A Krylov Subspace Approach to Modeling of Wave Propagation in Open Domains

Delft University of Technology, CAS Group

Jörn Zimmerling

Monday 2nd February, 2015

Introduction - Motivation

- Fast and robust modeling of wave-propagation essential to many areas of science

Introduction - Motivation

- Fast and robust modeling of wave-propagation essential to many areas of science
- Acoustic/seismic waves: Earth formations for exploration physics
- Electromagnetic waves: Induction logging of borehole

Introduction - Motivation

- Fast and robust modeling of wave-propagation essential to many areas of science
- Acoustic/seismic waves: Earth formations for exploration physics
- Electromagnetic waves: Induction logging of borehole
- Electromagnetic waves: Light matter interaction on the nano-scale
  - Periodic gratings for process control (ASML)
  - Sensors based on resonance shifts in plasmonic resonators

Introduction - Motivation

- Fast and robust modeling of wave-propagation essential to many areas of science
- Acoustic/seismic waves: Earth formations for exploration physics
- Electromagnetic waves: Induction logging of borehole
- Electromagnetic waves: Light matter interaction on the nano-scale
  - Periodic gratings for process control (ASML)
  - Sensors based on resonance shifts in plasmonic resonators

Summary

For the forward and inverse problem fast approximate solvers for wave equations in open domains are required.
forward problem: fast, low memory   inverse problem: low order

Introduction - Basic Idea

- Open wave equations can be expressed as

$$(\mathsf{A} + \mathsf{I}\partial_t)\mathsf{f} = \mathsf{b}, \tag{1}$$

with the sparse, system matrix A symmetric as $\mathsf{A}^T\mathsf{W} = \mathsf{WA}$.
Direct evaluation of Eq.1 not possible as A (Order(A) $> 10^6$)

Introduction - Basic Idea

- Open wave equations can be expressed as

$$(\mathsf{A} + \mathsf{I}\partial_t)\mathsf{f} = \mathsf{b}, \tag{1}$$

with the sparse, system matrix A symmetric as $\mathsf{A}^T\mathsf{W} = \mathsf{W}\mathsf{A}$.
Direct evaluation of Eq.1 not possible as A ($\text{Order}(\mathsf{A}) > 10^6$)

- Krylov approximation $\mathsf{A}\mathsf{V}_m \approx \mathsf{V}_m\mathsf{H}_m$ with $\text{Order}(\mathsf{A}) \gg m$
- Approximate solution $\mathsf{f}_m = \mathsf{V}_m\mathsf{q}$ via

$$(\mathsf{H}_m + \mathsf{I}\partial_t)\mathsf{q} = \mathsf{V}^T\mathsf{b} \tag{2}$$

Introduction - Basic Idea

- Open wave equations can be expressed as

$$(\mathsf{A} + \mathsf{I}\partial_t)\mathsf{f} = \mathsf{b}, \tag{1}$$

with the sparse, system matrix A symmetric as $\mathsf{A}^T\mathsf{W} = \mathsf{W}\mathsf{A}$.
Direct evaluation of Eq.1 not possible as A (Order(A) $> 10^6$)
- Krylov approximation $\mathsf{A}\mathsf{V}_m \approx \mathsf{V}_m\mathsf{H}_m$ with Order(A) $\gg m$
- Approximate solution $\mathsf{f}_m = \mathsf{V}_m\mathsf{q}$ via

$$(\mathsf{H}_m + \mathsf{I}\partial_t)\mathsf{q} = \mathsf{V}^T\mathsf{b} \tag{2}$$

Motivation for ROM approach

- Discretization of wave problems are oversampled w.r.t. Nyquist
- Approximation of a few resonances can be sufficient (e.g. violin)
- Frequency independent ABC/PML enables single ROM

Outline

1. From wave equation to discrete operator
   - System formulation
   - Approximation of open system by PML
2. Krylov methods for reduced order modeling
   - Construction
   - Projected solution
3. Examples
   - 2D box Problem TD
   - 3D cylinder Problem FD
4. Conclusion

Outline

TUDelft

From wave equation to discrete operator - System formulation 1

- Example of wave equation: the Maxwell equations

$$-\nabla \times \mathbf{H} + \sigma \mathbf{E} + \varepsilon \partial_t \mathbf{E} = -\mathbf{J}^{\text{ext}}, \tag{3}$$

$$\nabla \times \mathbf{E} + \mu \partial_t \mathbf{H} = -\mathbf{K}^{\text{ext}}. \tag{4}$$

Solve for $\mathbf{E}$ and $\mathbf{H}$ and given sources $\mathbf{J}^{\text{ext}}$ and $\mathbf{K}^{\text{ext}}$ and a spatially varying medium characterized by $\sigma(\mathbf{x}), \varepsilon(\mathbf{x})$ and $\mu(\mathbf{x})$.

From wave equation to discrete operator - System formulation 1

- Example of wave equation: the Maxwell equations

$$-\nabla\times\mathbf{H}+\sigma\mathbf{E}+\varepsilon\partial_t\mathbf{E}=-\mathbf{J}^{\text{ext}}, \tag{3}$$

$$\nabla\times\mathbf{E}+\mu\partial_t\mathbf{H}=-\mathbf{K}^{\text{ext}}. \tag{4}$$

  Solve for $\mathbf{E}$ and $\mathbf{H}$ and given sources $\mathbf{J}^{\text{ext}}$ and $\mathbf{K}^{\text{ext}}$ and a spatially varying medium characterized by $\sigma(\mathbf{x}),\varepsilon(\mathbf{x})$ and $\mu(\mathbf{x})$.
- General first order system formulation for all wave equations is

$$(\mathcal{D}+\mathcal{S}+\mathcal{M}\partial_t)\mathcal{F}=\mathcal{Q}'. \tag{5}$$

  Differentiation & medium matricees and field & source vector as

$$\mathcal{D}=\begin{bmatrix}0 & -\nabla\times\\ \nabla\times & 0\end{bmatrix},\ \mathcal{S}=\begin{bmatrix}\sigma & 0\\ 0 & 0\end{bmatrix},\ \mathcal{M}=\begin{bmatrix}\varepsilon & 0\\ 0 & \mu\end{bmatrix}, \tag{6}$$

$$\mathcal{F}=[\mathbf{E},\mathbf{H}]^T,\ \text{and}\ \mathcal{Q}'=-[\mathbf{J}^{\text{ext}},\mathbf{K}^{\text{ext}}]^T. \tag{7}$$

From wave equation to discrete operator - System formulation 2

- After discretization the Matrix equation

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t)\mathsf{f} = \mathsf{q}'. \tag{8}$$

describes the wave equation.

From wave equation to discrete operator - System formulation 2

- After discretization the Matrix equation

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t)\mathsf{f} = \mathsf{q}'. \tag{8}$$

describes the wave equation.

- We define $\mathsf{A} = (\mathsf{M}^{-1}\mathsf{D} + \mathsf{M}^{-1}\mathsf{S})$ and $\mathsf{q}'(\mathsf{x}, t) = \mathsf{q}(\mathsf{x})w(t)$,

$$(\mathsf{A} + \mathsf{I}\partial_t)\mathsf{f} = \mathsf{M}^{-1}\mathsf{q}(\mathsf{x})w(t), \tag{9}$$

From wave equation to discrete operator - System formulation 2

- After discretization the Matrix equation

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t)\mathsf{f} = \mathsf{q}'. \tag{8}$$

describes the wave equation.

- We define $\mathsf{A} = (\mathsf{M}^{-1}\mathsf{D} + \mathsf{M}^{-1}\mathsf{S})$ and $\mathsf{q}'(\mathsf{x}, t) = \mathsf{q}(\mathsf{x})w(t)$,

$$(\mathsf{A} + \mathsf{I}\partial_t)\mathsf{f} = \mathsf{M}^{-1}\mathsf{q}(\mathsf{x})w(t), \tag{9}$$

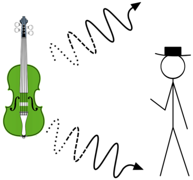
- Equation 9 is solved by

$$\mathsf{f} = w(t) * \eta(t) \exp(-\mathsf{A}t)\mathsf{M}^{-1}\mathsf{q}(\mathsf{x}), \tag{10}$$

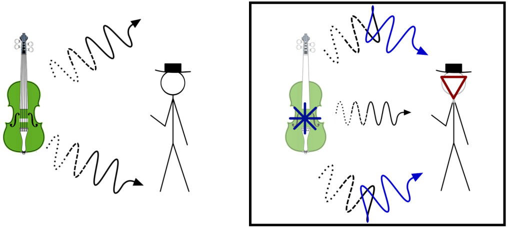
with $\eta(t)$ the Heaviside step function. The Laplace image is defined as

$$\hat{\mathsf{f}} = \hat{w}(s)(\mathsf{A} + s\mathsf{I})^{-1}\mathsf{M}^{-1}\mathsf{q}. \tag{11}$$

From wave equation to discrete operator - Approximation of open system by PML

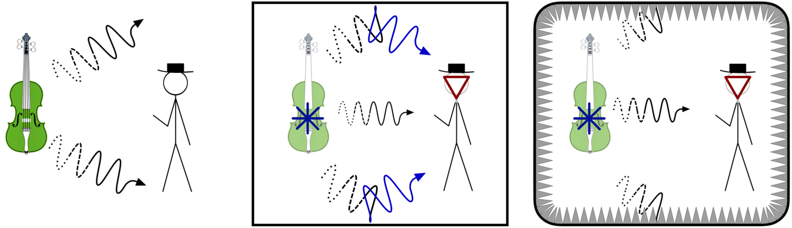


From wave equation to discrete operator - Approximation of open system by PML



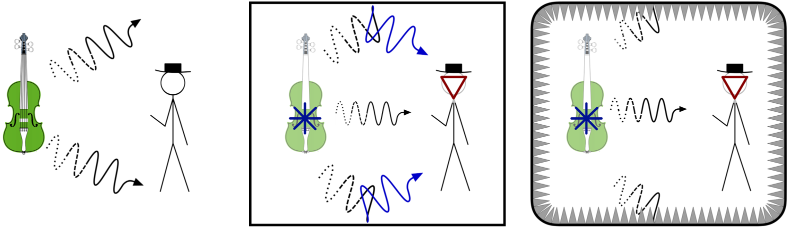
- Truncation of computational domain necessary

From wave equation to discrete operator - Approximation of open system by PML



- Truncation of computational domain necessary
- Perfectly matched layers (PML) absorb outgoing waves reflection less

From wave equation to discrete operator - Approximation of open system by PML



- Truncation of computational domain necessary
- Perfectly matched layers (PML) absorb outgoing waves reflection less
- Reformulation of PML to complex coordinate stretching
- Optimal frequency independent PML matched over spectral region of interest

From wave equation to discrete operator - Approximation of open system by PML

- After complex coordinate stretching A approximates outgoing waves and incoming waves

From wave equation to discrete operator - Approximation of open system by PML

- After complex coordinate stretching A approximates outgoing waves and incoming waves
  - $\mathfrak{Re}(\lambda) \geq 0$ contributes to the causal solution $t \geq 0$ (outgoing)
  - $\mathfrak{Re}(\lambda) \leq 0$ contributes to the anticausal solution $t \leq 0$ (incoming)

From wave equation to discrete operator - Approximation of open system by PML

- After complex coordinate stretching A approximates outgoing waves and incoming waves
  - $\mathfrak{Re}(\lambda) \geq 0$ contributes to the causal solution $t \geq 0$ (outgoing)
  - $\mathfrak{Re}(\lambda) \leq 0$ contributes to the anticausal solution $t \leq 0$ (incoming)
- Apply stability correction/radiation condition by using $\eta(\mathsf{A})$ as

$$\mathsf{f} = w(t) * \eta(t)\mathfrak{Re}\left[\eta(\mathsf{A})\exp\left(-\mathsf{A}t\right)\mathsf{M}^{-1}\mathsf{q}\right], \tag{12}$$

ensures causality.

From wave equation to discrete operator - Approximation of open system by PML

- After complex coordinate stretching A approximates outgoing waves and incoming waves
  - $\mathfrak{Re}(\lambda) \geq 0$ contributes to the causal solution $t \geq 0$ (outgoing)
  - $\mathfrak{Re}(\lambda) \leq 0$ contributes to the anticausal solution $t \leq 0$ (incoming)
- Apply stability correction/radiation condition by using $\eta(\mathsf{A})$ as

$$\mathsf{f} = w(t) * \eta(t)\mathfrak{Re}\left[\eta(\mathsf{A})\exp\left(-\mathsf{A}t\right)\mathsf{M}^{-1}\mathsf{q}\right], \tag{12}$$

  ensures causality.
- Numerical Greens function
- Symmetry condition $\mathsf{A}^T\mathsf{W} = \mathsf{WA}$ enables fast computation of Krylov basis

TU Delft

Outline

1. From wave equation to discrete operator
   - System formulation
   - Approximation of open system by PML
2. Krylov methods for reduced order modeling
   - Construction
   - Projected solution
3. Examples
   - 2D box Problem TD
   - 3D cylinder Problem FD
4. Conclusion

TUDelft

Krylov methods for ROM - Construction

- Polynomial, Extended and Rational Krylov subspace:

$$\mathcal{K}_m^{\mathsf{PKS}} = \mathrm{span}\{\mathsf{b}, \mathsf{Ab}, \mathsf{A}^2\mathsf{b}, \dots, \mathsf{A}^{\mathrm{m}-1}\mathsf{b}\}, \tag{13}$$

$$\mathcal{K}_{n;m}^{\mathsf{EKS}} = \mathrm{span}\{\mathsf{A}^{-\mathrm{n}+1}\mathsf{b}, \dots, \mathsf{A}^{-1}\mathsf{b}, \mathsf{b}, \mathsf{Ab}, \mathsf{A}^2\mathsf{b}, \dots, \mathsf{A}^{\mathrm{m}-1}\mathsf{b}\}, \tag{14}$$

$$\mathcal{K}_m^{\mathsf{RKS}} = \mathrm{span}\{(\mathsf{A} + \sigma_1 \mathsf{I})^{-1}\mathsf{b}, \dots, \prod_{\mathsf{i}=1}^{\mathrm{m}} (\mathsf{A} + \sigma_{\mathrm{i}} \mathsf{I})^{-1}\mathsf{b}\}. \tag{15}$$

Krylov methods for ROM - Construction

- Polynomial, Extended and Rational Krylov subspace:

$$\mathcal{K}_m^{\mathsf{PKS}} = \mathrm{span}\{b, Ab, A^2b, \ldots, A^{m-1}b\}, \tag{13}$$

$$\mathcal{K}_{n;m}^{\mathsf{EKS}} = \mathrm{span}\{A^{-n+1}b, \ldots, A^{-1}b, b, Ab, A^2b, \ldots, A^{m-1}b\}, \tag{14}$$

$$\mathcal{K}_m^{\mathsf{RKS}} = \mathrm{span}\{(A + \sigma_1 I)^{-1}b, \ldots, \prod_{i=1}^{m}(A + \sigma_i I)^{-1}b\}. \tag{15}$$

- In the case of a symmetry in A
  - PKS can be constructed via 3-term Lanczos algorithm
  - EKS can be constructed via 5-term Lanczos algorithm

Krylov methods for ROM - Construction

- Polynomial, Extended and Rational Krylov subspace:

$$\mathcal{K}_m^{\mathsf{PKS}} = \mathrm{span}\{b, Ab, A^2 b, \ldots, A^{m-1} b\}, \tag{13}$$

$$\mathcal{K}_{n;m}^{\mathsf{EKS}} = \mathrm{span}\{A^{-n+1} b, \ldots, A^{-1} b, b, Ab, A^2 b, \ldots, A^{m-1} b\}, \tag{14}$$

$$\mathcal{K}_m^{\mathsf{RKS}} = \mathrm{span}\{(A + \sigma_1 I)^{-1} b, \ldots, \prod_{i=1}^{m} (A + \sigma_i I)^{-1} b\}. \tag{15}$$

- In the case of a symmetry in A
  - PKS can be constructed via 3-term Lanczos algorithm
  - EKS can be constructed via 5-term Lanczos algorithm
- RKS can be constructed via rational Arnoldi algorithm
  Selection of shifts allow the adaption of the spectrum of H_m towards A

Krylov methods for ROM - Projected solution

- The projected solution of our wave equation is given by

$$\mathsf{f}_m(t) = w(t) * \eta(t)\mathfrak{Re}[\mathsf{V}_m \eta(\mathsf{H}_m) \exp(-\mathsf{H}_m t) \mathsf{V}_m^T \mathsf{M}^{-1} \mathsf{q}] \tag{16}$$

with Laplace image

$$\hat{\mathsf{f}}_m(s) = \hat{w}(s) \left[\mathsf{V}_m (\mathsf{H}_m + s\mathsf{I})^{-1} \mathsf{V}_m^T + \mathsf{V}_m^\dagger (\mathsf{H}_m^\dagger + s\mathsf{I})^{-1} \mathsf{V}_m^* \right] \mathsf{M}^{-1} \mathsf{q} \tag{17}$$

TU Delft

Krylov methods for ROM - Projected solution

- The projected solution of our wave equation is given by

$$\mathsf{f}_m(t) = w(t) * \eta(t)\mathfrak{Re}[\mathsf{V}_m\eta(\mathsf{H}_m)\exp(-\mathsf{H}_m t)\mathsf{V}_m^T\mathsf{M}^{-1}\mathsf{q}] \quad (16)$$

with Laplace image

$$\hat{\mathsf{f}}_m(s) = \hat{w}(s)\left[\mathsf{V}_m(\mathsf{H}_m + s\mathsf{I})^{-1}\mathsf{V}_m^T + \mathsf{V}_m^\dagger(\mathsf{H}_m^\dagger + s\mathsf{I})^{-1}\mathsf{V}_m^*\right]\mathsf{M}^{-1}\mathsf{q} \quad (17)$$

- Let $(\mathsf{s}_j, \lambda_j)$ be an eigenpair of H_m and satisfy $\mathfrak{Re}(\lambda_j) > 0$
- A resonance is given by $\mathsf{f}_{res} = \mathsf{V}_m\mathsf{s}_j$ with complex frequency λ_j

TU Delft

Krylov methods for ROM - Projected solution

- The projected solution of our wave equation is given by

$$\mathsf{f}_m(t) = w(t) * \eta(t)\mathfrak{Re}[\mathsf{V}_m \eta(\mathsf{H}_m) \exp(-\mathsf{H}_m t)\mathsf{V}_m^T \mathsf{M}^{-1}\mathsf{q}] \quad (16)$$

  with Laplace image

$$\hat{\mathsf{f}}_m(s) = \hat{w}(s)\left[\mathsf{V}_m(\mathsf{H}_m + s\mathsf{I})^{-1}\mathsf{V}_m^T + \mathsf{V}_m^\dagger(\mathsf{H}_m^\dagger + s\mathsf{I})^{-1}\mathsf{V}_m^*\right]\mathsf{M}^{-1}\mathsf{q} \quad (17)$$

- Let $(\mathsf{s}_j, \lambda_j)$ be an eigenpair of H_m and satisfy $\mathfrak{Re}(\lambda_j) > 0$
- A resonance is given by $\mathsf{f}_{res} = \mathsf{V}_m \mathsf{s}_j$ with complex frequency λ_j
  - $\mathfrak{Re}(\lambda_j)$ associated with losses (material and radiation)
  - $\mathfrak{Im}(\lambda_j)$ frequency of resonance

Krylov methods for ROM - Projected solution

- The projected solution of our wave equation is given by

$$\mathsf{f}_m(t) = w(t) * \eta(t)\mathfrak{Re}[\mathsf{V}_m\eta(\mathsf{H}_m)\exp(-\mathsf{H}_m t)\mathsf{V}_m^T\mathsf{M}^{-1}\mathsf{q}] \quad (16)$$

with Laplace image

$$\hat{\mathsf{f}}_m(s) = \hat{w}(s)\left[\mathsf{V}_m(\mathsf{H}_m + s\mathsf{I})^{-1}\mathsf{V}_m^T + \mathsf{V}_m^\dagger(\mathsf{H}_m^\dagger + s\mathsf{I})^{-1}\mathsf{V}_m^*\right]\mathsf{M}^{-1}\mathsf{q} \quad (17)$$

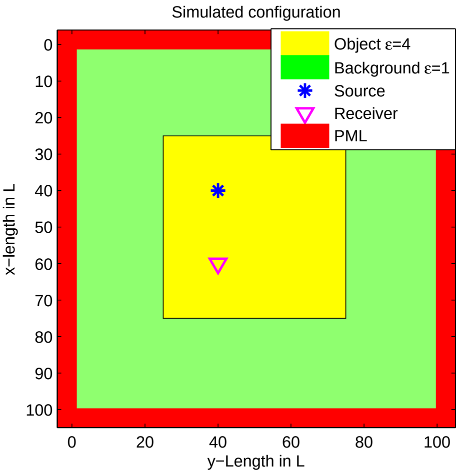
- Let $(\mathsf{s}_j, \lambda_j)$ be an eigenpair of H_m and satisfy $\mathfrak{Re}(\lambda_j) > 0$
- A resonance is given by $\mathsf{f}_{res} = \mathsf{V}_m\mathsf{s}_j$ with complex frequency λ_j
  - $\mathfrak{Re}(\lambda_j)$ associated with losses (material and radiation)
  - $\mathfrak{Im}(\lambda_j)$ frequency of resonance

Conclusion theoretical part

- Single ROM describes dynamics of A over whole frequency band
- After Krylov decomposition frequency sweeps possible in Eq. 17
- Evaluation of solution comes at negligible cost

Outline

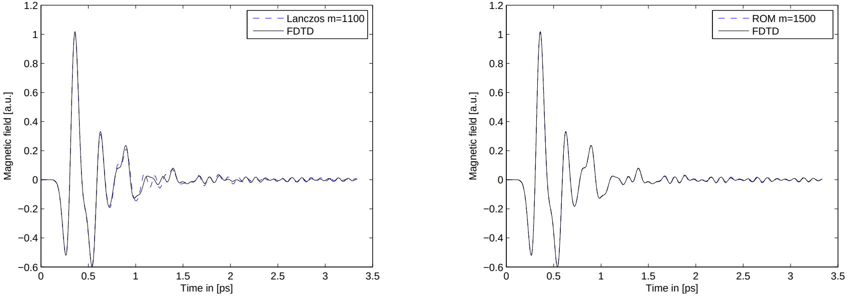
Examples - 2D box Problem



Configuration

- Dielectric box with contrast $c_0/c = 2$
- H-polarized 2D
- Derivative Gaussian pulse with $\lambda_{sc}^{max} = 94L$
- Small system of order $n = 36k$

Examples - 2D box Problem - Results

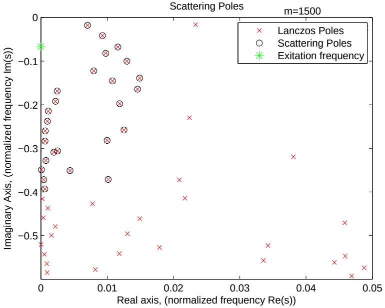


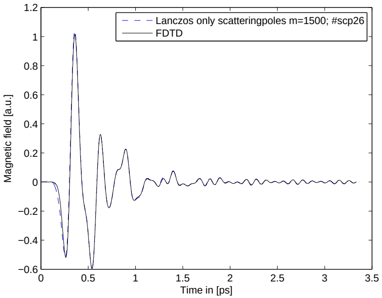
PKS Result

- Output compared with FDTD (time stepping)
- PKS converges within m=1500, RKS with m=48
- ROM allows convolution with arbitrary input wavelet

TU Delft

Examples - 2D box Problem - Ritz values



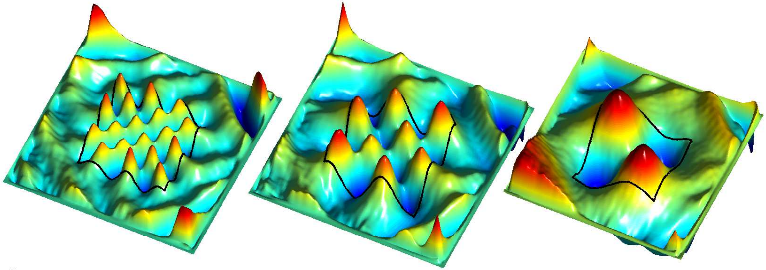


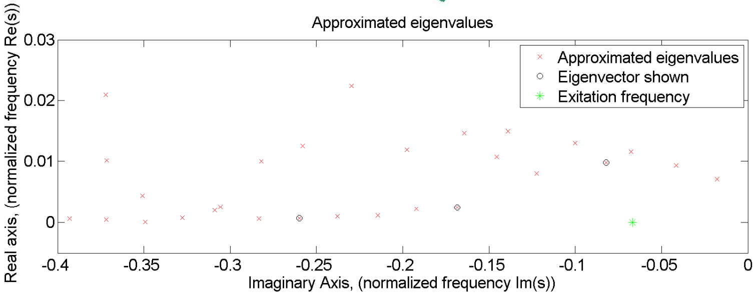
Resonance expansion

- Output can be expanded in just 26 approximate eigenpairs of A
- On time interval $[T_{min}, \infty)$ contributing Ritz values in $\Lambda^{\text{res}} := \{z \in \mathbb{C} : \ 0 \leq \text{Re}(z) < \sigma_{\text{max}}, \omega_{\text{min}} < -\text{Im}(z) < \omega_{\text{max}}\}$
- Error of approximation $O[\exp -\sigma_{max} T_{min}]$

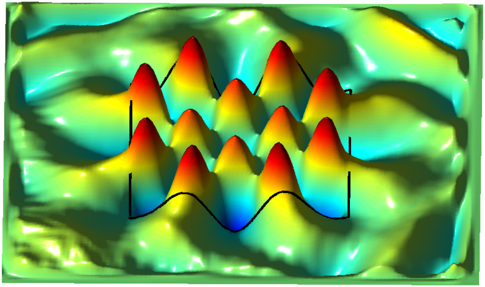
TUDelft

Examples - 2D box Problem - Ritz vectors

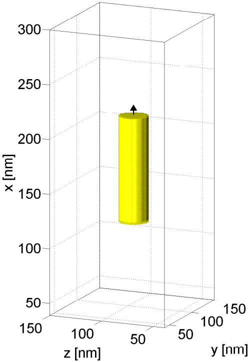




Examples - 2D box Problem - Resonance



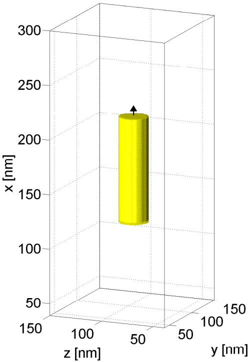
Examples - 3D box nanorod



PKS Results

- Spontaneous decay rate: quantum emitter close to resonator
- Electrical field at the source

Examples - 3D box nanorod

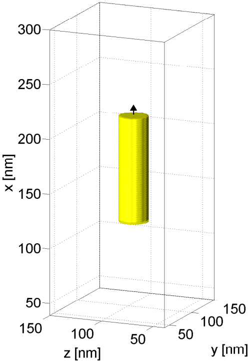


PKS Results

- Spontaneous decay rate: quantum emitter close to resonator
- Electrical field at the source
- Full 3D-Maxwell with second order dispersion relation
- $\beta_3 \partial_t^2 \tilde{\mathbf{P}} + \beta_2 \partial_t \tilde{\mathbf{P}} + \beta_1 \tilde{\mathbf{P}} = \beta_0 \mathbf{E}$

TUDelft

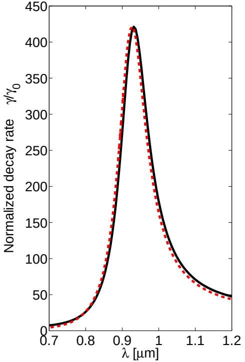
Examples - 3D box nanorod



PKS Results

- Spontaneous decay rate: quantum emitter close to resonator
- Electrical field at the source
- Full 3D-Maxwell with second order dispersion relation
- $\beta_3 \partial_t^2 \tilde{\mathbf{P}} + \beta_2 \partial_t \tilde{\mathbf{P}} + \beta_1 \tilde{\mathbf{P}} = \beta_0 \mathbf{E}$
- After discretization $n = 8.5 \cdot 10^6$

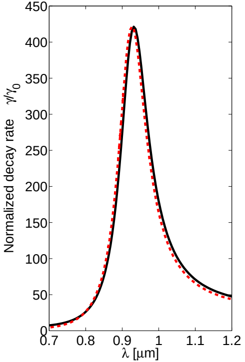
Examples - 3D box nanorod



Configuration

- Reduction to $m = 4500$
- $n/m = 2000$

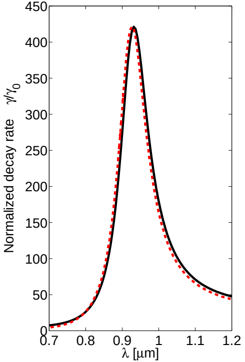
Examples - 3D box nanorod

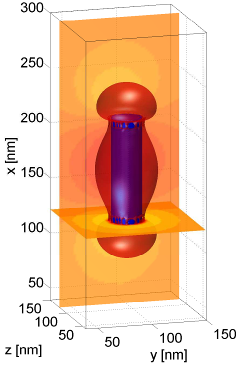


Configuration

- Reduction to $m = 4500$
- $n/m = 2000$
- Computation of ROM takes 45 min
- Evaluation of ROM at 100 frequencies takes 10 sec

Examples - 3D box nanorod





Configuration

- Reduction to $m = 4500$
- $n/m = 2000$
- Computation of ROM takes 45 min
- Evaluation of ROM at 100 frequencies takes 10 sec

TU Delft

Outline

Conclusion

- Krylov ROM can efficiently approximate wave propagation in open domains

TU Delft

Conclusion

- Krylov ROM can efficiently approximate wave propagation in open domains
- Significantly outperforms conventional methods:
  - TD: large time intervals, multiple wavelets
  - FD: multiple frequency solutions are needed

	PKS	EKS	RKS
Reduction n/m	low	medium	high

Conclusion

- Krylov ROM can efficiently approximate wave propagation in open domains
- Significantly outperforms conventional methods:
  - TD: large time intervals, multiple wavelets
  - FD: multiple frequency solutions are needed

	PKS	EKS	RKS
Reduction n/m	low	medium	high
Iteration Cost	low	medium	high

Conclusion

- Krylov ROM can efficiently approximate wave propagation in open domains
- Significantly outperforms conventional methods:
  - TD: large time intervals, multiple wavelets
  - FD: multiple frequency solutions are needed

	PKS	EKS	RKS
Reduction n/m	low	medium	high
Iteration Cost	low	medium	high
Memory Demand	$3n$	$5n$	$m \cdot n$

A Krylov Subspace Approach to Modeling of Wave Propagation in Open Domains

Delft University of Technology, CAS Group

Jörn Zimmerling

Monday 2[nd] February, 2015

TU Delft