Multi-scale S-fraction reduced-order models for large wave problems

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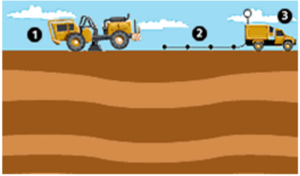
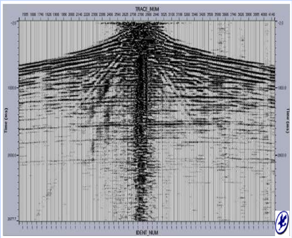
Outline

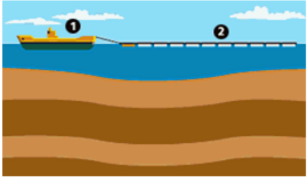
Seismic surveys in geophysics

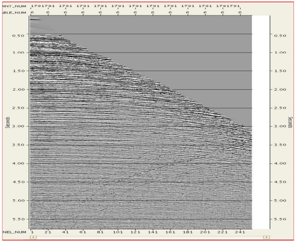
Land seismics





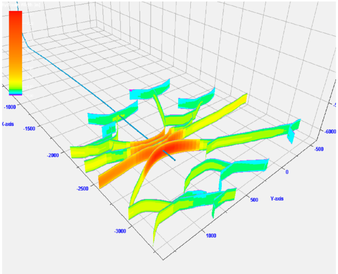
Marine seismics





Challenges in wavefield simulations

- Multiple spatial scales: survey domains vs thin waveguides
- Multiple time scales
- Consequently, discretized problem has up to of order 10^{10} unknowns
- Efficient parallelization is required



Elastic wave propagation

Linear wave equation

$$\mathbf{A}u + \frac{d^2u}{dt^2} = 0,\ \ u|_{t=0} = g,\ \ u'|_{t=0} = 0$$

$$A = A^* \geq 0,\ \ b, u(t) \in \mathcal{R}^N,\ \ \mathbf{A} \in \mathcal{R}^{N\times N}$$

$\mathbf{A}$ is of graph-Laplacian type, N is very large. Soluton can be expressed in terms of matrix function $u(t) = \cos(t\sqrt{A})g$

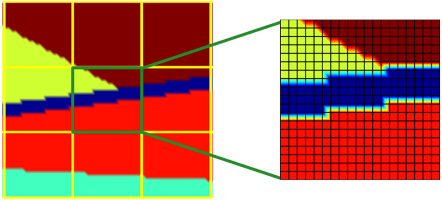
Goal: efficiently parallelizable reduced-order model for SPATIAL discretization with minimum number of state variables

Will exploit intimate connection between

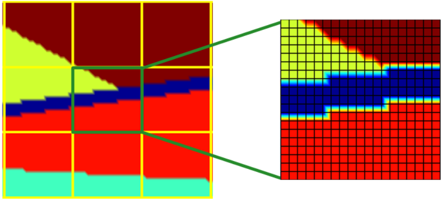
- Projection-based model reduction
- Rational approximation (of the transfer function)
- Stiltjes continued fraction
- Spectrally matched finite-difference grids

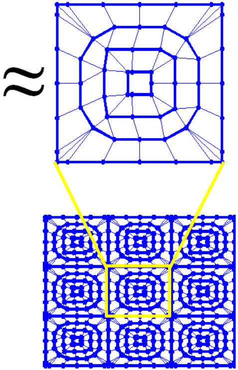
Outline

Multi-scale mimetic ROM at-a-glance



Multi-scale mimetic ROM at-a-glance





Details below:

- Sparse ROM construction
- Conjugation of adjacent ROMs

Outline

1D example with two subdomains

- We start with model problem for operator

$$(\sigma u_x)_x - \lambda u, \qquad x \in [-1;1],\ u|_{x=1} = u|_{x=-1} = 0$$

  with $\sigma(x) > 0$, $\lambda \in \mathbb{C} \setminus \mathbb{R}_-$ and two subdomains $[-1;0]$ and $[0;1]$
- Conjugation conditions: $u(0-) = u(0+) = u^0$ and $\sigma \frac{du}{dx}(0-) = \sigma \frac{du}{dx}(0+) = f$
- E.g., this eqn. can be obtained after the Laplace transform of wave problem on $[0,1] \times t$.
- Consider $[0;1]$. Let

$$Au - \lambda u = b,$$

  obtained from discretization of
  $(\sigma u_x)_x - \lambda u = 0,\ \sigma \frac{d}{dx} u|_{x=0} = -1, \quad u|_{x=1} = 0$
- We define the Neumann-to-Dirichlet (NtD) map a.k.a. current-to-voltage, transfer, impedance or Weyl function $f(\lambda)$ as

$$f(\lambda) = b^* u = b^*(A - \lambda I)^{-1} b.$$

1D example: SISO reduced order model

For projection subspace $\mathcal{V}_k$ and orthogonal basis V_k in it:
$f(\lambda) \approx f_k(\lambda) = b_k^*(A_k - \lambda I)^{-1} b_k$ where $b_k = V_k^* b,\ A_k = V_k^* A V_k$
f_k satisfies $2k$ matching conditions

Observation #1:

V_k can be chosen such that $A_k = T_k$ is tri-diagonal (Lanczos decomposition of arbitrary A_k: $T_k = Q^* A_k Q = Q^* V_k^* A V_k Q$) and $f_k(\lambda) = ||b_k||^2 e_1^*(T_k - \lambda I)^{-1} e_1$

Observation #2:

T_k can be diagonally transformed such that $f_k(\lambda) = u_1$ where $u_1, \ldots, u_k$ satisfy

$$\hat{\gamma}_i \left(\gamma_i(u_{i+1} - u_i) - \gamma_{i-1}(u_i - u_{i-1})\right) - \lambda u_i = 0,\ \ i > 0$$

with $\hat{\gamma}_0 \left(\gamma_0(u_1 - u_0)\right) - \lambda u_0 = -\hat{\gamma}_0,\ \ u_{k+1} = 0$

Takeaway

$f_k(\lambda) = u_1$ where $u_1, \dots, u_k$ satisfy

$$\hat{\gamma}_i \left(\gamma_i (u_{i+1} - u_i) - \gamma_{i-1}(u_i - u_{i-1}) \right) - \lambda u_i = 0, \; i > 0$$

with $\hat{\gamma}_0 \left(\gamma_0 (u_1 - u_0) \right) - \lambda u_0 = -\hat{\gamma}_0, \; u_{k+1} = 0$

- There is one-to-one correspondence between SISO ROM and three-point finite-difference scheme with positive steps
- Equivalent to representation of Stieltjes function $f_k(\lambda)$ in terms of continued s-fraction.
- For uniform medium $h_j = \frac{1}{\gamma_j}$ and $\hat{h}_j = \frac{1}{\hat{\gamma}_j}$ are grid steps of so-called spectrally–matched grid
- Time-domain equations: replace λ by $\frac{d^2}{dt^2}$

1D example: conjugation of two intervals

- Interval $[-1; 0]$:

$$\hat{\gamma}_i^1 \left(\gamma_i^1(u_{i+1}^1 - u_i^1) - \gamma_{i-1}^1(u_i^1 - u_{i-1}^1)\right) - \lambda u_i^1 = 0, \;\; i < 0$$

with $\hat{\gamma}_i^1 \left(-\gamma_i^1(u_{-1}^1 - u_0^1)\right) - \lambda u_0^1 = f\hat{\gamma}_0^1, \;\; u_{-k-1}^1 = 0$

- Interval $[0; 1]$:

$$\hat{\gamma}_i^2 \left(\gamma_i^2(u_{i+1}^2 - u_i^2) - \gamma_{i-1}^2(u_i^2 - u_{i-1}^2)\right) - \lambda u_i^2 = 0, \;\; i > 0$$

with $\hat{\gamma}_i^2 \left(\gamma_i^2(u_1^2 - u_0^2)\right) - \lambda u_0^2 = -f\hat{\gamma}_0^2, \;\; u_{k+1}^2 = 0$

- Eliminating flux f, we obtain

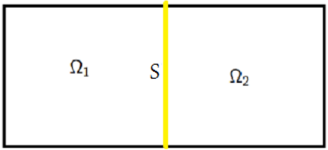
$$\hat{\gamma}_i \left(\gamma_i(u_{i+1} - u_i) - \gamma_{i-1}(u_i - u_{i-1})\right) - \lambda u_i = 0, \;\; |i| \leq k$$

with $u_{k+1} = u_{-k-1} = 0$, $\left(\hat{\gamma}_0\right)^{-1} = \left(\hat{\gamma}_0^1\right)^{-1} + \left(\hat{\gamma}_0^2\right)^{-1}$

- We can achieve spectral convergence of the NtD map using the simplest second order finite-difference (FD) scheme with the three-point stencil.

Outline

Multi-dimensional example: two subdomains



- For simplicity, consider nonsingular frequency-domain operator $\nabla \cdot (\Lambda \cdot \nabla u) - \lambda u$ on $\Omega \in \mathbb{R}^2$ with Dirichlet conditions.
- $\Omega = \Omega_1 \cup \Omega_2$, $S = \overline{\Omega}_1 \cap \overline{\Omega}_2$
- Conjugation conditions $u|_{S-0} = u|_{S+0} = U^0$, $\Lambda \cdot \nabla u|_{S+0} = \Lambda \cdot \nabla u|_{S-0} = f$
- Let $Au - \lambda u = b$ approximates $\nabla \cdot (\Lambda \cdot \nabla u) - \lambda u = b$, $\Lambda \cdot \nabla u|_S = 0$, $u_{\partial\Omega_1 \setminus S} = 0$
- We define the (approximate) transfer function $F(\lambda)$ at Ω_2 as

$$F(\lambda) = B^* u = B^*(A - \lambda I)^{-1} B$$

where *colspan*$\{B\}$ approximate solution on S

MIMO reduced order model

- For projection subspace $\mathcal{V}_k$ and orthogonal basis V_k in it: $F(\lambda) \approx F_k(\lambda) = B_k^*(A_k - \lambda I)^{-1} B_k$ where $B_k = V_k^* B, \; A_k = V_k^* A V_k$
- Similar to 1D, orthogonal+diagonal transform results in block tridiagonal finite-difference scheme

$$\hat{\Gamma}_i \left(\Gamma_i (U^{i+1} - U^i) - \Gamma_{i-1}(U^i - U^{i-1}) \right) - \lambda U^i = 0, \; i > 0$$

with $\hat{\Gamma}_0 \left(\Gamma_0 (U^1 - U^0) \right) - \lambda U^0 = -\hat{\Gamma}_0, \; U_{k+1} = 0$ and $F_k(\lambda) = U_1$

- Here Γ_i and $\hat{\Gamma}_i$ are block symmetric $m \times m$ matrices where $m = \dim\{colspan\{B\}\}$
- For efficient implementation, compressed set of input-output B is required
- Proper choice of $\mathcal{V}_k$ is crucial: we used $\mathcal{V}_k = span\{B, A^{-1}B, \ldots, A^{-k+1}B\}$

Examples of boundary basis functions

- Frequency-limited POD-type reduction
- Rigorously proven limit of 2ppw (compared to π ppw for polynomial even in homogeneous medium)

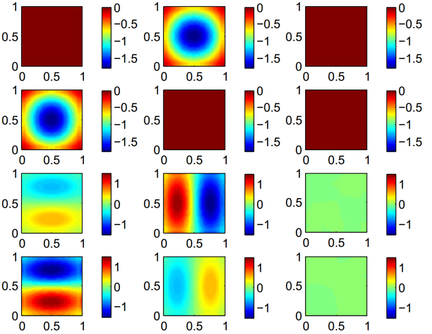


Figure: Homogeneous boundary

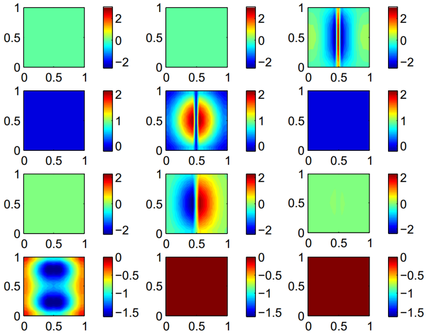


Figure: Fluid-filled fracture in homogeneous boundary

Conjugation of two subdomains

- Subdomain Ω_1:

$$\hat{\Gamma}_i^1 \left(\Gamma_i^1(U_{i+1}^1 - U_i^1) - \Gamma_{i-1}^1(U_i^1 - U_{i-1}^1)\right) - \lambda U_i^1 = 0, \ \ i < 0$$

with $\hat{\Gamma}_i^1 \left(-\Gamma_i^1(U_{-1}^1 - U_0^1)\right) - \lambda U_0^1 = \hat{\Gamma}_0^1 \tilde{f}, \ \ U_{-k-1}^1 = 0$

- Subdomain Ω_2:

$$\hat{\Gamma}_i^2 \left(\Gamma_i^2(U_{i+1}^2 - U_i^2) - \Gamma_{i-1}^2(U_i^2 - U_{i-1}^2)\right) - \lambda U_i^2 = 0, \ \ i > 0$$

with $\hat{\Gamma}_i^2 \left(\Gamma_i^2(U_1^2 - U_0^2)\right) - \lambda U_0^2 = -\hat{\Gamma}_0^2 \tilde{f}, \ \ U_{k+1}^2 = 0$

- Eliminating flux f, we obtain

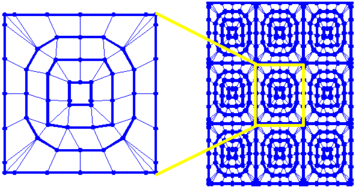
$$\hat{\Gamma}_i \left(\Gamma_i(U_{i+1} - U_i) - \Gamma_{i-1}(U_i - U_{i-1})\right) - \lambda U_i = 0, \ \ |i| \leq k$$

with $U_{k+1} = U_{-k-1} = 0, \ \left(\hat{\Gamma}_0\right)^{-1} = \left(\hat{\Gamma}_0^1\right)^{-1} + \left(\hat{\Gamma}_0^2\right)^{-1}$

- Time-domain formulation is obtained by replacing λ by $\frac{d^2}{dt^2}$

Outline

General formulation for multiple subdomains



- Assume that boundary basis functions at adjacent boundaries do not interact
- Interior nodes within subdomain Ω_α:

$$\hat{\Gamma}_i^\alpha \left(\Gamma_i^\alpha(U_{i+1}^\alpha - U_i^\alpha) - \Gamma_{i-1}^\alpha(U_i^\alpha - U_{i-1}^\alpha)\right) - \frac{d^2}{dt^2} U_i^\alpha = 0,$$

- For the unknown $U_0^{\alpha\beta}$ at boundary between subdomains Ω_α and Ω_β:

$$\hat{\Gamma}_i^{\alpha\beta} \left(\left(\Gamma_i^\alpha(U_1^\alpha - U_0^\alpha)\right)|_\beta + \left(\Gamma_1^\alpha(U_1^\beta - U_0^\beta)\right)|_\alpha\right) - \frac{d^2}{dt^2} U_0^{\alpha\beta} = 0,$$

MSMROM algorithm summary

Offline preprocessing

- A sparse ROM transfer function of every subdomain is computed. It accurately represents interaction of the subdomain with neighbors
- Costly but embarrassingly parallel
- Performed just ONCE for entire time-domain simulation for ALL SOURCES
- Compression of boundary basis functions is crucial
- Optimal ROM may allow to reduce the state variables up to a Nyquist limit of 2 ppw (work in progress)

Online computing

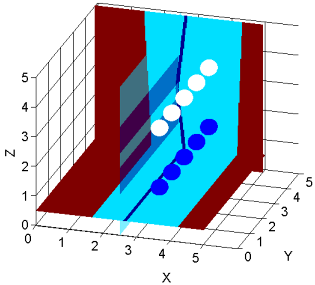
- Obtained reduced order spectrally convergent sparse system is solved via time-stepping (or any other solver)
- The minimal communication cost between subdomains. Ideal for HPC, in particular for GPU

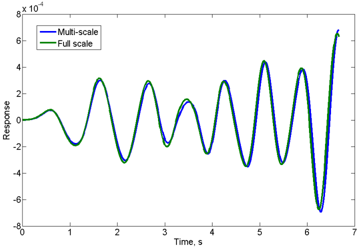
Drawing analogies

- Domain decomposition in the frequency domain: split the domain into subdomains interacting via NtD or DtN map, however then we reduce it and sparsify
- Spectral elements: partial case for homogeneous subdomains but can do significantly better, moreover applicable for heterogeneous ones
- Homogenization: constructs effective dispersive medium for domain sizes of order of the wavelength

Outline

Scattering by 3D liquid filled fractures in anisotropic elastic background with cavities





- Left: elastic model with water filled fracture; distances in meters; pulse Ricker wavelet. Right: simulation results for full and reduced models.
- Dimensionality reduction is 1800 vs 192000, speedup = 10 on serial processor

Outline

Conclusions

- We developed ROM-based sparse spatial discretization technique for wave equations
- Handles problems with unlimited complexity: arbitrary heterogeneuities, anisotropy
- Spectral convergence on arbitrary grid independent of the model
- Minimal interaction between ROMs in adjacent subdomain makes it perfect for HPC implementation, including GPU
- Can be formulated in terms of arbitrary non-negative matrix (no PDE is necessary)
- Future work
    - Optimal model reduction allows to reduce the unknowns up to Nyquist limit