## A model reduction approach to numerical inversion for a parabolic partial differential equation

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## A model reduction approach to numerical inversion for a parabolic partial differential equation

(9) Problem formulation
(2) Model order reduction and inversion
(3) Matching conditions
4. Non-linear preconditioner and its Jacobian
(5) Inversion method and numerical results

6 Extension to two dimensions
(7) Conclusions and future work

## Motivation

Problem: Time-domain Controlled Source Electromagnetic (CSEM) method in oil and gas exploration

- Determine the resistivity in the subsurface from time-resolved surface measurements
- Quasi-stationary parabolic Maxwell system
- Highly non-linear inverse problem, local minima, slow convergence
- Expensive forward modeling



Figures from: http://www.acceleware.com, http://www.engineerlive.com/Mining-Engineer/CSEM

## Continuum problem

- Layered medium, one-dimensional equation

$$
\frac{\partial}{\partial x}\left[r(x) \frac{\partial u(t, x)}{\partial x}\right]=\frac{\partial u(t, x)}{\partial t}, \quad x \in[0,1], \quad t>0
$$

- Boundary and initial conditions

$$
u_{x}(t, 0)=u(t, 1)=0, \quad u(0, x)=\delta(x)
$$

- Measurements: boundary time-domain response

$$
y(t)=u(t, 0), \quad t>0
$$

- Inverse problem: given $y(t)$ for $t>0$ find $r(x)$
- Inverse boundary value problems for parabolic (and elliptic) equations are typically ill-posed
- III-posedness in continuum leads to poor conditioning in numerics


## Model reduction framework: semi-discrete system

- Discretize on a fine (uniform) grid in space with spacing $h=1 /(N+1)$

$$
\begin{equation*}
\frac{\partial \mathbf{u}(t)}{\partial t}=A(\mathbf{r}) \mathbf{u}(t), \quad \mathbf{u}(0)=\frac{1}{h} \mathbf{e}_{1} \tag{1}
\end{equation*}
$$

- Discretization of the differential operator

$$
A(\mathbf{r})=-D^{T} \operatorname{diag}(\mathbf{r}) D, \quad \mathbf{r} \in \mathbb{R}_{+}^{N}
$$

- Time-domain response

$$
y(t ; \mathbf{r})=\mathbf{e}_{1}^{\top} \mathbf{u}(t)
$$

- Semi-discrete inverse problem: given $y(t ; \mathbf{r})$ find $\mathbf{r} \in \mathbb{R}_{+}^{N}$
- Treat (1) as a dynamical system, apply model reduction techniques
- Model reduction: given $\mathbf{r}$ find a reduced model that approximates $y$
- "Inverse" model reduction: obtain a reduced model from the $y$, then find $\mathbf{r}$ which has this reduced model


## Optimization formulation: non-linear preconditioning

- Noisy data

$$
d(t)=y\left(t ; \mathbf{r}^{\text {true }}\right)+\xi(t), \quad t>0
$$

where $\xi(t)$ is due to noise and discretization errors.

- Optimization formulation

$$
\mathbf{r}^{\star}=\underset{\mathbf{r} \in \mathcal{S}}{\arg \min } \frac{1}{2}\|\mathcal{Q}(d(t))-\mathcal{Q}(y(t ; \mathbf{r}))\|_{2}^{2}+\frac{\alpha}{2} \mathcal{P}(\mathbf{r})
$$

- Solution method: Gauss-Newton or non-linear CG
- Traditional approach: output least squares, no preconditioner $\mathcal{Q}$, regularization term $\mathcal{P}$ Tikhonov or TV
- Drawbacks: non-convexity, easy to get stuck in local minima, slow convergence, difficulties with high contrast, expensive
- Non-linear preconditioner $\mathcal{Q}: C(0,+\infty) \rightarrow \mathbb{R}^{q}$ with small $q$, the dimension of parameters of reduced models
- The mapping $\mathcal{Q}(y(\cdot ; \mathbf{r})): \mathbb{R}^{N} \rightarrow \mathbb{R}^{a}$ is an approximate identity


## Projection-based model reduction

- Transfer function of the full model $A(\mathbf{r}) \in \mathbb{R}^{N \times N}, \mathbf{b} \in \mathbb{R}^{N}$

$$
G(s ; \mathbf{r})=\int_{0}^{+\infty} y(t ; \mathbf{r}) e^{-s t} d t=\mathbf{b}^{T}(s l-A(\mathbf{r}))^{-1} \mathbf{b}, \quad s>0, \quad \mathbf{b}=\frac{1}{\sqrt{h}} \mathbf{e}_{1}
$$

- Transfer function of a reduced model $A_{m} \in \mathbb{R}^{m \times m}, \mathbf{b}_{m} \in \mathbb{R}^{m}$

$$
G_{m}(s)=\mathbf{b}_{m}^{T}\left(s l_{m}-A_{m}\right)^{-1} \mathbf{b}_{m}
$$

- Projection-based model reduction

$$
A_{m}=V^{\top} A V, \quad \mathbf{b}_{m}=V^{\top} \mathbf{b}, \quad V^{\top} V=I_{m}
$$

- Columns of $V \in \mathbb{R}^{N \times m}$ span the projection subspace
- Choice of subspace is dictated by matching conditions

$$
\left.\frac{\partial^{k} G_{m}}{\partial s^{k}}\right|_{s=\sigma_{j}}=\left.\frac{\partial^{k} G}{\partial s^{k}}\right|_{s=\sigma_{j}}, \quad j=1, \ldots, m, \quad k=0, \ldots, 2 M_{j}-1
$$

at interpolation nodes $\sigma_{j} \in[0,+\infty)$

## Rational Krylov Model Reduction

- Reduced order transfer function admits a partial fraction expansion

$$
G_{m}(s)=\sum_{j=1}^{m} \frac{c_{j}}{s+\theta_{j}}, \quad c_{j}>0, \quad \theta_{j}>0
$$

with negative poles $-\theta_{j}$ and positive residues $c_{j}$

- Rational $G_{m}$, hence rational interpolation
- Typical choices of projection subspaces in model reduction: rational Krylov subspaces

$$
\mathcal{K}_{m}(\boldsymbol{\sigma})=\operatorname{span}\left\{\left(\sigma_{j} I-A\right)^{-k} \mathbf{b} \mid j=1, \ldots, m ; k=1, \ldots, M_{j}\right\}
$$

- Popular special cases for forward modeling: moment matching

$$
\begin{aligned}
\mathcal{K}_{m}(+\infty) & =\operatorname{span}\left\{\mathbf{b}, A \mathbf{b}, \ldots, A^{m-1} \mathbf{b}\right\} \\
\mathcal{K}_{m}(0) & =\operatorname{span}\left\{A^{-1} \mathbf{b}, A^{-2} \mathbf{b}, \ldots, A^{-m} \mathbf{b}\right\}
\end{aligned}
$$

- $K_{m}(+\infty)$ is bad for inversion


## Inversion via model reduction: $\mathcal{H}_{2}$-optimality

- Proposed in [Druskin, Simoncini, Zaslavsky, 2011]
- Based on $\mathcal{H}_{2}$-optimal reduced models
- View reduced model as a function of interpolation nodes $\sigma$

$$
y_{m}(t ; \boldsymbol{\sigma})=\mathbf{b}^{T} V(\boldsymbol{\sigma}) e^{A_{m}(\boldsymbol{\sigma}) t} V(\boldsymbol{\sigma})^{T} \mathbf{b}, \quad \text { for } \quad A_{m}(\boldsymbol{\sigma})=V(\boldsymbol{\sigma})^{T} A(\mathbf{r}) V(\boldsymbol{\sigma})
$$

- Minimize time-domain error in $L_{2}$ sense

$$
\sigma^{\star}=\arg \min \left\|y(t ; \mathbf{r})-y_{m}(t ; \boldsymbol{\sigma})\right\|_{L_{2}[0,+\infty)}
$$

- Equivalent to $\mathcal{H}_{2}$-optimality in Laplace domain (solve with IRKA)

$$
\sigma^{\star}=\arg \min \left\|G(s ; \mathbf{r})-G_{m}(s)\right\|_{\mathcal{H}_{2}}
$$

- Use poles and residues of $G_{m}(s)$ as parameters in inversion
- Define the non-linear preconditioner with a chain of mappings

$$
\mathcal{Q}_{\mathcal{H}_{2}}(y(\cdot ; \mathbf{r})): \mathbf{r} \xrightarrow{(\mathrm{a})} A(\mathbf{r}) \xrightarrow{(\mathrm{b})} \boldsymbol{\sigma}^{\star} \xrightarrow{(\mathrm{c})} V\left(\boldsymbol{\sigma}^{\star}\right) \xrightarrow{(\mathrm{d})} A_{m} \xrightarrow{(\mathrm{e})}\left\{\left(c_{j}, \theta_{j}\right)\right\}_{j=1}^{m}
$$

## Inversion via model reduction: continued fraction

- We propose a different choice of parameters and matching conditions
- Write the reduced model response as a continued fraction

$$
G_{m}(s)=\frac{1}{\widehat{\kappa}_{1} s+\frac{1}{\kappa_{1}+\frac{1}{\ddots+\frac{1}{\widehat{\kappa}_{m} s+\frac{1}{\kappa_{m}}}}}}
$$

- This is a response $w_{1}(s)$ of a second-order finite difference scheme

$$
\frac{1}{\widehat{\kappa}_{j}}\left(\frac{w_{j+1}-w_{j}}{\kappa_{j}}-\frac{w_{j}-w_{j-1}}{\kappa_{j-1}}\right)-s w_{j}=0
$$

- Continued fraction coefficient are discrete resistivities
- Use $\left\{\left(\kappa_{j}, \widehat{\kappa}_{j}\right)\right\}_{j=1}^{m}$ as parameters in inversion, define $\mathcal{Q}$ as a chain

$$
\mathcal{Q}(y(\cdot ; \mathbf{r})): \mathbf{r} \xrightarrow{(\mathrm{a})} A(\mathbf{r}) \xrightarrow{(\text { b) }} \boldsymbol{V} \xrightarrow{(\mathrm{c})} \boldsymbol{A}_{m} \xrightarrow{\text { (d) }}\left\{\left(c_{j}, \theta_{j}\right)\right\}_{j=1}^{m} \xrightarrow{(\text { e })}\left\{\left(\kappa_{j}, \widehat{\kappa}_{j}\right)\right\}_{j=1}^{m}
$$

## Matching conditions for inversion

- The choice of matching conditions is important: what is good for forward modeling is not necessarily good for inversion
- Use the Jacobian of $\mathcal{Q}$ to quantify the quality of matching conditions

$$
(\mathcal{D Q})_{j, k}=\left\{\begin{array}{ll}
\frac{\partial \kappa_{j}}{\partial r_{k}}, & \text { for } j=1, \ldots, m \\
\frac{\partial \kappa_{j}}{\partial r_{k}}, & \text { for } j=m+1, \ldots, 2 m
\end{array} \quad, \quad k=1, \ldots, N .\right.
$$

- Proper matching conditions should give good conditioning and resolution
- Good conditioning of $\mathcal{D Q}$ is desirable for fast and robust performance of Gauss-Newton iteration, possible to achieve $\operatorname{cond}(\mathcal{D} \mathcal{Q}) \approx O(1)$
- Conditioning of $\mathcal{Q}(d(\cdot))$ always grows exponentially (unavoidable ill-posedness), slower growth is preferential
- Resolution is connected to optimal grids


## Connection to optimal grids

- Optimal (spectrally matched) grids were introduced in [Druskin, Knizhnerman, 2000] for exponential superconvergence of DtN maps
- Typically defined for $r(x) \equiv 1$

$$
\left(\kappa_{j}^{(0)}, \widehat{\kappa}_{j}^{(0)}\right)_{j=1}^{m}=\mathcal{Q}\left(y\left(\cdot, \mathbf{r}^{(0)}\right)\right), \quad \mathbf{r}^{(0)}=(1,1, \ldots, 1)^{T}
$$

- Continued fraction coefficients are the grid steps of FD scheme for

$$
\Delta w-s w=0
$$

- Staggered grid with primary and dual nodes

$$
x_{j}^{(0)}=\sum_{k=1}^{j} \kappa_{k}^{(0)}, \quad \widehat{x}_{j}^{(0)}=\sum_{k=1}^{j} \widehat{\kappa}_{k}^{(0)}, \quad j=1, \ldots, m
$$

- Optimal grids were used for inversion (Sturm-Liouville, EIT)
- Here we do not explicitly use optimal grids for inversion, but to quantify the resolution


## Optimal grids for different matching conditions



Compare three choices of matching conditions:
$(\circ, \times)$ Moment matching at zero, $\mathcal{K}_{m}(0)=\operatorname{span}\left\{A^{-1} \mathbf{b}, A^{-2} \mathbf{b}, \ldots, A^{-m} \mathbf{b}\right\}$
$(\square, \star)$ Interpolation $\mathcal{K}_{m}(\widetilde{\sigma})=\operatorname{span}\left\{\left(\widetilde{\sigma}_{j} I-A\right)^{-1} \mathbf{b} \mid j=1, \ldots, m\right\}$ at geometrically spaced nodes $\widetilde{\sigma}_{j}=\widetilde{\sigma}_{1}(1+C / m)^{j-1}$
$(*, \nabla)$ Interpolation at fast growing nodes $\boldsymbol{\sigma}^{\star}$

## Conditioning of the Jacobian



- Rows of $\mathcal{D Q}$ have the meaning of sensitivity functions
- Each row corresponds to one grid cell
- Sensitivity functions are localized
- Peak locations are at the optimal grid nodes
- Clustered nodes lead to (almost) linearly dependent rows of $\mathcal{D Q}$

Condition number growth for moment matching at zero (०), interpolation at $\widetilde{\boldsymbol{\sigma}}(\square)$, interpolation at $\boldsymbol{\sigma}^{\star}(\nabla)$

## Conditioning of rational approximation

- Optimization objective requires computing

$$
\left(\kappa_{j}, \widehat{\kappa}_{j}\right)_{j=1}^{m}=\mathcal{Q}(d(\cdot))
$$

- The most unstable step in inversion procedure
- Rational approximation (interpolation) problem
- Simple Padé for moment matching $\mathcal{K}_{m}(0)$

$$
\left.\frac{\partial^{j} G_{m}}{\partial s^{j}}\right|_{s=0}=\left.\frac{\partial^{j} G}{\partial s^{j}}\right|_{s=0}=(-1)^{j} \int_{0}^{+\infty} y(t ; \mathbf{r}) t^{j} d t, \quad j=0,1, \ldots, 2 m-1
$$

- Multipoint Padé for osculatory interpolation $\mathcal{K}_{m}(\widetilde{\boldsymbol{\sigma}})$

$$
G_{m}(s)=\frac{p(s)}{q(s)}, \quad\left\{\begin{array}{l}
p\left(\widetilde{\sigma}_{j}\right)-G_{m}\left(\widetilde{\sigma}_{j}\right) q\left(\widetilde{\sigma}_{j}\right)=0 \\
p^{\prime}\left(\widetilde{\sigma}_{j}\right)-G_{m}^{\prime}\left(\widetilde{\sigma}_{j}\right) q\left(\widetilde{\sigma}_{j}\right)-G_{m}\left(\widetilde{\sigma}_{j}\right) q^{\prime}\left(\widetilde{\sigma}_{j}\right)=0
\end{array}\right.
$$

$$
\text { for } j=1, \ldots, m
$$

- Once the coefficients of $p(s)$ and $q(s)$ are known, can compute the poles, residues and the continued fraction coefficients easily


## Conditioning of rational approximation: comparison

| $m$ | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\operatorname{cond}\left(T_{m}\right)$ | $5.28 \cdot 10^{1}$ | $1.26 \cdot 10^{5}$ | $1.84 \cdot 10^{9}$ | $9.14 \cdot 10^{13}$ | $2.86 \cdot 10^{16}$ |
| $\operatorname{cond}\left(R_{m}\right)$ | $4.43 \cdot 10^{2}$ | $6.73 \cdot 10^{4}$ | $1.85 \cdot 10^{7}$ | $6.95 \cdot 10^{9}$ | $3.83 \cdot 10^{12}$ |

- Both simple and multipoint Padé problems may be solved via SVD
- Simple Padé: SVD of Toeplitz matrix $T_{m} \in \mathbb{R}^{m \times(m+1)}$ of Taylor coefficients $\tau_{j}, j=1, \ldots, 2 m-1$ of

$$
\boldsymbol{G}(\boldsymbol{s})=\tau_{0}+\tau_{1} \boldsymbol{s}+\tau_{2} s^{2}+\ldots+\tau_{2 m-1} s^{2 m-1}+\ldots
$$

- Multipoint Padé: SVD of $R_{m} \in \mathbb{R}^{2 m \times(2 m+1)}$

$$
R_{m}=\left[\begin{array}{cc}
\Sigma_{1: m, 1: m} & -F \Sigma \\
\Sigma_{1: m, 1: m}^{\prime} & -F^{\prime} \Sigma-F \Sigma^{\prime}
\end{array}\right],
$$

with Vandermonde $\Sigma$ and $F=\operatorname{diag}(G(\widetilde{\sigma}))$

- Multipoint Padé is clearly superior


## Computing $\mathcal{Q}$ and $\mathcal{D}$ : chain of mappings

- Chain of mappings for computing $\mathcal{Q}$ and the Jacobian $\mathcal{D} \mathcal{Q}$

$$
\mathcal{Q}(y(\cdot ; \mathbf{r})): \mathbf{r} \xrightarrow{(\mathrm{a})} A(\mathbf{r}) \xrightarrow{(\mathrm{b})} \boldsymbol{V} \xrightarrow{(\mathrm{c})} \boldsymbol{A}_{m} \xrightarrow{\text { (d) }}\left\{\left(c_{j}, \theta_{j}\right)\right\}_{j=1}^{m} \xrightarrow{(\mathrm{e})}\left\{\left(\kappa_{j}, \widehat{\kappa}_{j}\right)\right\}_{j=1}^{m}
$$

(a) $A(\mathbf{r})=-D^{T}$ diag(r)D, trivial to differentiate.
(b) Requires differentiation of orthonormal basis $V$. Here we differentiate QR decomposition.
(c) $A_{m}=V^{\top} A V$, trivial to differentiate once $\mathcal{D} V$ is known.
(d) Differentiation of eigendecomposition

$$
c_{j}=\left(\mathbf{b}_{m}^{T} \mathbf{z}_{j}\right)^{2}, \quad A_{m} \mathbf{z}_{j}+\theta_{j} \mathbf{z}_{j}=0, \quad\left\|\mathbf{z}_{j}\right\|=1, \quad j=1, \ldots, m
$$

(e) Lanczos iteration. Explicit differentiation formulas derived in [Borcea, Druskin, Knizhnerman, 2005]

- Steps (d)-(e) can be combined into one using a variant of Lanczos. No explicit formulas, requires differentiation of the iteration.


## Differentiation of QR decomposition

- Krylov matrix $K=\left[\left(\widetilde{\sigma}_{1} I-A\right)^{-1} \mathbf{b}, \ldots,\left(\widetilde{\sigma}_{m} I-A\right)^{-1} \mathbf{b}\right] \in \mathbb{R}^{N \times m}$
- Compute V from QR decomposition: $K=V R, K^{\top} K=R^{\top} R=L L^{\top}$
- Need to differentiate Cholesky to get

$$
\frac{\partial V}{\partial r_{k}}=\left(\frac{\partial K}{\partial r_{k}}-V \frac{\partial L^{T}}{\partial r_{k}}\right) L^{-T}, \quad k=1, \ldots, N
$$

## Proposition (Differentiation of Cholesky factorization)

Let $M \in \mathbb{R}^{n \times n}$ be a matrix with Cholesky factorization $M=L L^{T}$. Given the perturbation $\delta M$ of $M$, the corresponding perturbation $\delta L$ of the Cholesky factor is computed by the following algorithm.

$$
\text { For } k=1, \ldots, n
$$

$$
\delta L_{k k}=\frac{1}{L_{k k}}\left(\frac{\delta M_{k k}}{2}-\sum_{j=1}^{k-1} \delta L_{k j} L_{k j}\right)
$$

$$
\text { For } i=k+1, \ldots, n
$$

$$
\delta L_{i k}=\frac{1}{L_{k k}}\left(\delta M_{i k}-\sum_{j=1}^{k} \delta L_{k j} L_{i j}-\sum_{j=1}^{k-1} \delta L_{i j} L_{k j}\right)
$$

## Regularization

- Traditional approaches require regularization for stability
- We use regularization only to improve the reconstruction quality
- Separate the fitting $\| \mathcal{Q}(d(\cdot))-\mathcal{Q}\left(y(\cdot ; \mathbf{r}) \|_{2}\right.$ step from regularization step
- Jacobian $\mathcal{D Q} \in \mathbb{R}^{2 m \times N}$ has a large null space $2 m \ll N$
- Minimze the regularization functional $\mathcal{P}(\mathbf{r})$ in $\operatorname{null}(\mathcal{D} \mathcal{Q})$
- Weighted discrete $H^{1}$ seminorm

$$
\mathcal{P}(\mathbf{r})=\frac{1}{2}\left\|W^{1 / 2} \Delta \mathbf{r}\right\|_{2}^{2}
$$

here $\Delta$ is the truncation of $D$ (first derivative, not second)

- Works for both smooth ( $W=I$ ) and piecewise constant resistivities (non-linear re-weighting at every iteration)
- Constrained optimization subproblem at each Gauss-Newton iteration

$$
\underset{\text { t. }[\mathcal{D Q} \mathcal{Q}](\mathrm{r}-\rho)=0}{\operatorname{minimize}} \rho^{T} \Delta^{T} W \Delta \rho
$$

## Regularization

- Regularization subproblem: quadratic with linear constraints
- First order optimality conditions, explicit solution from

$$
\begin{aligned}
\Delta^{T} W \Delta \rho+[\mathcal{D} \mathcal{Q}]^{\top} \boldsymbol{\lambda} & =0 \\
{[\mathcal{D Q}] \rho } & =[\mathcal{D} \mathcal{Q}] \mathbf{r}
\end{aligned}
$$

- May be ill-conditioned, SVD truncation, drop the smallest singular value
- Non-trivial weight $(W \neq I)$ is needed for piecewise constant resistivities
- Use weight introduced in [Abubakar, Habashy, Druskin, Knizhnerman, Alumbaugh, 2008]

$$
w_{j}=\left(\left([\Delta \mathbf{r}]_{j}\right)^{2}+\phi(\mathbf{r})^{2}\right)^{-1}, \quad j=1, \ldots, N-1,
$$

where

$$
\phi(\mathbf{r})=C_{\phi} \| \mathcal{Q}(d(\cdot))-\mathcal{Q}\left(y(\cdot ; \mathbf{r}) \|_{2}\right.
$$

- Sharp resolution of interfaces


## Inversion algorithm

(1) Solve the data fitting rational interpolation problem $\left(\kappa_{j}^{\star}, \widehat{\kappa}_{j}^{\star}\right)_{j=1}^{m}=\mathcal{Q}(d(\cdot))$
(2) Work with logarithms $\mathbf{I}^{\star}=\left(\log \kappa_{1}^{\star}, \ldots, \log \kappa_{m}^{\star}, \log \widehat{\kappa}_{1}^{\star}, \ldots, \log \widehat{\kappa}_{m}^{\star}\right)^{T}$
(3) Choose on initial guess $\mathbf{r}^{(1)} \in \mathcal{R}_{+}^{N}$
(4) For $p=1, \ldots, n_{G N}$ do
(0. Compute the non-linear preconditioner $\left(\kappa_{j}^{(p)}, \widehat{\kappa}_{j}^{(p)}\right)_{j=1}^{m}=\mathcal{Q}\left(y\left(t ; \mathbf{r}^{(p)}\right)\right)$ and its Jacobian $\mathcal{D} \mathcal{Q}^{(p)}=\mathcal{D} \mathcal{Q}\left(y\left(t ; \mathbf{r}^{(p)}\right)\right)$
(2) Work with logs $\mathbf{I}^{(p)}=\left(\log \kappa_{1}^{(p)}, \ldots, \log \kappa_{m}^{(p)}, \log \widehat{\kappa}_{1}^{(p)}, \ldots, \log \widehat{\kappa}_{m}^{(p)}\right)^{T}$
(3) Gauss-Newton step

$$
\boldsymbol{\rho}^{(p)}=-\left(\mathcal{D} \mathcal{Q}^{(p)}\right)^{\dagger} \operatorname{diag}\left(\kappa_{1}^{(p)}, \ldots, \kappa_{m}^{(p)}, \widehat{\kappa}_{1}^{(p)}, \ldots, \widehat{\kappa}_{m}^{(p)}\right)\left(\mathbf{I}^{(p)}-\mathbf{I}^{\star}\right)
$$

(4) Gauss-Newton update $\mathbf{r}^{G N}=\mathbf{r}^{(p)}+\zeta^{(p)} \rho^{(p)}$
(5) Compute the regularization weight for $\mathbf{r}^{G N}$
(6) Solve for next iterate $\mathbf{r}^{(p+1)}$ from

$$
\left[\begin{array}{cc}
\Delta^{T} W \Delta & \left(\mathcal{D} \mathcal{Q}^{(p)}\right)^{T} \\
\mathcal{D} \mathcal{Q}^{(p)} & 0
\end{array}\right]\left[\begin{array}{c}
\mathbf{r}^{(p+1)} \\
\lambda^{(p)}
\end{array}\right]=\left[\begin{array}{c}
0 \\
\left(\mathcal{D} \mathcal{Q}^{(p)}\right) \mathbf{r}^{G N}
\end{array}\right]
$$

## Numerical experiments: setup

- Time stepping over $\left[0, T_{\text {max }}\right]$ with $N_{T}$ steps to compute $\mathbf{y} \in \mathbb{R}^{N_{T}}$
- Systematic discretization errors even in the absence of noise

$$
y_{j}=y\left(t_{j} ; \mathbf{r}^{\text {tue }}\right)+\xi^{(s)}\left(t_{j}\right), \quad j=1, \ldots, N_{T}
$$

- Generate the data by adding noise $\mathbf{d}=\mathbf{y}+\boldsymbol{\xi}^{(n)}$
- Noise model

$$
\boldsymbol{\xi}^{(n)}=\epsilon \operatorname{diag}\left(\chi_{1}, \ldots, \chi_{N_{T}}\right) \mathbf{y},
$$

with independent $\chi_{k} \in \mathcal{N}(0,1)$

- Reduced model size $m$ chosen based on noise level $\epsilon$

| $m$ | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: |
| $\epsilon$ | $5 \cdot 10^{-2}$ | $5 \cdot 10^{-3}$ | $10^{-4}$ | 0 (noiseless) |

- Relative $\ell_{2}$ error to measure the quality

$$
\mathcal{E}=\frac{\left\|\mathbf{r}^{\star}-\mathbf{r}^{\text {true }}\right\|_{2}}{\left\|\mathbf{r}^{\text {tue }}\right\|_{2}}
$$

- Initial guess $\mathbf{r}^{1}=\mathbf{1}$, five Gauss-Newton iterations $n_{G N}=5$


## Numerical results: smooth resistivity




- True resistivity $\mathbf{r}^{\text {true }}$ (quadratic)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Numerical results: smooth resistivity




- True resistivity $\mathbf{r}^{\text {true }}$ (quadratic)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Numerical results: smooth resistivity




- True resistivity $\mathbf{r}^{\text {true }}$ (linear + Gaussian)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Numerical results: smooth resistivity



$$
m=6, \epsilon=0 \text { (noiseless) }
$$



- True resistivity $\mathbf{r}^{\text {rue }}$ (linear + Gaussian)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Numerical results: piecewise constant resistivity


$m=4, \epsilon=5 \cdot 10^{-3}$


- True resistivity $\mathbf{r}^{\text {true }}$ (jump of contrast 2)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Numerical results: piecewise constant resistivity


$m=6, \epsilon=0$ (noiseless)


- True resistivity $\mathbf{r}^{\text {true }}$ (jump of contrast 2)
$\times$ Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration
- Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations


## Approaches to higher dimensions

## Higher dimensions:

- One-dimensional problem is formally determined: 1D unknown $r(x)$ and 1D data $y(t)$
- In dimension two the problem is already overdetermined: 2D unknown $r(x, y)$, but 3D data $y_{i, j}(t)$, where $(i, j)$ are source-detector pairs
- Straightforward generalization: block Lanczos, block Krylov subspaces, matrix-valued continued fractions
- Block tridiagonal matrix with dense blocks, consequence of an overdetermined problem
- Dense blocks do not correspond directly to a finite-difference scheme
- Work with a subset of the data, make the problem formally determined


## Coinciding sources and receivers (transducers)

## Using one scalar continued fraction per transducer:

- Simplest reduction of the data $y_{i, j}(t)$ : take the diagonal $i=j$
- Sources and receivers coincide
- Excite at a point on the boundary at $t=0$, measure $y_{j}(t)$ at the same location for $t>0$ for each transducer $j=1, \ldots, n$
- Not the best setting in practice, measurements at source locations may be noisy
- Easier to work with theoretically, coinciding sources/receivers preserve the symmetry
- Construct separate scalar continued fractions interpolating each $y_{j}(t)$, $j=1, \ldots, n$
- Continued fractions are again Stieltjes due to the symmetry


## Sensitivities



Sensitivity functions of $\widehat{\kappa}_{j}$ (left) and $\kappa_{j}$ (right) for $j=1, \ldots, m$ (top to bottom), $m=5$ for a single transducer (black o) out of $n=8$ (red $\times$ ).
Simple Pade approximant at $\sigma=60$. Sensitivities resemble propagating spherical waves. Higher $\sigma$ means lower speed of propagation. Should avoid reflections from boundaries.

## Reconstructions: single low contrast inclusion



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Reconstructions: single high contrast inclusion



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Reconstructions: two adjacent inclusions



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Reconstructions: layered medium



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Reconstructions: skewed inclusion, low aperture



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Reconstructions: skewed inclusion, high aperture



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_{0}(x, y) \equiv 1$. Transducers: red $\times$.

## Conclusions and future work

## Conclusions:

- Non-linear preconditioning based on model reduction
- Data fitting: rational interpolation (unavoidably ill-conditioned)
- Reconstruction: well-conditioned
- Fast convergence, inexpensive
- Possible to extend to higher dimensions


## Future work:

- More work on 2D and 3D
- Non-coinciding source-receiver pairs
- Deal with the loss of symmetry

Preprint: A model reduction approach to numerical inversion for a parabolic partial differential equation. L. Borcea, V. Druskin, A.V. Mamonov and M. Zaslavsky, 2012, arXiv:1210.1257 [math.NA]

