Computational methods for distributed parameter estimation in dD

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with **Eldad Haber**

Outline

- Forward problems and distributed parameter estimation
- Solving the optimization problem
- 3D electromagnetic data inversion in frequency and time domain
- Discontinuous solutions and Huber's norm
- Outline

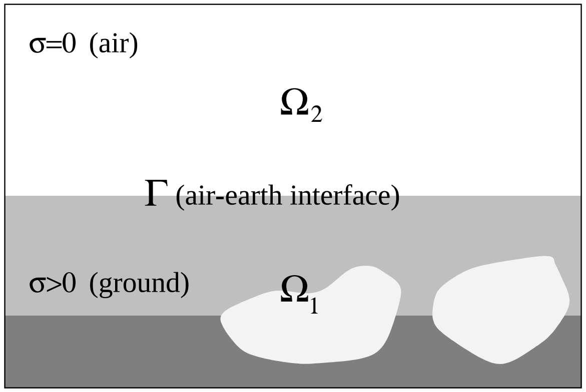
Forward problems and distributed parameter estimation - outline

- The forward problem (a discretized diffusive PDE system)
- The regularized inverse problem

Forward problem partial differential equation (PDE)

DC resistivity/ EIT/ Hydrology

$$\nabla \cdot (\sigma \boldsymbol{\nabla} \mathrm{u}) = \mathrm{q}$$



Electromagnetic prospecting

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \imath\omega\,\sigma\,\mathbf{E} = \imath\omega\mathbf{s}$$

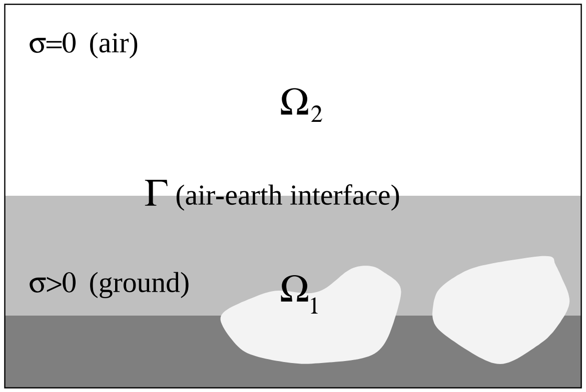
Forward problem partial differential equation (PDE)

Write PDE + BC as

$$\mathcal{A}(\mathrm{m})\mathrm{u} = \mathrm{q}$$

where

$$\sigma(\mathbf{x}) = e^{\mathrm{m}(\mathbf{x})} > 0, \ \mathbf{x} \in \Omega.$$

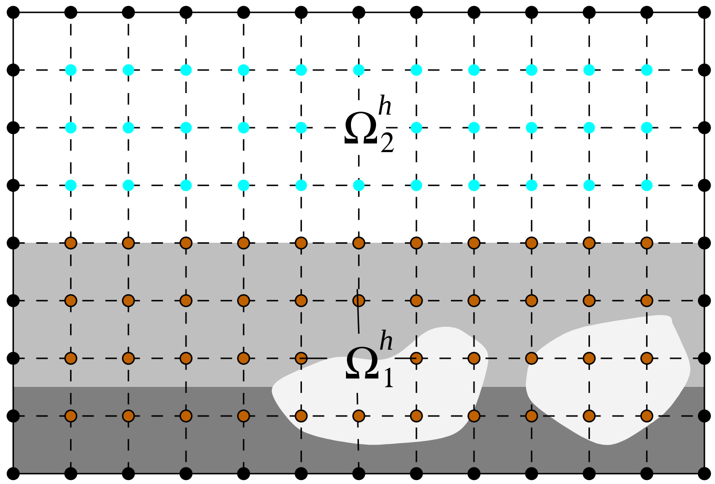


Forward problem

Discretize PDE on a grid:

$$A(m)u = q$$

A nonsingular, u, q vectors (grid functions).
Consider a tensor grid, not necessarily uniform:
e.g. assume the material properties to be constant in each cell. $\Rightarrow m$



The regularized inverse problem

Goal: Recover m given the measured data b subject to $A(m)u - q = 0$

The regularized inverse problem

Goal: Recover m given the measured data b subject to $A(m)u - q = 0$

But

- There is no unique solution to the inverse problem

- Solutions are very sensitive to noise

Must add information and isolate noise effects

The regularized inverse problem

Goal: Recover m given the measured data b subject to $A(m)u - q = 0$

From all the possible models choose the one closest to our *a priori* information.

$$\min \;\; \phi = \frac{1}{2}\|Qu - b\|^2 + \beta R(m)$$
$$\text{subject to} \quad A(m)u - q = 0$$

Where Q projects to data locations and $R(m)$ is a regularization term

The regularization term

$$R(m) = \left[\int_\Omega \rho(|\boldsymbol{\nabla} m|) + \alpha(m - m_{ref}) \right]_h$$

- Least squares

$$\begin{aligned} \rho(\tau) &= \frac{1}{2}\tau^2, \\ R'(m) &\leftarrow \nabla \cdot \boldsymbol{\nabla} m \end{aligned}$$

- Weighted least squares

$$R'(m) \leftarrow \nabla \cdot a \boldsymbol{\nabla} m$$

- Total variation

$$\begin{aligned} \rho(\tau) &= \tau, \\ R'(m) &\leftarrow \nabla \cdot \left(\frac{\boldsymbol{\nabla} m}{|\boldsymbol{\nabla} m|}\right) \end{aligned}$$

- Huber

$$
\begin{aligned}
\rho(\tau) &= \begin{cases} \tau, & \tau \geq \gamma, \\ \tau^2/(2\gamma) + \gamma/2, & \tau < \gamma \end{cases} \\
R'(m) &\leftarrow \nabla \cdot \left(\min\{\frac{1}{\gamma}, \frac{1}{|\boldsymbol{\nabla} m|}\} \, \boldsymbol{\nabla} m \right)
\end{aligned}
$$

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Solving the optimization problem - outline

- Unconstrained approach
- Constrained approach – reduced Hessian
- Balancing iteration accuracies
- Multigrid and preconditioned Krylov methods

Unconstrained approach

Common approach

[e.g. Tikhonov 1968, Parker 1973, Chan & Golub 1999, Vogel 2000] :

eliminate the constraints

$$u = A(m)^{-1}q$$

and obtain a large (dense) unconstrained minimization problem

$$\min \;\; \phi(m) = \frac{1}{2}\|QA(m)^{-1}q - b\|^2 + \beta R(m)$$

Unconstrained approach

$$\min \ \phi(m) = \frac{1}{2}\|QA(m)^{-1}q - b\|^2 + \beta R(m)$$

Newton and Gauss-Newton methods are well-known. Iterations involve positive definite linear systems of the form

$$(J^T J + \beta R'')\ \delta m = -p$$

Conventional wisdom: *it is good to have an unconstrained minimization problem*

But in the large, sparse context the superiority of this approach may be challenged.

Constrained approach

Introducing the Lagrangian

$$\mathcal{L}_{u,m,\lambda} = \frac{1}{2}||Qu - b||^2 + \beta R(m) + \lambda^T (A(m)u - q)$$

λ - Vector of Lagrange multipliers,

Need to find an extremum (saddle) point of the Lagrangian. i.e. solve large system of nonlinear equations

$$\begin{aligned}
\mathcal{L}_\lambda &= Au - q = 0, \\
\mathcal{L}_u &= Q^T(Qu - b) + A^T\lambda = 0, \\
\mathcal{L}_m &= \beta R'(m) + G^T\lambda = 0; \quad G = \frac{\partial A(m)u}{\partial m}
\end{aligned}$$

$$
\begin{aligned}
\mathcal{L}_\lambda &= Au - q = 0, \\
\mathcal{L}_u &= Q^T(Qu - b) + A^T\lambda = 0, \\
\mathcal{L}_m &= \beta R'(m) + G^T\lambda = 0; \quad G = \frac{\partial A(m)u}{\partial m}
\end{aligned}
$$

Use a variant of Newton's method (Lagrange-Newton, SQP, Gauss-Newton); e.g.

$$
\begin{pmatrix} A & 0 & G \\ Q^TQ & A^T & 0 \\ 0 & G^T & \beta R'' \end{pmatrix}
\begin{pmatrix} \delta u \\ \delta\lambda \\ \delta m \end{pmatrix}
= -\begin{pmatrix} \mathcal{L}_\lambda \\ \mathcal{L}_u \\ \mathcal{L}_m \end{pmatrix}
$$

Tasks at each iteration

1. Calculate the Gradients and Hessian
    -

2. Solve the large, sparse Hessian system
    -

3. Update
    -

Tasks at each iteration

1. Calculate the Gradients and Hessian
   - Calculation of the gradients and the Hessian is cheap with linear complexity.

2. Solve the large, sparse Hessian system
   -

3. Update
   - There are various well-known techniques for updating the iterate (damped Newton, trust region, directly updating λ, etc.)

Tasks at each iteration

1. Calculate the Gradients and Hessian

2. Solve the large, sparse Hessian system

   - To solve for the update direction, can
     - Eliminate $\delta u, \ \delta\lambda$ and solve a smaller positive system for δm (reduced Hessian approach).
     - Solve the whole thing simultaneously.

3. Update

Solving for the update direction - Reduced Hessian approach

Eliminating $\delta u,\ \delta\lambda$ obtain for δm

$$\begin{aligned} H_{red}\,\delta m &\equiv (J^T J + \beta R'')\,\delta m = -p \\ J &= -QA^{-1}G \end{aligned}$$

J is the *sensitivity matrix*

Solving for the update direction - Reduced Hessian approach

Eliminating $\delta u, \ \delta\lambda$ obtain for δm

$$\begin{aligned} H_{red}\, \delta m &\equiv (J^T J + \beta R'')\, \delta m = -p \\ J &= -QA^{-1}G \end{aligned}$$

J is the *sensitivity matrix*

To solve this use Preconditioned Conjugate Gradients, i.e. CG for

$$M^{-1}(J^T J + \beta R'')\delta m = -M^{-1}p \quad e.g.\ M = R''$$

But `evaluating` $H_{red}v$ is expensive!! The forward and adjoint problems are solved many times to a relatively high accuracy.

Balancing iteration accuracies

[Haber & Ascher '01], [Ascher & Haber '01]

- When the iterate is far from the optimal solution, it is wasteful to solve linearized problem to a high accuracy (i.e. balance accuracies of inner and outer iterations)

- When the iterate for the update direction is far from the solution to the linear system, it is wasteful to eliminate some variables accurately in terms of others (i.e. balance accuracies inside linear solver).

So

Balancing iteration accuracies

- When the iterate is far from the optimal solution, it is wasteful to solve linearized problem to a high accuracy (i.e. balance accuracies of inner and outer iterations)

Use `inexact Newton-type` methods, where linearized problem is not solved too accurately.

Balancing iteration accuracies

- When the iterate for the update direction is far from the solution to the linear system, it is wasteful to eliminate some variables accurately in terms of others (i.e. balance accuracies inside linear solver).

Solve for correction $\delta u,\ \delta\lambda,\ \delta m$ simultaneously.

Solving for the update direction simultaneously (all-at-once)

$$\begin{pmatrix} A & 0 & G \\ Q^TQ & A^T & 0 \\ 0 & G^T & \beta R'' \end{pmatrix} \begin{pmatrix} \delta u \\ \delta \lambda \\ \delta m \end{pmatrix} = - \begin{pmatrix} \mathcal{L}_\lambda \\ \mathcal{L}_u \\ \mathcal{L}_m \end{pmatrix}$$

No problem if β is large.. But it's small! Discretization of a strongly coupled PDE system.

Solving for the update direction simultaneously (all-at-once)

$$\begin{pmatrix} A & 0 & G \\ Q^T Q & A^T & 0 \\ 0 & G^T & \beta R'' \end{pmatrix} \begin{pmatrix} \delta u \\ \delta \lambda \\ \delta m \end{pmatrix} = - \begin{pmatrix} \mathcal{L}_\lambda \\ \mathcal{L}_u \\ \mathcal{L}_m \end{pmatrix}$$

Method we've considered:

- **Preconditioned QMR** for the symmetrized system

  See also [Biros & Ghattas, '99, '01]

- **Multigrid** for the linearized PDE system

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3D electromagnetic data inversion - outline

- The forward problem
  - Maxwell's equations in frequency domain
  - Reformulation and discretization
  - Maxwell's equations in time domain
- Examples

[Haber, Ascher & Oldenburg '02]

Maxwell's equations in frequency domain

$$
\begin{aligned}
&\nabla \times \mathbf{E} + \alpha\mu\mathbf{H} = \mathbf{s}_H \quad \text{in } \Omega,\\
&\nabla \times \mathbf{H} - \hat{\sigma}\mathbf{E} = \mathbf{s}_E \quad \text{in } \Omega,\\
&\mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \partial\Omega,
\end{aligned}
$$

where $\hat{\sigma} = \sigma + \alpha\epsilon$ and $\alpha = -\imath\omega$.

Typical parameter regimes in these applications satisfy $0 \leq \epsilon \ll 1$ and exclude high frequencies ω.

Reformulation and discretization

Helmholtz decomposition + Coulomb gauge :

$$\mathbf{E} = \mathbf{A} + \boldsymbol{\nabla}\phi$$
$$\nabla \cdot \mathbf{A} = 0$$

Thus, $\mathbf{A}$ is the electric field induced by magnetic fluxes, $\boldsymbol{\nabla}\phi$ is due to charge accumulation.

Next, differentiate like PPE in CFD and stabilize $\Rightarrow$

$$\nabla \times (\mu^{-1}\nabla \times \mathbf{A}) - \boldsymbol{\nabla}(\mu^{-1}\nabla \cdot \mathbf{A}) + \alpha\widehat{\sigma}(\mathbf{A} + \boldsymbol{\nabla}\phi) = \alpha\mathbf{s}$$
$$\nabla \cdot \widehat{\sigma}(\mathbf{A} + \boldsymbol{\nabla}\phi) = \nabla \cdot \mathbf{s}$$

For $\widehat{\sigma} = \sigma > 0$ this is an elliptic, diagonally dominant system.

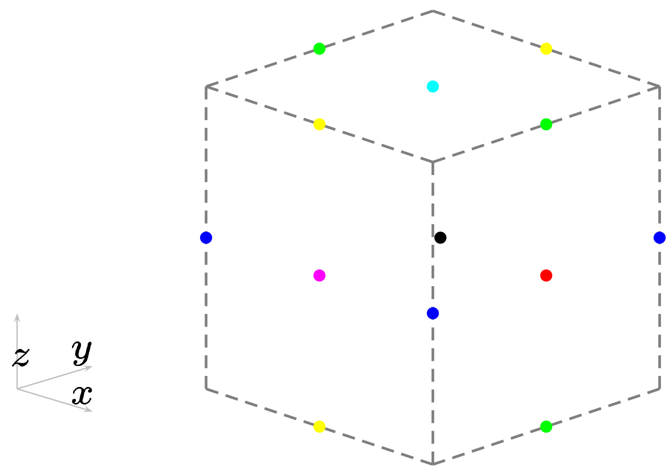
Boundary conditions:

$$
\begin{aligned}
-(\nabla \times \mathbf{A}) \times \mathbf{n}\Big|_{\partial\Omega} &= \mathbf{0}, \\
\mathbf{A} \cdot \mathbf{n}\Big|_{\partial\Omega} = \frac{\partial \phi}{\partial n}\Big|_{\partial\Omega} &= 0, \\
\int_\Omega \phi dV = 0.
\end{aligned}
$$

[Haber & Ascher ’01]

Elements of a finite volume discretization

- $\mathbf{A},\ \boldsymbol{\nabla}\phi,\ \mathbf{s}$ at face centers (like $\mathbf{E}$)
- $\phi, \nabla \cdot \mathbf{A}$ at cell center (like m)
- $\widehat{\sigma}$ by harmonic averaging at face centers
- μ by arithmetic averaging at edge centers (like $\mathbf{H}$)



One cell in a staggered grid

Discretized system - multi experiment

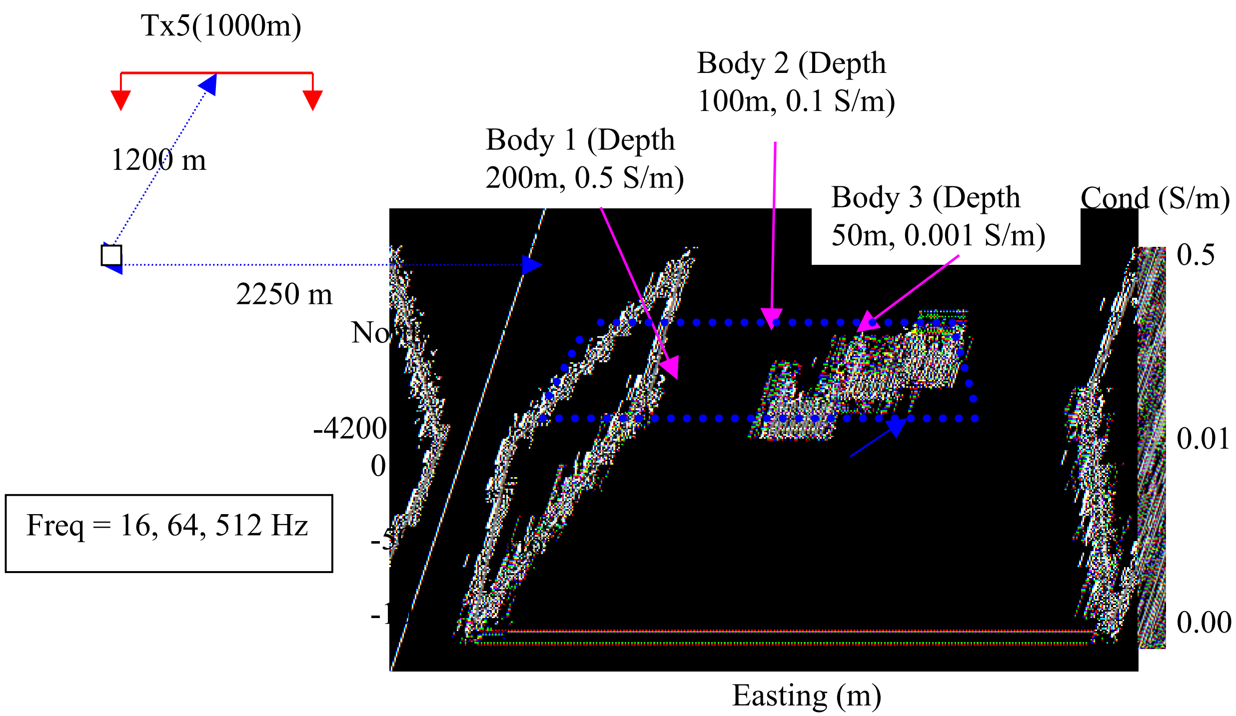
$$\begin{pmatrix} L_\mu + \alpha M_{\widehat{\sigma}} & \alpha M_{\widehat{\sigma}} \nabla_h \\ \nabla_h \cdot M_{\widehat{\sigma}} & \nabla_h \cdot M_{\widehat{\sigma}} \nabla_h \end{pmatrix} \begin{pmatrix} \mathbf{A} \\ \phi \end{pmatrix} = \begin{pmatrix} \alpha \mathbf{s} \\ \nabla_h \cdot s \end{pmatrix}$$

In a multiple source/frequency experiment, write above as $A_k(m)u_k = q_k$. Then forward problem is

$$A(m)u = \begin{pmatrix} A_1(m) & & & & \\ & A_2(m) & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & A_s(m) \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_s \end{pmatrix} = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ \vdots \\ q_s \end{pmatrix} = q.$$

Example - inversion of frequency domain data

Transmitter and receiver geometry from an actual CSAMT field survey (Penasquito, Mexico) but conductivity model synthesized.



- Transmitter is a 1km grounded wire a few km away from survey area – dealt with using a special procedure.

- Data on 5 field components at frequencies $16,\ 64$ and $512\ Hz$ at 28 stations spaced $50m$ apart on each of 11 lines with linespacing $100m$. (Total 308 data locations, 4620 data values.)

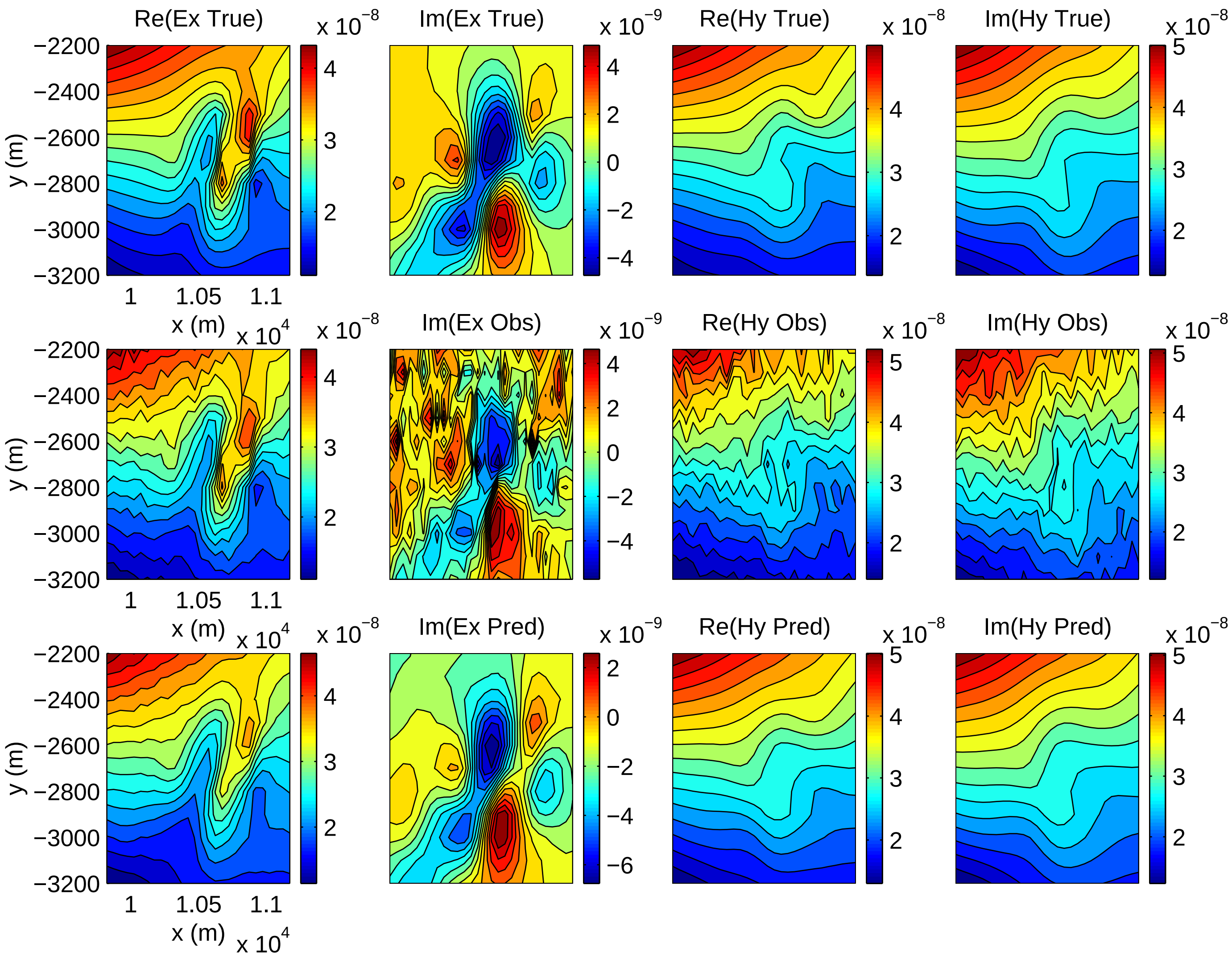
- "True model" has two conductive bodies and one resistive body

- Generate "true data" and contaminate by Gaussian noise, 2% in amplitude 2 degrees in phase.

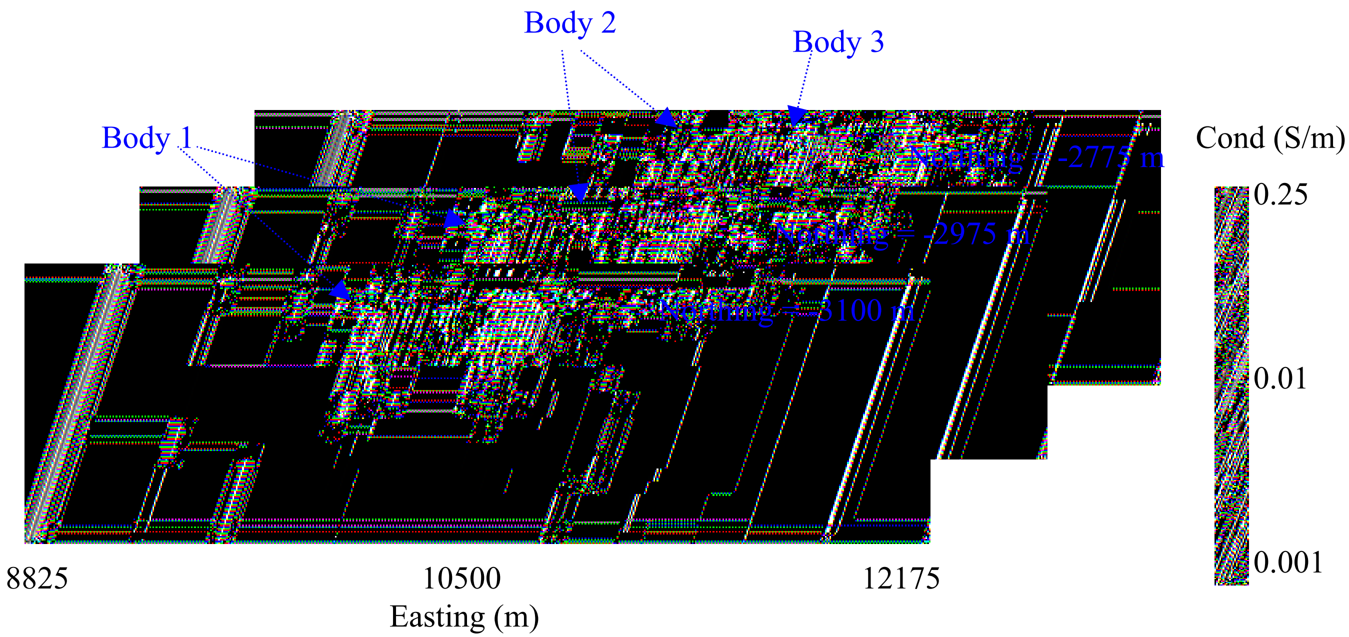
- The $3350m \times 3000m \times 2000m$ volume is discretized into $64 \times 50 \times 30 = 96,000$ cells.

$\beta = 100$	Final misfit = 0.06		
Nonlinear iter	KKT iter	$\|\|Au - q\|\|/\|\|q\|\|$	Rel-grad
1	4	$3e - 2$	2e-1
2	4	$2e - 4$	3e-2
3	3	$2e - 6$	5e-4

$\beta = 1e0$	Final misfit = 0.03		
Nonlinear iter	KKT iter	$\|\|Au - q\|\|/\|\|q\|\|$	Rel-rad
1	8	$1e - 6$	3e-3
2	6	$8e - 7$	9e-4



Re(Ex True)
Im(Ex True)
Re(Hy True)
Im(Hy True)
Im(Ex Obs)
Re(Hy Obs)
Im(Hy Obs)
Im(Ex Pred)
Re(Hy Pred)
Im(Hy Pred)
y (m)
x (m)
x 10^4
x 10^-8
x 10^-9



Body 2
Body 3
Body 1
Northing = -2775 m
Northing = -2975 m
Northing = -3100 m
Cond (S/m)
0.25
0.01
0.001
8825
10500
12175
Easting (m)

Maxwell's equations in time domain

$$\nabla \times \mathbf{E} + \mu \mathbf{H}_t = \mathbf{0} \quad \text{in } \Omega,$$
$$\nabla \times \mathbf{H} - \sigma \mathbf{E} - \epsilon \mathbf{E}_t = \mathbf{s}_r(t) \quad \text{in } \Omega,$$
$$\mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \partial\Omega.$$

- Parameter regime over non-short time scales yields heavy dissipation – very stiff problems.
- Measure field only beyond initial, transient layer.

Maxwell's equations in time domain

$$\nabla \times \mathbf{E} + \mu \mathbf{H}_t = \mathbf{0} \quad \text{in } \Omega,$$
$$\nabla \times \mathbf{H} - \sigma \mathbf{E} - \epsilon \mathbf{E}_t = \mathbf{s}_r(t) \quad \text{in } \Omega,$$
$$\mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \partial\Omega.$$

- Cannot expect high accuracy, as sources are typically only continuous in time.
- Lagrange multipliers (solution of adjoint problem) are of low continuity.

$\Rightarrow$ Discretize in time using backward Euler.

$$\begin{aligned} \alpha_n &= (t_n - t_{n-1})^{-1} \\ \hat{\sigma}_n &= \sigma + \alpha_n \epsilon \end{aligned}$$

$$\begin{aligned} \nabla \times \mathbf{E}^n + \alpha_n \mu \mathbf{H}^n = \alpha_n \mathbf{H}^{n-1} \equiv \mathbf{s}_H \\ \nabla \times \mathbf{H}^n - \hat{\sigma}_n \mathbf{E}^n = \mathbf{s}_r^n - \alpha_n \epsilon \mathbf{E}^{n-1} \equiv \mathbf{s}_E \\ \mathbf{n} \times \mathbf{H}^n = 0. \end{aligned}$$

This has the same form as in frequency domain. Apply the same treatment!

Discretized system - s time steps

$$\begin{pmatrix} L_\mu + \alpha_n M_{\widehat{\sigma}} & \alpha_n M_{\widehat{\sigma}} \nabla_h & 0 \\ \nabla_h \cdot M_{\widehat{\sigma}} & \nabla_h \cdot M_{\widehat{\sigma}} \nabla_h & 0 \\ \alpha_n^{-1} M_\mu^{-1} \nabla_h \times & 0 & I \end{pmatrix} \begin{pmatrix} \mathbf{A}_n \\ \phi_n \\ \mathbf{H}_n \end{pmatrix} = \begin{pmatrix} \alpha_n \mathbf{s} \\ \nabla_h \cdot s \\ \mathbf{H}_{n-1} \end{pmatrix}$$

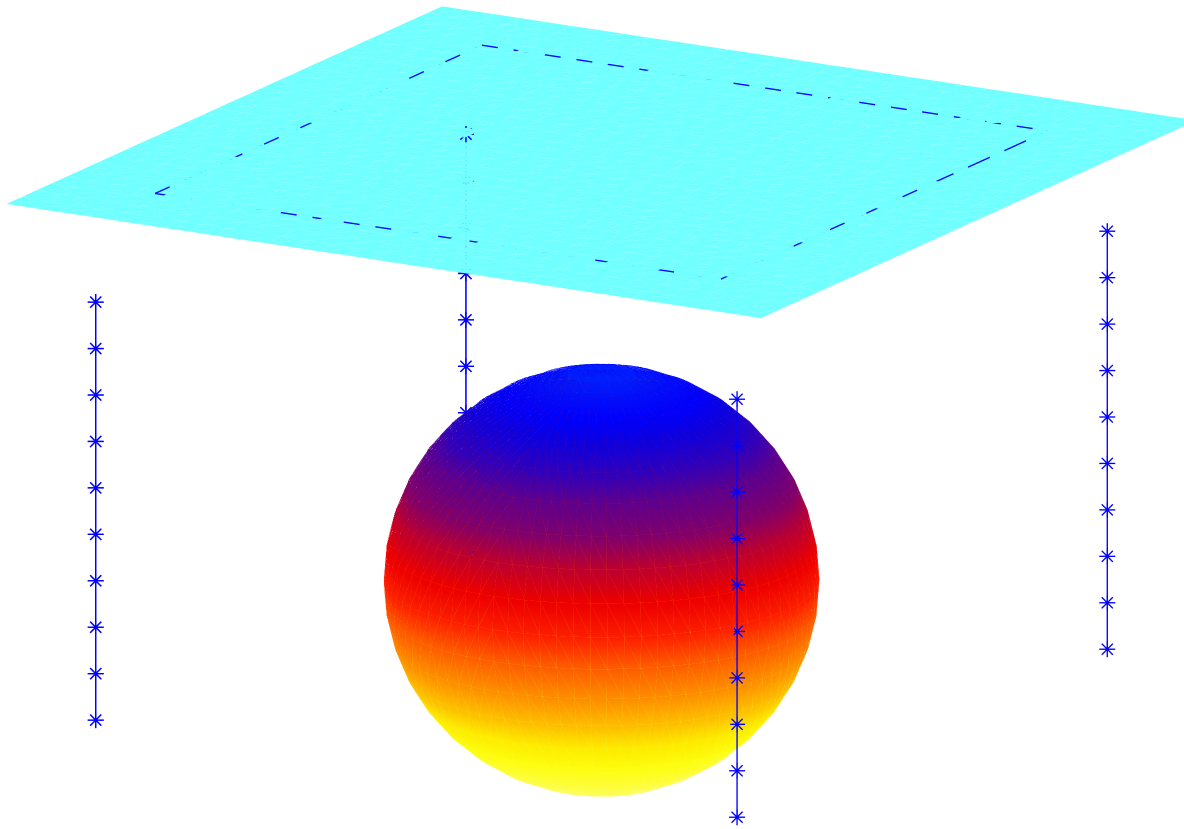
For the nth time step, write above as $B_n u_{n-1} + A_n(m) u_n = q_n$. Then forward problem is

$$A(m)u = \begin{pmatrix} A_1(m) & & & & \\ B_2 & A_2(m) & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & B_s & A_s(m) \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_s \end{pmatrix} = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ \vdots \\ q_s \end{pmatrix} = q.$$

Example - inversion of time domain data

A square loop $50m \times 50m$ just above earth's surface. Data acquired at 20 depths in each of 4 boreholes surrounding conductive body at 18 logarithmically spaced times between $10^{-4} - 10^{-1}\ sec$.

"True model" is a conductive sphere radius $15m$ buried in a uniform halfspace.



- Time discretization: 32 steps equally spaced on a log-grid $10^{-7} - 10^{-1}\ sec$.

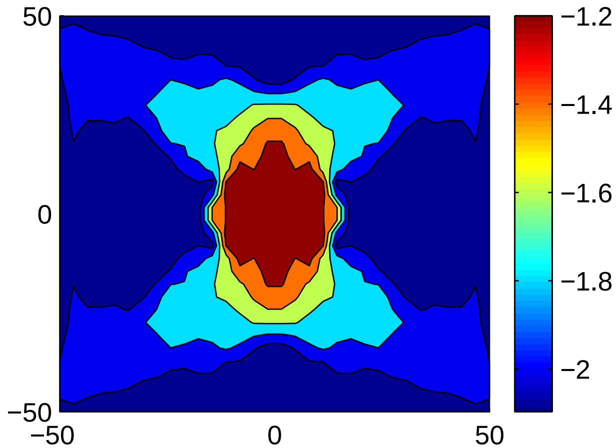
- Inversion grid in space $40 \times 40 \times 32$.

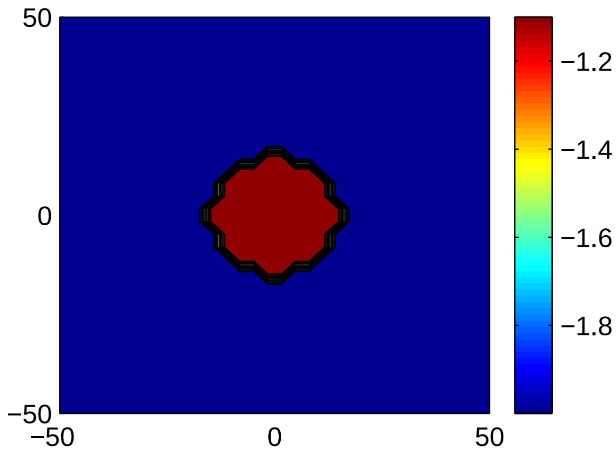
- Initial guess is uniform halfspace equal to true background conductivity.

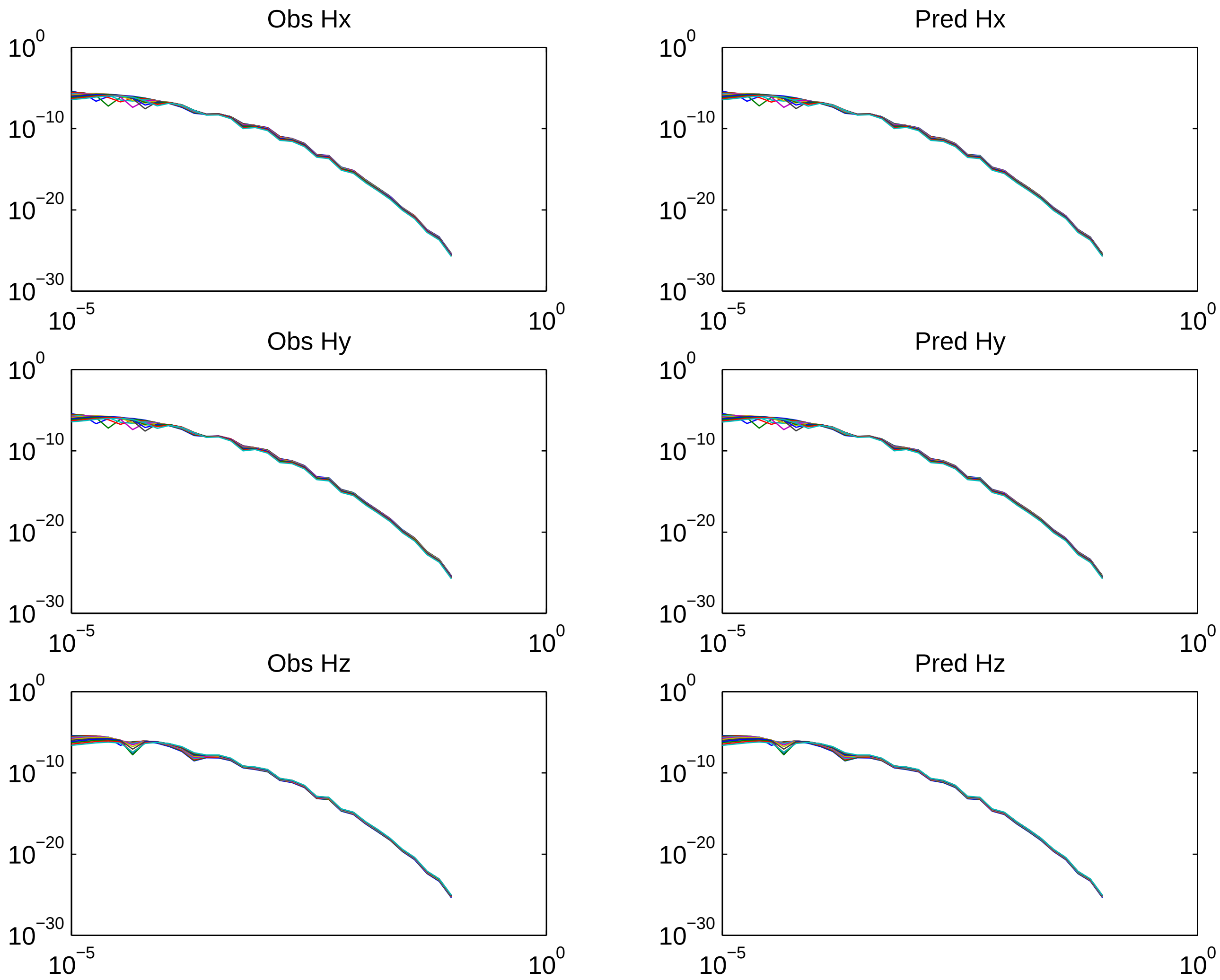
$\beta = 1e-1$	Final misfit = 0.1		
Nonlinear iter	KKT iter	$\|\|Au-q\|\|/\|\|q\|\|$	Rel-grad
1	2	$3e-3$	1e-2
2	3	$2e-4$	4e-3
3	2	$7e-6$	1e-3
4	2	$9e-7$	3e-4

$\beta = 1e-2$	Final misfit = 0.04		
Nonlinear iter	KKT iter	$\|\|Au-q\|\|/\|\|q\|\|$	Rel-grad
1	7	$4e-6$	2e-3
2	5	$6e-7$	7e-4

$\beta = 1e-3$	Final misfit = 0.02		
Nonlinear iter	KKT iter	$\|\|Au-q\|\|/\|\|q\|\|$	Rel-grad
1	8	$2e-6$	3e-3
2	7	$8e-7$	9e-4


50
0
−50
−50
0
50
−1.2
−1.4
−1.6
−1.8
−2


50
0
−50
−50
0
50
−1.2
−1.4
−1.6
−1.8


Obs Hx
Pred Hx
Obs Hy
Pred Hy
Obs Hz
Pred Hz
10^0
10^-10
10^-20
10^-30
10^-5

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Discontinuous solutions and Huber's norm - outline

- Least squares, TV and Huber
- Choosing the Huber parameter
- Lagged diffusivity, Gauss-Newton and all-at-once
- Example in 2D

Least squares, TV and Huber

A priori knowledge: model probably contains jump discontinuities!

So, in regularization term

$$R(m) = \left[\int_\Omega \rho(|\nabla m|) + \alpha(m - m_{ref}) \right]_h$$

want to limit effect of penalty through jump. Note:

- For $|\nabla m| \to \infty$, $\int |\nabla m|$ integrable but $\int |\nabla m|^2$ is not.
- For $|\nabla m| \to 0$, $\int |\nabla m|$ yields problems but $\int |\nabla m|^2$ does not.

So, combine: use Huber's norm

$$\begin{aligned} \rho(\tau) &= \begin{cases} \tau, & \tau \geq \gamma, \\ \tau^2/(2\gamma) + \gamma/2, & \tau < \gamma \end{cases} \\ R'(m) &\leftarrow \nabla \cdot \left(\min\{\frac{1}{\gamma}, \frac{1}{|\boldsymbol{\nabla} m|}\} \, \boldsymbol{\nabla} m \right) \end{aligned}$$

Choosing the Huber parameter

We choose, depending on the solution,

$$\gamma = \frac{h}{|\Omega|_h} \left[\int_{\Omega} |\boldsymbol{\nabla} m| \right]_h .$$

Others choose this parameter using an expression from robust statistics involving medians of $|\boldsymbol{\nabla} m|$.

Question: Why not choose to penalize less through discontinuities?

Answer: This leads to non-convex functionals and local minima even when forward problem is the identity, $J = I$.

Lagged diffusivity, Gauss-Newton and all-at-once

In the **Gauss-Newton** iteration step

$$\begin{pmatrix} A & 0 & G \\ Q^T Q & A^T & 0 \\ 0 & G^T & \beta R'' \end{pmatrix} \begin{pmatrix} \delta u \\ \delta \lambda \\ \delta m \end{pmatrix} = - \begin{pmatrix} \mathcal{L}_\lambda \\ \mathcal{L}_u \\ \mathcal{L}_m \end{pmatrix}$$

use **lagged diffusivity** approximation: at current iterate,

$$R'' \delta m \approx \nabla \cdot \left(\min\{\frac{1}{\gamma}, \frac{1}{|\boldsymbol{\nabla} m|}\} \, \boldsymbol{\nabla} \delta m \right).$$

Our **all at once** discussion now extends directly, although nonlinear problem becomes harder.

Note that for denoising $J = I$ there is essentially a global convergence proof.

[e.g. Vogel, 2002; Sapiro, 2001]

But is there really enough accurate data in applications to allow honest identification of discontinuities with our diffusive forward operators?!

Example in 2D

Forward mother problem $\nabla \cdot m^{-1} \boldsymbol{\nabla} u = q$

Domain $\Omega = [-1, 1]^2$

Right hand side with source and sink

$$q = exp(-10((x + 0.6)^2 + (y + 0.6)^2)) - exp(-10((x - 0.6)^2 + (y - 0.6)^2))$$

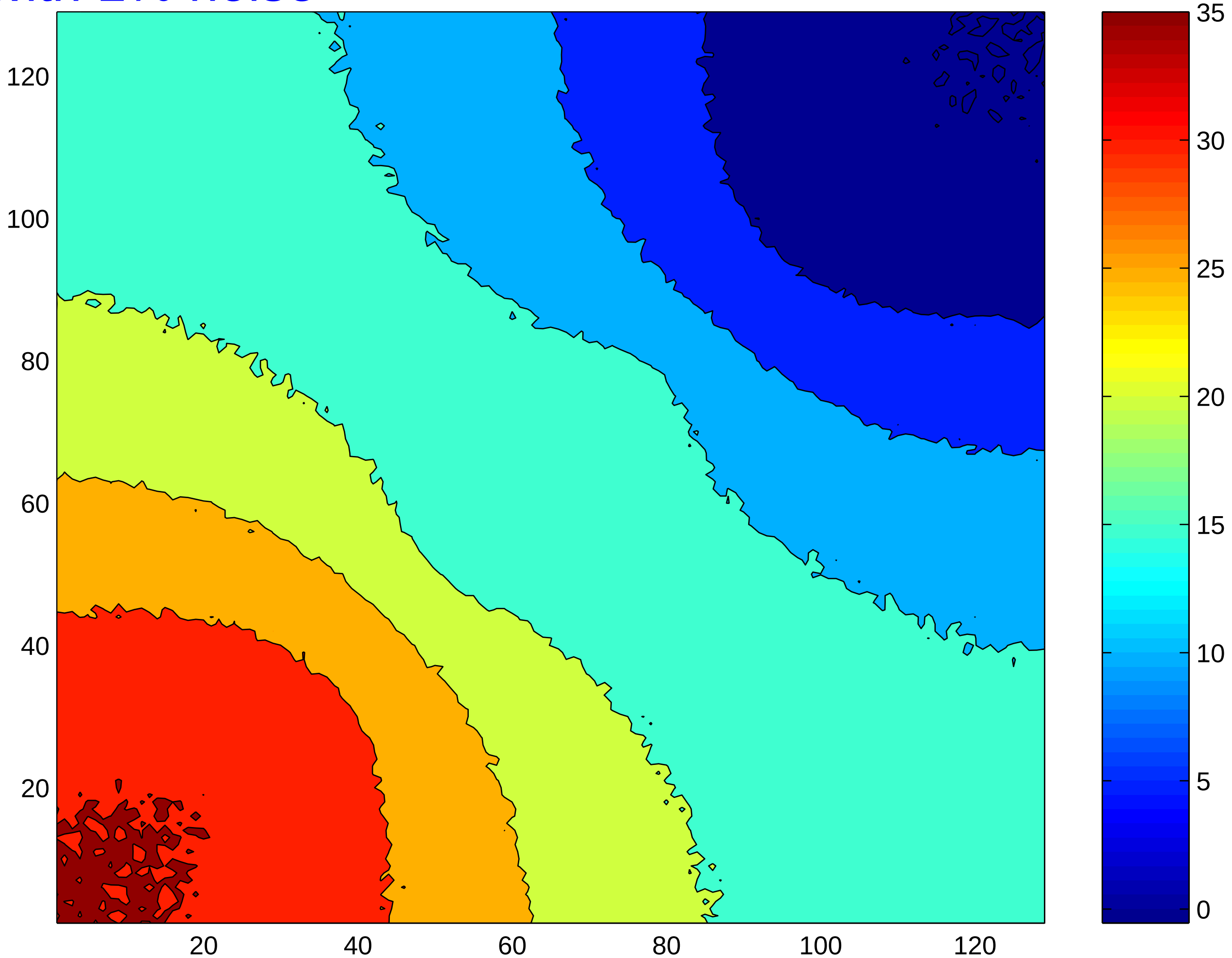
“True model” with discontinuities

Data everywhere with 1% noise

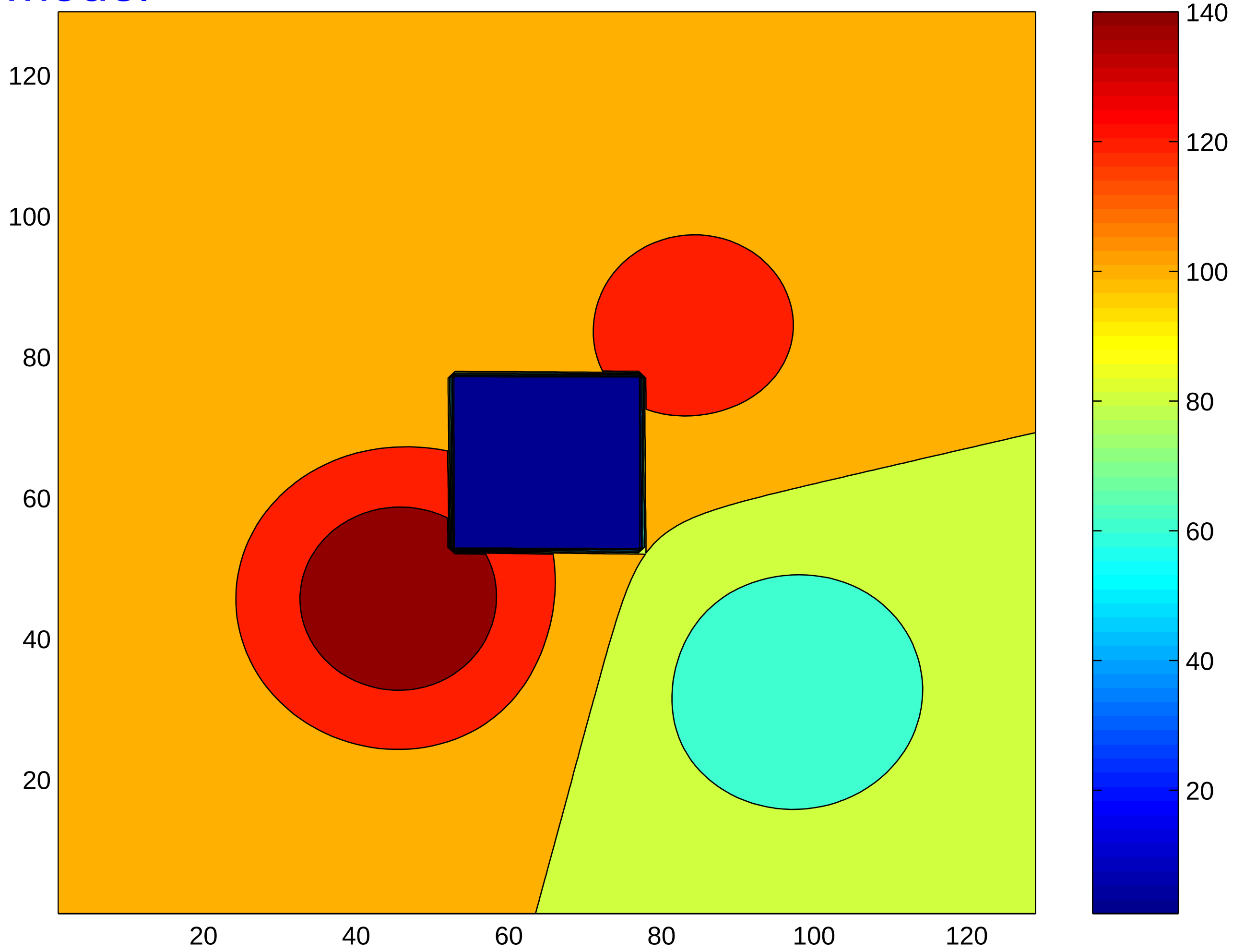
Uniform cell-centered discretization 129×129

Iterative solver with a multigrid preconditioner

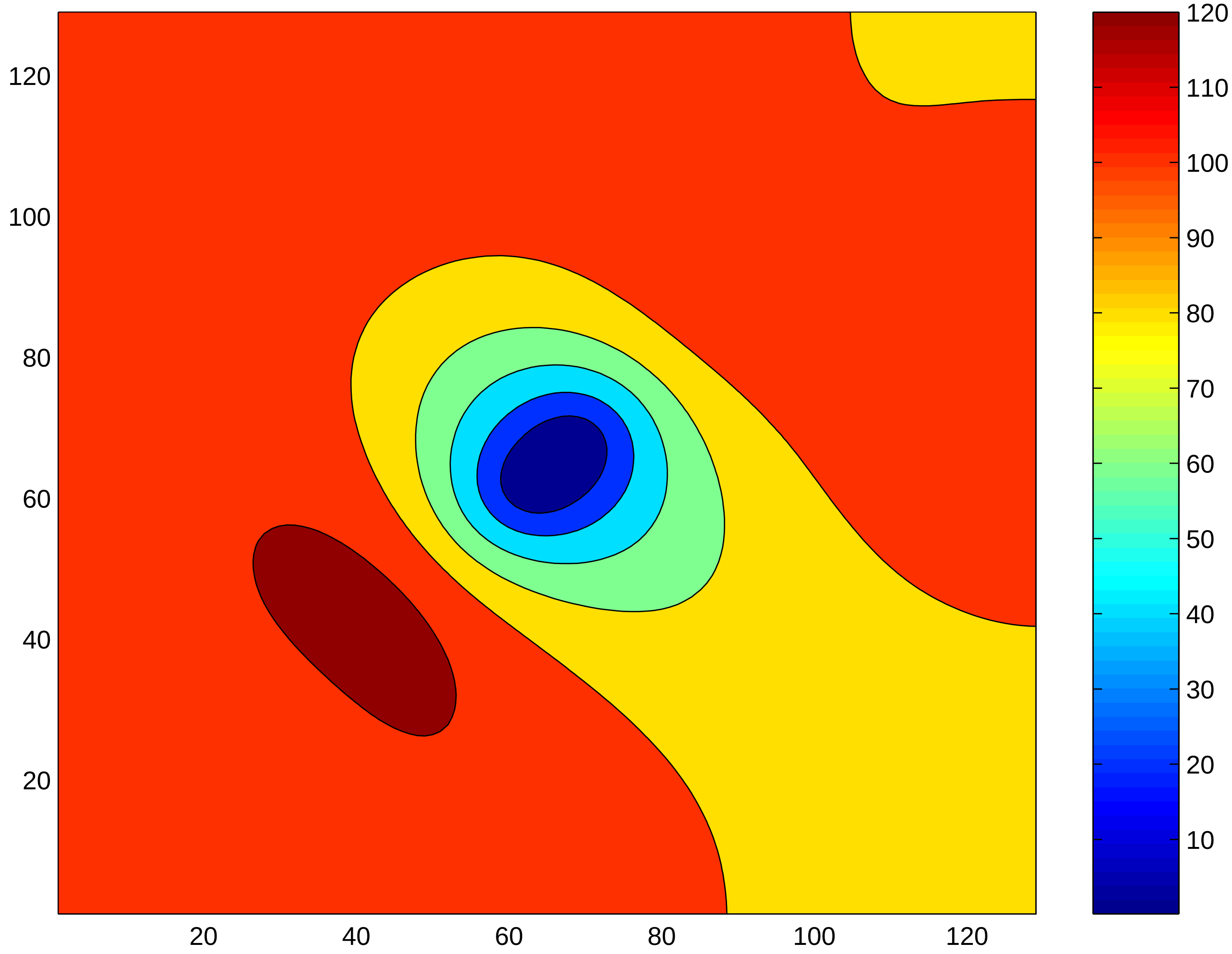
Data with 1% noise



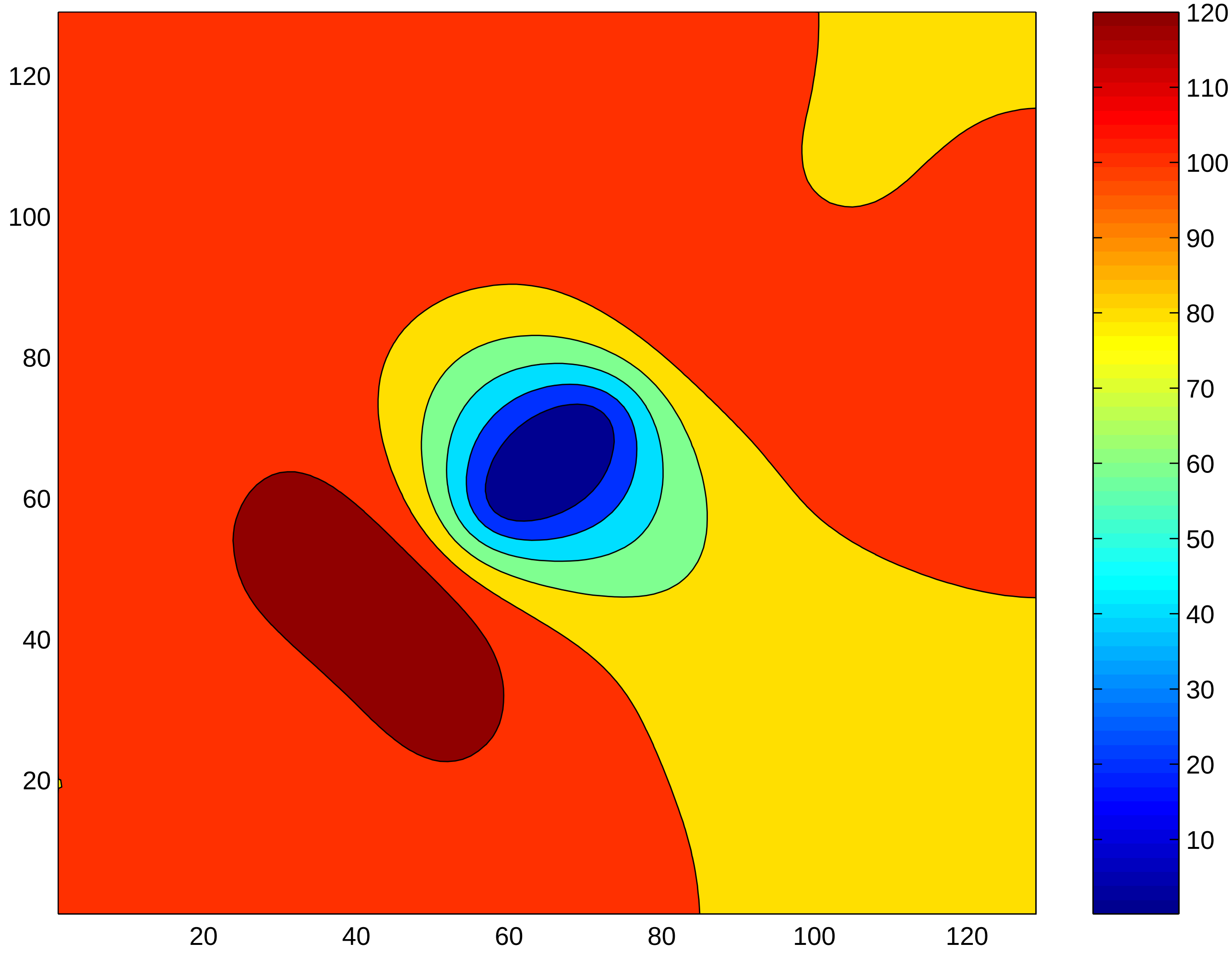
“True model”



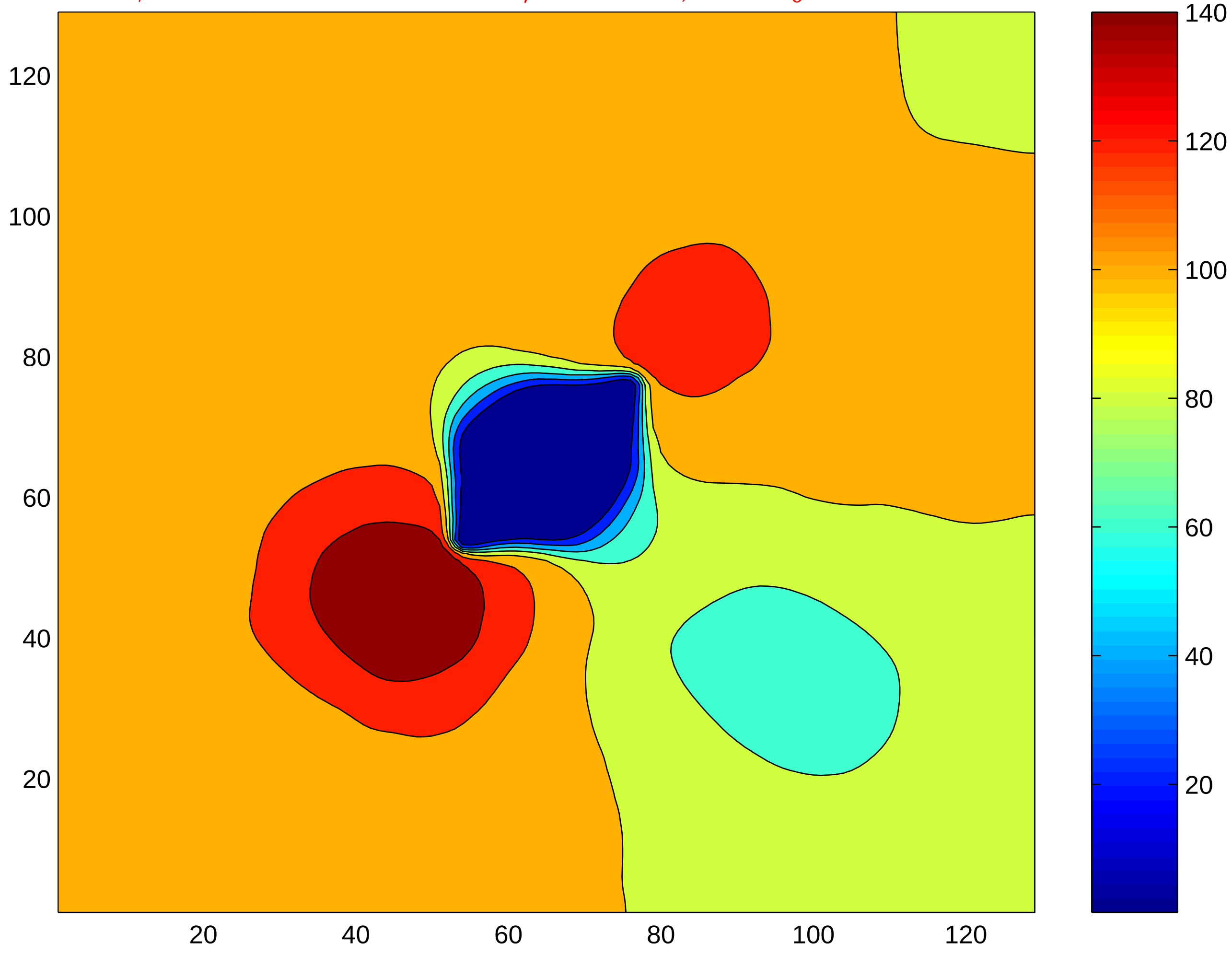
Least squares with $\beta = 1.e - 5 \ \Rightarrow \ misfit = 1.66e - 2$



Least squares with $\beta = 3.e-6 \;\Rightarrow\; misfit = 1.50e-2$



Huber with $\beta = 1.e-5 \;\Rightarrow\; \gamma = 4.6, misfit = 1.01e-2$



Outline

- Forward problems and distributed parameter estimation
- Solving the optimization problem
- 3D electromagnetic data inversion in frequency and time domain
- Discontinuous solutions and Huber’s norm
- Outline