Pros and Cons of Full- and Reduced-space Methods for Wavefield Reconstruction Inversion

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SIAM Conference on Mathematical and Computational Issues in the Geosciences
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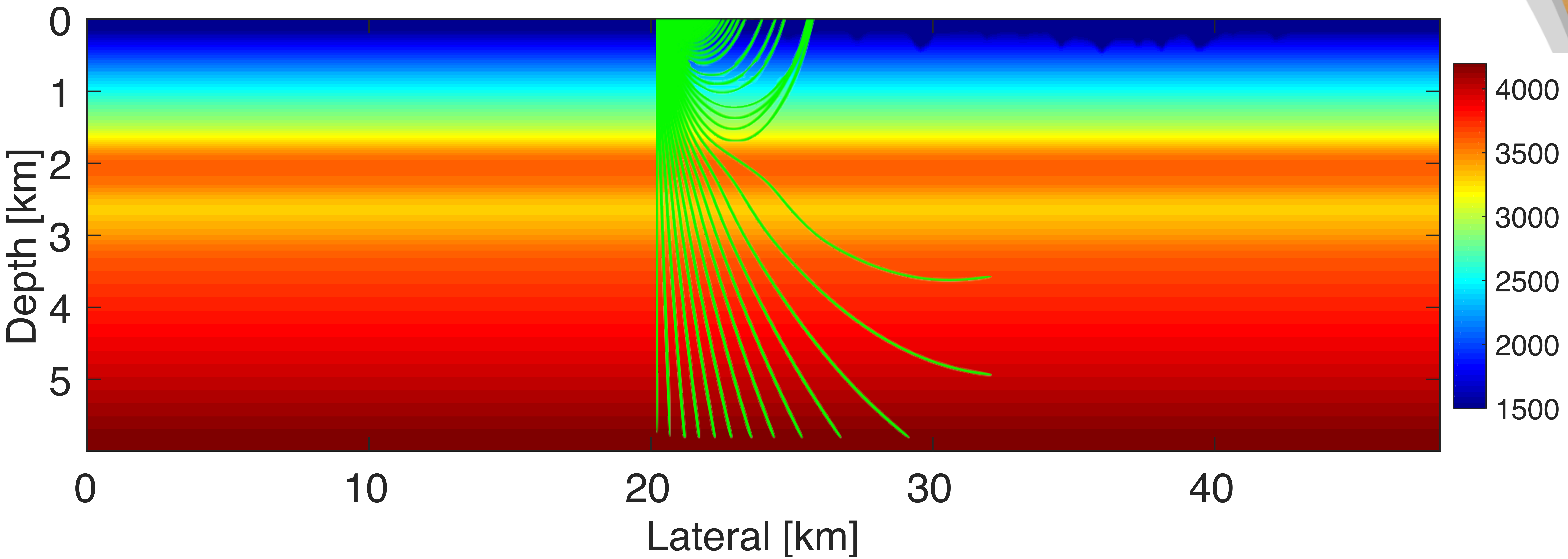
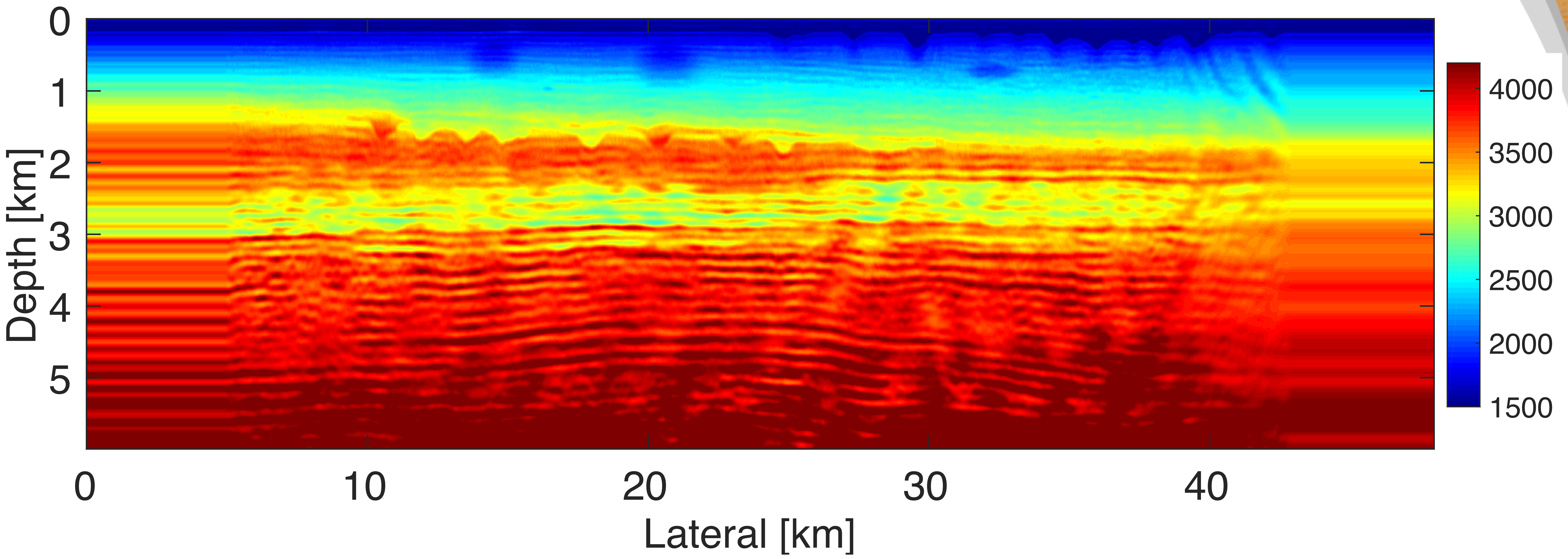
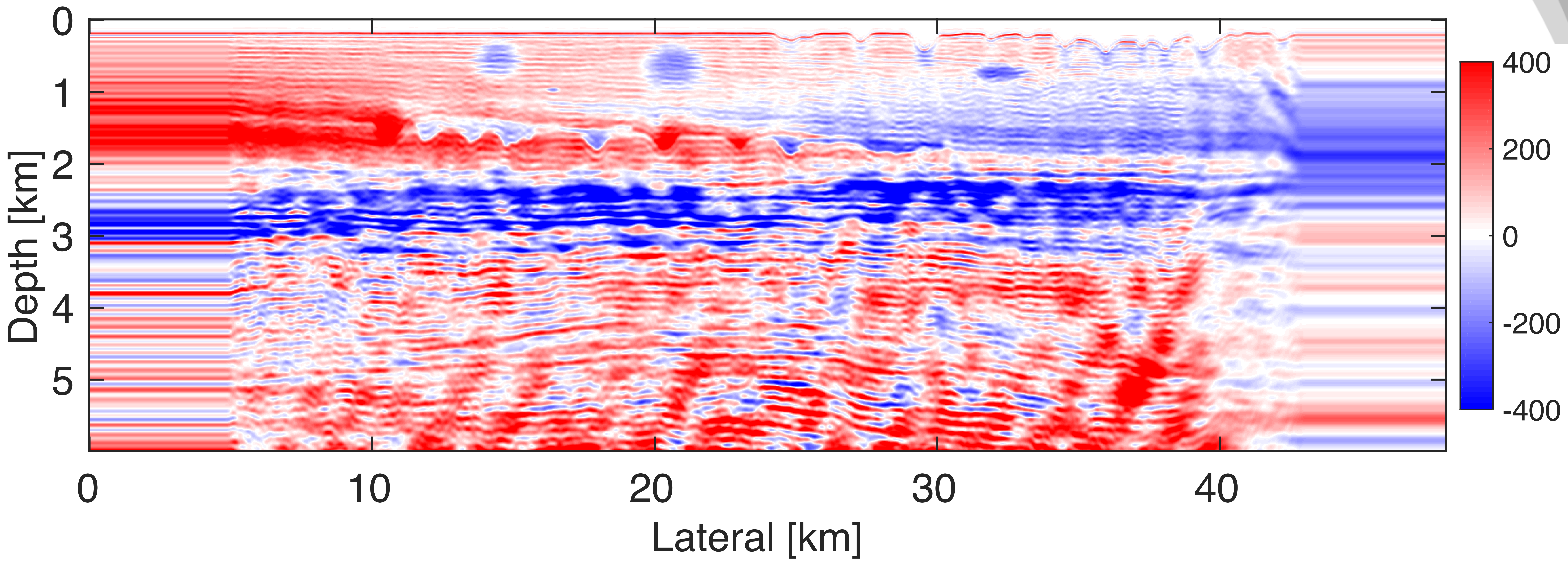
Initial model



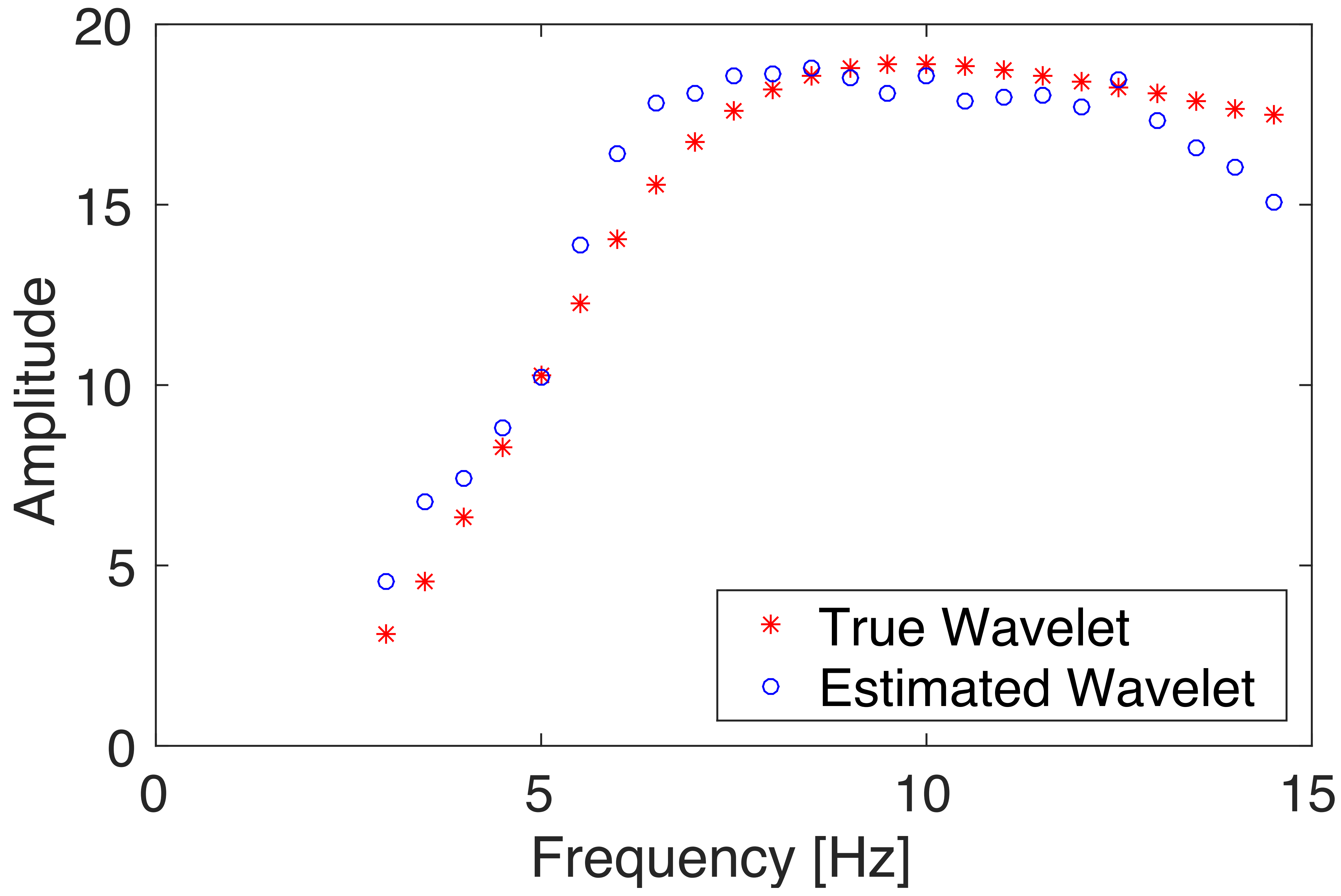
Inversion result



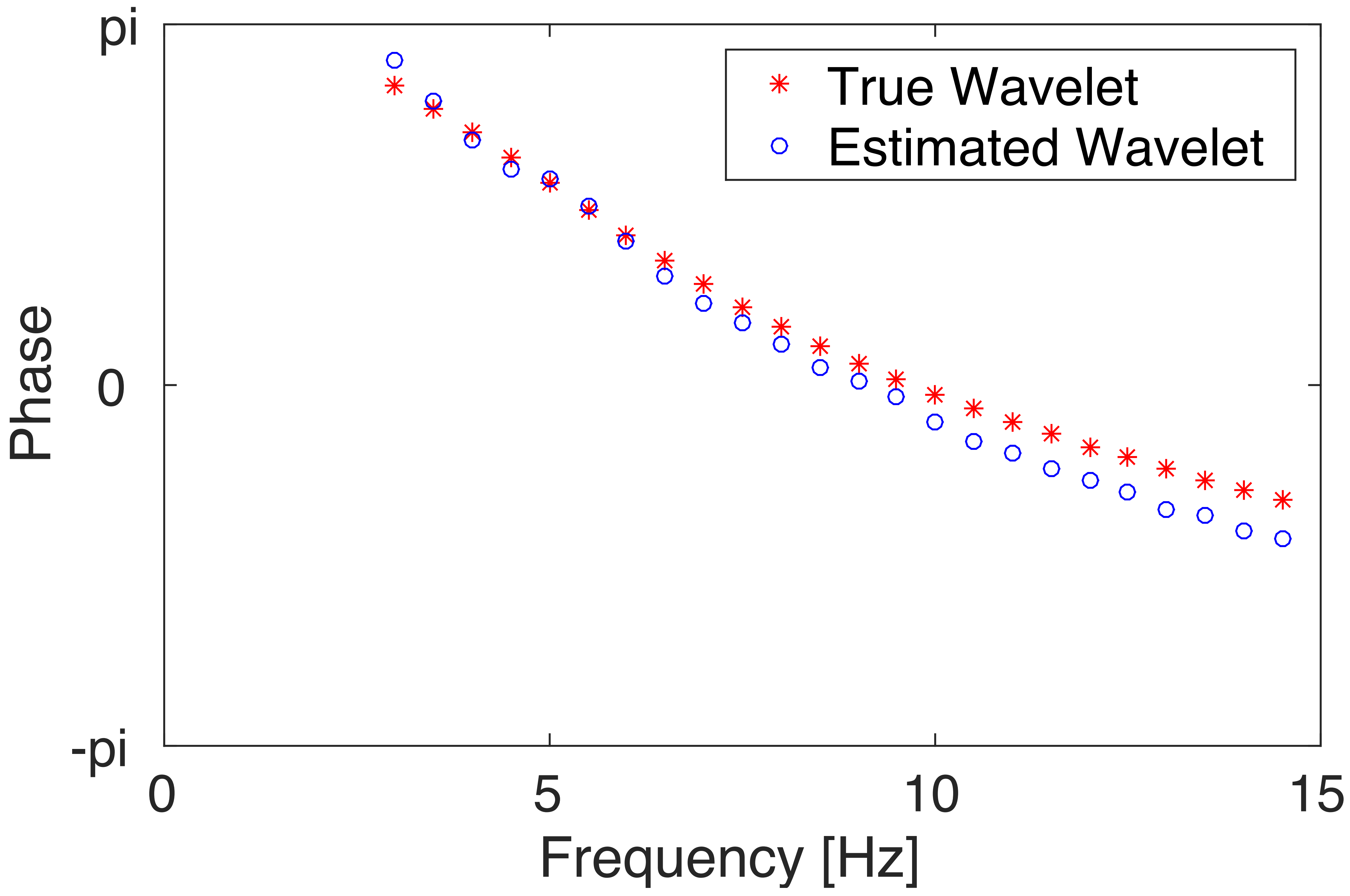
Model update



Source wavelet comparison



Amplitude



Phase

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

PDE-constrained optimization

Use the 'discretize-then-optimize' framework:

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

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

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

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

All-at-once full-space: [E. Haber & U.M. Ascher, 2001 ; G. Biros & O. Ghattas , 2005 ; Grote et. al., 2011]

- update fields, medium parameters & multipliers simultaneously
- function value, gradient, Hessian evaluation is ~free & exact
- sparse Hessian
- requires storage of all fields & multipliers + working memory (gradients, Hessian & update direction)
- updates are computationally demanding

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

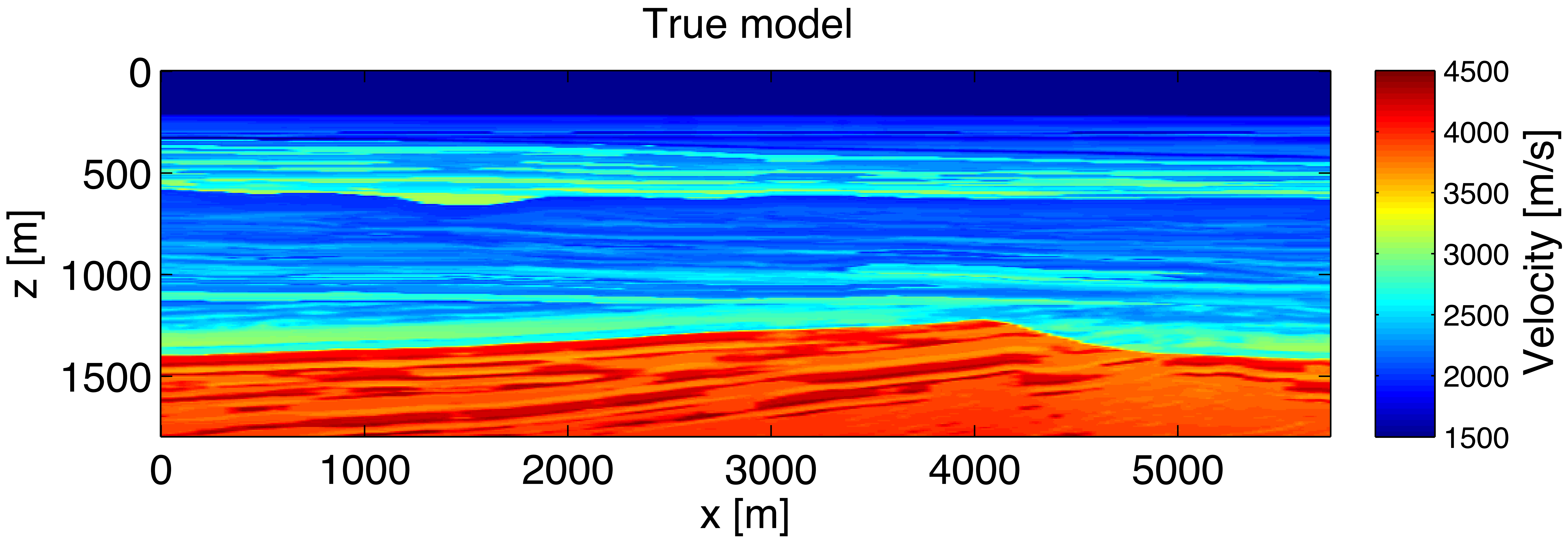
$$\mathcal{L}(\mathbf{m},\mathbf{u},\mathbf{v}) = \frac{1}{2}\|P\mathbf{u}-\mathbf{d}\|_2^2 + \mathbf{v}^*\left(H(\mathbf{m})\mathbf{u}-\mathbf{q}\right)$$

eliminate field variables

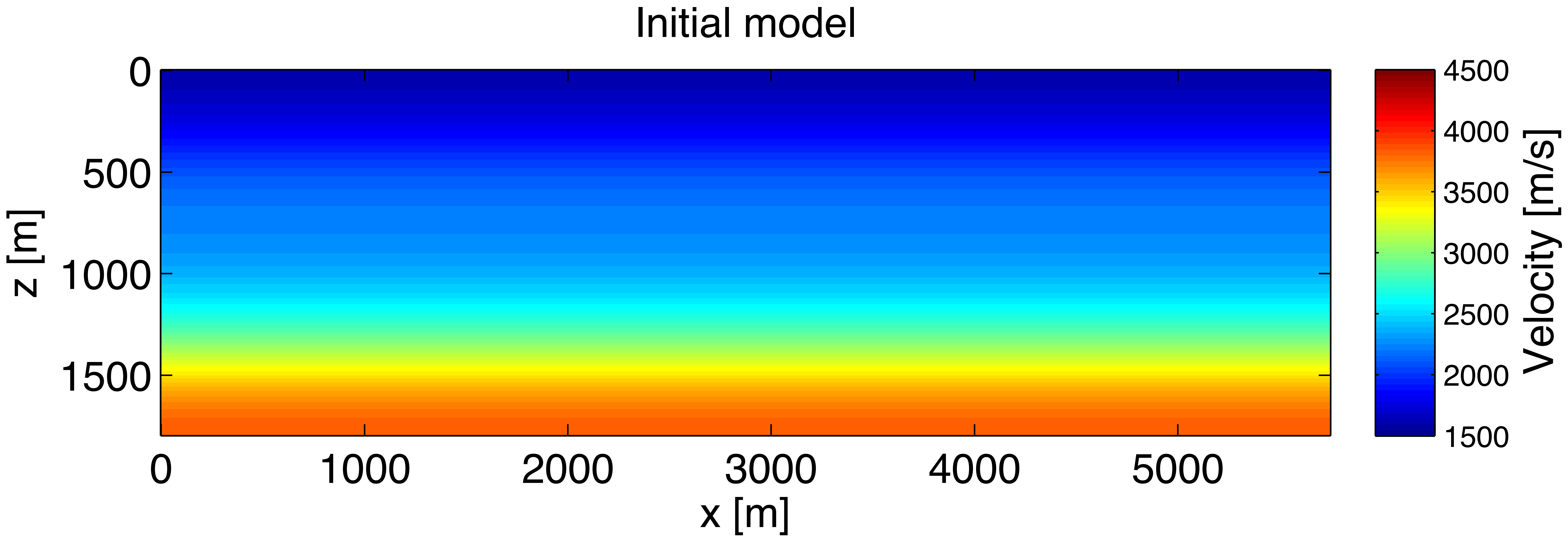
$$\min_{\mathbf{m}} \frac{1}{2}\|PH(\mathbf{m})^{-1}\mathbf{q}-\mathbf{d}\|_2^2$$

Reduced space: [Tarantola, ’84; Haber et al., ‘00; Epanomeritakis et al., ‘08]

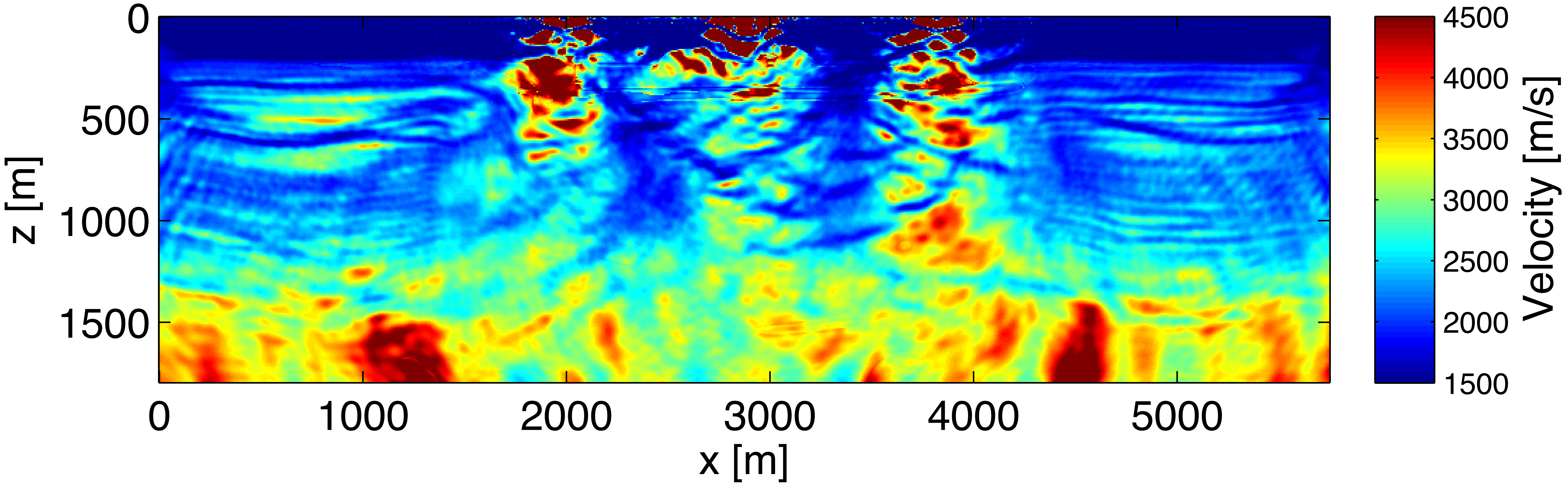
- storage as low as two fields at a time
- highly nonlinear in **m** & non-convex
  - expensive “exact” forward & adjoint solves for each iteration
  - inexact when sub-problems are solved iteratively
- dense reduced-Hessian
- requires extra safeguards/accuracy control [T. van Leeuwen & F.J. H ‘14]
- **reliance on accurate starting models to avoid cycle skipping**



Example from **[Peters et al. 2014]**



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



Few algorithms have quadratic-penalty form:
[R.E. Kleinman & P.M. van den Berg, '92 ; T. van Leeuwen & F.J.H, '13]

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

$$\downarrow$$

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

$$\downarrow$$

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

[T. van Leeuwen & F.J.H. '13,'15]

$$\downarrow$$

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

reduced quadratic-penalty

Penalty method:

- no need to store all the fields (u)
- no adjoint solves
- sparse approximation of Gauss-Newton Hessian for small λ
- less non-linear in **m**
- **need to solve data-augmented wave equation**

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

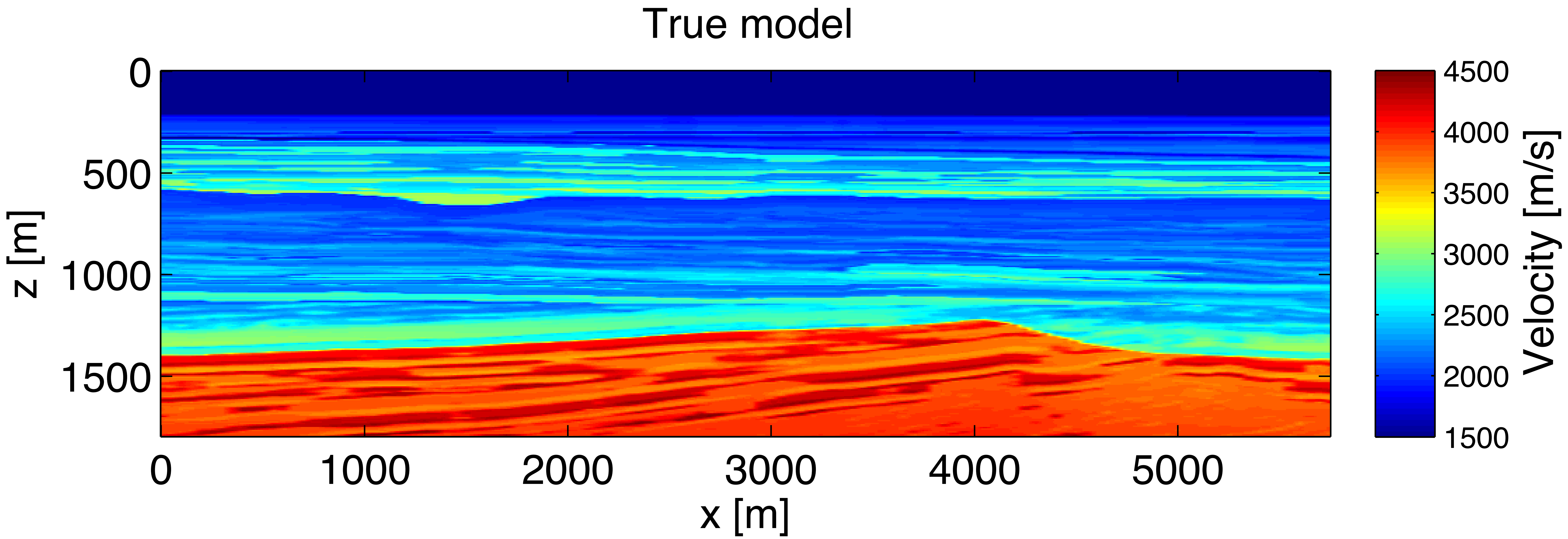
Reduced-space quadratic-penalty method
– Wavefield Reconstruction Inversion (WRI)

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

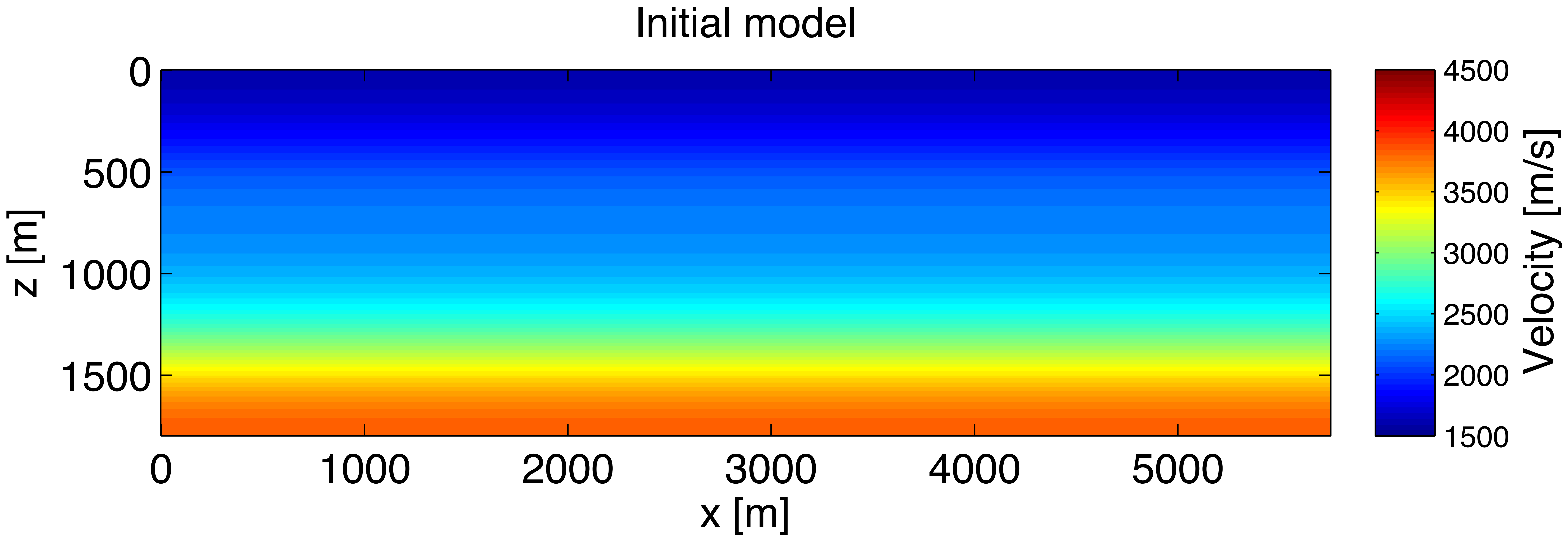
at every iteration

- 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 $\mathbf{m}$

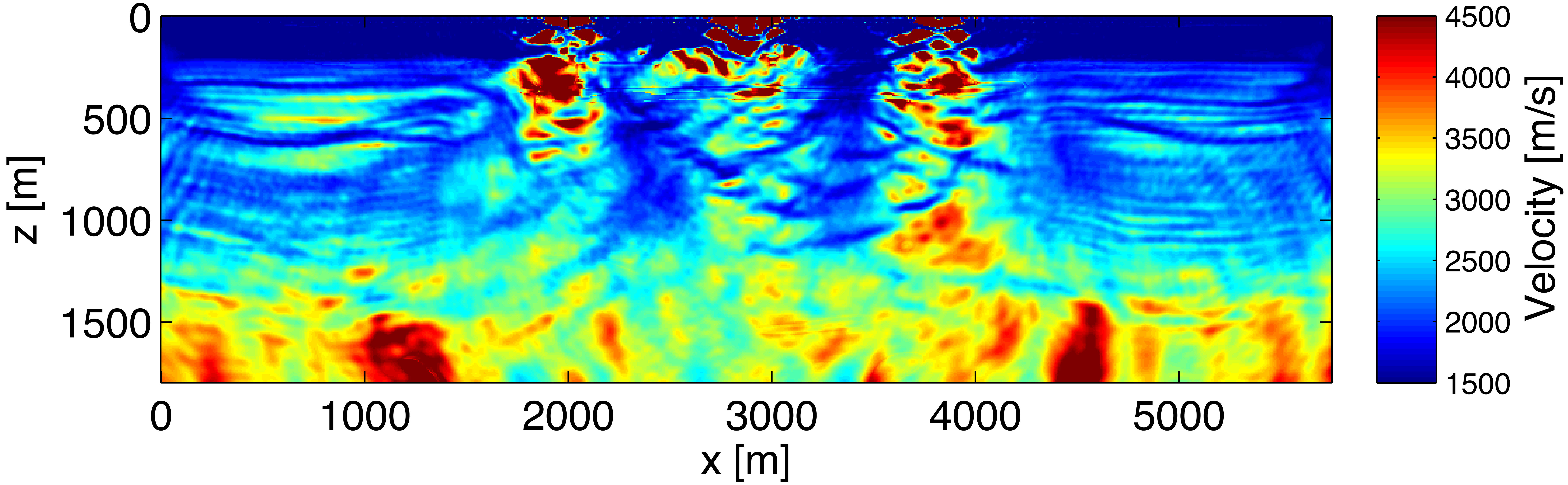
+ trust-region / line-search



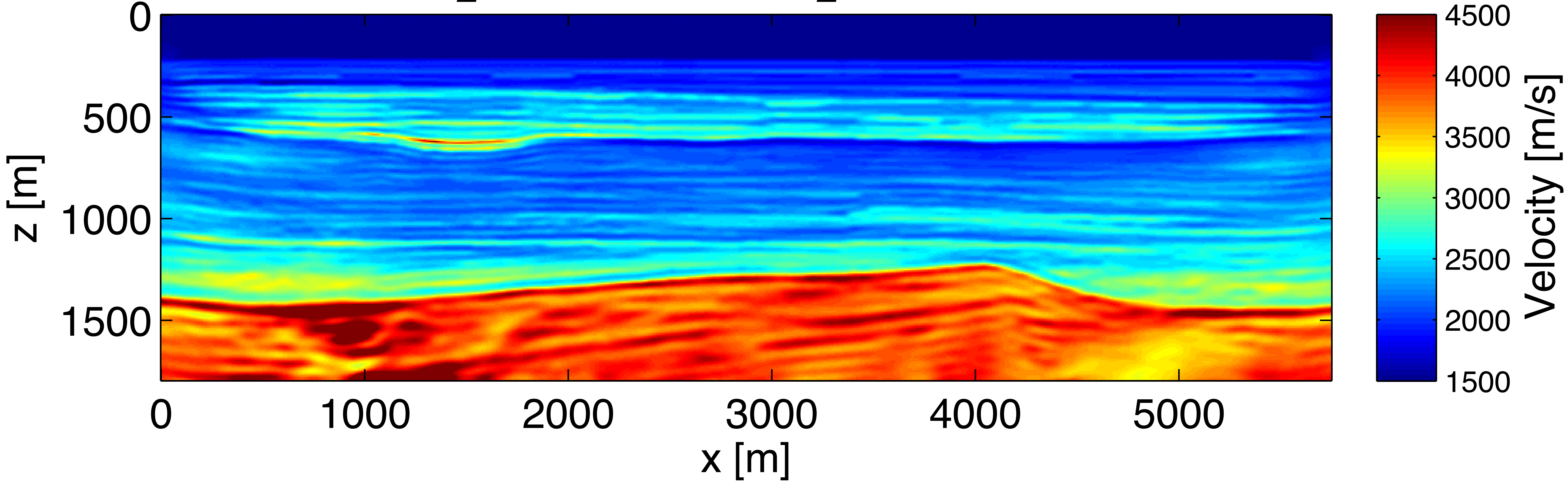
Example from [Peters et al. 2014]



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



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



Reduced-space sub-problems

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

In 3D we have iterative & inexact solves:

- variable elimination & projection are assumed exact
- inaccuracy may cause problems in reduced-space methods
  - how accurate do we need to be?
  - can we change the accuracy per iteration?
- costs are dominated by accuracy & # of source experiments
- heuristic solutions proposed in frugal approaches
  [T. van Leeuwen & F.J. Herrmann, 2014]

Inexact PDE solves
– full-space vs reduced-space

reduced-space:

- error in objective function value
- error in gradient
- error in Hessian

→ error in medium parameter update

full-space:

- objective function value always exact
- gradient always exact
- Hessian always exact

→ globally convergent inexact Newton methods
[S.C. Eisenstat & H.F. Walker, 1994]

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Quadratic-penalty full space methods

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

Newton's method:

$$\begin{pmatrix} P^*P + \lambda^2 H^* H & \nabla^2_{\mathbf{u},\mathbf{m}}\phi \\ \nabla^2_{\mathbf{m},\mathbf{u}}\phi & \lambda^2 G^*_{\mathbf{m}} G_{\mathbf{m}} \end{pmatrix} \begin{pmatrix} \delta\mathbf{u} \\ \delta\mathbf{m} \end{pmatrix} = -\begin{pmatrix} P^*(P\mathbf{u}-\mathbf{d}) + \lambda^2 H^*(H\mathbf{u}-\mathbf{q}) \\ \lambda^2 G^*_{\mathbf{m}}(H\mathbf{u}-\mathbf{q}) \end{pmatrix}$$

updates for medium parameters

updates for all fields

How to solve?

Quadratic-penalty based full space methods

Initial attempt: block diagonal approximation

$$\begin{pmatrix} P^*P + \lambda^2 H^*H & 0 \\ 0 & \lambda^2 G_{\mathbf{m}}^* G_{\mathbf{m}} \end{pmatrix} \begin{pmatrix} \delta\mathbf{u} \\ \delta\mathbf{m} \end{pmatrix} = - \begin{pmatrix} P^*(P\mathbf{u} - \mathbf{d}) + \lambda^2 H^*(H\mathbf{u} - \mathbf{q}) \\ \lambda^2 G_{\mathbf{m}}^*(H\mathbf{u} - \mathbf{q}) \end{pmatrix}$$

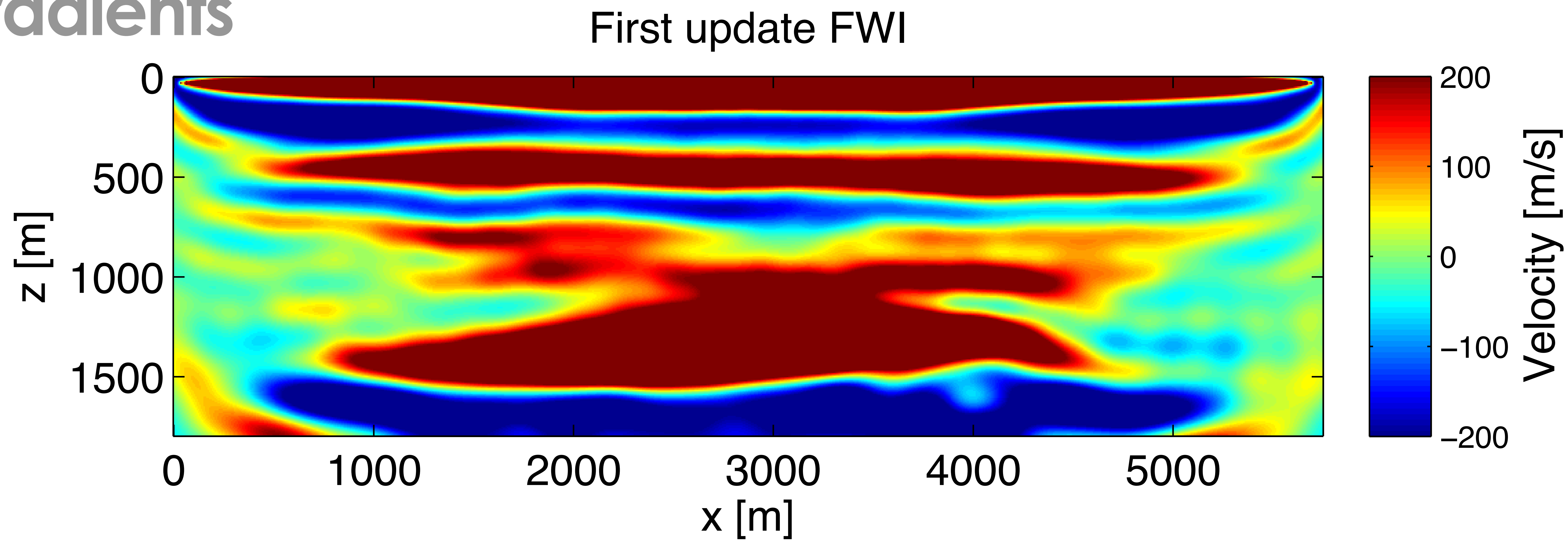
Give up some of Newton's method properties.

Update computation intrinsically parallel per field.

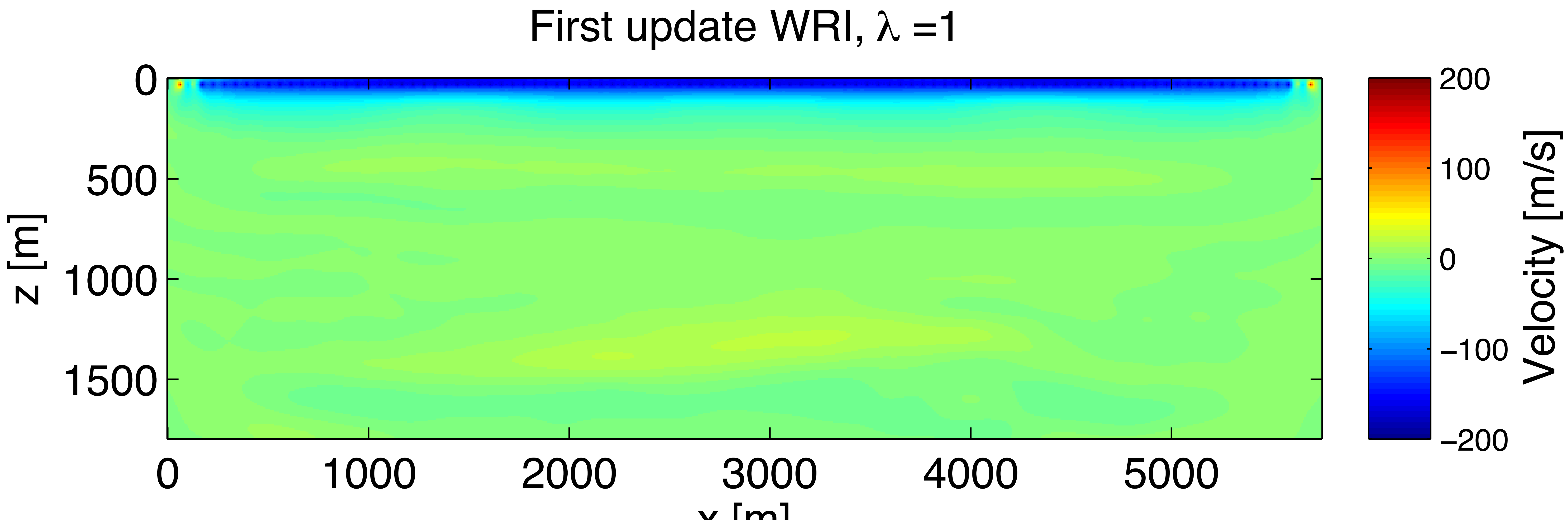
Same as WRI

- if system is solved exactly, and
- fields are initialized by data fit via exact solve data-augmented system

Gradients



First update FWI
z [m]
x [m]
0
500
1000
1500
0
1000
2000
3000
4000
5000
200
100
0
−100
−200
Velocity [m/s]

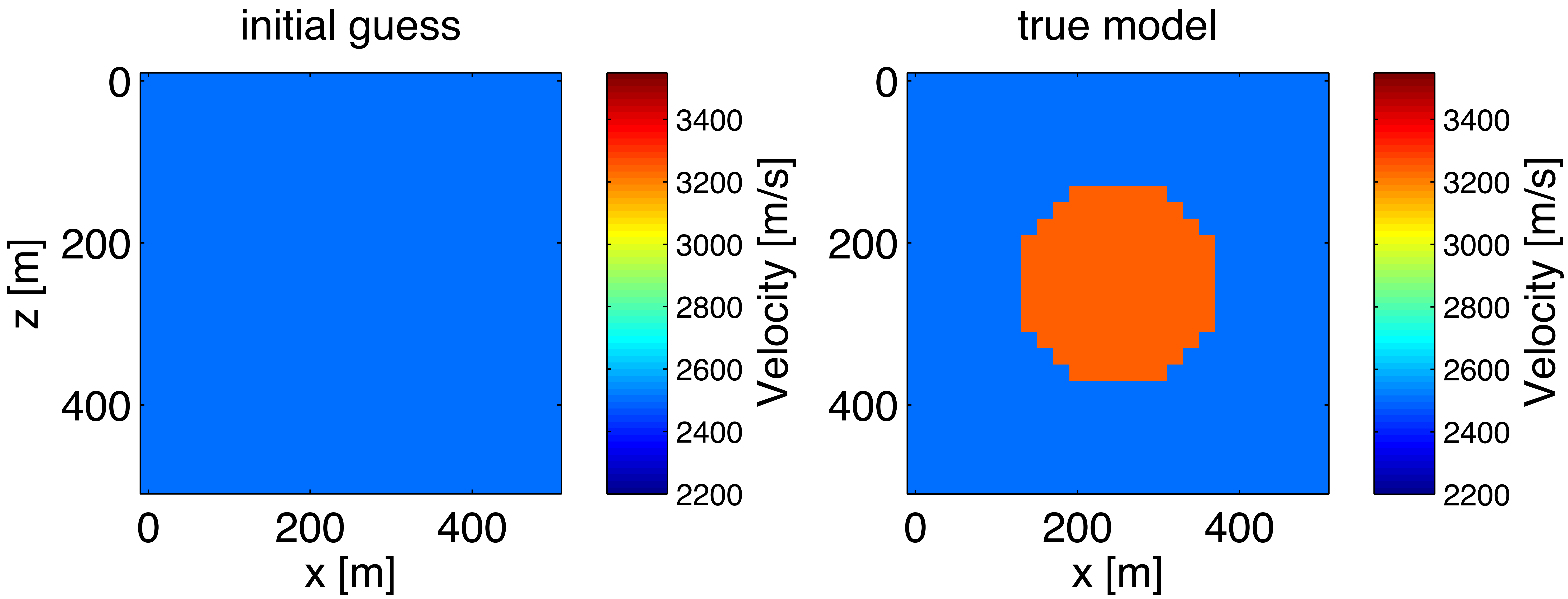


First update WRI, λ =1
z [m]
x [m]
0
500
1000
1500
0
1000
2000
3000
4000
5000
200
100
0
−100
−200
Velocity [m/s]

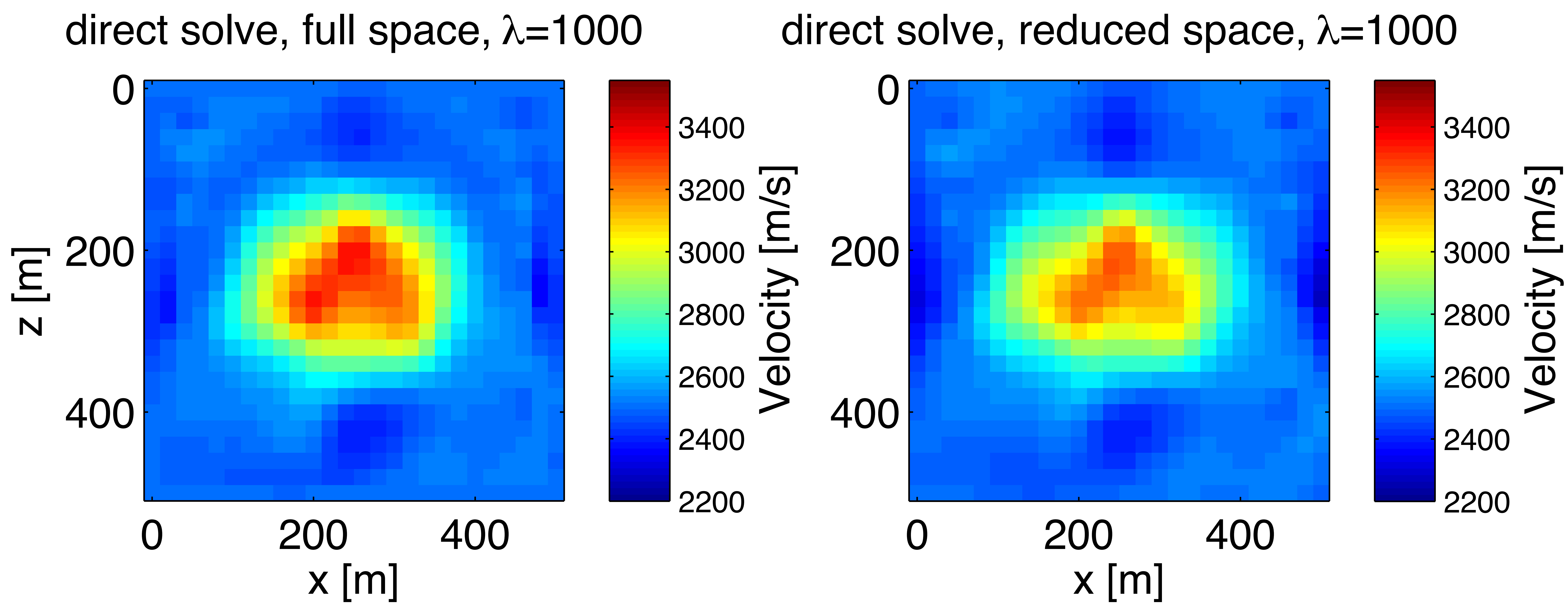
Toy problem

- cross-well setting
- 4 frequencies [6-10] Hz
- 5 simultaneous sources
- 5 receivers

Toy problem

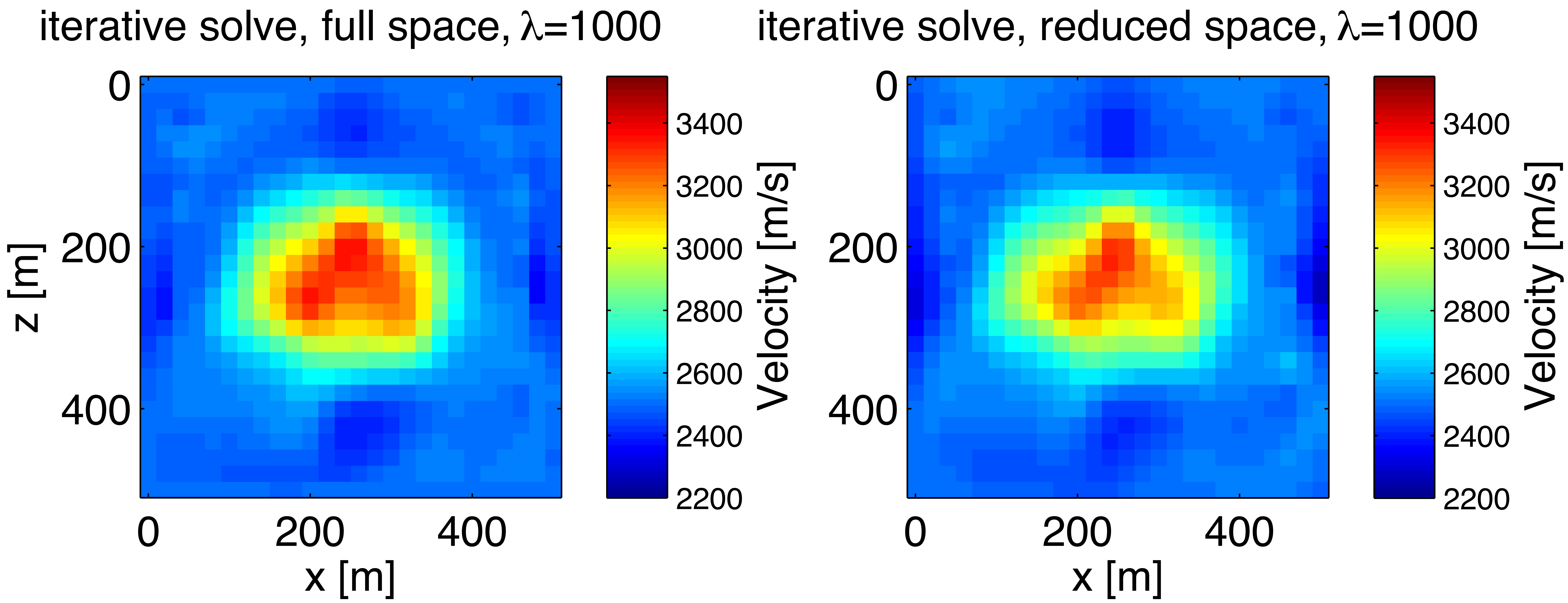

initial guess
true model
z [m]
0
200
400
x [m]
0
200
400
Velocity [m/s]
3400
3200
3000
2800
2600
2400
2200

Toy problem



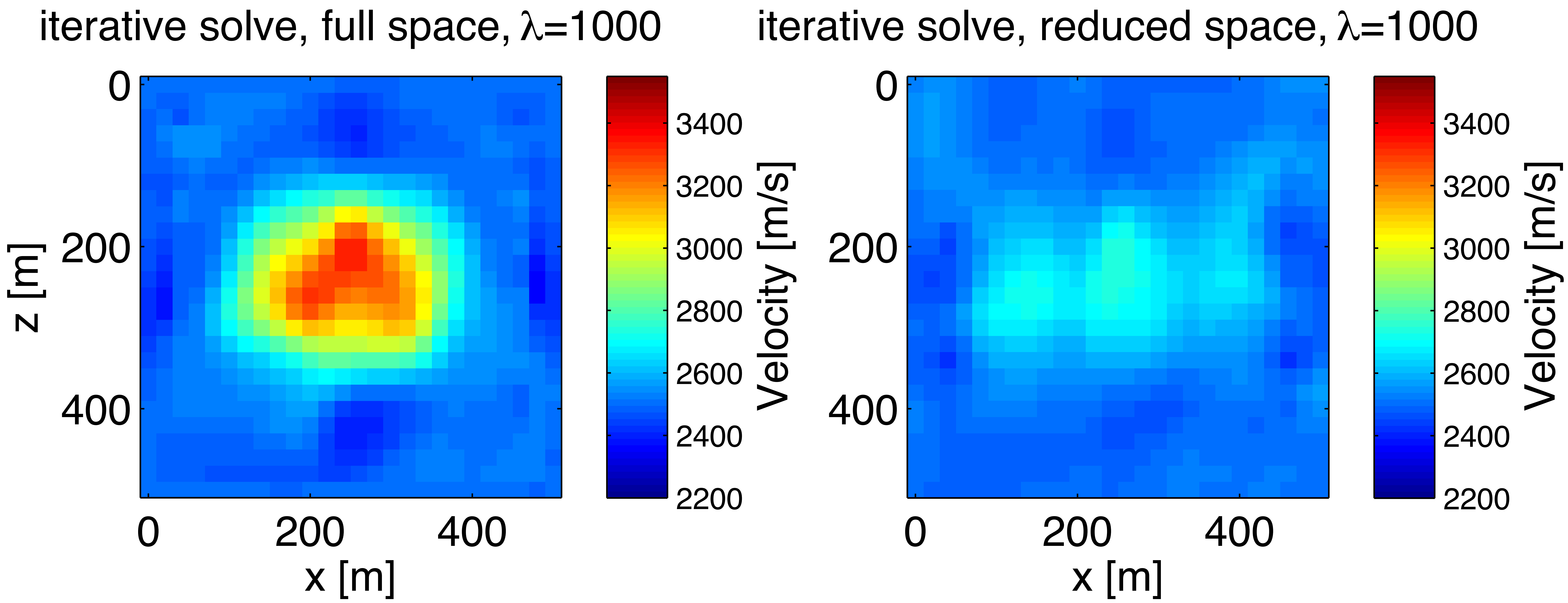
direct solution for least-squares problems

Toy problem



accurate iterative solution for least-squares problems

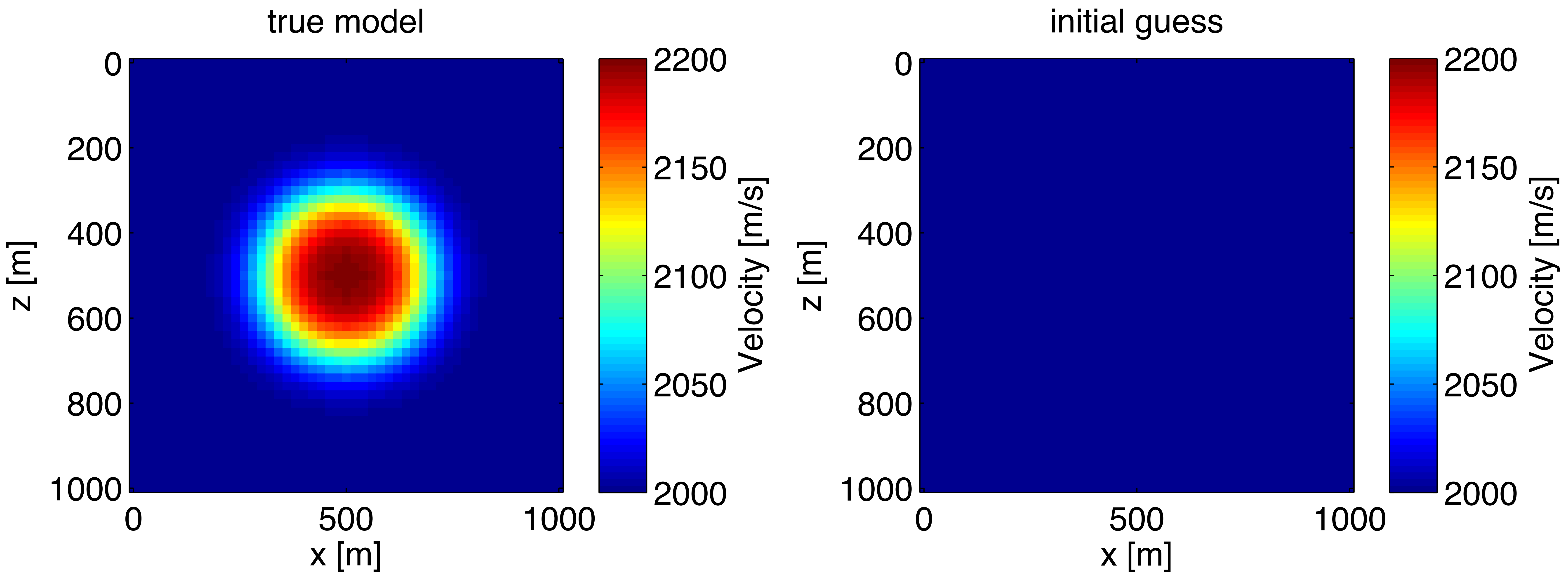
Toy problem



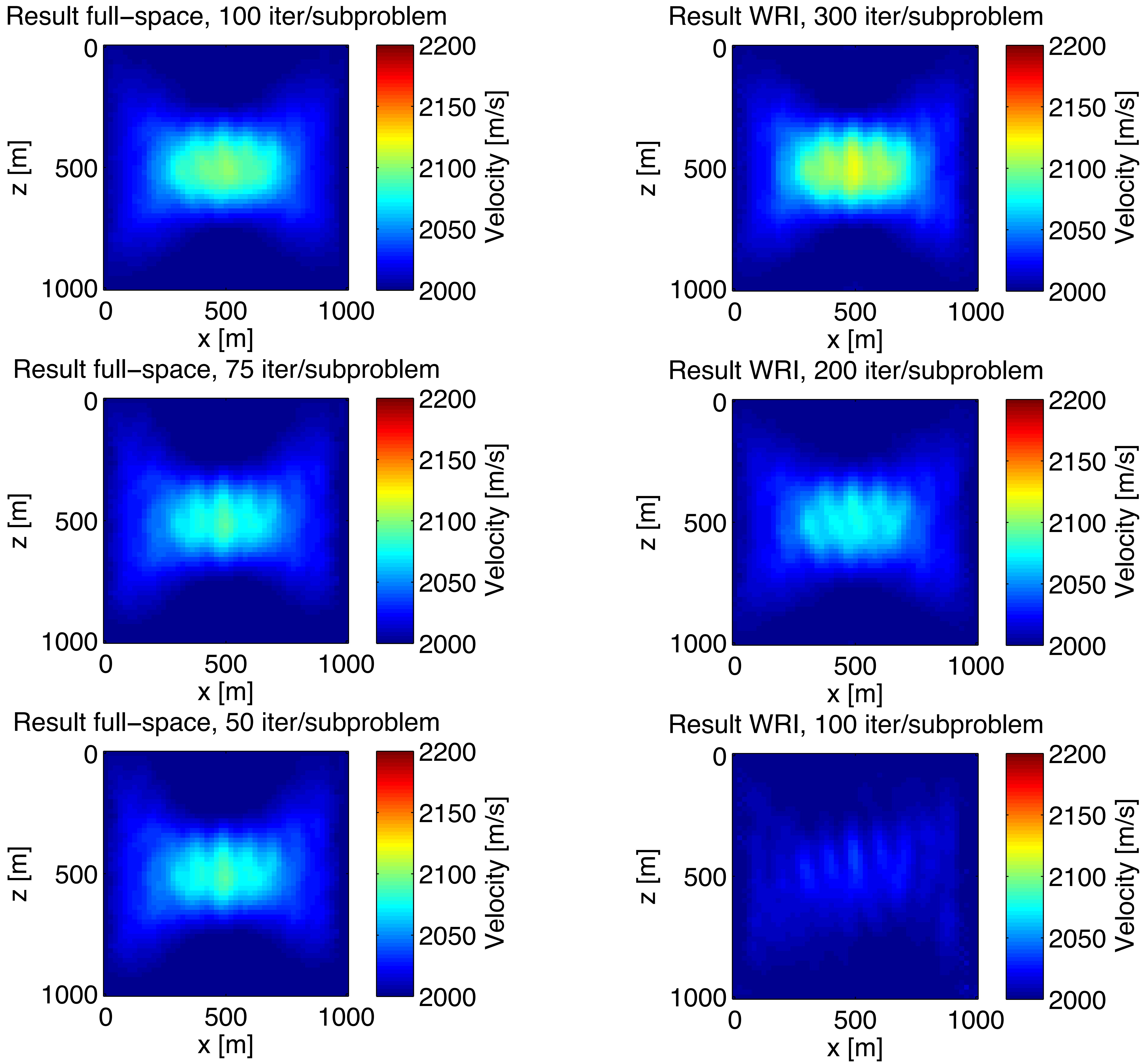
inaccurate iterative solution for least-squares problems

Toy problem

- cross-well setting
- 4 frequencies [4-10] Hz
- 20 sources, 9 receivers

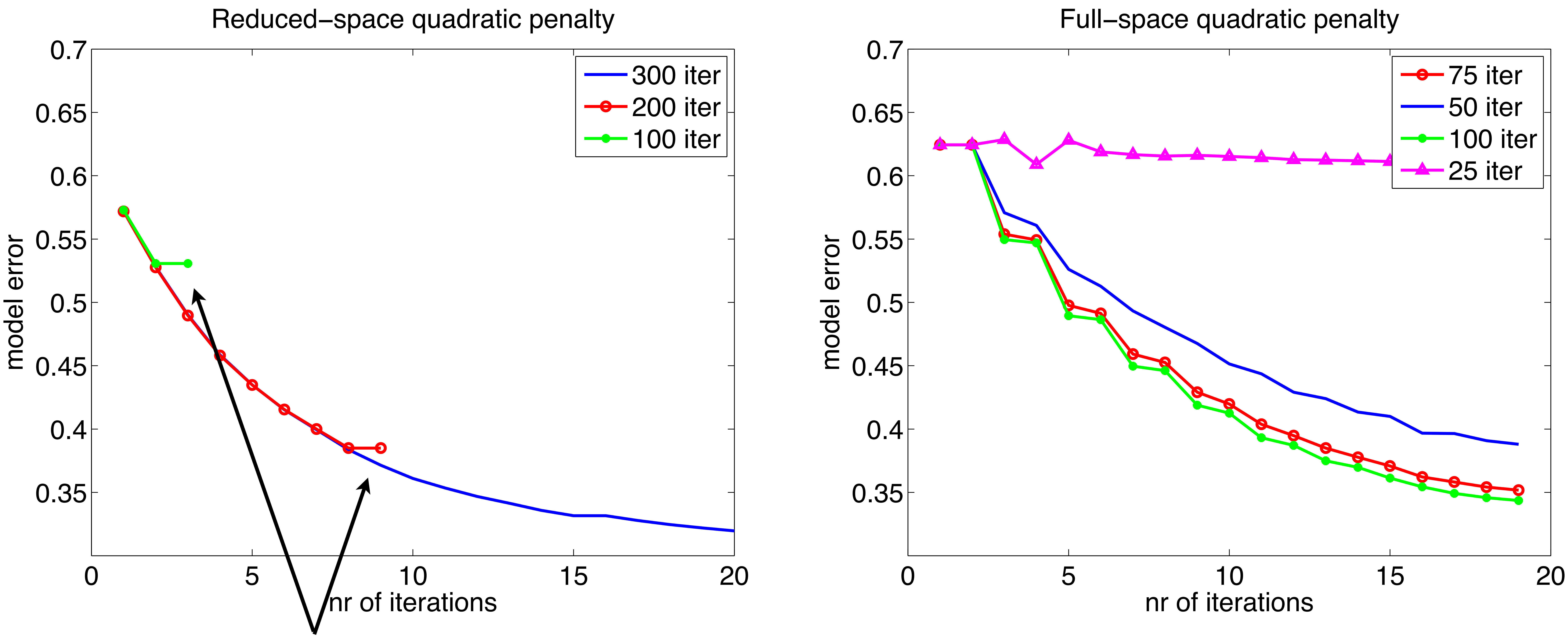


Results



Result full–space, 100 iter/subproblem
Result WRI, 300 iter/subproblem
Result full–space, 75 iter/subproblem
Result WRI, 200 iter/subproblem
Result full–space, 50 iter/subproblem
Result WRI, 100 iter/subproblem
z [m]
x [m]
Velocity [m/s]
0
500
1000
2000
2050
2100
2150
2200

Results:
model error for various iteration budgets for sub-problems



no descent direction found for inaccurate sub-problem solves

Memory requirements

Keep in memory all fields for all frequencies & sources

Can be distributed over multiple nodes

Quadratic-penalty based full-space avoids storage of multipliers, but may not be enough by itself

Feasible? Need

- parallel computing
- simultaneous sources
- stochastic optimization to reduce the working memory
- small frequency batches

Full vs Reduced-space

	Reduced-space FWI	Reduced-space WRI	Full-space
Hessian, gradient & function evaluation	solve PDE's	solve 1 least-squares problem	~free
Hessian, gradient & function evaluation	inexact	inexact	exact
Hessian	dense	sparse + dense	sparse
memory for fields	2 fields per parallel process	1 field per parallel process	all fields in memory (can be distributed over nodes)
working memory	1 gradient & update direction	1 gradient & update direction	update directions & gradients in memory

~free = sparse matrix-vector products

Conclusions

WRI's extends the search space

- less reliant on starting models
- but requires accurate solves

All-at-once methods remain memory intensive

- but less reliant on accurate solves
- still need accurate initialization wavefields by guaranteeing data fits

Bottom line. Not clear which one will perform better... yet.

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

SINBAD

NSERC CRSNG

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