Model Order Reduction for Wave Equations

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General solution and symmetry

- Semidiscrete Maxwell/wave field system

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t)\, \mathsf{f}(t) = -\mathsf{q}'(t), \quad t > 0$$

  Field and source vector vanish for $t < 0$

- Time dependence of source can be factored out:

$$\mathsf{q}'(t) = w(t)\tilde{\mathsf{q}}$$

- $w(t)$ is called the *source wavelet* or *source signature* and vanishes for $t < 0$

General solution and symmetry

- Semidiscrete Maxwell/wave field system

$$(\mathsf{D}+\mathsf{S}+\mathsf{M}\partial_t)\,\mathsf{f}(t) = -w(t)\tilde{\mathsf{q}}, \quad t>0$$

- Symmetry properties of matrix D:
    - Matrix D is *skew-symmetric* w.r.t. W:

$$\mathsf{D}^T\mathsf{W} = -\mathsf{W}\mathsf{D}$$

    - Matrix D is *symmetric* w.r.t. $\mathsf{W}\delta^-$:

$$\mathsf{D}^T\mathsf{W}\delta^- = \mathsf{W}\delta^-\mathsf{D}$$

General solution and symmetry

- Multiply system by M^{-1} to obtain

$$(\mathsf{A} + \mathsf{I}\partial_t)\,\mathsf{f}(t) = -w(t)\mathsf{q}, \quad t > 0$$

with

$$\mathsf{q} = \mathsf{M}^{-1}\tilde{\mathsf{q}} \quad \text{and} \quad \mathsf{A} = \mathsf{M}^{-1}(\mathsf{D} + \mathsf{S})$$

- solution can be written in terms of the matrix exponential function (evolution operator)

$$\mathsf{f}(t) = -w(t) * U(t)\exp(-\mathsf{A}t)\mathsf{q}, \quad t > 0$$

  - $U(t)$: Heaviside unit step function
  - $*$: convolution in time

General solution and symmetry

- Initial-value problem:

$$(\mathsf{A} + \mathsf{I}\partial_t)\,\mathsf{f}(t) = 0, \quad t > 0$$

with $\mathsf{f}(0) = \mathsf{f}_0$.

- Solution:

$$\mathsf{f}(t) = \exp(-\mathsf{A}t)\mathsf{f}_0 \quad t \geq 0$$

General solution and symmetry

- Lossless media: $A = M^{-1}D$
  - **A.** Matrix A is *skew-symmetric* w.r.t. WM

$$A^T WM = -WMA$$

- General case: $A = M^{-1}(D + S)$
  - **B.** Matrix A is *symmetric* w.r.t. $WM\delta^-$

$$A^T WM\delta^- = WM\delta^- A$$

General solution and symmetry

- Symmetry property **A** is related to *energy conservation*
- Solution initial value problem:

$$\mathrm{f}(t) = \exp(-\mathrm{A}t)\mathrm{f}_0, t \geq 0$$

- Stored energy in initial field is given by

$$\mathcal{E}_0 = \frac{1}{2}\mathrm{f}_0^T \mathrm{WMf}_0$$

General solution and symmetry

- Stored energy at time instant t:

$$\begin{aligned}\mathcal{E}(t) &= \frac{1}{2}\mathrm{f}^T(t)\mathrm{WMf}(t)\\ &= \frac{1}{2}\mathrm{f}_0^T\exp(-\mathrm{A}^T t)\mathrm{WM}\exp(-\mathrm{A}t)\mathrm{f}_0\\ &= \frac{1}{2}\mathrm{f}_0^T\mathrm{WM}\exp(+\mathrm{A}t)\exp(-\mathrm{A}t)\mathrm{f}_0\\ &= \mathcal{E}_0\end{aligned}$$

General solution and symmetry

- WM is diagonal positive definite
- Energy inner product

$$\langle \mathrm{x}, \mathrm{y} \rangle_{\mathrm{en}} = \mathrm{y}^T \mathrm{WMx}$$

- Inner product induces the energy norm

$$\|\mathrm{f}\|_{\mathrm{en}} = \langle \mathrm{f}, \mathrm{f} \rangle_{\mathrm{en}}^{1/2} \qquad \mathcal{E}(t) = \frac{1}{2} \|\mathrm{f}\|_{\mathrm{en}}^2$$

General solution and symmetry

- Symmetry property **B** is related to *reciprocity*
- Introduce the matrices

$$\delta^{\mathsf{e}} = \frac{1}{2}(\mathsf{I} + \delta^{-}) \quad \text{and} \quad \delta^{\mathsf{h}} = \frac{1}{2}(\mathsf{I} - \delta^{-})$$

- We have

$$\delta^{\mathsf{e}}\delta^{-} = \delta^{-}\delta^{\mathsf{e}} = \delta^{\mathsf{e}}$$

and

$$\delta^{\mathsf{h}}\delta^{-} = \delta^{-}\delta^{\mathsf{h}} = -\delta^{\mathsf{h}}$$

General solution and symmetry

- Electric-type vector:
$$\mathsf{u} = \delta^{\mathsf{e}}\mathsf{u}$$
- Magnetic-type vector:
$$\mathsf{u} = \delta^{\mathsf{h}}\mathsf{u}$$
- Source vector is of the electric-type:
$$\mathsf{q} = \delta^{\mathsf{e}}\mathsf{q}$$

General solution and symmetry

- Solution:

$$\mathrm{f}_q(t) = -w(t) * U(t)\exp(-\mathrm{A}t)\mathrm{q}$$

- Measurement:

$$\mathrm{r}^T\mathrm{WMf}_q(t)$$

  for some receiver vector r
- Using symmetry property B, we have
  - Electric-field measurement, $\mathrm{r} = \delta^{\mathrm{e}}\mathrm{r}$:

$$\mathrm{r}^T\mathrm{WMf}_q(t) = \mathrm{q}^T\mathrm{WMf}_r(t)$$

  - Magnetic-field measurement, $\mathrm{r} = \delta^{\mathrm{h}}\mathrm{r}$:

$$\mathrm{r}^T\mathrm{WMf}_q(t) = -\mathrm{q}^T\mathrm{WMf}_r(t)$$

General solution and symmetry

- Recall

$$\frac{1}{2}\mathrm{f}^T\mathrm{WMf} = \text{stored field energy in the domain}$$
$$\frac{1}{2}\mathrm{f}^T\mathrm{WMf} = \textit{sum} \text{ of electric and magnetic field energy}$$

- $\mathrm{WM}\delta^-$ is *not* positive definite

$$\frac{1}{2}\mathrm{f}^T\mathrm{WM}\delta^-\mathrm{f} = \textit{difference} \text{ of electric and magnetic field energy}$$

- Free-field Lagrangian:

$$\mathcal{L}(t) = \frac{1}{2}\mathrm{f}^T(t)\mathrm{WM}\delta^-\mathrm{f}(t)$$

General solution and symmetry

- Bilinear form

$$\langle \mathsf{x}, \mathsf{y} \rangle_{\mathsf{la}} = \mathsf{y}^T \mathsf{W} \mathsf{M} \delta^- \mathsf{x} \qquad (\textit{not}\ \text{an inner product})$$

- Energy and Lagrangian:

$$\mathcal{E}(t) = \frac{1}{2}\langle \mathsf{f}, \mathsf{f} \rangle_{\mathsf{en}} \quad \text{and} \quad \mathcal{L}(t) = \frac{1}{2}\langle \mathsf{f}, \mathsf{f} \rangle_{\mathsf{la}}$$

General solution and symmetry

- Symmetry:
  - Lossless case ($\mathsf{S} = 0$): A is skew-symmetric w.r.t. $\langle\cdot,\cdot\rangle_{\mathsf{en}}$
  - General case: A is symmetric w.r.t. $\langle\cdot,\cdot\rangle_{\mathsf{la}}$
- General solution (again):

$$\mathsf{f}(t) = -w(t) * U(t)\exp(-\mathsf{A}t)\mathsf{q}, \quad t > 0$$

Krylov MOR

- Power series expansion matrix exponential function

$$\exp(-\mathrm{A}t) = \sum_{k=0}^{\infty} \frac{(-\mathrm{A}t)^k}{k!}$$

- Solution consists of a superposition of powers of A acting on q
- It makes sense to look for approximations that belong to the *Krylov subspace*

$$\mathcal{K}_m = \mathrm{span}\{\mathrm{q}, \mathrm{Aq}, ..., \mathrm{A}^{m-1}\mathrm{q}\}$$

Krylov MOR

- **Lossless case:** $\mathsf{A} = \mathsf{M}^{-1}\mathsf{D}$
- Let v_1, v_2, ...,v_m be a basis of $\mathcal{K}_m$ orthonormal w.r.t. WM

$$\langle \mathsf{v}_i, \mathsf{v}_j \rangle_{\mathsf{en}} = \delta_{i,j}$$

- Expand approximation $\mathsf{f}_m(t)$ in terms of these basis vectors

$$\begin{aligned} \mathsf{f}_m(t) &= \alpha_1(t)\mathsf{v}_1 + \alpha_2(t)\mathsf{v}_2 + \ldots + \alpha_m(t)\mathsf{v}_m \\ &= \mathsf{V}_m \mathsf{a}_m(t) \end{aligned}$$

with

$$\mathsf{V}_m = [\mathsf{v}_1, \mathsf{v}_2, \ldots, \mathsf{v}_m]$$

and

$$\mathsf{a}_m(t) = [\alpha_1(t), \alpha_2(t), \ldots, \alpha_m(t)]^T$$

Krylov MOR

- V_m is a tall matrix having the basis vectors as its columns
- Residual of the field approximation

$$\begin{aligned} r_m(t) &= -w(t)q - Af_m(t) - \partial_t f_m(t) \\ &= -w(t)q - AV_m a_m(t) - V_m \partial_t a_m(t) \end{aligned}$$

- We determine the expansion coefficients from the *Galerkin condition*

$$V_m^T W M r_m(t) = 0$$

Krylov MOR

- Using the orthonormality of the basis vectors w.r.t. WM, we obtain

$$(\mathsf{T}_m + \mathsf{I}_m \partial_t)\,\mathsf{a}_m(t) = -w(t)\mathsf{V}_m^T \mathsf{WMq}, \quad t > 0$$

with I_m identity matrix order m, and

$$\mathsf{T}_m = \mathsf{V}_m^T \mathsf{WMAV}_m$$

- Note that T_m is skew-symmetric

Krylov MOR

- In addition, we take

$$v_1 = \|q\|_{en}^{-1} q$$

- Note that v_1 is first column of matrix V_m

$$v_1 = V_m e_1$$

- Consequently,

$$q = \|q\|_{en} V_m e_1$$

Krylov MOR

- and we have

$$(\mathsf{T}_m + \mathsf{I}_m \partial_t)\, \mathsf{a}_m(t) = -w(t) \|\mathsf{q}\|_{\mathrm{en}} \mathsf{e}_1, \quad t > 0$$

- Solution:

$$\mathsf{a}_m(t) = -\|\mathsf{q}\|_{\mathrm{en}}\, w(t) * U(t) \exp(-\mathsf{T}_m t) \mathsf{e}_1, \quad t > 0$$

- Field approximation or ROM:

$$\mathsf{f}_m(t) = -\|\mathsf{q}\|_{\mathrm{en}}\, w(t) * U(t) \mathsf{V}_m \exp(-\mathsf{T}_m t) \mathsf{e}_1, \quad t > 0$$

Krylov MOR

- The basis vectors can be generated using the algorithm

$$\beta_{i+1} \mathrm{v}_{i+1} = \mathrm{A}\mathrm{v}_i + \beta_i \mathrm{v}_{i-1}, \quad i = 1, 2, ..., m$$

with $\mathrm{v}_0 = 0$, $\beta_1 = \|\mathrm{q}\|_{\mathrm{en}}$, and the β_i, $i \geq 2$, are determined from the condition

$$\langle \mathrm{v}_i, \mathrm{v}_i \rangle_{\mathrm{en}} = 1, \quad i = 1, 2, ..$$

- Proof is by induction
- This is the *Lanczos algorithm for skew-symmetric matrices*

Krylov MOR

- After m steps of this algorithm we have the summarizing equation

$$\mathsf{A}\mathsf{V}_m = \mathsf{V}_m \mathsf{T}_m + \beta_{m+1} \mathsf{v}_{m+1} \mathsf{e}_m^T$$

with

$$\mathsf{T}_m = \begin{pmatrix} 0 & -\beta_2 & & & \\ \beta_2 & 0 & & & \\ & & \ddots & & \\ & & & & -\beta_m \\ & & & \beta_m & 0 \end{pmatrix} = \mathsf{V}_m^T \mathsf{W}\mathsf{M}\mathsf{A}\mathsf{V}_m$$

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- Compared with an explicit leap-frog time-stepping scheme

$$1/\beta_i \text{ act as a time step}$$

- For the general case proceed in a similar manner
- Basis vectors are "orthonormal" w.r.t. $\langle \cdot, \cdot \rangle_{\mathrm{la}}$
- Matrix T_m is tridiagonal and (complex/sign) symmetric in this case
- *Remark:* the resulting Lanczos algorithm may break down, since $\langle \cdot, \cdot \rangle_{\mathrm{la}}$ is not an inner product

Krylov MOR

- Frequency-domain modeling
- A Laplace transform gives

$$\hat{\mathrm{f}}(s) = -\hat{w}(s)(\mathrm{A} + s\mathrm{I})^{-1}\mathrm{q}$$

- Matrix resolvent instead of matrix exponential needs to be evaluated
- ROM:

$$\hat{\mathrm{f}}_m(s) = -\|\mathrm{q}\|_{\mathrm{en}}\hat{w}(s)\mathrm{V}_m(\mathrm{T}_m + s\mathrm{I})^{-1}\mathrm{e}_1$$

Krylov MOR

- Convergence, what to expect?
- High-frequency expansion of resolvent:

$$(\mathsf{A} + s\mathsf{I})^{-1} = s^{-1}(\mathsf{I} + s^{-1}\mathsf{A})^{-1} = s^{-1}\sum_{k=0}^{\infty}(-s^{-1}\mathsf{A})^k$$

- Powers of A: Early times/high frequencies are approximated first

Krylov MOR

- When it exists, the group inverse $A^{\#}$ of A is uniquely defined by the conditions

$$AA^{\#}A = A, \quad A^{\#}AA^{\#} = A, \quad \text{and} \quad AA^{\#} = A^{\#}A$$

- $AA^{\#}$ projector onto the range of A
- Source vector belongs to the range of A: $q = AA^{\#}q$

$$\begin{aligned}
\hat{f}(s) &= -\hat{w}(s)(A + sI)^{-1}q \\
&= -\hat{w}(s)(A + sI)^{-1}AA^{\#}q \\
&= -\hat{w}(s)A^{\#}(I + sA^{\#})^{-1}q \\
&= -\hat{w}(s)A^{\#}\sum_{k=0}^{\infty}(-sA^{\#})^{k}q
\end{aligned}$$

- Low-frequency expansion
- Inverse powers of A: late-times/low-frequencies are approximated first

Krylov MOR

- Construct ROMs belonging to the Krylov space

$$\mathcal{K}_m = \mathrm{span}\{\mathsf{q}, \mathsf{A}^{\#}\mathsf{q}, \ldots, (\mathsf{A}^{\#})^{m-1}\mathsf{q}\}$$

- $\mathsf{A}^{\#}$ inherits symmetry properties of A
- Lanczos algorithms with $\mathsf{A}^{\#}$
- $\mathsf{A}^{\#}$ can be determined explicitly
- Action of $\mathsf{A}^{\#}$ on a vector requires solution of Poisson equation(s)

Krylov MOR

- Early- and late-time field approximations
- Construct a ROM that belongs to the *extended Krylov space*

$$\mathcal{K}_{k,m} = \mathrm{span}\{(\mathsf{A}^{\#})^{k-1}\mathsf{q}, (\mathsf{A}^{\#})^{k-2}\mathsf{q}, \ldots, \mathsf{A}^{\#}\mathsf{q}, \mathsf{q}, \mathsf{A}\mathsf{q}, \ldots, \mathsf{A}^{m-1}\mathsf{q}\}$$

- By exploiting symmetry, a basis of this space can again be generated via short recurrence relations

Krylov MOR

- Standard Krylov: field approximated by a polynomial in A
- Extended Krylov: field approximated by a Laurent polynomial in A
- Rational Krylov: field approximated by a rational function in A