A *penalty* method for *PDE*-constrained optimization with applications to *wave*-equation based *seismic* inversion

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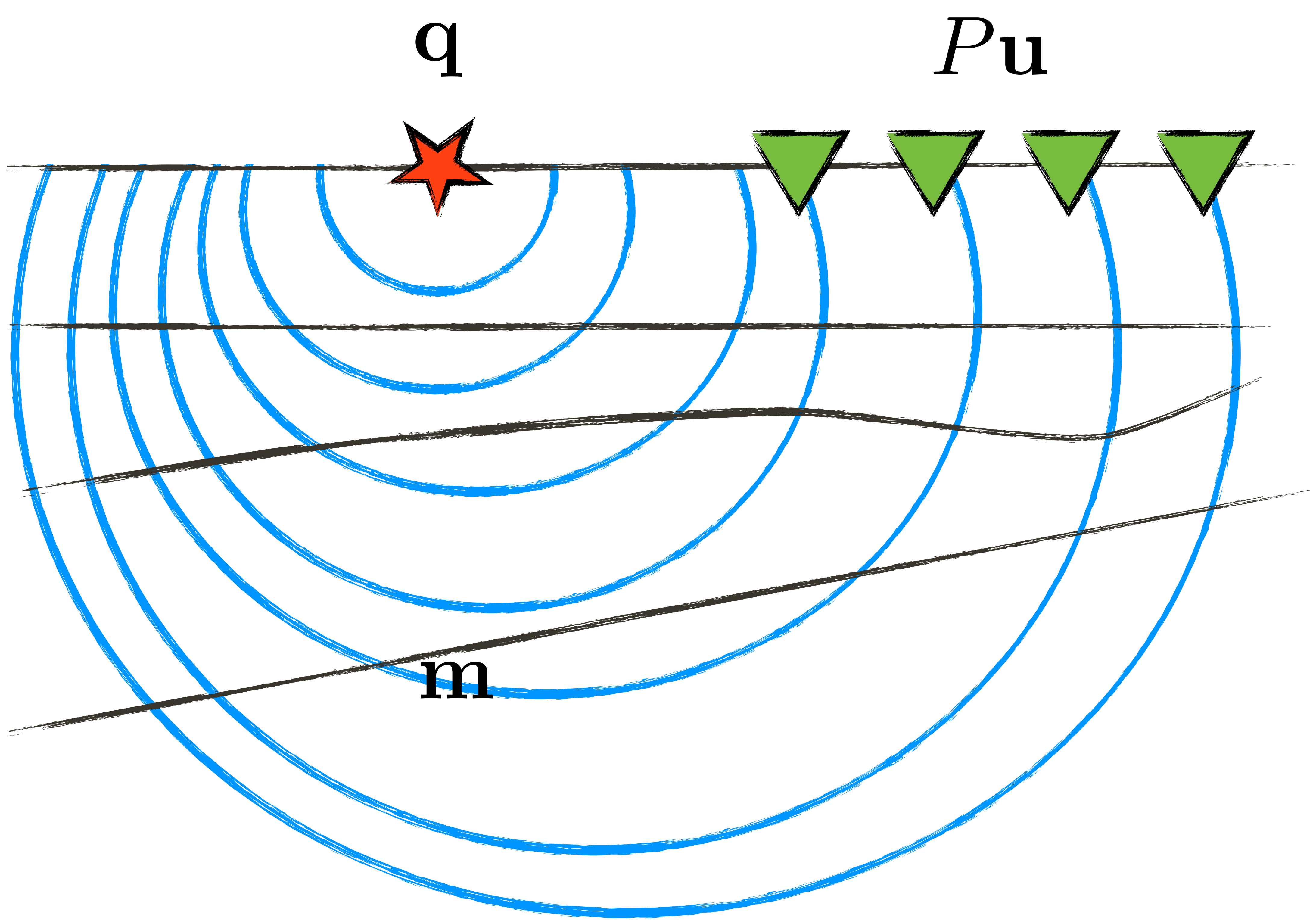
van Leeuwen, T and Herrmann, F J (2013). Mitigating local minima in full-waveform inversion by expanding the search space. Geophysical Journal International.
van Leeuwen, T and Herrmann, F J (2013).A penalty method for PDE-constrained optimization. Submitted for publication
van Leeuwen, T and Herrmann, F J (2013). US Provisional Patent Application No. 61/815,533. A Penalty Method for PDE-Constrained Optimization with Applications to Wave-Equation Based Seismic Inversion

Seismic waveform inversion

Given observed data, $\mathbf{d}$, find *model* parameters, $\mathbf{m}$, and a *wavefield*, $\mathbf{u}$, such that, $P\mathbf{u} \approx \mathbf{d}$ and $A(\mathbf{m})\mathbf{u} \approx \mathbf{q}$



Observation

If we measure the wavefield *everywhere*, we can *trivially* solve

$$P\mathbf{u} = \mathbf{d}$$

Given $\mathbf{u}$ we *can* calculate the *medium* parameters by *solving*

$$A(\mathbf{m})\mathbf{u} = \mathbf{q}$$

for $\mathbf{m}$ *knowing* $\mathbf{q}$.

This leads to $$\min_{\mathbf{m}} ||A(\mathbf{m})P^{-1}\mathbf{d} - \mathbf{q}||_2^2$$

compared to $$\min_{\mathbf{m}} ||PA(\mathbf{m})^{-1}\mathbf{q} - \mathbf{d}||_2^2$$

Question

When P is *not* invertible, can we *reconstruct* a *wavefield* from the *observed* data that can act as a *proxy*?

For a given $\mathbf{m}$, we want the *proxy* wavefield to

I. *fit* the data–i.e., $P\mathbf{u} \approx \mathbf{d}$, and

II. *obey* the *wave*-equation–i.e., $A(\mathbf{m})\mathbf{u} \approx \mathbf{q}$

Why *not* use the least-squares solution of the *data*-augmented system?

$$\begin{pmatrix} P \\ A(\mathbf{m}) \end{pmatrix} \mathbf{u} \approx \begin{pmatrix} \mathbf{d} \\ \mathbf{q} \end{pmatrix}$$

Naive algorithm

1. Reconstruct the *unknown* wavefield by *solving*

$$\mathbf{u}_k = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} P \\ A(\mathbf{m}_k) \end{pmatrix} \mathbf{u} - \begin{pmatrix} \mathbf{d} \\ \mathbf{q} \end{pmatrix} \right\|_2^2$$

2. Reconstruct the *model* by *solving*

$$\mathbf{m}_{k+1} = \arg\min_{\mathbf{m}} \|A(\mathbf{m})\mathbf{u}_k - \mathbf{q}\|_2^2$$

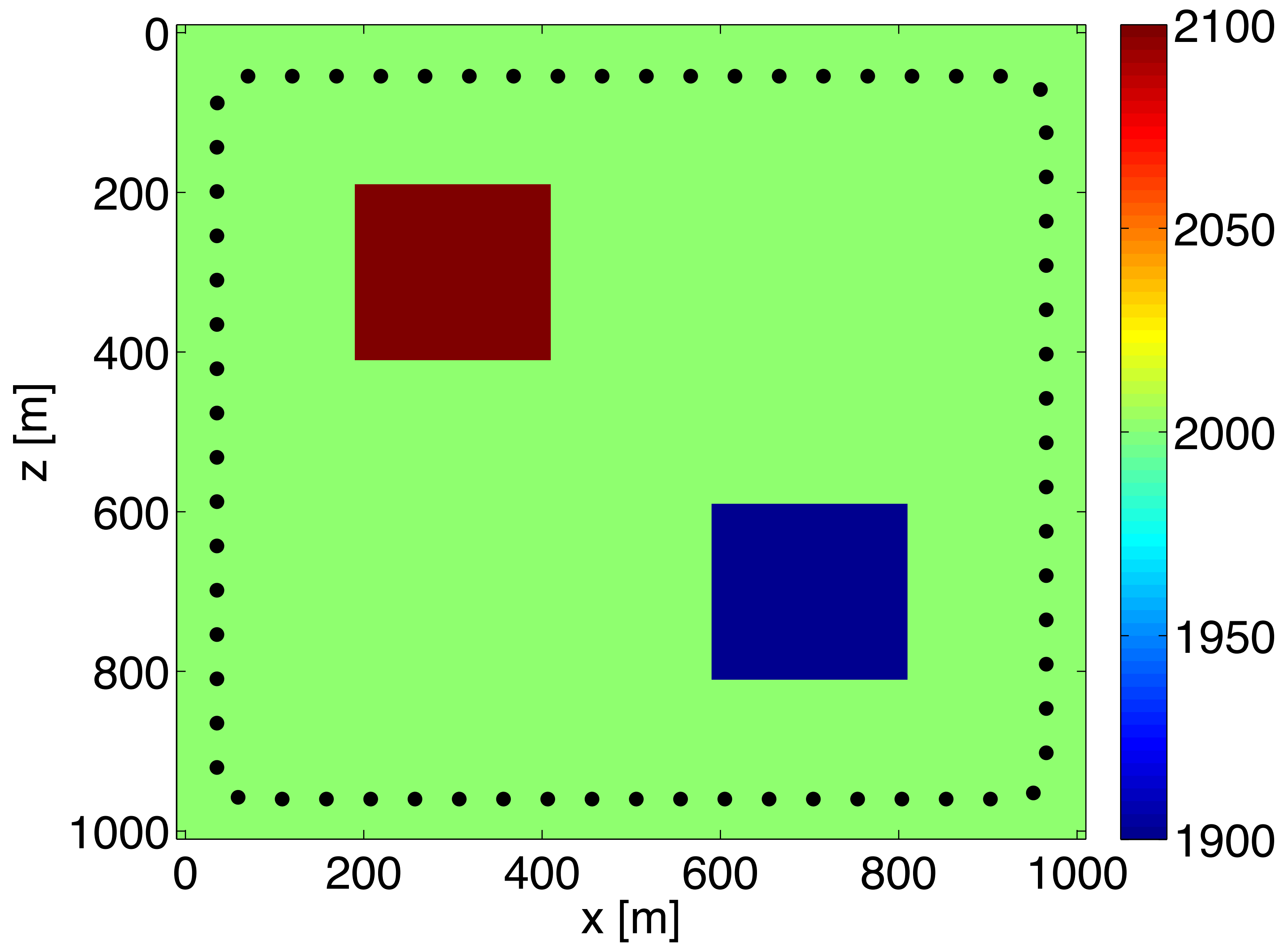
3. Repeat

Simple example

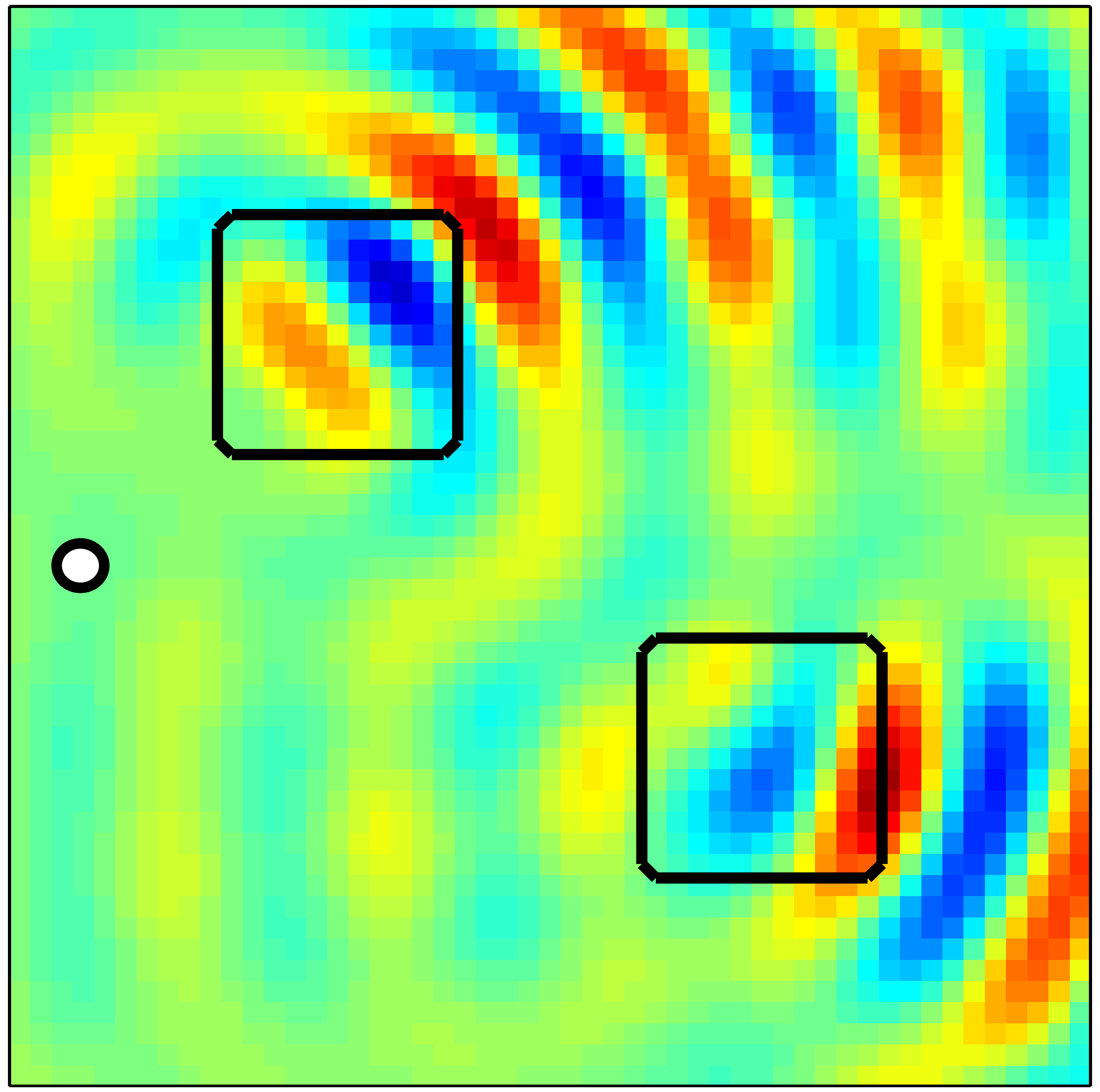
- Invert *monochromatic* data (10 Hz) with transducers *all* around
- *constant* velocity *initial* velocity *model*
- *5*-point discretization of Helmholtz system

$$A(\mathbf{m}) = \omega^2 \mathrm{diag}(\mathbf{m}) + L$$

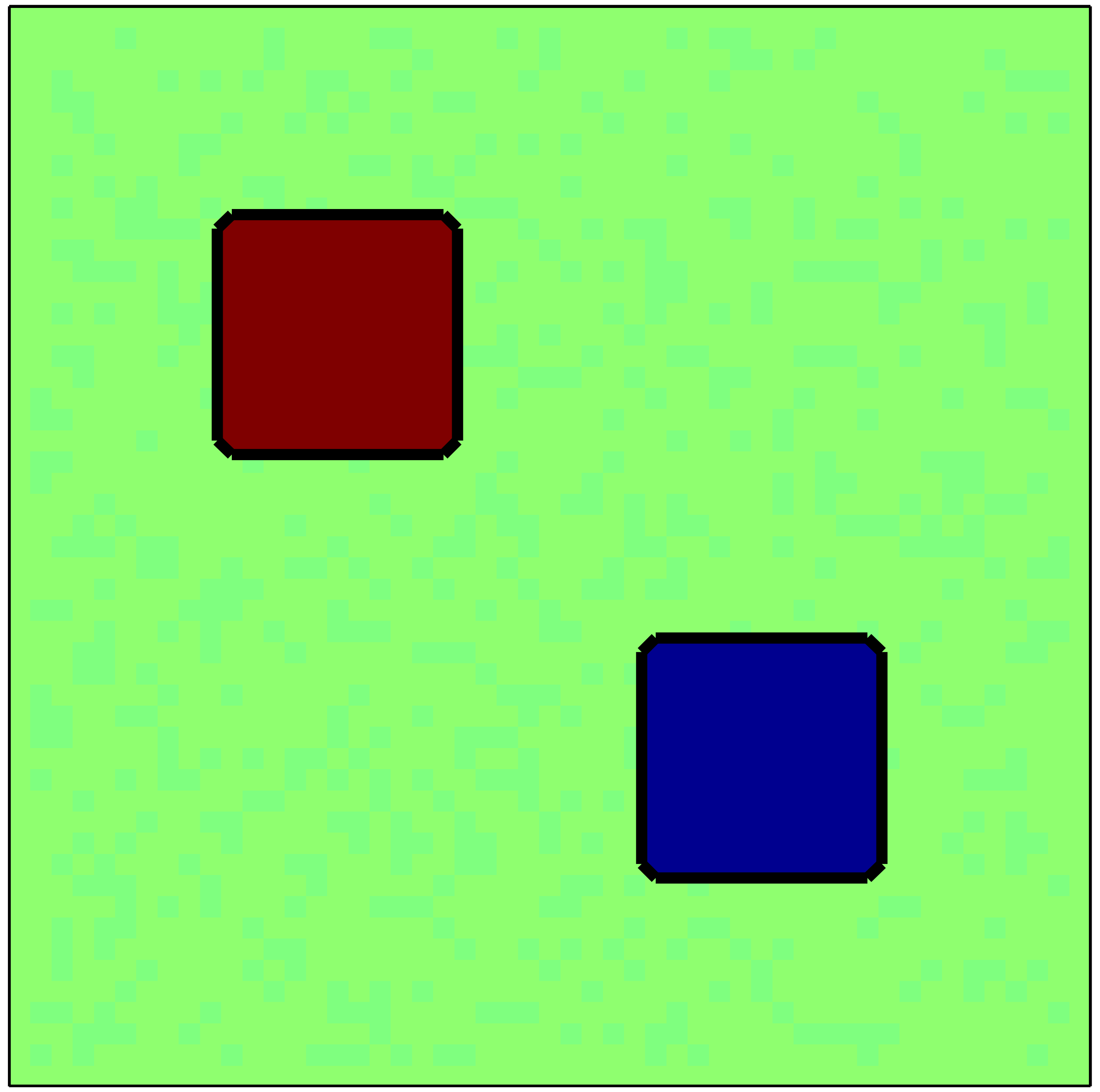
- two *subproblems* are both *linear* (in $\mathbf{m}$ and $\mathbf{u}$)



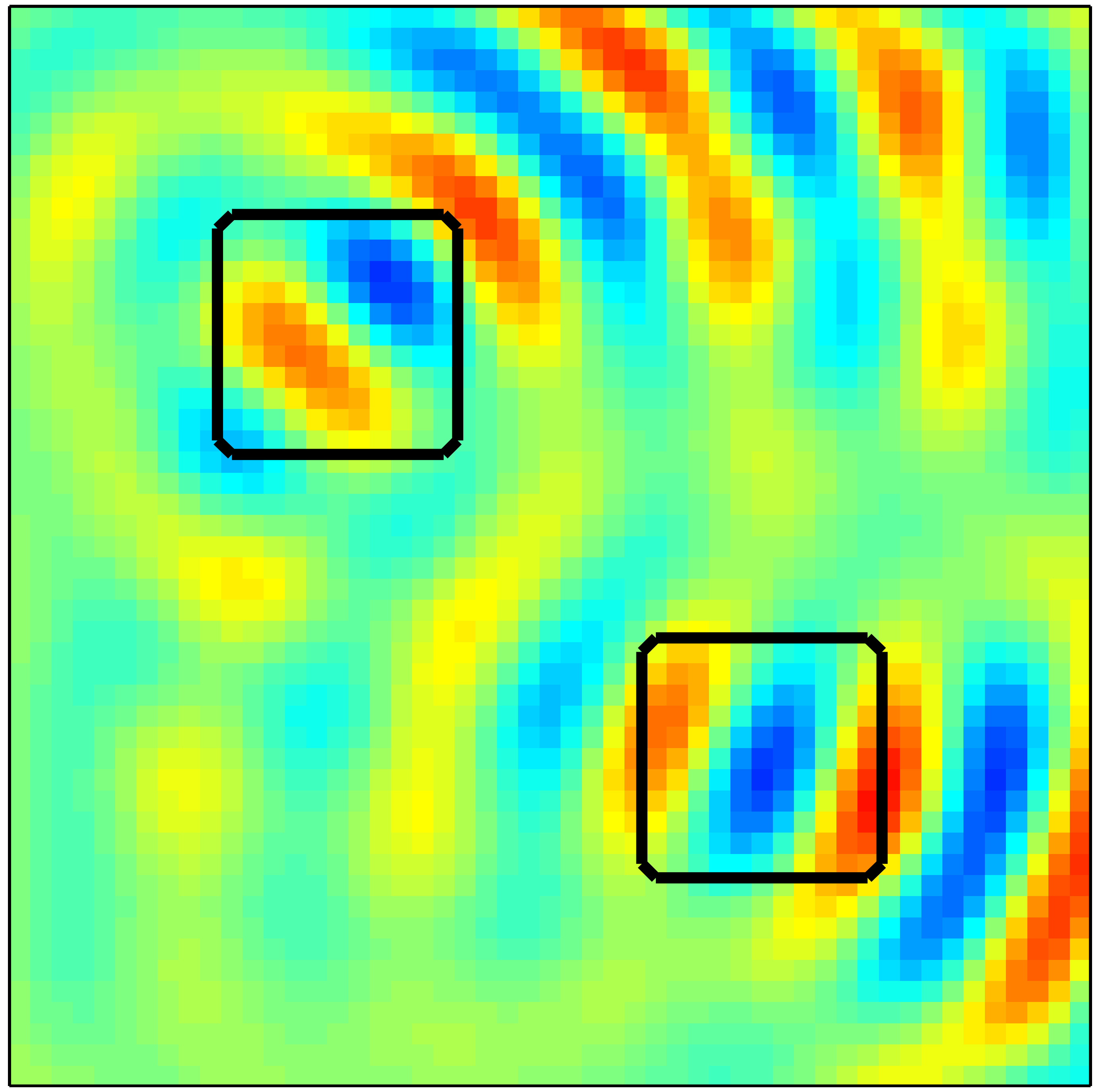
true wavefield



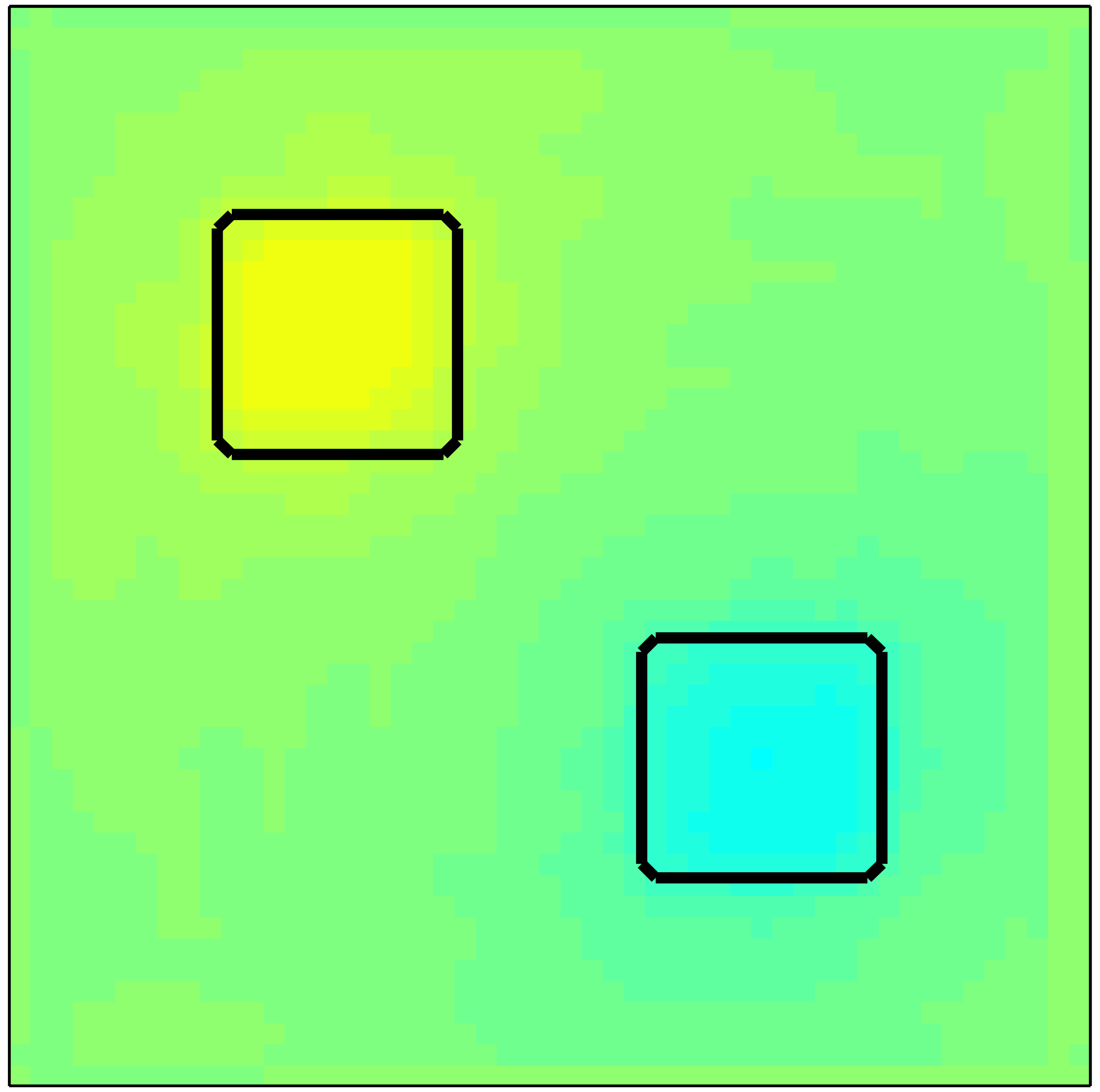
true model



iteration 1

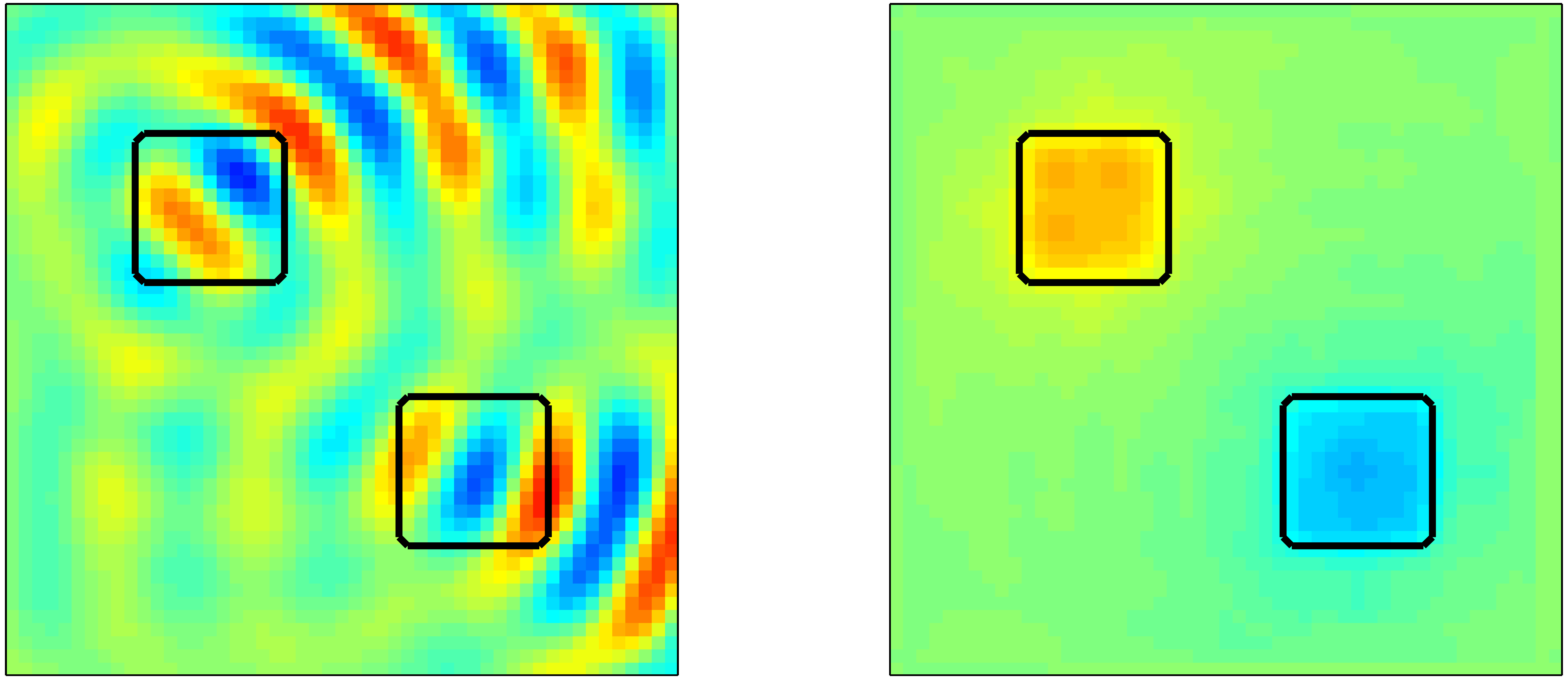


$$\mathbf{u}_0 = (P^*P + A_0^*A_0)^{-1}(P^*\mathbf{d} + A_0^*\mathbf{q})$$



$$\mathbf{m}_1 = \mathrm{diag}(|\mathbf{u}_0|^2)^{-1}\mathrm{diag}(\mathbf{u}_0)^*(\mathbf{q} - L\mathbf{u}_0)$$

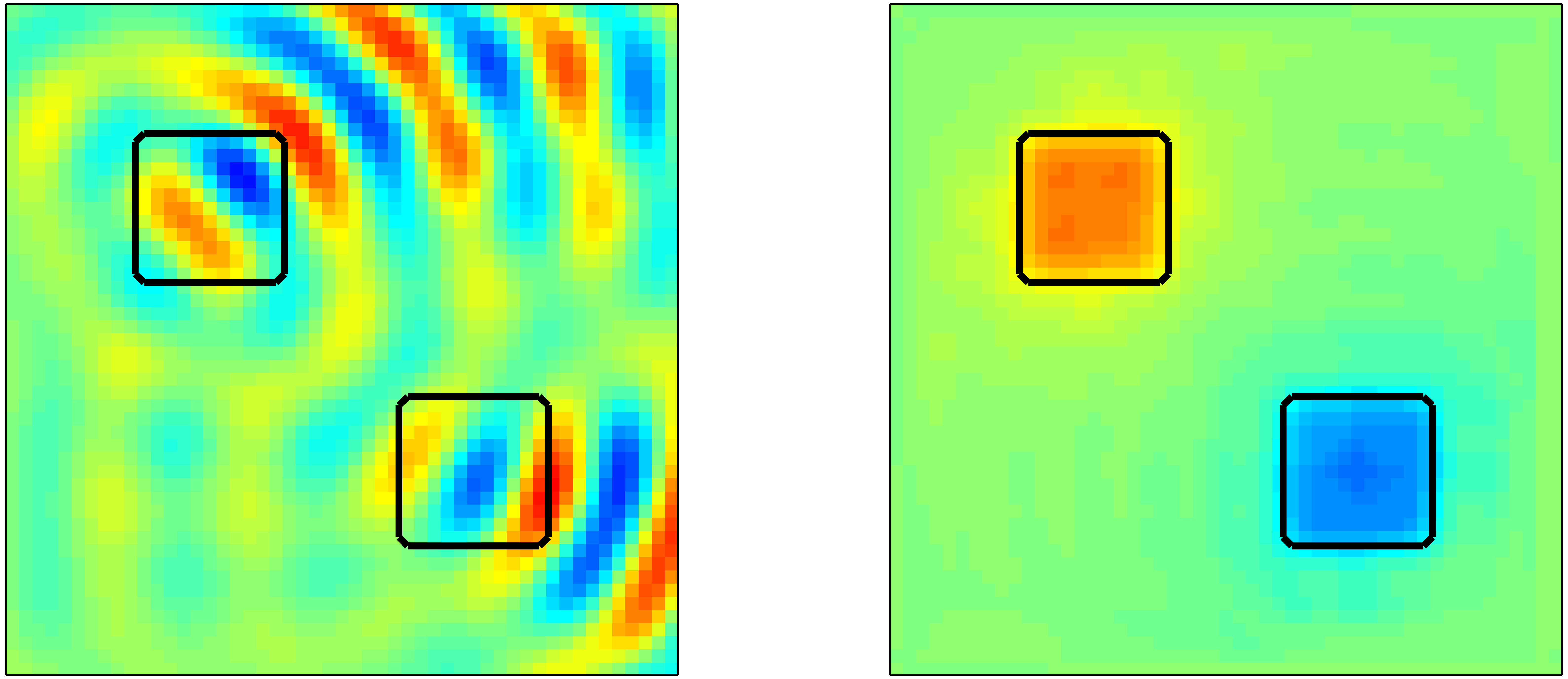
iteration 2



$$\mathbf{u}_1 = (P^*P + A_1^*A_1)^{-1}(P^*\mathbf{d} + A_1^*\mathbf{q})$$

$$\mathbf{m}_2 = \mathrm{diag}(|\mathbf{u}_1|^2)^{-1}\mathrm{diag}(\mathbf{u}_1)^*(\mathbf{q} - L\mathbf{u}_1)$$

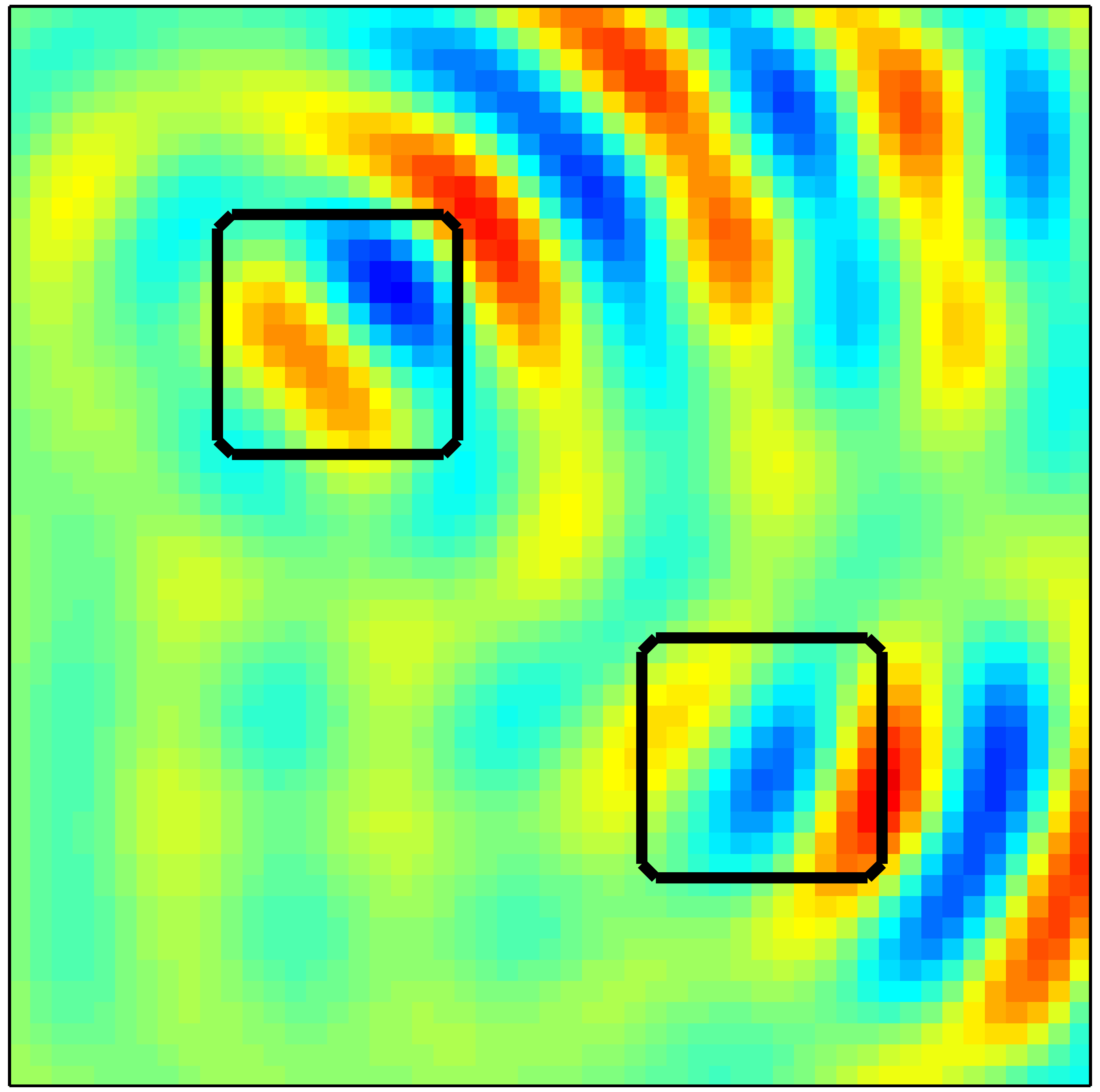
iteration 3

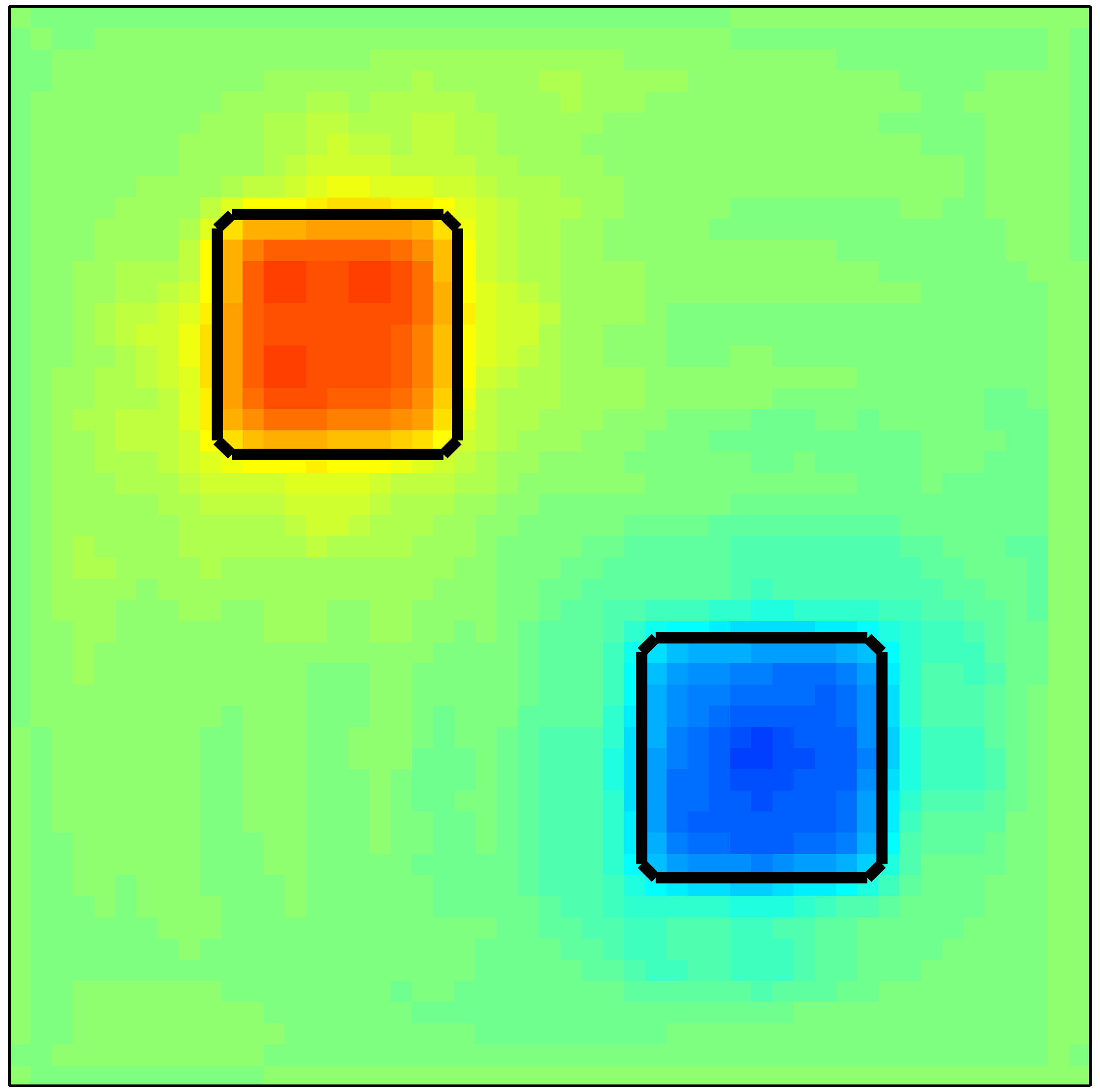


$$\mathbf{u}_2 = \left(P^*P + A_2^*A_2\right)^{-1}\left(P^*\mathbf{d} + A_2^*\mathbf{q}\right)$$

$$\mathbf{m}_3 = \mathrm{diag}(|\mathbf{u}_2|^2)^{-1}\mathrm{diag}(\mathbf{u}_2)^*\left(\mathbf{q} - L\mathbf{u}_2\right)$$

iteration 4

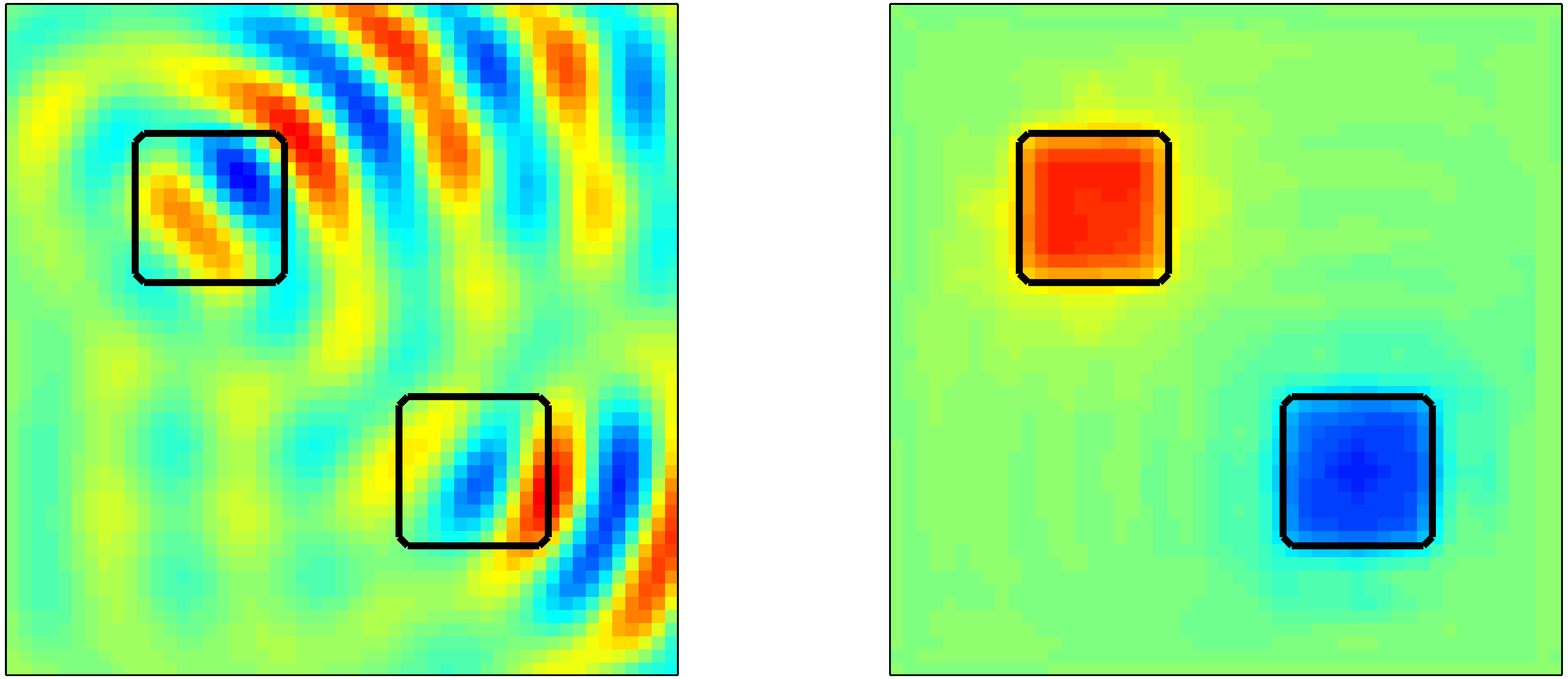




$$\mathbf{u}_3 = (P^*P + A_3^*A_3)^{-1}(P^*\mathbf{d} + A_3^*\mathbf{q})$$

$$\mathbf{m}_4 = \mathrm{diag}(|\mathbf{u}_3|^2)^{-1}\mathrm{diag}(\mathbf{u}_3)^*(\mathbf{q} - L\mathbf{u}_3)$$

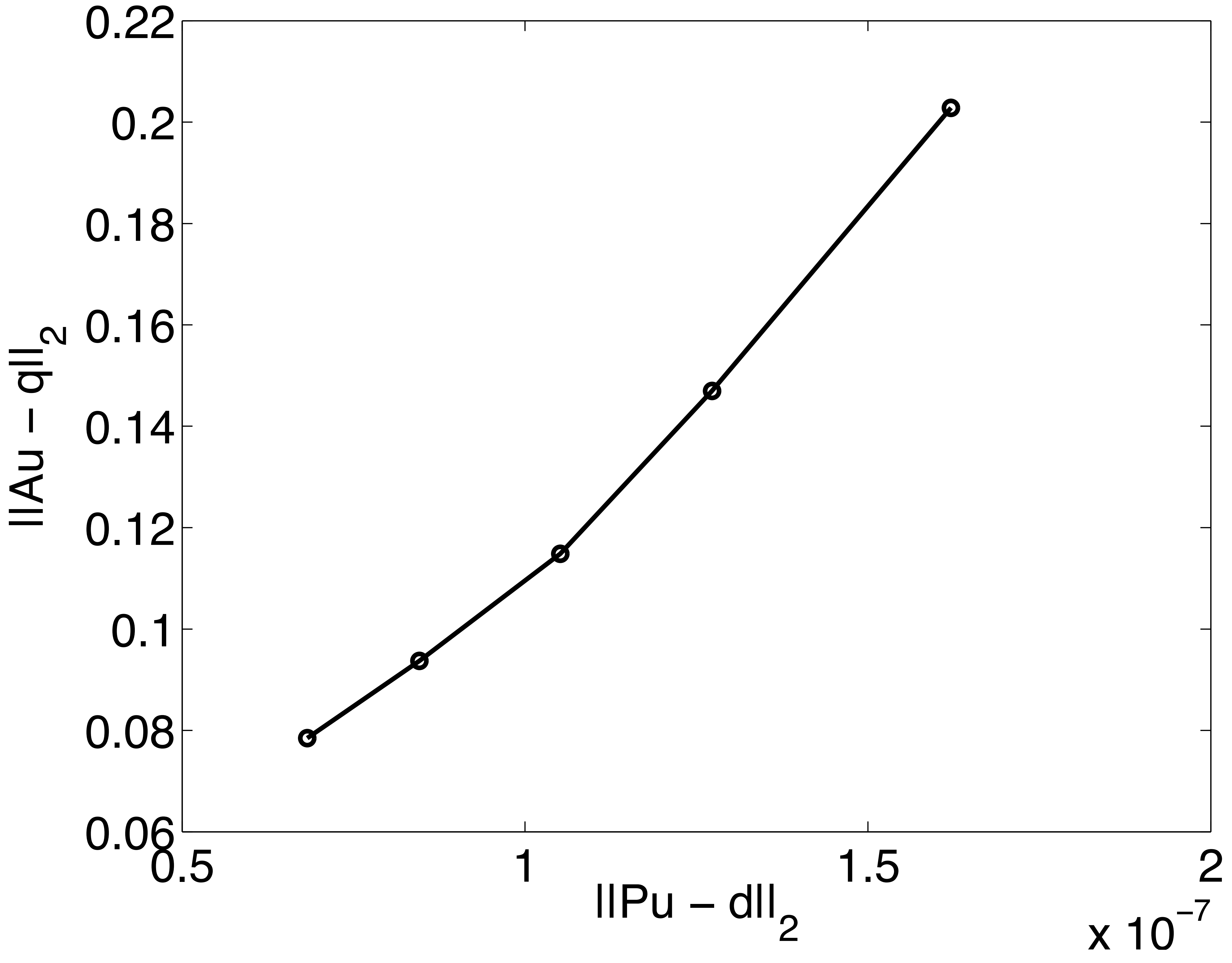
iteration 5



$$\mathbf{u}_4 = \left(P^*P + A_4^*A_4\right)^{-1}\left(P^*\mathbf{d} + A_4^*\mathbf{q}\right)$$

$$\mathbf{m}_5 = \mathrm{diag}(|\mathbf{u}_4|^2)^{-1}\mathrm{diag}(\mathbf{u}_4)^*\left(\mathbf{q} - L\mathbf{u}_4\right)$$

Convergence
in terms of *data*-fit & *PDE*-fit



Outline

PDE-constrained optimization

- *full* & *reduced*-space approaches
- KKT system & adjoint formulation

Penalty formulation

- *augmented* system
- gradient & GN Hessian

Numerical examples

Future work & conclusions

PDE-*constrained* optimization
multi-experiment data

$$\min_{\mathbf{m},\mathbf{u}} \sum_{i=1}^{M} \frac{1}{2}\|P_i\mathbf{u}_i - \mathbf{d}_i\|_2^2 \quad \text{subject to} \quad A_i(\mathbf{m})\mathbf{u}_i = \mathbf{q}_i, \quad i = 1\cdots M,$$

- wavefields collected in $\mathbf{u} = [\mathbf{u}_1; \cdots ; \mathbf{u}_M]$ are typically *much bigger* than $\mathbf{m}$
- *solving* these problems for *large* models & large *M* is
  - *computationally* expensive
  - requires *lots* of *RAM* to store wavefields for *each* source

All-at-once approach [Haber & Asher ’01]

Cast into *Lagrangian form*

adjoint wavefields

$$\min_{\mathbf{m},\mathbf{u},\mathbf{v}} \mathcal{L}(\mathbf{m},\mathbf{u},\mathbf{v}) = \sum_{i=1}^{M} \frac{1}{2}\|P_i\mathbf{u}_i - \mathbf{d}_i\|_2^2 + \langle \mathbf{v}_i, A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i\rangle$$

Solve by *iterations* on *sparse* KKT system

$$\begin{pmatrix} * & * & G^* \\ * & P^*P + * & A \\ G & A & 0 \end{pmatrix} \begin{pmatrix} \delta\mathbf{m} \\ \delta\mathbf{u} \\ \delta\mathbf{v} \end{pmatrix} = - \begin{pmatrix} G^*\mathbf{v} \\ A^*\mathbf{v} + P^*(P\mathbf{u} - \mathbf{d}) \\ A\mathbf{u} - \mathbf{q} \end{pmatrix}$$

* higher order terms

All-at-once approach

Involves actions of *block*-diagonal matrices $A,\ P,\ G$ with

$$G_i(\mathbf{m}, \mathbf{u}_i) = \frac{\partial A_i(\mathbf{m})\mathbf{u}_i}{\partial \mathbf{m}}$$

Pros:

- *no* explicit PDE solves
- iterations w/ *sparse* (KKT) system
- GN Hessian is *sparse*
- search-space *expansion* – *mitigates* local *minima*
- *"more"* linear in $\mathbf{m}$

Cons:

- introduces *extra* variable
- *indefinite* system so *challenge* to *precondition*
- requires *simultaneous* access= storage of *forward & adjoint wavefields* for *all* sources
- That's a show *stopper*...

Reduced approach

[A. Tarantola & Valette ‘82; Plessix ’06; Epanomeritakis et al. ‘08]

For each $i = 1 \cdots M$ experiments *eliminate* the PDE *constraint*–i.e,.

$$\min_{\mathbf{m}} \phi_{\mathrm{red}}(\mathbf{m}) = \sum_{i=1}^{M} \frac{1}{2} \| P_i A_i(\mathbf{m})^{-1} \mathbf{q}_i - \mathbf{d}_i \|_2^2$$

Solve by *accumulating* gradients

$$\nabla \phi_{\mathrm{red}}(\mathbf{m}) = \sum_{i=1}^{M} G_i(\mathbf{m}, \mathbf{u}_i)^* \mathbf{v}_i$$

$$= \sum_{i=1}^{M} \omega_i^2 \mathrm{diag}(\mathbf{u}_i)^* \mathbf{v}_i$$

Reduced approach

Involves solutions of *forward* & *adjoint* for $i = 1 \cdots M$

$$\begin{aligned} A_i(\mathbf{m})\mathbf{u}_i &= \mathbf{q}_i \\ A_i(\mathbf{m})^*\mathbf{v}_i &= -P_i^*(P_i\mathbf{u}_i - \mathbf{d}_i) \end{aligned}$$

Accumulate reduced GN Hessian

$$\nabla^2\phi_{\mathrm{red}}(\mathbf{m}) \approx H_{GN} = \sum_{i=1}^{M} G_i^* A_i^{-*} P_i^T P_i A_i^{-1} G_i$$

Pros:

- *no* need to have *simultaneous* access to *all* wavefields
- *accumulate* gradients & Hessians
- *adjoint*-state method has *intuitive* interpretation

Cons:

- PDEs need to be solved *explicitly*
- Jacobian & GN Hessian are *dense* matrices
- *smaller* search space – *local* minima
- *highly* nonlinear in $\mathbf{m}$

Challenge

Can we find an *alternative* approach that has *best* of both *worlds*?

- *expanded* search space as in all-at-once method w/o needing *simultaneous* access to *all* wavefields for each *iteration*
- *sparse* matrices
- *mundane* nonlinearity
- *accumulation* of *gradients* & GN *Hessians*

Probabilistic argument

In Tarantola's formulation the least-squares misfit ϕ_{reduced}

- allows for *errors* in the data *residual*
- *but,* considers wave-equation *physics* as *infallible*

Instead, we consider both *physics* & *observed* data as *fallible*...

- *least-squares* penalties for *model* & *data* errors

New approach [van Leeuwen & FJH '13]

Penalty formulation:

$$\min_{\mathbf{m},\mathbf{u}} \phi_\lambda(\mathbf{m},\mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2}\|P_i\mathbf{u}_i - \mathbf{d}_i\|_2^2 + \frac{\lambda^2}{2}\|A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i\|_2^2$$

Solution coincides [Bertsekas '96] with solution of original *constrained* formulation as $\lambda \uparrow \infty$

Penalty approach

For each $i = 1 \cdots M$ *eliminate* the wavefield by solving $\nabla_{\mathbf{u}_i} \phi_\lambda(\mathbf{m}, \mathbf{u}_i) = 0$

Define *modified* objective

$$\phi_{\text{pen}}(\mathbf{m}) = \overline{\phi}_\lambda(\mathbf{m}, \overline{\mathbf{u}}(\mathbf{m}))$$

Calculate derivates

$$\nabla \phi_{\text{pen}} = \nabla_{\mathbf{m}} \overline{\phi}_\lambda$$

$$\nabla^2 \phi_{\text{pen}} = \nabla^2_{\mathbf{m}} \overline{\phi}_\lambda - \nabla^2_{\mathbf{m},\mathbf{u}} \overline{\phi}_\lambda \left(\nabla^2_{\mathbf{u}} \overline{\phi}_\lambda \right)^{-1} \nabla^2_{\mathbf{u},\mathbf{m}} \overline{\phi}_\lambda$$

(*all* evaluated at *optimal* $\overline{\mathbf{u}}$)

SLIM

Penalty approach

A *local* minimizer of $\phi_{\mathrm{pen}}(\mathbf{m})$, together with the corresponding $\overline{\mathbf{u}}$ are also *local* minimizers of $\overline{\phi}_{\lambda}(\mathbf{m}, \overline{\mathbf{u}}(\mathbf{m}))$ and *vice versa*.

Penalty approach

Solve for *wavefields* by *inverting*

$$\min_{\mathbf{u}_i} \left\| \begin{pmatrix} P_i \\ \lambda A_i(\mathbf{m}) \end{pmatrix} \mathbf{u}_i - \begin{pmatrix} \mathbf{d}_i \\ \lambda \mathbf{q}_i \end{pmatrix} \right\|_2^2$$

Compute gradient–***no*** adjoint wavefield required!

$$\nabla \phi_{\mathrm{pen}}(\mathbf{m}) = G(\mathbf{m}, \overline{\mathbf{u}})^* (A(\mathbf{m})\overline{\mathbf{u}} - \mathbf{q})$$

GN–Hessian

$$\begin{aligned} \nabla^2 \phi_{\mathrm{pen}}(\mathbf{m}) = \lambda^2 G^* G \\ + \lambda^4 G^* A \left(P^* P + \lambda^2 A^* A\right)^{-1} A^* G \end{aligned}$$

Penalty approach

Accumulate gradients

$$\nabla_{\mathbf{m}}\phi_{\text{pen}}(\mathbf{m},\overline{\mathbf{u}}) = \sum_{i=1}^{M} G_i(\mathbf{m},\overline{\mathbf{u}}_i)^* \left(A_i(\mathbf{m})\overline{\mathbf{u}}_i - \mathbf{q}_i\right)$$

Accumulate (approximate for small λ) Gauss-Newton Hessians:

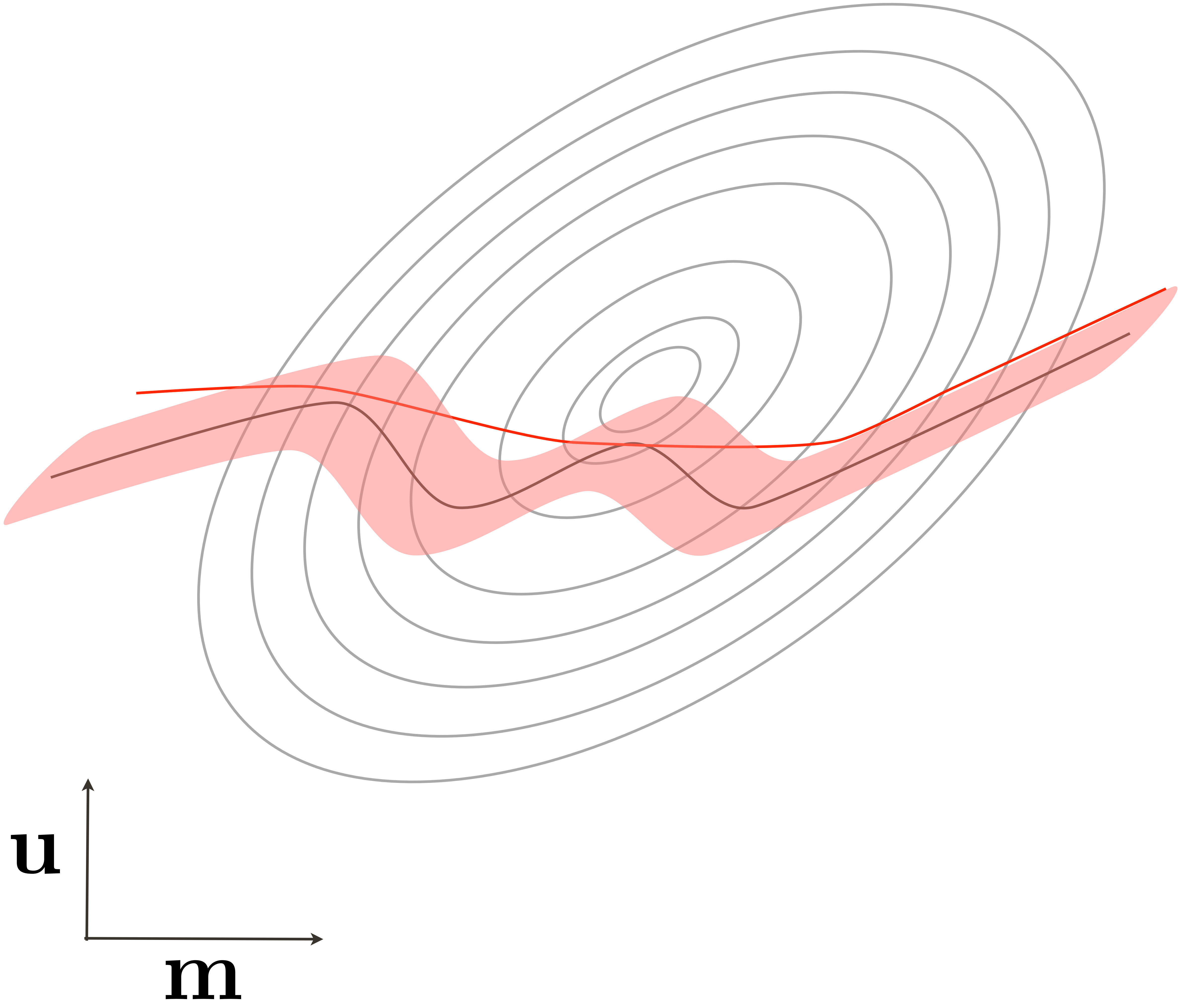
$$\nabla^2\phi_{\text{pen}}(\mathbf{m}) \approx \sum_{i=1}^{M} \lambda^2 G_i^* G_i$$

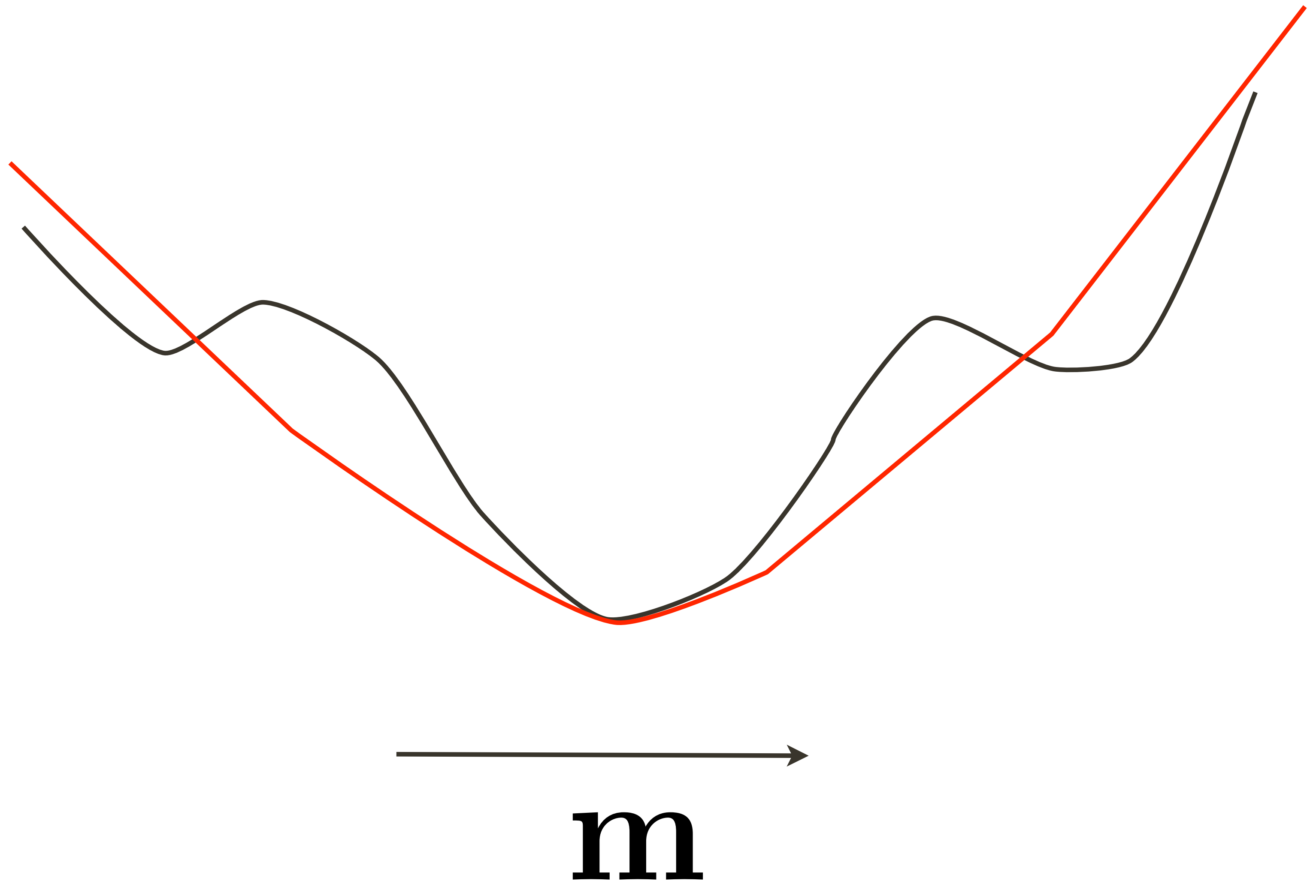
Penalty approach

Algorithm 1 FWI algorithm based on the penalty formulation

for $t = 0$ to N **do**
  $\mathbf{g}_t = 0$
  $H_t = 0$
  for $k = 1$ to N_f **do**
    for $l = 1$ to N_s **do**
      solve $\begin{pmatrix} \lambda_t A_k(\mathbf{m}_t) \\ P \end{pmatrix} \mathbf{u}_{kl} = \begin{pmatrix} \lambda_t \mathbf{q}_{kl} \\ \mathbf{d}_{kl} \end{pmatrix}$
      $\mathbf{g}_t = \mathbf{g}_t + \lambda_t^2 G_k(\mathbf{m}_t, \mathbf{u}_{kl})^* (A_k(\mathbf{m}_t)\mathbf{u}_{kl} - \mathbf{q}_{kl})$
      $H_t = H_t + \lambda_t^2 G_k(\mathbf{m}_t, \mathbf{u}_{kl})^* G_k(\mathbf{m}_t, \mathbf{u}_{kl})$
    end for
  end for
  solve $H_t \Delta\mathbf{m}_t = -\mathbf{g}_t$
  update $\mathbf{m}_{t+1} = \mathbf{m}_t + \Delta\mathbf{m}_t$
  update λ_t.
end for

Penalty vs. Reduced





Penalty vs. Reduced

Pros:

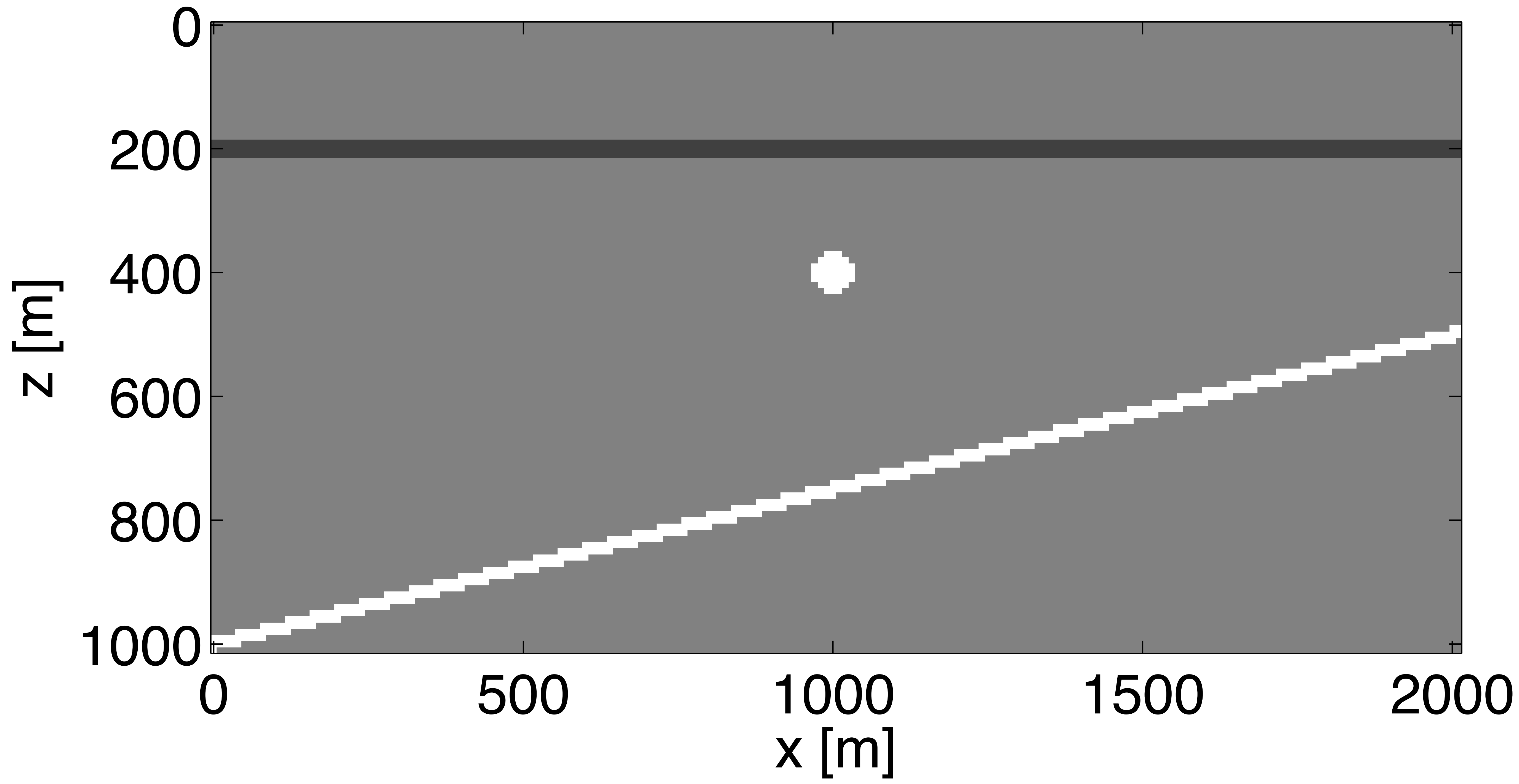
- *expansion* of *search* space
- *no* need to have *simultaneous* access to *all* wavefields for *each* iteration
- *no* adjoint wavefields
- *sparse* approximation of Hessian at *small* λ
- less *non*-linear in $\mathbf{m}$

Cons:

- *accurate* solutions of overdetermined *data*-augmented system
- cooling *strategy* for λ

Numerical examples

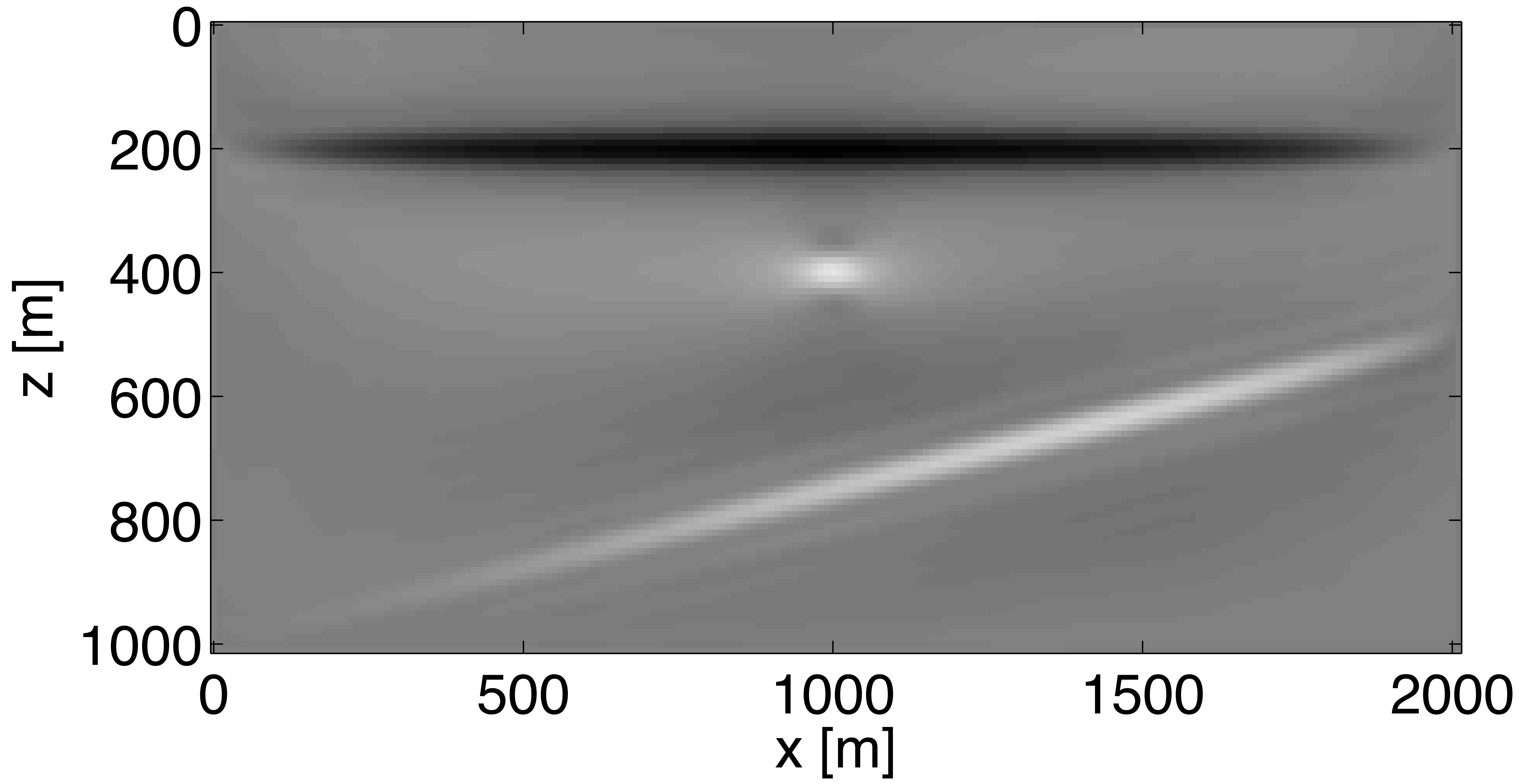
- Imaging
- Local minima
- Full-waveform inversion
- DC resistivity
- Optical tomography



Original image

Imaging

The *gradient* of the reduced objective yields an *image* of the subsurface..



RTM-migration

Imaging

***Conventional* RTM:**

1. solve forward wave-equation
2. solve adjoint wave-equation
3. apply `imaging condition’

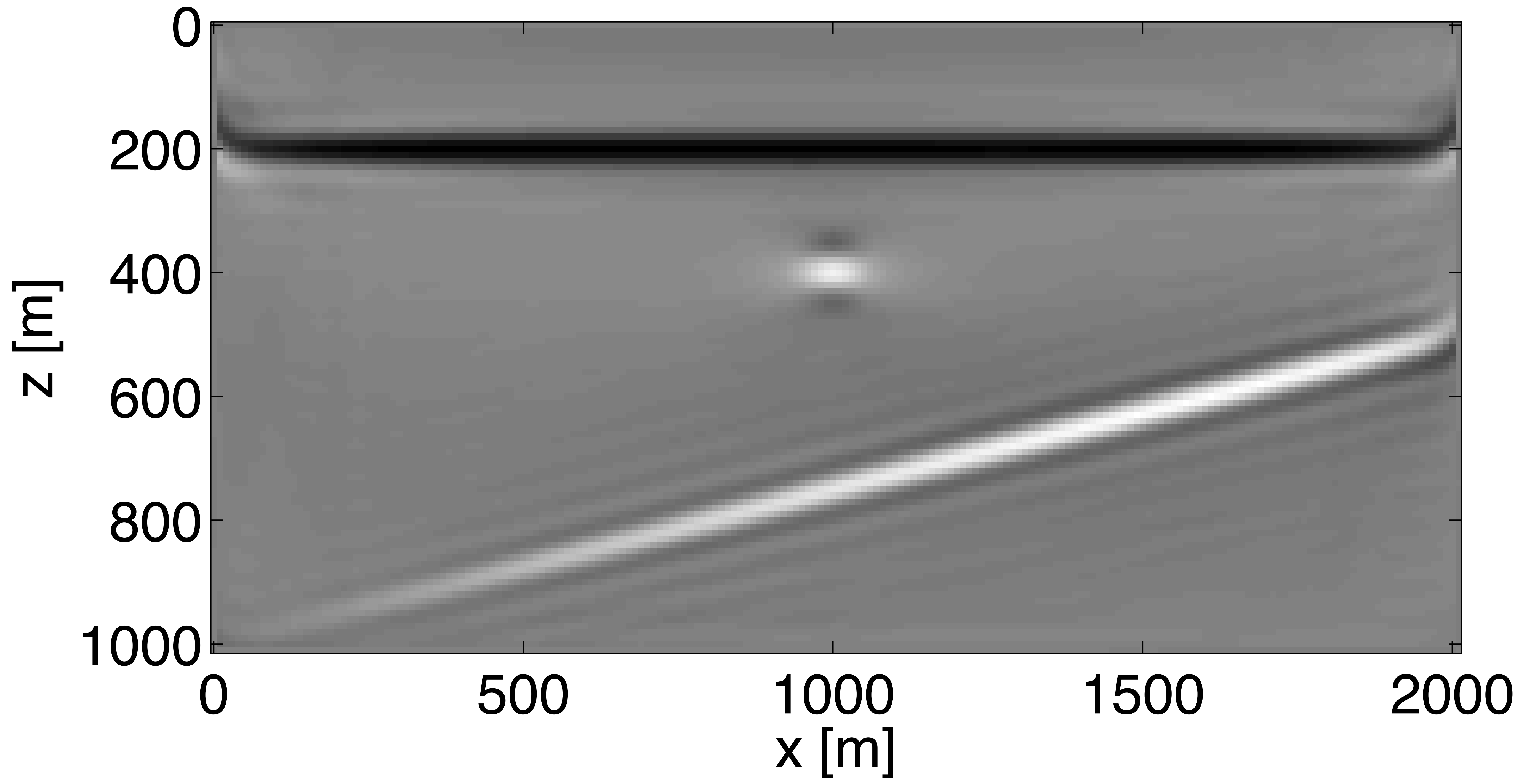


Image w/ penalty method

Imaging

***Penalty*-method reverse-time migration:**

1. solve overdetermined wave-equation
2. go for lunch
3. apply `imaging condition’

Penalty vs. reverse-time

Reverse-time migration w/ *adjoint* state:

$$\delta \mathbf{m}_{\mathrm{red}} = \sum_{i=1}^{M} \omega_i^2 \mathrm{diag}(\mathbf{u}_i)^* \mathbf{v}_i$$

$$\mathbf{v}_i := \overbrace{A_i(\mathbf{m})^{-*}\left(P_i^*(\mathbf{d}_i - P_i\mathbf{u}_i)\right)}^{\text{back prop. data residue}}$$

$$H_{\mathrm{red}}^{GN} = \sum_{i=1}^{M} G_i^* A_i^{-*} P_i^T P_i A_i^{-1} G_i$$

"*Forward*"–time migration w/ penalty formulation

$$\delta \mathbf{m}_{\mathrm{pen}} = \lambda^2 \sum_{i=1}^{M} \omega_i^2 \mathrm{diag}(\mathbf{u}_i)^* \delta \mathbf{u}_i$$

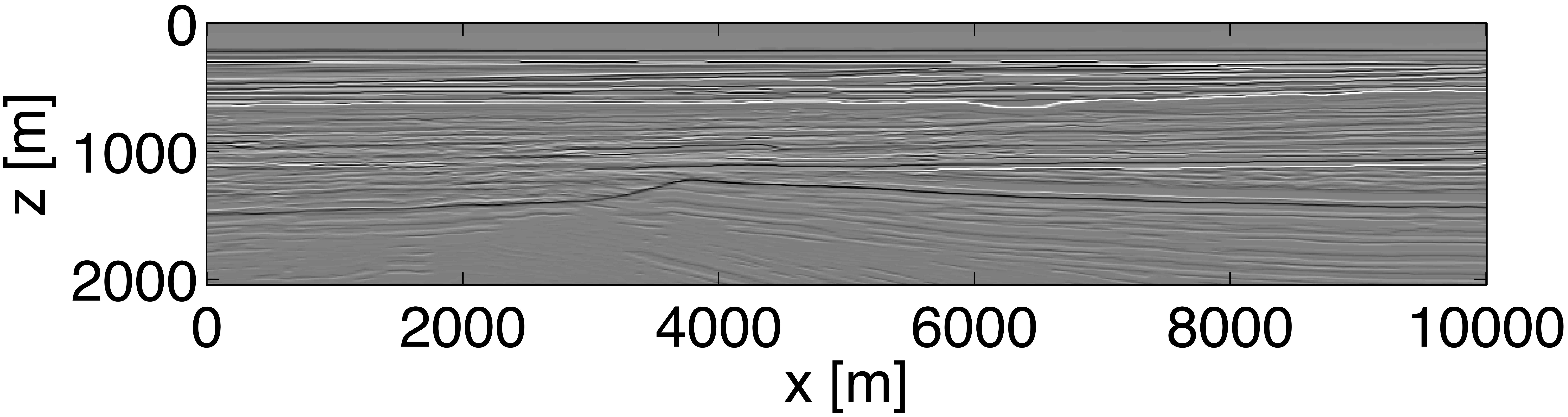
$$\delta \mathbf{u}_i := \overbrace{\left(A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i\right)}^{\text{PDE residue}}$$

with *trivial* sparse GN–Hessian

$$H_{\mathrm{pen}}^{GN} = \lambda^2 \sum_{i=1}^{M} \omega_i^4 \mathrm{diag}(\mathbf{u}_i)^* \mathrm{diag}(\mathbf{u}_i)$$

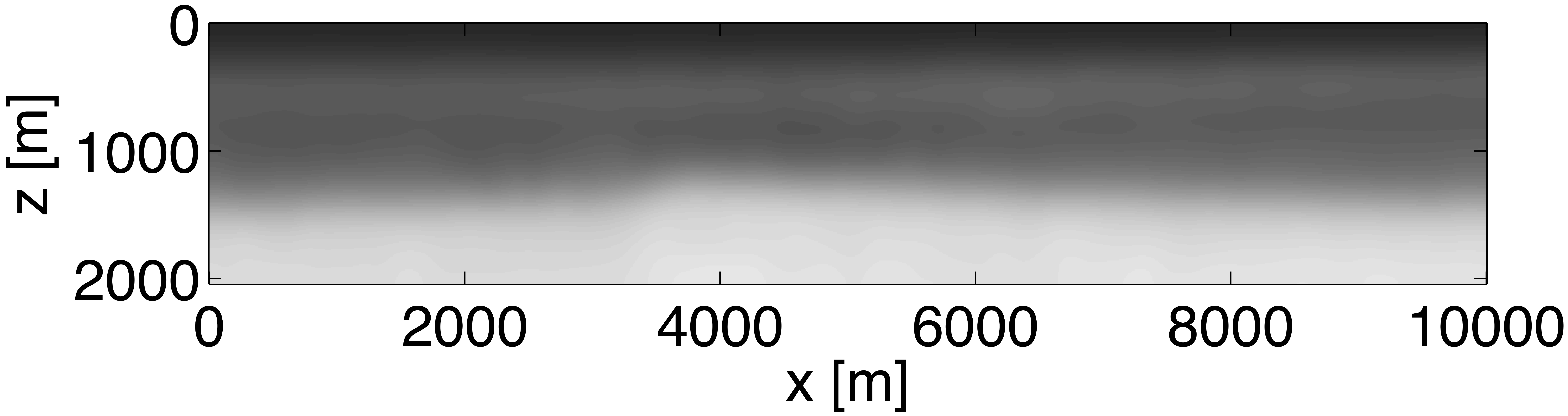
Imaging
[BG Compass model]

Perturbation
model grid spacing: 10m
inversion crime
split spread w/ 50m source & receiver spacing
57 frequencies 2-30Hz



Imaging

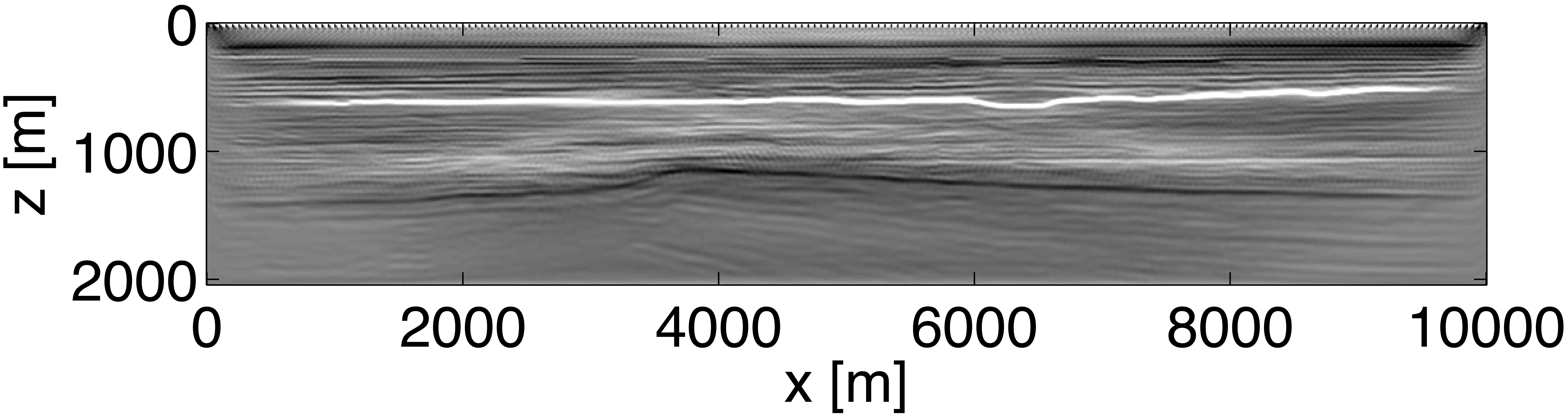
Background model



Imaging

Conventional **RTM:**

1. solve forward wave-equation
2. solve adjoint wave-equation
3. apply `imaging condition’



Imaging

***Penalty*-method reverse-time migration:**

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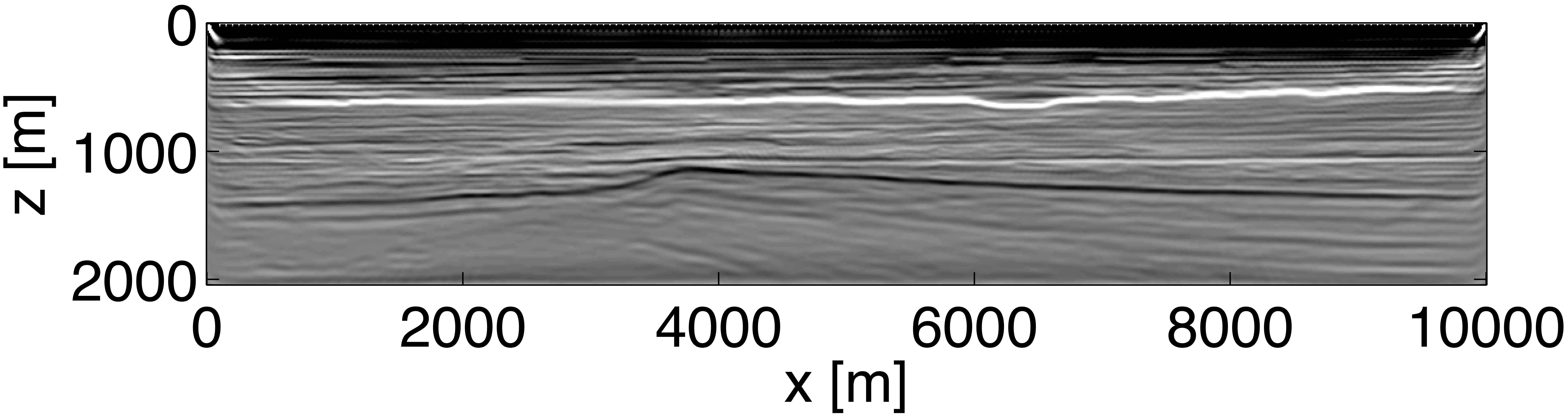

Imaging
[BG Compass model]

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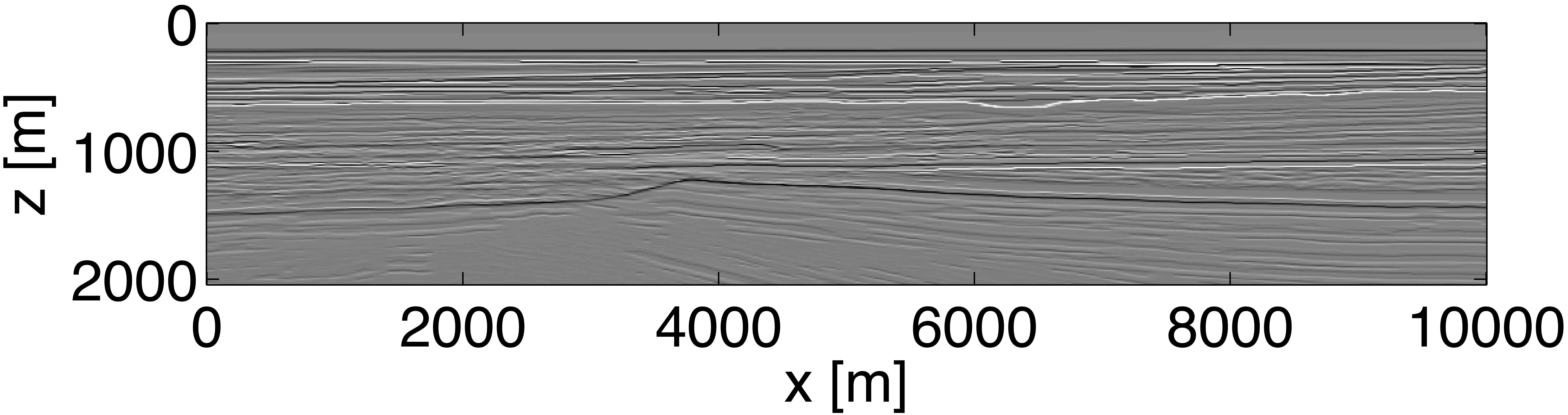
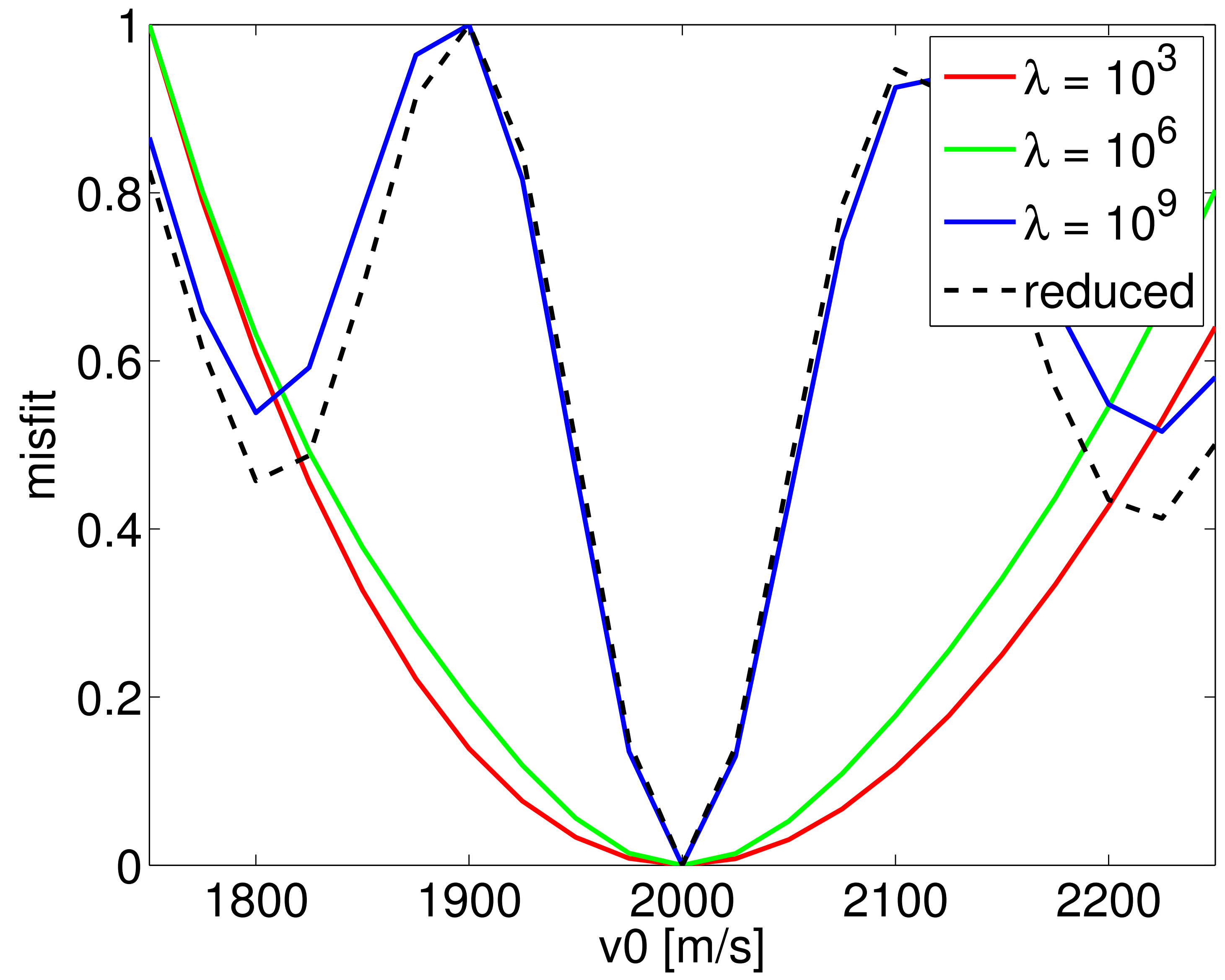
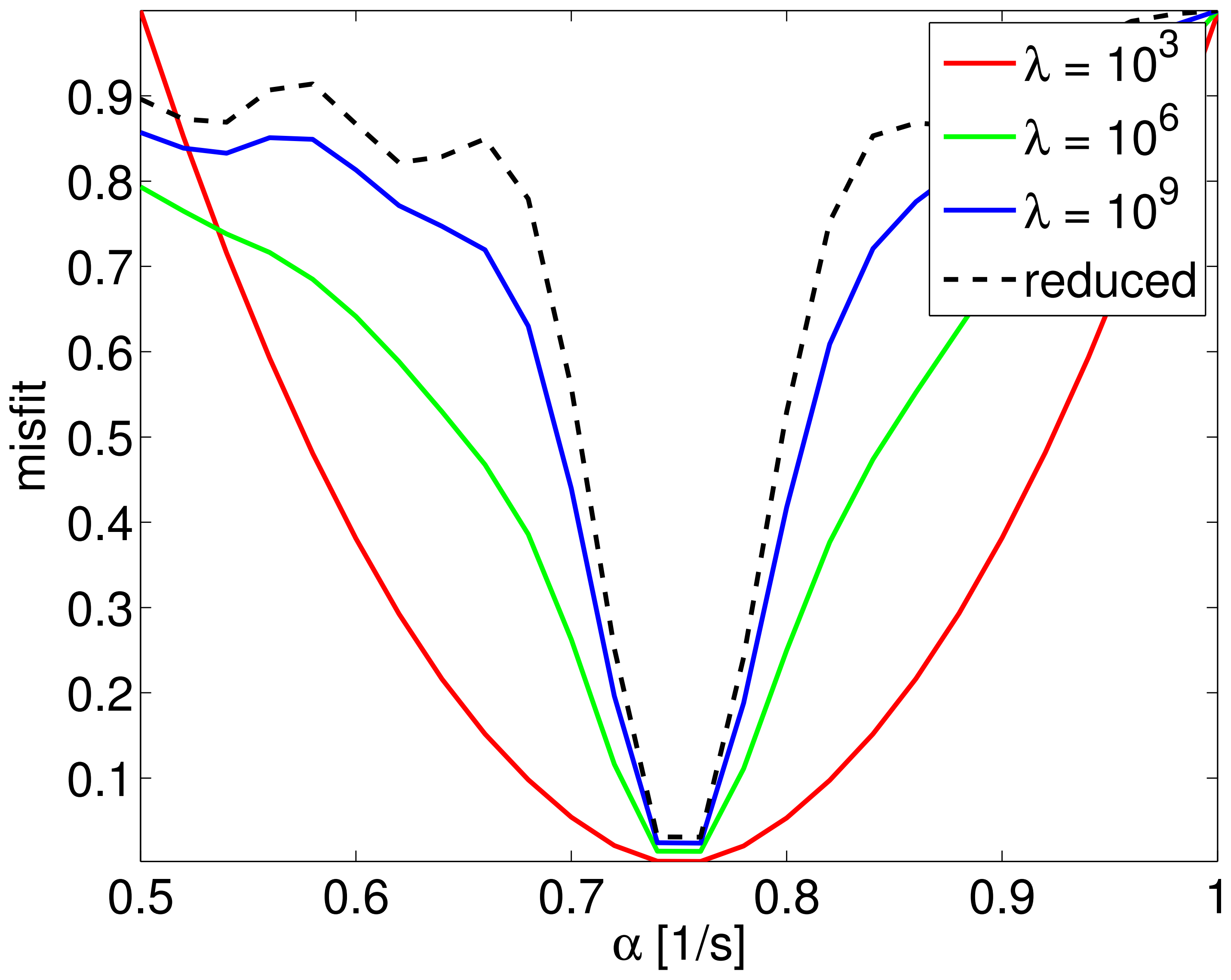


Local minima

single shot, single frequency data for *linear* velocity profile $v(z) = v_0 + \alpha z$, misfit as function of (v_0, α)



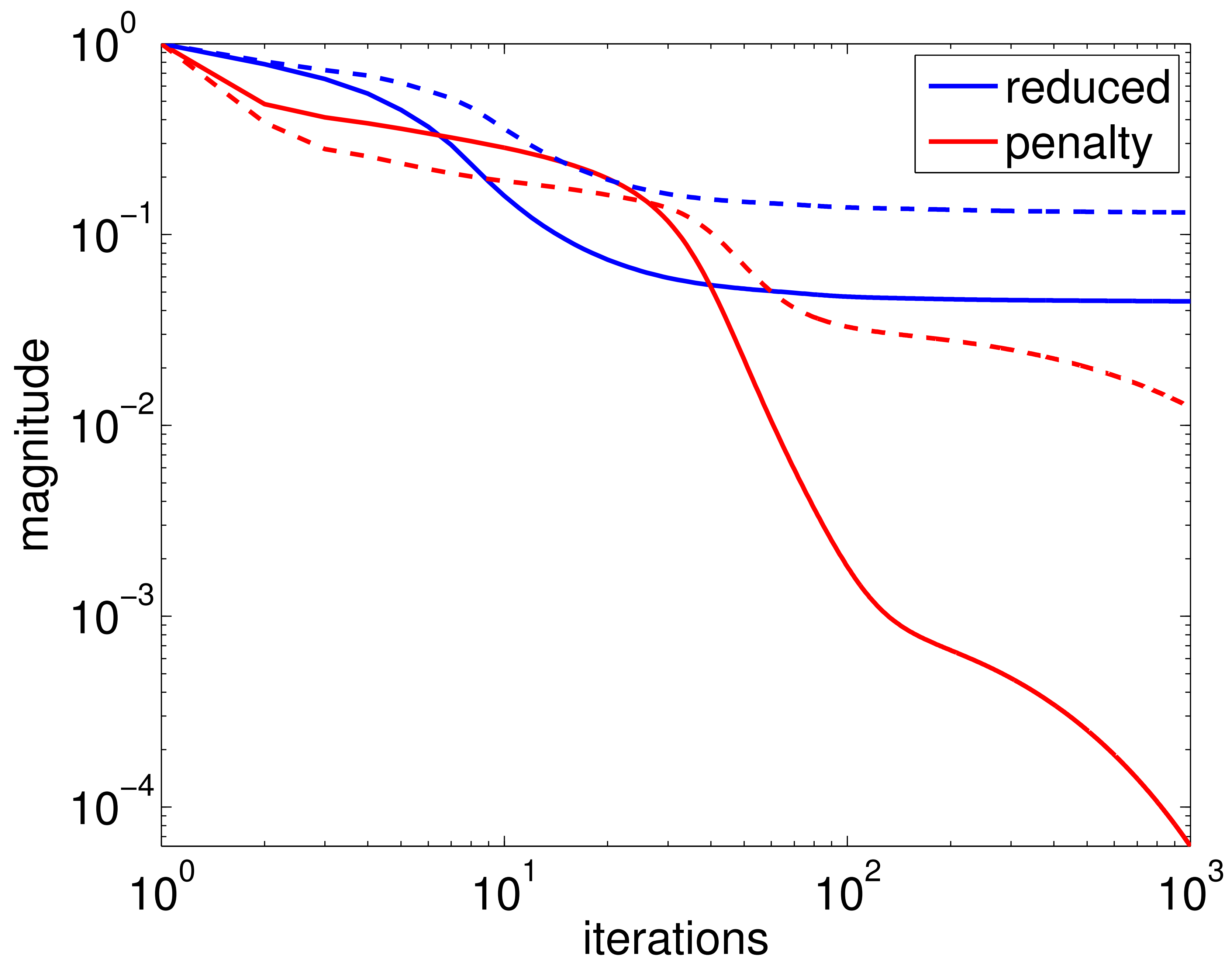
constant



slope

Local minima

Invert *single* shot, *single* frequency data for 1D velocity profile using *steepest* descent.

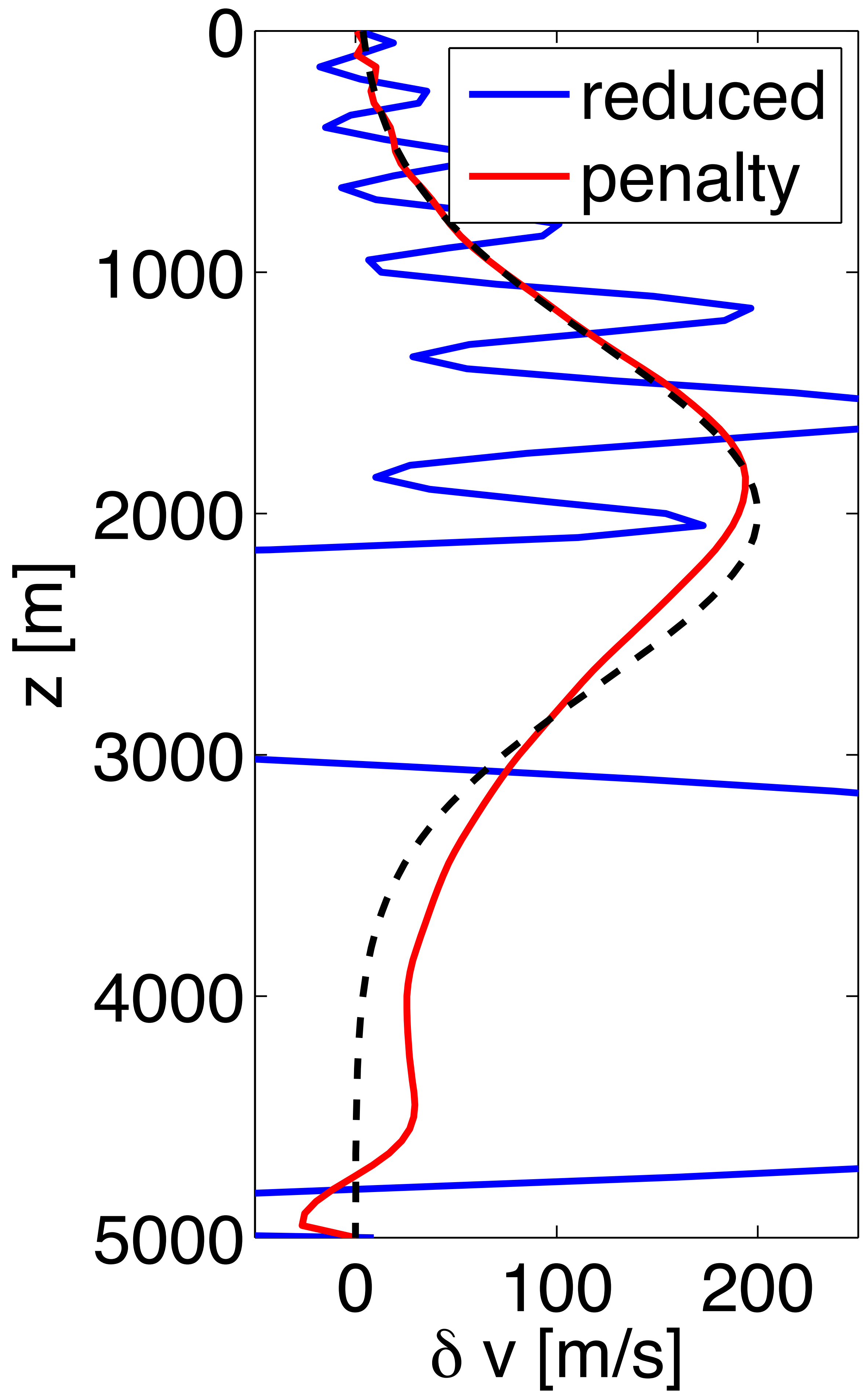


- misfit

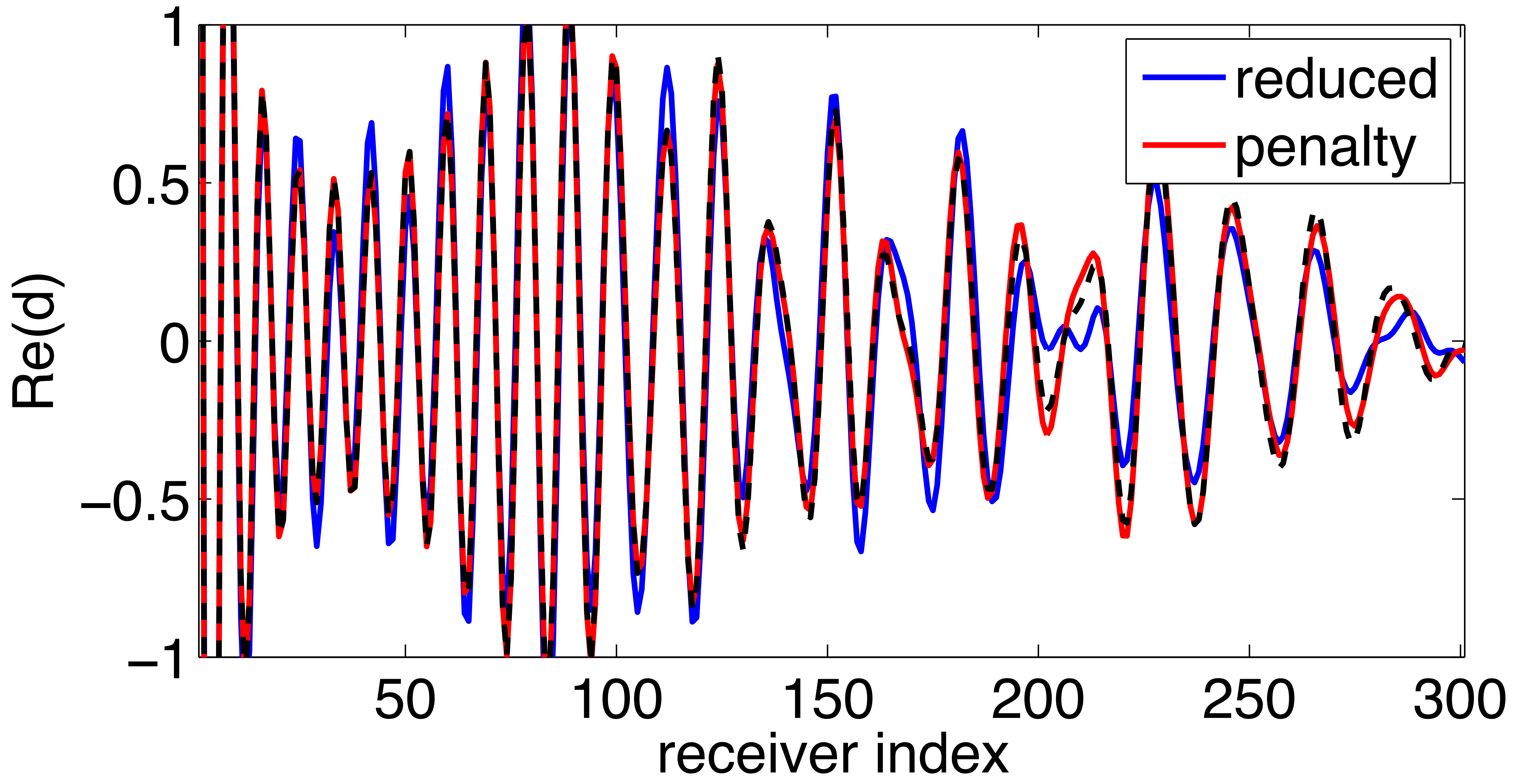
-- gradient

misfit & gradient as function # iterations

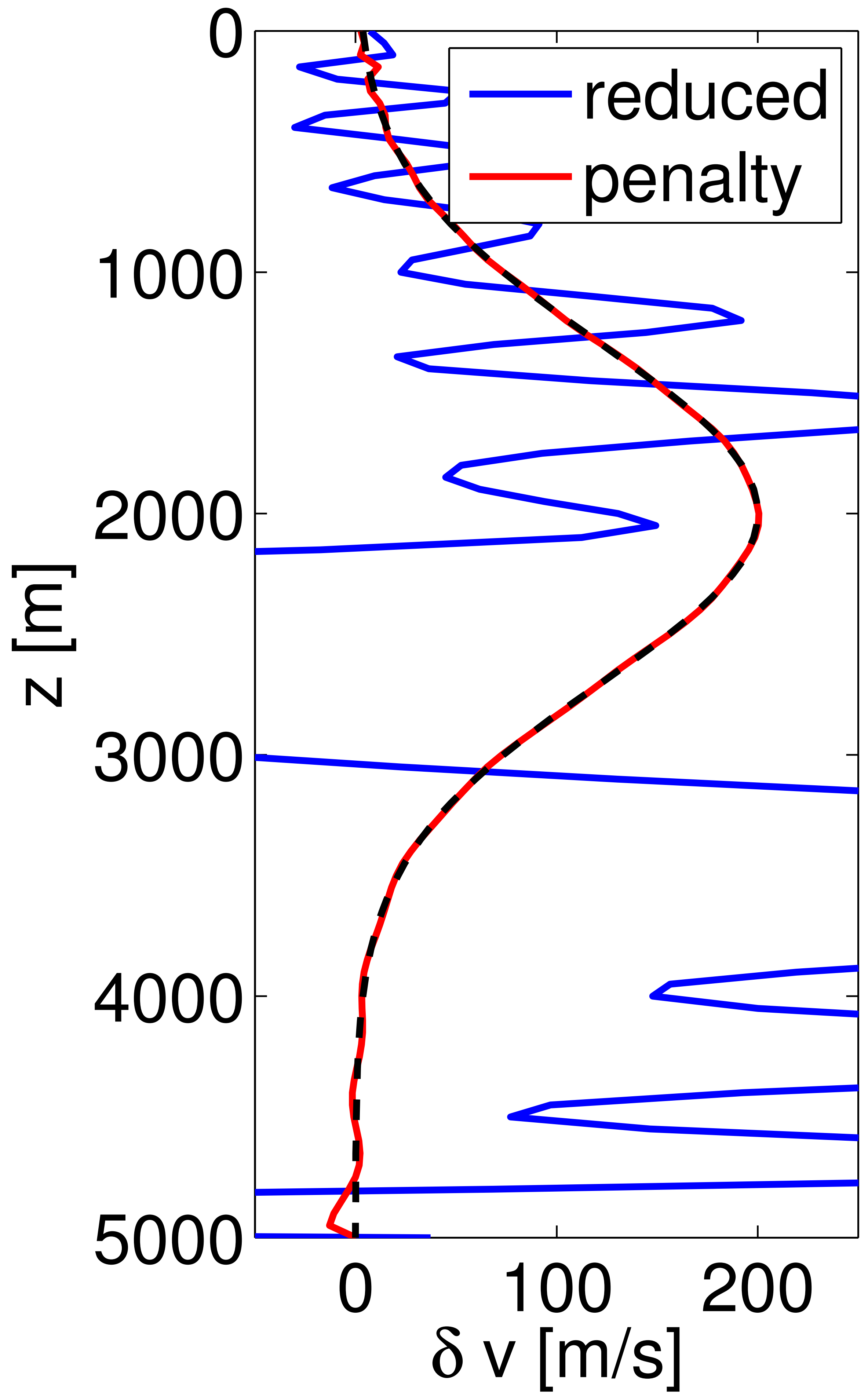
Local minima



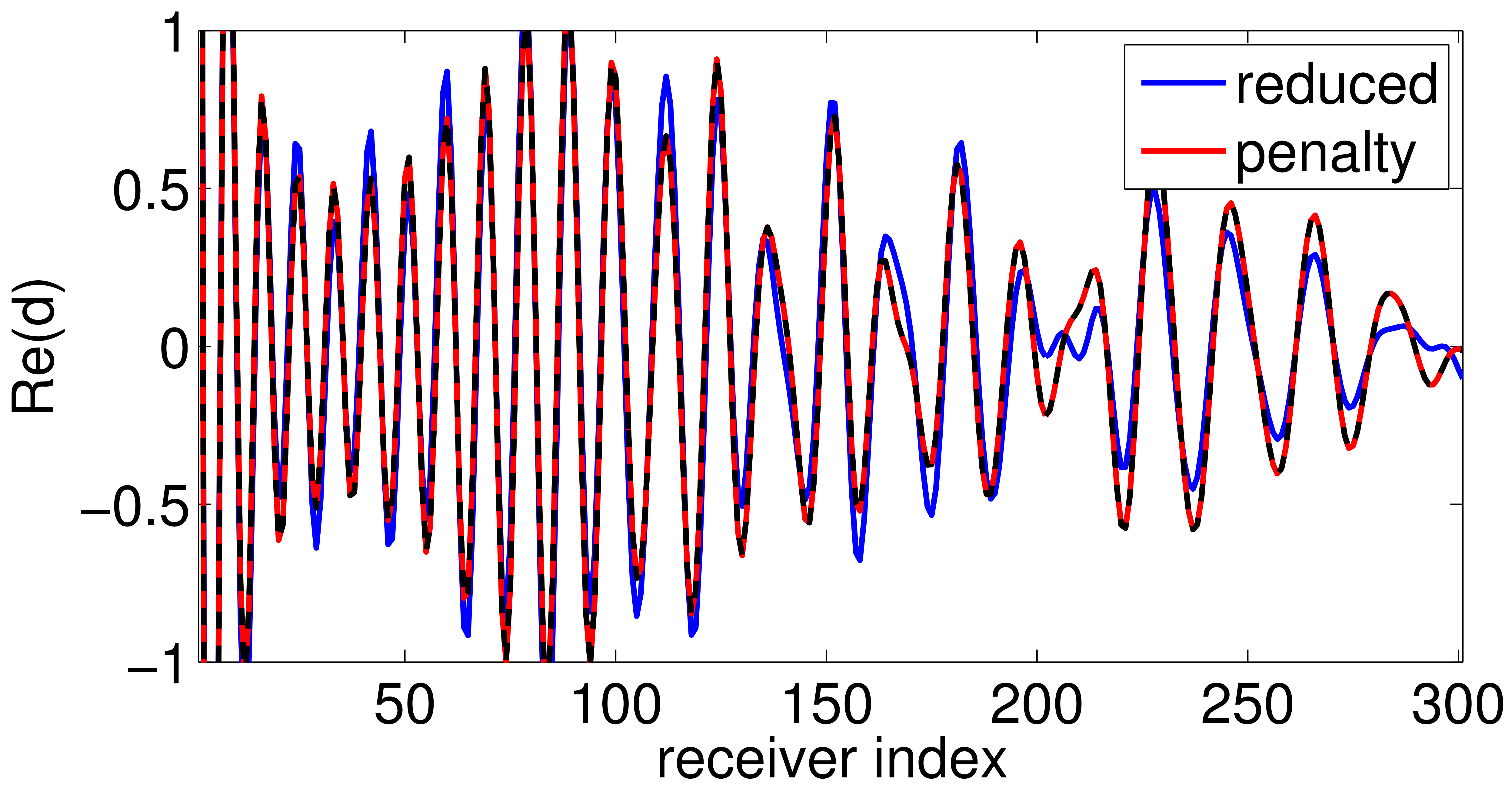
After 100 iterations



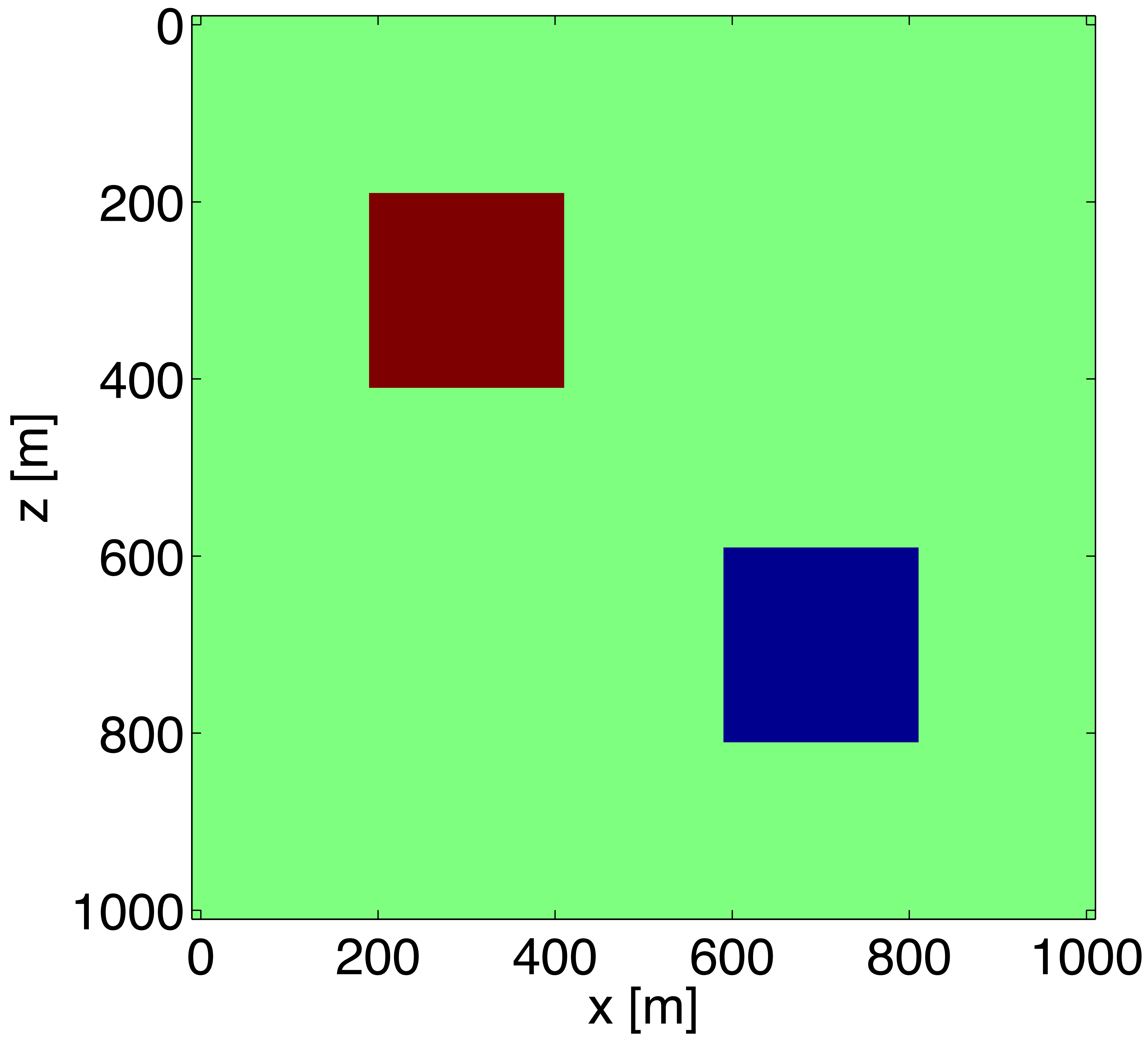
Local minima



After 1000 iterations



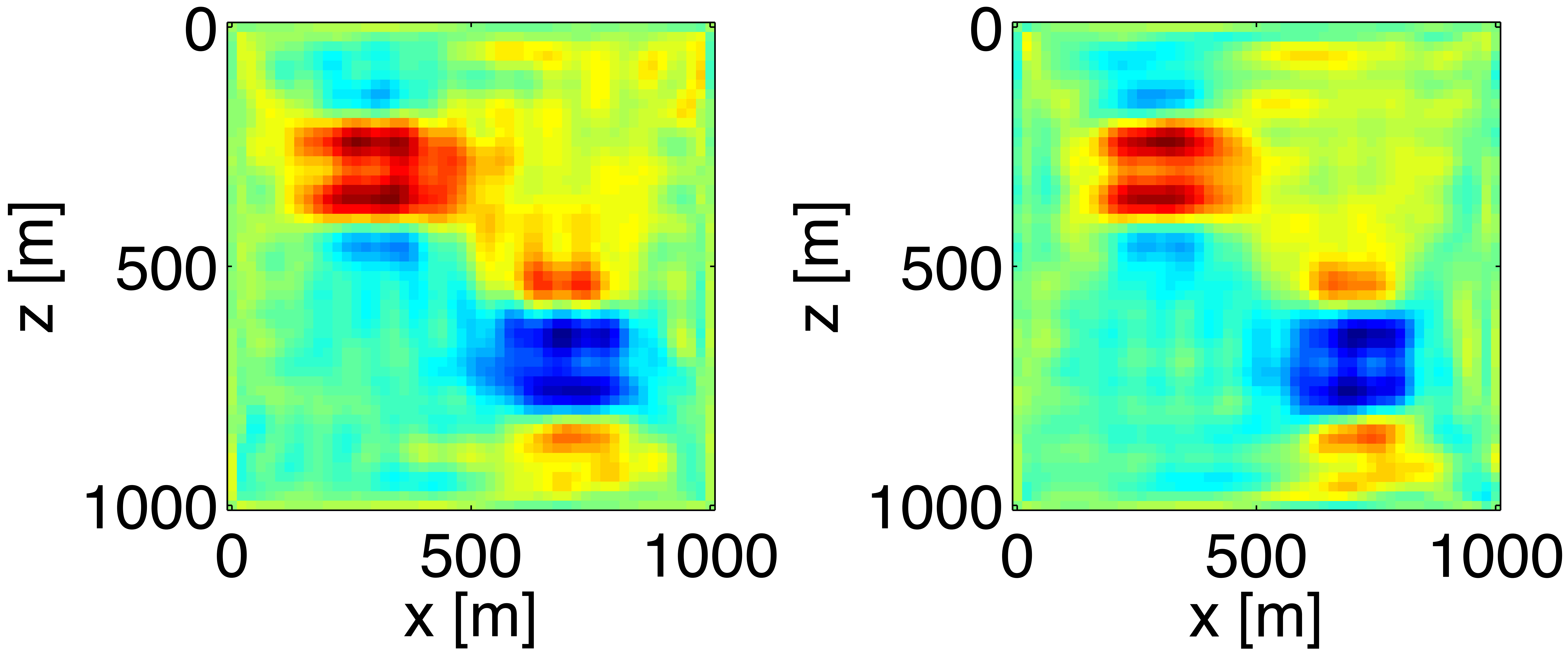
Cross well



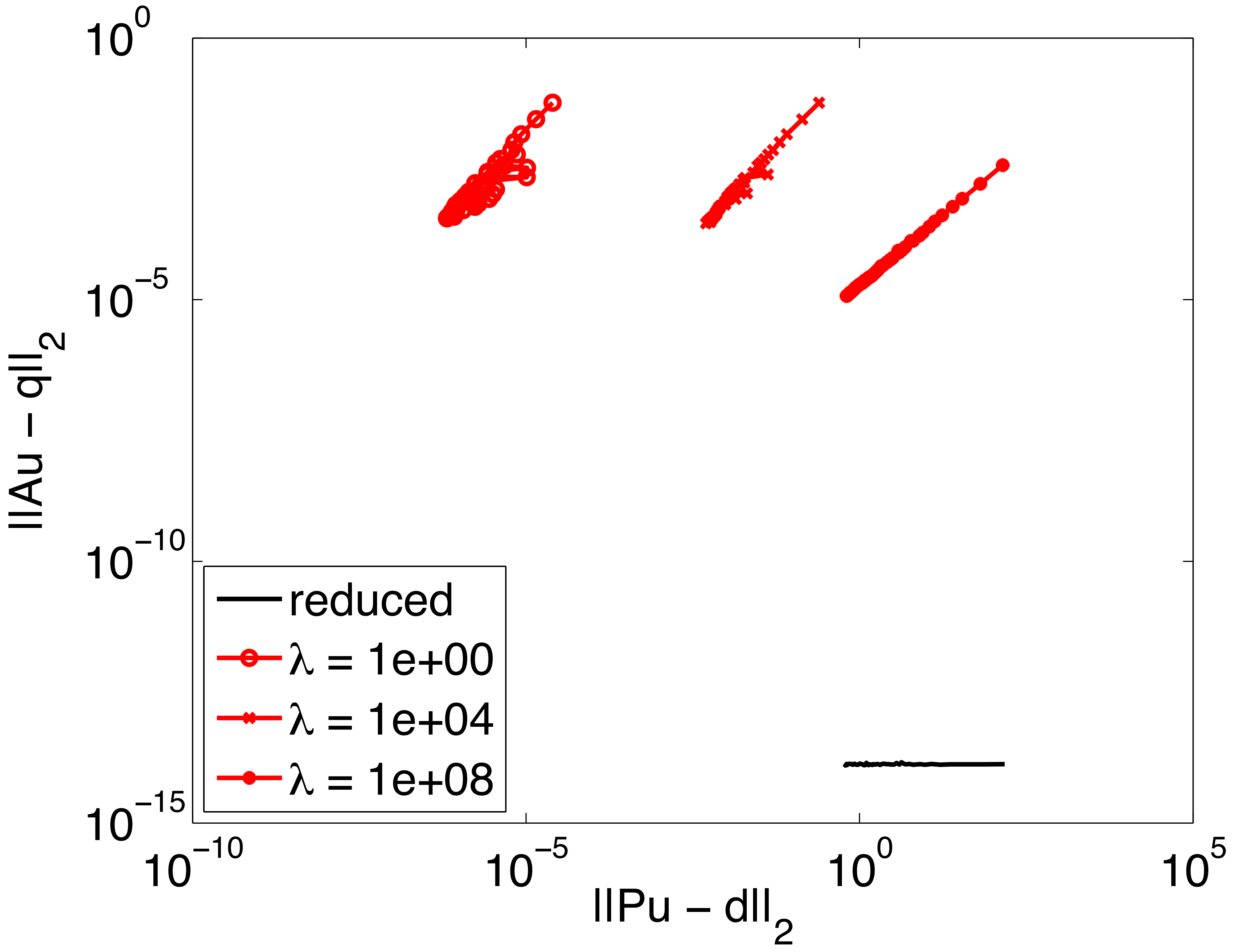
original medium

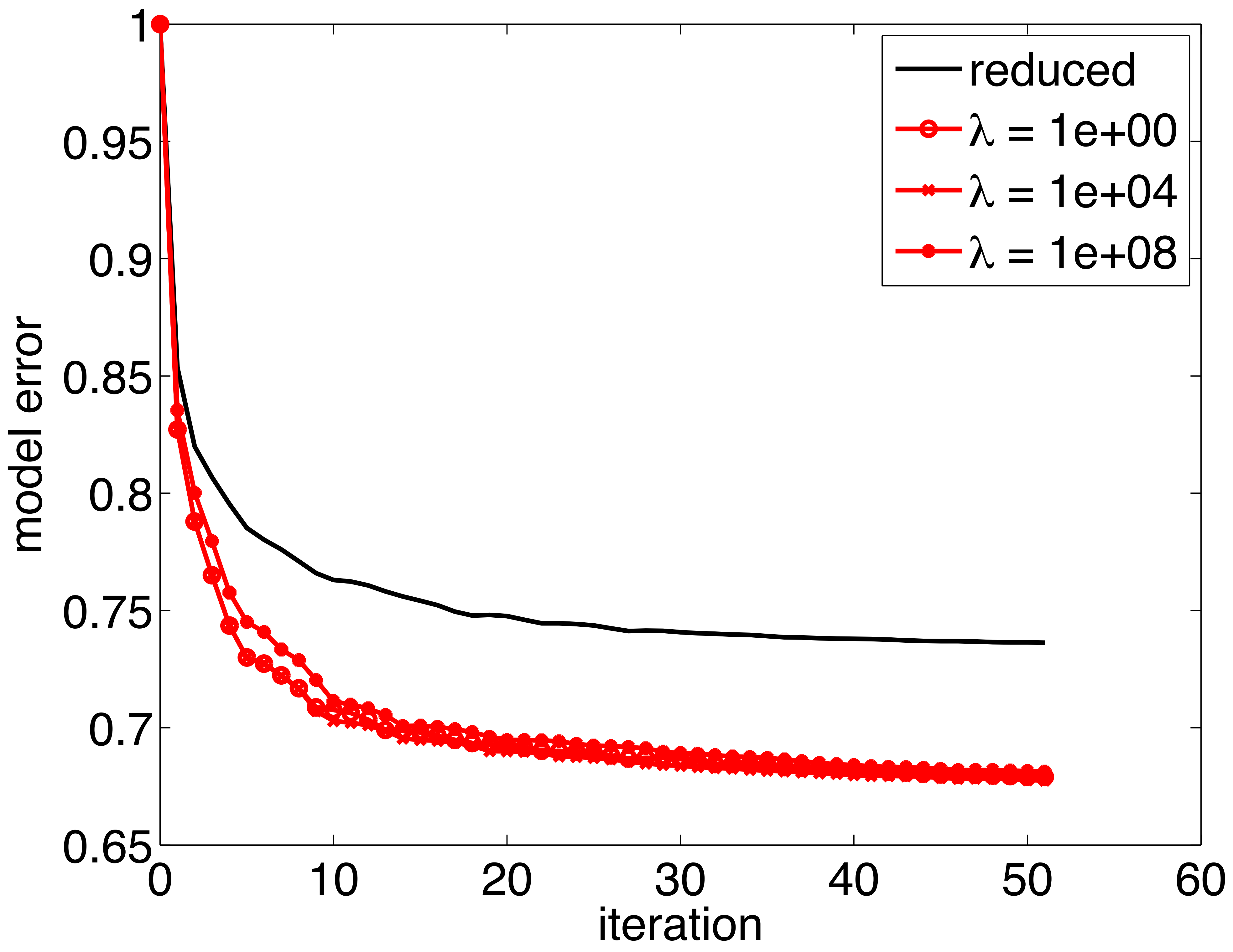
- 2D cross-well configuration
- 5 point Helmholtz FD operator with abc
- Direct solver for PDEs (A\b)
- invert a single frequency (10 Hz)
- L-BFGS

Cross well FWI

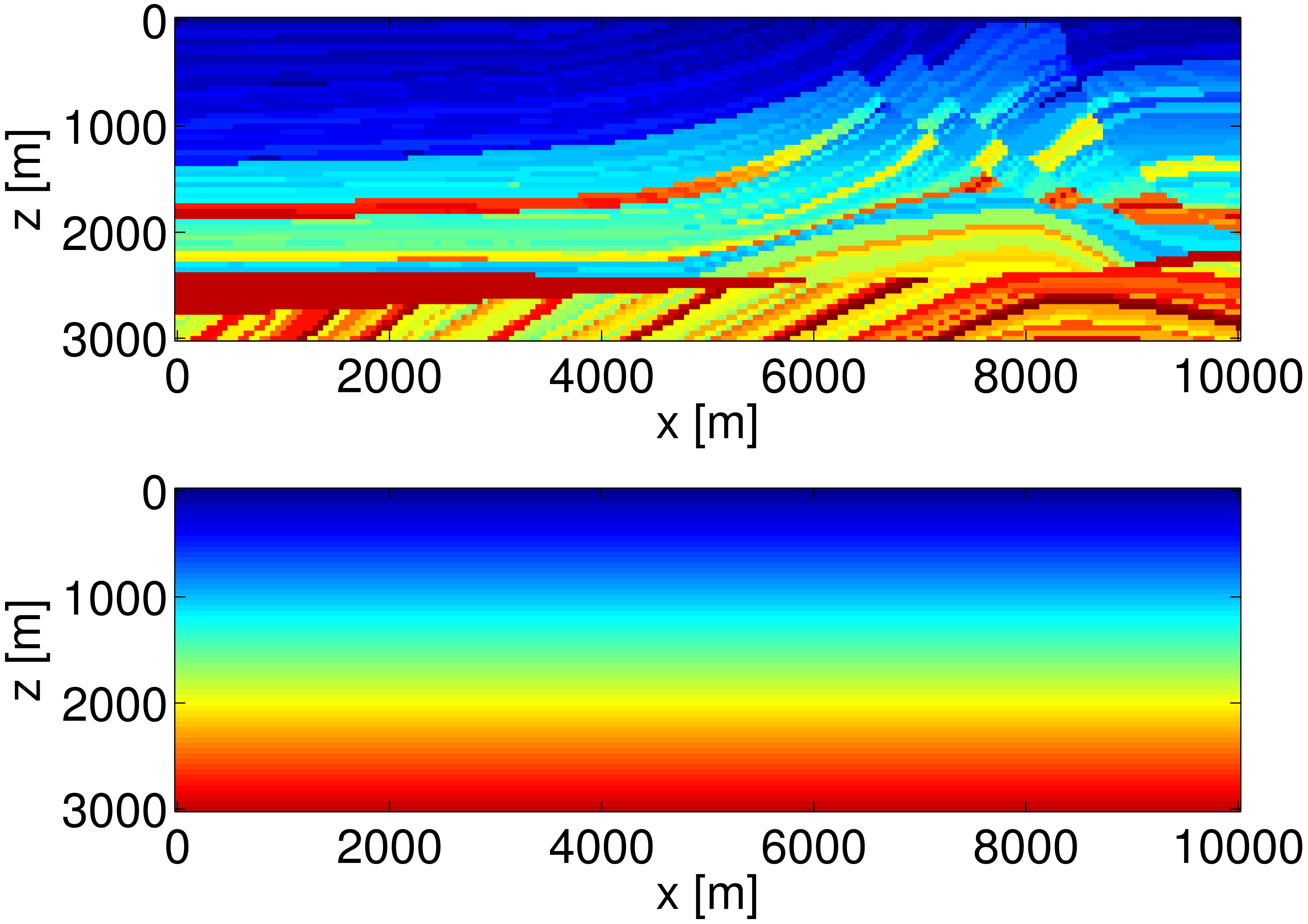


Cross well FWI





Waveform inversion



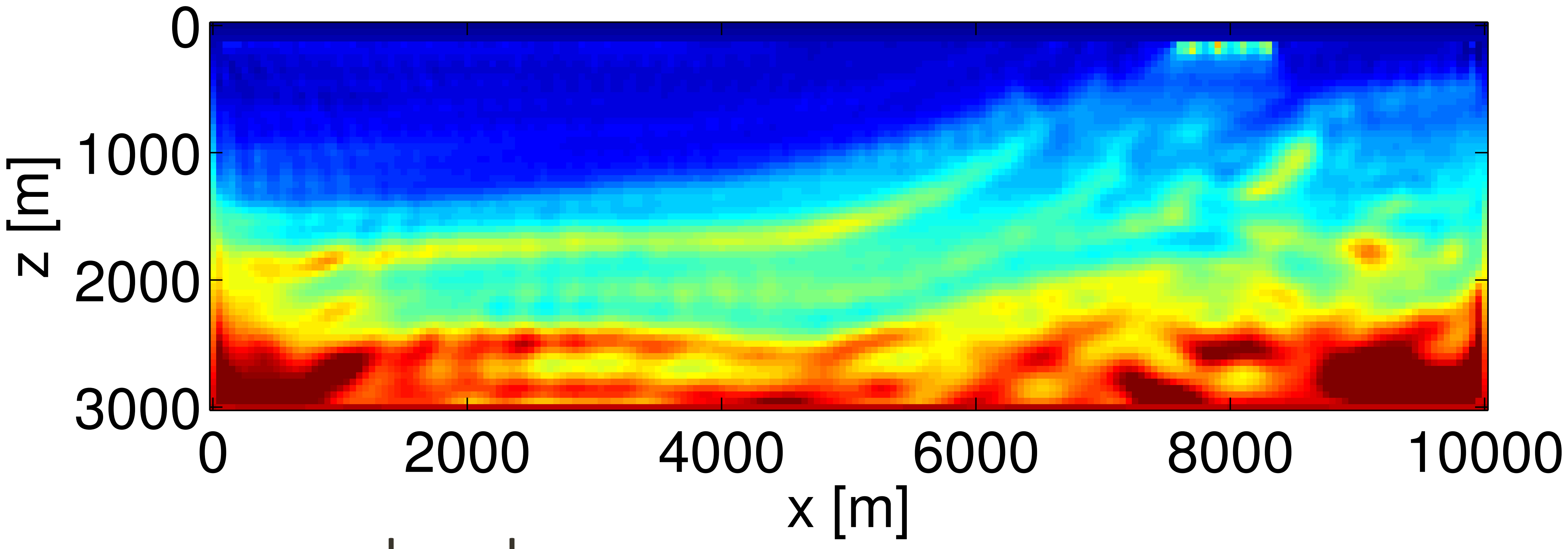
original + initial model

- 2D reflection configuration
- 5 point Helmholtz FD operator with abc
- Direct solver for PDEs (A\b)
- frequency continuation
- L-BFGS

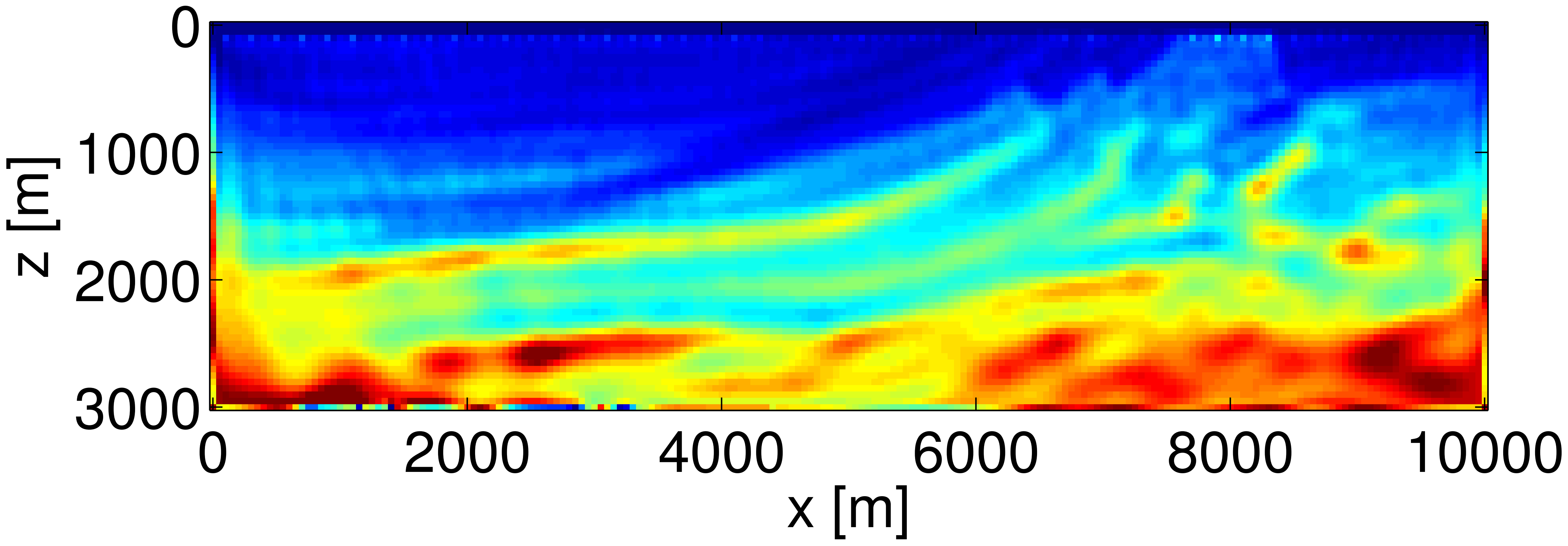
Waveform inversion

frequencies 1-5 Hz, no noise

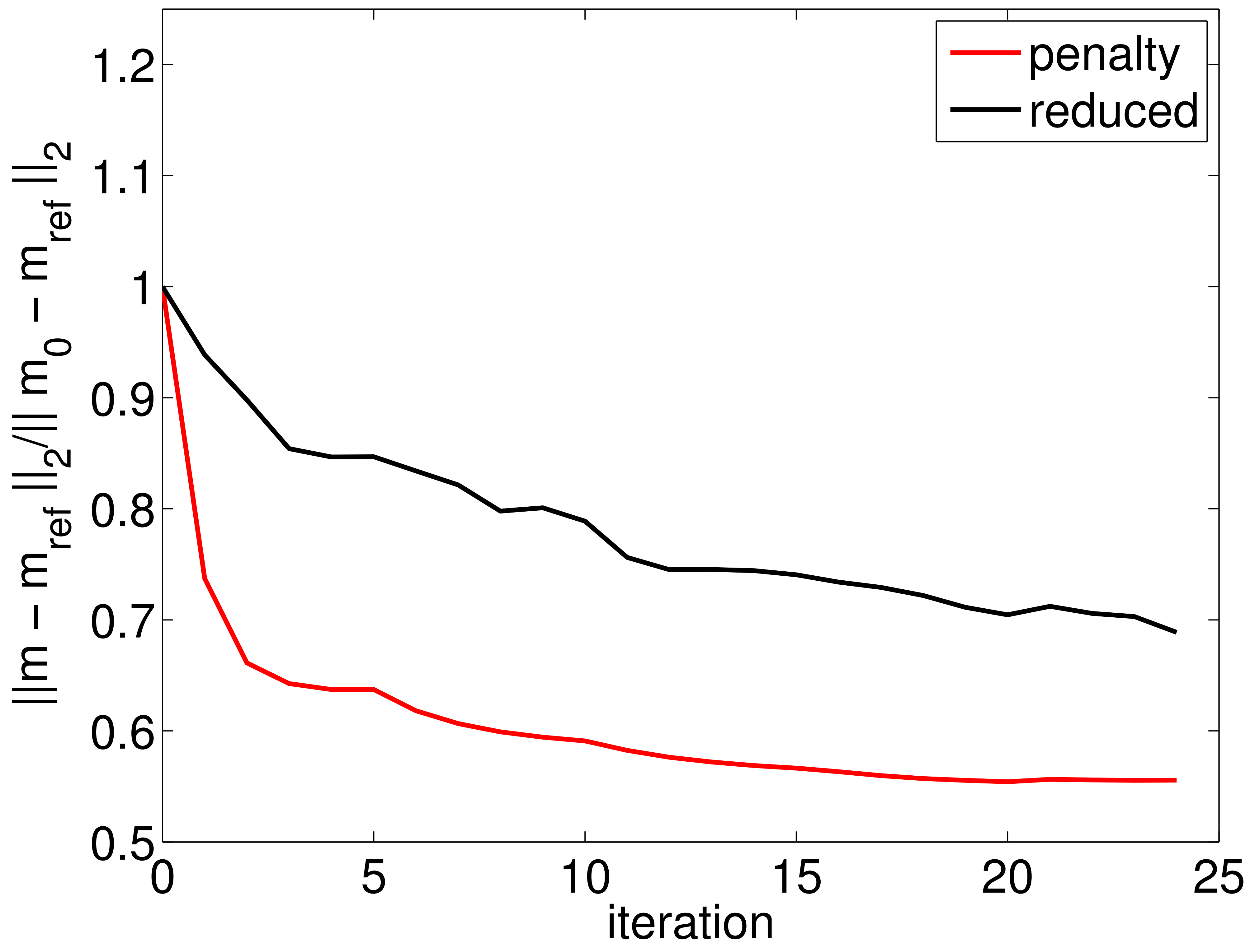
penalty



reduced

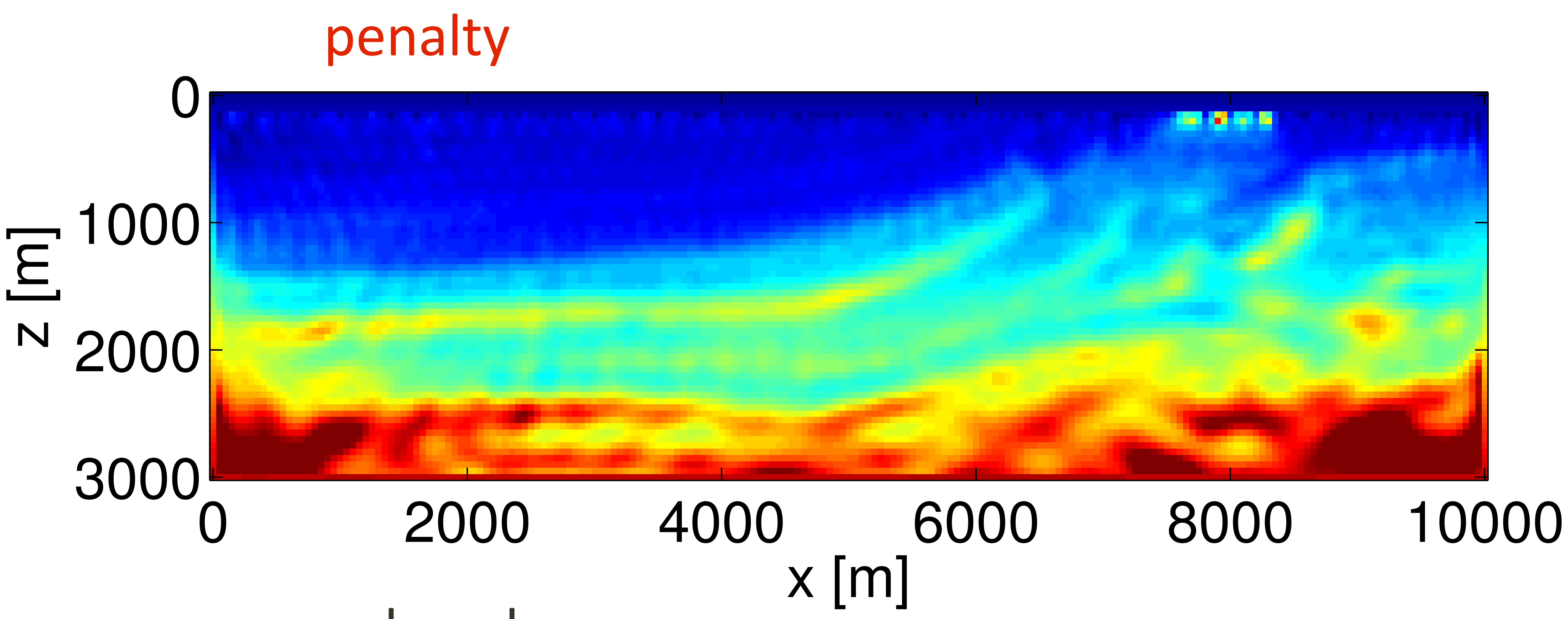


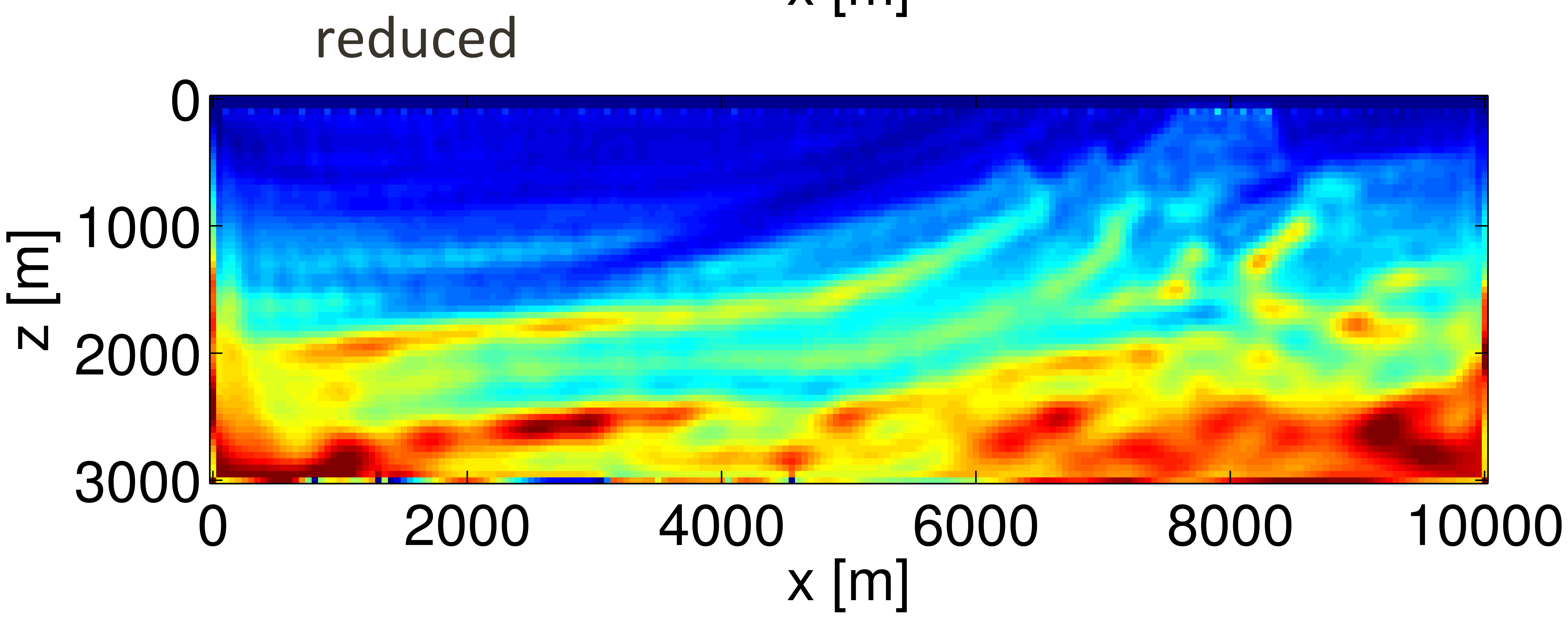
model error

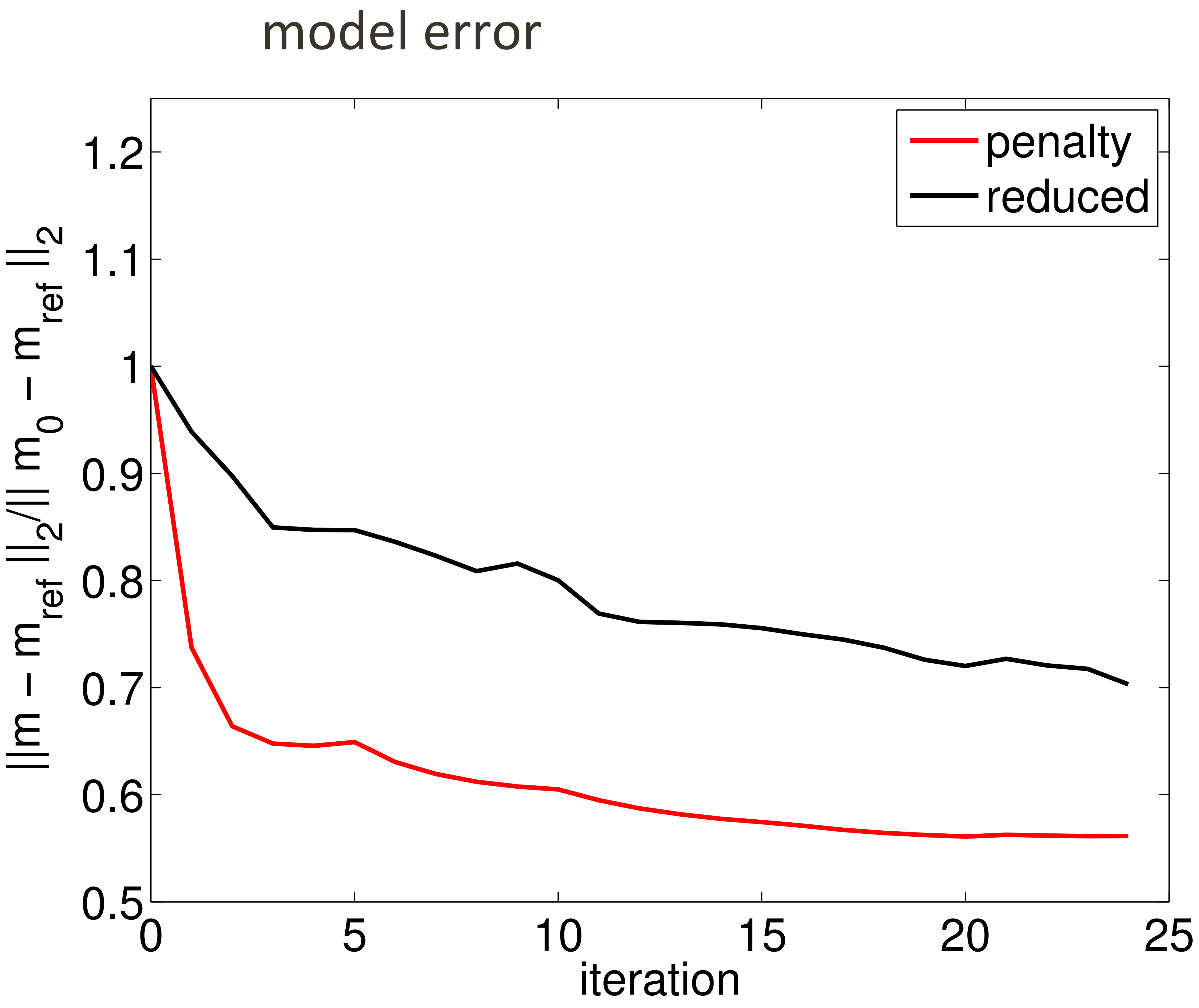


Waveform inversion

frequencies 1-5 Hz, 10 % Gaussian noise

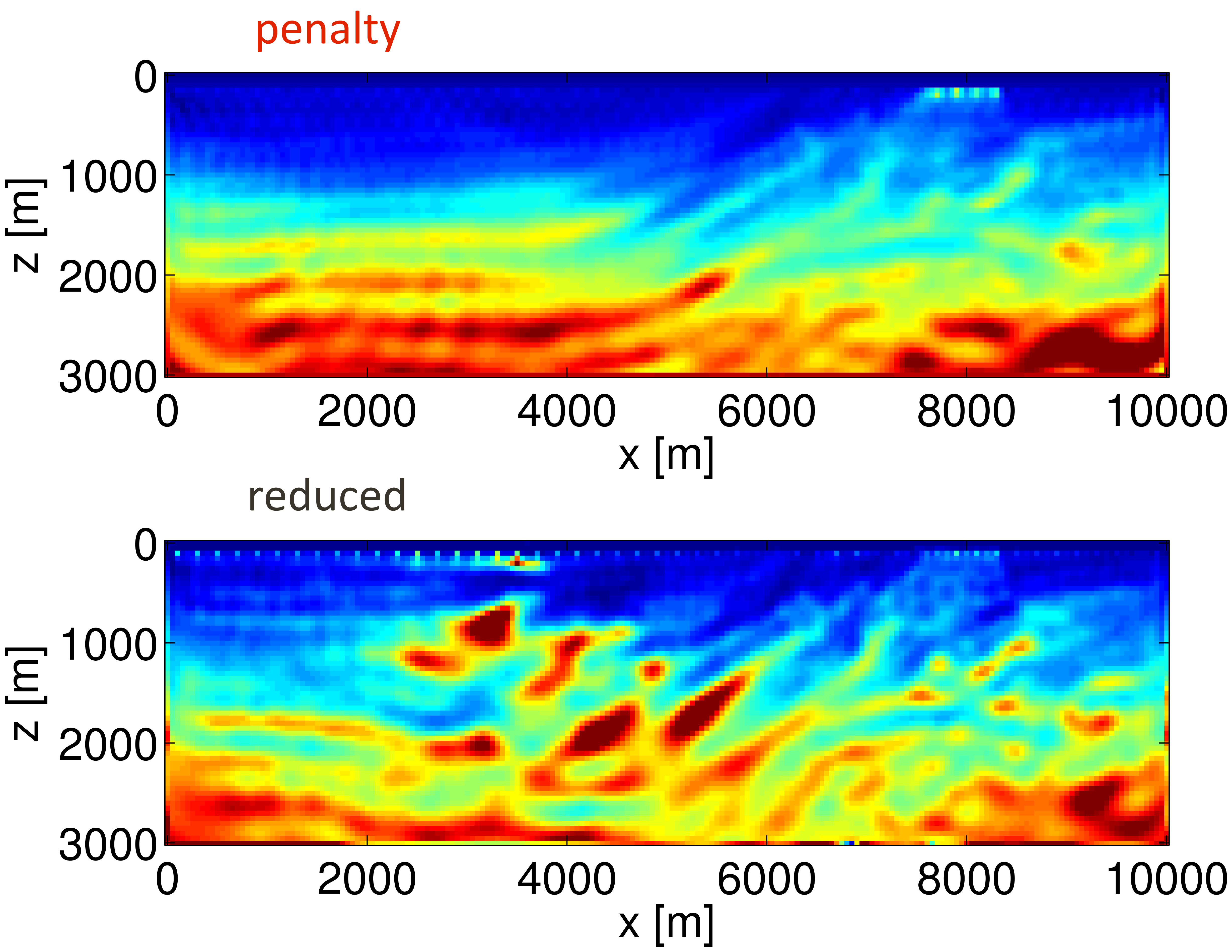


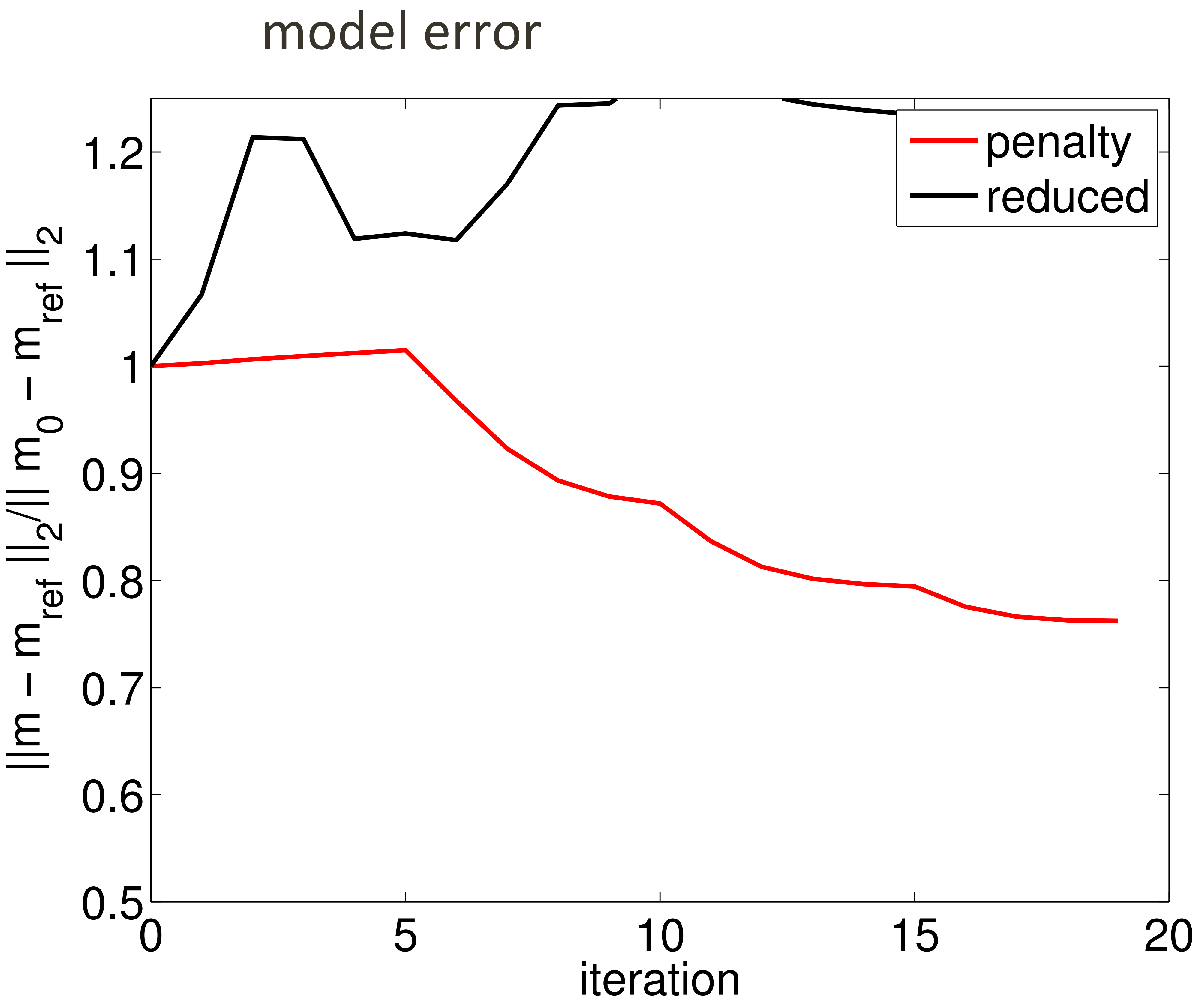




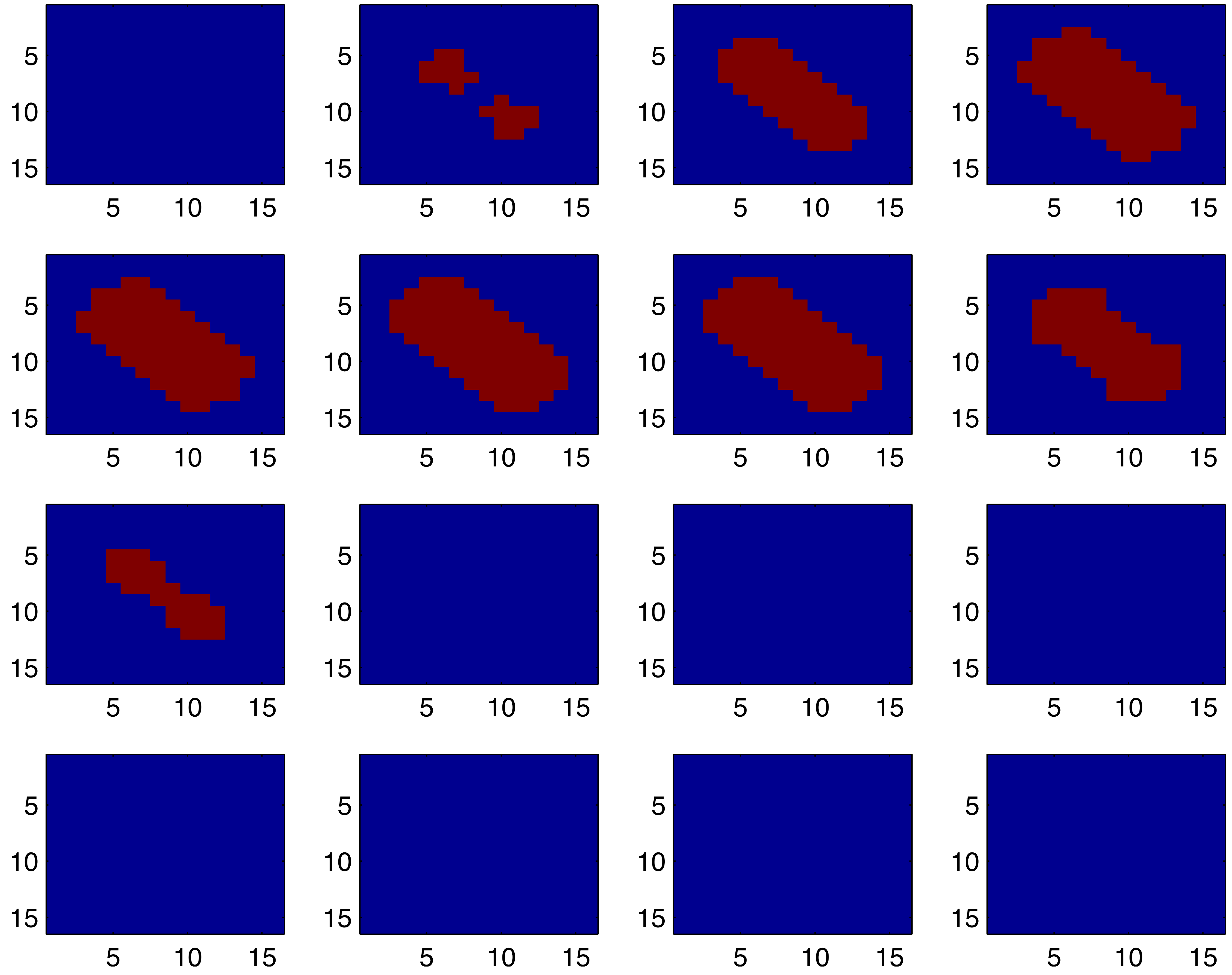
Waveform inversion

frequencies 2-5 Hz, 10 % Gaussian noise





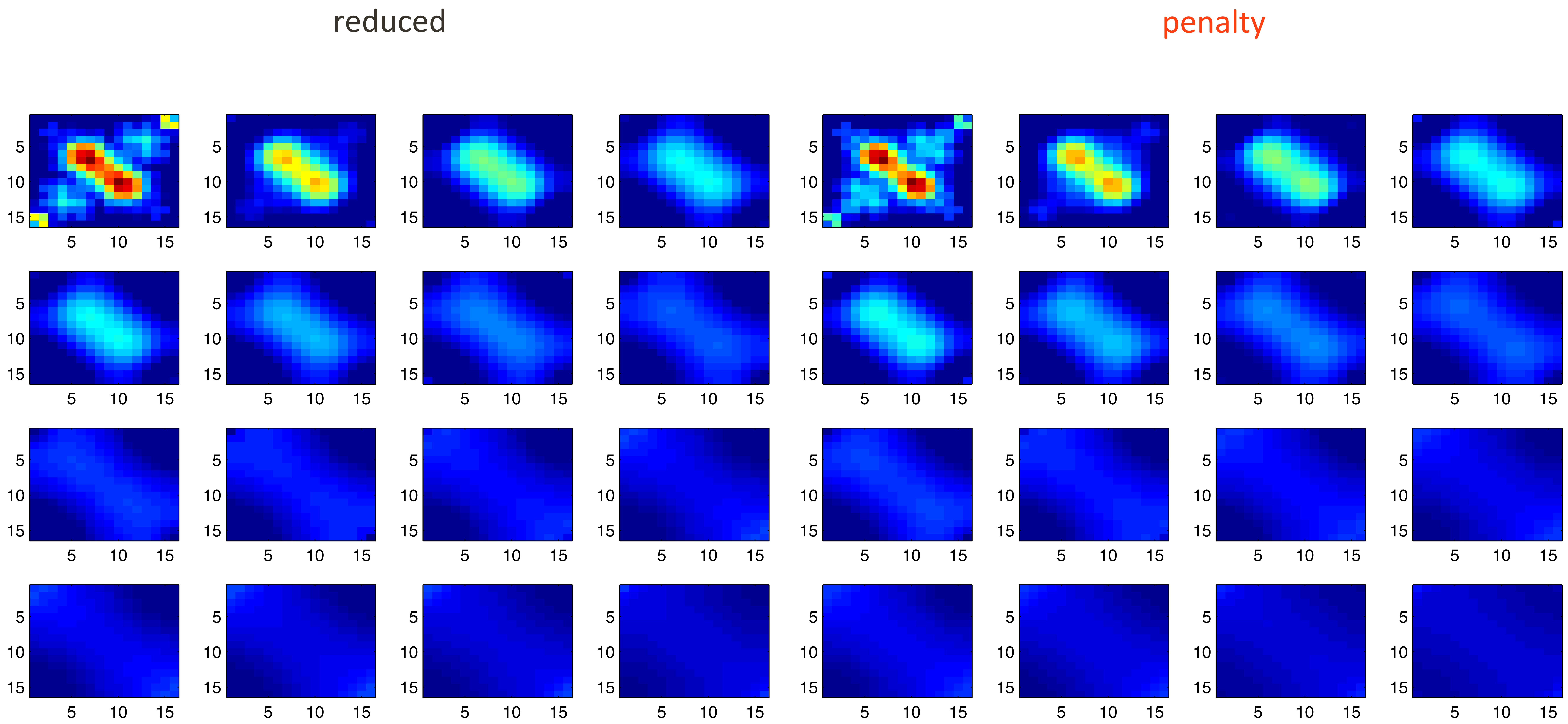
3D DC resistivity



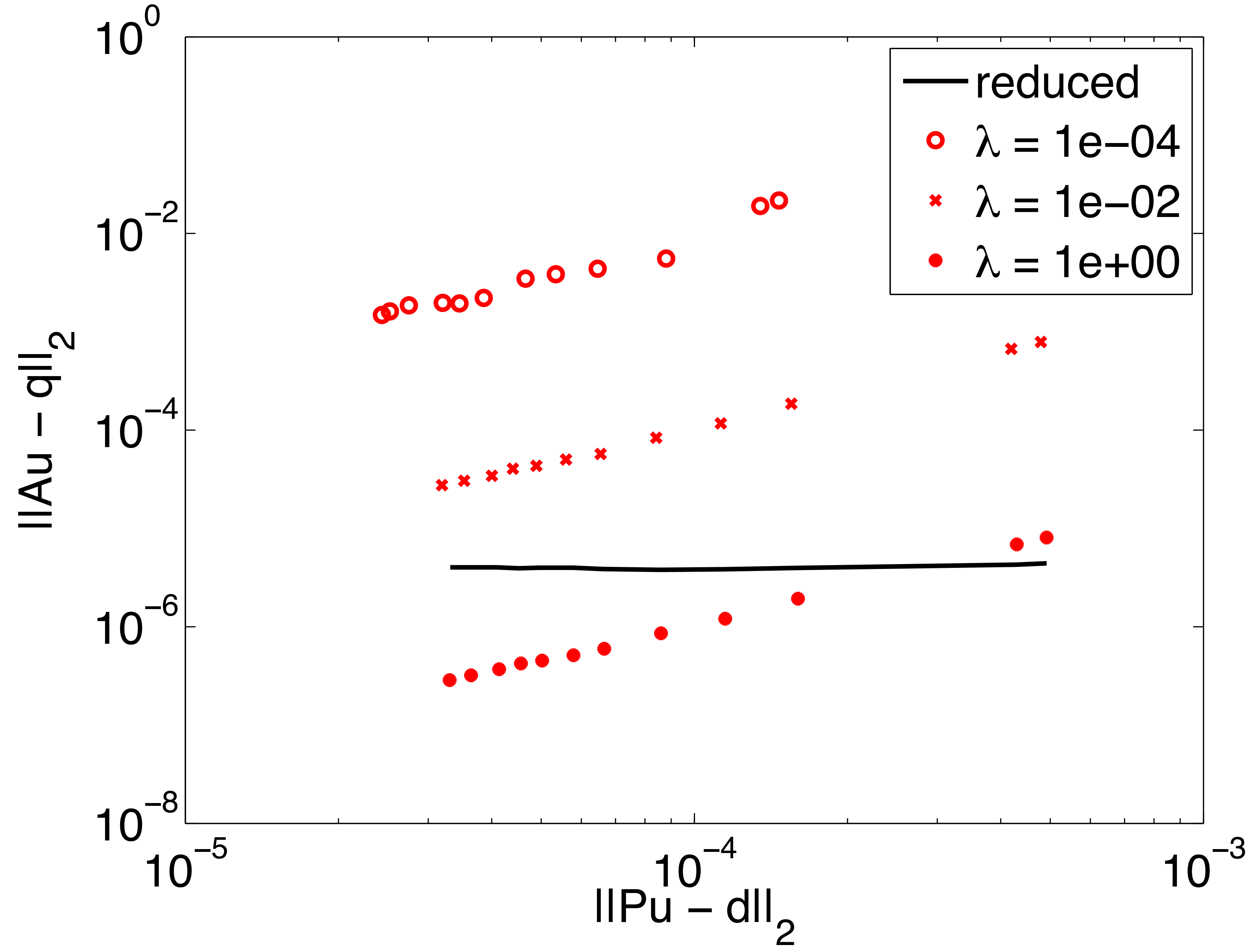
conductivity

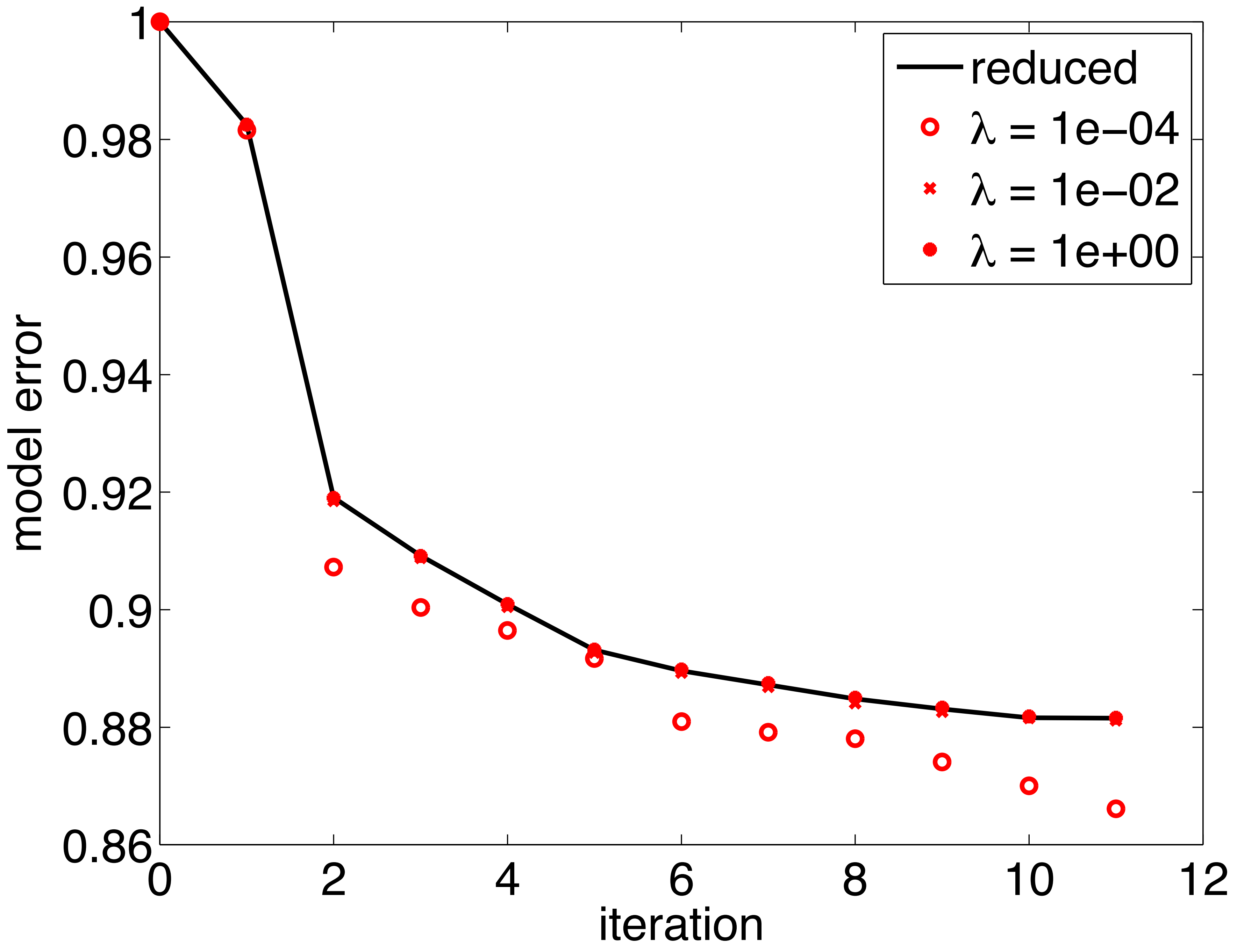
- PDE: $\nabla \cdot \sigma \nabla u = q$
- 16x16x16 grid
- 83 sources (crosswell)
- rec. on the surface
- FD discretization [Haber '07]
- iterative solvers for PDEs
- L-BFGS

3D DC resistivity

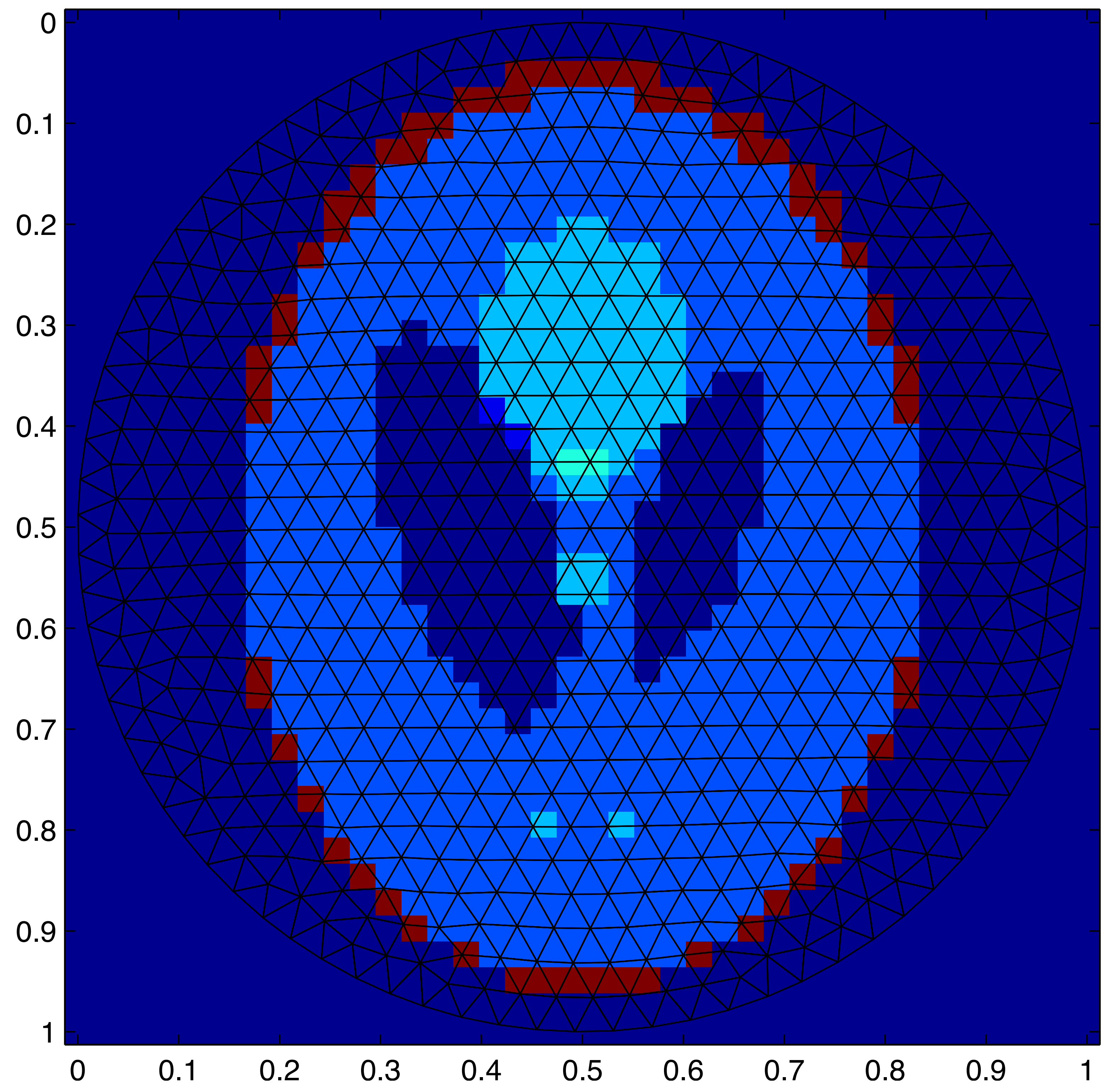


3D DC resistivity



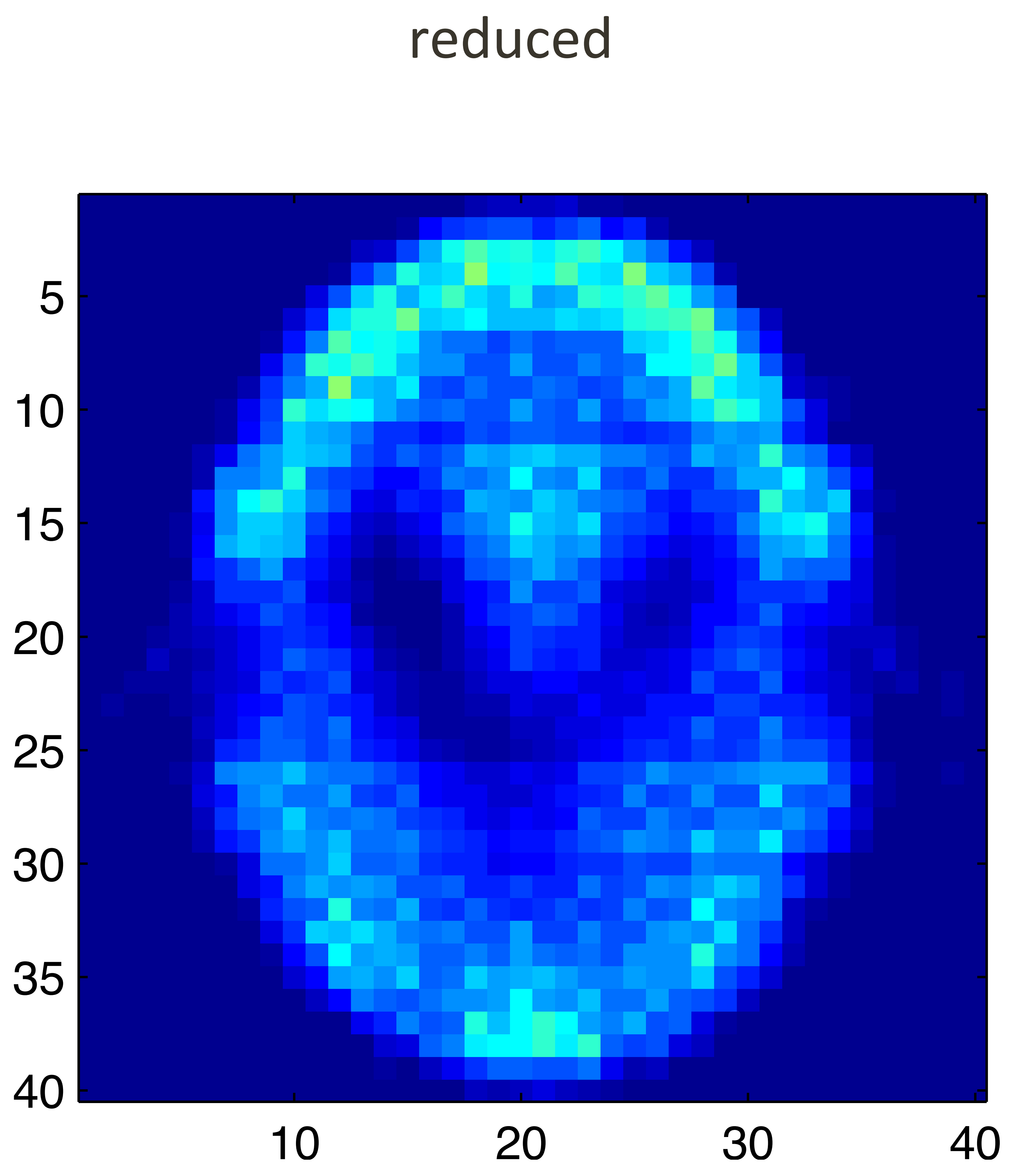


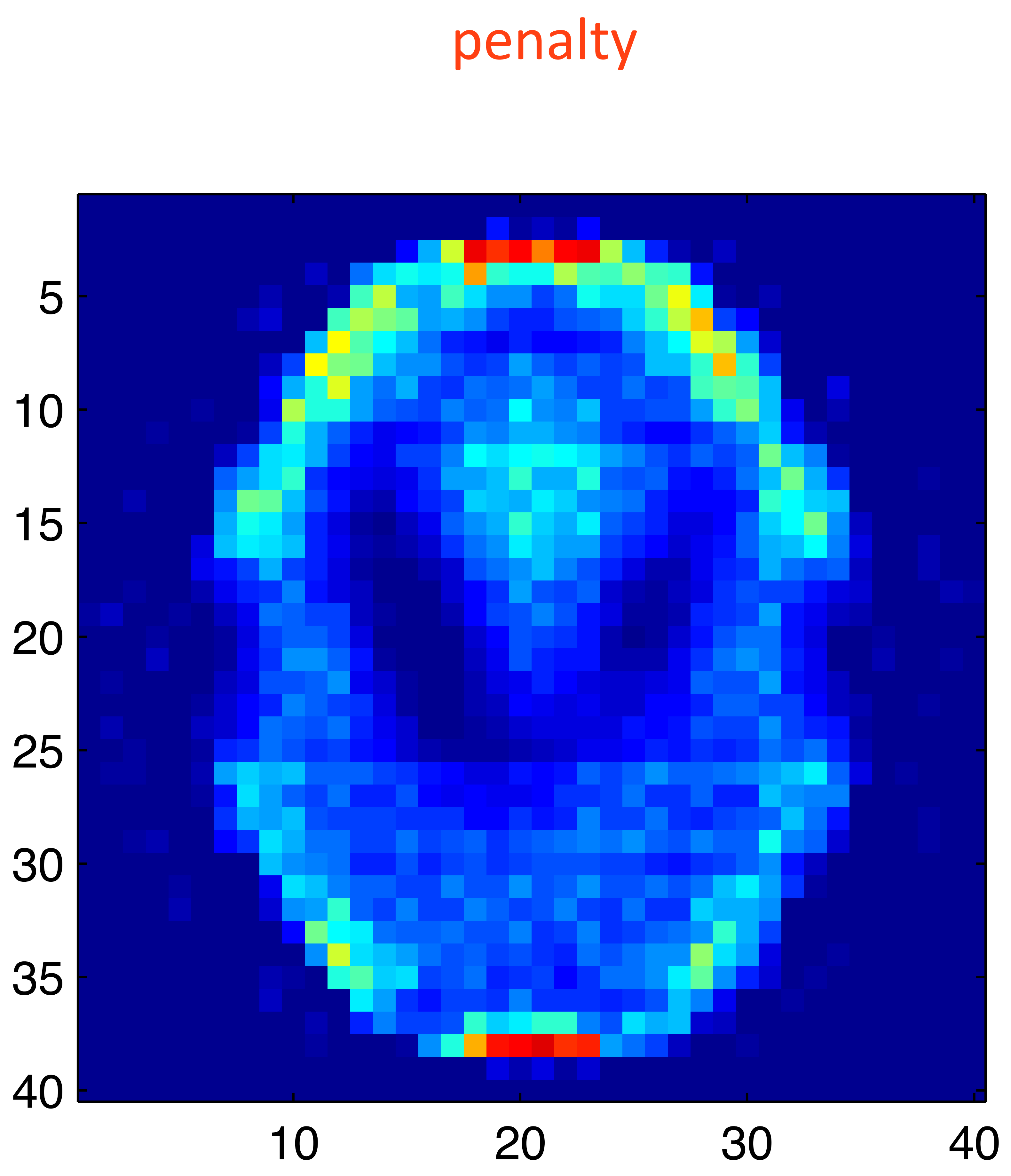
Optical tomography



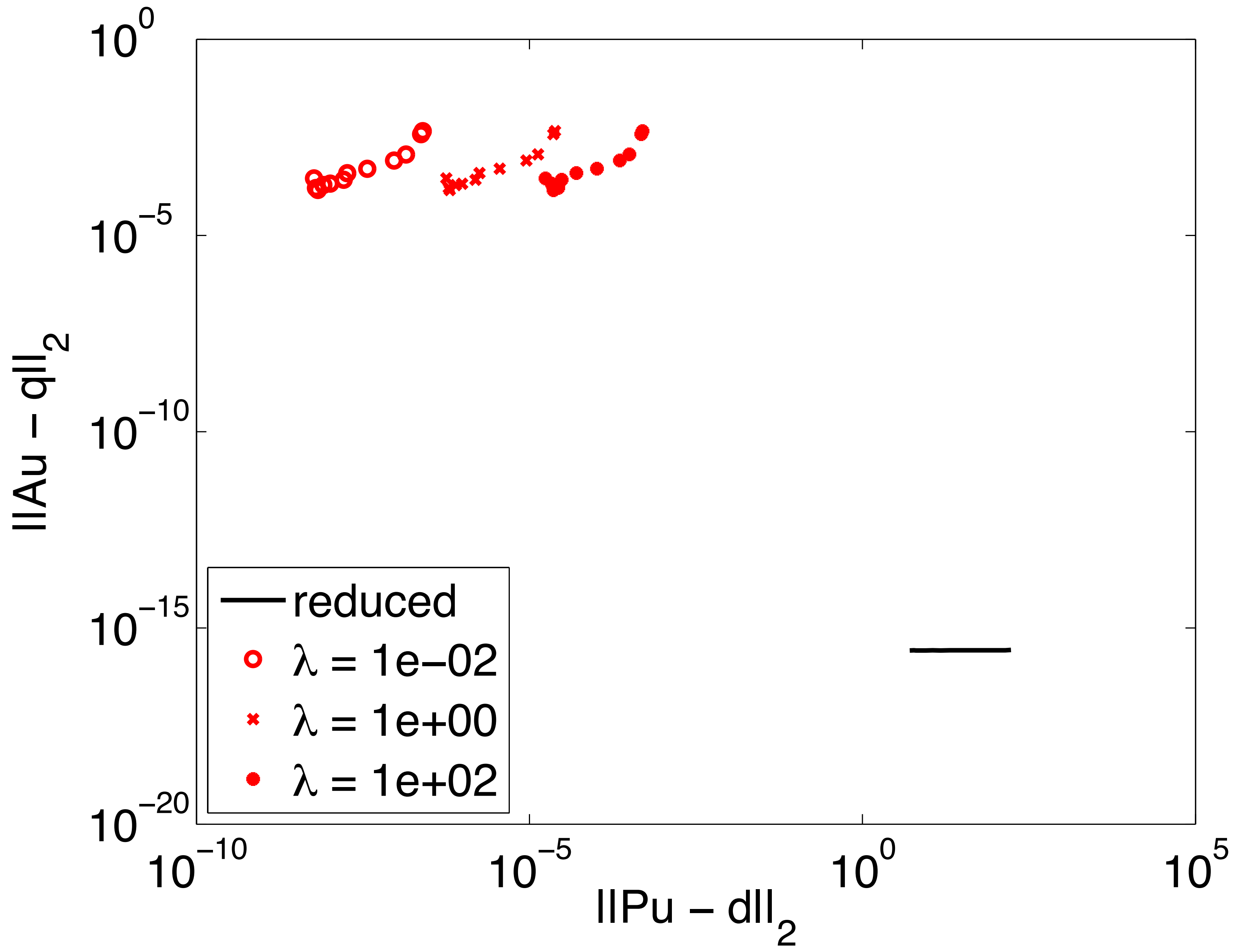
- PDE: $(-\imath\omega/c + \Omega \cdot \nabla + \mu_t)u = 0$
- FV discretization [Abdoulaev '05]
- 1 frequency (400 MHz), 21 angles
- Direct solvers for PDEs
- L-BFGS

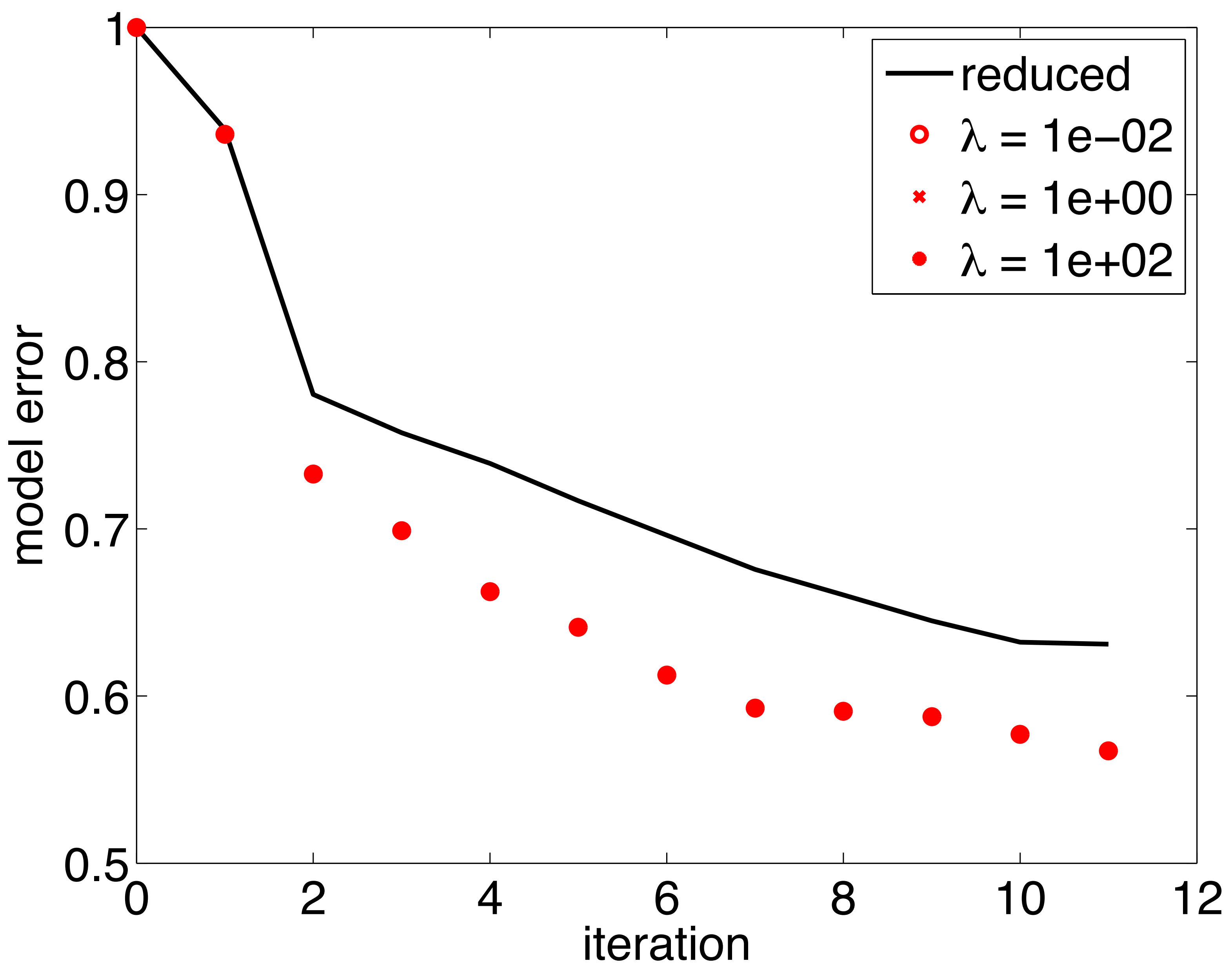
Optical tomography





Optical tomography





Conclusions

New method for *wave*-equation based inversion:

- *extended* search space as in *all-at-once* similar but with memory & CPU requirements as in *reduced* approach
- *no* adjoints & *sparse* GN-Hessian approximation
- `*less* non-linear' problem

Applicable to other PDE-constrained problems:

- DC resistivity
- Optical tomography

Future work

- *fast* solves for *augmented* PDE, preconditioning
- (GN) Hessian approximations
- misfit penalties & (sparse) regularization
- other PDEs
- *extensions* to combat *non*-uniqueness
- ...

Acknowledgements

Thank you for your attention !

https://www.slim.eos.ubc.ca/

SINBAD

NSERC CRSNG

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