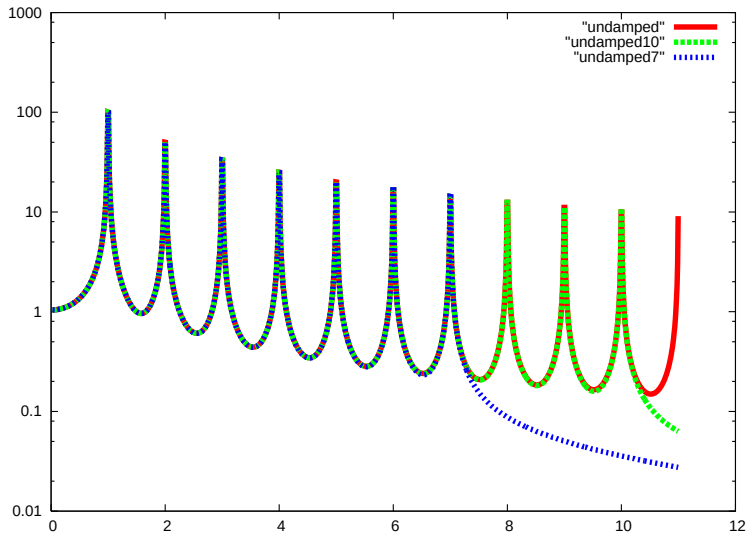
- The solution of $(K - \omega^2 M)x = f$ is

$$x = \sum_{j=1}^{n} u_j \frac{u_j^T f}{\lambda_j - \omega^2}$$

- Rational function with poles λ_j.

Modal superposition, cont.

$$x = \sum_{j=1}^{n} u_j \frac{u_j^T f}{\lambda_j - \omega^2} \approx \sum_{j=1}^{k} u_j \frac{u_j^T f}{\lambda_j - \omega^2}$$



Vector-Padé approximation

Approximation of $x = (K - \alpha M)^{-1} f$ by

$$\tilde{x} = \frac{x_0 + \alpha x_1 + \cdots + \alpha^{k-1} x_{k-1}}{(\alpha - \lambda_1) \cdots (\alpha - \lambda_k)}$$

This is a rational function with k poles.

Determine the coefficients so that

- the first k derivatives in σ match

Frequency sweeping

For each ω precondition

$$(K - \omega^2 M)x = f$$

into

$$(K - \sigma M)^{-1}(K - \omega^2 M)x = (K - \sigma M)^{-1} f$$

and solve by an iterative method.

- Use linear system solver for applying $(K - \sigma M)^{-1}$
- For the AMLS method, $K - \sigma M$ is a diagonal matrix.

Input-output system

- SISO

$$\begin{aligned}(K - \omega^2 M)x &= b \\ y &= d^T x\end{aligned}$$

- Compute y accurately and fast
- Use MOR as fast solver
- Often many outputs (100's or 1000's)
- Twosided methods (MOR) are not often used in this case

Summary

- Modal truncation:

$$\tilde{x} = \sum_{j=1}^{k} u_j \frac{u_j^T f}{\lambda_j - \alpha}$$

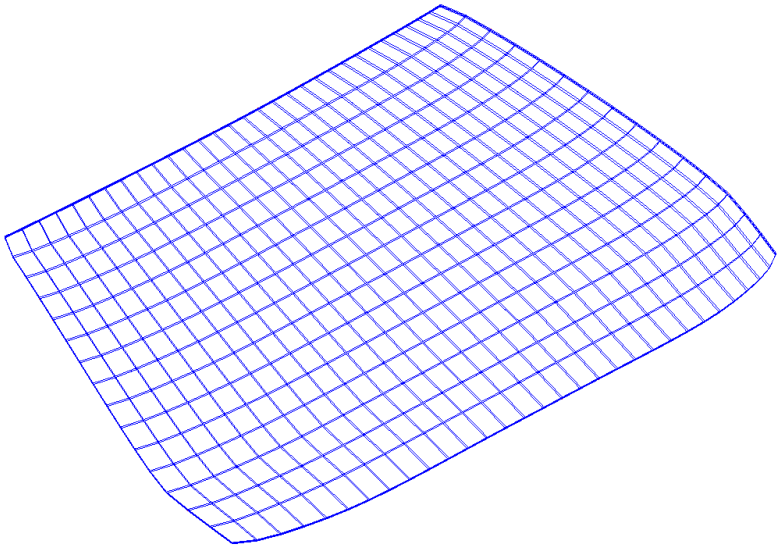
- Padé approximation:

$$\tilde{x} = \frac{x_0 + \alpha x_1 + \cdots + \alpha^{k-1} x_{k-1}}{(\alpha - \mu_1) \cdots (\alpha - \mu_k)}$$

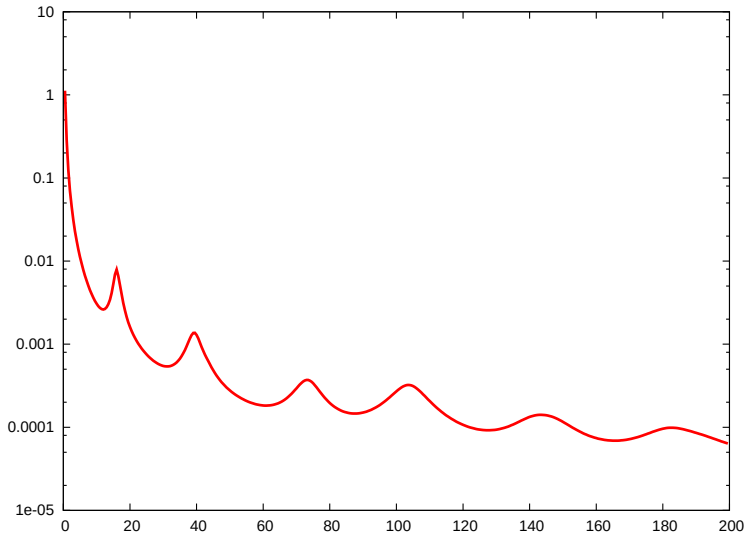
- Frequency sweeping
  Solve $(M - \omega^2 M)x = f$ by an iterative method
- MOR: find reduced model for linear system

$$\begin{aligned} (K - \omega^2 M)x &= b \\ y &= d^T x \end{aligned}$$

Numerical example: BMW Windscreen



- Glaverbel-BMW windscreen with 10% structural damping
- Direct method : 2653 seconds
- Lanczos method : 14 seconds



Notation

- Define $\alpha = \omega^2$
- $A = (K - \sigma M)^{-1} M$ and $b = (K - \sigma M)^{-1} f$
- Assume $\sigma = 0$ and

then we solve

$$(K - \alpha M)x = f$$

or

$$\begin{aligned} (K - \sigma)^{-1}(K - \alpha M)x &= (K - \sigma)^{-1} f \\ (I - \alpha A)x &= b \end{aligned}$$

Eigenvalue problem:

$$Ku_j = \lambda_j M u_j$$

Assume A symmetric.

Lanczos method

- Krylov space: $\text{span}\{b, Ab, \ldots, A^{k-1}b\}$

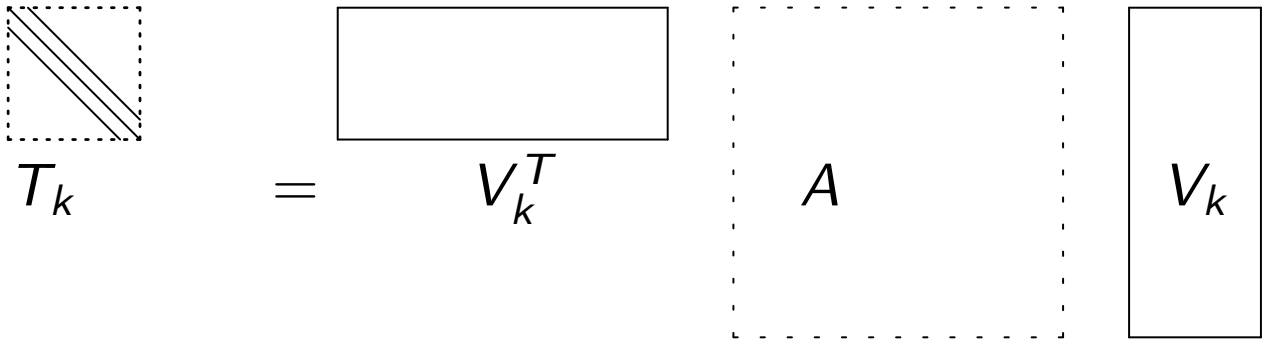
- Lanczos method builds orthogonal basis $V_k = [v_1, \ldots, v_k]$.

$$\text{Range}(V_k) = \text{span}\{b, Ab, \ldots, A^{k-1}b\}$$

- and a tridiagonal matrix $T_k = V_k^T A V_k$
- major cost: k matrix vector products with A : $w = Av$
- small cost when k is small
- Also called Ritz vector technique (mechanical engineering)

Lanczos method

Transform a large size matrix into a small size matrix



Shift-invariance property

- Krylov spaces

$$\{v, Av, A^2v, \ldots\}$$

and

$$\{v, (I - \alpha A)v, (I - \alpha A)^2 v, \ldots\}$$

are equal, since $(I - \alpha A)v = v - \alpha Av$

- Applying the Lanczos method to A, applies it for free to $A + \alpha I$ for all α.

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- Applying the Lanczos method to A, applies it for free to $A + \alpha I$ for all α.

- As, a consequence,

$$\begin{aligned} V_k^T A V_k &= T_k \\ V_k^T (I - \alpha A) V_k &= I - \alpha T_k \end{aligned}$$

- Therefore, no need to build Krylov space for different values of α

Shifted or parameterized linear systems

- Analyzed in the context of model reduction methods (Connection with rational approximation)
  [Gallivan, Grimme, Van Dooren 1994], [Feldman, Freund 1995], [Gallivan, Grimme, Van Dooren 1996], [Grimme, Sorensen, Van Dooren 1996], [Ruhe & Skoogh 1998], [Bai & Freund 2000], [Bai & Freund 2001] [Bai & Su 2006]
- in the context of parameterized linear systems
  [Freund 1993], [Frommer & Glässner, 1993], [Simoncini & Gallopoulos 1998], [Simoncini, 1999, 2010], [Simoncini & Perotti 2002], [M. 2003], [Edema, Vuik 2008], [M. 2008], [M. & Bai, 2010]

Undamped vibration problem

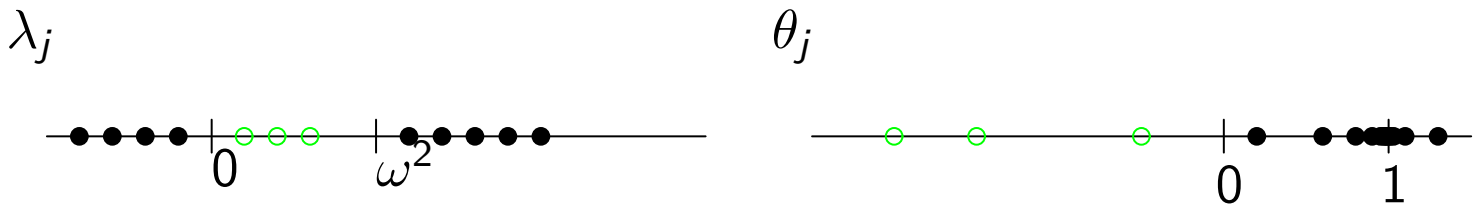
- When $A = K^{-1}M$, A is non-symmetric.
- However, $x^T MAy = y^T MAx$ for all x, y. So, A is self-adjoint with the M inner product
- Use the Lanczos method with M orthogonalization:

$$V_k^T M V_k = I$$

- Matrix vector products with A:
  - One matrix factorization of $K = LDL^T$
  - k solves of the form $LDL^T w = Mv$

Iterative solver connection

- Lanczos method (Conjugate gradients) is iterative linear system solver for
$$(I - \alpha A)x = b$$
- Let $A = K^{-1}M$
- Let $Ku_j = \lambda_j Mu_j$
- Eigenvalues of $K^{-1}(K - \omega^2 M)$ are $\theta_j = \dfrac{\lambda_j - \omega^2}{\lambda_j}$
- Fast convergence when most eigenvalues are clustered around one:
  - ω close to 0



- When there are no eigenvalues λ between 0 and ω^2, then we have a positive definite linear system

MINRES versus Lanczos

- Lanczos:

$$\tilde{x} = \sum \frac{y_j}{\alpha - \mu_j}$$

  - Vertical asymptotes

MINRES versus Lanczos

- Lanczos:

$$\tilde{x} = \sum \frac{y_j}{\alpha - \mu_j}$$

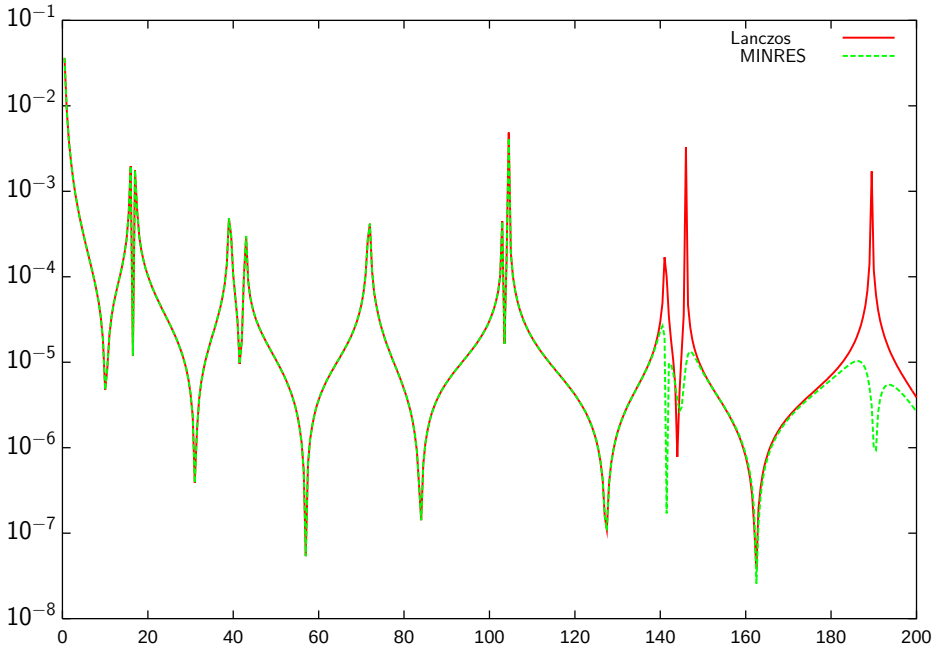
  - Vertical asymptotes

- MINRES:

$$\tilde{x} = \sum \frac{y_j(\alpha)}{\alpha - \mu_j(\alpha)}$$

  - Denominator is never zero
  - No vertical asymptotes

Example


Lanczos
MINRES
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
0
20
40
60
80
100
120
140
160
180
200

Eigenvalue and Padé connection

- Lanczos method produces k eigenvalue estimates: eigenvalues of T_k
  We can show that the Lanczos method computes

$$\tilde{x} = \sum_{j=1}^{k} \tilde{u}_j \frac{\tilde{w}_j^T f}{\lambda_j - \alpha}$$

  where $\tilde{u}_j$ is a Ritz vector (i.e. approximate eigenvector).

  - There are k terms, so we can only compute k vertical asymptotes in the function
  - The number of eigenvalues in the frequency range should be smaller than k.

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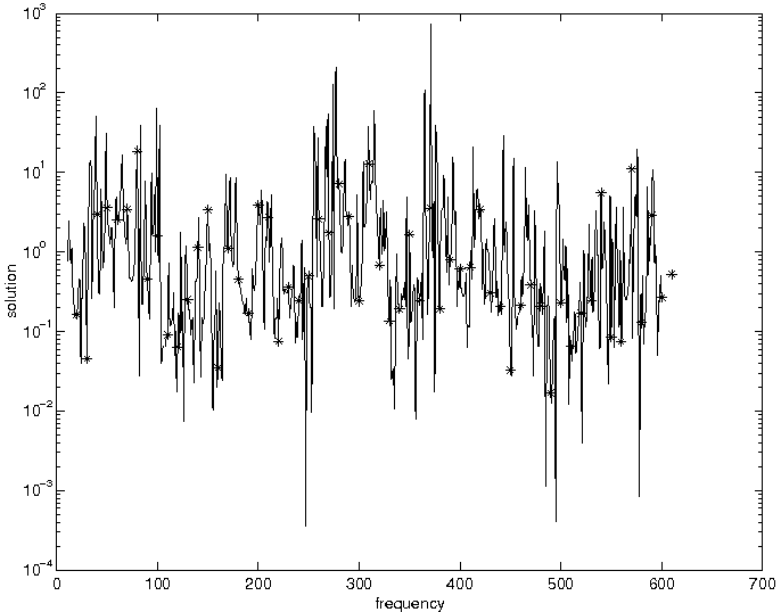
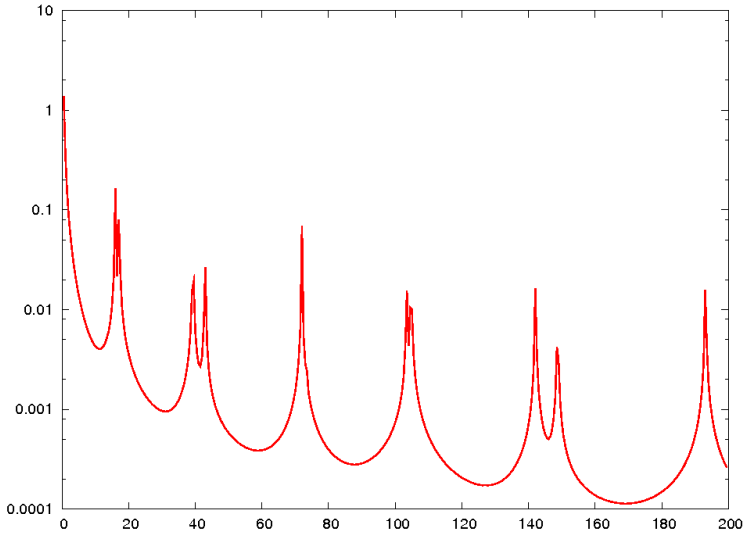
  - There are k terms, so we can only compute k vertical asymptotes in the function
  - The number of eigenvalues in the frequency range should be smaller than k.
- Padé connection: $\tilde{x}$ is a rational approximation with

$$x^{(j)}(0) = \tilde{x}^{(j)}(0) \quad \text{for} \quad j = 0, \ldots, k-1$$

Eigenvalue connection: example



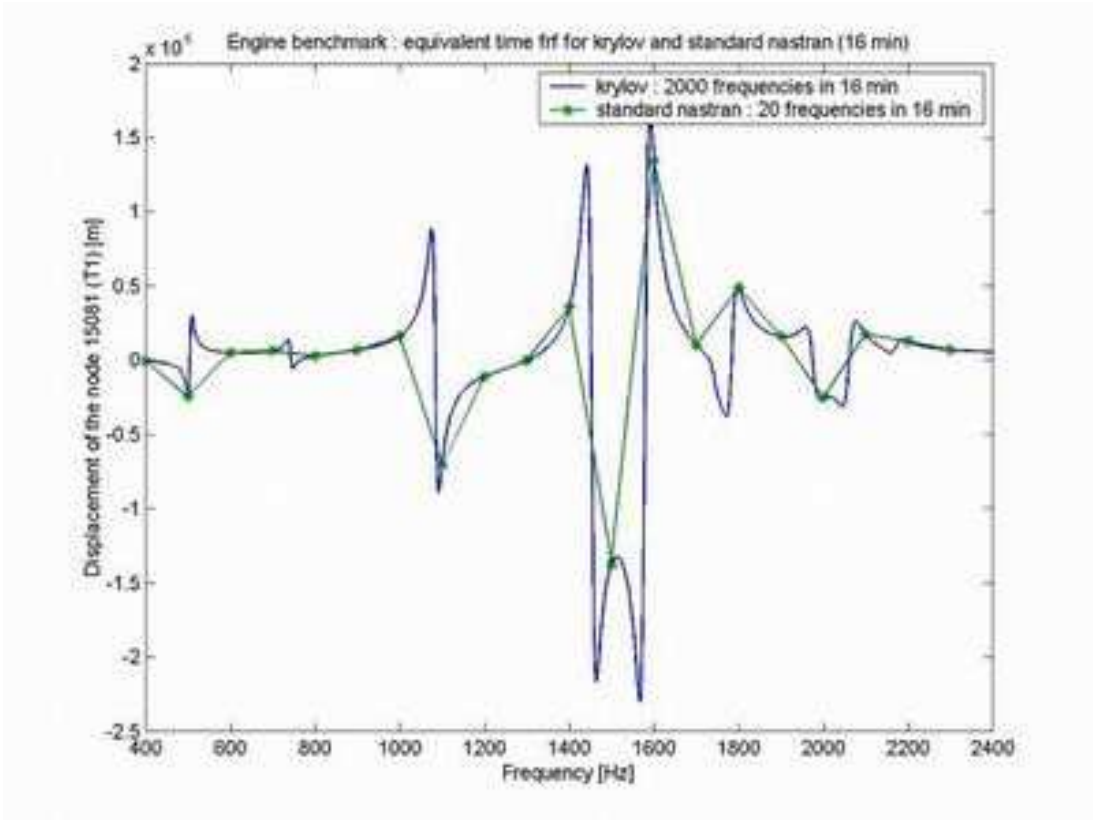


Hard problem: more than 10,000 eigenvalues

Easy problem: less than 20 eigenvalues

Industrial example with NASTRAN

- Traditional computation
  - For each frequency, perform factorization of $K - \omega^2 M$ and solve
- Lanczos computation
  - One matrix factorization of $K - \sigma M$ and solve
  - k solves.



Nonlinear frequency dependence

$$(K + i\omega C - \omega^2 M)x = f$$

- 'Linearization':
  - Define matrices A and B

$$A = \begin{bmatrix} K & \\ & I \end{bmatrix} \qquad B = \begin{bmatrix} iC & -M \\ I & \end{bmatrix}$$

so that

$$(A - \omega B)\begin{pmatrix} x \\ \omega x \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

This is called a linearization, a similar trick as the solution of second order ODE's.

Linearizations

- Linearizations have been studied for the solution of the quadratic eigenvalue problem

$$(K + \lambda C + \lambda^2 M)u = 0$$

[Gohberg, Lancaster, Rodman, 1982] [Tisseur, M. 2001] [Mackey,Mackey,Mehl,Mehrmann,2006]

- Methods based on Companion 'linearization'
- Higher order polynomials

$$(A_0 + \omega A_1 + \cdots + A_p \omega^p)x = f$$

Transform to

$$\left(\begin{bmatrix} A_0 & & & \\ & -I & & \\ & & \ddots & \\ & & & -I \end{bmatrix} + \omega \begin{bmatrix} A_1 & A_2 & \cdots & A_p \\ I & 0 & & \\ & \ddots & \ddots & \\ & & I & 0 \end{bmatrix} \right) \begin{pmatrix} x \\ \omega x \\ \vdots \\ \omega^{p-1} x \end{pmatrix} = \begin{pmatrix} f \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Methods

- [Parlett & Chen 1990] Pseudo Lanczos method (pretends B is positive definite)
- [Simoncini & al, 2005] similar
- [Freund, 2005]: analysis of Krylov spaces
- [Bai & Su, 2005] SOAR: based on Arnoldi's method
- [M. 2008] Q-Arnoldi: based on Arnoldi's method (for eigenvalue problems)
- [Amiraslani, Corless, Lancaster, 2009] Other polynomials than powers of ω.
- [Jarlebring, M., Michiels 2010] Infinite-Arnoldi: based on Arnoldi's method (for delay eigenvalue problem)

Multiple right-hand sides

$$(K - \omega^2 M)[x_1, \ldots, x_s] = [f_1, \ldots, f_s]$$

for $\omega \in \Omega = [\omega_{\min}, \omega_{\max}]$.
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- Use Lanczos method for each f_j separately
  - Low memory cost
  - The cost is proportional to s

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- Use block-Lanczos method for each all f_j together
  - Fast method
  - High memory cost

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- Recycling Ritz vectors in Krylov methods [Giraud,Ruiz & Touhami, 2006] [Kilmer & de Sturler 2006] [Darnell, Morgan, Wilcox 2007] [Stathopoulos & Orginos, 2009][M. & Bai, 2010]

Recycling

- Compute the FRF for the first right-hand side
- Extract eigenvalues / eigenvectors
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$$\hat{x} = \sum_{j=1}^{k} \hat{u}_j \frac{\hat{u}_j^T f}{\hat{\lambda}_j - \omega^2}$$

    - ★ First k moments of $\hat{x}$ and x match.

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    - ★ First k moments of $\hat{x}$ and x match.
  - With reuse of eigenvalues:

$$\hat{x} = \sum_{j=1}^{p} u_j \frac{u_j^T f}{\lambda_j - \omega^2} + \sum_{j=p+1}^{k} \hat{u}_j \frac{\hat{u}_j^T f}{\hat{\lambda}_j - \omega^2}$$

    - ★ First $k - p$ moments of $\hat{x}$ and x match.
    - ★ Interpolation in the p deflated eigenvalues.

Frequency sweeping with modal acceleration

The solution of

$$(I - \omega^2 A)x = b \tag{1}$$

for $\omega \in \Omega$ is split into two parts.

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- Compute

$$x_p = \sum_{j=1}^{p} u_j \frac{u_j^T f}{\lambda_j - \omega^2}$$

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$$x_p = \sum_{j=1}^{p} u_j \frac{u_j^T f}{\lambda_j - \omega^2}$$

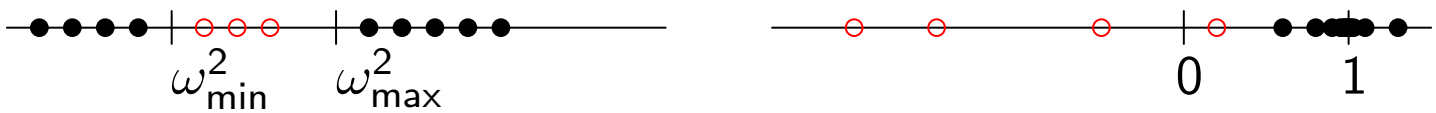
- Solve (1) iteratively using starting vector x_p, i.e. $x = x_p + y$ with y the solution of

$$\begin{aligned} (I - \omega^2 A)y &= b - (I - \omega^2 A)x_p \\ &= (I - U_p U_p^T M)b \end{aligned}$$

Modal acceleration

- We can prove that eigenvalues in the frequency range are computed to machine precision
- As a result, the right-hand side has 'no' components in the associated eigenvalues
- This significantly improves the condition number

Eigenvalues of $Kx = \lambda Mx$ Eigenvalues of A



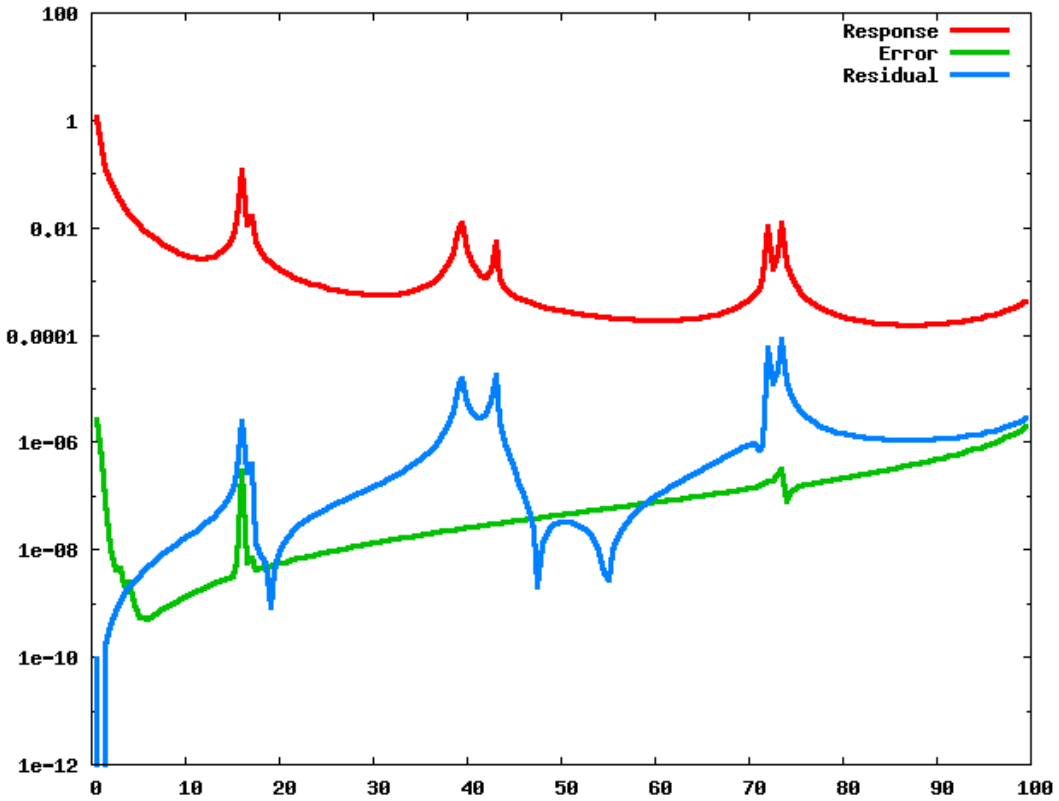
  - Most eigenvalues of A lie near one.
  - The number of required iterations is the number of isolated eigenvalues of A away from one.
  - Convergence for all $\omega^2 \in \Omega^2$ requires the number of iterations, k, to be at least the number of eigenvalues in Ω^2.
  - Remove the red eigenvalues: positive definite matrix, and small condition number

Windscreen

- Glaverbel-BMW windscreen
- grid : 3 layers of 60×30 HEX08 elements ($n = 22,692$)
- $\Omega = [0, 100]$
- First run:
  - unit point force at one of the corners
  - Use Lanczos method with $k = 20$ vectors.
  - We keep the Ritz values in $[0, 2 \times 100^2]$: $p = 14$

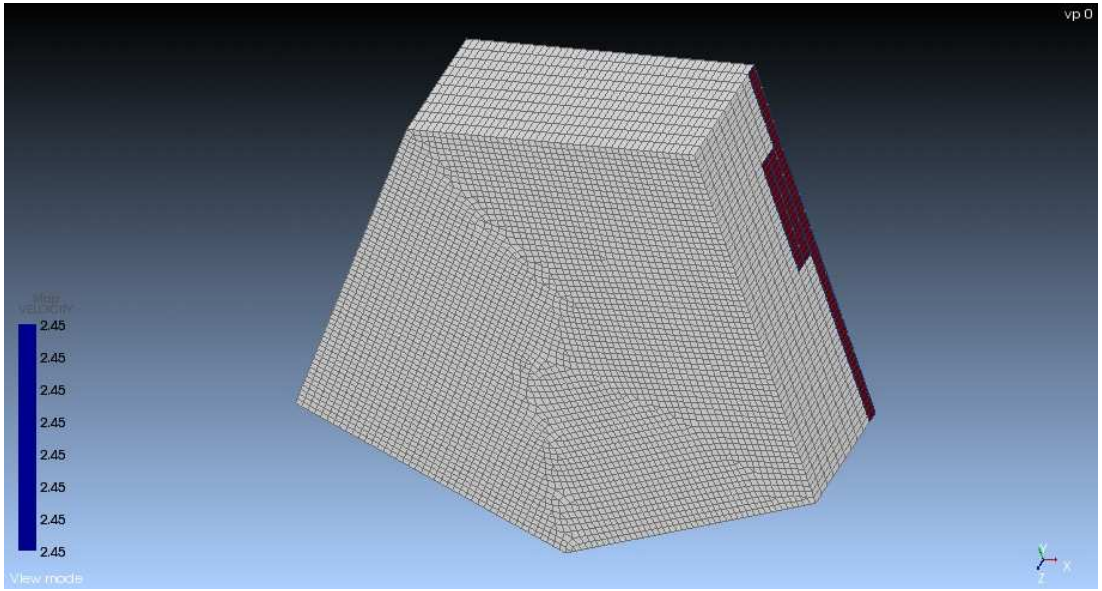
Windscreen

- Second run with other right-hand side
  - Perform 6 additional Lanczos steps



  - The largest condition number of linear system is 1.9813.
  - Six iterations reduce the error by $2 \cdot 10^{-5}$.

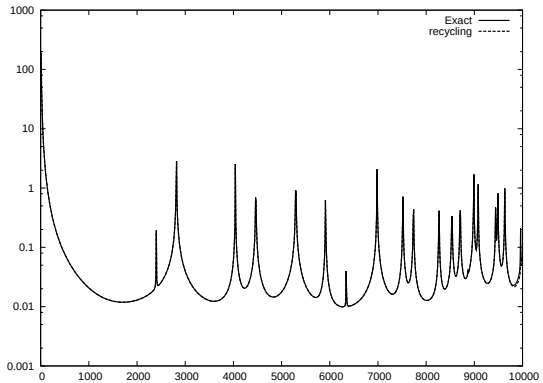
Acoustic cavity



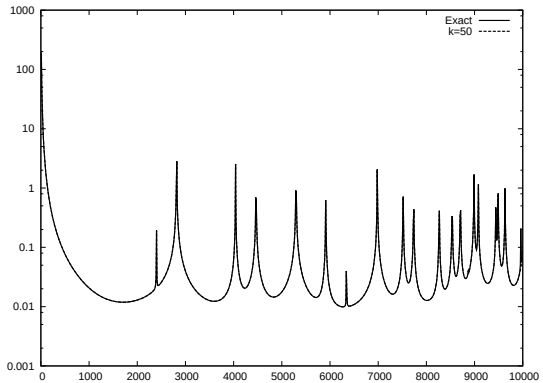
- $n = 48,158$
- Frequency range : $[0, 10000]$
- 202 right-hand sides
- matrix factorization: 8 seconds
- Lanczos method with 40 vectors: 6 seconds

Acoustic cavity (cont.)

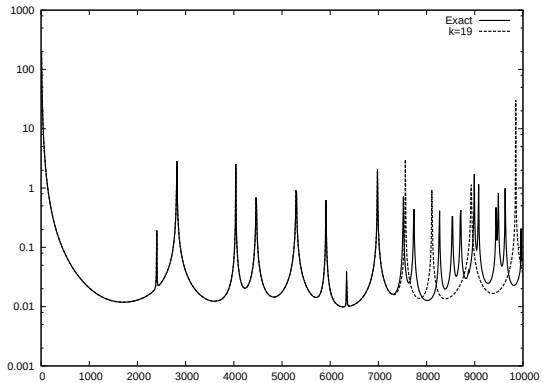
- 2nd right-hand side: keep the 31 Ritz values in $[0, 2 \times 10.000^2]$.
- 9 additional Lanczos iterations recycling 31 Ritz vectors: 2 seconds



With recycling

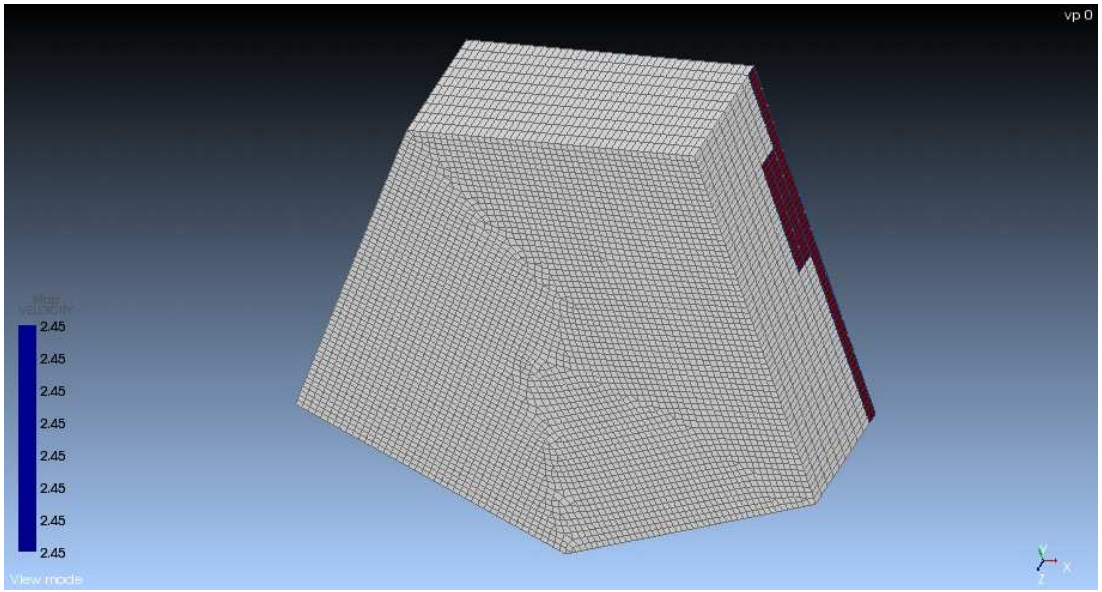


Lanczos $k = 50$



Lanczos $k = 19$

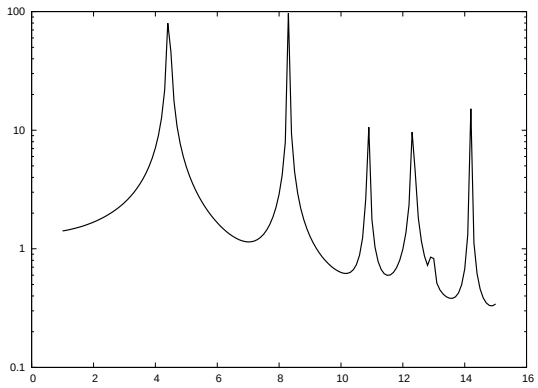
Acoustic cavity



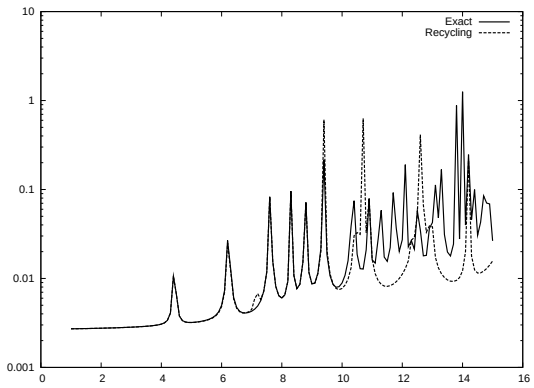
- $n = 140,228$
- Frequency range : $[0, 10000]$
- 202 right-hand sides
- matrix factorization: 13 seconds
- Lanczos method with 50 vectors: 15 seconds
- Recycling 36 vectors: only 4 seconds
- For 201 right-hand sides: 800 instead of 3000 seconds.

Multiple eigenvalues

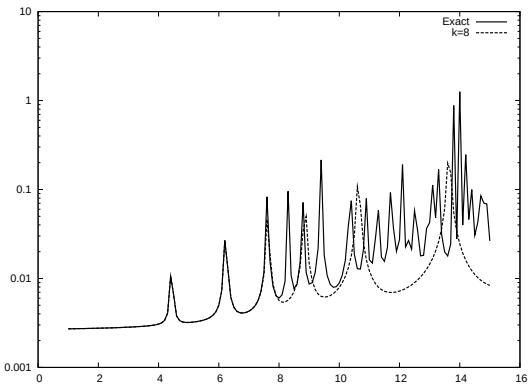
- 3D Laplacian on a cube.
- 30 Lanczos iterations with first right-hand side
- Recycle 22 Ritz pairs
- Run 8 iterations with the second right-hand side



Lanczos for f_1



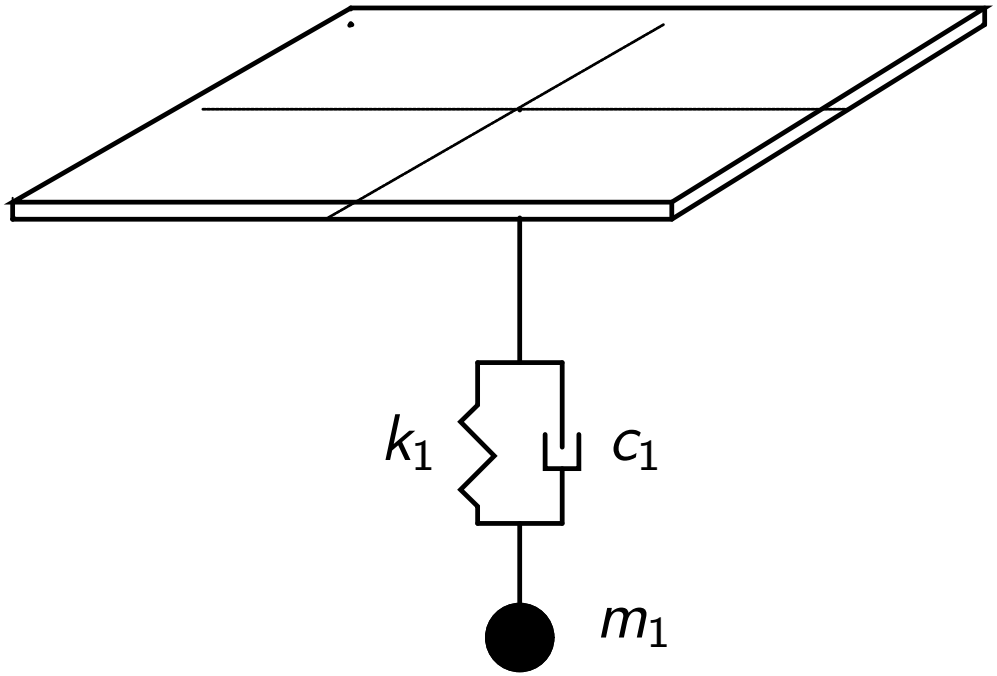
Recylcing for f_2



Lanczos $k = 8$ for f_2

Gradient computation

- Determination of optimal parameters of a vibrating system
- Example: optimal parameters for a damper of a floor in a building near a noisy road



Optimization problem

- Parametrized linear system:

$$\begin{cases} (K(p) + i\omega C(p) - \omega^2 M(p))x &= f \\ y &= d^T x \end{cases}$$

- Find parameters p so that
  - $\|y\|_2 = \int_0^{\omega_{\max}} |y|^2 d\omega$ is minimal
  - $\|y\|_\infty = \sup_0^{\omega_{\max}} |y|^2$ is minimal
- This is, in general, a non-smooth optimization problem
- Expensive evaluation of y and the gradient
- Model order reduction is an important tool to reduce the computational cost
  - Both function value and gradient should be computed by the reduced model

Gradient computation

- [Antoulas, Beattie, Gugercin 2010] [Yue, M. 2010] show interpolation properties on derivatives for two-sided MOR:

$$\begin{cases} (K(p) + i\omega C(p) - \omega^2 M(p))x &= f \\ y &= d^T x \end{cases}$$

  - $Z(\omega) = K + i\omega - \omega^2 M$
  - $x = Z(\omega)^{-1} f$
  - $y = d^T x$
  - $\dfrac{\partial y}{\partial p} = (Z(\omega)^{-1} d)^T \dfrac{\partial Z(\omega)}{\partial p} Z(\omega)^{-1} f$
- $Z(\omega)^{-T} d$ and $Z(\omega)^{-1} f$ are computed by two-sided Krylov methods

Numerical example

- Floor with damper ($n = 29800$)
- Reduced model $k = 25$
- Determine optimal parameters

	Direct method	Krylov
Matrix size	29800	25
Optimizer computed	(14007181,42404)	(14007225, 42410)
Function value	134.5477989	134.5479496
CPU time	Several Days	3735s

Conclusions

- Krylov methods usually work well for acoustic simulation
- Recycling Ritz vectors is a reliable and efficient method for the solution with multiple right-hand sides
- Parametrized models with many parameters are current challenges

- Solving parameterized linear systems with multiple right-hand sides can benefit from recycling Ritz vectors
- Does not work well when eigenvalues are multiple
- Also works for Rayleigh damping

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