ON SOLUTION OF LARGE-SCALE MAXWELL'S EQUATIONS IN THE TIME DOMAIN

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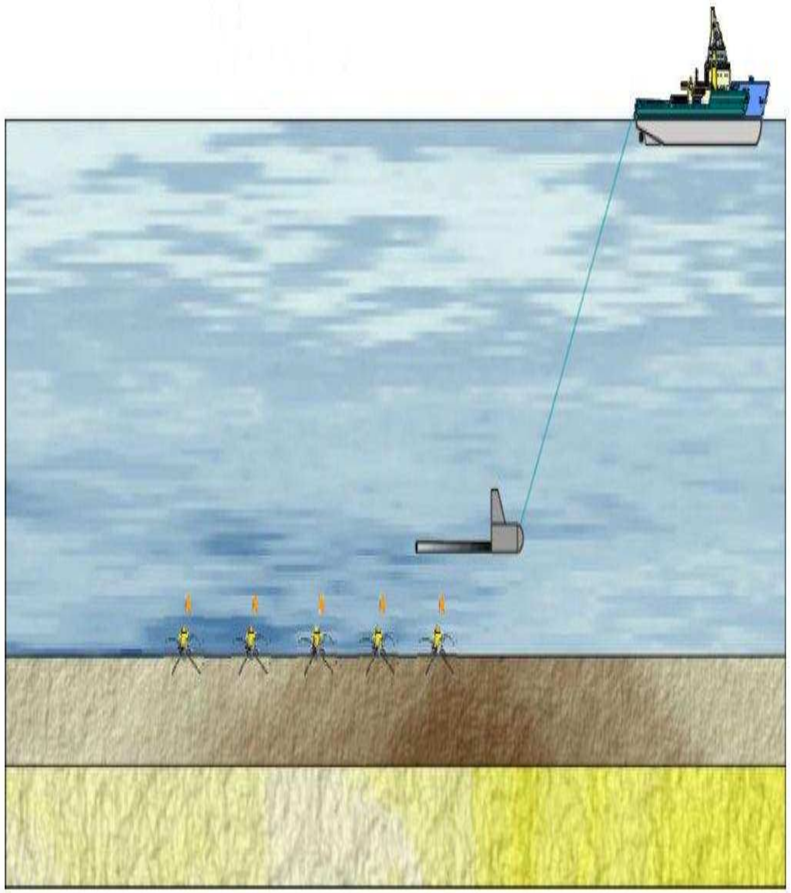
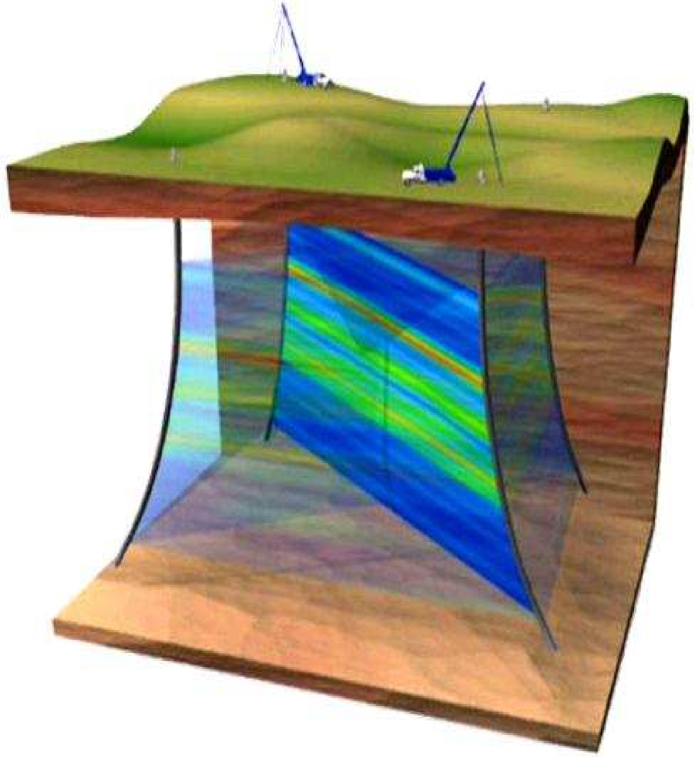
Outline

- Formulation of the problem
- Spatial discretization
- Time-domain solution of non-dispersive problem
- Time-domain solution of dispersive problem

Configuration





Maxwell's equations in dispersive medium

Time-convolution equations:

$$\begin{aligned} \nabla \times E &= -\mu \frac{\partial H}{\partial t}, \\ \nabla \times H &= J_c + J_d + J', \\ J_c &= \sigma(t, \mathbf{r}) * E, \\ J_d &= \epsilon(t, \mathbf{r}) * \frac{\partial E}{\partial t} \end{aligned} \tag{1}$$

Laplace domain:

$$\left(A + \mu\tilde{\sigma}(z, \mathbf{r})z + \mu\tilde{\epsilon}(z, \mathbf{r})z^2\right)\tilde{E} = \tilde{g},$$

$$0 < A = A^* = \nabla \times \nabla \times, \ \tilde{g} = -\mu \frac{\partial \tilde{J}'}{\partial t}$$

Motivations

- Number of unknowns $\approx 10^6 - 10^7$. Large condition numbers
- Multiple scales: large time intervals in order to address near and far heterogeneities
- For dispersive problems solution depends on all previous states
- Multiple matrices inversions are the most time consuming part
- Way to accelerate: projection to the subspace of small dimension (important: preserve properties of initial system)

Examples, non-dispersive medium

Models:

$\tilde{\sigma}(z,\mathbf{r}) = \sigma_\infty(\mathbf{r}), \tilde{\epsilon}(z,\mathbf{r}) = \epsilon_\infty(\mathbf{r})$ $\qquad$ $\tilde{\sigma}(z,\mathbf{r}) = \sigma_\infty(\mathbf{r}), \epsilon(z,\mathbf{r}) = 0$

Laplace domain:

$\left(A + z\sigma_\infty(\mathbf{r}) + z^2\epsilon_\infty(\mathbf{r})\right)\tilde{E} = \tilde{g}$ $\qquad$ $\left(A + z\sigma_\infty(\mathbf{r})\right)\tilde{E} = \tilde{g}$

Time domain:

$\left(A + \sigma_\infty(\mathbf{r})\frac{\partial}{\partial t} + \epsilon_\infty(\mathbf{r})\frac{\partial^2}{\partial t^2}\right)\tilde{E} = g$ $\qquad$ $\left(A + \sigma_\infty(\mathbf{r})\frac{\partial}{\partial t}\right)\tilde{E} = g$

Examples, Cole-Cole dispersive model

$$\tilde{\sigma}(z,\mathbf{r}) = \sigma_\infty(\mathbf{r})\left(1 - \frac{\eta(\mathbf{r})}{1+(z\tau(\mathbf{r}))^{c(\mathbf{r})}}\right), \ \tilde{\epsilon}(z,\mathbf{r}) = 0$$

Ohm's law may be rewritten as a fractional order differential equation:

$$\mathbf{J}_c + \tau^c D_t^c \mathbf{J}_c = \sigma_\infty(1-\eta)\mathbf{E} + \tau^c \sigma_\infty D_t^c \mathbf{E}$$

Expanding is series near $z = z_0$: $\tilde{\sigma}(z) = \sum_{i=0}^{\infty} \tilde{\sigma}_i \left(z - z_0\right)^i$

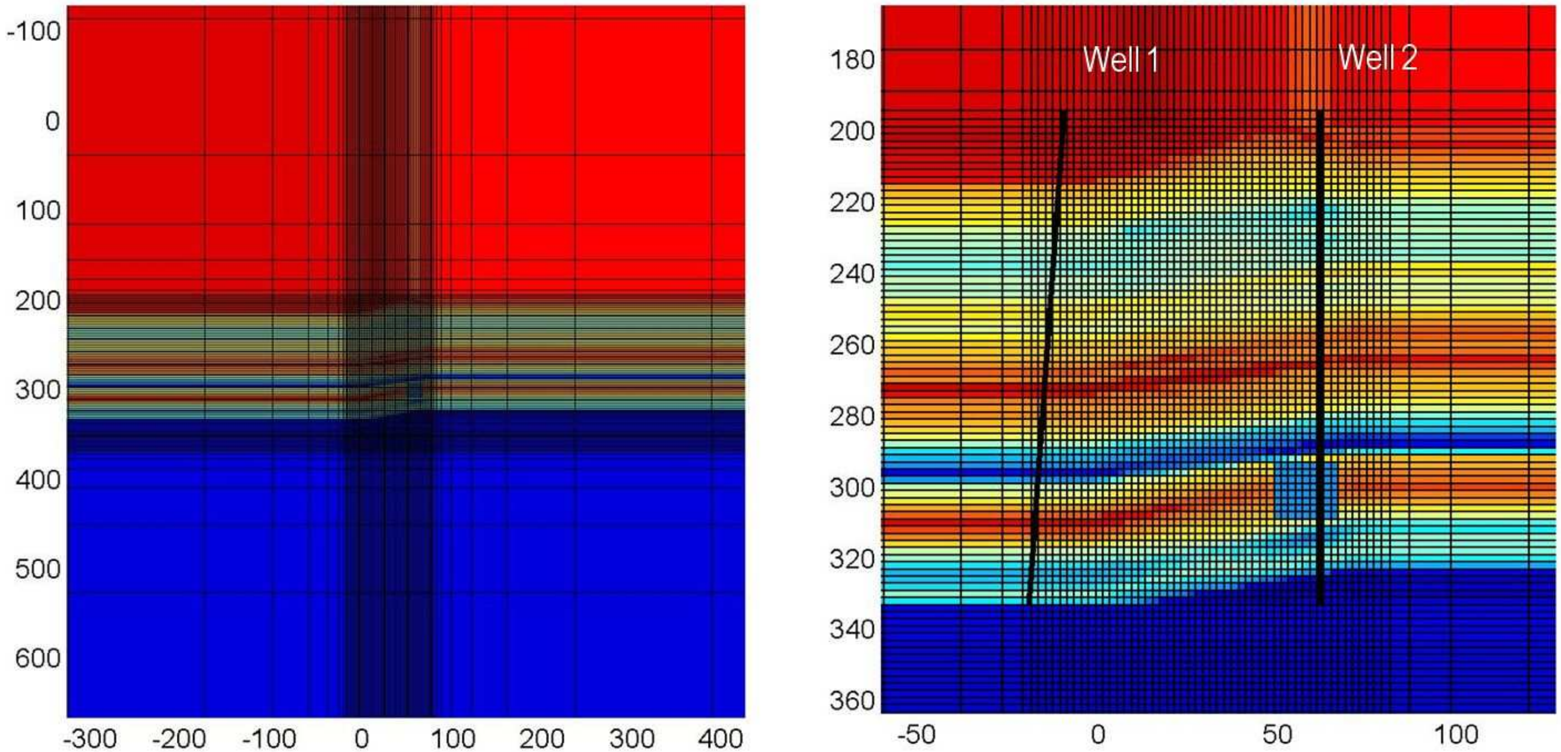
we obtain infinite order dynamical system

$$\left(A + \sum_{i=0}^{\infty} a_i \left(z - z_0\right)^i\right)\tilde{E} = \tilde{g},$$

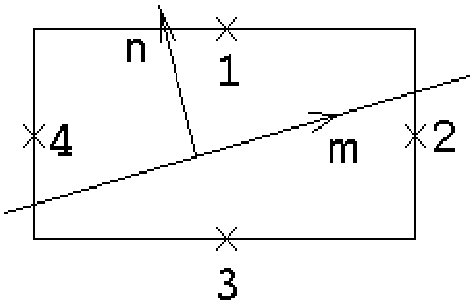
$$\left(A + \sum_{i=0}^{\infty} a_i \left(\frac{\partial}{\partial t} - z_0 I\right)^i\right) E = g.$$

Spectrally matched grid for outer domain

Ingerman, Dr., Kn. [CPAM, 2000]



Nodal homogenization



Moskow et al [SINUM, 1999]

$$-\nabla \cdot \sigma \nabla \varphi = J'$$

The solution may be approximated in cell H by a function from

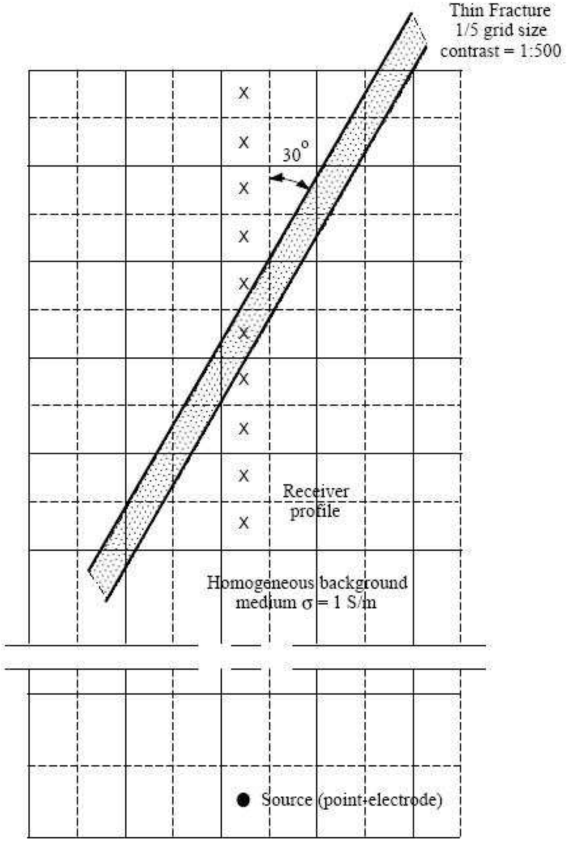
$$L(H) = span(\varphi_0 = 1, \varphi_1 = m \cdot r, \varphi_2 = \int_0^{n \cdot r} \frac{ds}{\sigma})$$

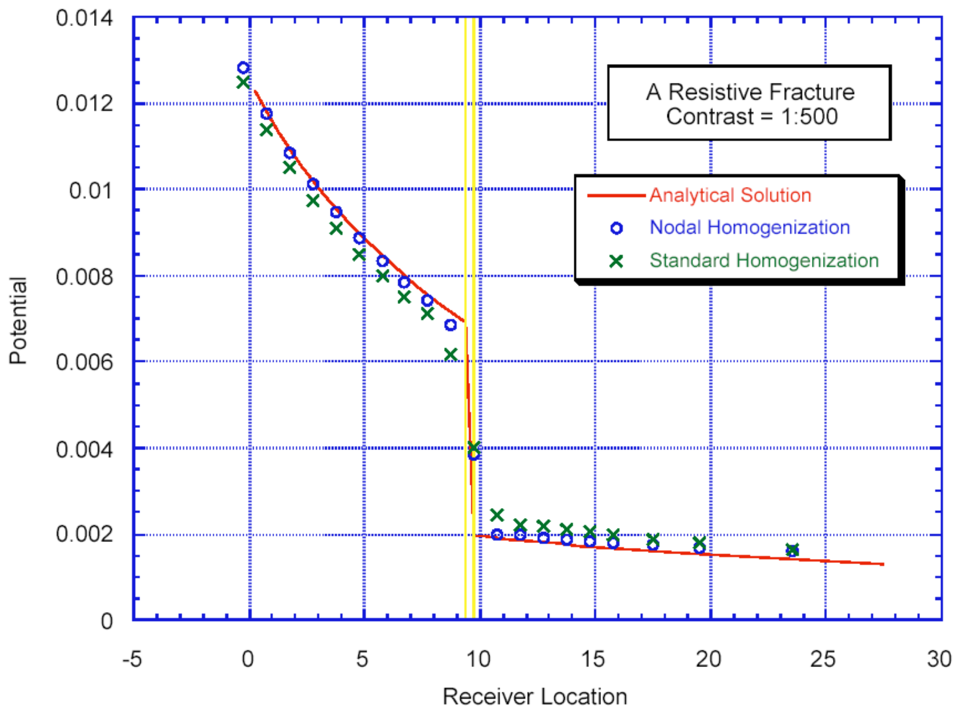
Effective tensor Σ_{ij}: energy matching for functions from $L(H)$.

$$\int_H \sigma \varphi^{\alpha},_i \varphi^{\beta},_j \, dV = |H| \Sigma_{ij}^{H} \bar{\varphi},_i^{\alpha} \bar{\varphi},_j^{\beta} \;, \alpha, \beta = 1, 2$$

Theorem (convergence in weak sense) $(u - u_h, v)_{\Sigma} \leq Ch$

Fracture. Results





Existing approaches for time domain problems

Semi-discrete time-domain equations

$AE(t) + \frac{dE(t)}{dt} = g$

$AE(t) + \frac{d(\sigma * E(t))}{dt} = g$

- **Time stepping**
- **Contour integration for TD problems**

  Quadrature formula for $u(t) = \int_\Gamma e^{-\lambda t} \left(A_- \sigma_\infty z I\right)^{-1} \tilde{g} dz$,
- Krylov subspace methods

Non-dispersive problem, subspace reduction

Compute matrix exponential: for $g(t) = \delta(t) f(\mathbf{r})$

$$E(t) = \exp\left(-\tilde{A}t\right) f$$

$E(t) \approx E_m(t) \in colspan V_m$, where $V_m \in \mathbb{R}^{n\times m}$, $m \ll n$ and $(V_m)^* V_m = I$

Projection based methods:

$$E_m(t) = V_m \exp(-T_m t) V_m^* f$$

$$T_m = V_m^* \tilde{A} V_m \in \mathbb{R}^{m\times m}$$

Subspace reductions, non-dispersive case

Polynomial Krylov subspace reduction:

$$V_m \in span\{\tilde{g}, A\tilde{g}, A^2\tilde{g}, ..., A^{m-1}\tilde{g}\}$$

Rational Krylov Subspace Reduction

$$V_m \in \text{span}\{b, Ab, \ldots, A^{m-1}b\}, \qquad b = \prod_{j=1}^{n}(A + z_j\sigma_\infty I)^{-1}\tilde{g}$$

If all shifts are different then

$$V_m \in \text{span}\{(A+z_1\sigma_\infty I)^{-1}\tilde{g}, (A+z_2\sigma_\infty I)^{-1}\tilde{g}, \ldots, (A+z_m\sigma_\infty I)^{-1}\tilde{g}\}$$

Requires solution of m shifted linear systems

$$E_m = R_{m-1,m}(A)\tilde{g}$$

Subspace choice. Non-dispersive problem

We use iterative solver for 3D large scale system, thus there is no advantage in using the same shifts

Third Zolotarev problem in the complex plane:

$$\sigma_m = \min_{\lambda_1,\ldots,\lambda_m, z_1,\ldots,z_m} \frac{\sup_{\lambda\in\Lambda} |r(\lambda)|}{\inf_{z\in i\mathbb{R}} |r(z)|},$$

where

$$r(z) = \prod_{j=1}^{m} \frac{z-\lambda_j}{z+z_j},$$

and λ_i are auxiliary parameters.

Error estimate (*Dr., Kn., Z. [SISN, 2008]*):

$$\sqrt[m]{||E-E_m||_{L_2[0;+\infty)}} \lessapprox \sqrt[m]{\sigma_m} \approx e^{-\frac{\pi^2}{2\log\frac{4\lambda_{\max}}{\lambda_{\min}}}},$$

Nested subspaces

Sequences $\{z_j\}_{j=1}^m$ are not nested

$$\frac{1}{m}\sum_{j=1}^{m}\delta(z-z_j)\to\alpha(z),$$

where $\alpha(z)$ is equilibrium measure on $[\lambda_{min};\lambda_{max}]$.

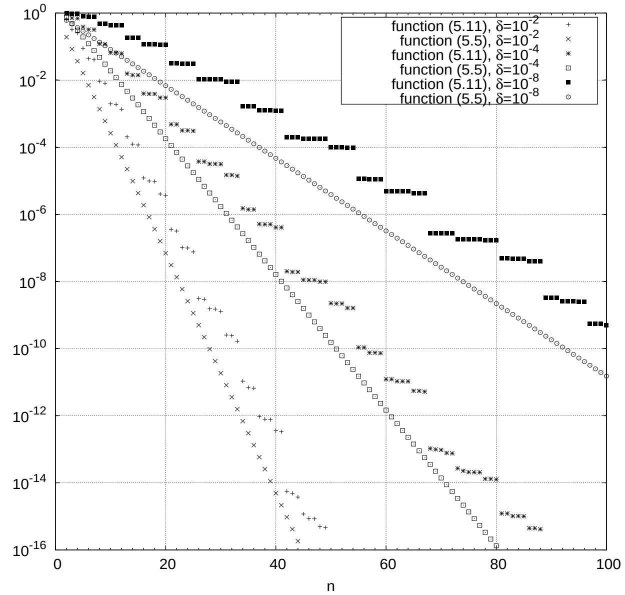
We choose nested $\{\bar{z}_j\}_{j=1}^m$

$$\frac{1}{m}\sum_{j=1}^{m}\delta(z-\bar{z}_j)\to\alpha(z).$$

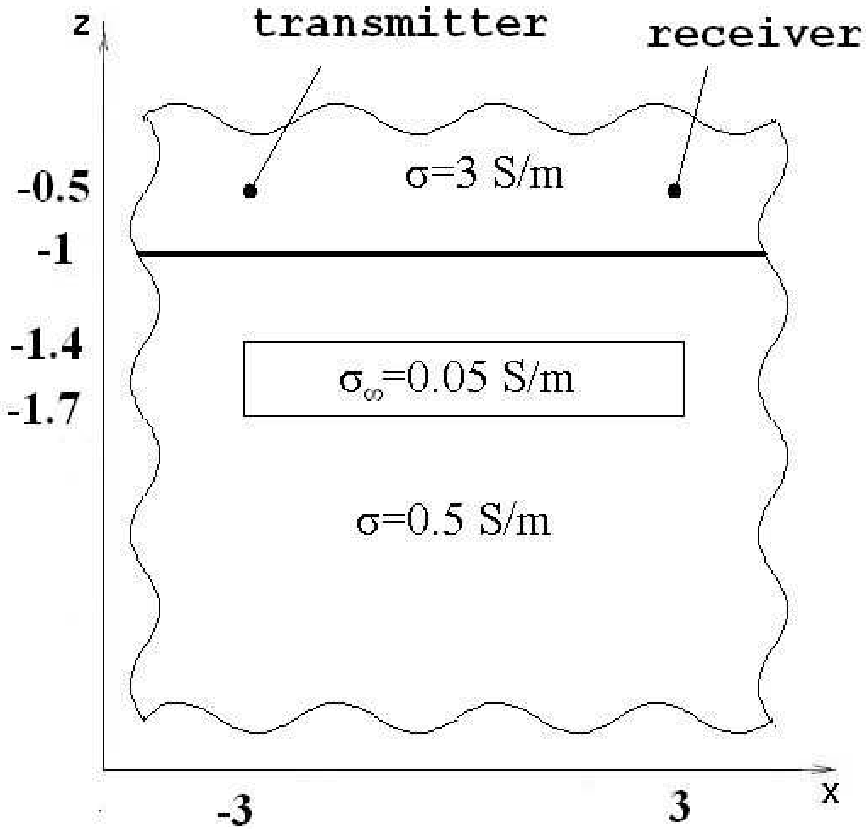
$\alpha(z_j)=t_j$, t_j is EDS on $[0;1)$

$$t_j=\{j\xi\},$$

where ξ is any irrational number

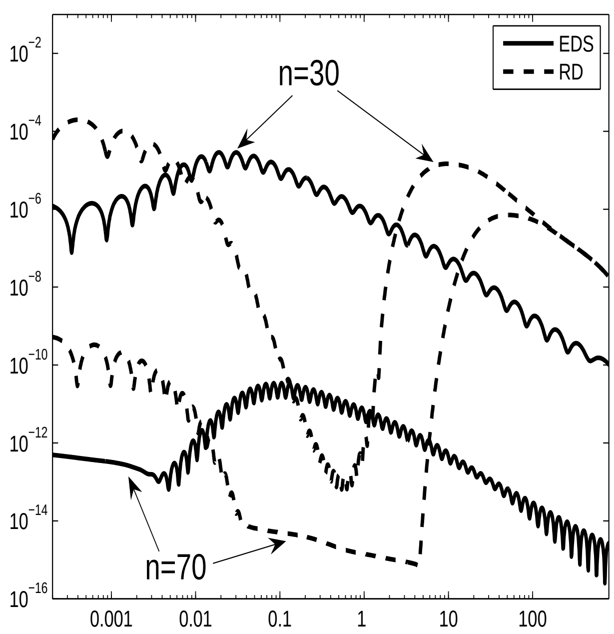


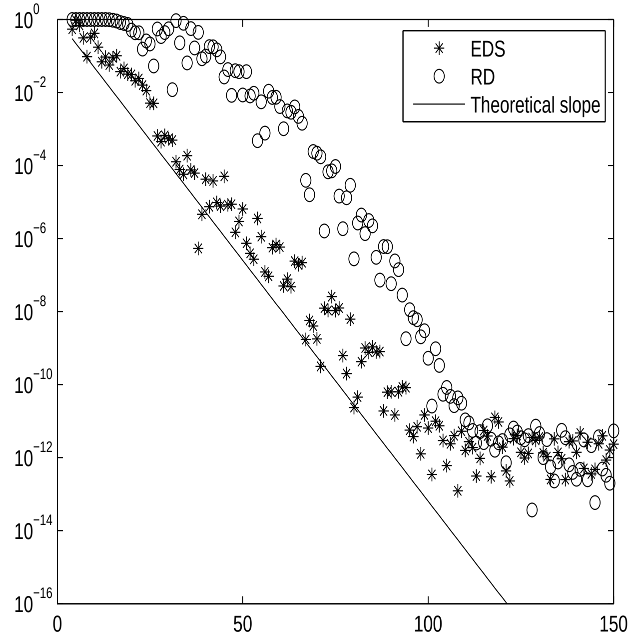
Synthetic example



Multiple shifts vs single shift

Single shift: Anderson [JAT, 1981]





Parameter-dependent Krylov subspace reduction

$$\tilde{A}(z)\tilde{E} := (A + \mu\tilde{\sigma}(z, \mathbf{r})z)\,\tilde{E} = \tilde{g},$$

Similar to rational Krylov subspace,

$$V_m \in \text{span}\{(\tilde{A}(z_1))^{-1}\tilde{g}, (\tilde{A}(z_2))^{-1}\tilde{g}, \ldots, (\tilde{A}(z_m))^{-1}\tilde{g}\}$$

Stability: $\tilde{A}(z)$ doesn't have spectrum in $\mathcal{C}_+$. So does $\tilde{T}_m$

Passivity: $\Re\frac{1}{z}\tilde{A}(z) \succ 0$ in $\mathcal{C}_+$. Similarly $\Re\frac{1}{z}\tilde{T}_m \succ 0$ in $\mathcal{C}_+$.

Error estimate, pseudospectrum

Let $[\alpha_{min}(z), \alpha_{max}(z)]$ and $[\beta_{min}(z), \beta_{max}(z)]$ be the spectral intervals of $\Re\tilde{A}(z)$ and $\Im\tilde{A}(z)$ respectively. We denote

$$\alpha(z) = \text{dist}\,\{[\alpha_{min}(z), \alpha_{max}(z)], 0\}\,,\ \beta(z) = \text{dist}\,\{[\beta_{min}(z), \beta_{max}(z)], 0\}$$

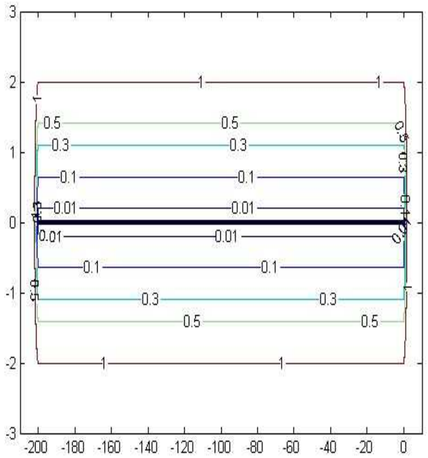
and isolines $\sqrt{\alpha^2(z) + \beta^2(z)} = \epsilon$ as Γ_ϵ.

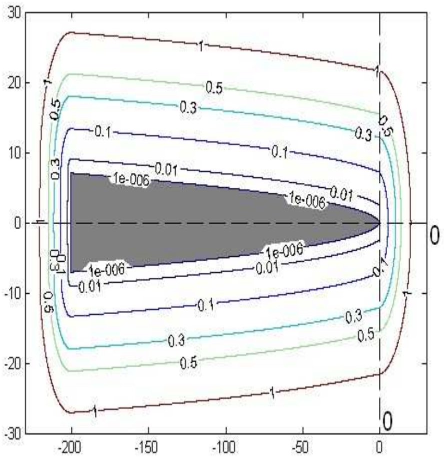
Error estimate(*Dr., Z. [2009]*): for $g(t) = \delta(t)f(\mathbf{r})$

$$||E - E_m||_{L_2[0;+\infty)} \lessapprox C\frac{|\Gamma_\epsilon|}{\epsilon}\sigma_m$$

$$\sigma_m = \min_{\lambda_1,\ldots,\lambda_m,z_1,\ldots,z_m} \frac{\sup_{\lambda\in\Gamma_\epsilon}|r(\lambda)|}{\inf_{z\in i\mathbb{R}}|r(z)|},\ r(z) = \prod_{j=1}^{m}\frac{z-\lambda_j}{z+z_j}$$

Subspace choice. Examples



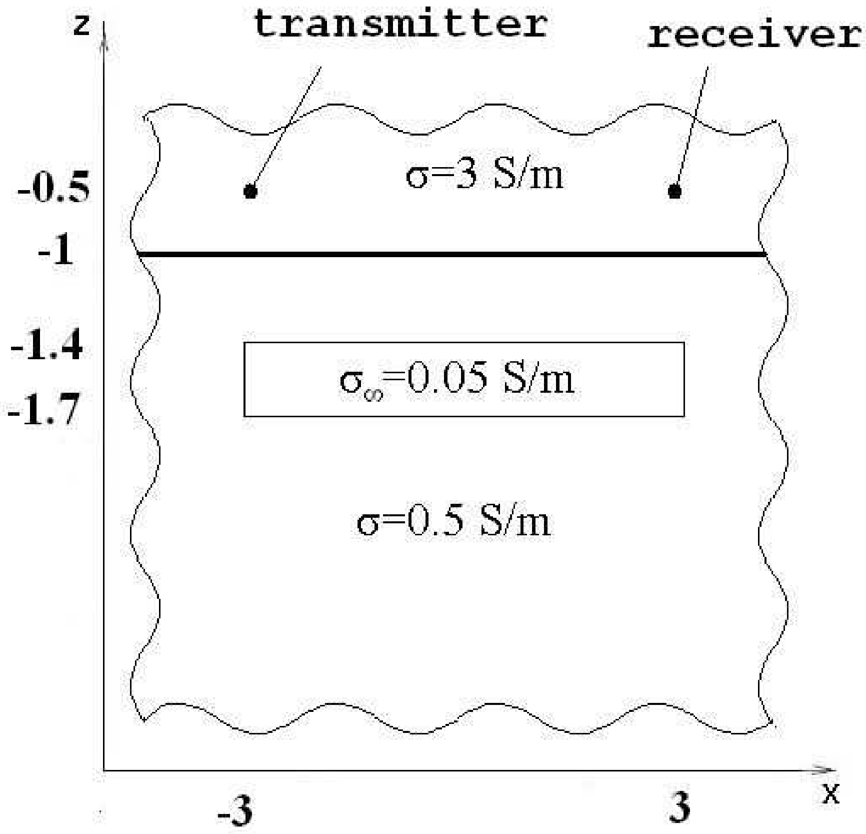


$$\sigma_n = \min_{\lambda_1,\dots,\lambda_n,z_1,\dots,z_n} \frac{\sup_{\lambda\in\Gamma_\epsilon} |r(\lambda)|}{\inf_{z\in i\mathbb{R}} |r(z)|},$$

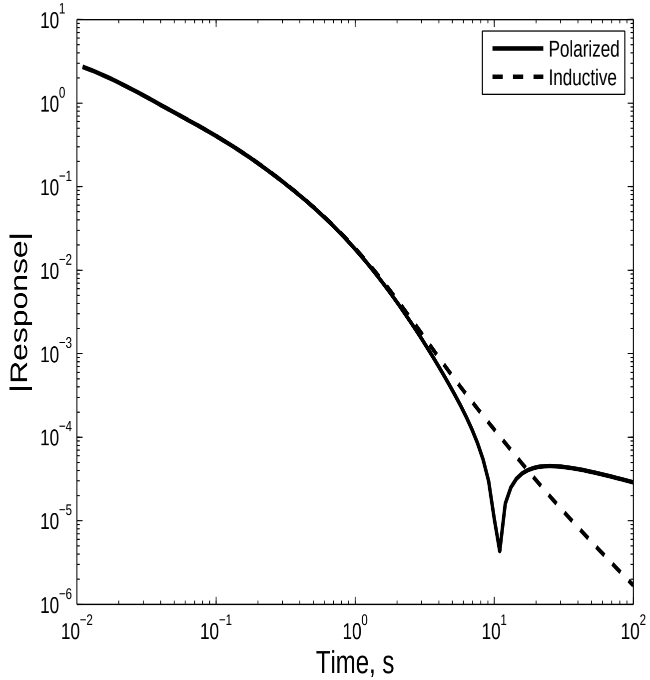
$$r(z) = \prod_{j=1}^{n} \frac{z-\lambda_j}{z+z_j}$$

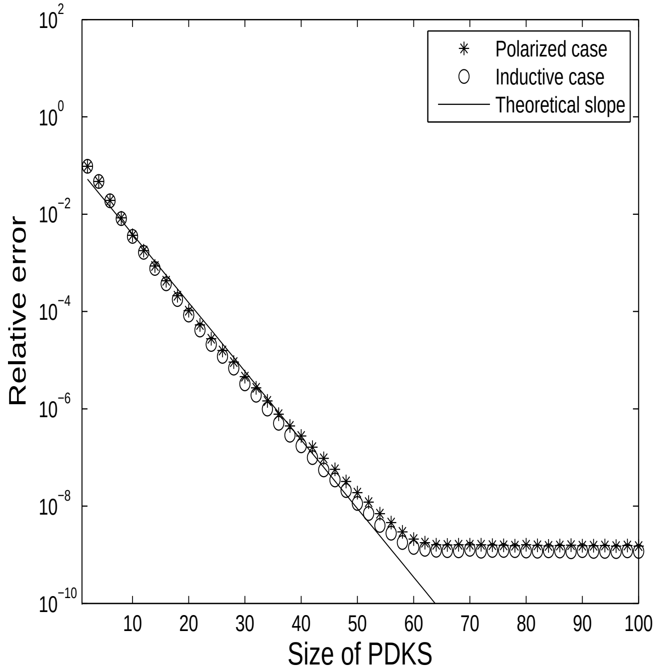
- For dispersive problem spectrum is complex
- For large scale problems Zolotarev points from non-dispersive problems may be used for dispersive problems too
- General case: open question

Synthetic example



Solutions and convergence rates





Conclusions and open questions

- We developed a powerful tool for solution of large scale convolutionary problems
- The cost of any time interval is no more than 10-15 conventional complex frequency problems.
- Orthogonalization is performed using explicit computation of residual. Rational Arnoldi may be used instead for non-dispersive problem. Open question: analogue for dispersive problems
- The reduction to the Zolotarev problem allows to design optimal shifts in the Laplace domain for non-dispersive problems as well as Cole-Cole large scale dispersive problems. Open question: solution for more general dispersive problem