# Reduced Order Models For A Few Problems with Parameter Sweeps

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- Frequency Response Problem
  - Work in collaboration with C. Farhat and R. Tezaur (Stanford U.)
- Coherent Transport using Green function
  - Work in collaboration with M. P. Anantram and D. Ji (U. Washington EE)
- Incompressible flow simulations with varying viscosity
  - Work in collaboration with Y. Wu (U. Washington)

Discrete problems of the form

$$\begin{bmatrix} \mathsf{M}_{s} & \mathbf{0} \\ -\rho_{f}\mathsf{C} & \frac{1}{c_{f}^{2}}\mathsf{M}_{f} \end{bmatrix} \begin{bmatrix} \ddot{\mathsf{u}}_{s} \\ \ddot{\mathsf{p}}_{f} \end{bmatrix} + \begin{bmatrix} \mathsf{D}_{s} & \mathbf{0} \\ \mathbf{0} & \mathsf{D}_{f} \end{bmatrix} \begin{bmatrix} \dot{\mathsf{u}}_{s} \\ \dot{\mathsf{p}}_{f} \end{bmatrix} \\ + \begin{bmatrix} \mathsf{K}_{s} & \mathsf{C}^{\mathsf{T}} \\ \mathbf{0} & \mathsf{K}_{f} \end{bmatrix} \begin{bmatrix} \mathsf{u}_{s} \\ \mathsf{p}_{f} \end{bmatrix} = \begin{bmatrix} \mathsf{f}_{s} \\ \mathsf{g}_{f} \end{bmatrix}$$

- Very large sparse matrices ( $\geq 10^6$ ).
- M<sub>s</sub>, K<sub>s</sub>, M<sub>f</sub>, and K<sub>f</sub> are usually real symmetric matrices.
- D<sub>s</sub> and D<sub>f</sub> are damping matrices.
- C is the coupling matrix between the structure and fluid.

These matrices typically depend on geometry, topology, and material parameters.

Time-harmonic excitation

$$\begin{bmatrix} \mathbf{f}_s \\ \mathbf{g}_f \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} e^{i\omega t} \quad \Rightarrow \quad \begin{bmatrix} \mathbf{u}_s \\ \mathbf{p}_f \end{bmatrix} = \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} e^{i\omega t}$$

The model becomes a frequency-dependent linear system

$$-\omega^{2} \begin{bmatrix} \mathbf{M}_{s} & \mathbf{0} \\ -\rho_{f} \mathbf{C} & \frac{1}{c_{f}^{2}} \mathbf{M}_{f} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} + i\omega \begin{bmatrix} \mathbf{D}_{s} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{f} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{s} & \mathbf{C}^{T} \\ \mathbf{0} & \mathbf{K}_{f} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix}$$

Discrete problems of the form

$$(\mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega))\mathbf{x}(\omega) = \mathbf{f}(\omega)$$

Frequency response problems have to be solved for many parameters.

- Very large sparse matrices ( $\geq 10^6$ )
- Problem with multiple frequencies (100+  $\omega$ ) in an interval  $[\omega_l, \omega_r]$
- Interested in the whole field  $x(\omega)$
- Linear systems are increasingly difficult to solve when  $\omega$  grows

# Applications of Frequency Response Problems

Structural vibrations and interior noise acoustics
 Elastodynamics
 Interior Helmholtz



Scattering
 Exterior Helmholtz





Maxwell



- Straightforward Algorithm
  - Sample the interval of interest  $[\omega_l, \omega_r]$ :  $\hat{\omega}_0, \cdots, \hat{\omega}_S$
  - Solve the linear system

$$(\mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega))\mathbf{x}(\omega) = \mathbf{f}(\omega)$$

- CPU intensive
- Reduced-order model can speed up the simulation time.

- Many techniques have been proposed with a similar goal.
  - Reviews: Freund (2003), Bai-Dewilde-Freund (2005), Antoulas (2005), ...
- Interpolatory Reduced Order Models (Padé approximation or moment matching)
  - Freund (2003), Bai-Su (2005), Beattie-Gugercin (2005), Patera et al. (2006), Olsson-Ruhe (2006), Avery-Farhat-Reese (2007), Meerbergen (2008), Tuck Lee-Pinsky (2008), ...

Consider

$$\mathbf{x}(\omega) = \left(\mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega)\right)^{-1} \mathbf{f}(\omega)$$

A Galerkin approximation in the subspace  $\boldsymbol{\mathsf{V}}$  is such that

$$\begin{aligned} \mathbf{V}^{H}\left[\left(\mathbf{K}-\omega^{2}\mathbf{M}+\mathbf{S}(\omega)\right)\mathbf{V}\tilde{\mathbf{x}}(\omega)-\mathbf{f}(\omega)\right]&=\mathbf{0}\\ \mathbf{V}^{H}\left(\mathbf{K}-\omega^{2}\mathbf{M}+\mathbf{S}(\omega)\right)\mathbf{V}\tilde{\mathbf{x}}(\omega)&=\mathbf{V}^{H}\mathbf{f}(\omega)\\ \tilde{\mathbf{x}}(\omega)&=\left(\mathbf{V}^{H}\mathbf{K}\mathbf{V}-\omega^{2}\mathbf{V}^{H}\mathbf{M}\mathbf{V}+\mathbf{V}^{H}\mathbf{S}(\omega)\mathbf{V}\right)^{-1}\mathbf{V}^{H}\mathbf{f}(\omega)\\ \mathbf{x}(\omega)&\approx\mathbf{V}\tilde{\mathbf{x}}(\omega)=\mathbf{V}\left(\mathbf{V}^{H}\mathbf{K}\mathbf{V}-\omega^{2}\mathbf{V}^{H}\mathbf{M}\mathbf{V}+\mathbf{V}^{H}\mathbf{S}(\omega)\mathbf{V}\right)^{-1}\mathbf{V}^{H}\mathbf{f}(\omega)\end{aligned}$$

A one-point matching approximation of x at  $\omega_0$  is defined as a function  $x_{(\omega_0;J)}$  satisfying

$$\mathbf{x}_{(\omega_0;J)}(\omega_0) = \mathbf{x}(\omega_0) \quad \frac{d^j \mathbf{x}_{(\omega_0;J)}}{d\omega^j}(\omega_0) = \frac{d^j \mathbf{x}}{d\omega^j}(\omega_0), \quad \forall j < J$$

The Taylor expansion of  $\mathbf{x}_{(\omega_0;J)}$  around  $\omega_0$  matches the first J terms of the Taylor expansion of  $\mathbf{x}$  around the same point,

$$\mathbf{x}(\boldsymbol{\omega}) = \mathbf{x}_{(\boldsymbol{\omega}_0;J)}(\boldsymbol{\omega}) + \mathscr{O}\left((\boldsymbol{\omega} - \boldsymbol{\omega}_0)^J\right)$$

Local convergence around the expansion point  $\omega_0$ .

The derivatives of  ${\bf x}$  are solutions of a system of linear equations with the same left-hand side

$$\left(\mathsf{K} - \omega^2 \mathsf{M} + \mathsf{S}(\omega)\right) \frac{d\mathsf{x}}{d\omega}(\omega) = \frac{d\mathsf{f}}{d\omega}(\omega) - \left(\frac{d\mathsf{S}}{d\omega}(\omega) - 2\omega\mathsf{M}\right)\mathsf{x}(\omega)$$

and

$$\left( \mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega) \right) \frac{d^j \mathbf{x}}{d\omega^j}(\omega) = \frac{d^j \mathbf{f}}{d\omega^j}(\omega) - \sum_{k=1}^j \frac{j!}{k!(j-k)!} \frac{d^k}{d\omega^k} \left( \mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega) \right) \frac{d^{j-k} \mathbf{x}}{d\omega^{j-k}}(\omega)$$

Consider the matching frequency  $\omega_0$ . If

$$\operatorname{span}\left\{\mathsf{x}(\omega_0),\frac{d\mathsf{x}}{d\omega}(\omega_0),\ldots,\frac{d^{J-1}\mathsf{x}}{d\omega^{J-1}}(\omega_0)\right\}\subset\operatorname{span}\mathsf{V}$$

Then,

$$\begin{aligned} \mathsf{x}(\omega) &= \mathsf{V}\left(\mathsf{V}^{H}\mathsf{K}\mathsf{V} - \omega^{2}\mathsf{V}^{H}\mathsf{M}\mathsf{V} + \mathsf{V}^{H}\mathsf{S}(\omega)\mathsf{V}\right)^{-1}\mathsf{V}^{H}\mathsf{f}(\omega) \\ &+ \mathscr{O}\left((\omega - \omega_{0})^{J}\right) \end{aligned}$$

• Freund-Feldmann (1995), Beattie-Gugercin (2009), ...

#### Interpolatory Model Reduction in a Frequency Band

A Galerkin projection-based method for approximating

$$\mathsf{x}(\omega) = \left(\mathsf{K} - \omega^2 \mathsf{M} + \mathsf{S}(\omega)
ight)^{-1}\mathsf{f}(\omega)$$

in a frequency interval consists in

• Building V that satisfies the property

$$\operatorname{span}\left\{\mathbf{x}(\omega_0), \frac{d\mathbf{x}}{d\omega}(\omega_0), \dots, \frac{d^{J-1}\mathbf{x}}{d\omega^{J-1}}(\omega_0)\right\} \subset \operatorname{span} \mathbf{V}$$

• Evaluating, in the frequency interval,

$$ilde{\mathbf{x}}(\omega) = \left( \mathbf{V}^H \mathbf{K} \mathbf{V} - \omega^2 \mathbf{V}^H \mathbf{M} \mathbf{V} + \mathbf{V}^H \mathbf{S}(\omega) \mathbf{V} 
ight)^{-1} \mathbf{V}^H \mathbf{f}(\omega)$$

• Approximating  $\mathbf{x}(\omega)$  with  $\mathbf{V}\tilde{\mathbf{x}}(\omega)$ 

# Towards Multi-Point Matching

- A single point approximation converges first around the expansion point.
- To get a better approximation over an interval, multiple expansion points can be used at the same time.



 Example for frequency sweep analysis of a thick spherical steel shell submerged in water and excited by a point load on its inner surface.

#### Multi-Point Matching via Galerkin Projection

Consider the matching frequencies  $\omega_0, \cdots, \omega_{P-1}$ . If

$$\operatorname{span}\left\{\mathbf{x}(\omega_{0}), \frac{d\mathbf{x}}{d\omega}(\omega_{0}), \dots, \frac{d^{J-1}\mathbf{x}}{d\omega^{J-1}}(\omega_{0})\right\} + \dots$$
$$\operatorname{span}\left\{\mathbf{x}(\omega_{P-1}), \frac{d\mathbf{x}}{d\omega}(\omega_{P-1}), \dots, \frac{d^{J-1}\mathbf{x}}{d\omega^{J-1}}(\omega_{P-1})\right\} \subset \operatorname{span}\mathbf{V}$$

Then, formally,

$$\begin{split} \mathsf{x}(\omega) &= \mathsf{V}\left(\mathsf{V}^{H}\mathsf{K}\mathsf{V} - \omega^{2}\mathsf{V}^{H}\mathsf{M}\mathsf{V} + \mathsf{V}^{H}\mathsf{S}(\omega)\mathsf{V}\right)^{-1}\mathsf{V}^{H}\mathsf{f}(\omega) \\ &+ \mathscr{O}\left(\prod_{p=0}^{P-1}(\omega - \omega_{p})^{J}\right) \end{split}$$

• Gallivan-Grimme-van Dooren (1996), Beattie-Gugercin (2009), ...

## Multi-Point Matching via Galerkin Projection

Consider

$$\mathbf{x}(\omega) = \left(\mathbf{K} - \omega^2 \mathbf{M} + \mathbf{S}(\omega)\right)^{-1} \mathbf{f}(\omega)$$

- Loop on frequencies:  $\omega_0, \cdots, \omega_{P-1}$ 
  - Set  $\mathbf{x}(\omega_p) = \left(\mathbf{K} \omega_p^2 \mathbf{M} + \mathbf{S}(\omega_p)\right)^{-1} \mathbf{f}(\omega_p)$
  - Compute the derivatives of x at  $\omega_p$  (systems with same matrix)
  - Augment  ${\boldsymbol{\mathsf{V}}}$  with these new derivatives
  - Form an orthonormal basis
- Compute the projected matrices:  $V^H K V$ ,  $V^H M V$ ,  $V^H S(\omega) V$
- Approximate the frequency response over  $[\omega_l, \omega_r]$

$$\mathbf{x}(\omega) \approx \mathbf{V} \left( \mathbf{V}^H \mathbf{K} \mathbf{V} - \omega^2 \mathbf{V}^H \mathbf{M} \mathbf{V} + \mathbf{V}^H \mathbf{S}(\omega) \mathbf{V} 
ight)^{-1} \mathbf{V}^H \mathbf{f}(\omega)$$

Frequency sweep analysis of a thick spherical steel shell submerged in water and excited by a point load on its inner surface. FE model using isoparametric cubic elements incorporates a perfectly matched layer (PML) and roughly 400,000 dofs





## Fluid-Structure Acoustic Vibration Analysis

• Frequency sweep analysis of a submerged thick spherical shell



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### Fluid-Structure Acoustic Vibration Analysis

• Frequency sweep analysis of a submerged thick spherical shell



## Solutions of Linear Systems

• Iterative domain-decomposition algorithm for solving

$$(\mathbf{K} - \boldsymbol{\omega}^2 \mathbf{M}) \mathbf{x} = \mathbf{b}$$

- K and M are complex symmetric matrices
- FETI-DPH
- GMRES on Lagrange multipliers
- Matching of 72 (= 24 + 24 + 24) values at 3 points on 16 nodes (with 8 cores)
  - "Straightforward" sweep with FETI-DPH and 240 samples  $\approx 240 \times 20 \textit{s} = 4,800 \textit{s}$
  - Average of 41 iterations per right hand side (128 subdomains, coarse grid size 30,039)
  - CPU time for reduced order model and "reduced" sweep: 313s

- The quality of interpolatory reduced-order models depends on the selection of interpolation points and on the number of matched derivatives.
- This selection has mostly been heuristic, which remains the main disadvantage of interpolatory model reduction.

- Starting from P<sub>0</sub> sampling frequencies, build a first model matching J derivatives per point.
- Monitor the residual norms

$$\boldsymbol{\omega} \mapsto \frac{\left\| \left( \mathsf{K} - \boldsymbol{\omega}^2 \mathsf{M} + \mathsf{S}(\boldsymbol{\omega}) \right) \mathsf{V} \tilde{\mathsf{x}}(\boldsymbol{\omega}) - \mathsf{f}(\boldsymbol{\omega}) \right\|_2}{\|\mathsf{f}(\boldsymbol{\omega})\|_2}$$

on every interval  $[\omega_p, \omega_{p+1}] \subset [\omega_l, \omega_r].$ 

- Add a new sampling frequency if one norm value is greater than tolerance *τ*.
  - Check values at a few points in  $[\omega_p, \omega_{p+1}]$ .
- Create a new interpolatory reduced order model (if needed).

# 2. Selecting Matching Points and Number of Derivatives

• Use the adaptive scheme for placing points described previously and monitoring the residual norms

$$\omega \mapsto \frac{\left\| \left(\mathsf{K} - \omega^2 \mathsf{M} + \mathsf{S}(\omega)\right) \mathsf{V}\tilde{\mathsf{x}}(\omega) - \mathsf{f}(\omega) \right\|_2}{\|\mathsf{f}(\omega)\|_2} \quad \text{ on } \left[ \omega_l, \omega_r \right]$$

- For every sampling frequency  $\omega_p$ ,
  - Compute J<sub>max</sub> derivatives
  - Keep a number of derivatives between  $J_{min}$  and  $J_{max}$  such that
    - the residual norms decrease sufficiently with the new directions
    - the residual norms are just below tolerance au

 $(1 \leq J_{\min} \leq J_{\max})$ 

### Example: Helmholtz Scattering Problem



$$(\mathbf{K} - \omega^2 \mathbf{M})\mathbf{p}_f(\omega) = \mathbf{g}_f(\omega) \quad \omega \in [9, 36]$$

- K and M are complex symmetric matrices of size 777,650 (cubic elements).
- A frozen perfectly matched layer is used.

#### Automatic Adaptivity



• 
$$J_{min} = 16$$
 and  $J_{max} = 64$ .

# Automatic Adaptivity



•  $J_{min} = 16$  and  $J_{max} = 64$ .

#### Automatic Adaptivity



• 
$$J_{min} = 16$$
 and  $J_{max} = 64$ .

$J_{min}, J_{max}, \Delta J$		8,8,0	16,16,0	32,32,0	48,48,0	64,64,0	16,64,4
# of interpolation points		7	5	4	4	4	4
Size of approximation subspace		56	80	128	192	256	112
Average relative residual		1.2e-7	7.2e-8	3.3e-7	2.1e-8	9.1e-8	5.2e-7
Maximum relative residual		1.9e-6	9.7e-7	4.9e-6	1.1e-7	1.4e-6	7.6e-6
Maximum relative error		5.9e-7	4.7e-7	2.0e-7	2.6e-7	1.6e-7	8.5e-7
CPU time (s)	Subspace construction	712.7	534.9	471.0	509.8	573.6	448.1
	Projection setup	23.7	27.8	49.5	95.3	154.6	49.9
	Post-processing	38.0	48.6	68.6	97.0	125.4	62.1
	Total	774.3	611.3	589.1	774.4	853.6	560.1

Table I. Acoustic scattering problem: performance of the adaptive DGP method in terms of CPU cost and accuracy ( $\tau = 10^{-3}$ , 33 CPU cores).

• Brute force time with 541 samples: 49,339 s

### Non-Equilibrium Green's Functions (NEGF)

The retarded Green's function  $\mathbf{G}^r$  is defined

$$(EI - H - \Sigma_{lead}(E))G^{r}(E) = AG^{r} = I$$

The electron density at point q and energy E is

$$n_q(E) = 2 \int \frac{dE}{2\pi} G_{qL}^r \Sigma_{LL}^< \left(G_{qL}^r\right)^H + G_{qR}^r \Sigma_{RR}^< \left(G_{qR}^r\right)^H$$

and the current from lead L to R is

$$J_{L\to R} = \frac{2e}{h} \int dE T_{LR}(E) \left( f_L(E) - f_R(E) \right)$$

$$T_{LR}(E) = \operatorname{tr}\left[\Gamma_{LL}(E) G_{LR}^{r}(E) \Gamma_{RR}(E) (G_{LR}^{r}(E))^{H}\right]$$

## Non-Equilibrium Green's Functions (NEGF)

The problem is to solve

$$(E\mathbf{I} - \mathbf{H} - \Sigma_{lead}(E))\mathbf{G}_{L}^{r}(E) = \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

and

$$(EI - H - \Sigma_{lead}(E)) \mathbf{G}_{R}^{r}(E) = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{I} \end{bmatrix}$$

over a wide range of energy values.

- Build an interpolatory reduced-order model to approximate columns of G<sup>r</sup> over [E<sub>min</sub>, E<sub>max</sub>]
- Select the matching energies adaptively.
- Select the columns to interpolate adaptively.



Figure: Potential for the rectangular nanodevice



Figure: Sampling Values



Figure: Absolute Error between FOM and ROM

$N_{x}$	Size of FOM	Time Brute Force	Size of ROM	Time ROM
26	<i>n</i> = 1014	23 <i>s</i>	<i>s</i> = 86	7 <i>s</i>
50	<i>n</i> = 3750	182 <i>s</i>	<i>s</i> = 113	39 <i>s</i>
100	n = 15000	1828 <i>s</i>	<i>s</i> = 156	252 <i>s</i>

Table: Evolution of timings as the number of grid points  $N_x$  is increased (with evaluation of transmission at 768 energy points).

• Tolerance  $\tau = 10^{-2}$ 

• 
$$N_y = 3N_x/2$$

### **Problem Formulation**

Consider the incompressible Navier-Stokes equation in a bounded domain  $\Omega \in \mathbb{R}^2$ 

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - v\Delta \mathbf{u} = \mathbf{f} \quad \text{in } \Omega \times (0, T]$$
$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \times (0, T]$$
$$\mathbf{u} = \mathbf{b} \quad \text{on } \Gamma_D \times (0, T]$$
$$-p\mathbf{n} + v\nabla u \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, T]$$
$$\mathbf{u}(0) = \mathbf{u}_0$$

where  $\mathbf{u}(\mathbf{x}, t)$  and  $p(\mathbf{x}, t)$  denote the velocity and pressure fileds.  $\Omega$  is a bounded domain in  $\mathbb{R}^2$  whose boundary is denoted by  $\partial \Omega = \Gamma_D \cup \Gamma_N$ . v denote the kinematic viscosity of the fluid,  $\mathbf{u}_0$  a given initial velocity, and  $\mathbf{b}$  a specified boundary velocity.

- **1** Build the snapshot database for two viscosity values  $S = \bigcup_{j=1}^{n_x} \{x_j(v_1)\} \bigcup_{j=1}^{n_x} \{x_j(v_P)\}.$
- **2** Set the number of clusters  $N_V = 2$ .
- **3** Construct the local ROBs  $\Phi_i$  by partition *S* into  $N_v$  overlapping clusters
- Evaluate the residuals at all the check points using ROM model
- **6** Find the viscosity value giving the largest residuals.
- 6 If the residuals are larger than a tolerance,
  - Set  $S \leftarrow S \cup \{\mathbf{x}_1(v_{j_{max}}), \mathbf{x}_2(v_{j_{max}}), \dots, \mathbf{x}_{n_x}(v_{j_{max}})\}$
  - $N_V \leftarrow N_V + 1$
  - Go to Step 3

#### Numerical experiments

• Incompressible Navier-Stokes flow on a T-shaped domain



• Inlet velocity 
$$\mathbf{b} = \begin{bmatrix} 100(1 + 4sin(20\pi t))(1 - y)(y - 0.5) \\ 0 \le t \le 0.05 \end{bmatrix}$$
 for

• Full order model: 11,203 degrees of freedom

#### Solution at training configuration v = 1

• 
$$S = {x^j (v = 1)}_{j=1}^{n_x}$$
 and  $n_x = 500$ 

Approach	Error	Speedup	
ROM	2.5e-04	1.71	
ROM + 2 Clusters	5.8e-05	1.61	
ROM + 3 Clusters	2.6e-05	1.51	
ROM + NL Reduction	3.0e-04	104	
ROM + 2 Clusters + NL Reduction	6.7e-05	106	
ROM + 2 Clusters + NL Reduction	3.3e-05	100	

Table: Performance of ROM of dimension 15.

#### Predictive ROM simulation



Figure: Parameter sweep for the T-shaped problem: POD size = 30

- We studied interpolatory reduced-order model.
- We designed adaptive schemes for selecting the matching points.

