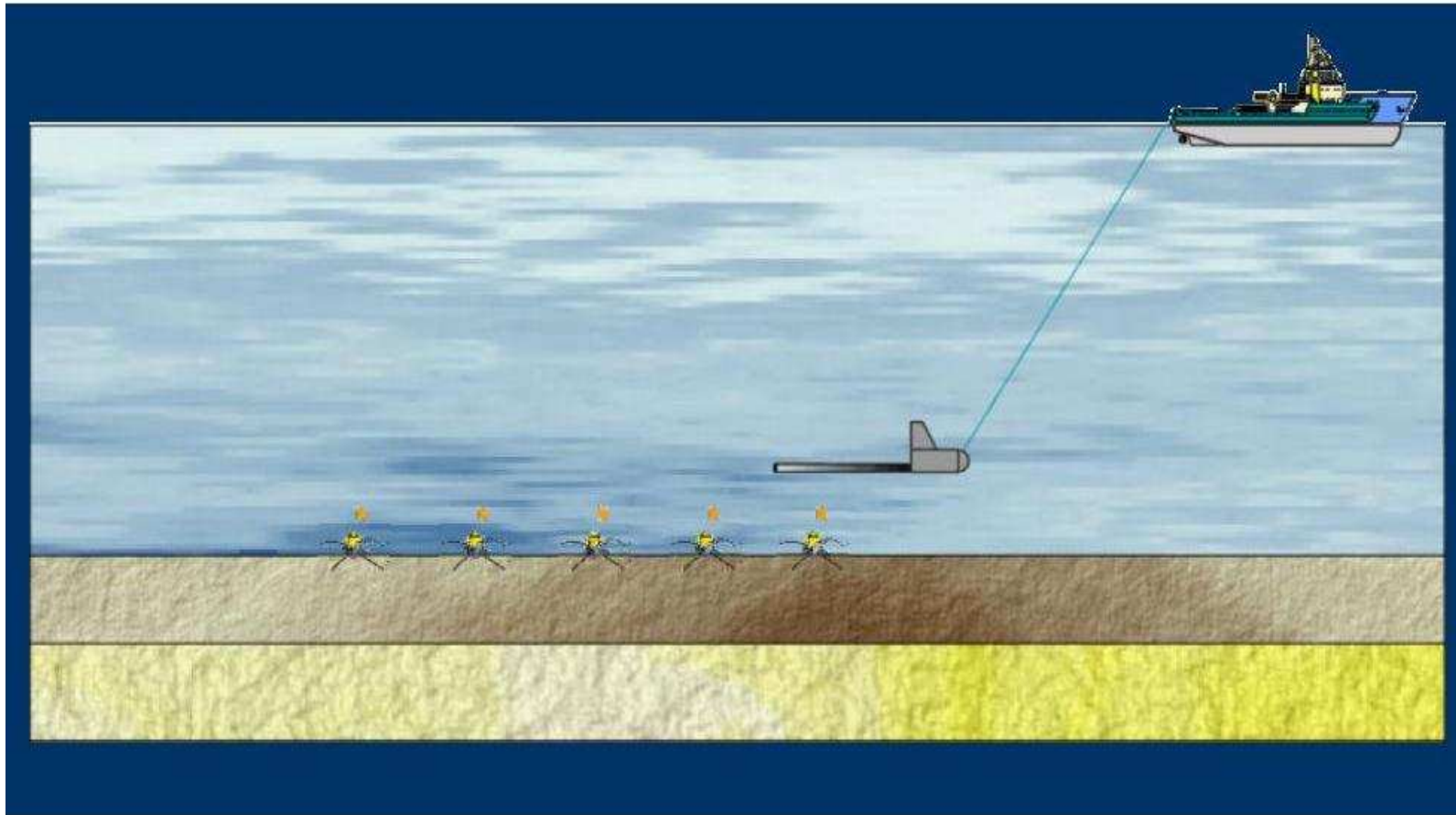


MODEL REDUCTION APPROACHES FOR
FORWARD AND INVERSE PROBLEMS OF
GEOPHYSICAL EXPLORATION

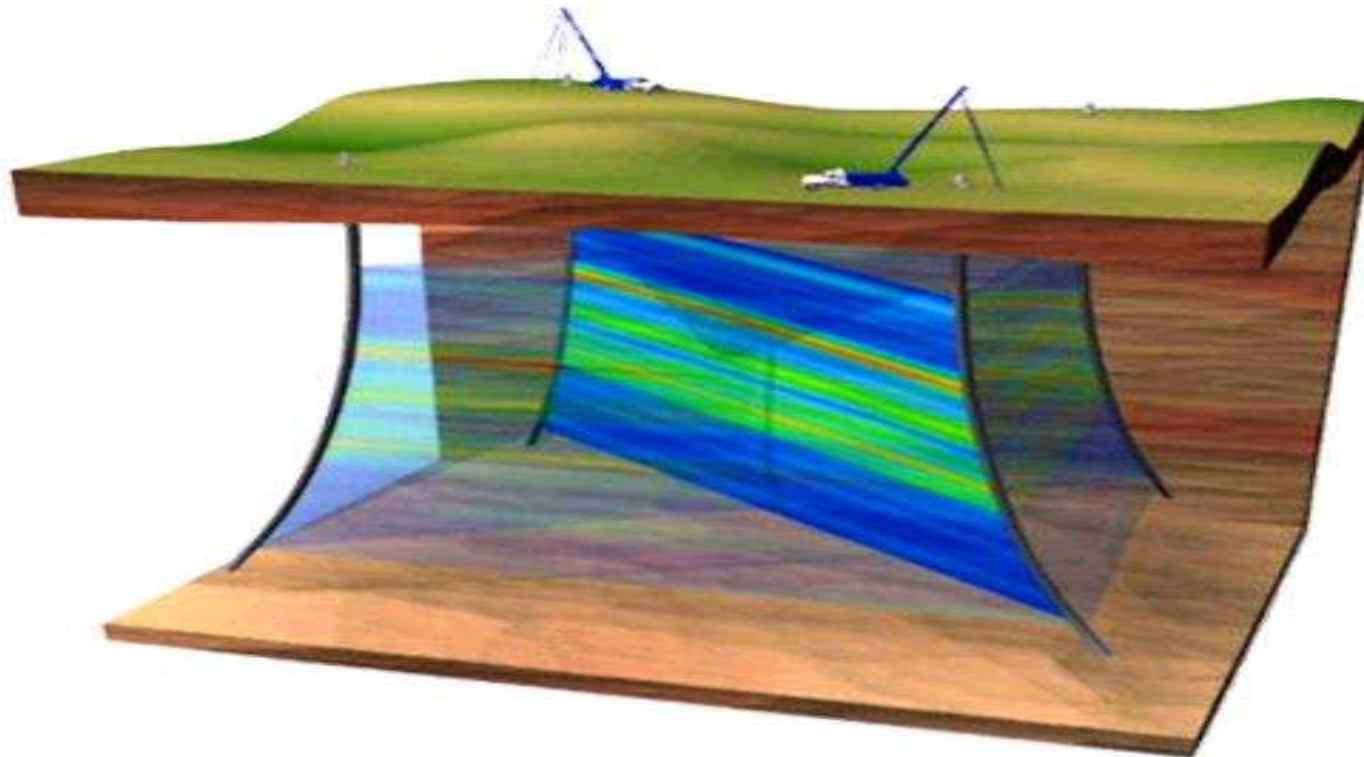
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Cross-well configuration



Motivations

- The most time consuming part is multiple computations of forward solutions
- Way to accelerate: design fast and accurate self-learning surrogate of the forward solver, which efficiently uses the information from all the previous calls

Outline

- Multi-frequency problems
- Inverse problems (multi-parametric model reduction)

Multi-frequency problems.

Optimization of Rational Krylov Subspace
Reduction

Existing approaches (incomplete)

- Krylov subspace reduction for time and frequency domain Maxwell equations (SLDM) [Druskin, Knizhnerman, 1988]
- Circuit theory: approximation of transit function in the frequency domain via Pade-Lanczos connection [Freund et al, 1995; Bai, 2003]
- Rational Krylov projection [Ruhe, 1994; Gugercin, Willcox, 2007], H^∞ -optimal [Megretski, 2006] and H^2 -optimal [Gugercin, Antoulas, Beattie, 2006]

Frequency domain Maxwell equations

$$\begin{aligned}\nabla \times E &= i \omega \mu H, \\ \nabla \times H &= \sigma E + J', \\ J &= \sigma E + J'\end{aligned}\tag{1}$$

Magnetic field formulation

$$\nabla \times \sigma^{-1} \nabla \times H - i \omega \mu H = \nabla \times \sigma^{-1} J'\tag{2}$$

Discretization and linear solver

- Lebedev grid (superposition of Yee grids)
- Spectrally Matched Grids for approximation in infinite domains (MOR based, will be discussed by Vladimir)
- Homogenization
- Divergence-free preconditioner and QMR for complex symmetric linear system

But we still need acceleration

Rational Krylov subspace

Purpose: solve

$$A_\omega H_\omega = S$$

for any frequency from $[\omega_l; \omega_r]$, where

$$A_\omega = A_0 + i\omega I$$

Reduced model: solve for certain frequencies ω_j , $j = 1, \dots, m$ and then use real and imaginary parts of the obtained solutions

$$u_j = \Re(A_{\omega_j}^{-1} S) = A(A^2 + \omega^2 I)^{-1} S,$$

$$u_{j+m} = \Im(A_{\omega_j}^{-1} S) = \omega(A^2 + \omega^2 I)^{-1} S,$$

i.e. we consider the problem of approximating u_ω by rational Krylov subspace $K_{2m} = \text{span}\{u_1, \dots, u_{2m}\}$.

Reduced order model

Rational $2m - 1/2m$ interpolation matching solution at source and its derivative

$u_\omega \in M^{2m}$ such that

$$(A_\omega u_\omega; v) = (S; v)$$

for any $v \in M^{2m}$.

Choice of interpolation points:

- geometric grid
- Zolotaryov nodes (asymptotically optimal in Cauchy-Hadamard sense)

Skeleton approximations

Scalarizing the problem, i.e., consider it in the spectral coordinates, we will seek the Galerkin approximant $\tilde{w} \in V$ to the function

$$\frac{1}{\lambda + i\omega}, \quad \lambda \in \mathbb{R}, \quad \lambda \geq 0, \quad \omega \in [\omega_l; \omega_r],$$

where $V = \text{span}\{v_1, \dots, v_n\}$ and $v_l = (\lambda + i\omega_l)^{-1}$.

$$f_{\text{skel}}(\lambda, s) = \left(\frac{1}{\lambda + i\omega_1}, \quad \dots, \quad \frac{1}{\lambda + i\omega_n} \right) M^{-1} \begin{pmatrix} \frac{1}{i\omega + \lambda_1} \\ \vdots \\ \frac{1}{i\omega + \lambda_n} \end{pmatrix}, \quad M = (M_{kl}) \text{ is}$$

the $n \times n$ matrix with the entries $M_{kl} = 1/(\lambda_k + i\omega_l)$.

Asymptotically optimal choice of frequencies

Relative approximation error:

$$\delta = \left[\frac{1}{\lambda + i\omega} - f_{\text{skel}}(\lambda, \omega) \right] / \frac{1}{\lambda + i\omega} = \prod_{j=1}^n \frac{\lambda - \lambda_j}{\lambda + i\omega_j} \cdot \prod_{j=1}^n \frac{i\omega - i\omega_j}{\omega + \lambda_j},$$

i.e, λ_j and ω_j are interpolating points.

$$\delta = \frac{r(\lambda)}{r(-i\omega)}, \quad r(z) = \prod_{j=1}^n \frac{z - \lambda_j}{z + i\omega_j}.$$

Minimization problem $\sigma_n = \min_{\lambda_1, \dots, \lambda_n, \omega_1, \dots, \omega_n} \frac{\max_{\lambda \geq 0} |r(\lambda)|}{\min_{\omega \in [\omega_l; \omega_r]} |r(i\omega)|}$ is a partial case of the third Zolotaryov problem in the complex plane, and it has the unique solution with noncoinciding nodes

Convergence rate

Introduce the full elliptic integral of modulus $\kappa = \sqrt{1 - \frac{\omega_l}{\omega_r}}$

$$K = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-\kappa^2 t^2)}}.$$

Theorem: With the number $\rho = \exp \left[-\frac{\pi K(\sqrt{1-\kappa^2})}{2K(\kappa)} \right]$ the following assertions are valid:

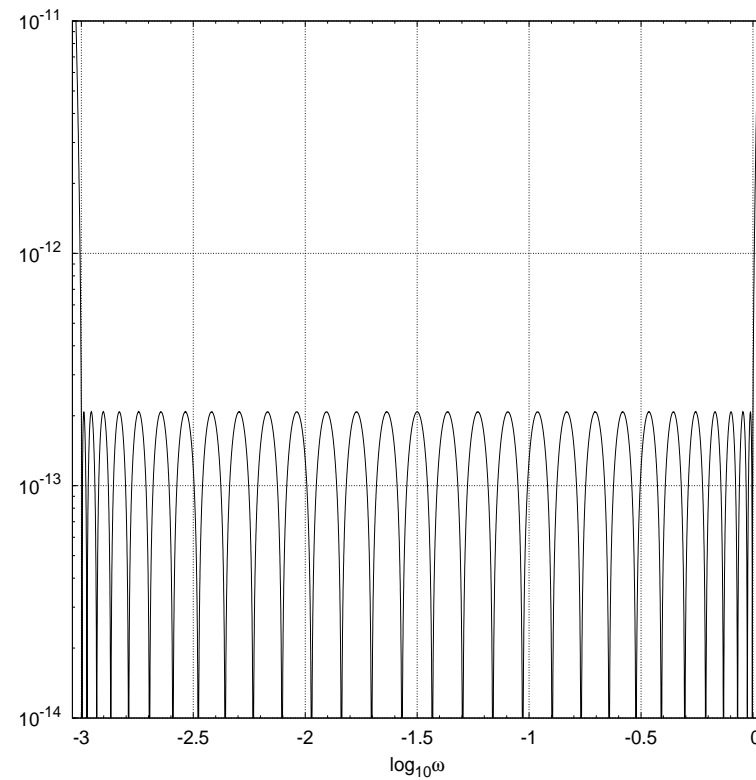
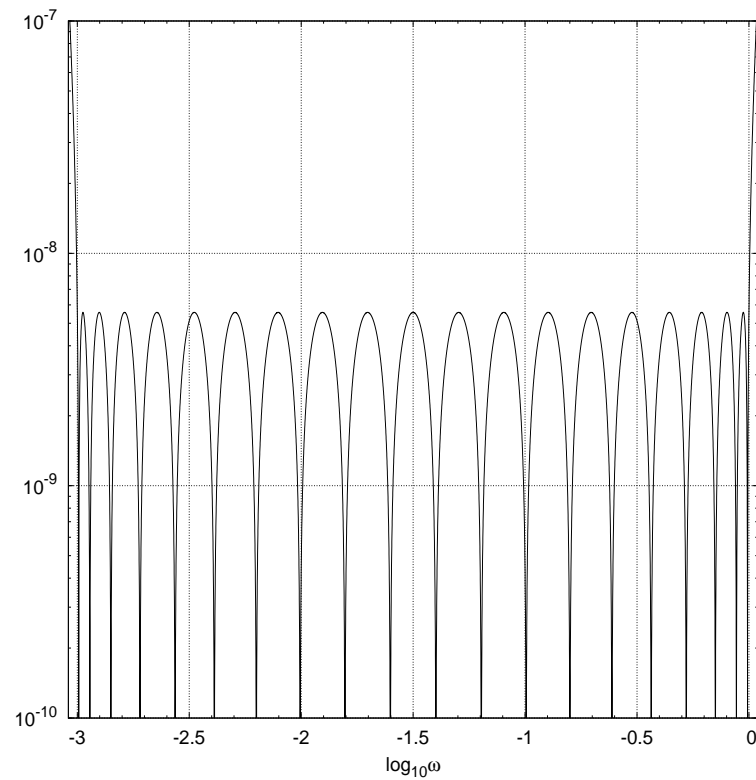
$$\sigma_n \geq \rho^n, \quad n \in \mathbb{N},$$

$$\lim_{n \rightarrow \infty} \sqrt[n]{\sigma_n} = \rho.$$

Explicit formula:

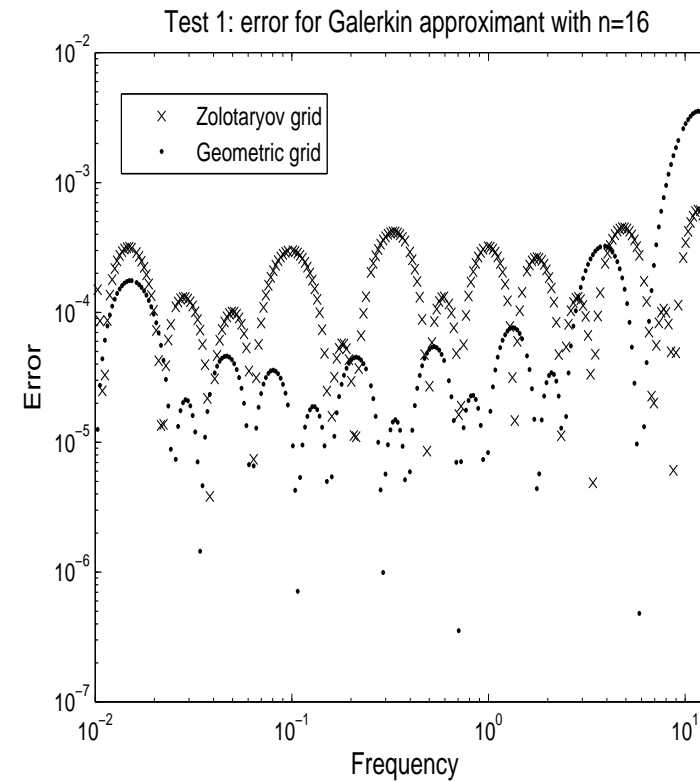
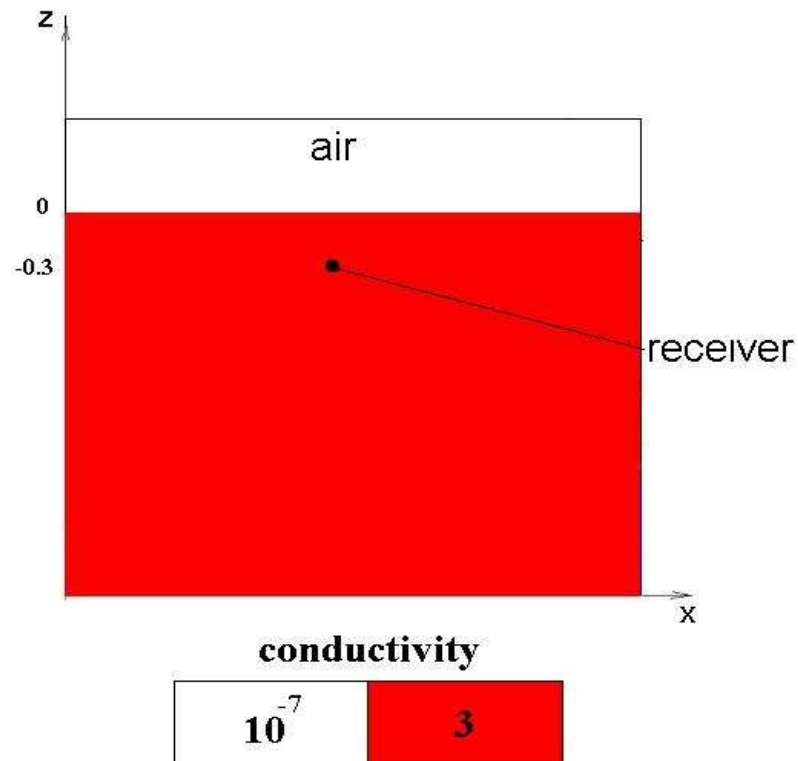
$$\omega_j = 1 - (1 - \kappa^2) \operatorname{sn} \left(\frac{2j-1}{n}, \kappa \right)^2, \quad \omega_{\frac{n}{2}+j} = -\omega_j, \quad j = 1, \dots, \frac{n}{2}$$

$$\mathbf{Error} \frac{\max_{\lambda \geq 0} |r(\lambda)|}{|r(i\omega)|} \cdot$$



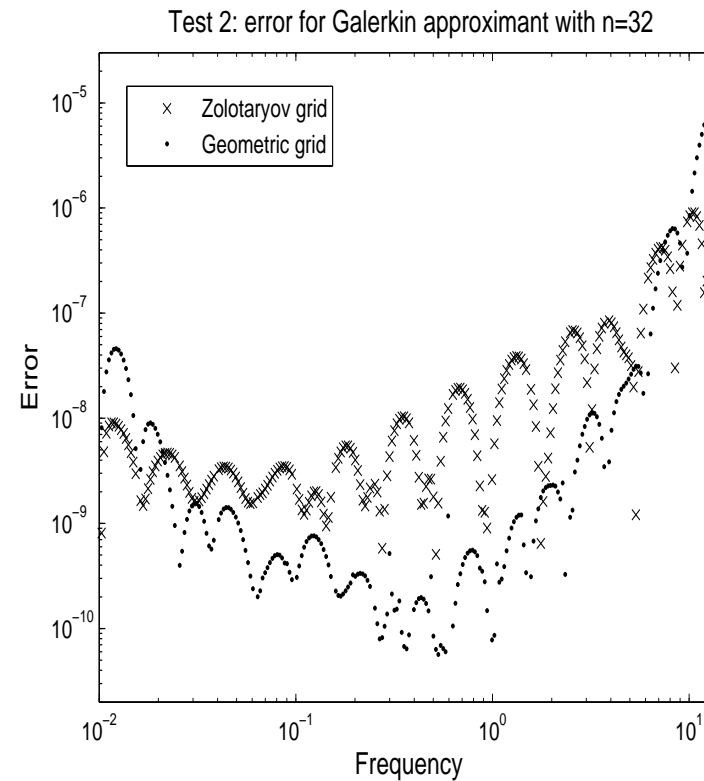
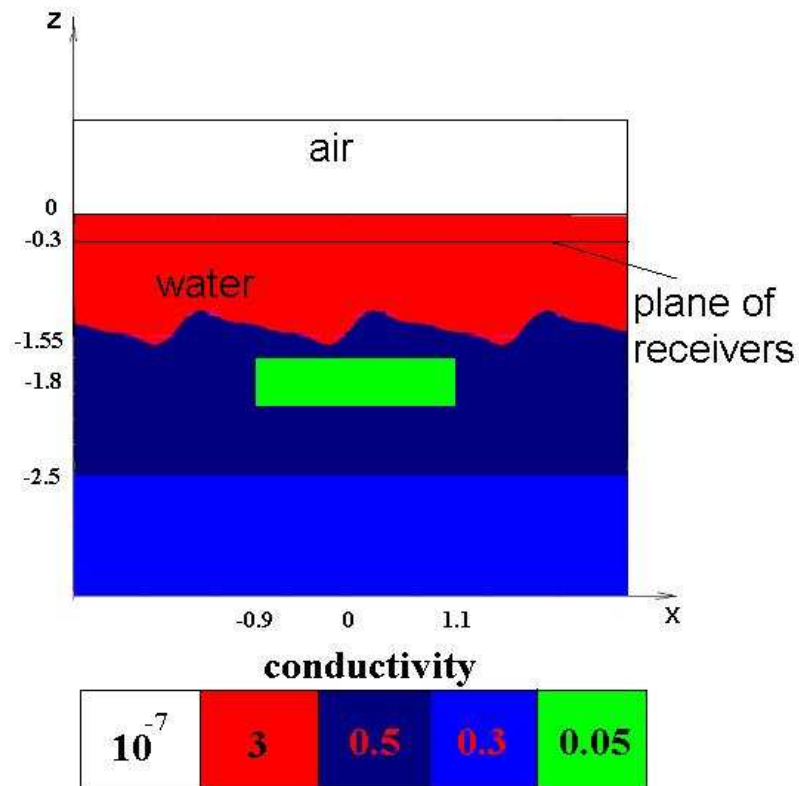
$n = 40$ (left) and $n = 60$ (right)

Homogeneous half-space



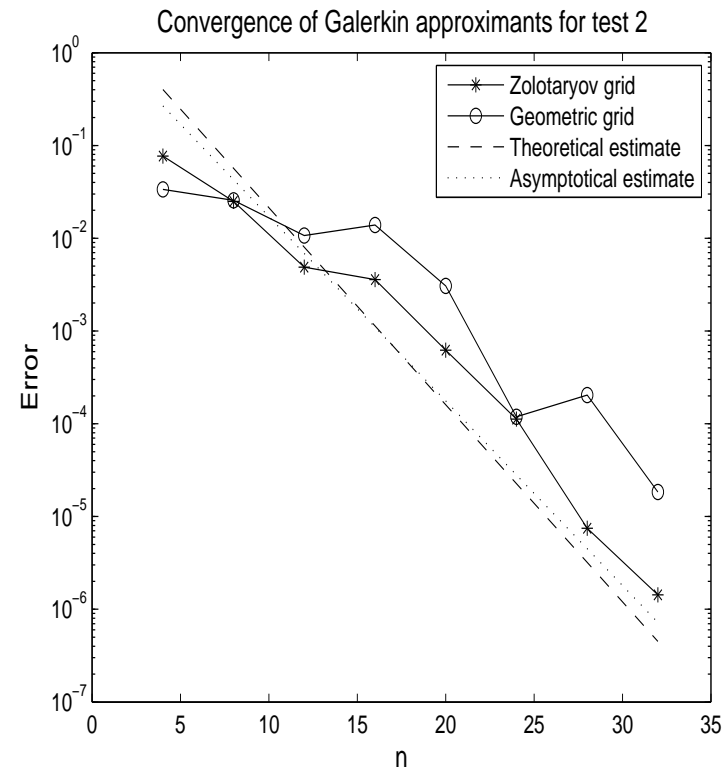
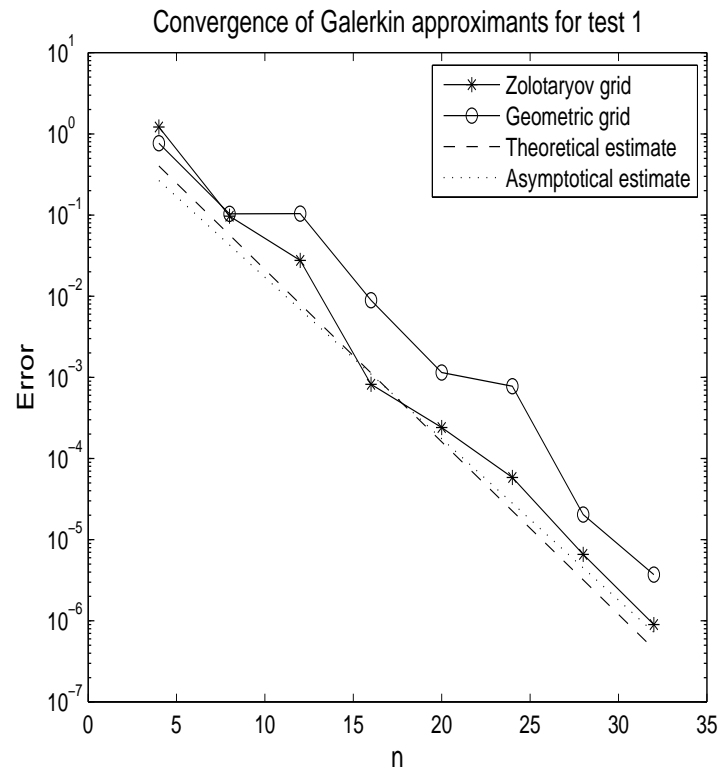
Medium structure (left) and approximation error using M^{16}

More complex medium



Medium structure (left) and approximation error using M^{32}

Convergence of reduced order models



Homogeneous half-space (left) and more complex case (right)

Inverse problems.

Multi-parametric model reduction

Existing approaches (incomplete)

- One-parametric inversion [Remis, Budko, 2005]
- Multi-parametric model reduction [Weile et al, 1999; J.H. Lee et al, 2005; Cuyt et al, 2006]
- Multi-parametric inversion [L. Daniel, O.C. Siong, L.S. Chay, K. H. Lee, J. White, 2004]

Formulation of the forward problem

Let

$$A(\rho)u_k = s_k, \quad k = 1, \dots, m_s \quad (3)$$

be FE or FD approximation of the linear second order PDE problem with symmetric (or complex symmetric) operator, i.e.

$$u_k, s_k \in C^N, \quad A(\rho) \in C^{N \times N},$$

N is very large. ρ is a finite-dimensional vector of the discrete PDE coefficient and $A(\rho)$ is linear with respect to it, m_s is the number of (linearly independent) sources.

Examples of the problems

- A is real symmetric: 3D EIT, DC equation for electric potential

$$A \approx -\nabla \cdot (\rho \nabla u),$$

where u is the electric potential, $\rho > 0$ is the variable electrical conductivity distribution of the medium.

- A is complex symmetric: frequency domain Maxwell system

$$A \approx \nabla \times (\rho \nabla \times H) - \kappa H, \quad (4)$$

where H is the magnetic field, $\rho > 0$ is variable electrical resistivity of the medium (the inverse of the electrical conductivity in the EIT), $\kappa = \sqrt{-1}\omega\mu$ is a (constant) complex wave number, ω is radial frequency, μ is magnetic permeability.

Formulation of the inverse problem

For simplicity we assume (can be extended for any measurements), that the measurements are given by impedance matrix with elements

$$m_{lk} = s_l^T u_k^\rho, \quad k, l = 1, \dots, m_s.$$

Total we have m_s^2 unknowns.

Let $F(\rho)$ be the forward operator mapping the model ρ to the measurements.

The inverse problem as a minimization of the residual functional:

$$\|F(\rho) - M\| \rightarrow \min,$$

assuming Euclidean norm.

Assumptions for simplicity

Assumption 1: The solution of our inverse problem is unique, and can be obtained by the GN algorithm.

Assumption 2: The number of measurements m and the dimension of ρ are not large, so the problem is stable and does not require regularization or any constraints. Although the same techniques can be applied for regularized and constrained inverse problems.

Reduced Order Model (ROM), I

Let ρ^i be iterates of our inversion algorithm. For every iteration we need to obtain solutions $u_l^{\rho^i}$, $l = 1, \dots, m_s$.

Let U^n be the $N \times n \cdot m_s$ matrix of the solutions $u_l^{\rho^i}$, $l = 1, \dots, m_s$, $i = 1, \dots, n - 1$ as a columns:

$$U^n = \left(u_1^{\rho^0}, \dots, u_{m_s}^{\rho^0}, \dots, u_1^{\rho^{n-1}}, \dots, u_{m_s}^{\rho^{n-1}} \right).$$

Reduced Order Model (ROM), II

For a given ρ we want to compute an approximant v_l^ρ to u_l^ρ for $l = 1, \dots, m_s$ using U^n .

Galerkin method:

$$v_i^\rho = U^n B^{-1} (U^n)^T s_i,$$

where $B = (U^n)^T A(\rho) U^n \in C^{m_s n \times m_s n}$ is the projection matrix.

Reduction of model order: from N to $m_s n$. We define our reduced order model $F^n(\rho) \approx F(\rho)$ as the matrix with elements $m_{lk}^n = s_l^T v_k^\rho$, $k, l = 1, \dots, m_s$.

Properties of ROM: interpolation

Theorem 1: $F^n(\rho)$ matches $F(\rho)$ and its derivative at points $\rho^0, \dots, \rho^{n-1}$:

$$F^n(\rho^i) = F(\rho^i), \quad i = 0, \dots, n - 1,$$

and

$$\frac{\partial F^n}{\partial \rho}(\rho^i) = \frac{\partial F}{\partial \rho}(\rho^i), \quad i = 0, \dots, n - 1.$$

Properties of ROM: monotonic error decrease

Theorem 2: If $s_i, i = 1, \dots, m_s$ are real and $A(\rho)$ is a real symmetric positive definite operator, then

$$F - F^1 \geq \dots \geq F - F^n \geq 0. \quad (5)$$

Model Reduction Gauss Newton algorithm

Initialization: consider initial guess ρ^0 ; compute $u_l^{\rho^0}$, $l = 1, \dots, m_s$ and form U^1

Now any i – *th* iteration ($i > 1$) consists of the following two steps:

1. Find ρ^n by minimizing approximate residual:

$$\|F^n(\rho) - M\| \rightarrow \min.$$

2. Compute $u_l^{\rho^n}$, $l = 1, \dots, m_s$, form U^{n+1} ;

Continue until convergence

Truncation of MRGN

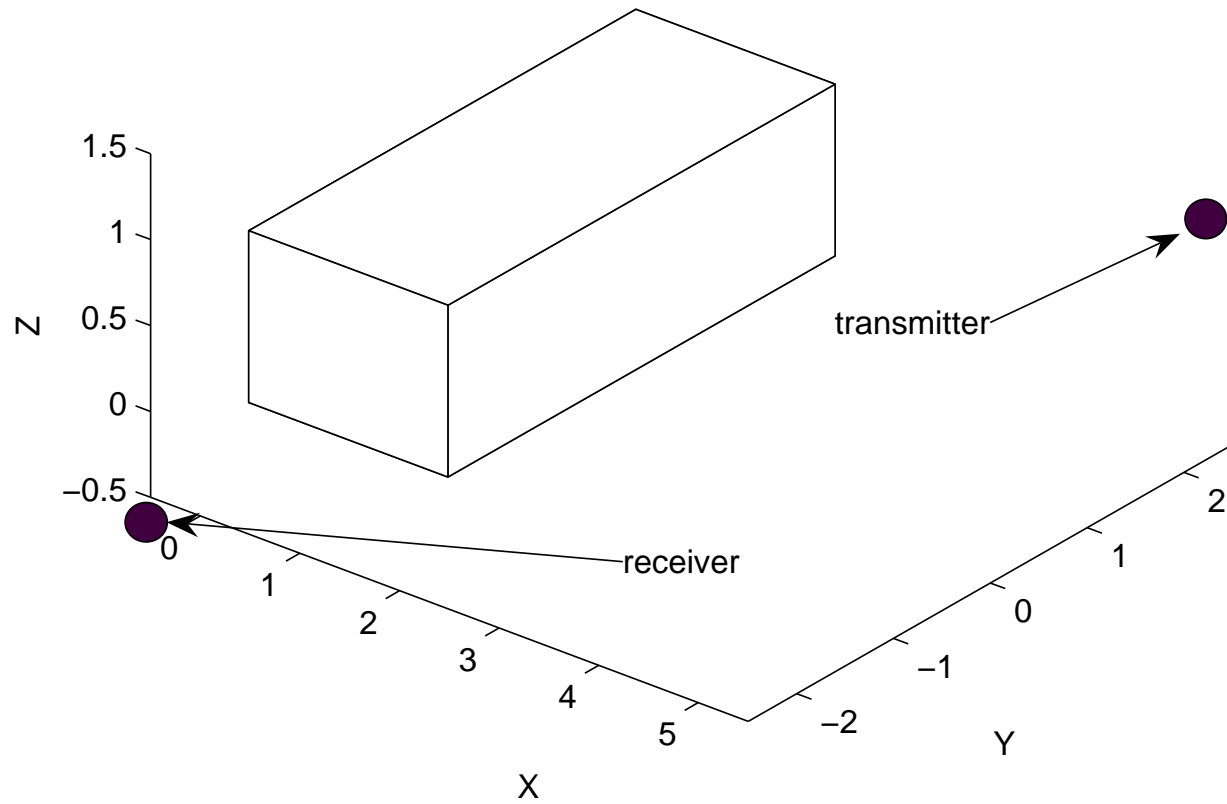
One may keep not all previous solutions but just a part of them.

Advantages: memory usage is reduced, computation of ROM is cheaper

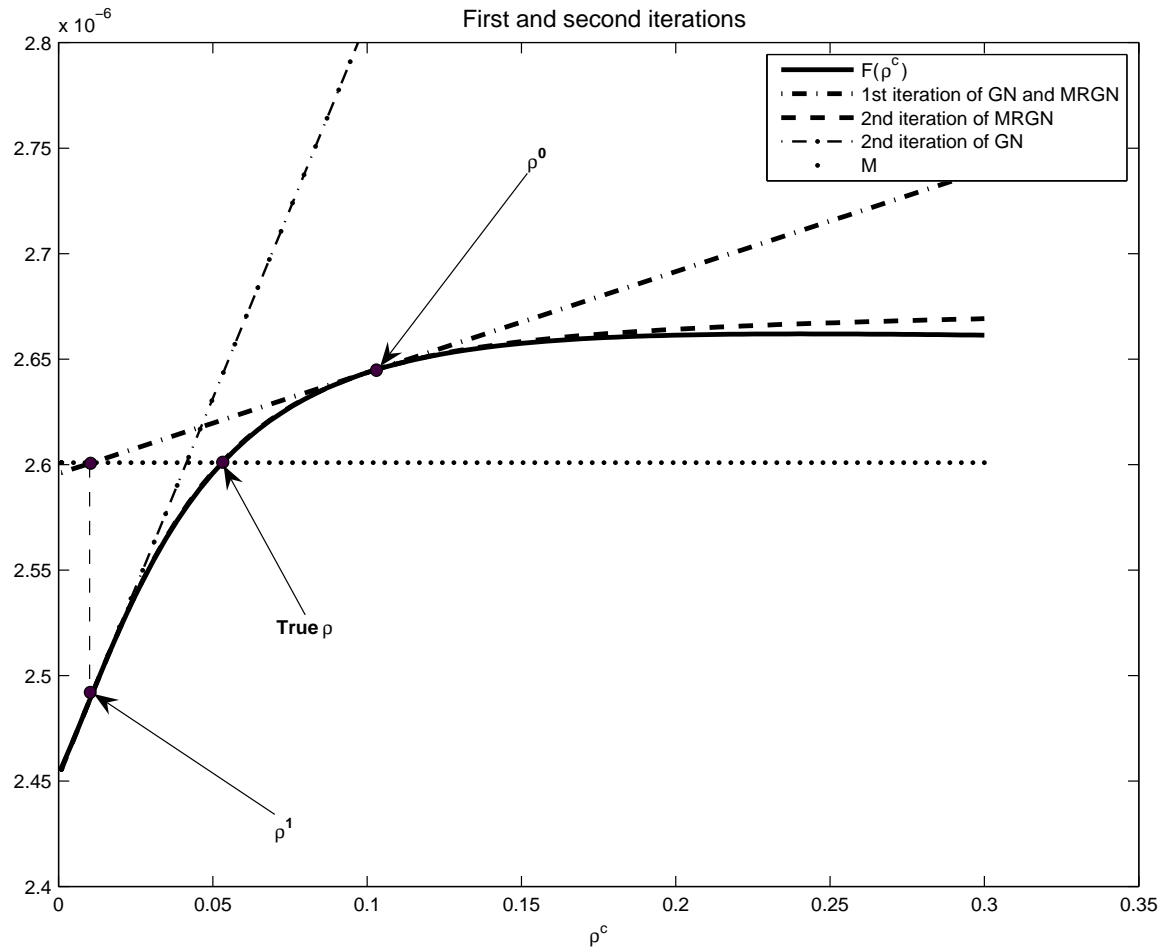
Disadvantage: worse approximation properties of ROM

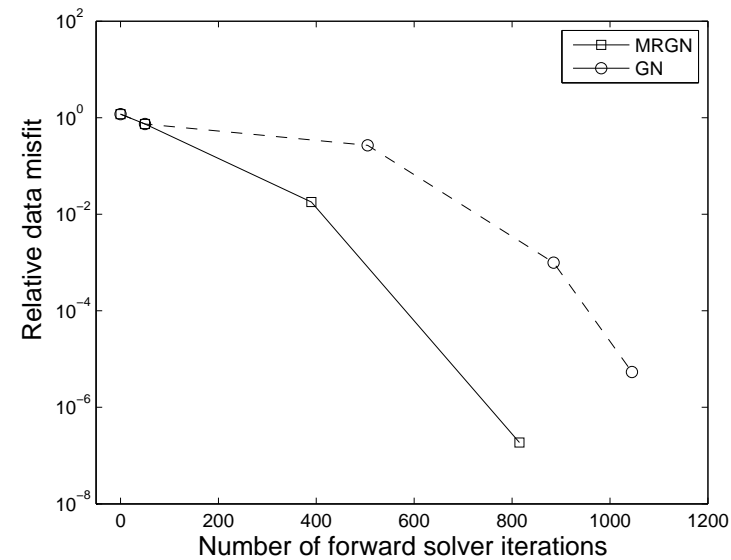
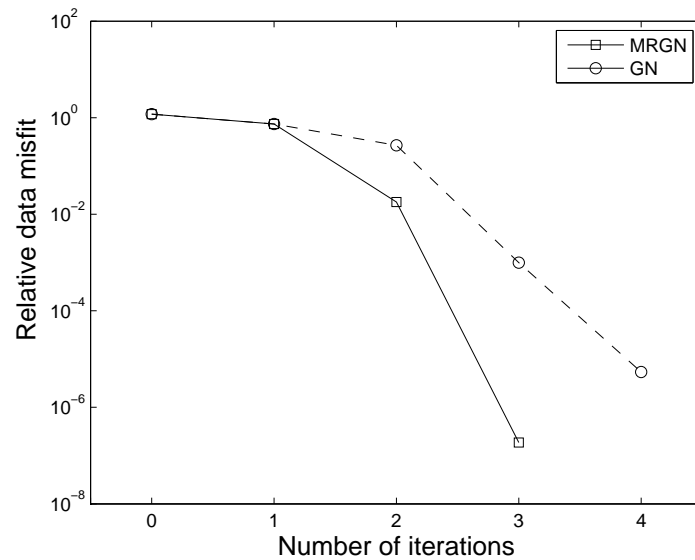
If one keeps just the last solution the MRGN reduces to standard GN

Inversion model for test 1

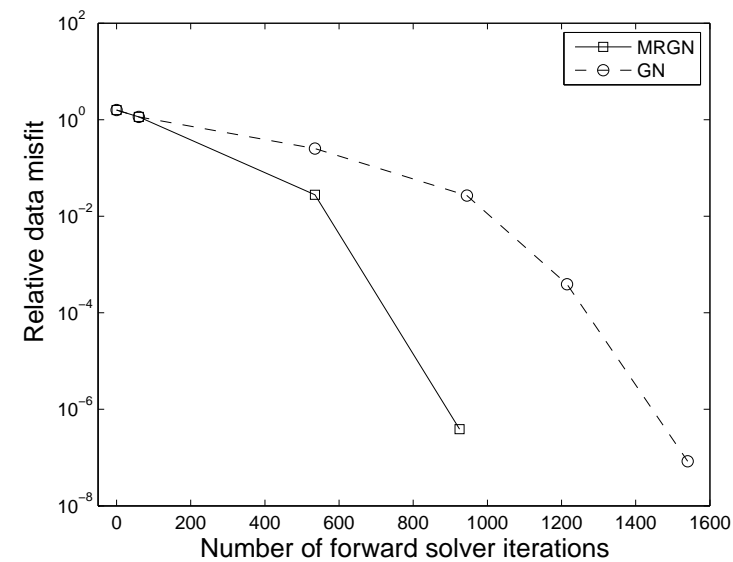
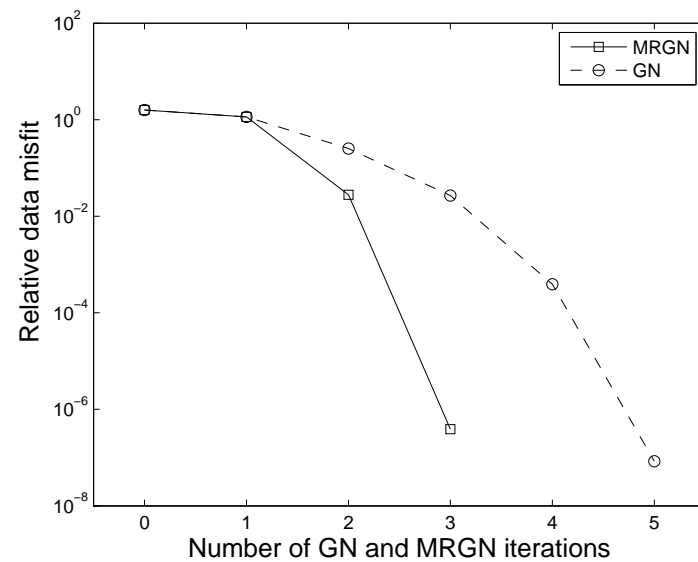


Typical behavior of reduced models



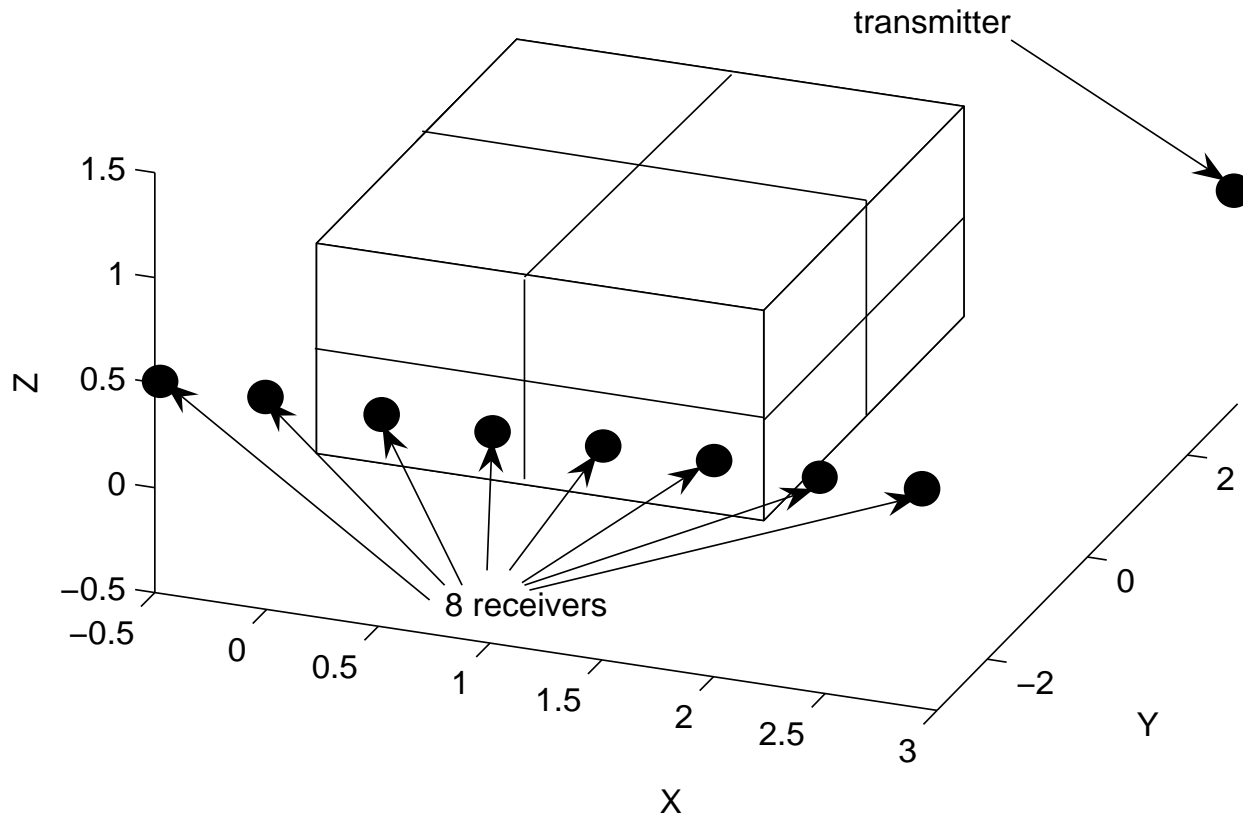
Test 1. Contrast=100. Exact data

Relative data misfit of the GN and the MRGN for the one parameter inversion. Left: as a function of the number of external iterations (n). Right: as a function of the total number of QMR iterations.

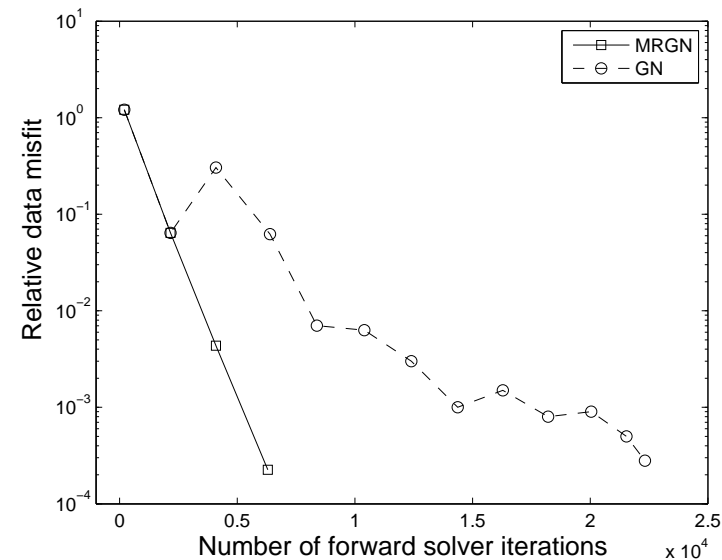
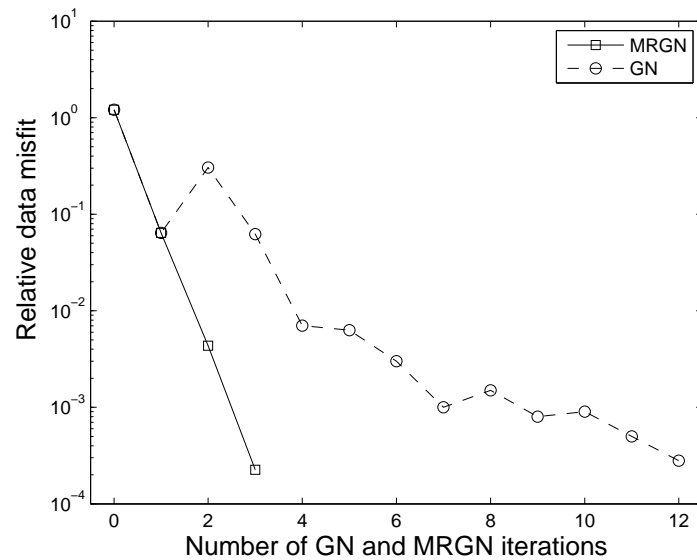
Test 1. Contrast=1000. Exact data

Relative data misfit of the GN and the MRGN for the one parameter inversion. Left: as a function of the number of external iterations (n). Right: as a function of the total number of QMR iterations.

Inversion model for test 2

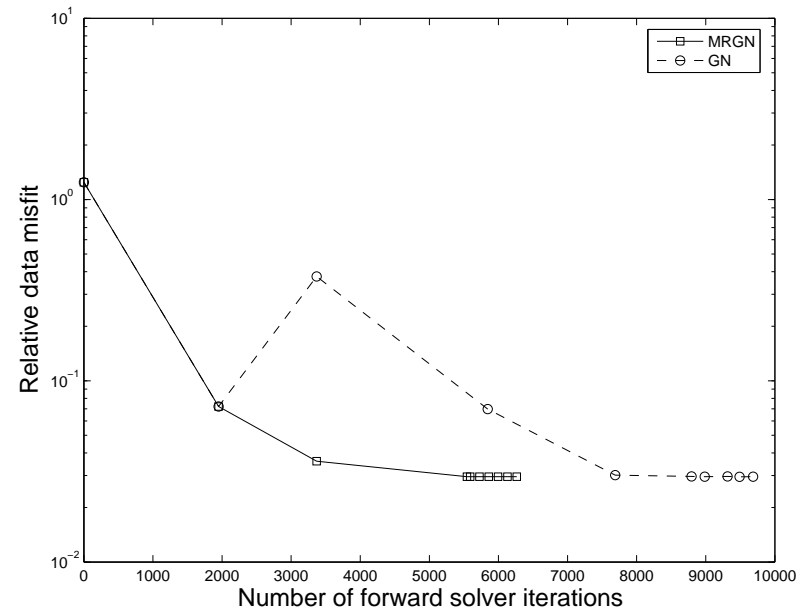
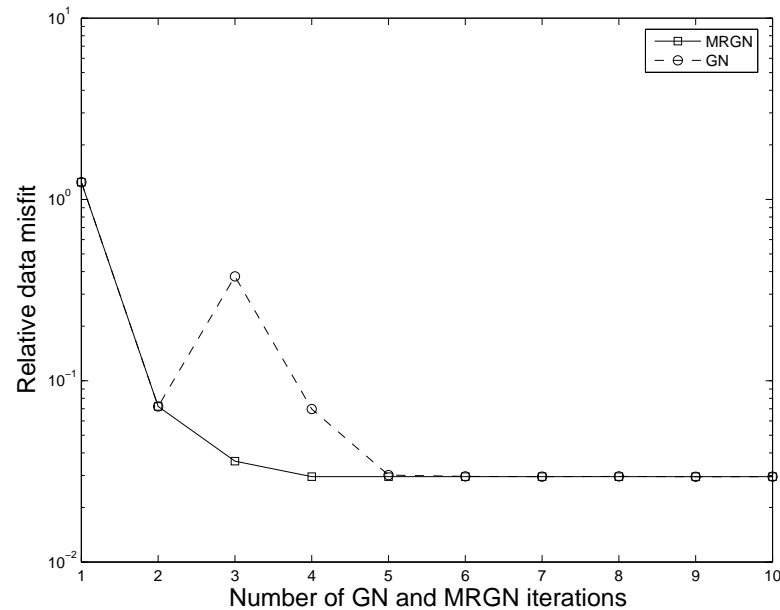


Test 2. Exact data



Relative data misfit of the GN and the MRGN for the eight parameter inversion. Left: as a function of the number of external iterations (n). Right: as a function of the total number of QMR iterations.

Test 2. Noisy data (4%)



Relative data misfit of the GN and the MRGN for the eight parameter inversion. Left: as a function of the number of external iterations (n). Right: as a function of the total number of QMR iterations.

Conclusions

- Reduced Order models for multi-frequency problems were developed and optimal choice of frequencies was established for Galerkin formulation.
- We have developed a method to speed up solutions of nonlinear inverse PDE problems by designing efficient multivariate rational interpolant of the forward solver with respect to the PDE coefficients
- Numerical experiments show significant acceleration on examples of 3D Maxwell's equations, however the method can be applied to practically all inverse PDE problems currently employing the Gauss-Newton algorithm or its modifications as well as to multi-frequency problems