An algorithm for solving least-squares problems with a Helmholtz block and multiple right-hand-sides

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SLIM
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Problem of interest

$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

Originates from the 'discretize-then-optimize' framework for PDE-constrained optimization:

$$\min_{\mathbf{m},\mathbf{u}} \frac{1}{2}\|P\mathbf{u} - \mathbf{d}\|_2^2 \quad \text{s.t.} \quad H(\mathbf{m})\mathbf{u} = \mathbf{q}$$

[E. Haber & U.M. Ascher, 2001 ; G. Biros & O. Ghattas , 2005 ; Grote et. al., 2011]

$H(\mathbf{m}) \in \mathbb{C}^{N\times N}$ discrete PDE

$\mathbf{m} \in \mathbb{R}^N$ medium parameters

$P \in \mathbb{R}^{m\times N}$ selects field at receivers

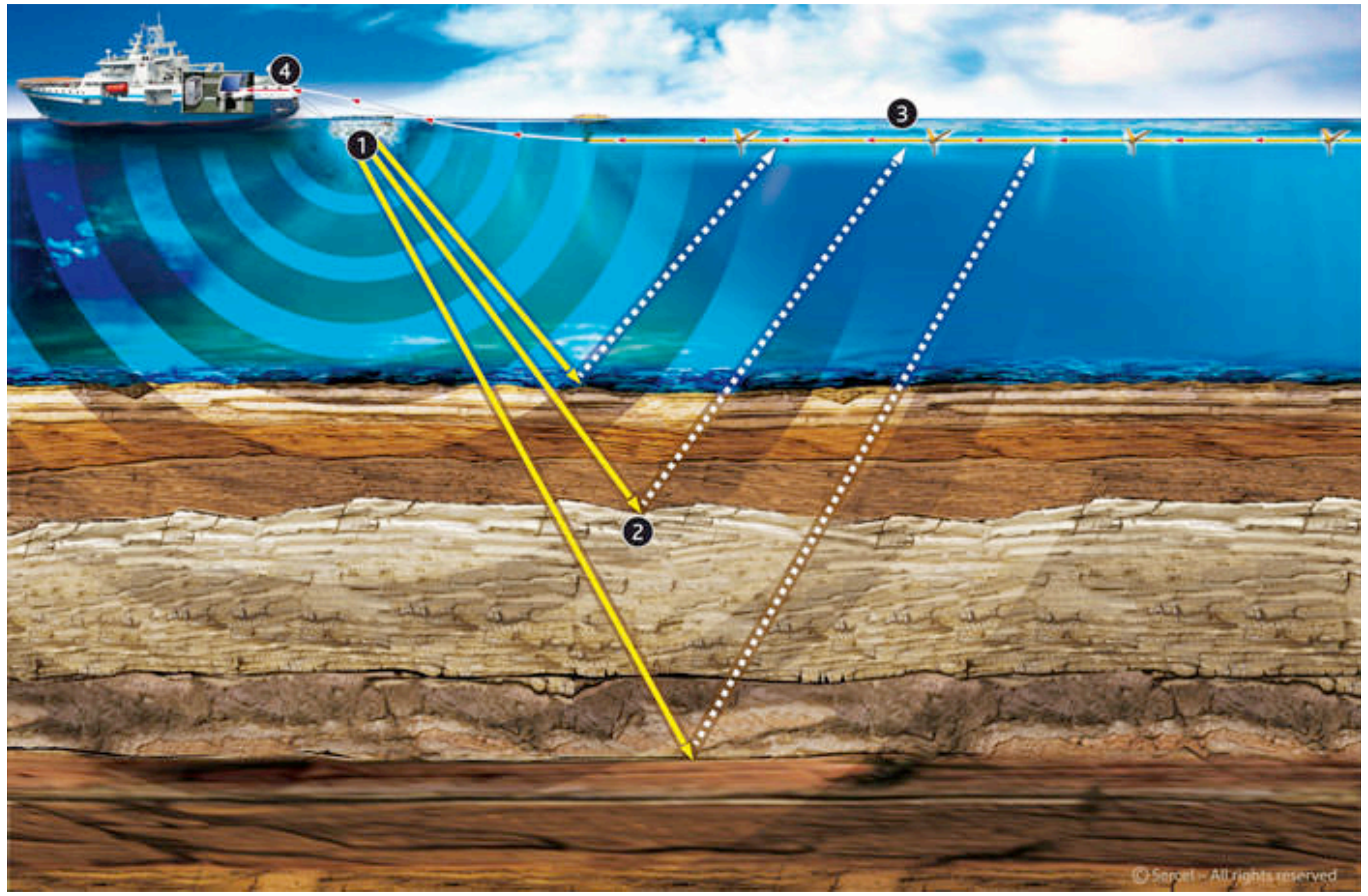
$\mathbf{u} \in \mathbb{C}^N$ field

$\mathbf{d} \in \mathbb{C}^m$ observed data

$\mathbf{q} \in \mathbb{C}^N$ source

PDE-constrained optimization

The PDE of interest in this talk is the scalar Helmholtz equation



[from:http://www.sercel.com/about/Pages/what-is-geophysics.aspx]

PDE-constrained optimization

Multi-experiment structure:

$$\min_{\mathbf{m},\mathbf{u}} \frac{1}{2}\|P\mathbf{u}-\mathbf{d}\|_2^2 \quad \text{s.t.} \quad H(\mathbf{m})\mathbf{u}=\mathbf{q}$$

$$\begin{pmatrix} P_1 & & & \\ & P_2 & & \\ & & \ddots & \\ & & & P_k \end{pmatrix}\begin{pmatrix}\mathbf{u}_1\\ \mathbf{u}_2\\ \vdots \\ \mathbf{u}_k\end{pmatrix} - \begin{pmatrix}\mathbf{d}_1\\ \mathbf{d}_2\\ \vdots \\ \mathbf{d}_k\end{pmatrix} \qquad \begin{pmatrix} H_1 & & & \\ & H_2 & & \\ & & \ddots & \\ & & & H_k \end{pmatrix}\begin{pmatrix}\mathbf{u}_1\\ \mathbf{u}_2\\ \vdots \\ \mathbf{u}_k\end{pmatrix} - \begin{pmatrix}\mathbf{q}_1\\ \mathbf{q}_2\\ \vdots \\ \mathbf{q}_k\end{pmatrix}$$

$k \times N$ field parameters

- 1 PDE: *N* ~ [1e6 - 1e9] grid points
- [1 - 100] right-hand-sides (*k* sources)
- [1 - 100] *m* receivers ($P \in \mathbb{R}^{m\times N}$)

PDE-constrained optimization

$$\min_{\mathbf{m},\mathbf{u}} \frac{1}{2}\|P\mathbf{u}-\mathbf{d}\|_2^2 \quad \text{s.t.} \quad H(\mathbf{m})\mathbf{u}=\mathbf{q}$$

↓

$$\mathcal{L}(\mathbf{m},\mathbf{u},\boldsymbol{\gamma}) = \frac{1}{2}\|P\mathbf{u}-\mathbf{d}\|_2^2 + \boldsymbol{\gamma}^*\big(H(\mathbf{m})\mathbf{u}-\mathbf{q}\big)$$

↓

eliminate field variables

↓

[E Haber et al., 2000 ; I Epanomeritakis et al., 2008]
[T. van Leeuwen & F.J. Herrmann, 2014]

$$\min_{\mathbf{m}} \frac{1}{2}\|PH(\mathbf{m})^{-1}\mathbf{q}-\mathbf{d}\|_2^2$$

reduced gradient method / adjoint-state / reduced Lagrangian

$$\min_{\mathbf{m},\mathbf{u}} \|H(\mathbf{m})\mathbf{u}-\mathbf{q}\|_2 \quad \text{s.t.} \quad \|P\mathbf{u}-\mathbf{d}\|_2 \le \sigma$$

↓

$$\min_{\mathbf{m},\mathbf{u}} \frac{1}{2}\|P\mathbf{u}-\mathbf{d}\|_2^2 + \frac{\lambda^2}{2}\|H(\mathbf{m})\mathbf{u}-\mathbf{q}\|_2^2$$

↓

eliminate field variables $\nabla_{\mathbf{u}}\phi(\mathbf{m},\bar{\mathbf{u}},\lambda)=0$

[T. van Leeuwen & F.J. Herrmann, 2013]

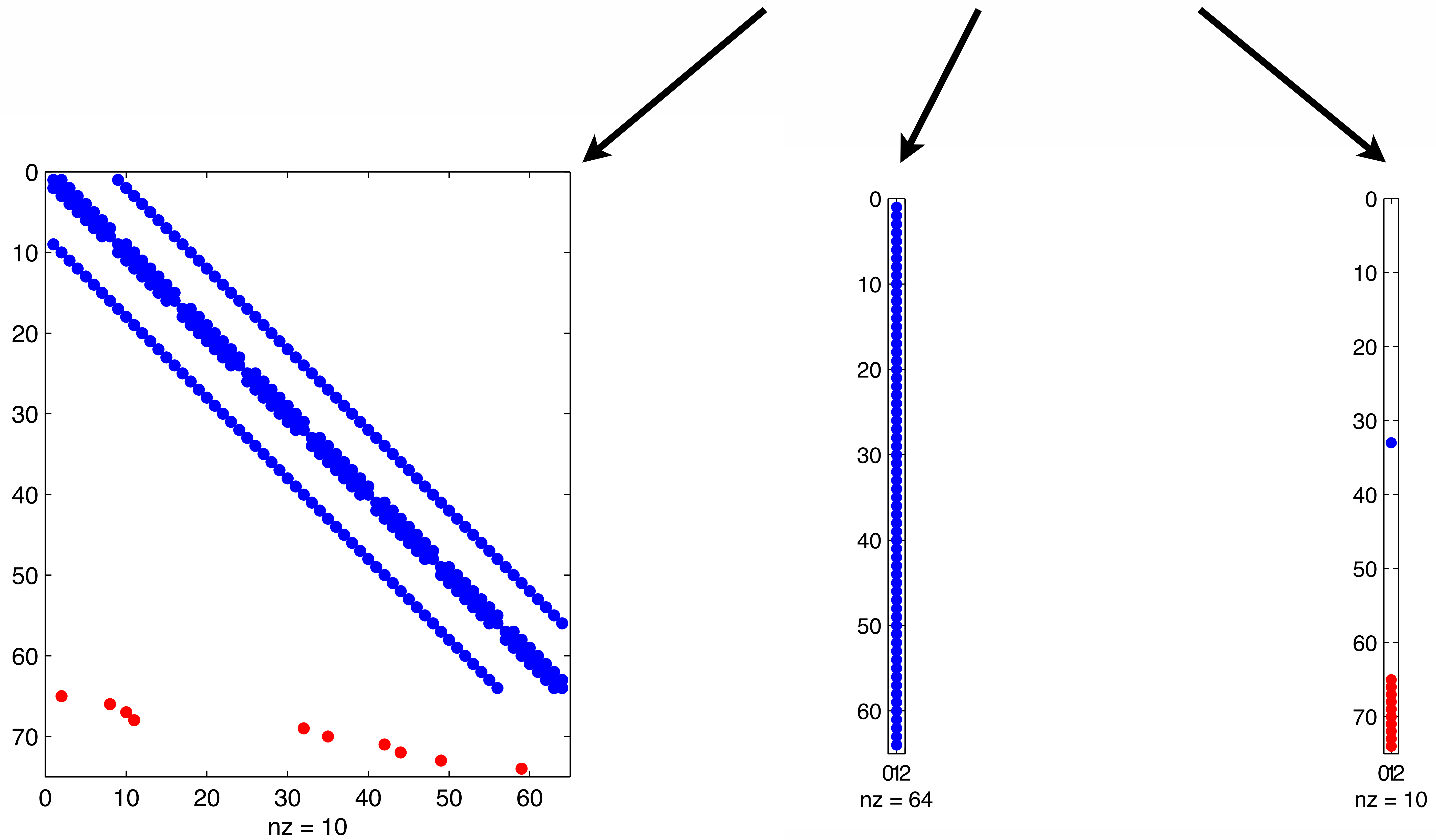
↓

$$\min_{\mathbf{m}} \frac{1}{2}\|P\bar{\mathbf{u}}-\mathbf{d}\|_2^2 + \frac{\lambda^2}{2}\|H(\mathbf{m})\bar{\mathbf{u}}-\mathbf{q}\|_2^2$$

reduced quadratic-penalty

reduced quadratic-penalty: $\bar{\phi}(\mathbf{m}, \bar{\mathbf{u}}, \lambda) = \frac{1}{2}\|P\bar{\mathbf{u}} - \mathbf{d}\|_2^2 + \frac{\lambda^2}{2}\|H(\mathbf{m})\bar{\mathbf{u}} - \mathbf{q}\|_2^2$

$$\nabla_{\mathbf{u}}\phi(\mathbf{m}, \bar{\mathbf{u}}, \lambda) = 0 \longleftrightarrow \bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$



[T. van Leeuwen & F.J. Herrmann, 2013]

A reduced-space quadratic-penalty method

To minimize: $$\min_{\mathbf{m}} \frac{1}{2}\|P\bar{\mathbf{u}} - \mathbf{d}\|_2^2 + \frac{\lambda^2}{2}\|H(\mathbf{m})\bar{\mathbf{u}} - \mathbf{q}\|_2^2$$

at every outer iteration:

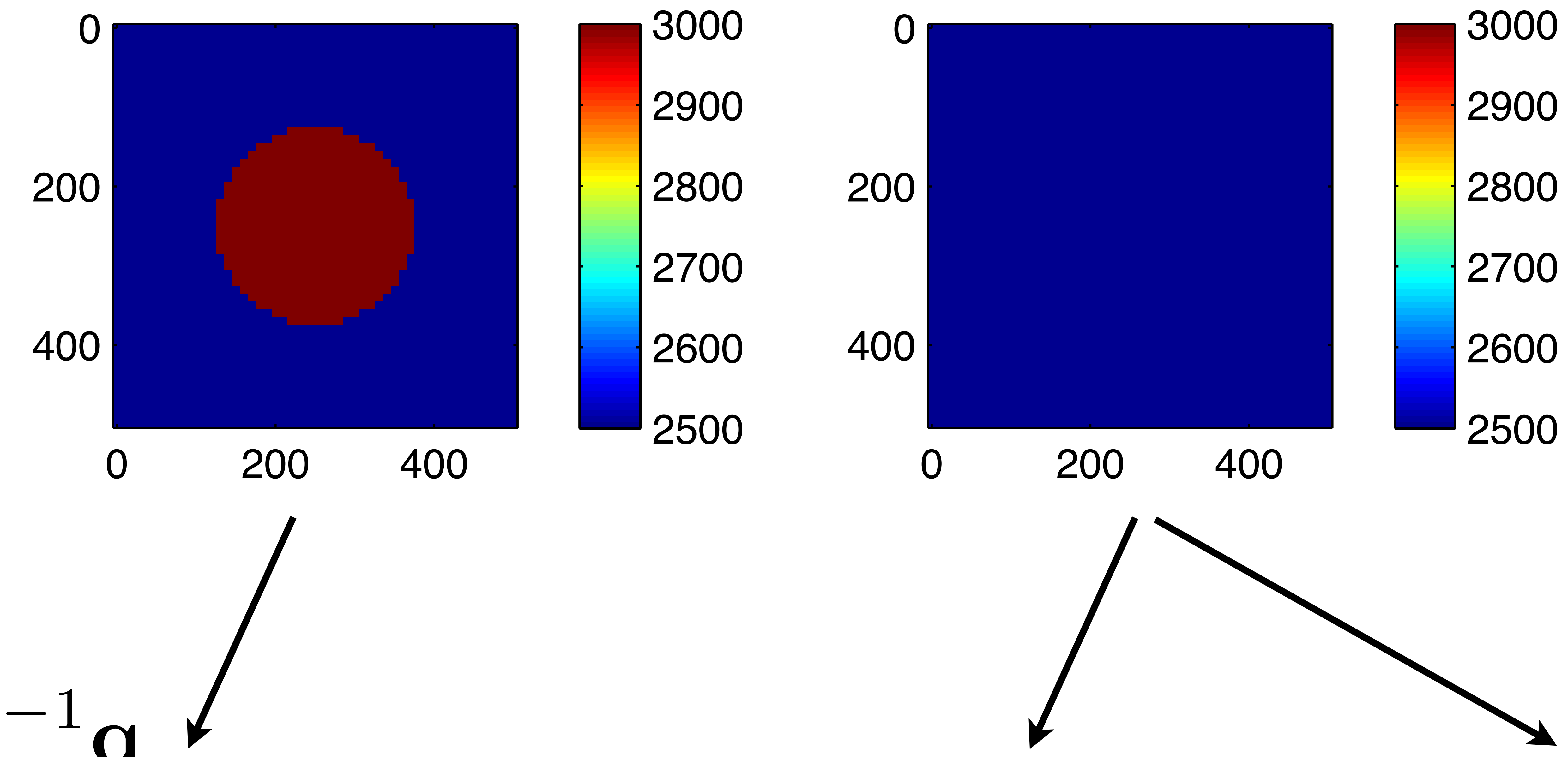
- compute $$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$
- evaluate $\bar{\phi}(\mathbf{m}, \bar{\mathbf{u}}, \lambda)$ & $\nabla_{\mathbf{m}}\bar{\phi}(\mathbf{m}, \bar{\mathbf{u}}, \lambda)$
- update $\mathbf{m}$

Properties of the problem

$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

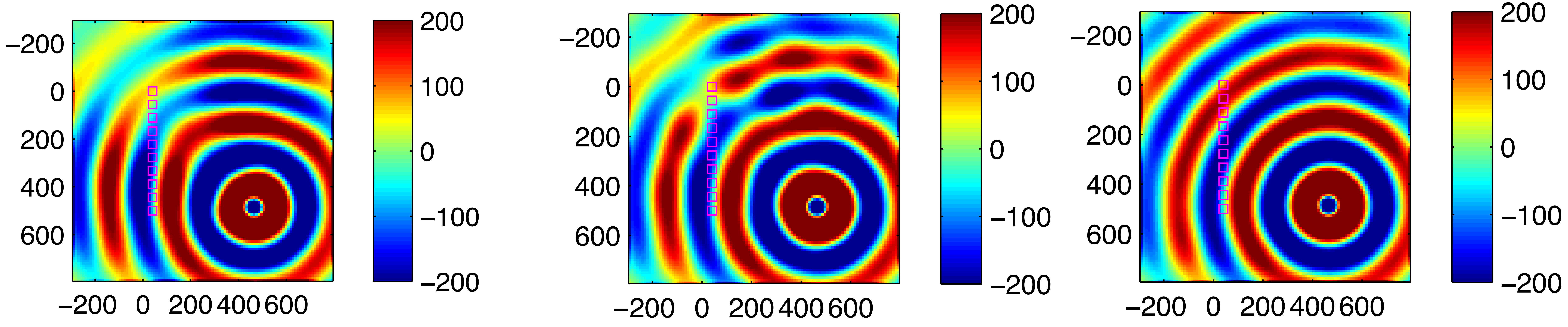
- H is indefinite, not Hermitian
- inconsistent
- full column rank
- may lose symmetry when using a Perfectly Matched Layer (PML)

2D example



$$\mathbf{u} = H(\mathbf{m}_*)^{-1}\mathbf{q}$$

$$\mathbf{u} = H(\mathbf{m}_0)^{-1}\mathbf{q}$$



$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}_0) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

Algorithms

Main challenge: solve $$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

- iteratively & matrix-free
- no QR or LU factorizations
- at cost cost of a few PDE solves

Algorithms

What about preconditioned LSQR, CGLS? (preconditioner: λH)

$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} (\lambda H(\mathbf{m}))^{-1}\mathbf{u} - \begin{pmatrix} \lambda\mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

using exact preconditioning this solves

$$(I + H_\lambda^{-*}P^*PH_\lambda^{-1})\mathbf{y} = \lambda\mathbf{q} + (H_\lambda^*)^{-1}P^*\mathbf{d}, \quad \text{with} \quad H_\lambda\bar{\mathbf{u}} = \mathbf{y}$$

- $m+1$ distinct eigenvalues (identity + low-rank) $\qquad (m = n_{\text{rec}})$

Algorithms

What about preconditioned LSQR, CGLS? (preconditioner: λH)

$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ P \end{pmatrix} (\lambda H(\mathbf{m}))^{-1} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

- expected computational cost: $n_{\text{src}} \times 2(1 + n_{\text{rec}})$ PDE solves
- not competitive with Lagrangian based reduced-space algorithms which require $2n_{\text{src}}$ PDE solves
- more PDE solves required in case of inexact PDE solves

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Proposed algorithm

LS-problem in normal-equation form:

$$\left(\lambda^2 H(\mathbf{m})^* H(\mathbf{m}) + P^* P\right)\bar{\mathbf{u}} = \lambda^2 H(\mathbf{m})\mathbf{q} + P^*\mathbf{d}$$

Split-preconditioning by λH without computations

$$(I + H_\lambda^{-*} P^* P H_\lambda^{-1})\mathbf{y} = \lambda\mathbf{q} + (H_\lambda^*)^{-1} P^*\mathbf{d}, \quad \text{with} \quad H_\lambda \bar{\mathbf{u}} = \mathbf{y}$$

- $m+1$ distinct eigenvalues (identity + low-rank), even for inexact PDE solves
- Exploit identity + low-rank structure by solving $H^{-*}P^* = W$

Proposed algorithm

identity + low-rank factorization:

$$(I + WW^*)\mathbf{y} = \lambda\mathbf{q} + W\mathbf{d}, \quad \text{with} \quad H_\lambda\bar{\mathbf{u}} = \mathbf{y}$$

and invert system matrix as (Sherman-Morrison)

$$\mathbf{y} = (I - W(I + W^*W)^{-1}W^*)(\lambda\mathbf{q} + W\mathbf{d}), \quad \text{with} \quad H_\lambda\bar{\mathbf{u}} = \mathbf{y}$$

so we only need to invert the dense matrix $(I + W^*W) \in \mathbb{C}^{m\times m}$

(this is alway small enough to do explicitly, $m \leq 100$)

Proposed algorithm

identity + low-rank factorization:

$$(I + WW^*)\mathbf{y} = \lambda\mathbf{q} + W\mathbf{d}, \quad \text{with} \quad H_\lambda \bar{\mathbf{u}} = \mathbf{y}$$

Stability of Sherman-Morrison is a concern in general, but was found to be sufficiently accurate for some Helmholtz test problems.

In case Sherman-Morrison is not accurate enough:

$$\arg\min_{\mathbf{y}} \left\| \begin{pmatrix} I \\ W^* \end{pmatrix} \mathbf{y} - \begin{pmatrix} \lambda\mathbf{q} \\ \mathbf{d} \end{pmatrix} \right\|_2$$

Proposed algorithm

for angular frequency ω **do**

  // solve m Helmholtz problems

  $H_\lambda^* W = P^*$

  $M = (I + W^* W)^{-1}$

  for right hand side i **do**

    $\mathbf{y}_i = \left(I - WMW^*\right)\left(\lambda \mathbf{q}_i + W\mathbf{d}_i\right)$

    // solve for $\bar{\mathbf{u}}_i$

    $H_\lambda \bar{\mathbf{u}}_i = \mathbf{y}_i$

  end for

end for

Proposed algorithm

Matrix-free algorithm

- no direct solves
- related mildly overdetermined systems **[L. M. Delves & I. Barrodale, 1979]**

Computational cost:

- 1 PDE per receiver
- 1 PDE per source

Memory requirements:

- 1 vector per receiver (W)
- system matrix (H)
- storage for solving systems with H

Proposed algorithm

Inexact solutions to the linear systems:

for angular frequency ω **do**
  // solve m Helmholtz problems inexactly
→ $H_\lambda^* \hat{W} = P^* + R_W$
  $\hat{M} = (I + \hat{W}^* \hat{W})^{-1}$
  for right hand side $\mathbf{b}_i$ **do**
    $\hat{\mathbf{y}}_i = \left(I - \hat{W}\hat{M}\hat{W}^*\right)\left(\lambda \mathbf{q}_i + \hat{W}\mathbf{d}_i\right)$
    // solve for $\bar{\mathbf{u}}_i$ inexactly
→ $H_\lambda \hat{\mathbf{u}}_i = \hat{\mathbf{y}}_i + \mathbf{r}_\mathbf{u}$
  end for
end for

Proposed algorithm

error propagation (1 right-hand-side, 1 receiver case):

$$H_\lambda^* \hat{\mathbf{w}} = \mathbf{p}^* + \mathbf{r}_{\mathbf{w}}$$

$$(I + \hat{\mathbf{w}}\hat{\mathbf{w}}^*)\hat{\mathbf{y}} = \lambda \mathbf{q} + \hat{\mathbf{w}} d$$

$$H_\lambda \hat{\mathbf{u}} = \hat{\mathbf{y}} + \mathbf{r}_{\mathbf{u}}$$

Proposed algorithm

error propagation (1 right-hand-side, 1 receiver case):

$$H_\lambda^* \hat{\mathbf{w}} = \mathbf{p}^* + \mathbf{r}_\mathbf{w}$$

$$(I + \hat{\mathbf{w}}\hat{\mathbf{w}}^*)\hat{\mathbf{y}} = \lambda \mathbf{q} + \hat{\mathbf{w}} d \quad \longrightarrow \quad \text{solve as: } \hat{\mathbf{y}} = (I - \hat{m}\hat{\mathbf{w}}\hat{\mathbf{w}}^*)(\lambda \mathbf{q} + \hat{\mathbf{w}} d)$$

with $\hat{m} = \dfrac{1}{1 + \hat{\mathbf{w}}^* \hat{\mathbf{w}}}$

$$H_\lambda \hat{\mathbf{u}} = \hat{\mathbf{y}} + \mathbf{r}_\mathbf{u}$$

derivation of error bounds based on observable quantities is work in progress

Suggested PDE-solver

Need to store 1 vector per receiver

-> use PDE-solver with low-memory & setup requirements

Helmholtz:

- CGMN (only 4 vectors) / CARP-CG — [A. Bjorck & T. Elfving, 1979; D. Gordon & R. Gordon, 2010; T. van Leeuwen & F.J. Herrmann, 2014]
- Shifted-Laplacian w/ multi-grid — [Y.A. Erlangga, 2008; H. Calandra et al., 2013]
- combination of the above — [R. Lago & F.J. Herrmann, 2015]

Randomization and subsampling

What is the number of receivers is too large, storage wise?

Can we approximate the least-squares problem using randomization & subsampling?

Use ideas from algorithms such as

- **[V Rokhlin & M Tygert, 2008]**
- Blendenpik **[H. Avron et. al., 2010]**
- LSRN **[X. Meng, M. A. Saunders, M. W. Mahoney, 2014]**

Randomization and subsampling

Initial attempt in this work:

apply randomization and subsampling to the receiver block only for a one-step approximation:

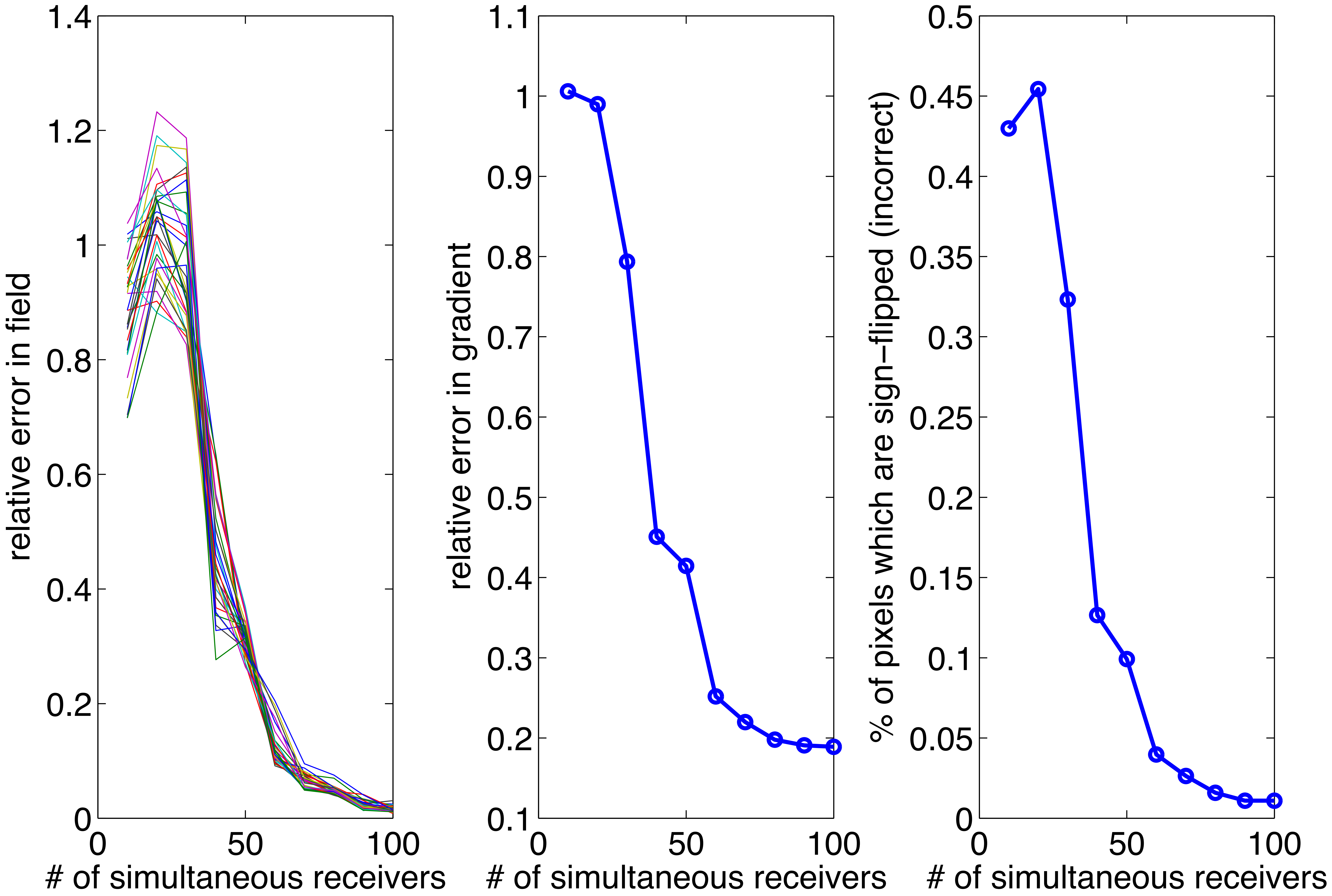
$$\bar{\mathbf{u}} = \arg\min_{\mathbf{u}} \left\| \begin{pmatrix} \lambda H(\mathbf{m}) \\ VP \end{pmatrix} \mathbf{u} - \begin{pmatrix} \lambda \mathbf{q} \\ V\mathbf{d} \end{pmatrix} \right\|_2$$

$V \in \mathbb{C}^{l \times m}, \quad l < m$ (complex, random, flat)

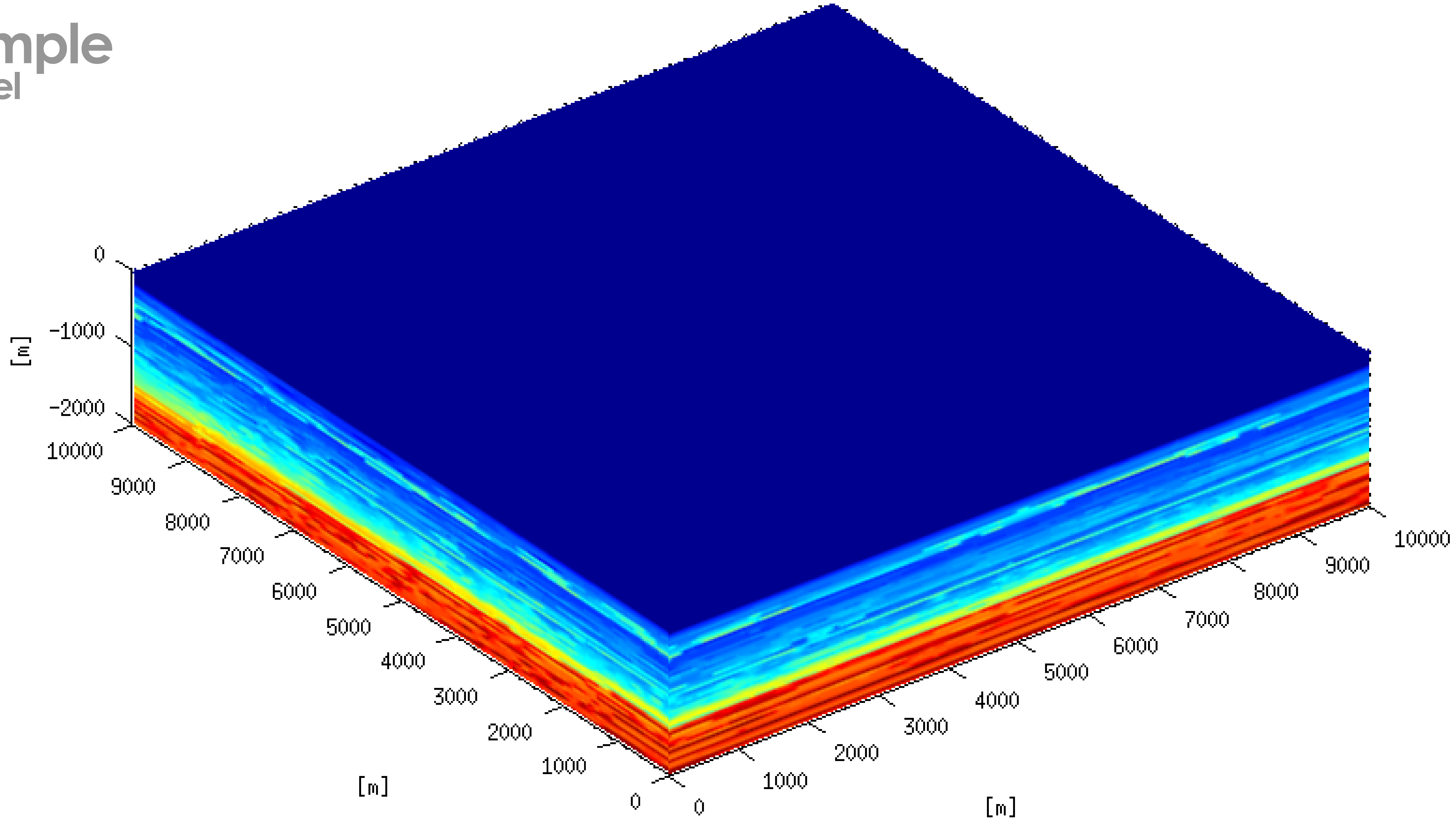
reduces

- # of PDE solves
- # vectors to be stored

Simultaneous receivers

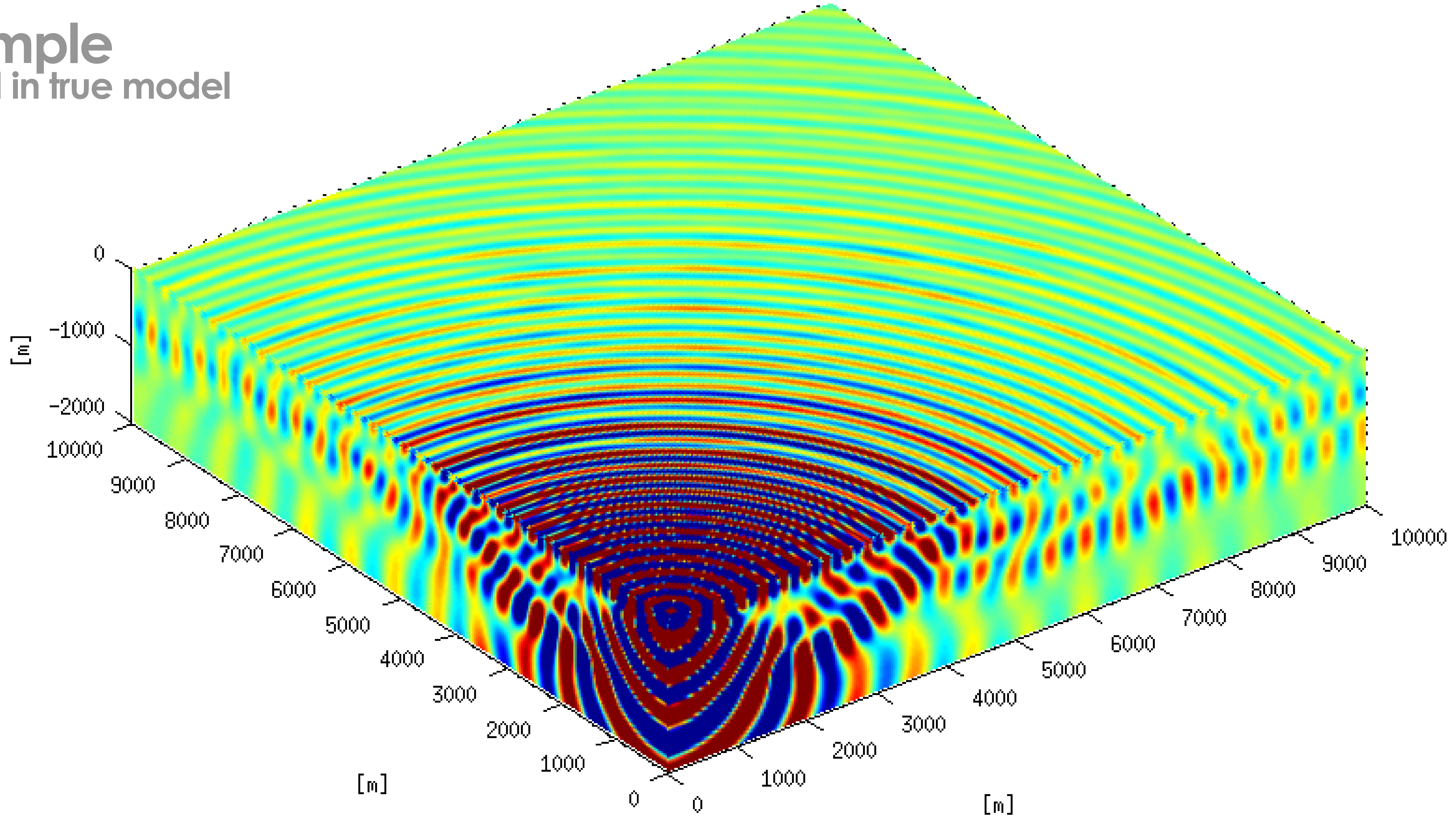


3D Example
– true model

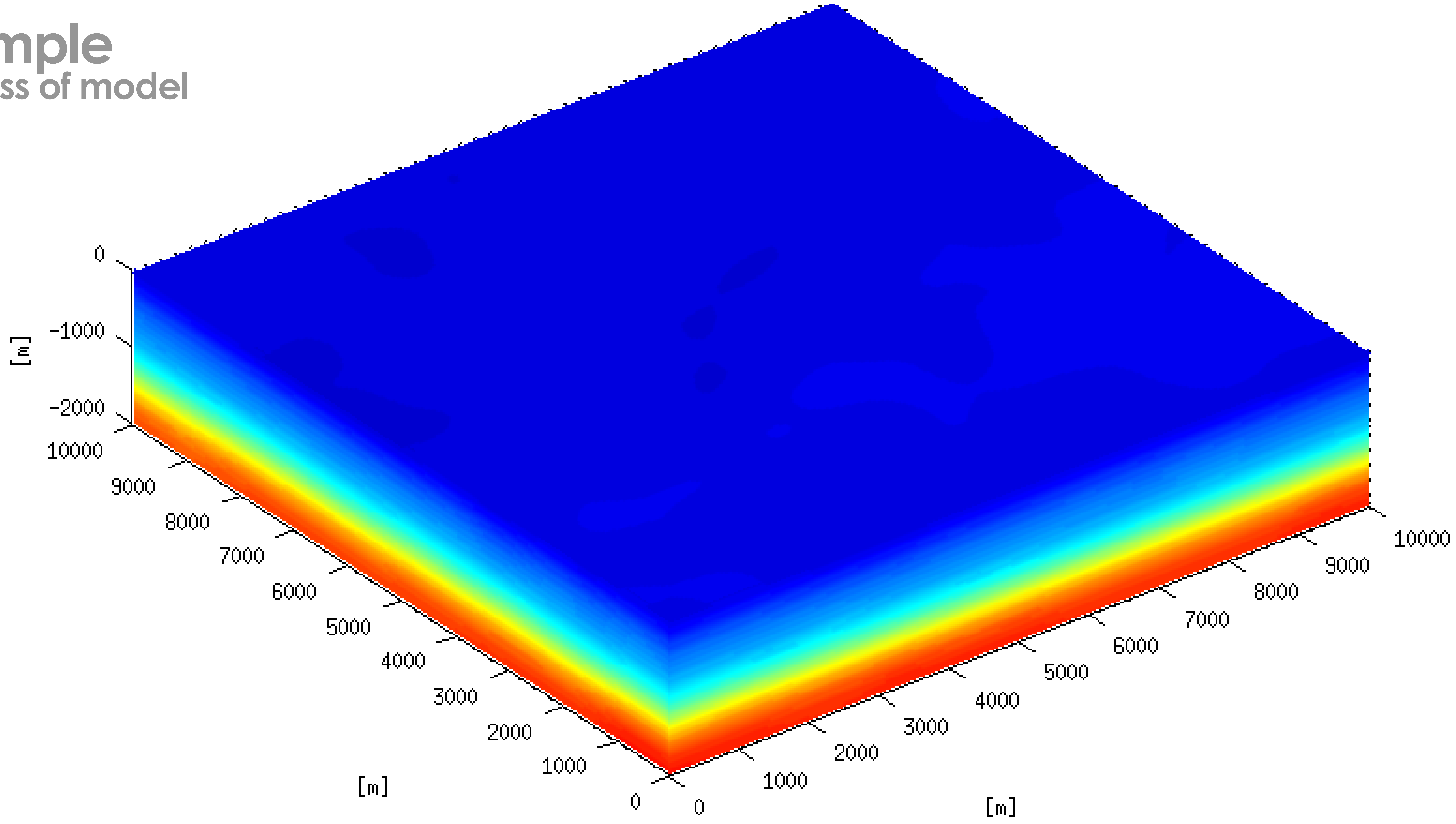


10 x 10 x 2 km, 5 Hz, 27-point discretization, ~1e7 grid points, source at [0,0,0]

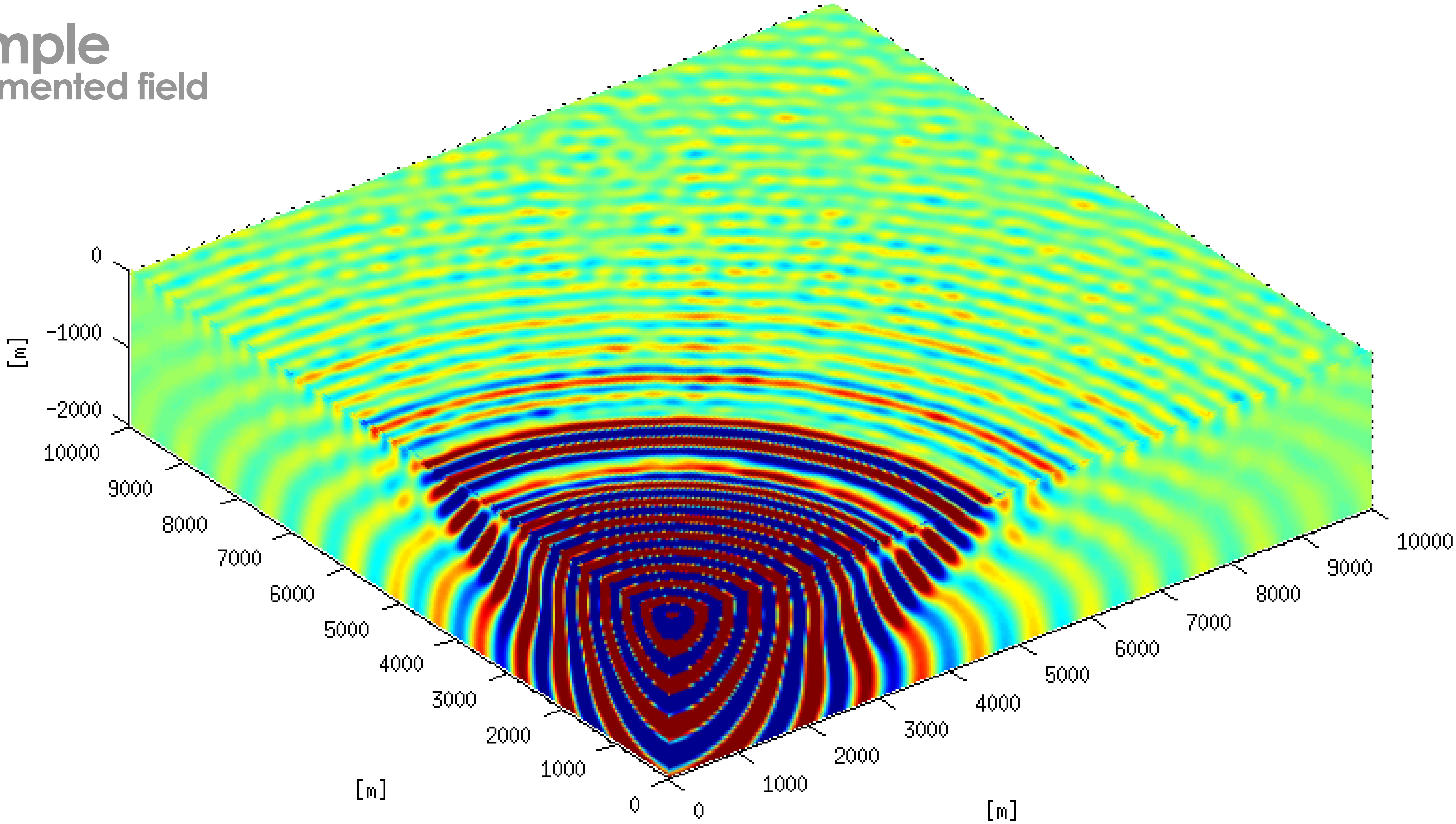
3D Example
– wavefield in true model



3D Example
– initial guess of model



3D Example
– data-augmented field



Conclusions

- Enabler for 3D parameter estimation using a quadratic-penalty method.

- There is potential for randomization and subsampling to reduce the computational cost and memory requirements.

- Proposed algorithm might be used for other large-scale mildly overdetermined problems with many variables & few constraints.

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