

Simultaneous estimation of wavefields & medium parameters reduced-space versus full-space waveform inversion

Bas Peters, Felix J. Herrmann

Workshop W-12, The limit of FWI in subsurface parameter recovery.
SEG 85TH annual meeting, Friday, 23 October

Motivation

Full-Waveform Inversion (FWI) works well when a good start model and/or low-frequency data is available.

$$\min_{\mathbf{m}} \frac{1}{2} \|PH(\mathbf{m})^{-1}\mathbf{q} - \mathbf{d}\|_2^2 = \frac{1}{2} \|\mathbf{d}_{\text{pred}}(\mathbf{m}) - \mathbf{d}_{\text{obs}}\|_2^2$$

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

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If iterative solvers in frequency domain are used, we cannot compute:

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

Instead we obtain:

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

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Instead we obtain:

$$\hat{\mathbf{u}} = H(\mathbf{m})^{-1}(\mathbf{q} + \mathbf{r}_{\mathbf{u}}) = \underbrace{H(\mathbf{m})^{-1}\mathbf{r}_{\mathbf{u}}}_{\text{error}} + \mathbf{u}$$

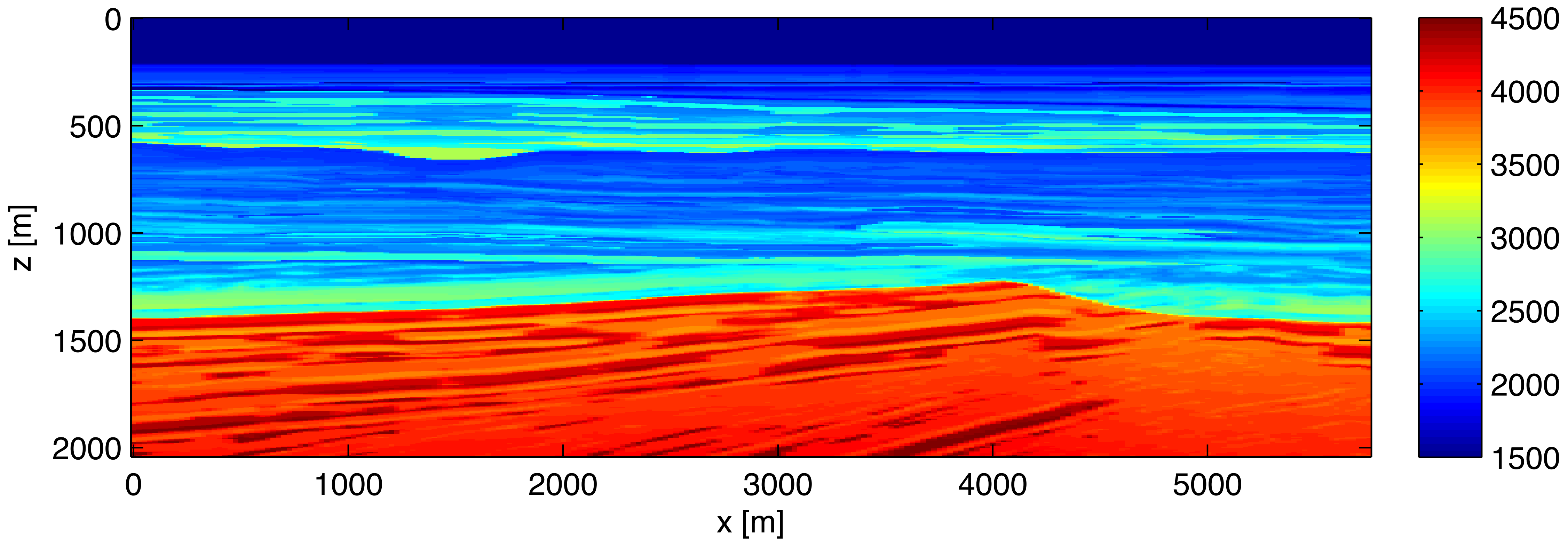
residual
↓

Example

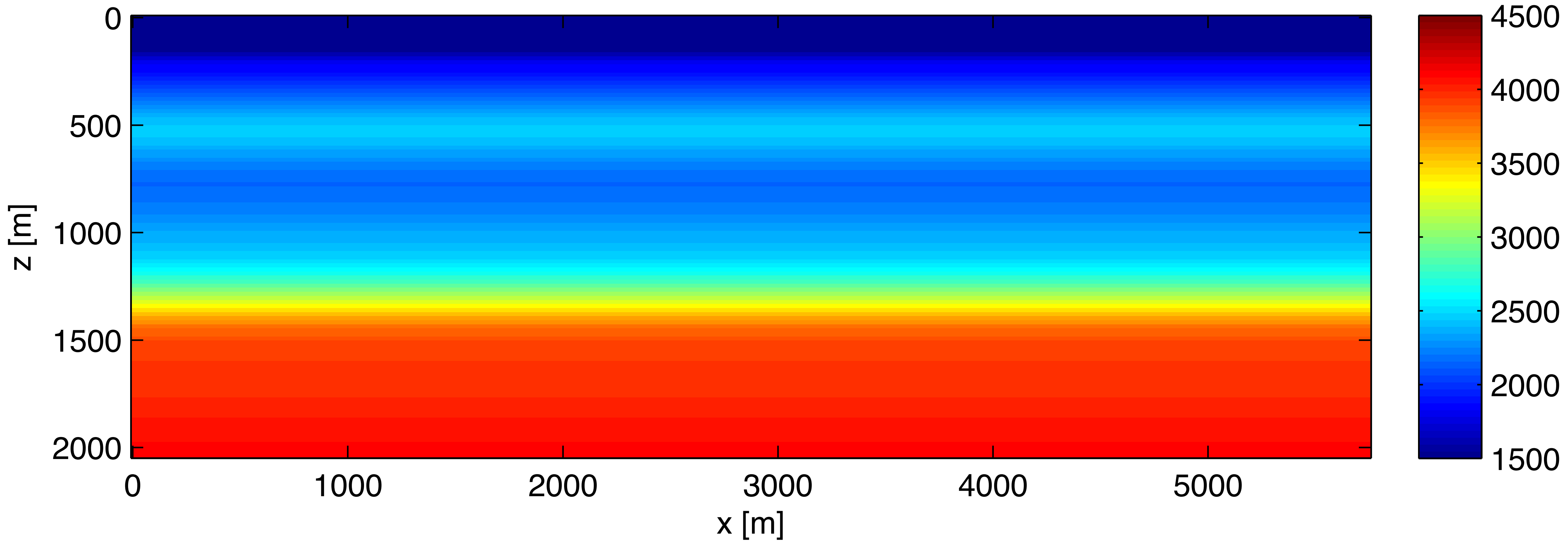
Illustration of what happens when PDE's are solved inaccurately

- 3-15Hz
- good start model
- full-offset source & receiver array
- noise free data

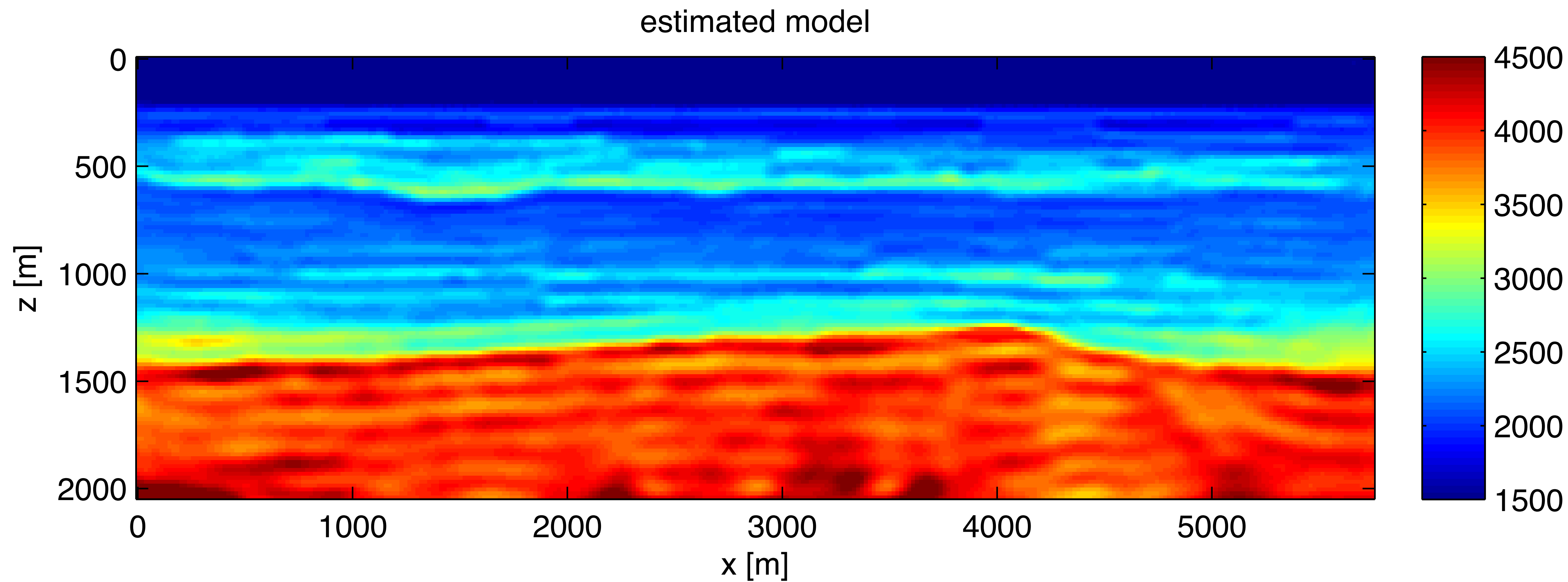
True velocity model



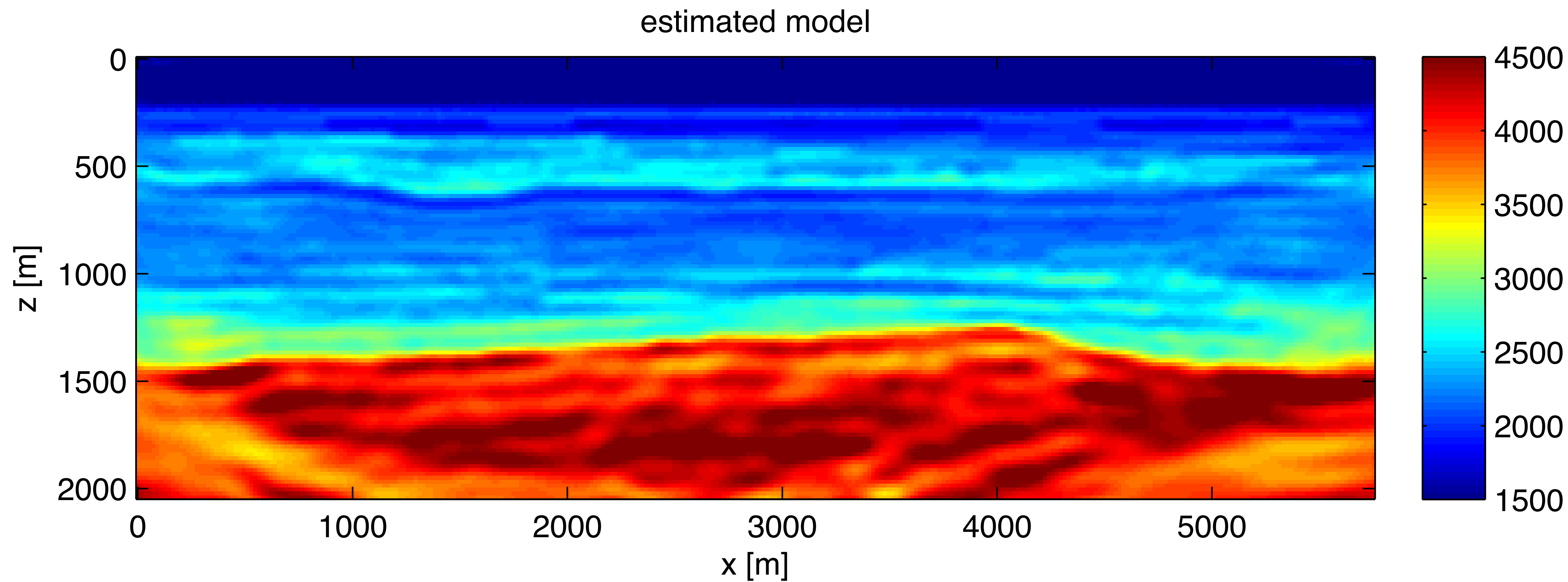
Initial velocity model



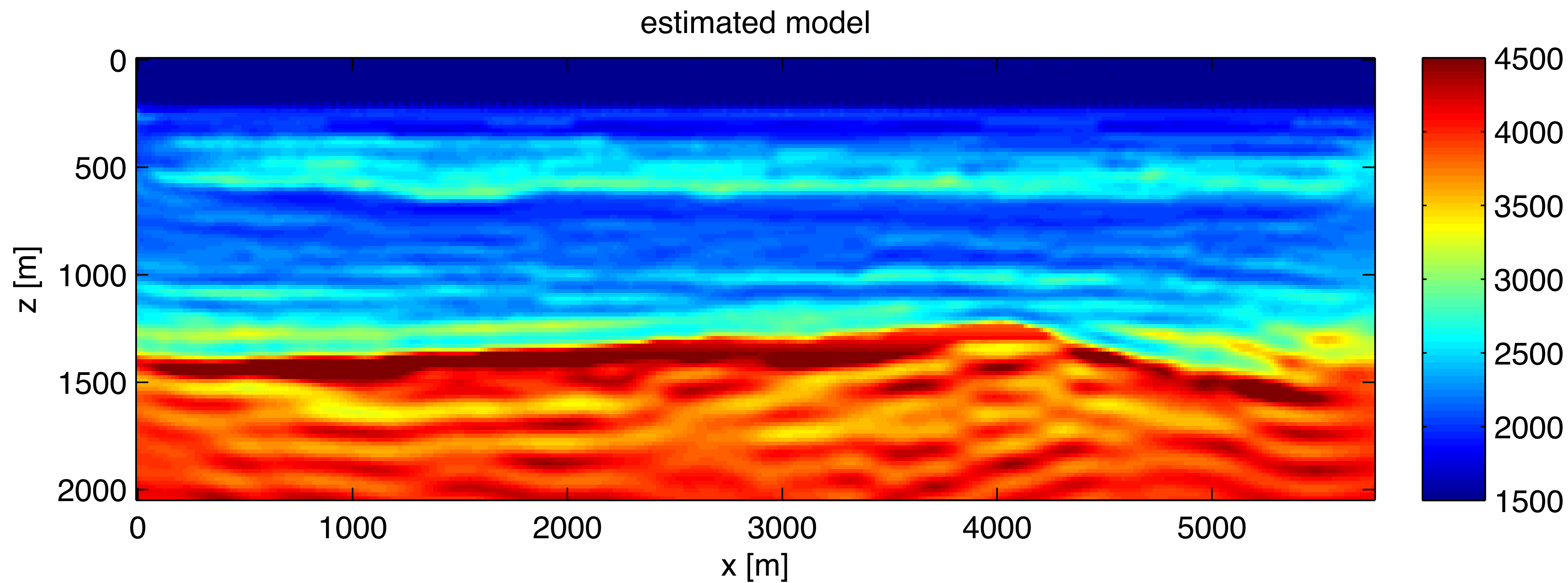
FWI using very accurate iterative solver & LBFGS



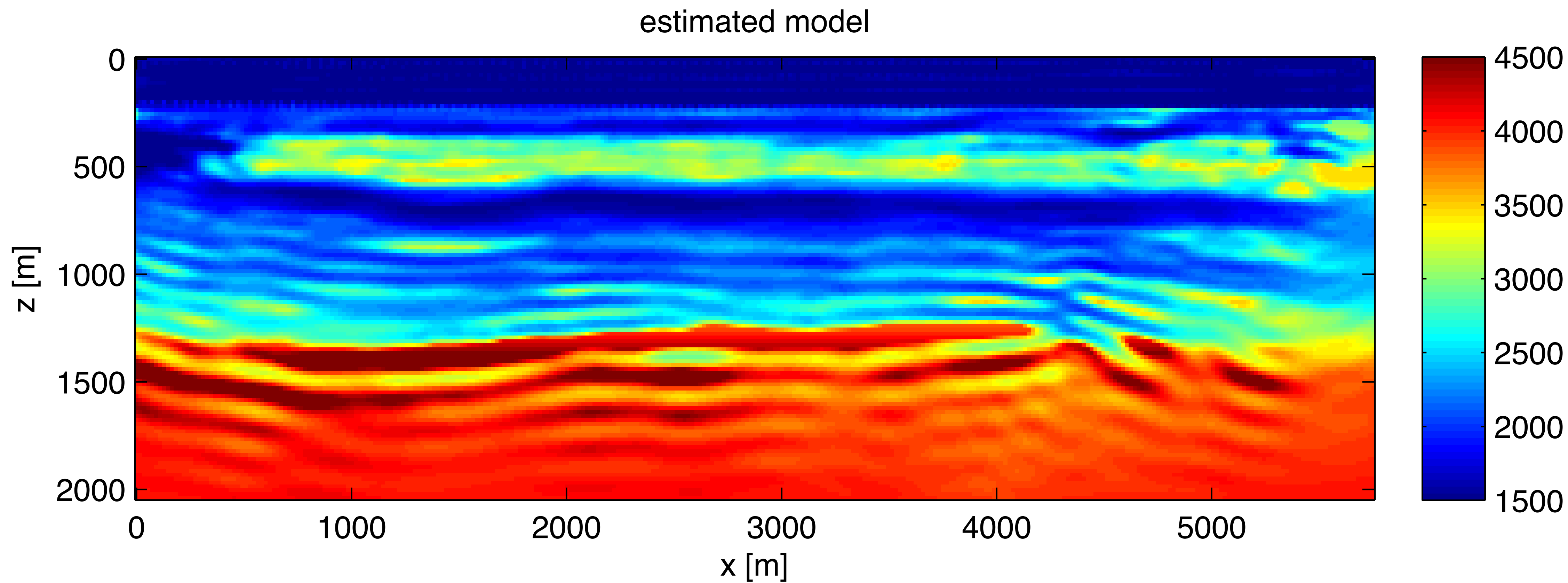
FWI using accurate iterative solver & LBFGS



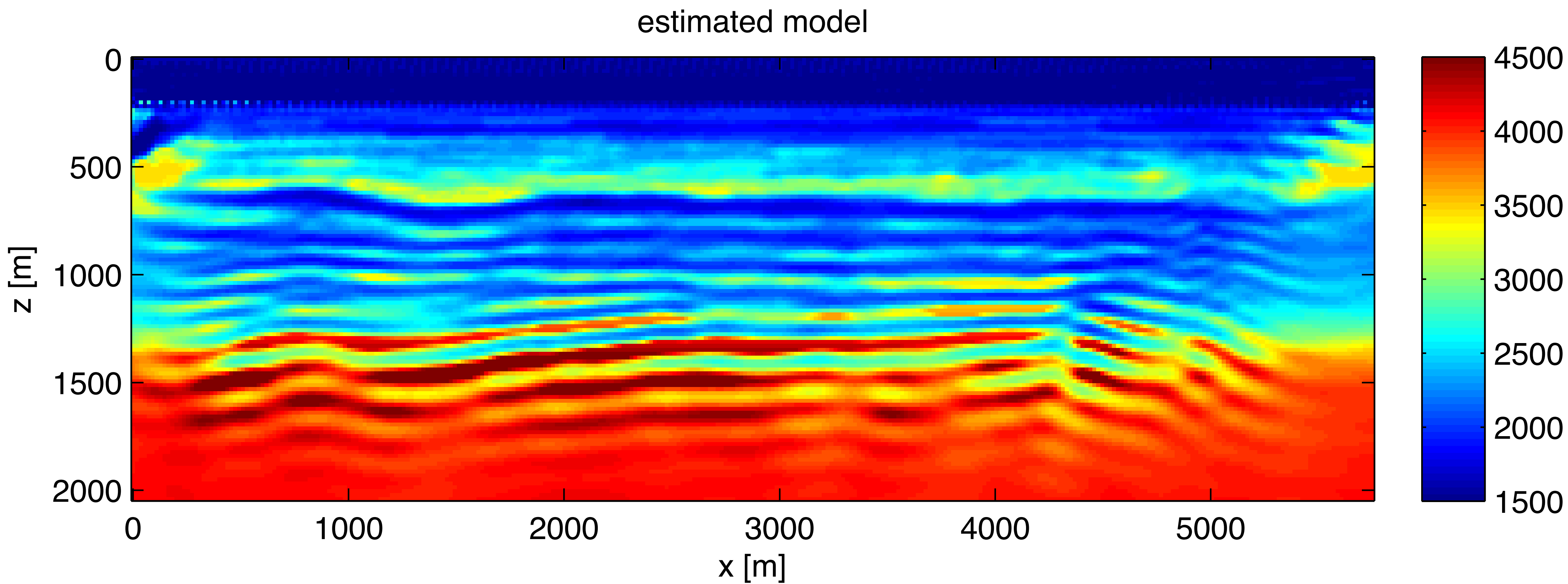
FWI using less accurate iterative solver & LBFGS



FWI using inaccurate accurate iterative solver & LBFGS



FWI using very inaccurate accurate iterative solver & LBFGS



Inexact PDE solves

reduced-space: (includes FWI) [A Tarantola, 1984; E Haber et al., 2000; I Epanomeritakis et al., 2008]

- error in objective function value
 - error in gradient
 - error in Hessian
- error in medium parameter update

- storage as low as two fields at a time
- dense reduced-Hessian
- requires extra safeguards/accuracy control [T. van Leeuwen & F.J. Herrmann, 2014]

Goal

This talk is about deriving an algorithm which:

- allows for inexact solutions of linear systems
- enjoys similar parallelism and memory requirements as FWI

Data, PDE's and constraints

For the true medium parameters and true fields we know that:

$$H(\mathbf{m})\mathbf{u} = \mathbf{q} \ \& \ P\mathbf{u} = \mathbf{d}$$

Many ways to use these equations to form:

- objectives,
- constraints
- algorithms

Adjoint-state based FWI is just one algorithm.

Data, PDE's and constraints

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

Data, PDE's and constraints

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

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

Data, PDE's and constraints

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

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

$$\min_{\mathbf{m}} \frac{1}{2} \|\mathbf{P}\mathbf{H}(\mathbf{m})^{-1}\mathbf{q} - \mathbf{d}\|_2^2 = \frac{1}{2} \|\mathbf{d}_{\text{pred}}(\mathbf{m}) - \mathbf{d}_{\text{obs}}\|_2^2$$

Data, PDE's and constraints

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

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

Data, PDE's and constraints

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

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Multi-experiment structure:

$$\begin{array}{ccc}
 & P\mathbf{u} - \mathbf{d} & H(\mathbf{m})\mathbf{u} - \mathbf{q} \\
 & \downarrow & \downarrow \\
 \begin{pmatrix} P_1 & & & \\ & P_2 & & \\ & & \dots & \\ & & & P_k \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_k \end{pmatrix} - \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \vdots \\ \mathbf{d}_k \end{pmatrix} & \begin{pmatrix} H_1 & & & \\ & H_2 & & \\ & & \dots & \\ & & & H_k \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_k \end{pmatrix} - \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \\ \vdots \\ \mathbf{q}_k \end{pmatrix} & \\
 & & \downarrow \\
 k = n_{\text{src}} \times n_{\text{freq}} & & k \times N \text{ field parameters}
 \end{array}$$

A quadratic-penalty based full space method

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

σ - λ relation is known
[W. Gander, 1980; A. Bjork, 1996]

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

A quadratic-penalty based full space method

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

Newton's method:

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


 updates for for working subset of fields & medium parameters

A quadratic-penalty based full space method

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

- update fields & medium parameters simultaneously
- function value, gradient, Hessian evaluation is ~free & exact
- sparse Hessian
- theory allows for inexact updates computations
- requires storage of working subset of fields
+ working memory (gradients, Hessian & update)
- update computation is challenging

A quadratic-penalty based full space method

Approximate: block diagonal & positive (semi) definite

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

- give up some of Newton's method properties
- update computation intrinsically parallel per field
- no need to form off-diagonal blocks

philosophy: more & cheaper iterations

Memory requirements

save fields for the working subset of frequencies & sources
can be distributed over multiple nodes

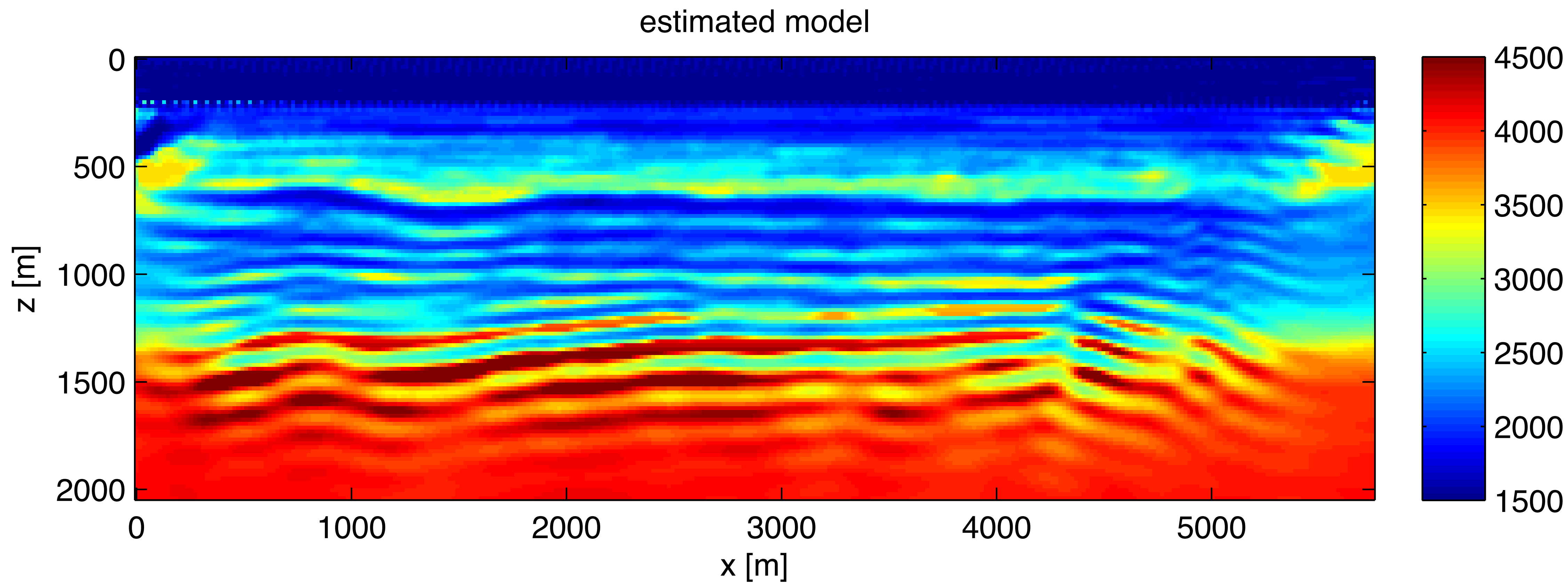
feasible? need

- parallel computing
- **simultaneous sources** (redrawing is possible)
- small frequency batches

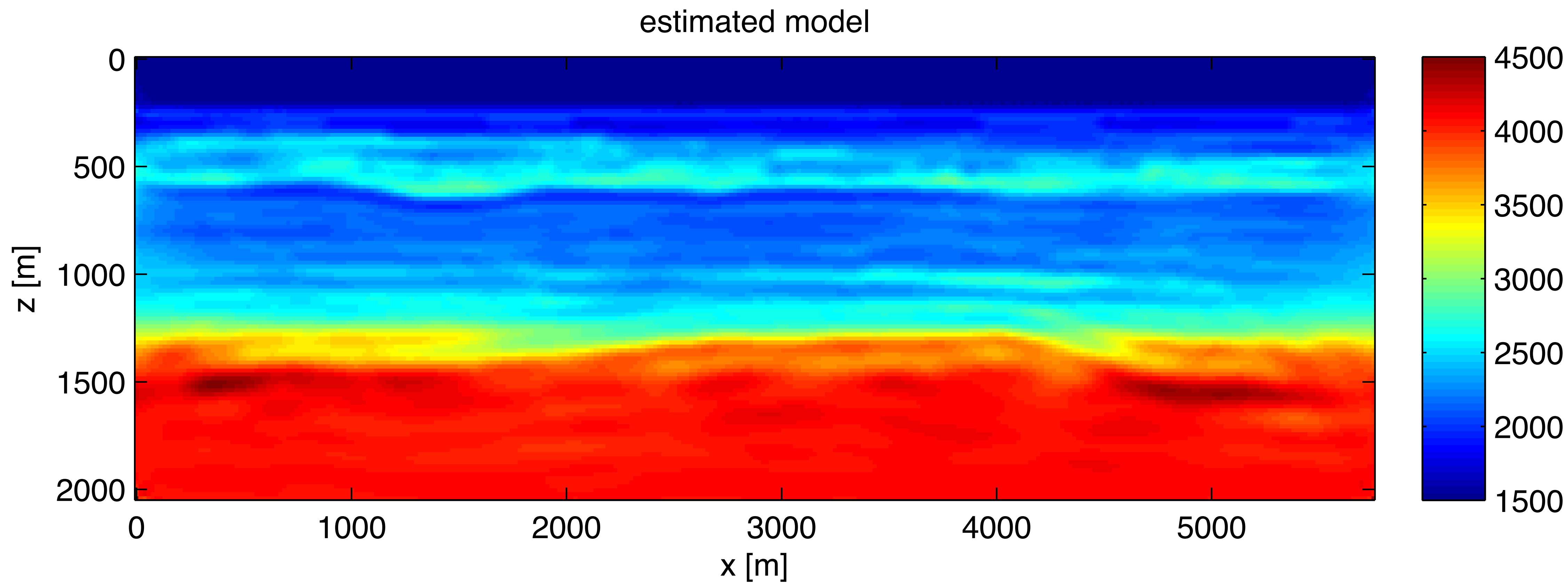
Algorithm

0. construct initial guess \mathbf{m} for medium and \mathbf{u}_i for each field
 - while** not converged **do**
 1. form Hessian and gradient // form (~free)
 2. ignore the $\nabla_{\mathbf{u},\mathbf{m}}^2\phi$, $\nabla_{\mathbf{m},\mathbf{u}}^2\phi$ blocks // approximate
 3. find $\delta\mathbf{m}$ & each $\delta\mathbf{u}_i$ in parallel // solve
 4. find steplength α using linesearch // evaluate (~free)
 5. $\mathbf{m} = \mathbf{m} + \alpha\delta\mathbf{m}$ & $\mathbf{u} = \mathbf{u} + \alpha\delta\mathbf{u}$ // update model and fields
 - end**
-

FWI using very inaccurate accurate iterative solver & LBFGS



Full-space method of this talk using very inaccurate accurate iterative solver



Related work

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

The presented algorithm is a quadratic-penalty version of Lagrangian-based all-at-once algorithms:

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

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

solve (inexactly) at every iteration: Newton-KKT system

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

Related work

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

Lagrangian based full-space methods also store the multipliers + corresponding gradient & Hessian blocks.

no intrinsic parallel structure

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

* higher order terms

number of field variables: $2 \times n_{\text{src}} \times n_{\text{freq}} \times n_{\text{grid}}$

Inexact PDE solves

– full-space vs reduced-space

reduced-space (FWI):

- error in objective function value
 - error in gradient
 - error in Hessian
- error in medium parameter update

full-space (this talk):

- objective function value always exact
 - gradient always exact
 - Hessian always exact
- globally convergent inexact Newton methods
[S.C. Eisenstat & H.F. Walker, 1994]

Full vs Reduced-space

	Reduced-space	Full-space
Hessian, gradient & function evaluation	solve PDE's	~free
Hessian, gradient & function evaluation	inexact	exact
Hessian	dense	sparse
memory for fields	2 fields per parallel process	working subset of simultaneous source fields in memory
working memory	1 gradient & update direction	update directions & gradients in memory

~free = sparse matrix-vector products

Conclusions

Constructed a quadratic-penalty based full-space method which:

- updates fields & medium parameters simultaneously
- main computations are intrinsically parallel
- suitable for frequency domain waveform inversion with iterative solvers
- con: need to store working subset of simultaneous source fields
- but, less storage needed compared to Lagrangian full-space methods

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SINBAD



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