A Unified 2D/3D Software Environment for Large Scale Time-Harmonic Full Waveform Inversion

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3D Full Waveform Inversion

Complicated process

- computationally intensive
- requires lots of memory, time
- large amount of programmer effort to get things *fast*
- often speed is the trade off for *correctness*

3D Full Waveform Inversion

Industry codebases, while fast

- are *inflexible* - hard to integrate new changes
- are *incorrect* - no ‘true derivatives’ of the underlying modelling code
- are *poorly maintained* - a new hire will have no idea what’s going on

3D Full Waveform Inversion

As a result

- codes are disconnected from mathematical underpinnings
- bugs are hard to diagnose
- difficult to incorporate new ideas from academia, research labs in to production-level codes

Software organization

Software hierarchy manages complexity

- human brains have very limited working memory
- if a particular part of a program only has one function, people using/debugging it only have to think about that one function
- if software is easier to reason about -> it’s easier to work with, easier to test

Software organization

Software hierarchy manages complexity

- we don't have to sacrifice performance
  - lowest level operations implemented in C w/multithreading

- hiding irrelevant details at each level
  - higher level functions don't have any idea about C/fortran/that gross stuff

Software organization

Anything that we do that isn’t solving PDEs is essentially irrelevant, computation time-wise

Software organization

Anything that we do that isn't solving PDEs is essentially irrelevant, computation time-wise

- advantageous for software design -> any overhead introduced is negligible compared to solving PDEs

  - if a single wavefield can be stored in RAM - true for low frequency time harmonic FWI

Software organization

PDEs are the computational bottleneck

- design our software for maximum ease of use + “plug and play” components
- speedups made to solving PDEs propagate to whole framework

FWI Problem

$$\min_{m} \frac{1}{2N_s} \sum_{i=1}^{N_s} \|P_r H(m)^{-1} q_i - d_i\|_2^2$$

m - discrete model vector
N_s - number of shots
P_r - receiver restriction operator
$H(m)u_i = q_i$ - monochromatic Helmholtz system for shot i
d_i - measured data for shot

New way to organize FWI Software

opAbstractMatrix

Modeling matrix : multiplication/division

opAbstractMatrix

A SPOT operator

- linear operator class - behaves like a matrix
- knows how to multiply, divide itself
- can handle matrix-free operations or form sparse matrix for 2D problems

Extensions

- Kaczmarz sweeps
- Jacobi iterations

opAbstractMatrix

Particular matrix-vector products specified at construction

discrete_helmholtz - constructs Helmholtz operator with particular parameters

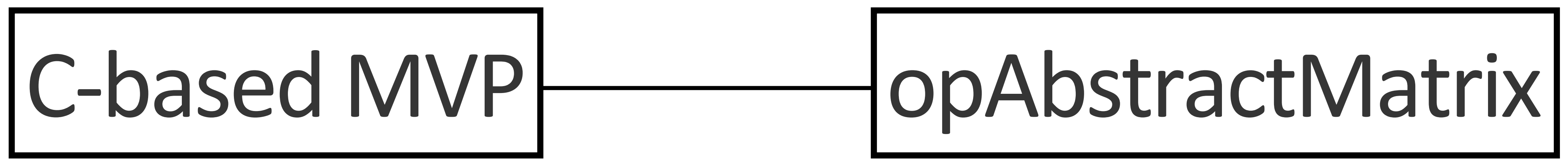
- can swap between stencils
- construct multigrid preconditioner

Excerpt from discrete_helmholtz

```
wn = param2wavenum(v_pml,freq,model.unit);
switch scheme
  case PDEopts.HELM3D_STD7
    Hmvp = FuncObj(@helm3d_7pt_mvp_mex,{vec(wn),vec(dt),vec(nt),npml,freq,[],[]});
    jacobi = FuncObj(@helm3d_7pt_jacobi_mex,{vec(wn),vec(dt),vec(nt),npml,freq,[],[],[],[]});
    kacz_sweep = [];
  case PDEopts.HELM3D_OPERTO27
    Hmvp = FuncObj(@helm3d_operto27_mvp,{wn,dt,nt,npml,[],n_threads,[],false});
    jacobi = [];
    kacz_sweep = FuncObj(@helm3d_operto27_kaczswp,{wn,dt,nt,npml,[],[],[],[],[]});
    if nargout >= 3
        [~,wn] = param2wavenum(v_pml,freq,model.unit);
        dHmvp = FuncObj(@helm3d_operto27_mvp,{wn,dt,nt,npml,[],n_threads,[],true});
        [~,~,wn] = param2wavenum(v_pml,freq,model.unit);
        ddHmvp = FuncObj(@helm3d_operto27_mvp,{wn,dt,nt,npml,[],n_threads,[],true});
    end
end
helm_params = struct;
helm_params.multiply = Hmvp;
helm_params.jacobi = jacobi;
helm_params.kacz_sweep = kacz_sweep;
helm_params.N = prod(nt);
helm_params.iscomplex = true;
H = opAbstractMatrix(mat_mode,helm_params,opts.solve_opts);
```

New way to organize FWI Software

Multithreaded
Mat-vec multiply



Modeling matrix :
multiplication/division

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Te

[1] Operto et. al. “3D finite-difference frequency-domain modeling of visco-acoustic wave propagation using a massively parallel direct solver: A feasibility study”, Geophysics 2007

C-based Matrix Vector Product

Implementation of 27-pt compact stencil [1]

Multi-threaded along the z-coordinate with openMP

Forward, adjoint modes

Te

[1] Chen, et. al. “An Optimal 9-Point Finite Difference Scheme For The Helmholtz Equation With PML.”, 2013

Helmholtz matrix

In 2D, we can afford to use explicit sparse matrices + fast direct solvers

- implementation of [1]

Explicit matrices VS implicit matrices is opaque to the user

- interface remains the same

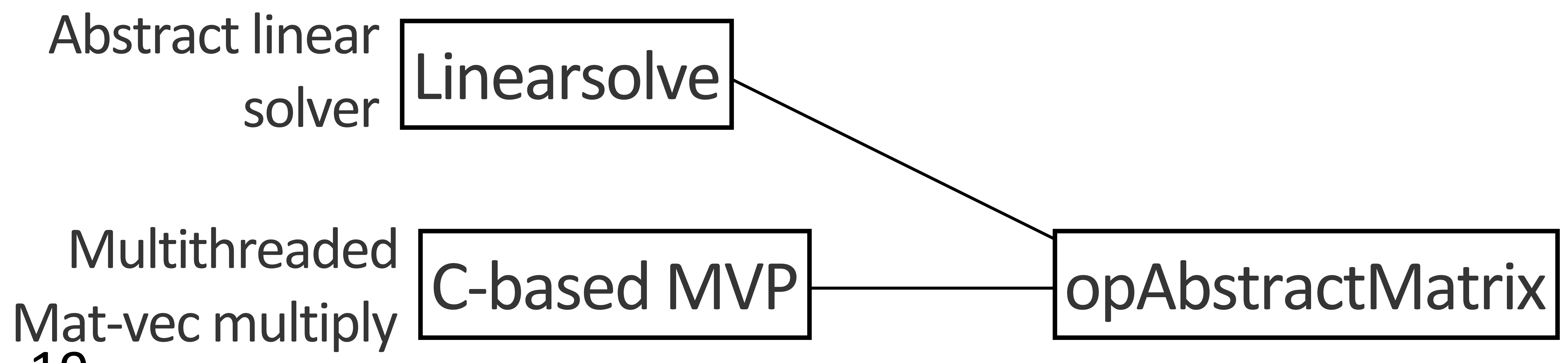
C-based Matrix Vector Product

Matlab Compiler

- write stencil-based code in Matlab -> C code with openMP multithreading

- nearly as fast as native C code, much easier to develop

New way to organize FWI Software



Modeling matrix : multiplication/division

Linearsolve

Abstract interface for “Solve Ax = b with a specified method”

- encourages code reuse - smoothers for multigrid, preconditioner applications

- calls the specified method (GMRES,CG, etc.) with the prescribed number of iterations, right hand side, initial guess, tolerance, and preconditioner

LinSolveOpts

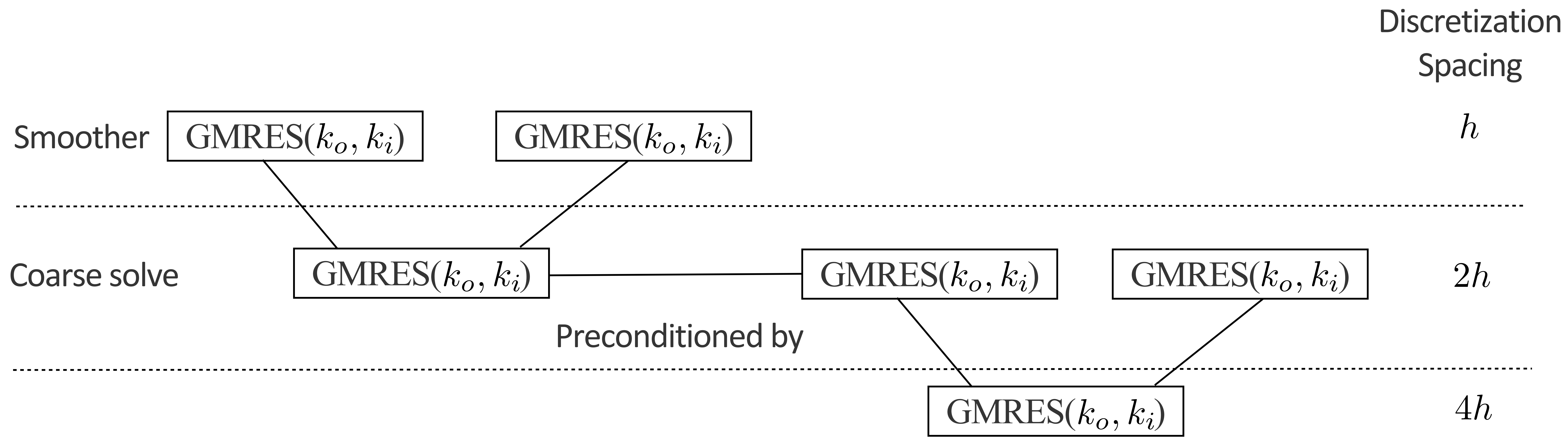
Object for storing

- linear solver method
- maximum outer iterations
- maximum inner iterations (for some solvers)
- tolerance
- preconditioner

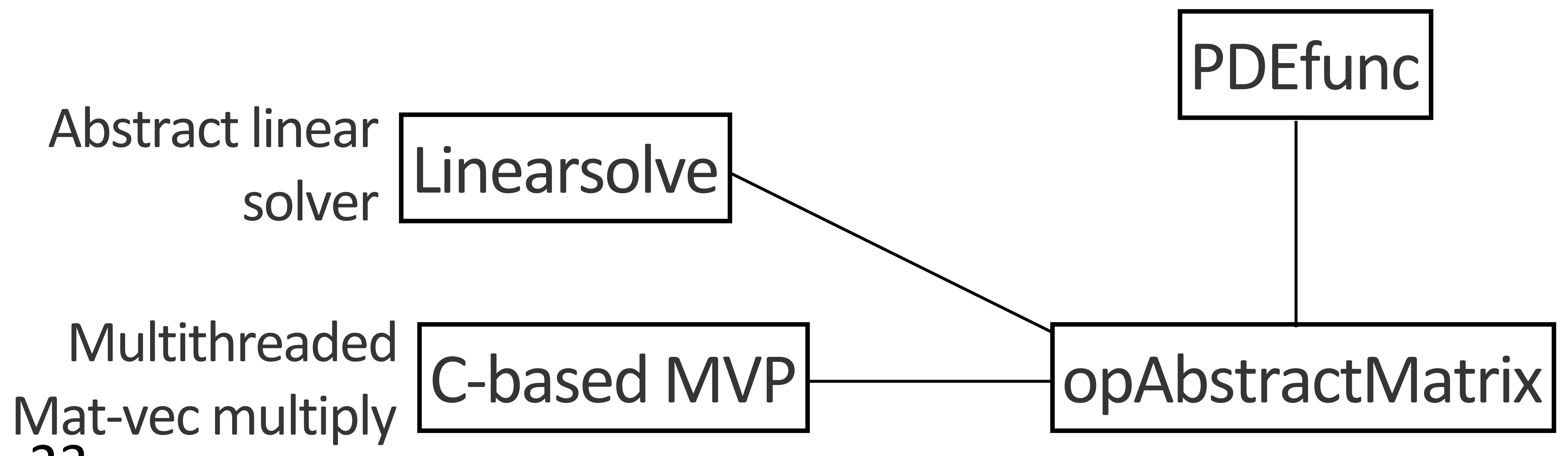
As well as default options for these

- Solvers: CG, FGMRES, LU, etc.
- Preconditioners: ML-GMRES, Shifted Laplacian, etc.

Multilevel-GMRES



New way to organize FWI Software



PDE-related quantities
Serial version

Modeling matrix : multiplication/division

PDEfunc

Main workhorse function

For each source index

- solve the Helmholtz equation - don't care how
- use solution to compute objective + gradient, demigration/ migration, hessian/GN hessian matrix vector product - whatever the user requests

Serial code, implicitly multithreaded

Excerpt from PDEfunc

```
Uk = Hk \ Qk_i;
switch func
   case OBJ
      [phi,dphi] = misfit(Pr*Uk,Dobs(:,data_idx),current_src_idx,freq_idx);
      f = f + phi;
      if nargout >= 2
        Vk = Hk' \ ( -Pr'* dphi);
          g = g + sum(real(conj(Uk) .* (dH'*Vk)),2);
      end

    case FORW_MODEL
      output(:,data_idx) = Pr*Uk;

   case JACOB_FORW
      dUk = Hk\(dHdm*(-Uk));
      output(:,data_idx) = Pr*dUk;

   case JACOB_ADJ
      Vk = Hk'\( -Pr'* input(:,data_idx) );
      output = output + sum(real(conj(Uk) .* (dH'*Vk)),2);
end
```

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PDEfunc

Extensions to Wave-equation Reconstruction Inversion

Standard FWI

$$\min_m \frac{1}{2}\|P_r u(m) - d\|_2^2$$
$$\text{s.t.} H(m)u(m) = q$$

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PDEfunc

Extensions to Wave-equation Reconstruction Inversion

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

$$u(m) = \arg\min_{u} \left\| \begin{bmatrix} Pr \\ \lambda H(m) \end{bmatrix} u - \begin{bmatrix} d \\ \lambda q \end{bmatrix} \right\|_2$$

Song and Williamson,“Frequency-domain acoustic-wave modeling and inversion of crosshole data: Part I-2.5-D modeling method.” Geophysics (1995)

PDEfunc

Extensions to 2.5D FWI

- When the velocity is y-invariant

$$v(x,y,z) = h(x,z)$$

- After a Fourier transform in y-, the Helmholtz equation reads as

$$(\partial_x^2 + \partial_z^2 + \omega^2 h(x,z) - k_y^2)u_{k_y}(x,z) = S(\omega)\delta(x-x_s)\delta(z-z_s)$$

Song and Williamson,"Frequency-domain acoustic-wave modeling and inversion of crosshole data: Part I-2.5-D modeling method." Geophysics (1995)

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PDEfunc

Extensions to 2.5D FWI

- we can reconstruct the 3D wavefield $u(x,y,z)$ as

$$u(x,y,z) = \frac{1}{\pi}\int_0^{k_{nyq}} \tilde{u}_{k_y}(x,z)\cos(k_y(y-y_s))dk_y$$

$$= \sum_{j=1}^{N} w_j u_{k_y^j}(x,z)$$

Song and Williamson,“Frequency-domain acoustic-wave modeling and inversion of crosshole data: Part I-2.5-D modeling method.” Geophysics (1995)

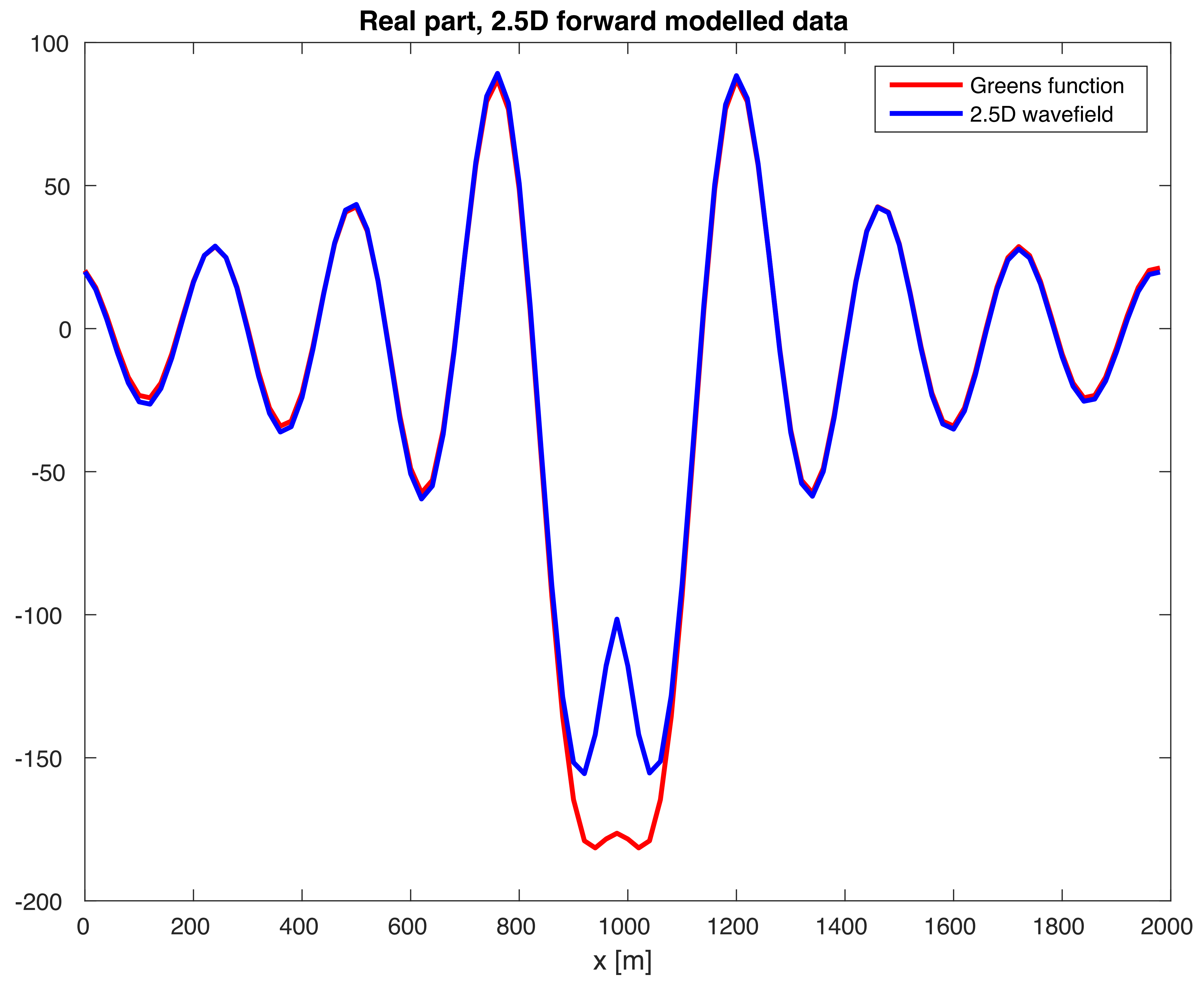
PDEfunc

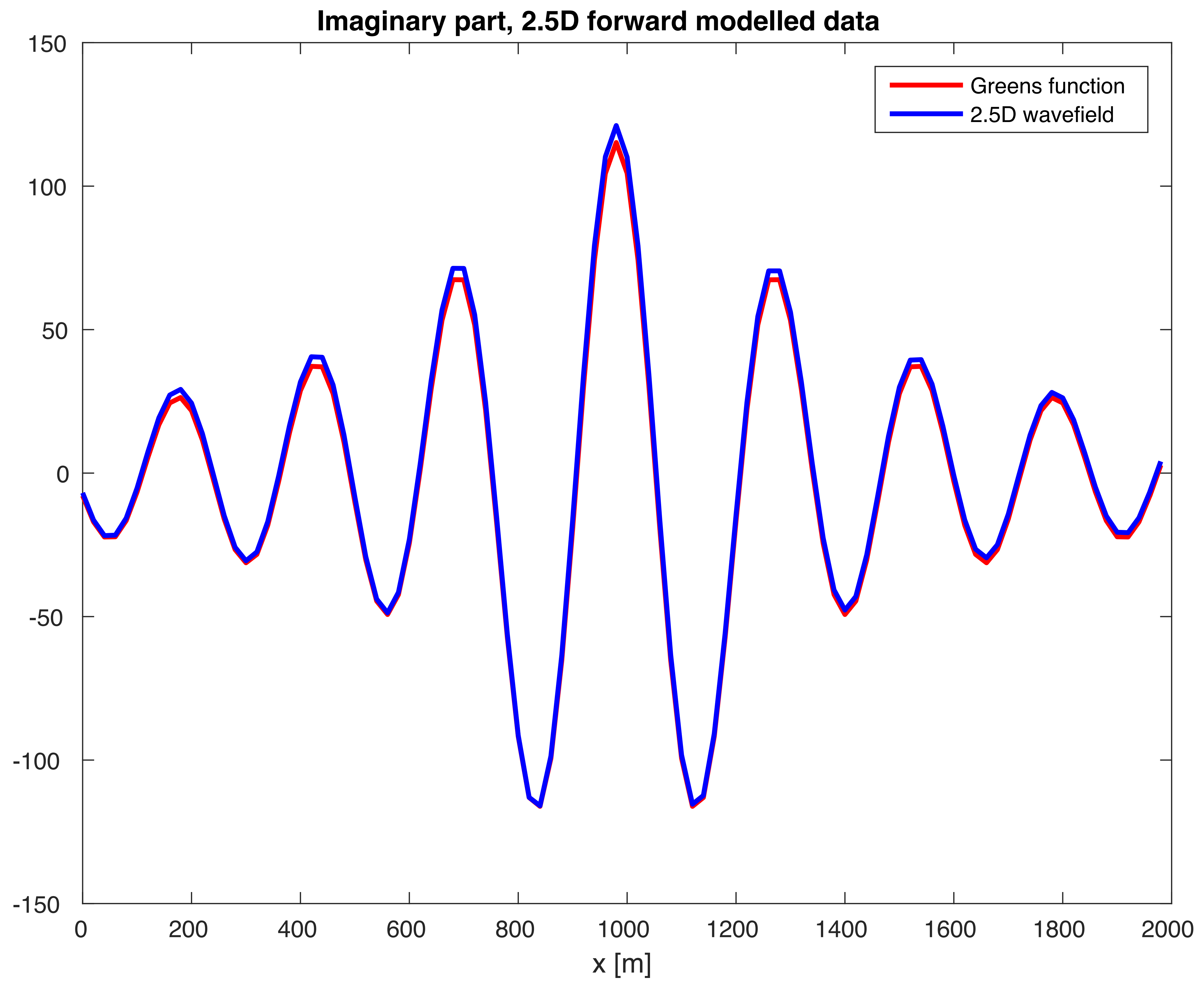
Extensions to 2.5D FWI

- weighted sum structure of the wavefield
  -> weighted sum structure for gradient, hessian, etc.

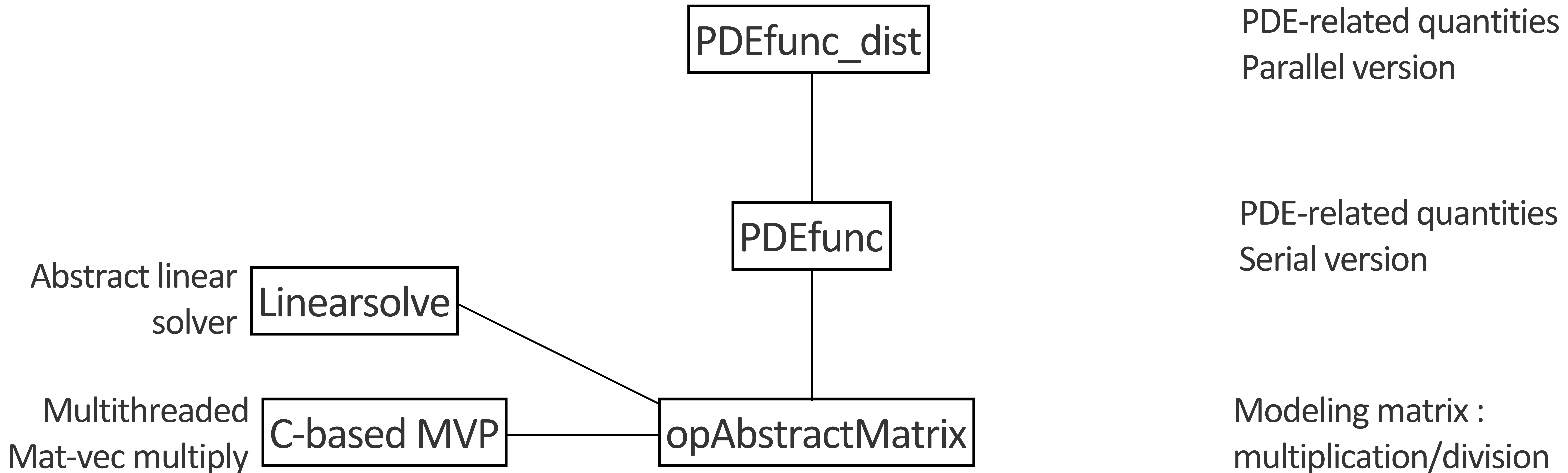
- correct 3D physics without full 3D costs

2.5D Modeling





New way to organize FWI Software



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Separable objective function

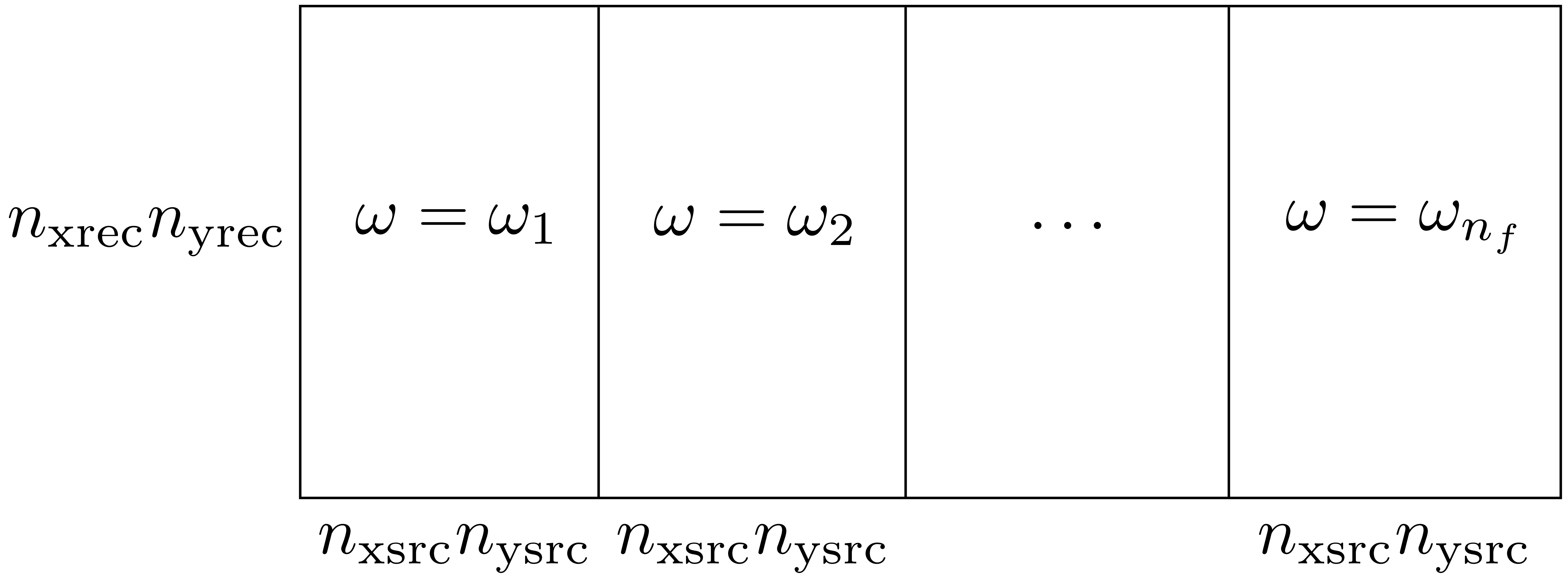
$$f_I(m) = \frac{1}{2|I|} \sum_{i \in I} \|P_r H(m)^{-1} q_i - d_i\|_2^2$$
$$= \frac{1}{2|I|} \sum_{i \in I} f_i(m)$$

The objective function is *separable* over shots/frequencies
- distribute indices to parallel workers

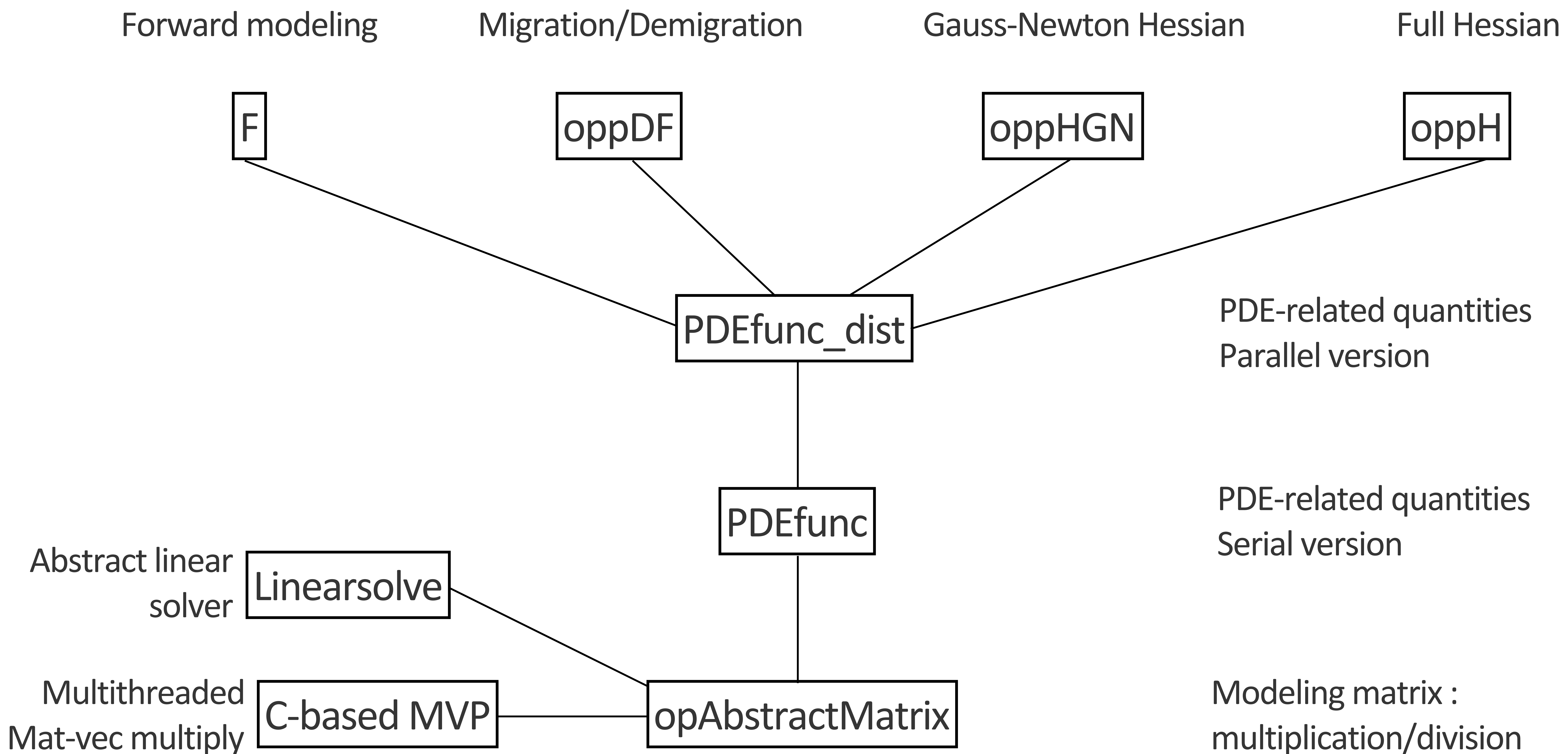
Objective separable -> gradient, GN Hessian, Hessian are separable

PDEfunc_dist does no computation, just parallel distribution + summation
- separate computation from parallelization
- easiest component to 'swap out' with your own parallelization scheme

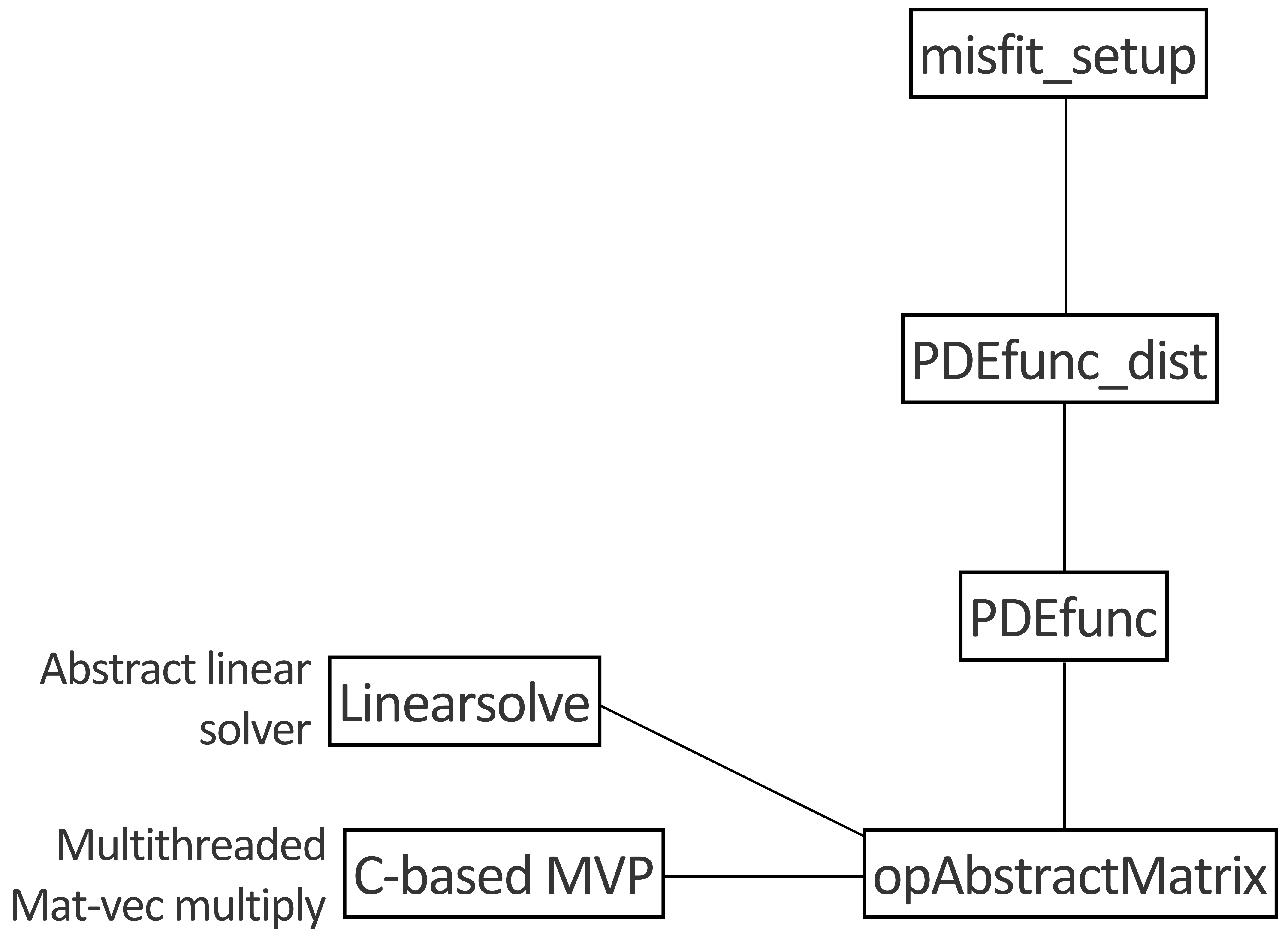
Data volume


$n_{\text{xrec}}n_{\text{yrec}}$
$\omega = \omega_1$
$\omega = \omega_2$
$\dots$
$\omega = \omega_{n_f}$
$n_{\text{xsrc}}n_{\text{ysrc}}$
$n_{\text{xsrc}}n_{\text{ysrc}}$
$n_{\text{xsrc}}n_{\text{ysrc}}$

New way to organize FWI Software



New way to organize FWI Software



FWI objective setup

PDE-related quantities
Parallel version

PDE-related quantities
Serial version

Modeling matrix : multiplication/division

misfit_setup

Constructs function handle for objective

- velocity subsampling
- frequency slice distribution

Batch mode interface to the objective

- stochastic inversion algorithm can specify which source indices to use

Fancy wrapper around PDEfunc_dist

PDEopts

Options for specifying

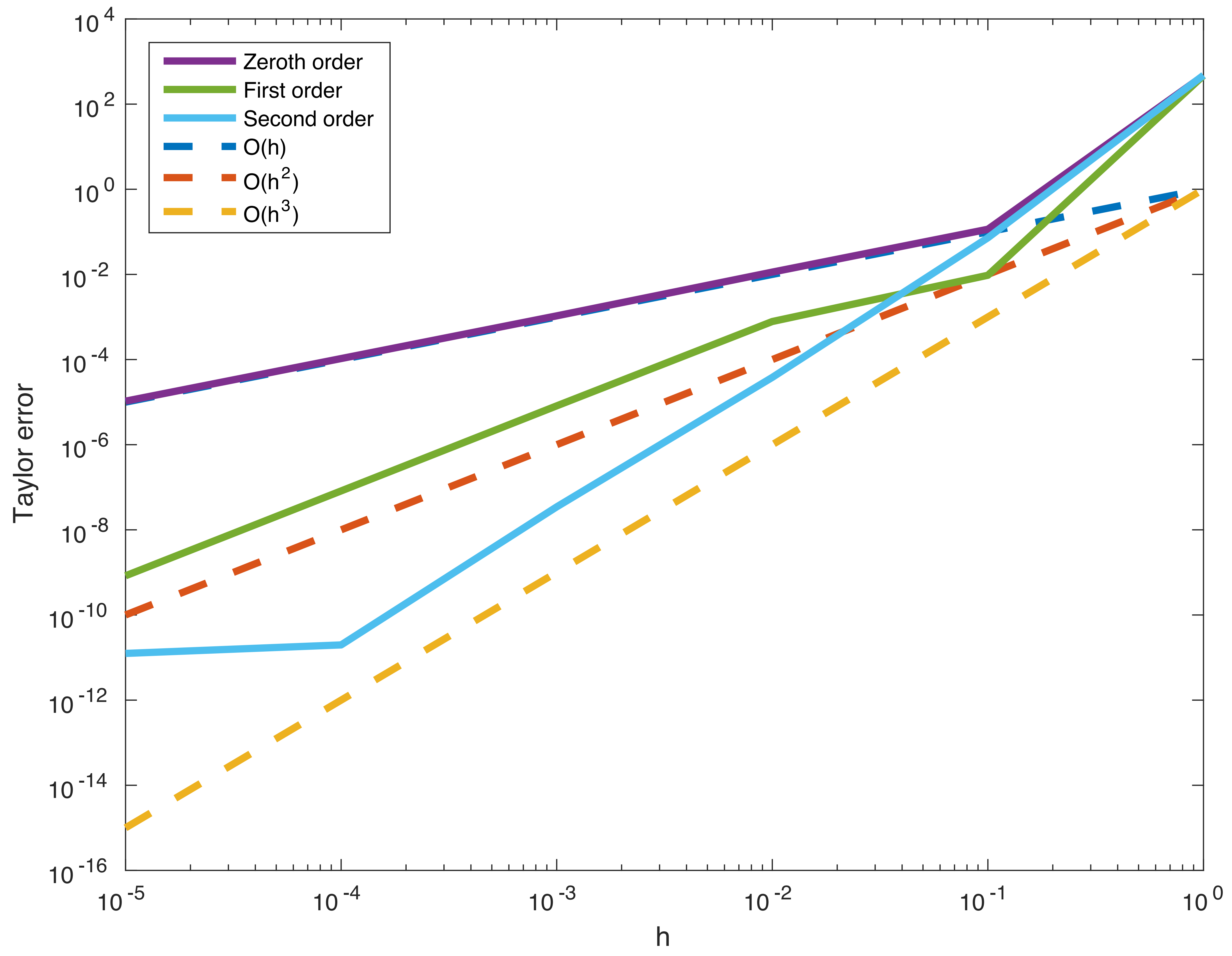
- PDE stencil
- PML width/layout
- preconditioner
- source/receiver interpolation
- source estimation
- ...

Taylor error test

$$f(m + h\delta m) - f(m) = O(h)$$

$$f(m + h\delta m) - f(m) - h\nabla f(m)^T \delta m = O(h^2)$$

$$f(m + h\delta m) - f(m) - h\nabla f(m)^T \delta m - \frac{h^2}{2}\delta m^T \nabla^2 f(m) \delta m = O(h^3)$$



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Adjoint Test

	$\langle Ax, y \rangle$	$\langle x, A^H y \rangle$	Relative Difference
Helmholtz system matrix	$1.903020 + 2.087502i \cdot 10^1$	$1.903020 + 2.087502i \cdot 10^1$	$1.51 \cdot 10^{-15}$
Jacobian	$-6.204229 \cdot 10^{-2}$	$-6.204229 \cdot 10^{-2}$	$6.8525 \cdot 10^{-10}$
Hessian	$-5.842717 \cdot 10^{-3}$	$-5.842717 \cdot 10^{-3}$	$7.9767 \cdot 10^{-11}$

Results

Algorithm

$$\min_m \frac{1}{N_s}\sum_{i=1}^{N_s} f_i(m)$$
$$\text{s.t.} \quad m_L \leq m \leq m_U$$

m - discrete model vector

m_L, m_U - point-wise model bounds (water layer + constant min/max velocities)

$f_i(m) = \frac{1}{2}\|P_r H(m)^{-1} q_i - d_i\|_2^2$ - per-shot misfit function

P_r - receiver restriction operator

$H(m)u_i = q_i$ - discrete Helmholtz system for shot i

d_i - measured data for shot

Algorithm

$$\min_m \frac{1}{N_s} \sum_{i=1}^{N_s} f_i(m)$$
$$\text{s.t.} \quad m_L \leq m \leq m_U$$

We have too many shots to process at once

- Can process p shots at a time when we have p Matlab workers

Typically $N_s \gg p$

Schmidt, et. al., “Optimizing Costly Functions with Simple Constraints: A Limited-Memory Projected Quasi-Newton Algorithm”, 2009

Algorithm

$$m_k = \arg\min_m \frac{1}{|I_k|} \sum_{i \in I_k} f_i(m)$$

$$\text{s.t.} \quad m_L \leq m \leq m_U$$

At the kth iteration, randomly draw a subset of sources $I_k \subset \{1, \ldots, N_s\}$ with $|I_k| = p$

Approximately solve the above problem with constrained LBFGS or spectral projected gradient

Repeat for T iterations

Algorithm

Inner subproblem

- solved with $\frac{N_s}{p}$ function evaluations
- each subproblem is equivalent to one pass over the full data

We use three outer iterations

- equivalent to three gradient steps with all the shots

3D FWI Example

Overthrust model

- 20 km x 20 km x 4.6 km - 50 m spacing, 500m water layer
- 50 x 50 sources, 200m spacing - 2500 shots
- 401 x 401 receivers, 50m spacing
- 3Hz - 6Hz frequency range, single freq. inverted at a time

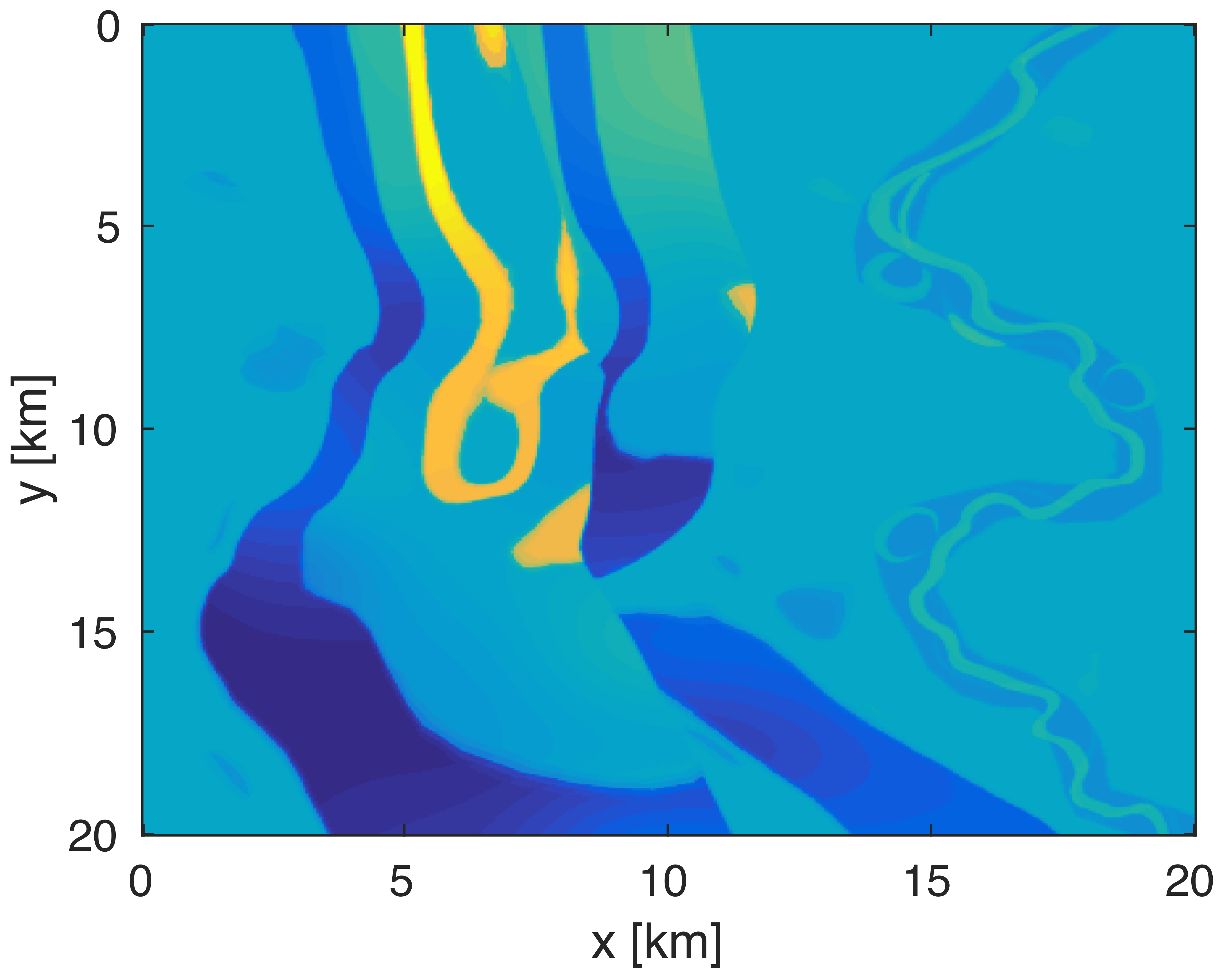
Computational Environment

SENAI Yemoja cluster

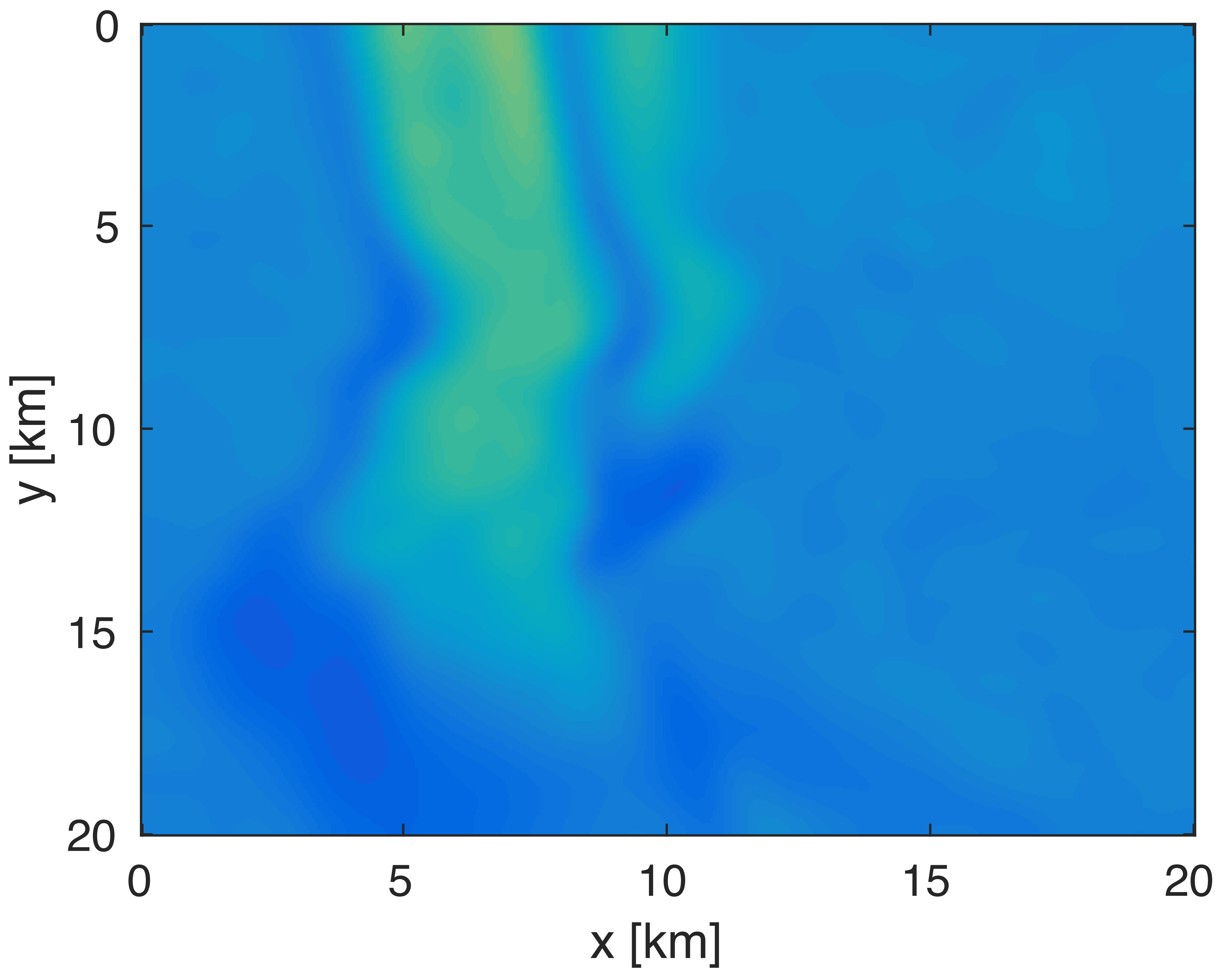
- 100 nodes, 128 GB RAM each, 20-core processors

- 400 Parallel Matlab workers (4 per node), Helmholtz MVP uses 5 threads - full core utilization

z=1000m slice

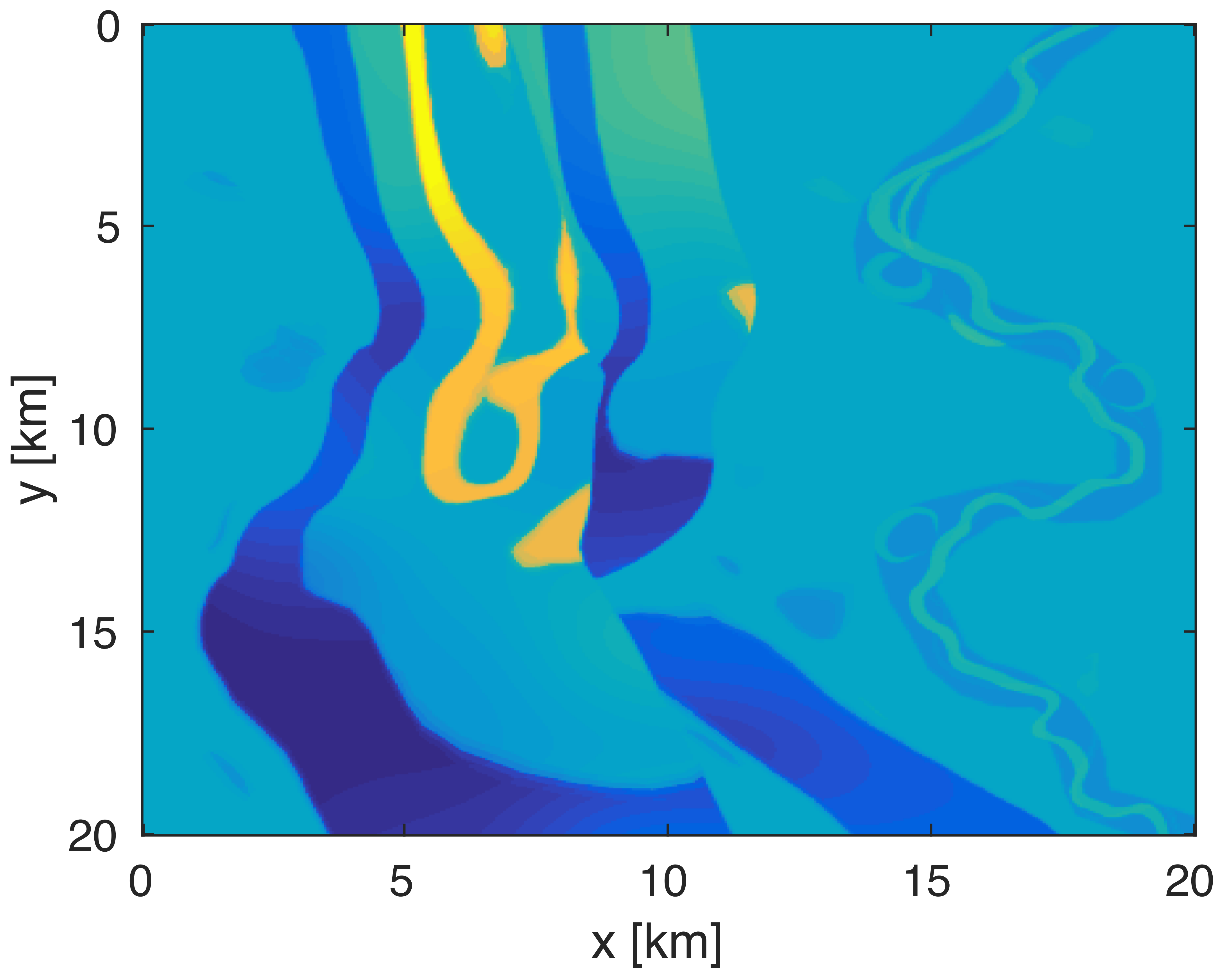


True model

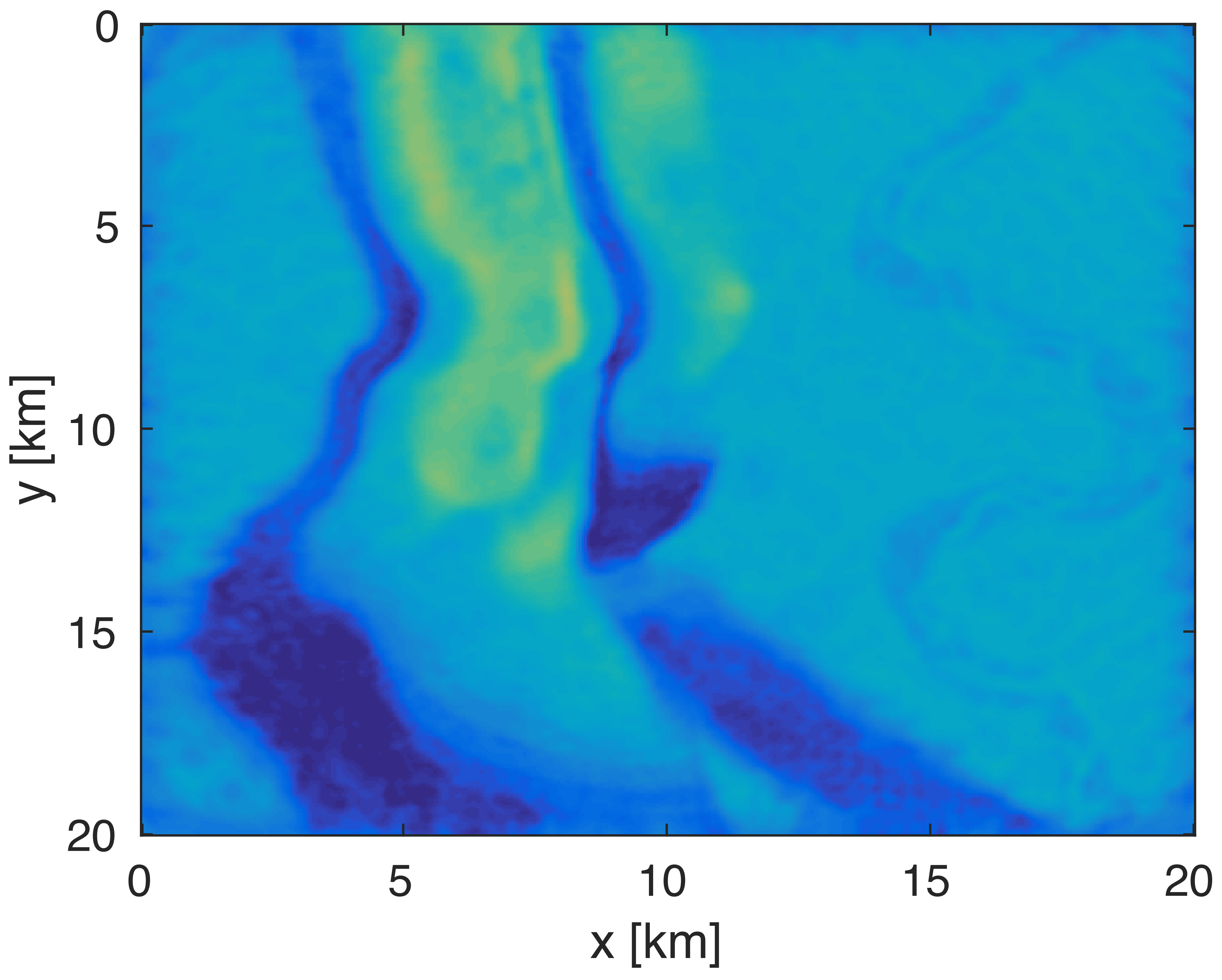


Initial model

z=1000m slice

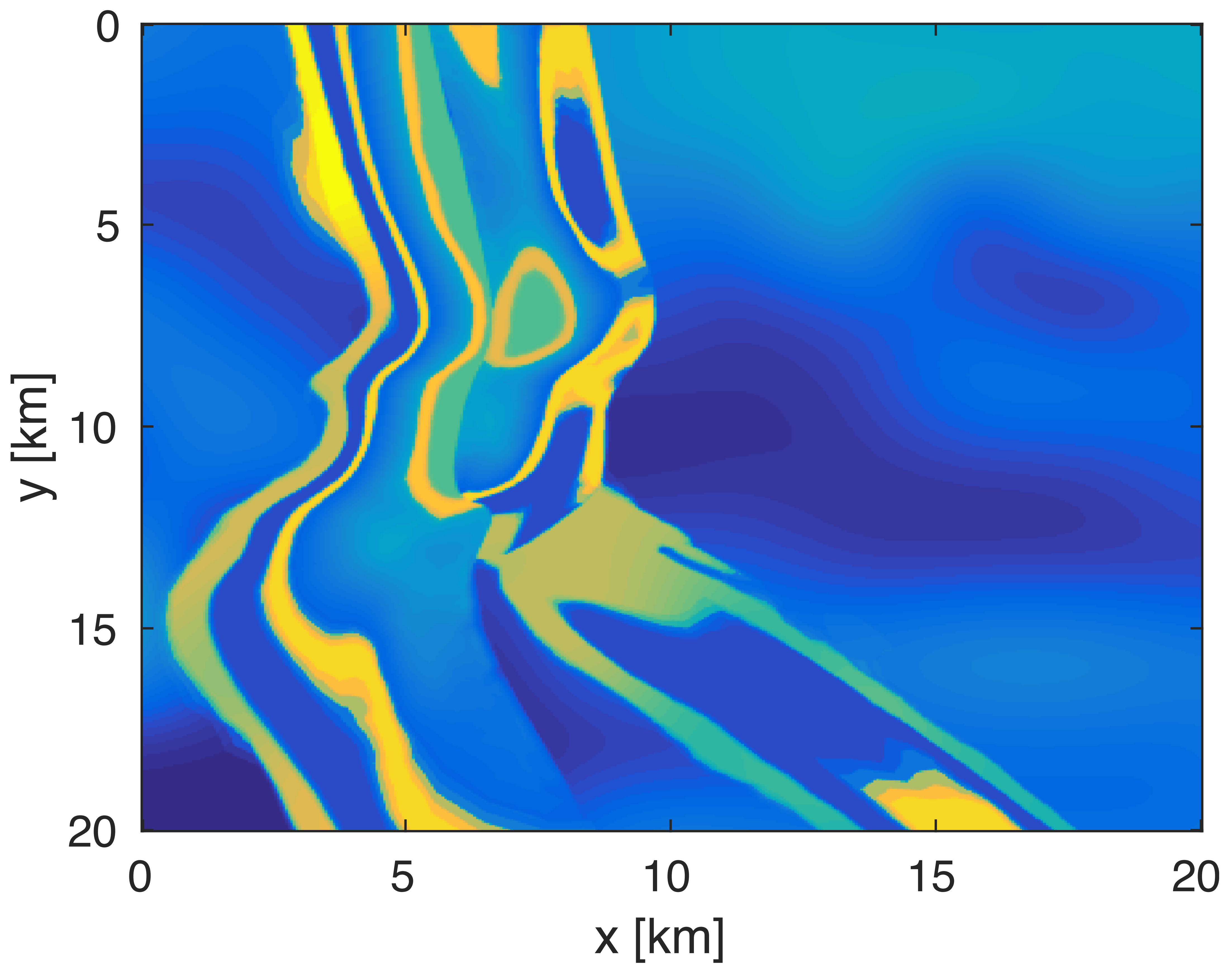


True model

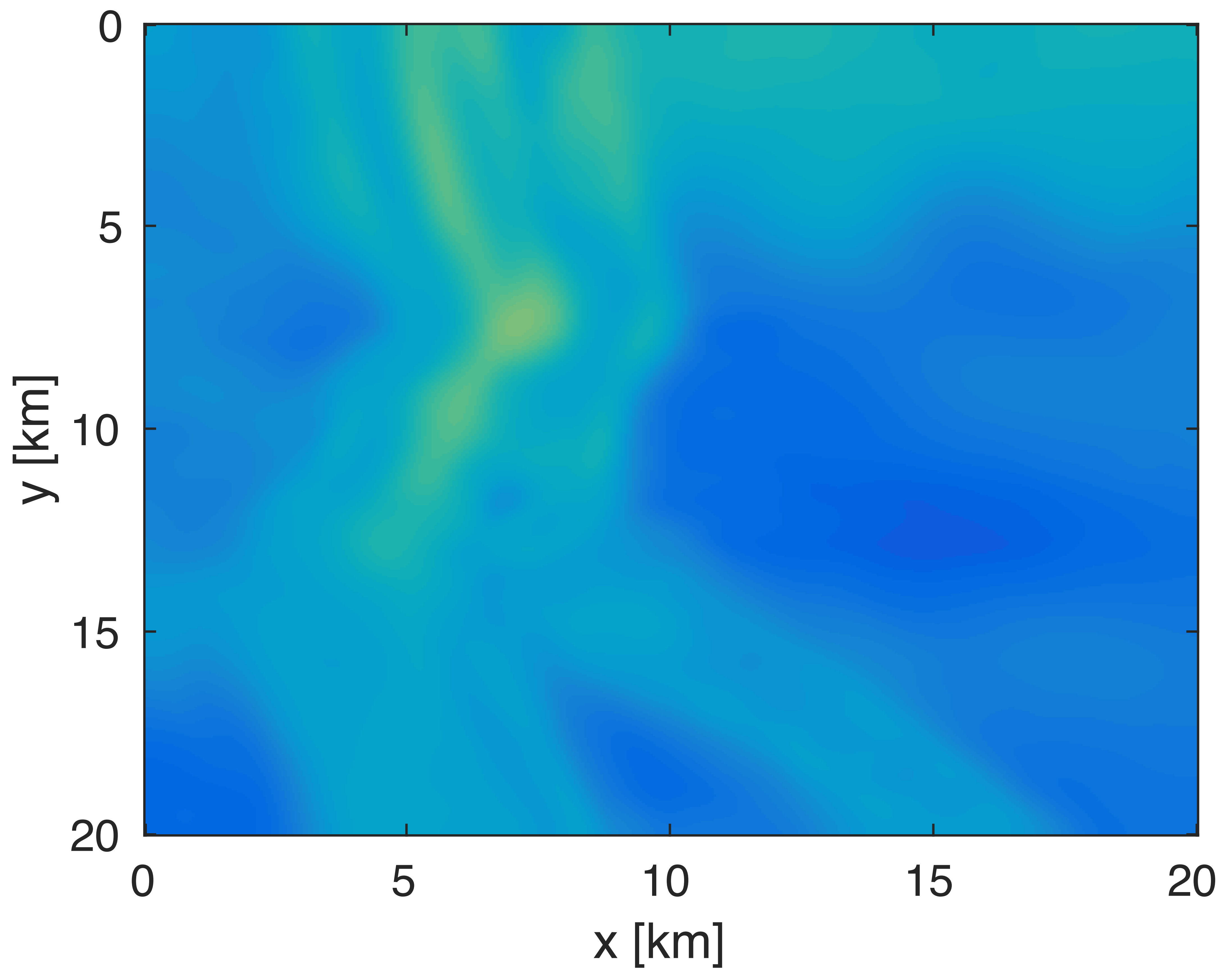


Stochastic LBFGS

z=2000m slice

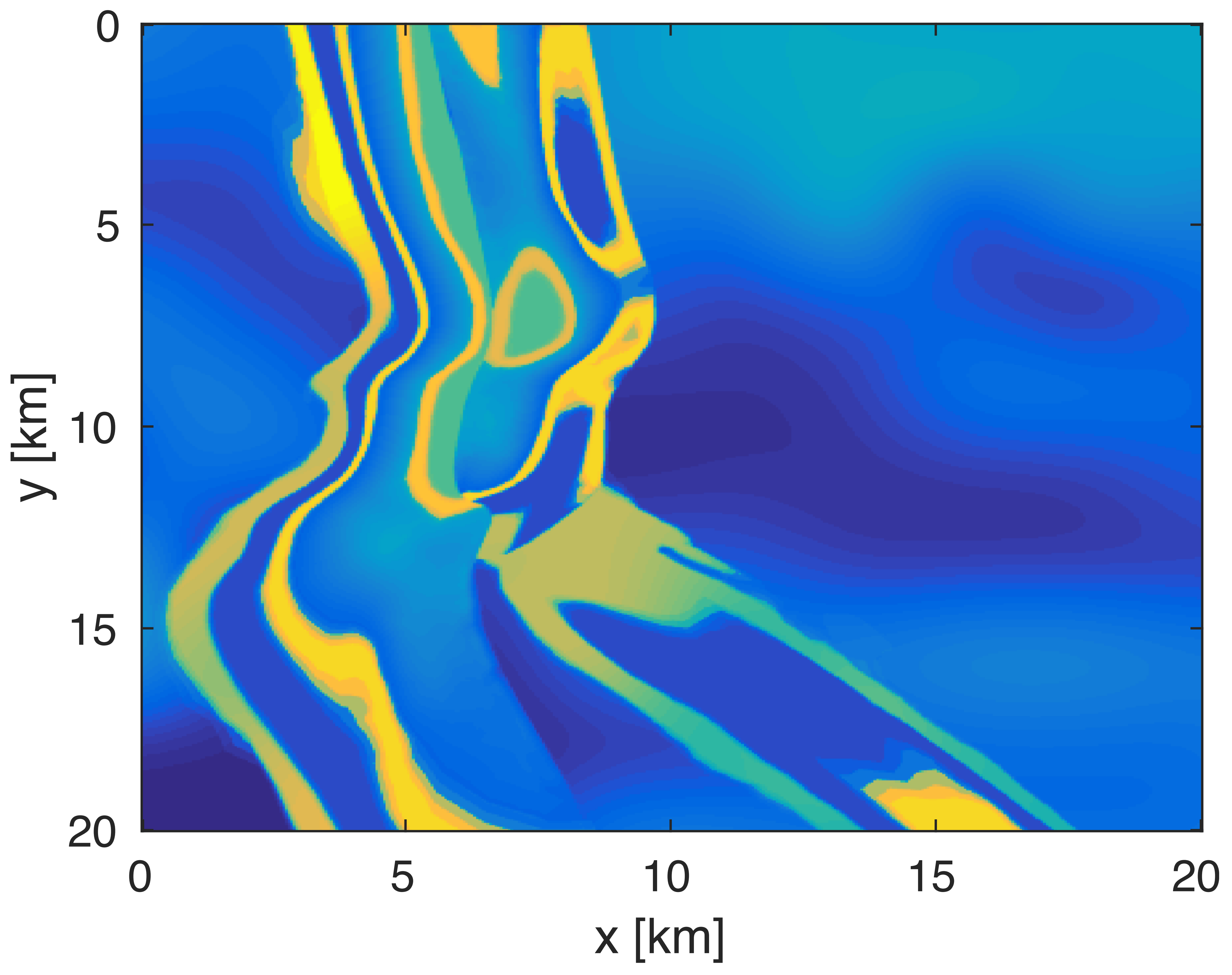


True model

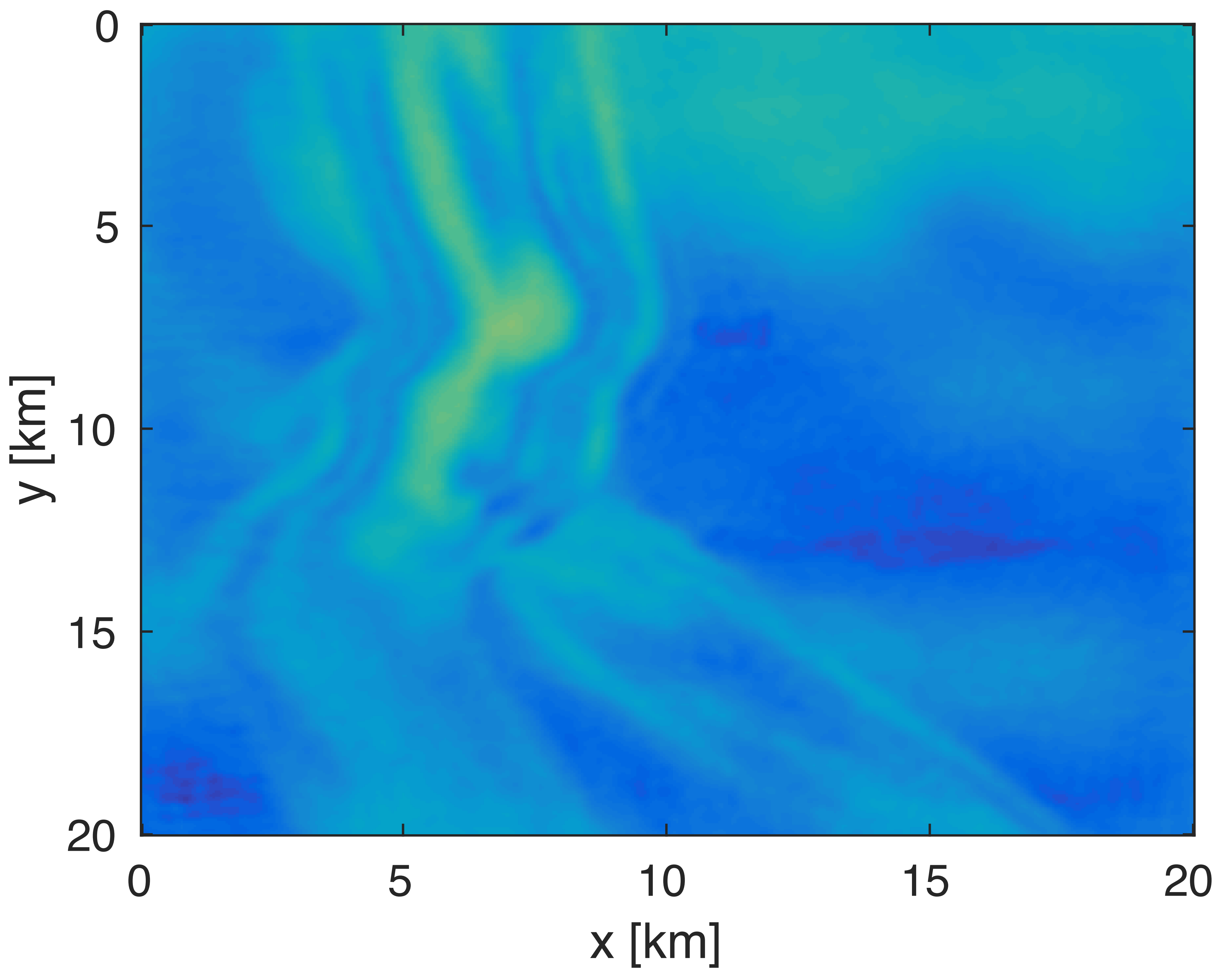


Initial model

z=2000m slice

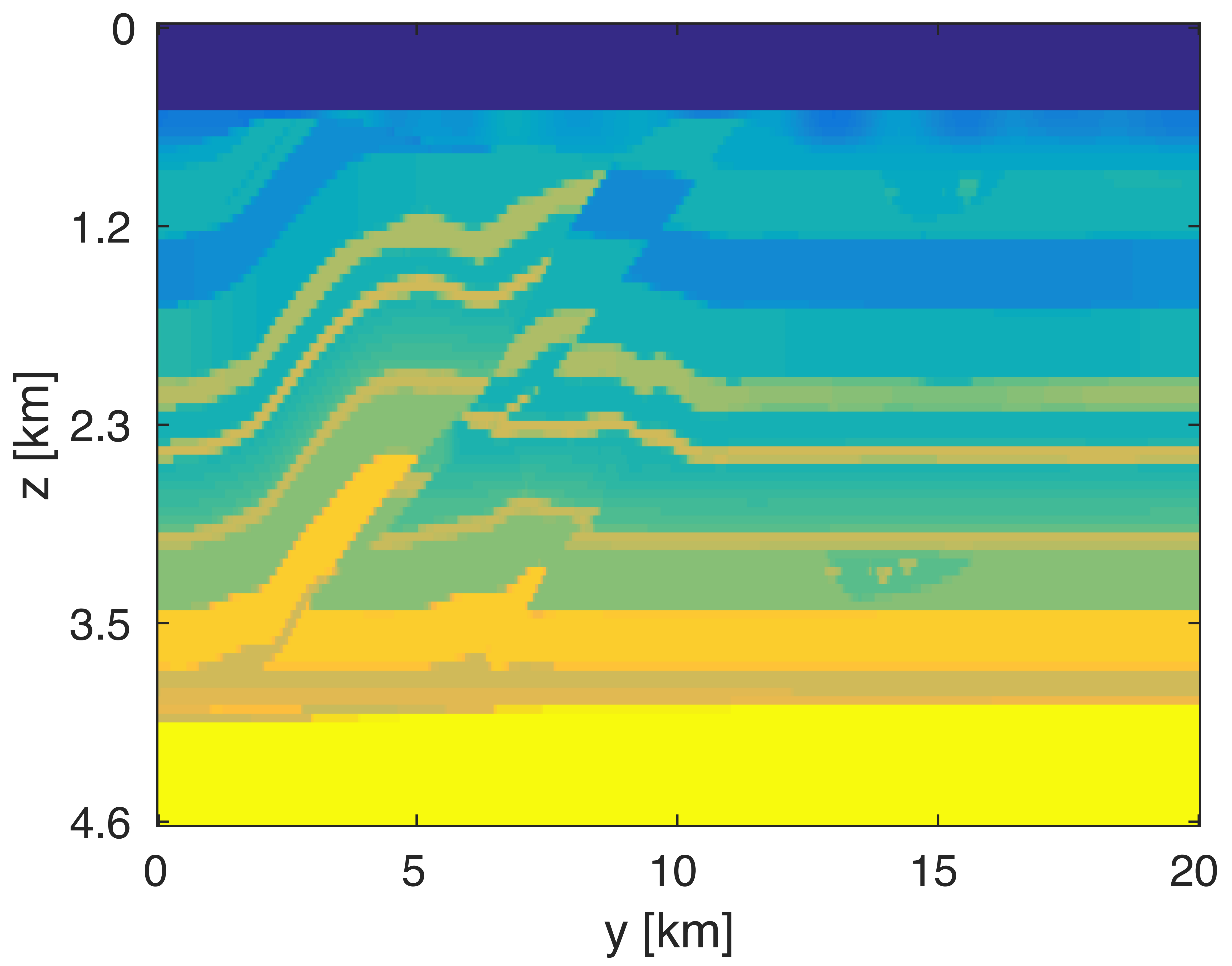


True model

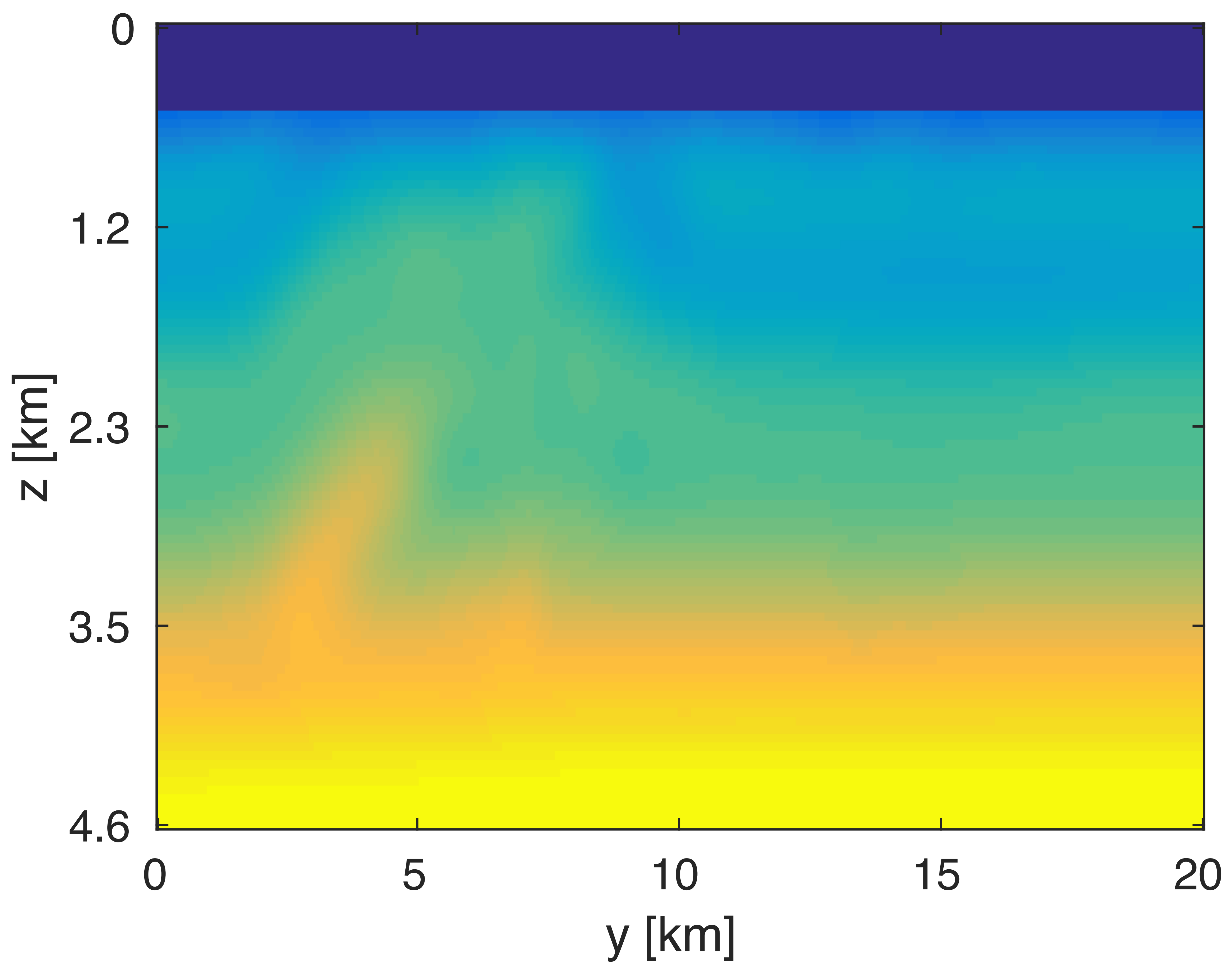


Stochastic LBFGS

x=12.5km slice

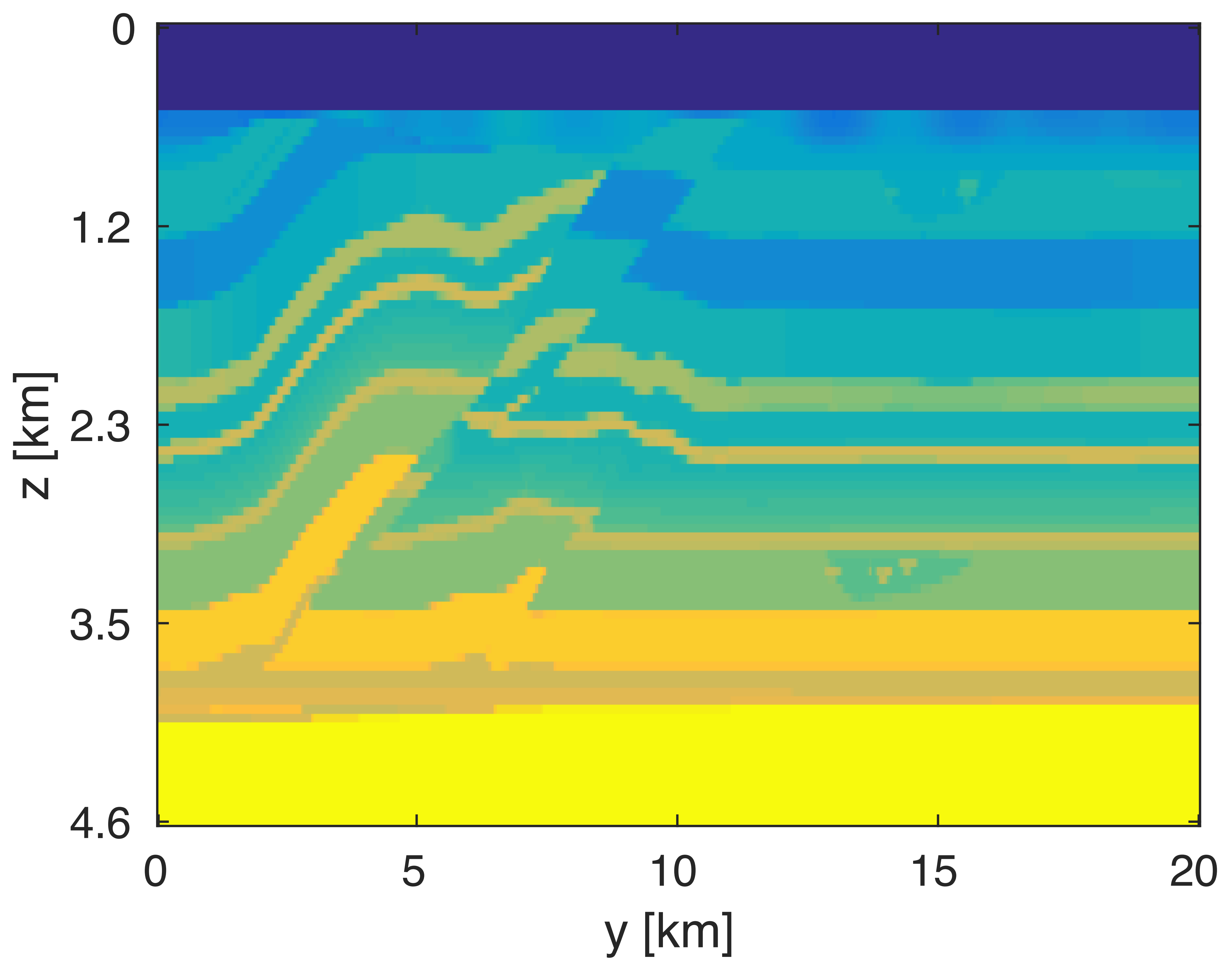


True model

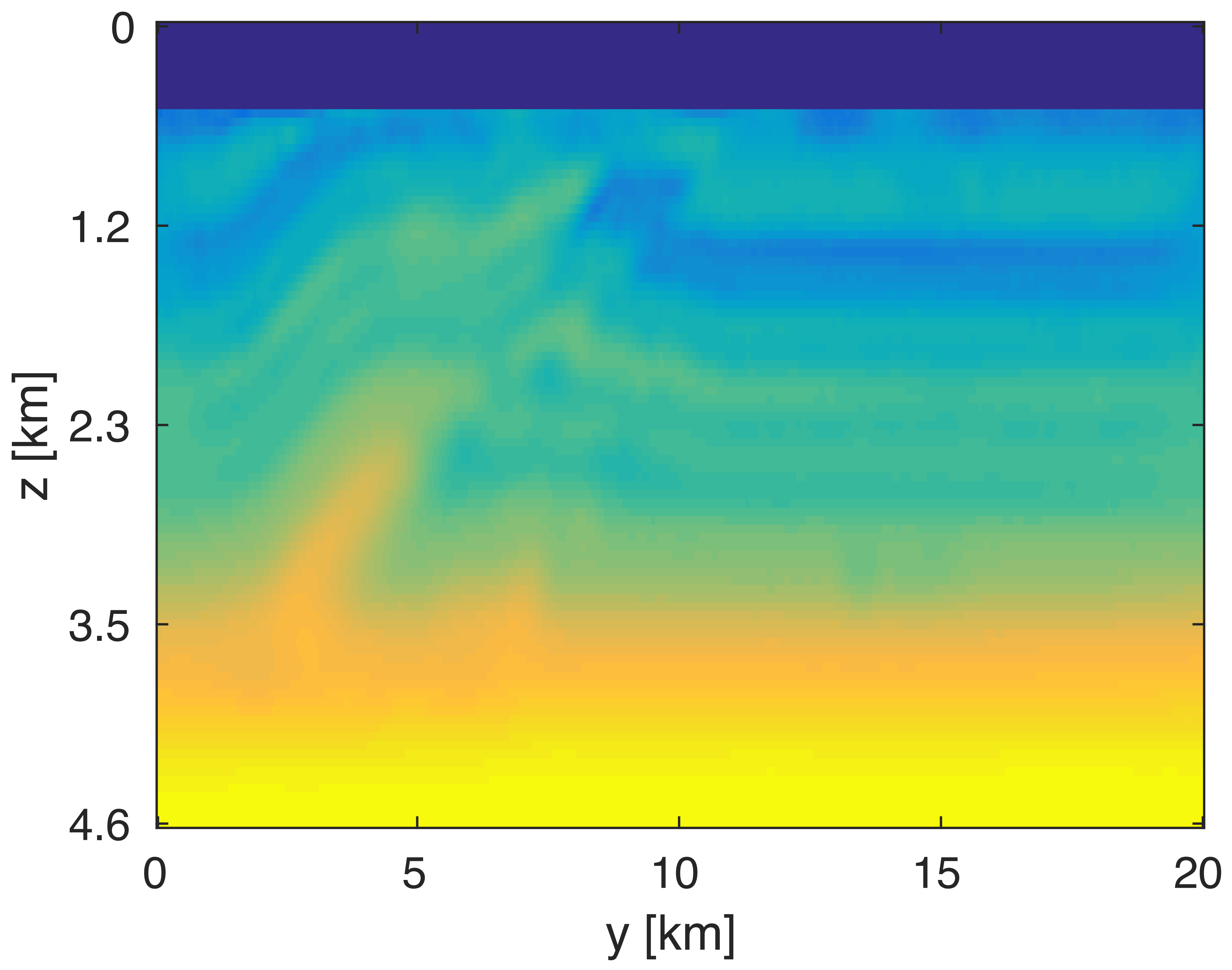


Initial model

x=12.5km slice

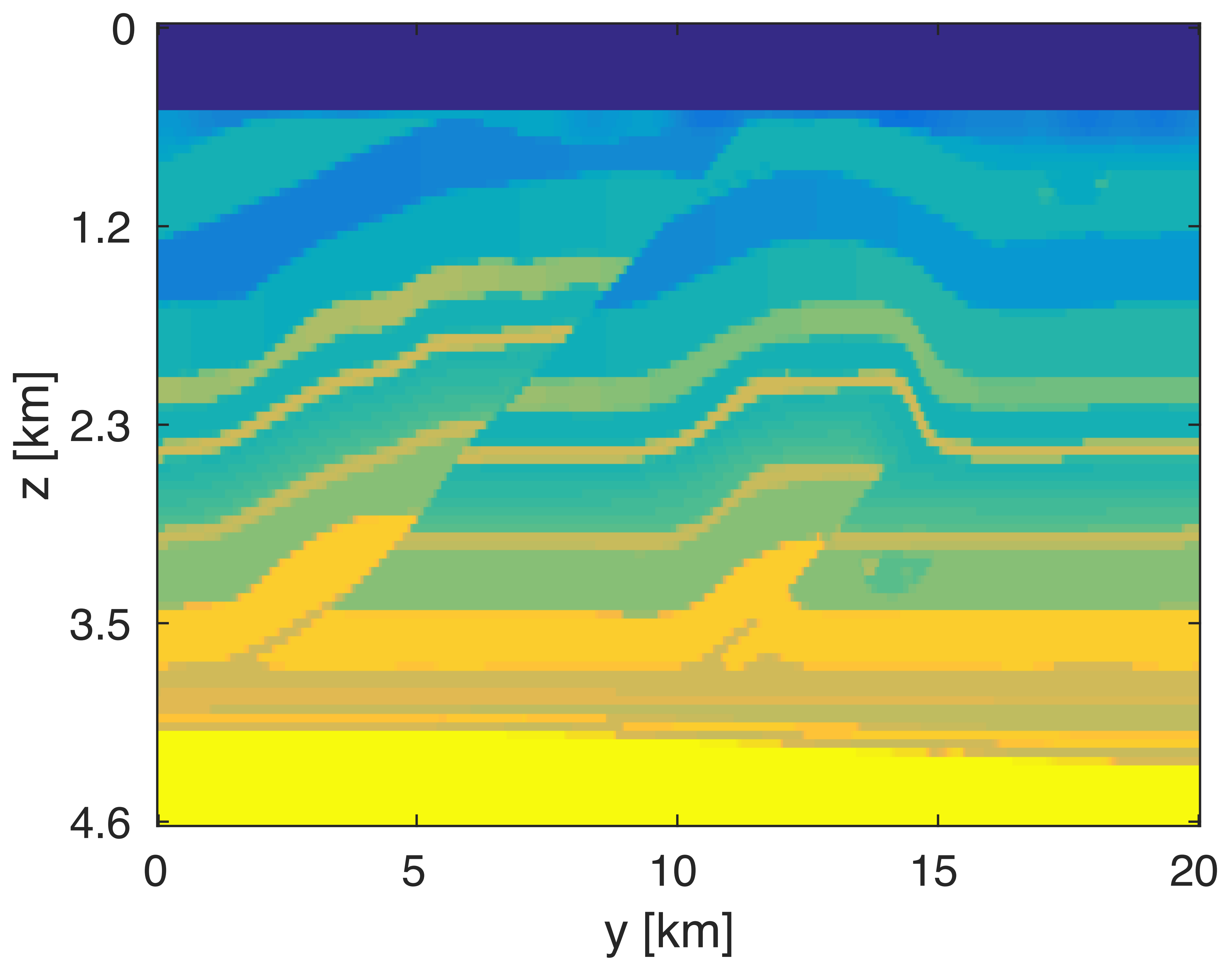


True model

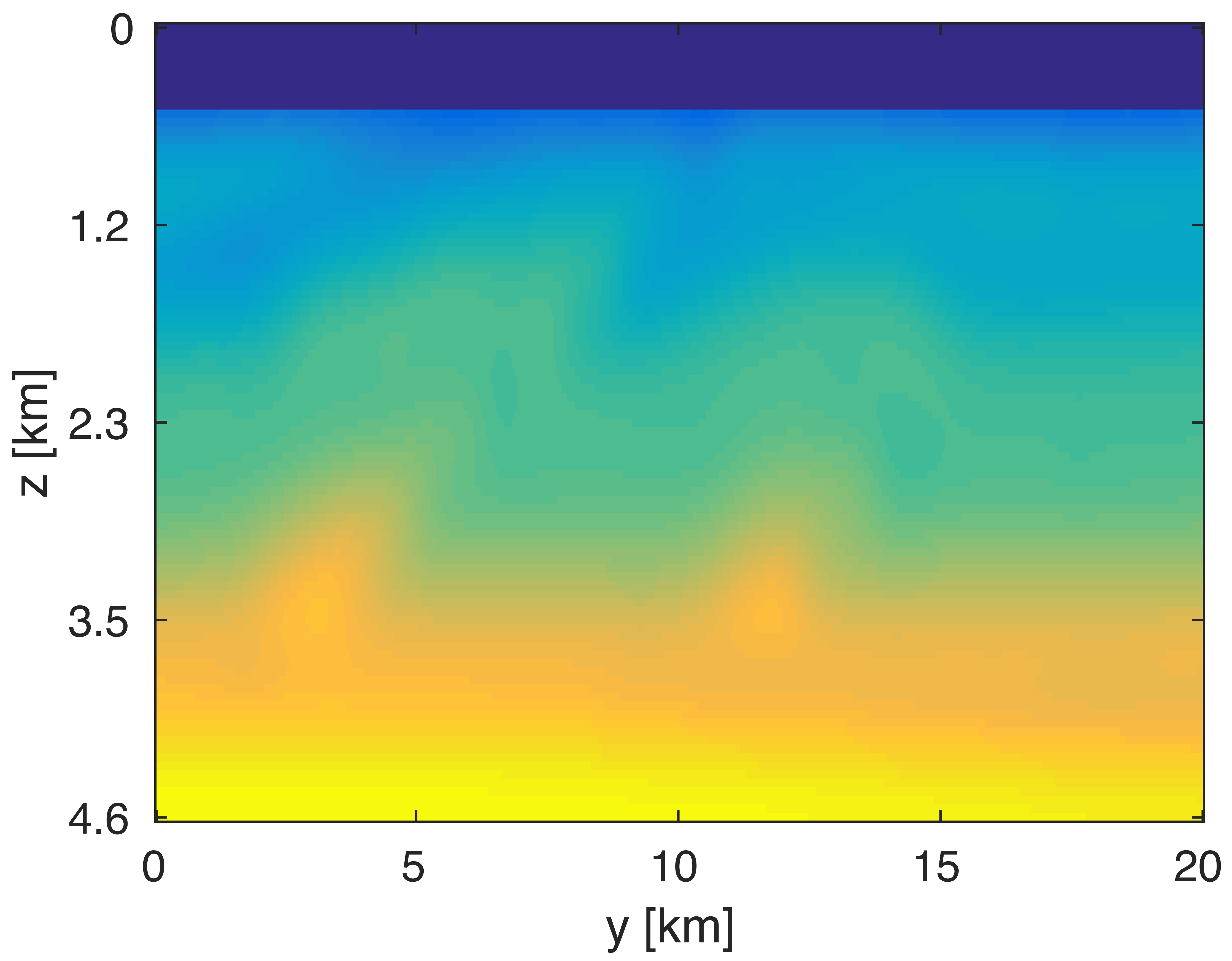


Stochastic LBFGS

x=17.5km slice

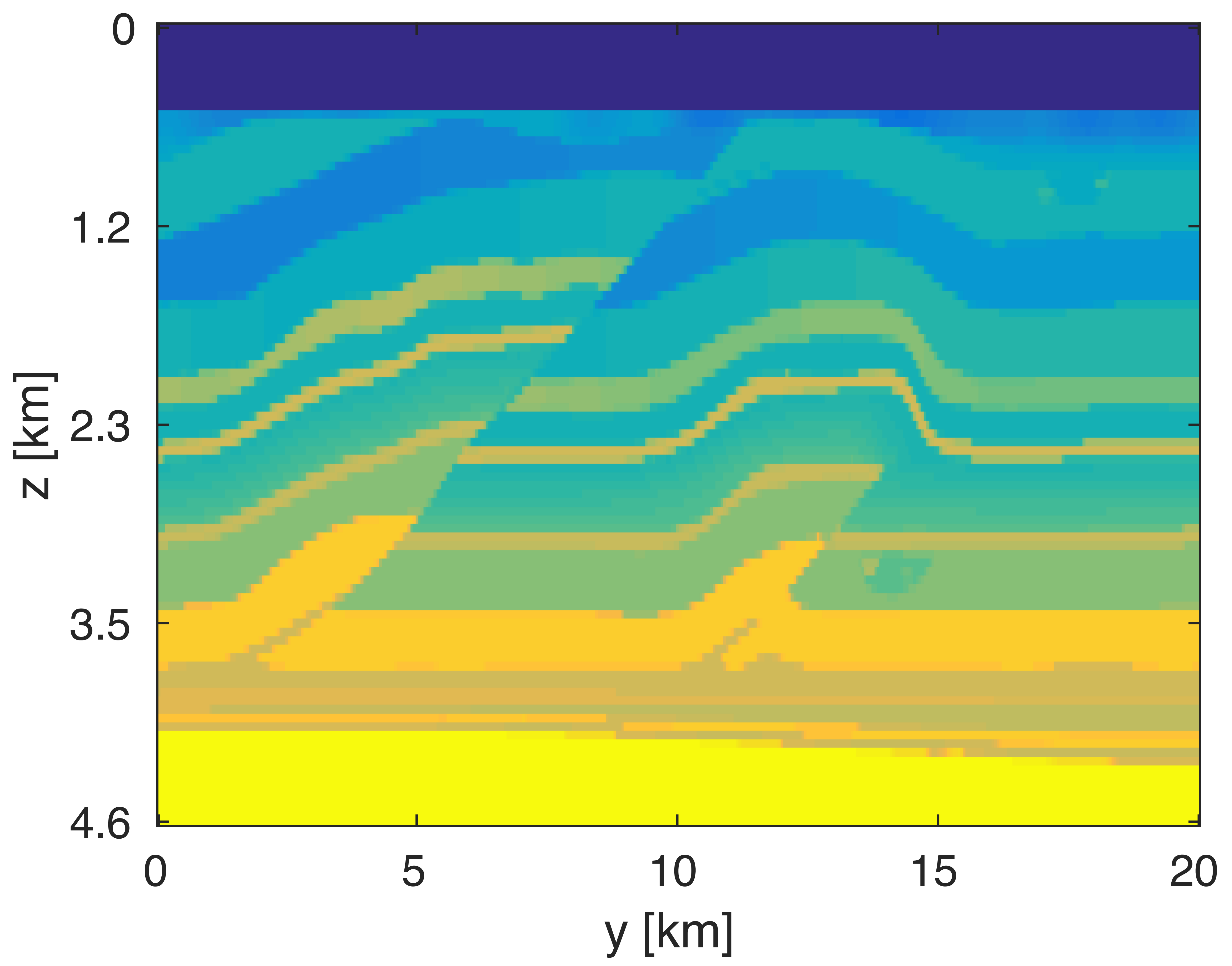


True model

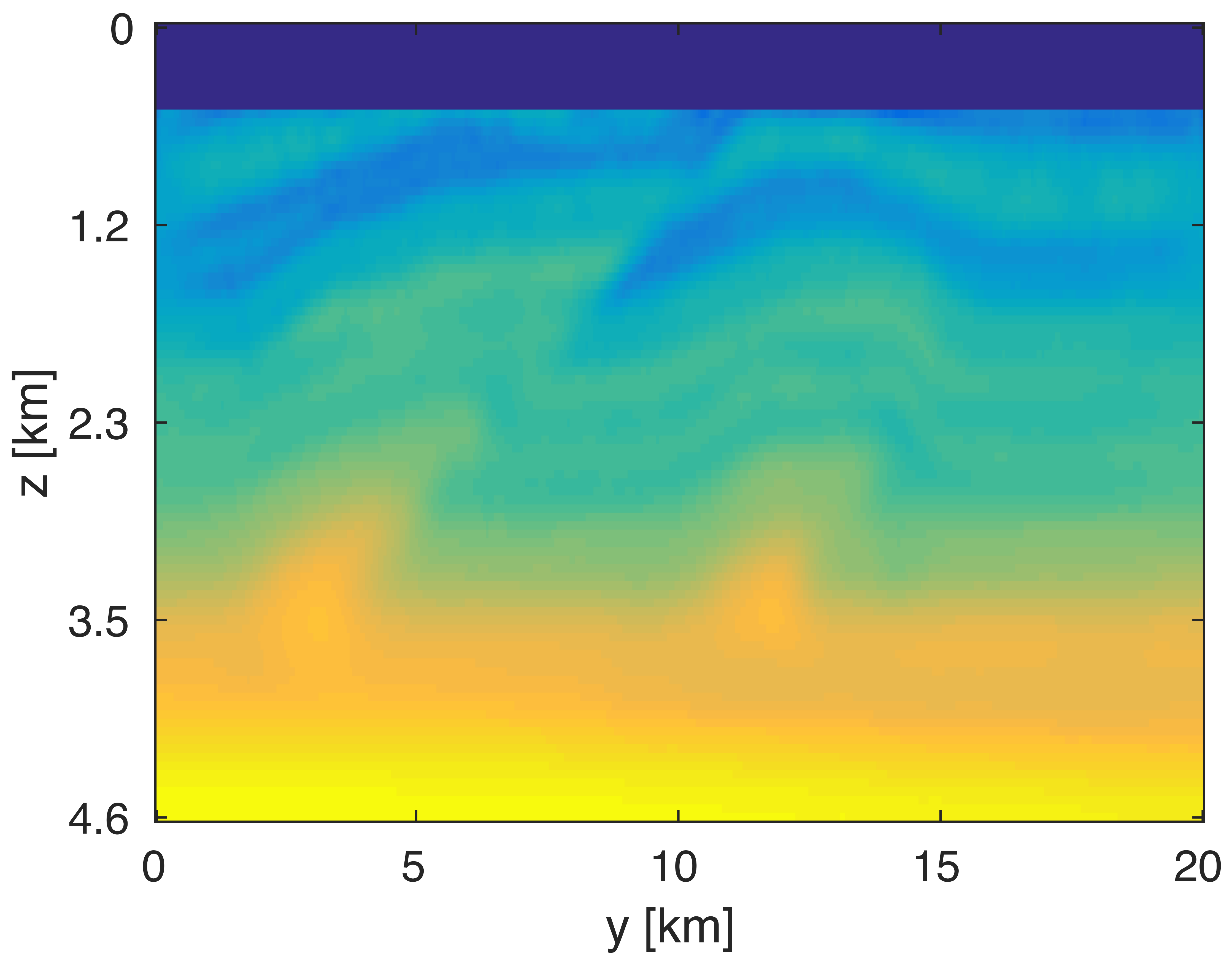


Initial model

x=17.5km slice

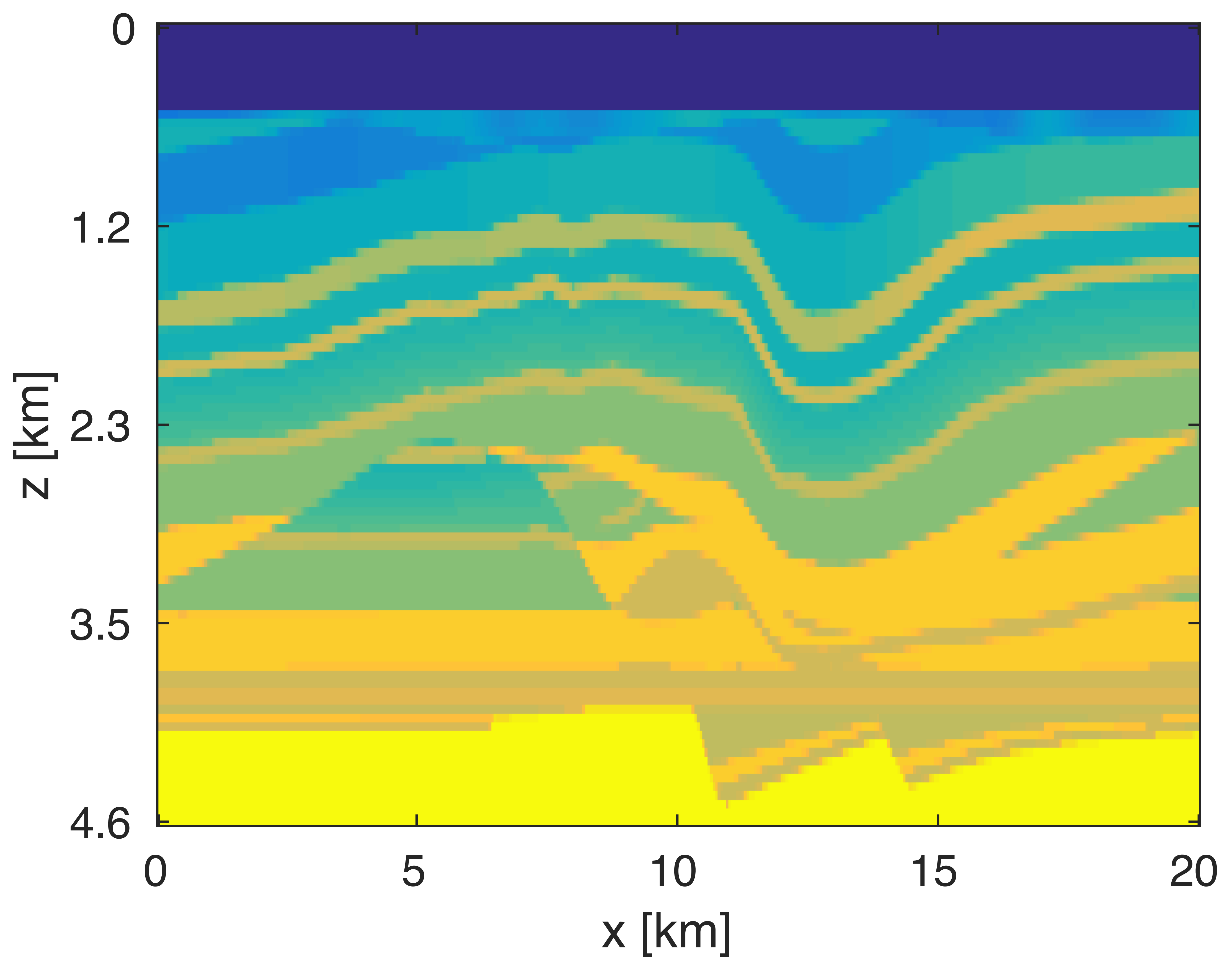


True model

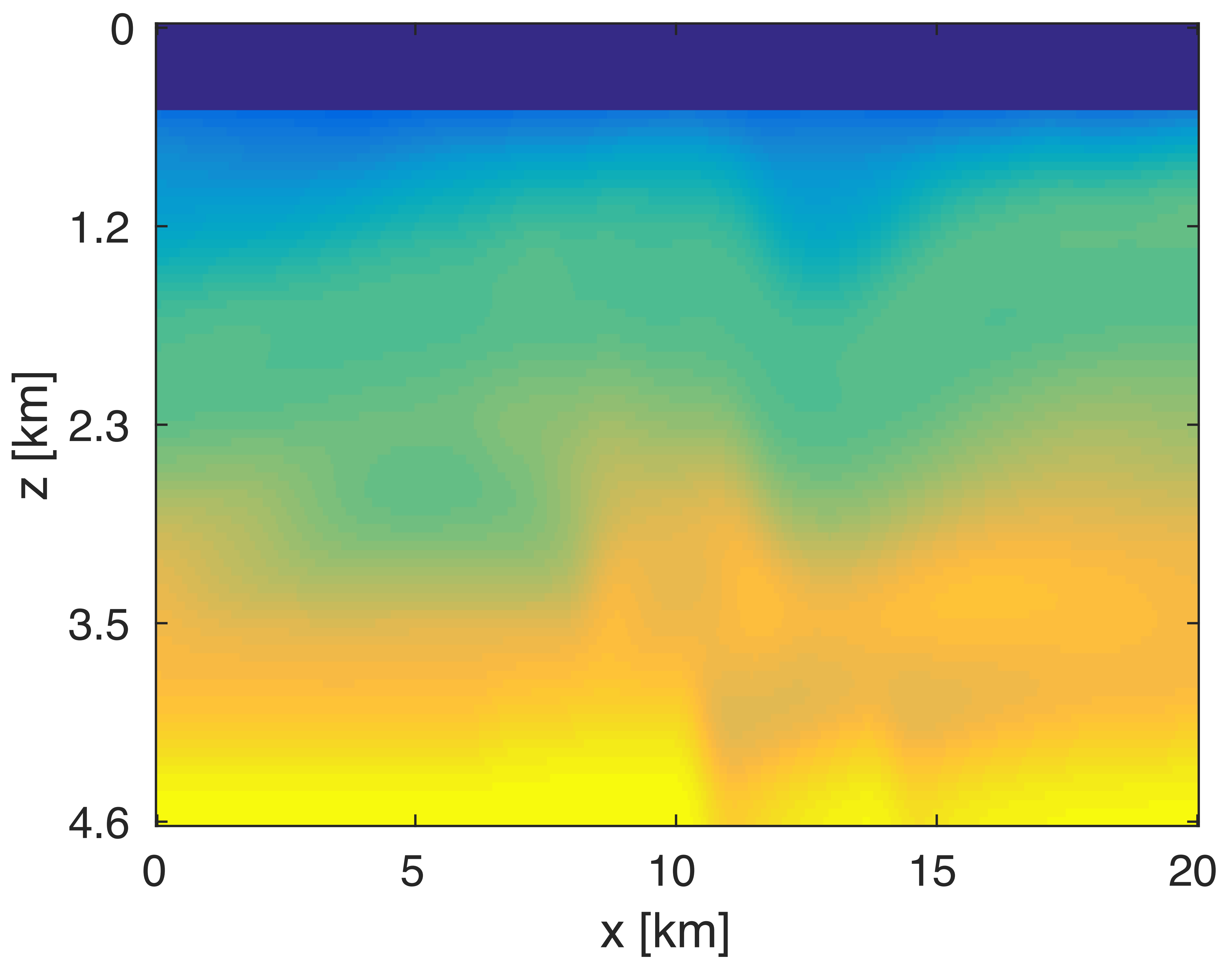


Stochastic LBFGS

y=5km slice

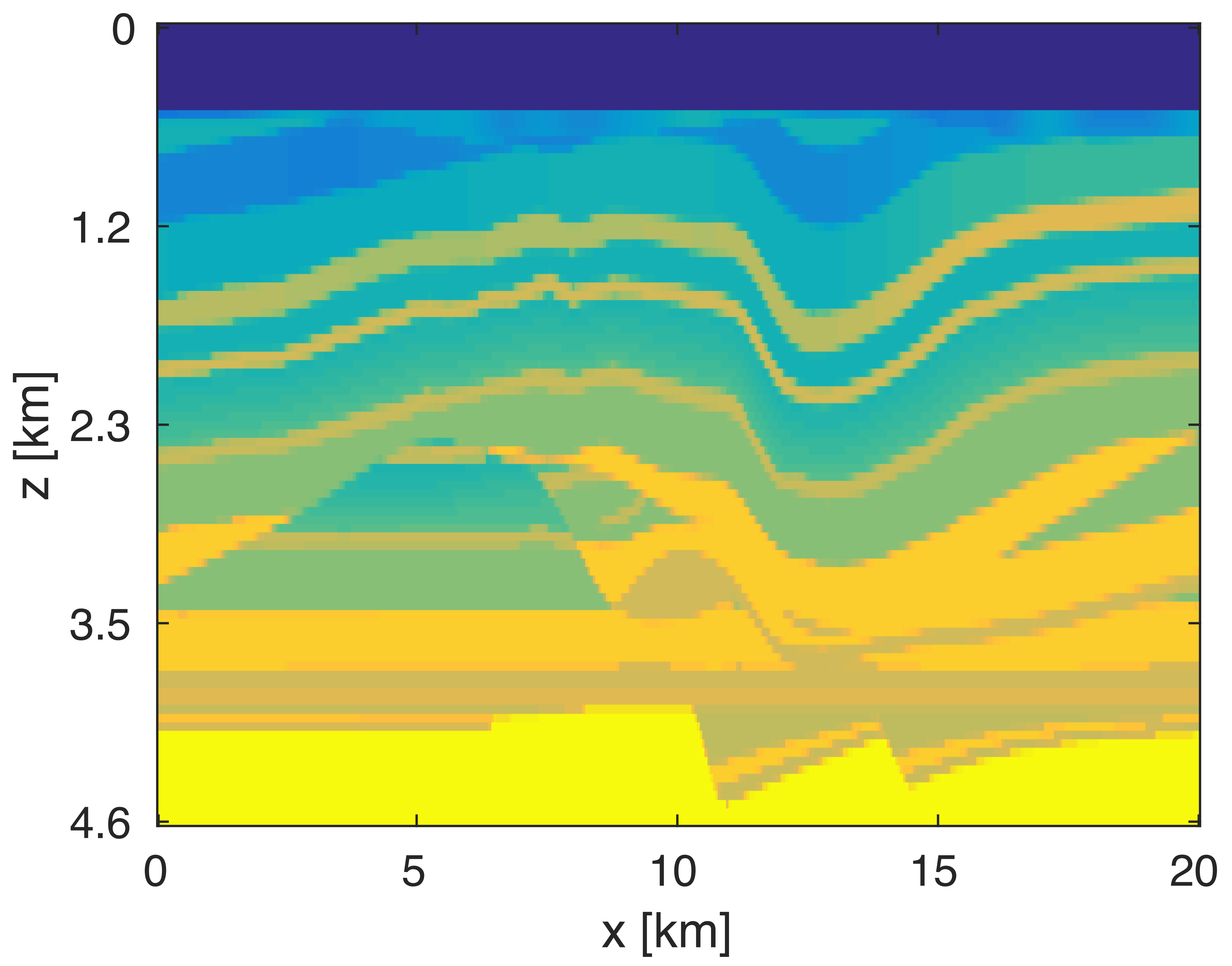


True model

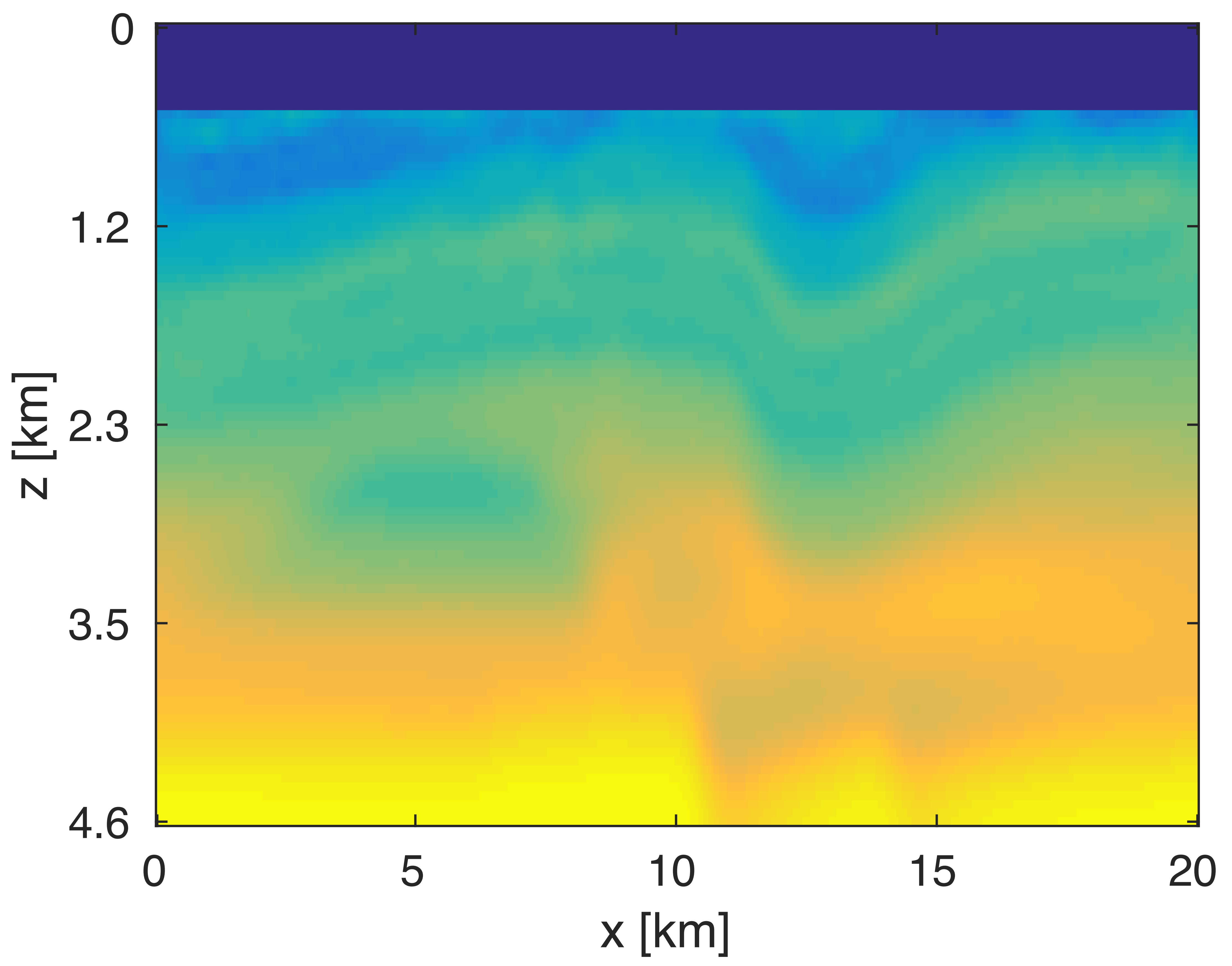


Initial model

y=5km slice

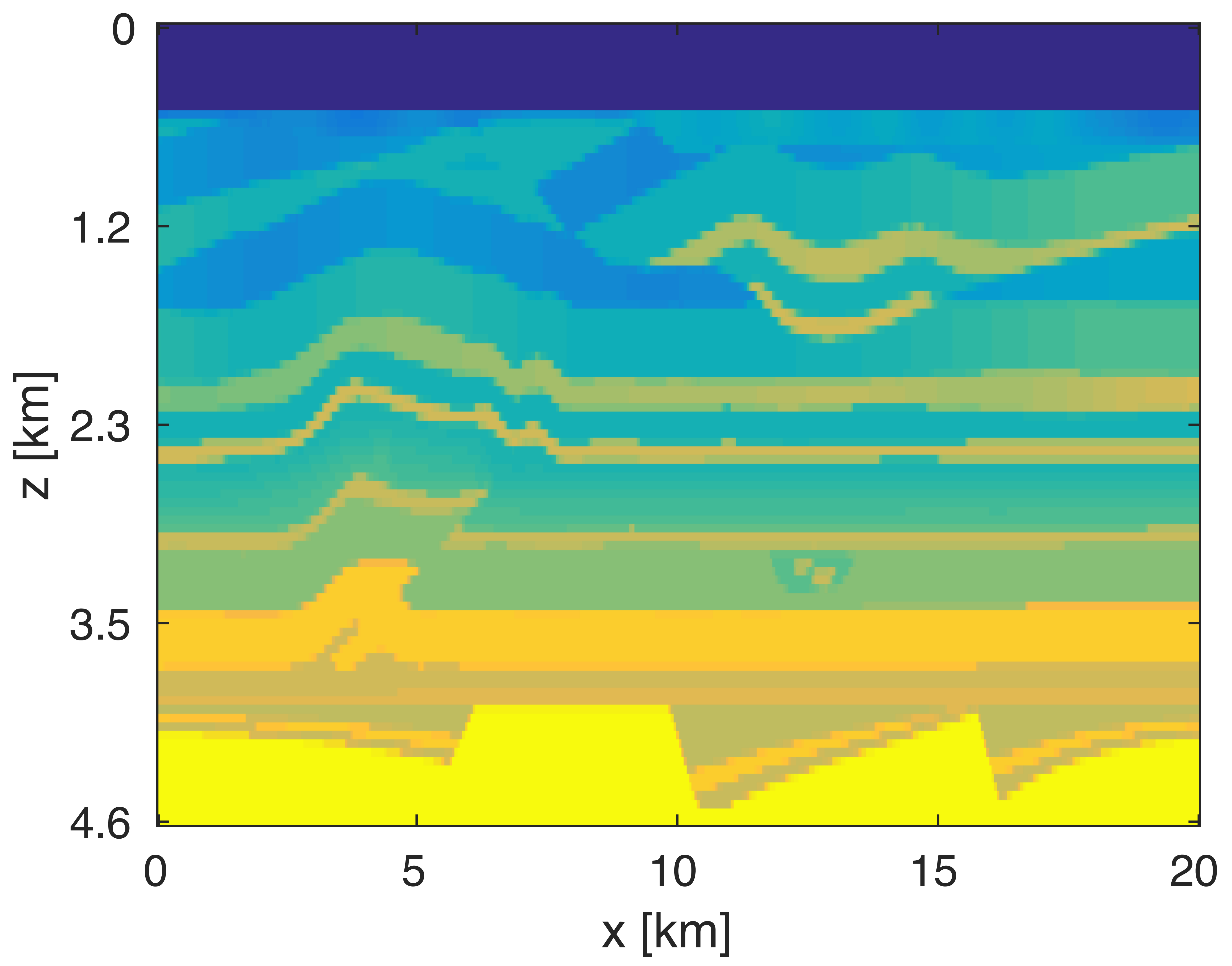


True model

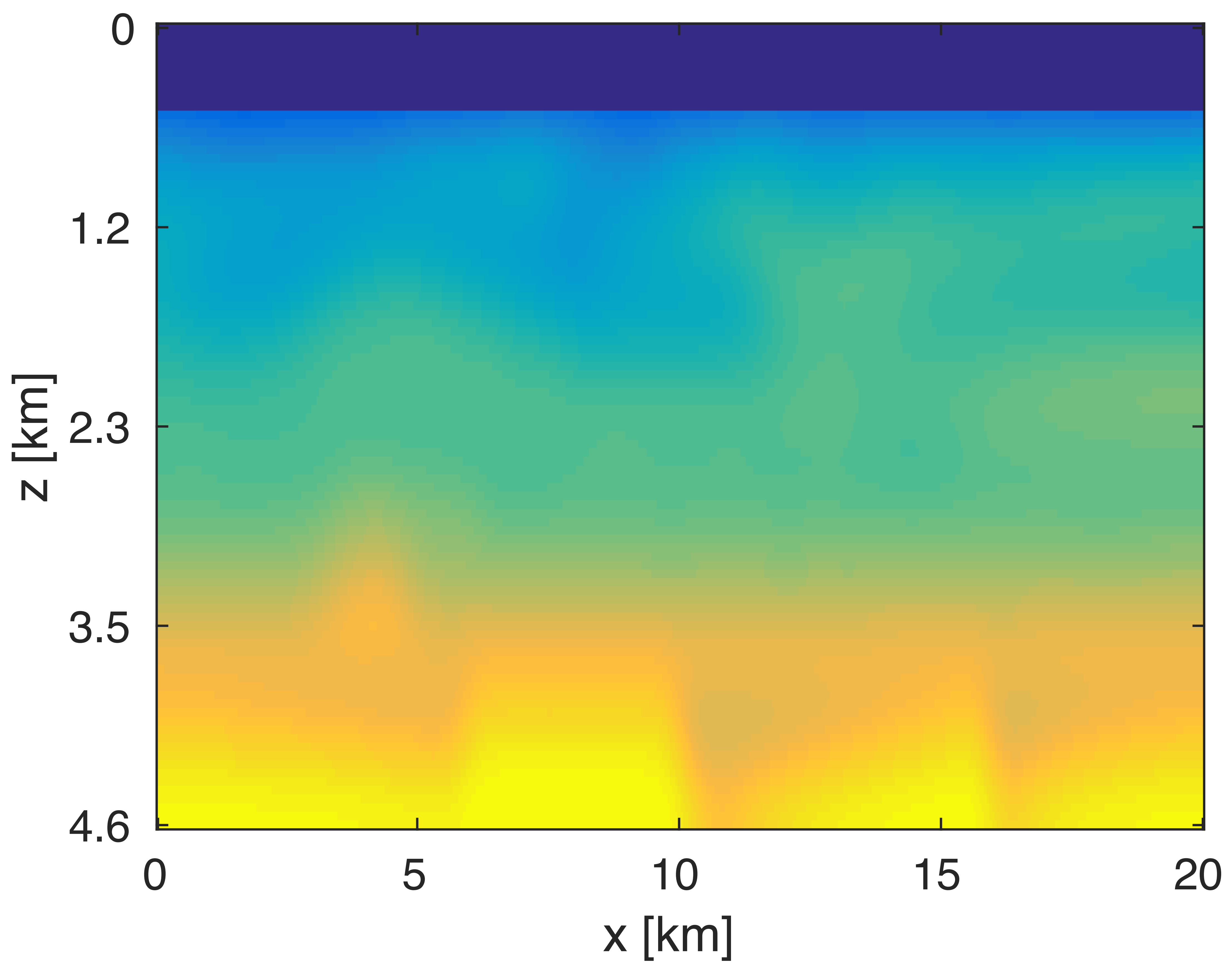


Stochastic LBFGS

y=10km slice

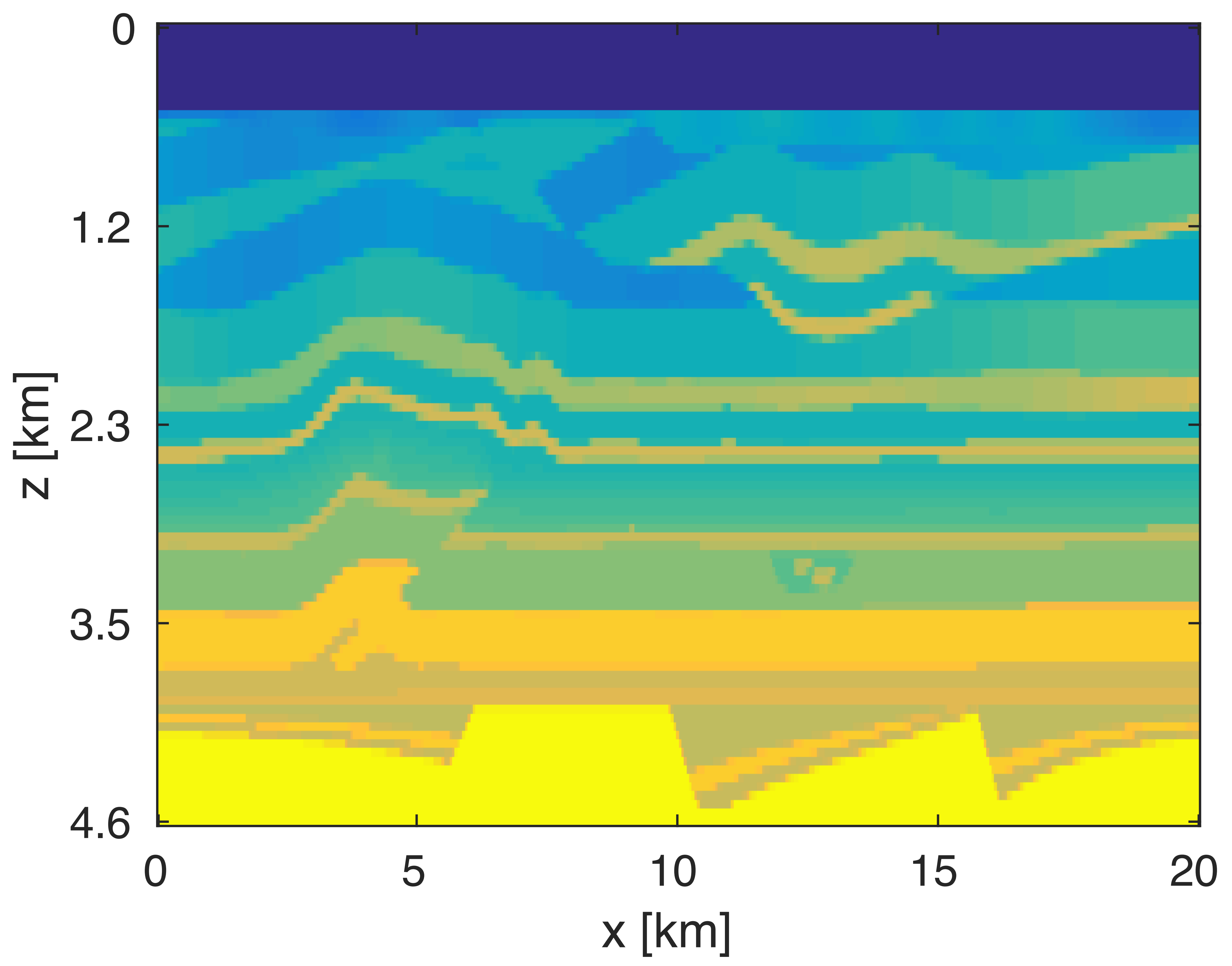


True model

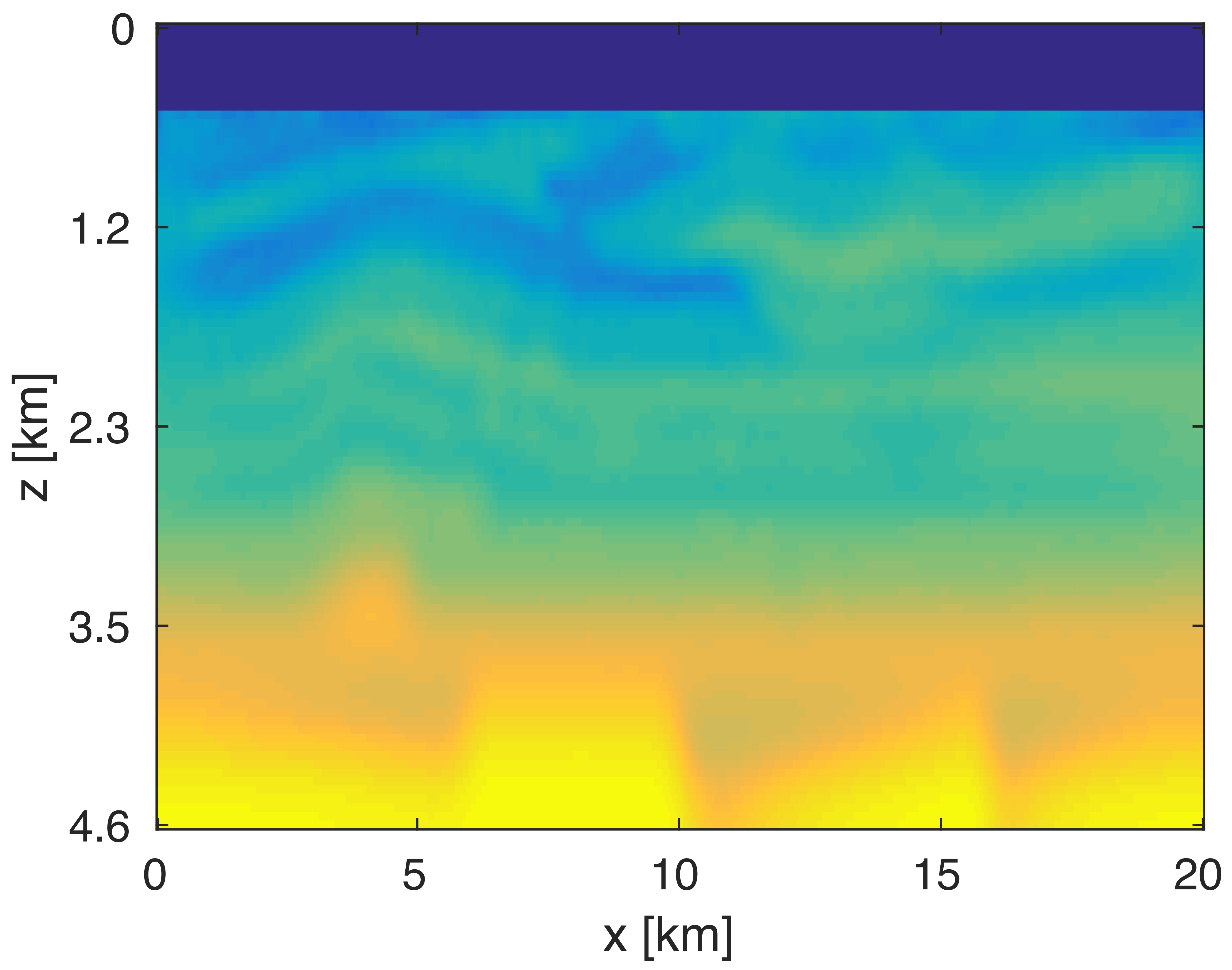


Initial model

y=10km slice



True model



Stochastic LBFGS

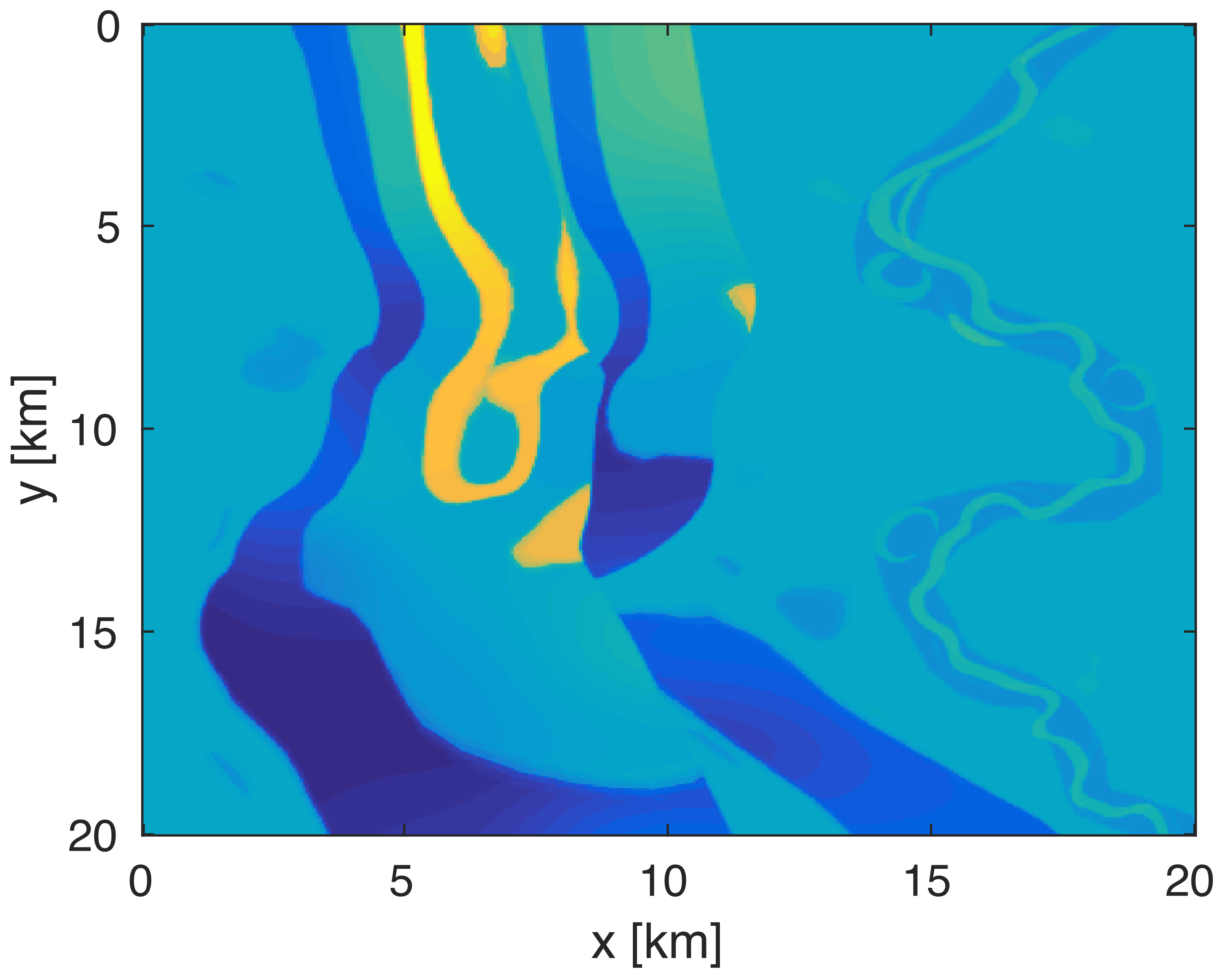
3D Overthrust Model

Same model as before, no water layer (SEG abstract results)

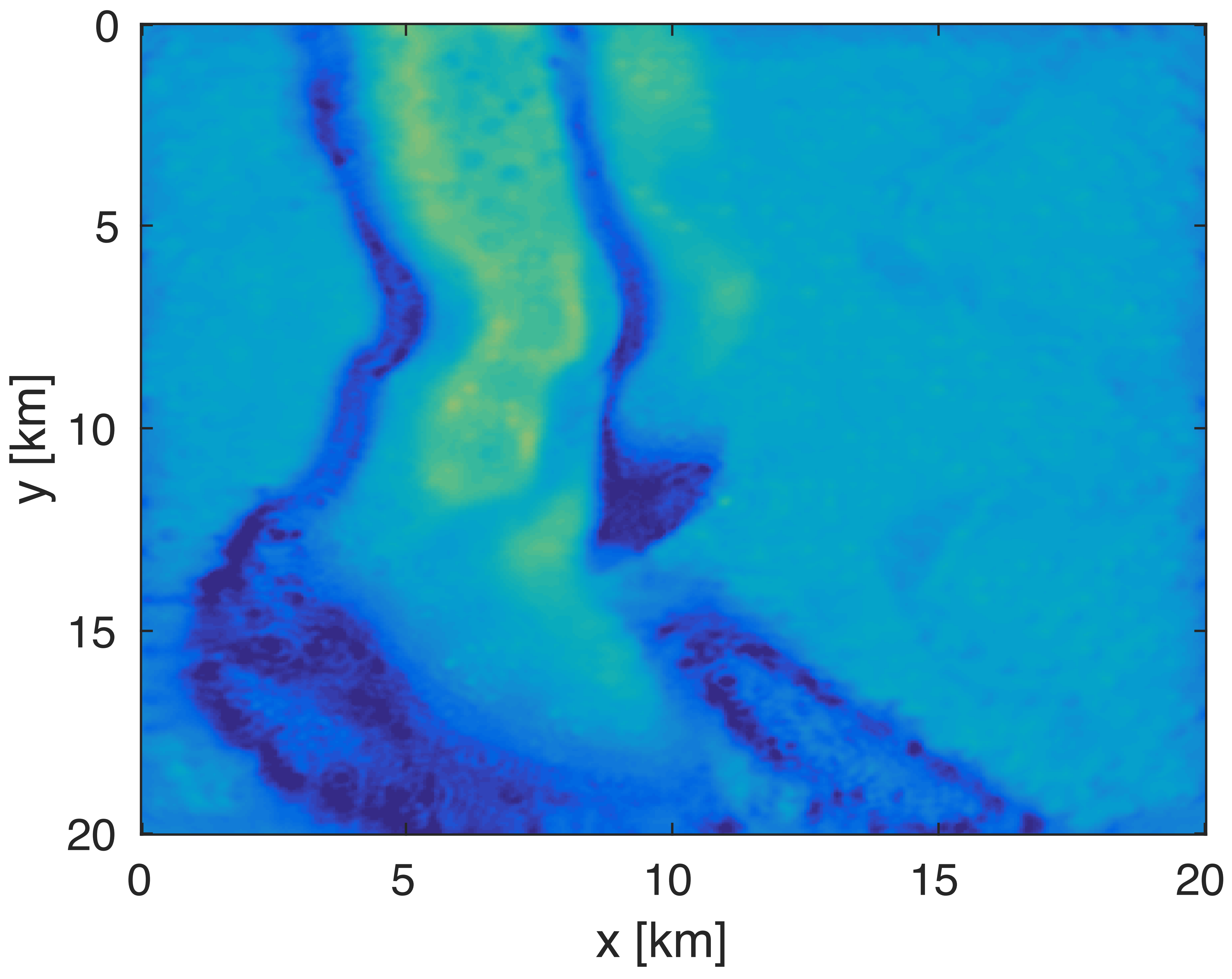
3Hz - 8Hz, inverted one frequency at a time

Compare the stochastic approach to the full-data approach (equivalent # of PDEs solved)

z=500m slice

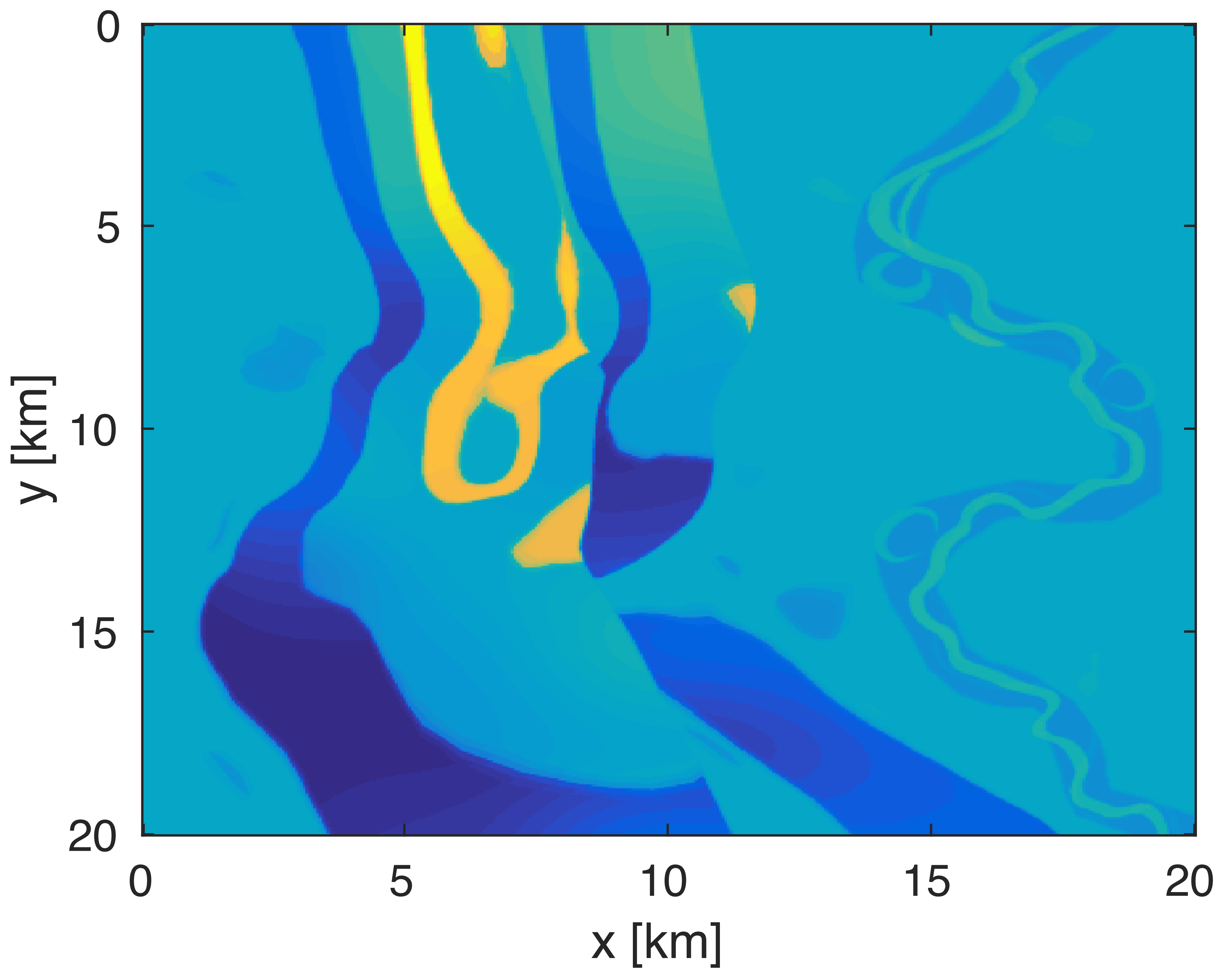


True model

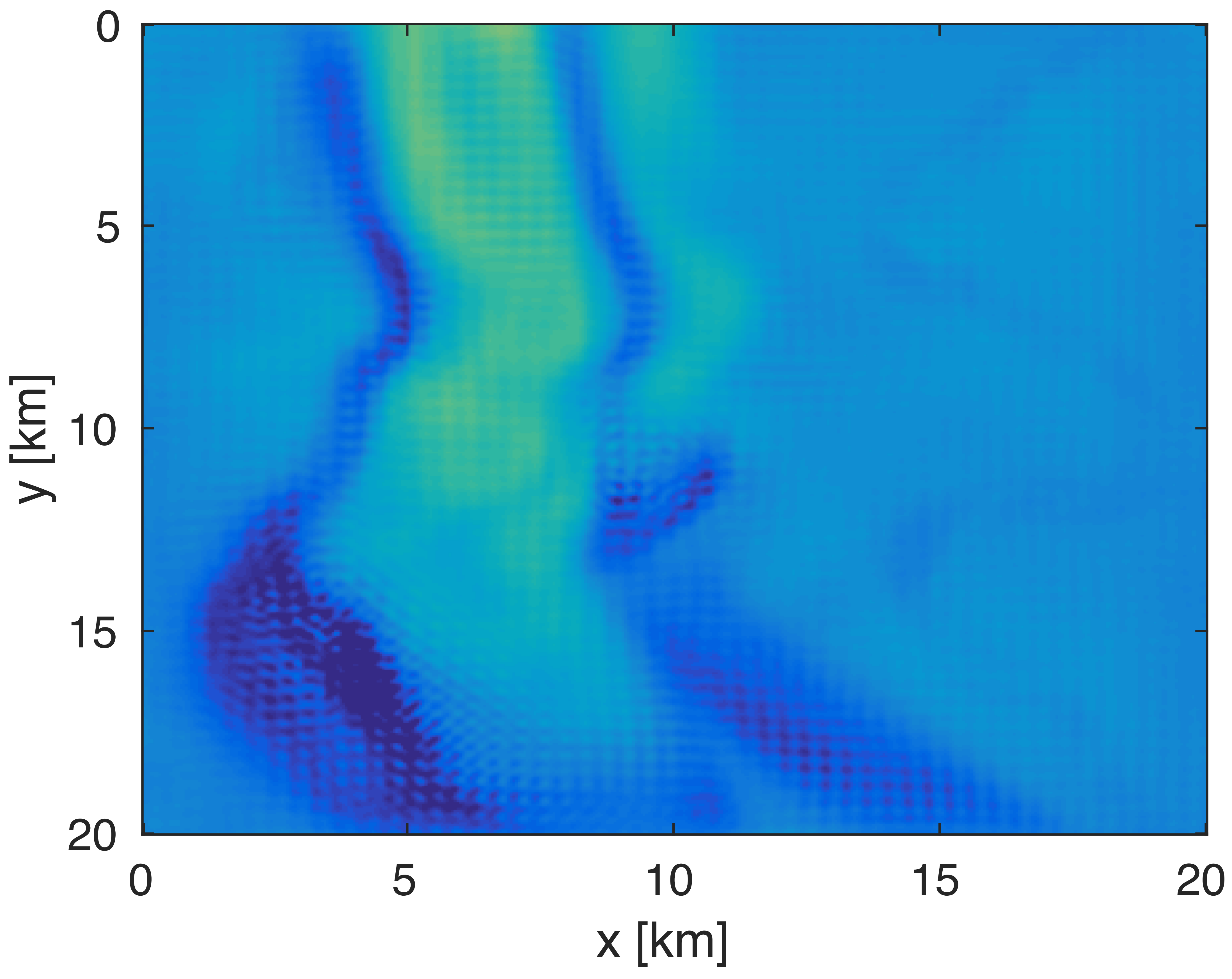


Stochastic LBFGS

z=500m slice

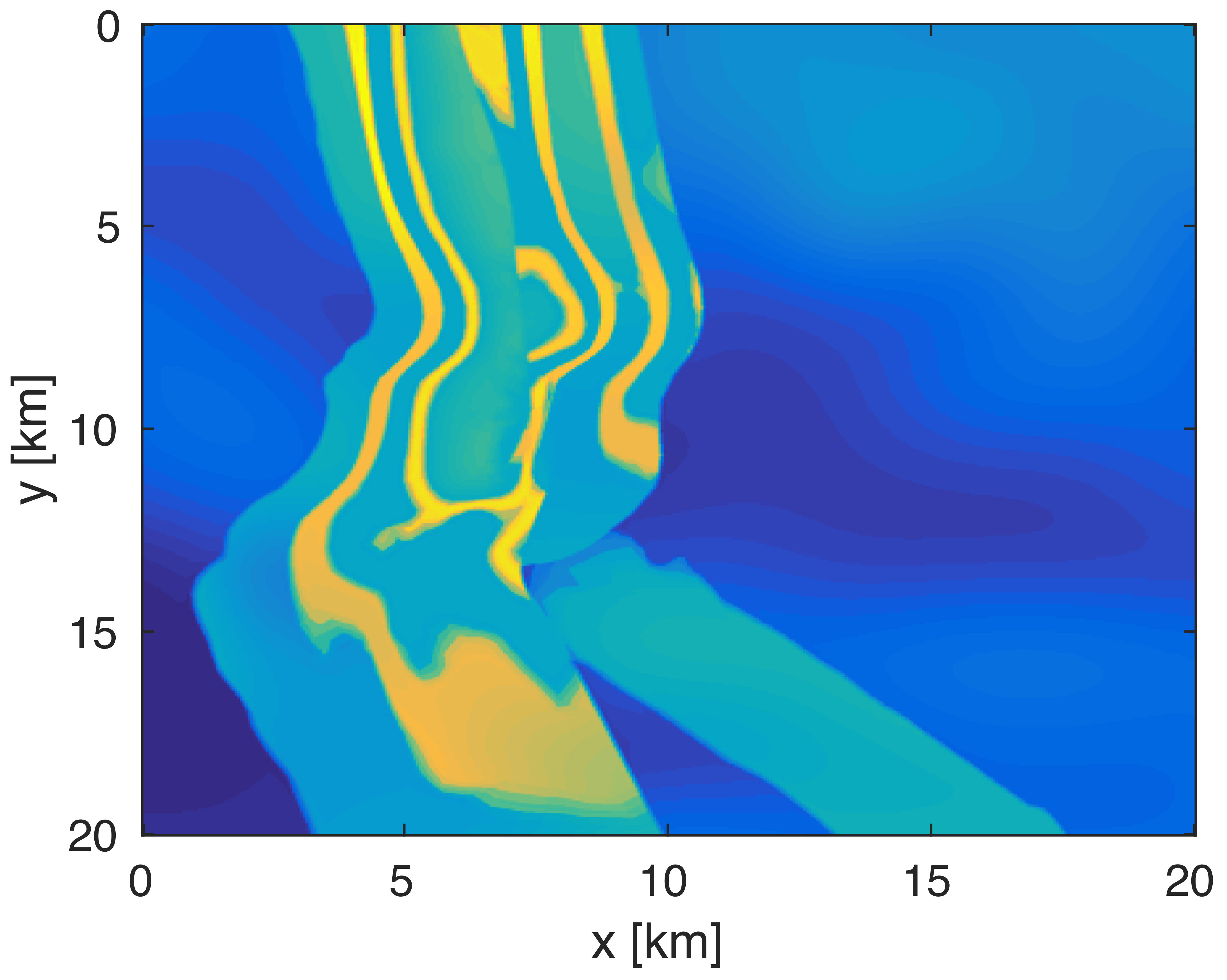


True model

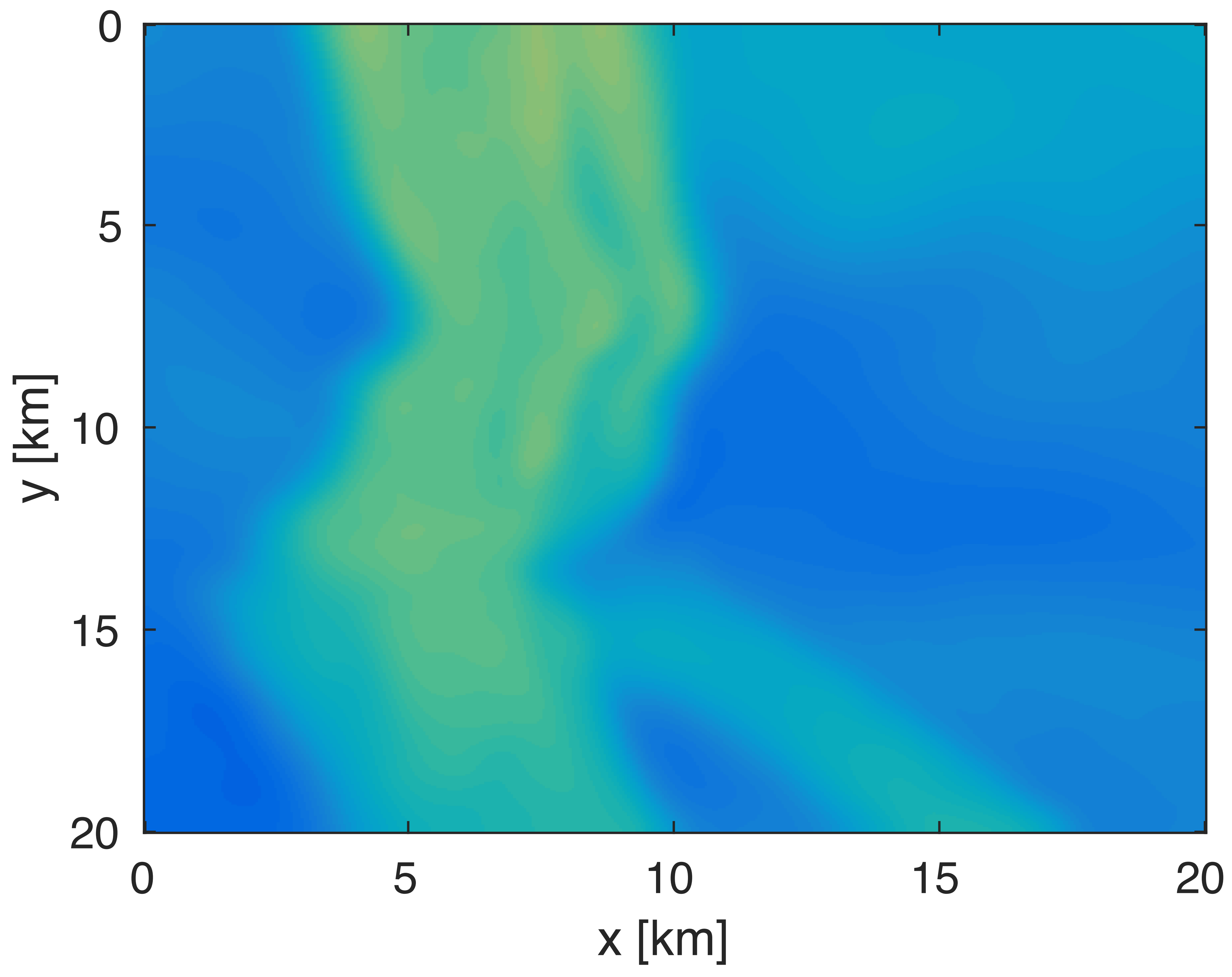


Full data

z=1000m slice

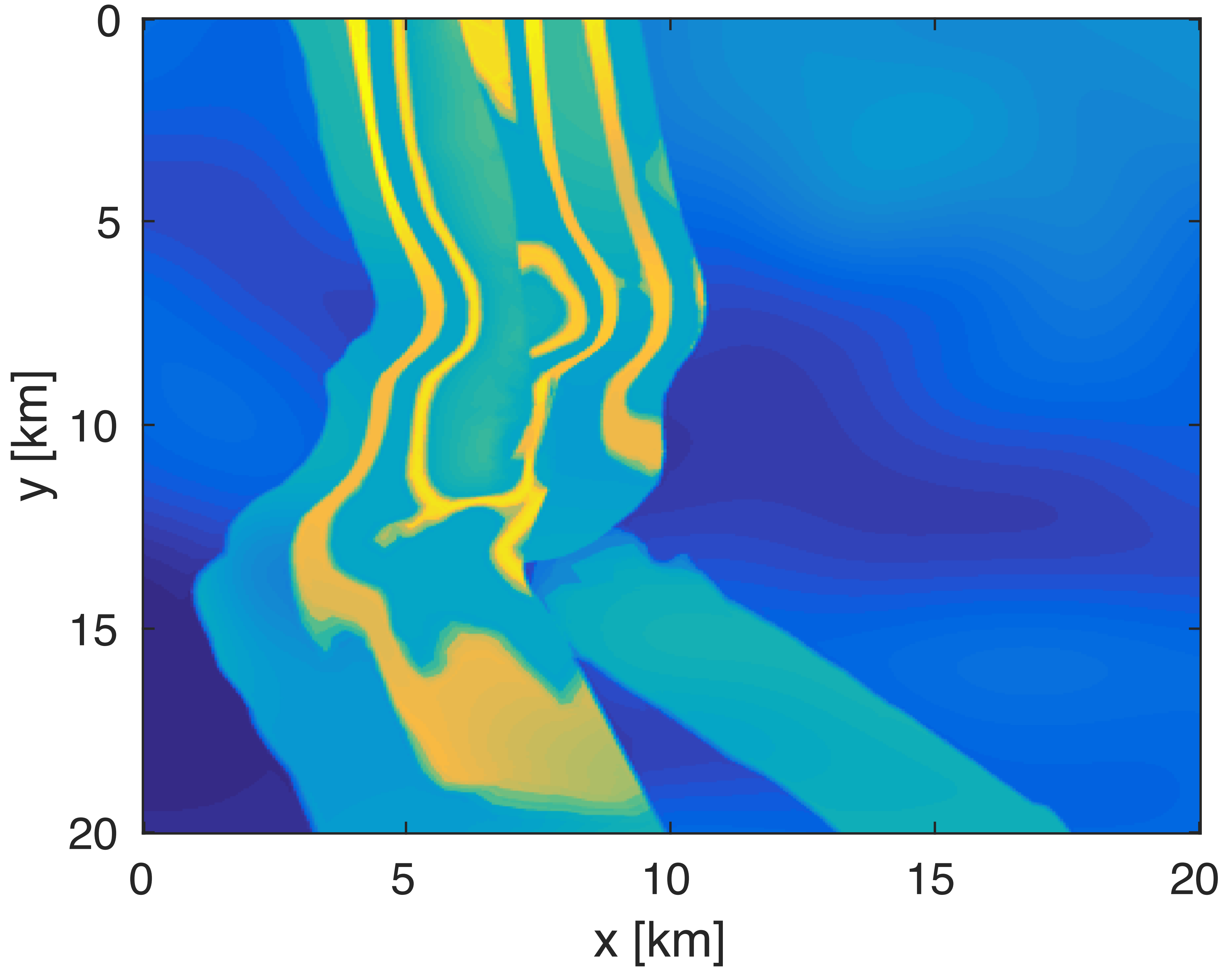


True model

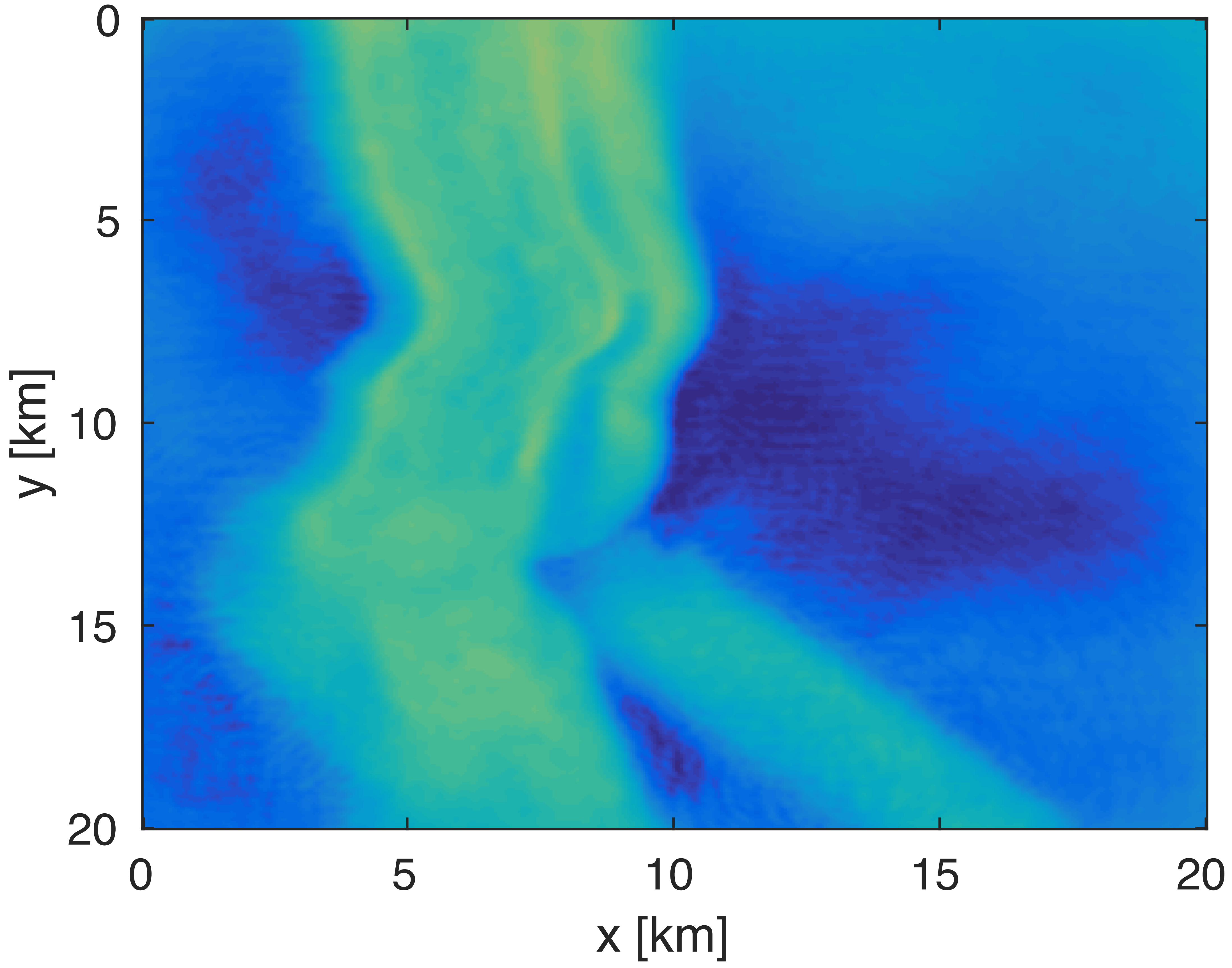


Initial Model

z=1000m slice

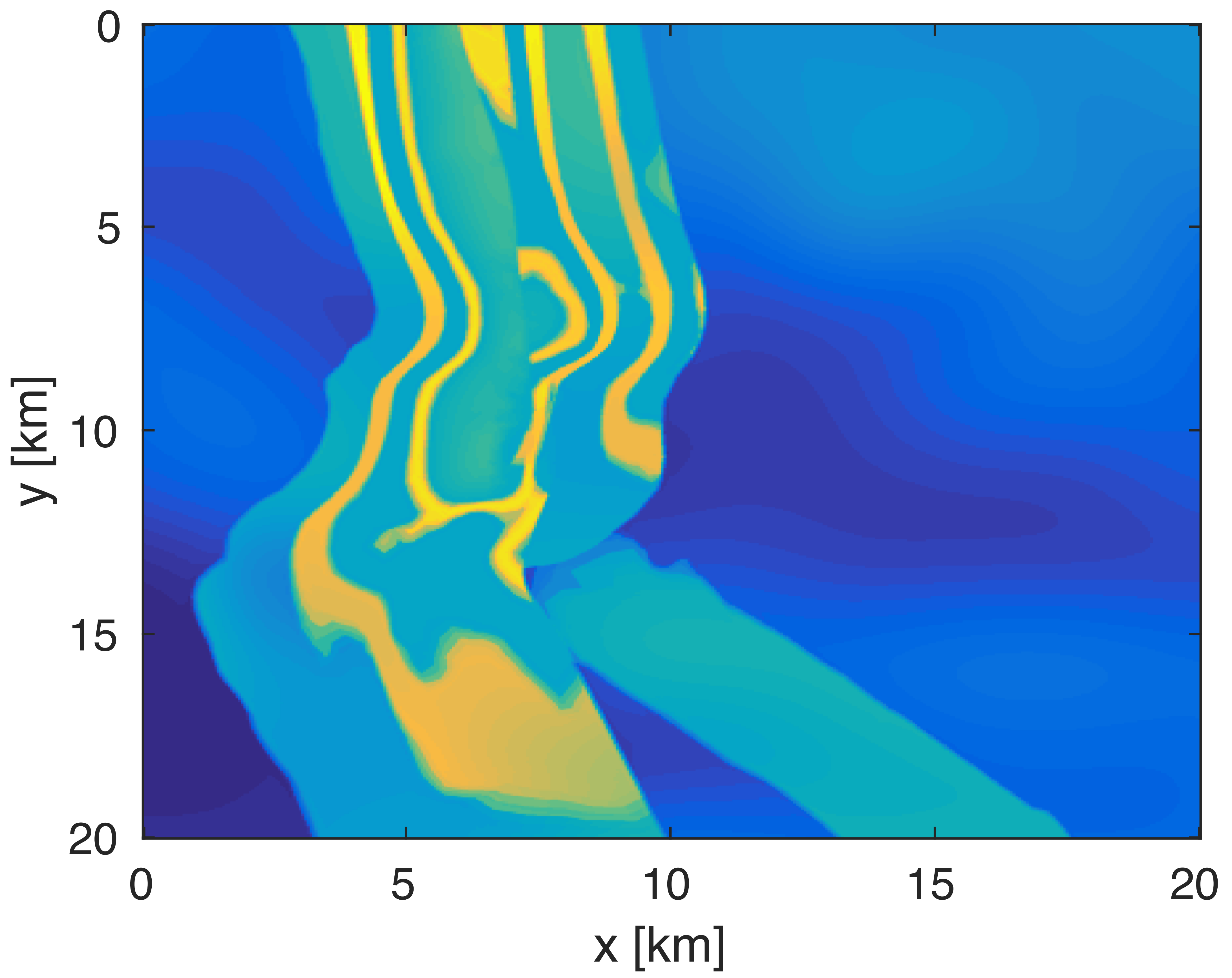


True model

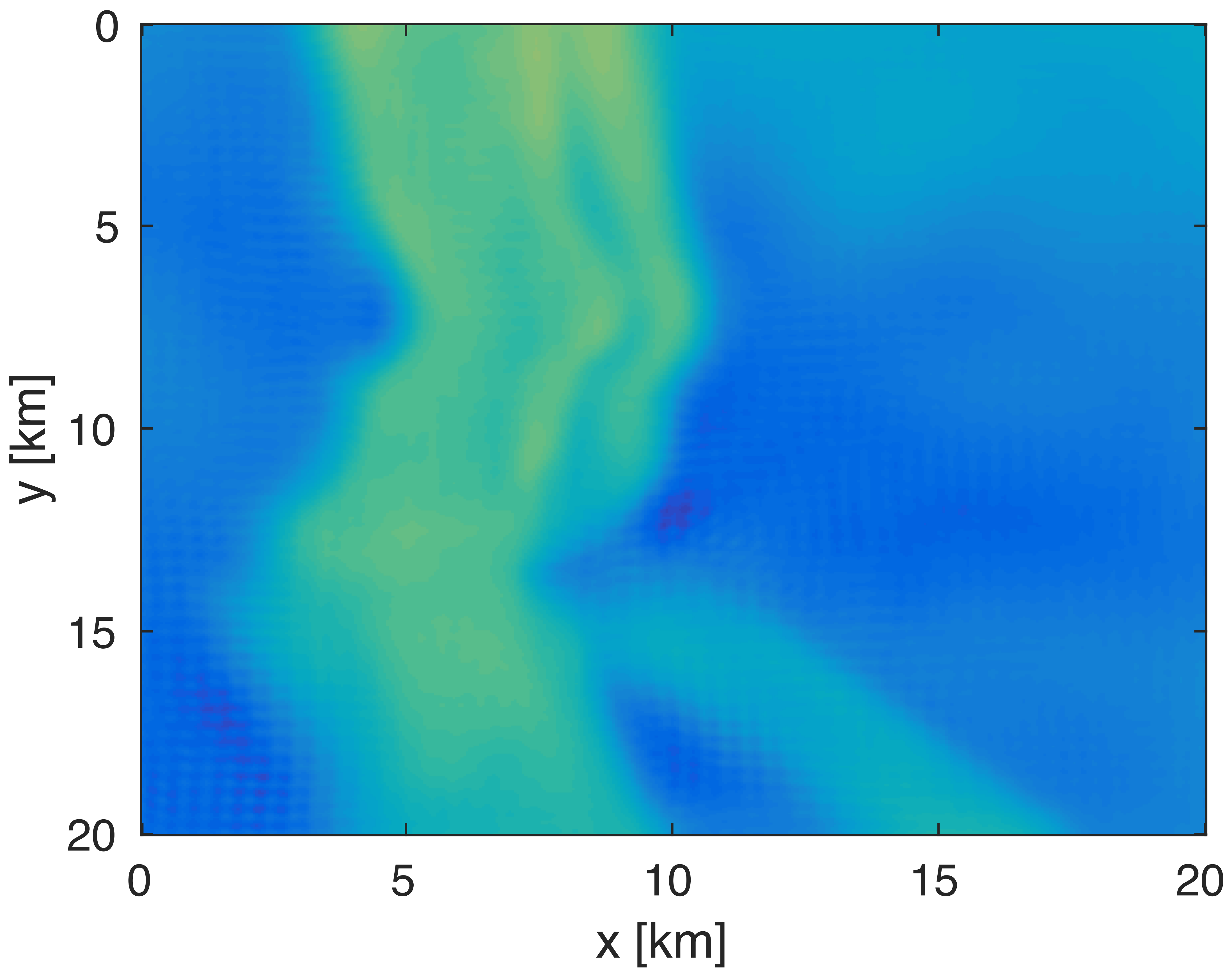


Stochastic LBFGS

z=1000m slice

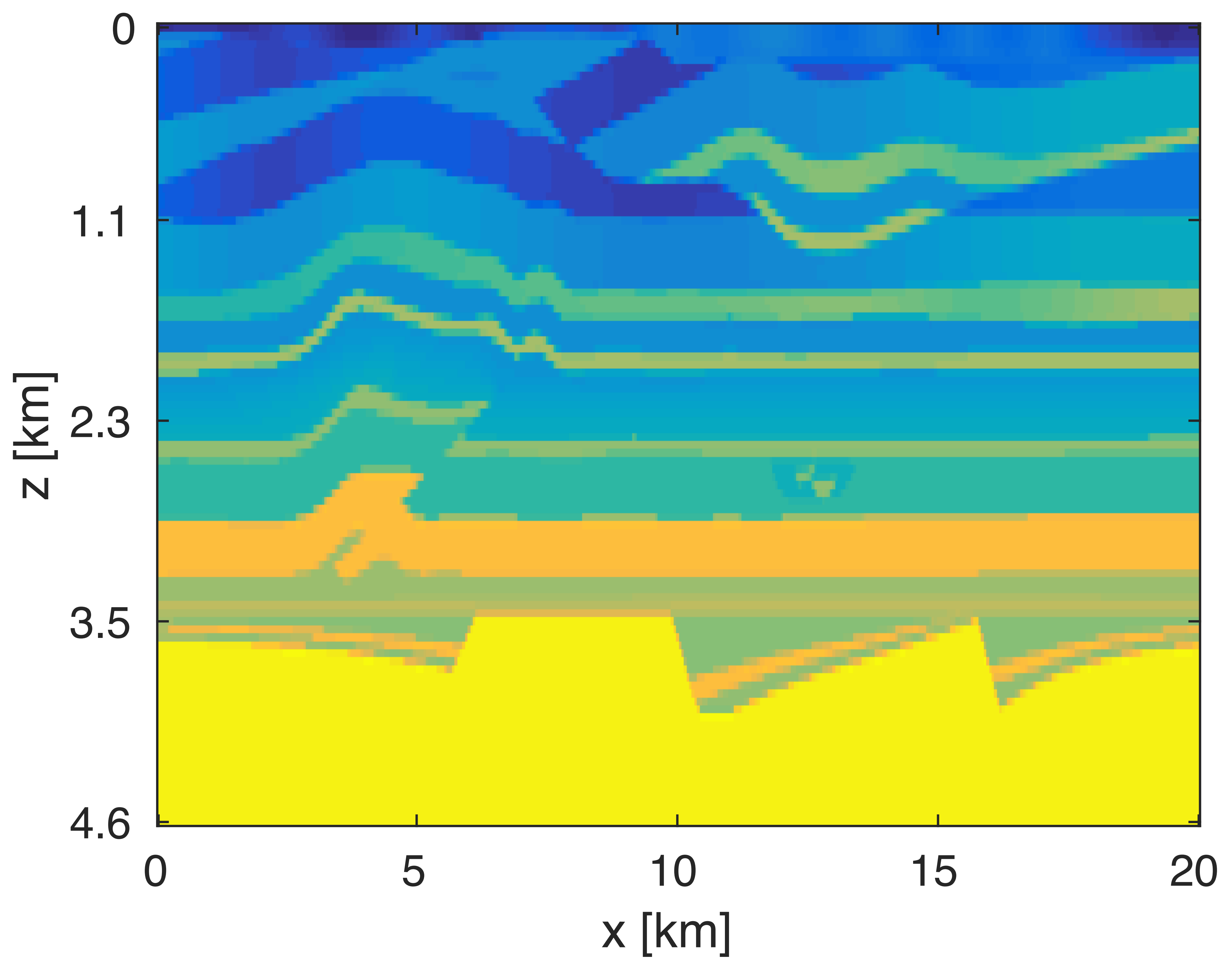


True model

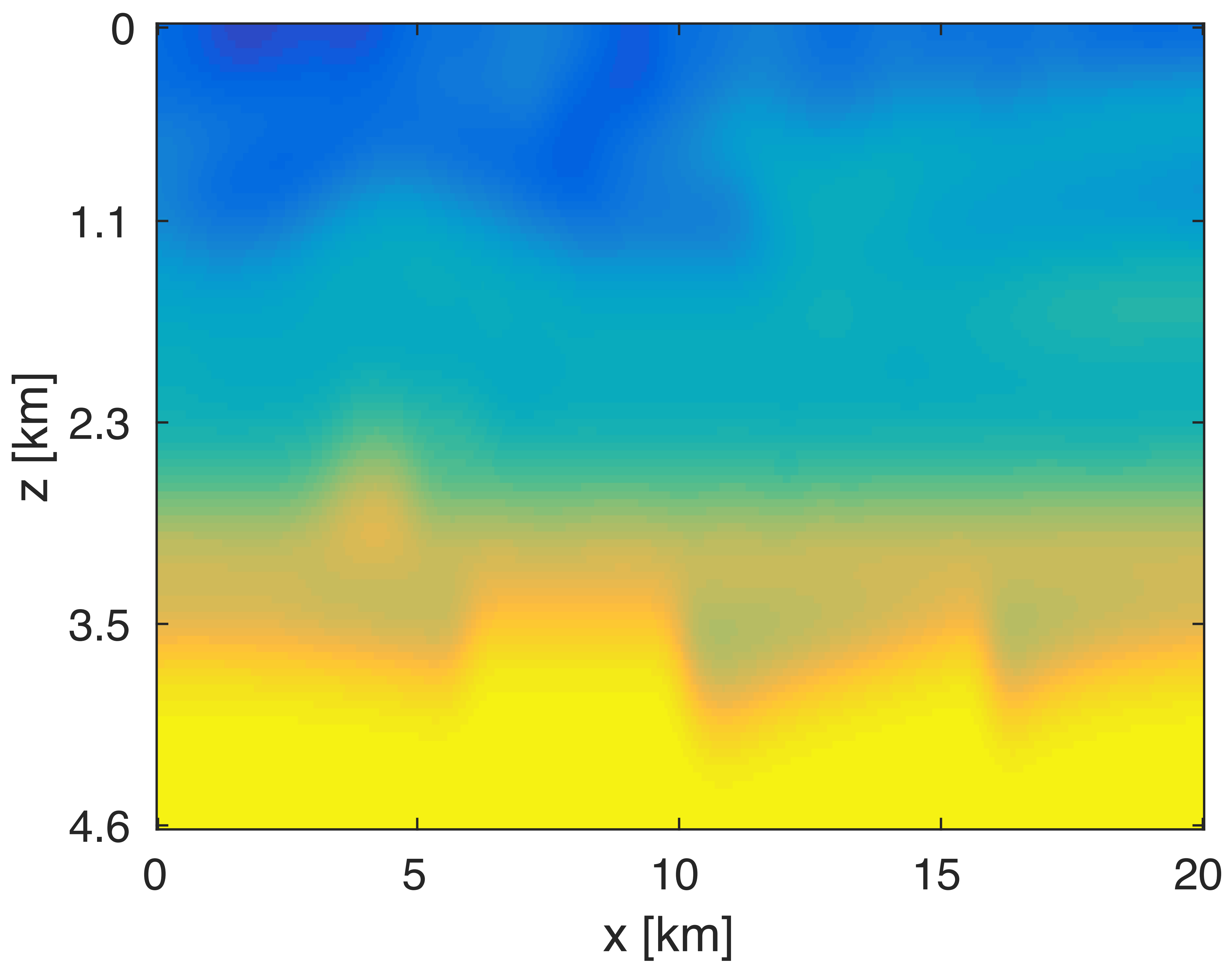


Full data

y=10000m slice

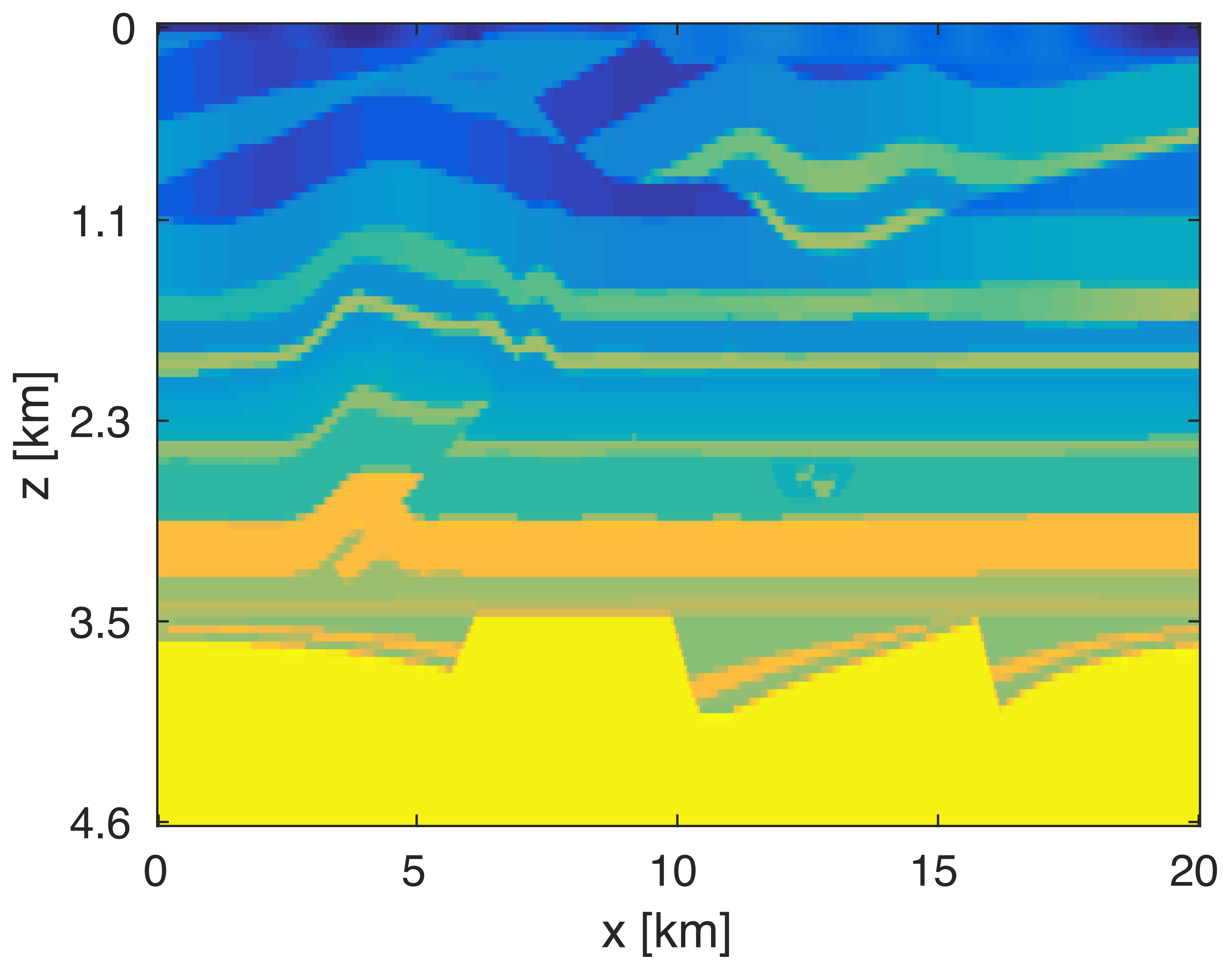


True model

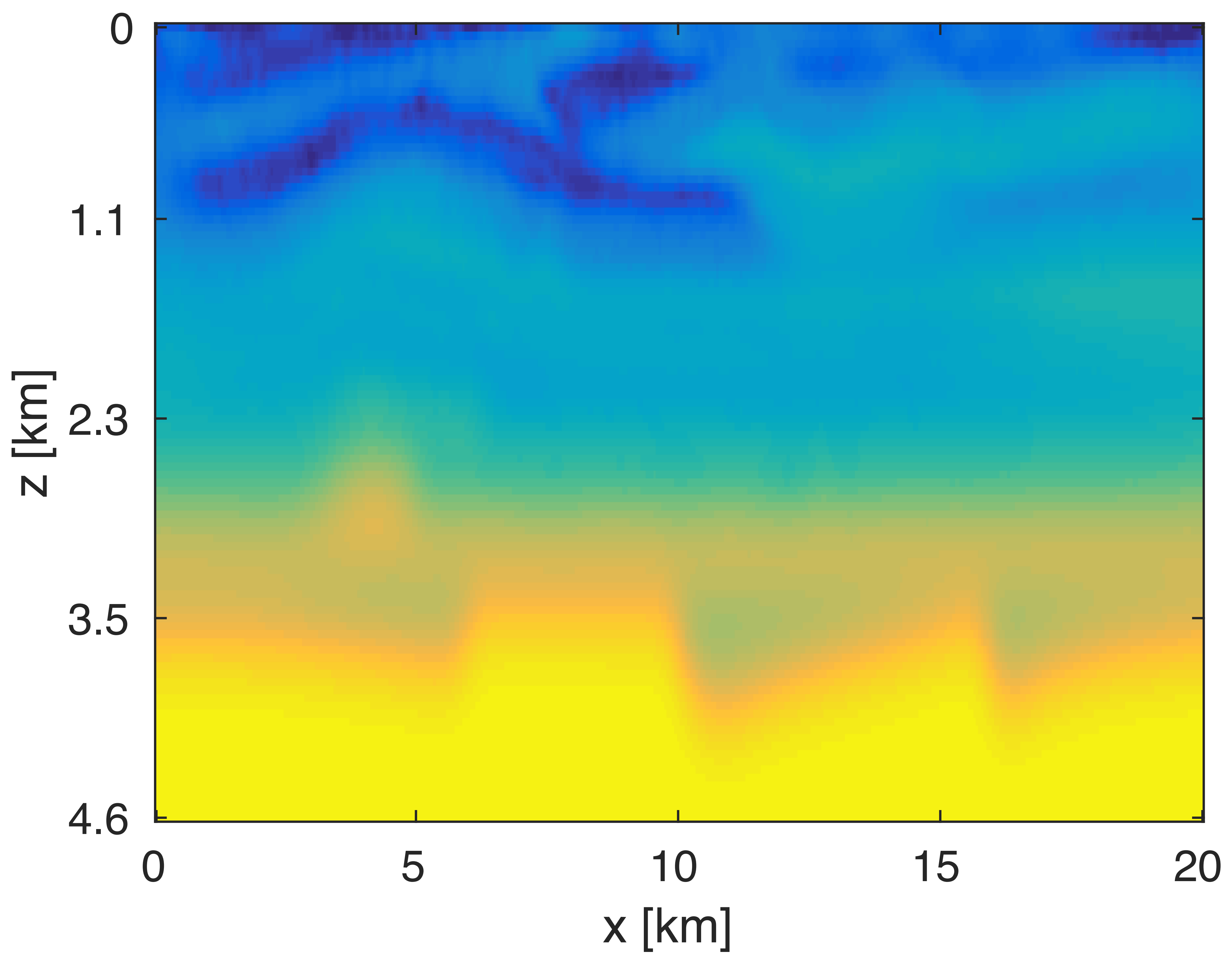


Initial model

y=10000m slice

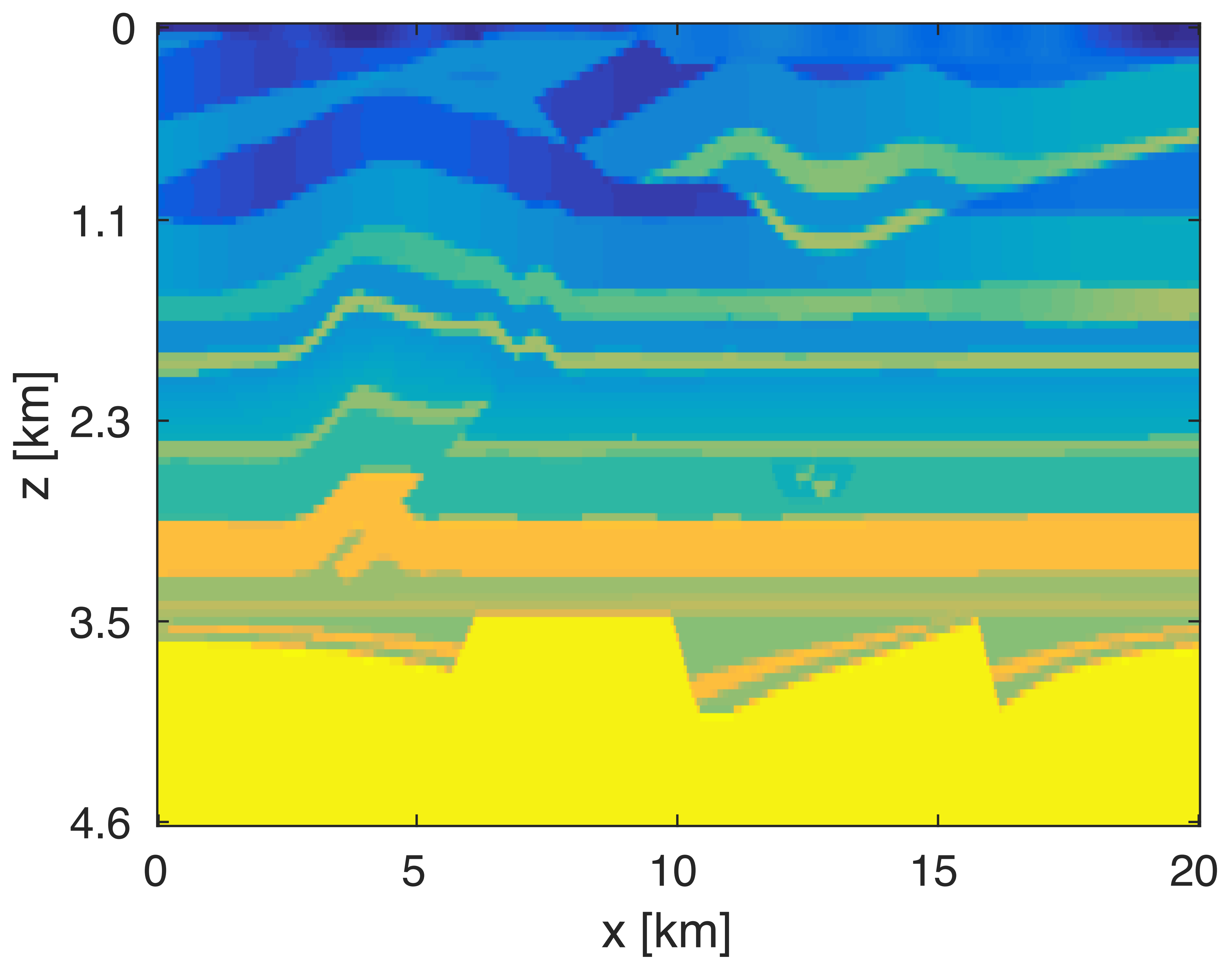


True model

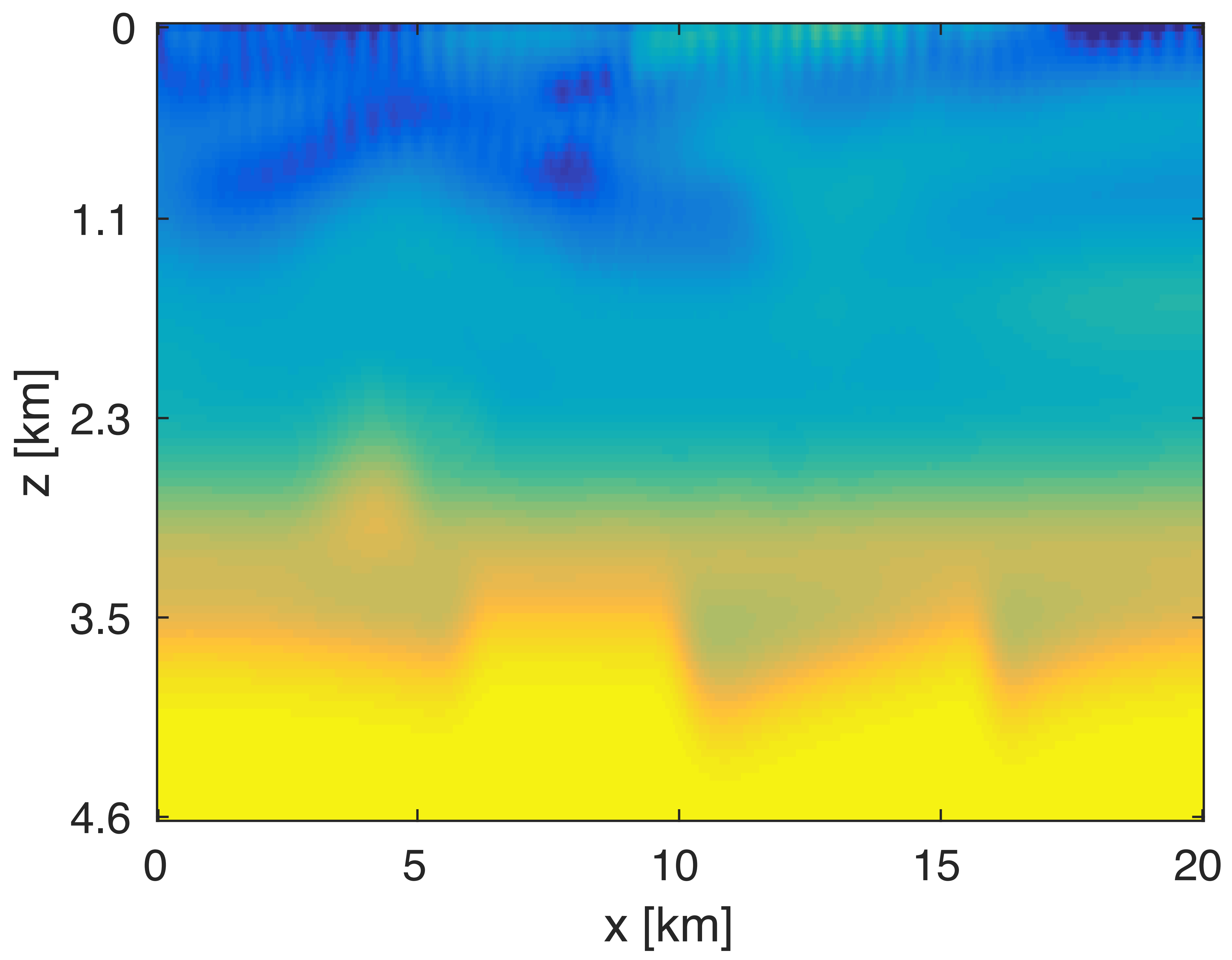


Stochastic LBFGS

y=10000m slice



True model



Full data

Summary

Performance and correctness don’t have to be mutually exclusive

- Design software in a modular, hierarchical way yields benefits of both

Modularity -> flexibility

- Very easy to swap out modules (PDE discretizations, preconditioners) without changing code

Summary

Modularity -> Easier to test

- Easier to test -> easier to get right

We can design code that is *demonstrably* correct

- Reduce scope of potential problems in FWI

Summary

Right abstractions for FWI ->

- ease of use
- computationally efficient
- flexible
- easy to extend, understand, optimize
- can prototype algorithms in 2D, run immediately in 3D

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Thank you for your attention