# Uncertainty quantification for Wavefield Reconstruction Inversion using a PDE free semi-definite Hessian and randomize-then-optimize method

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2016/10/17

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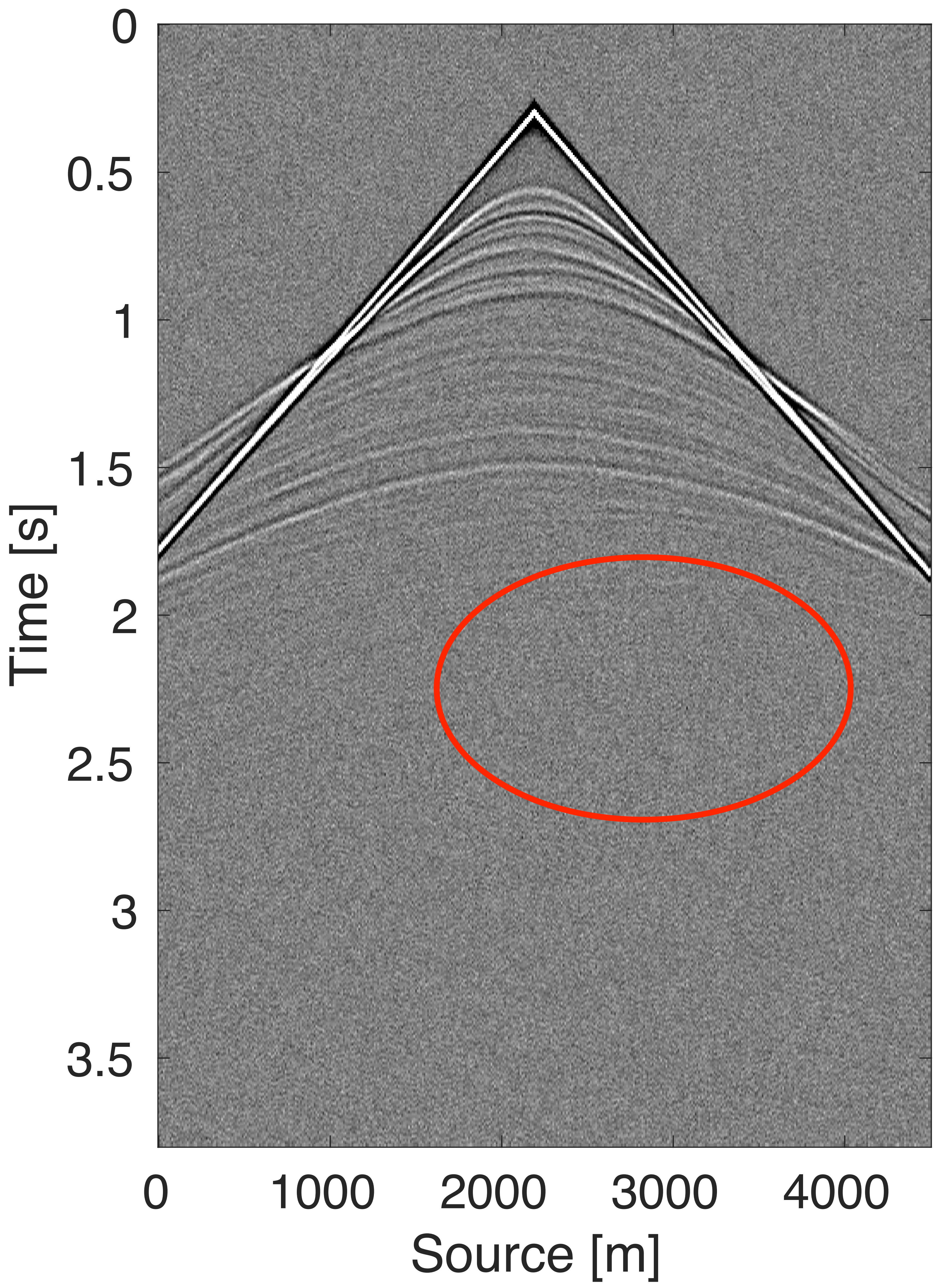
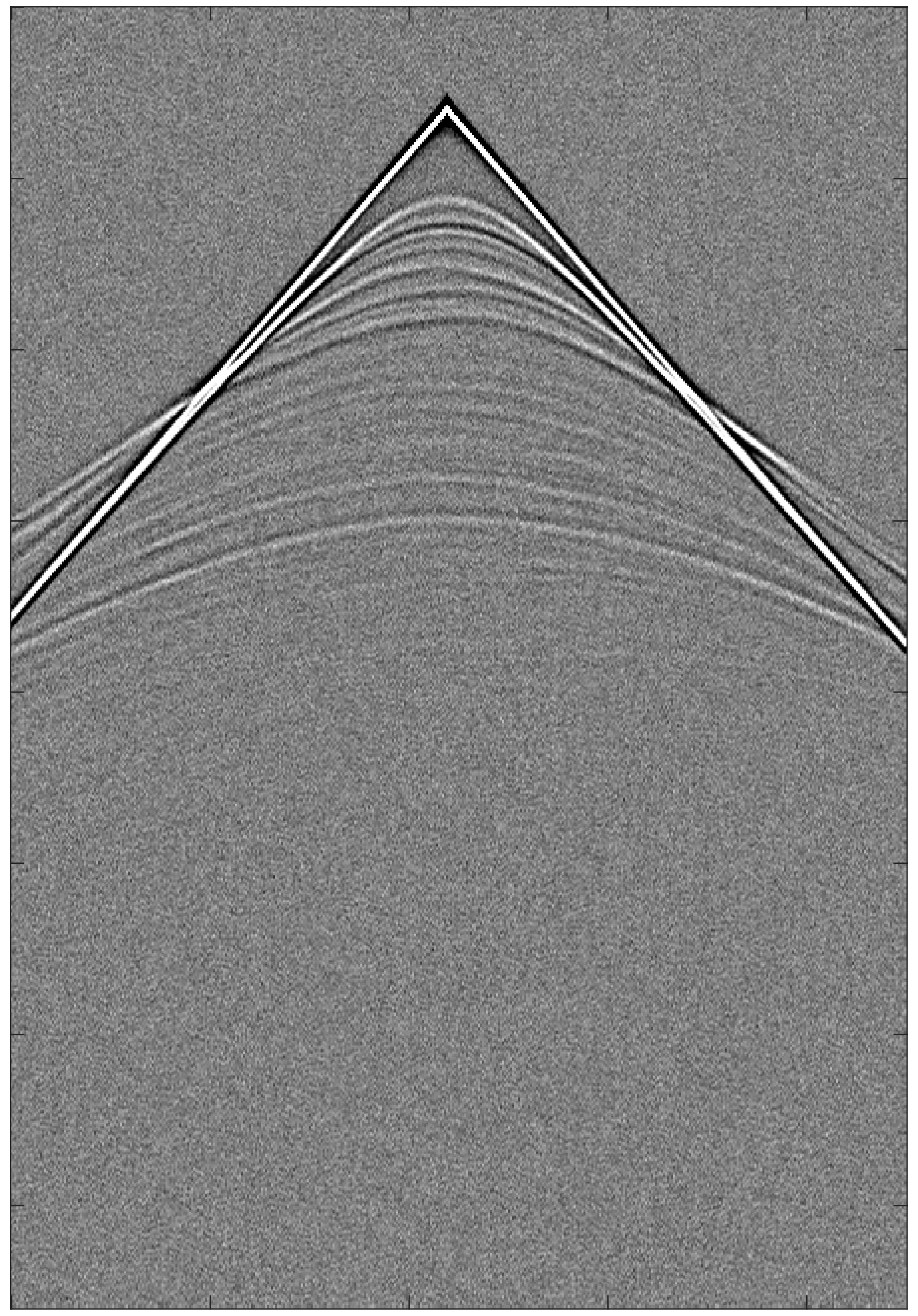
University of British Columbia

# Motivation

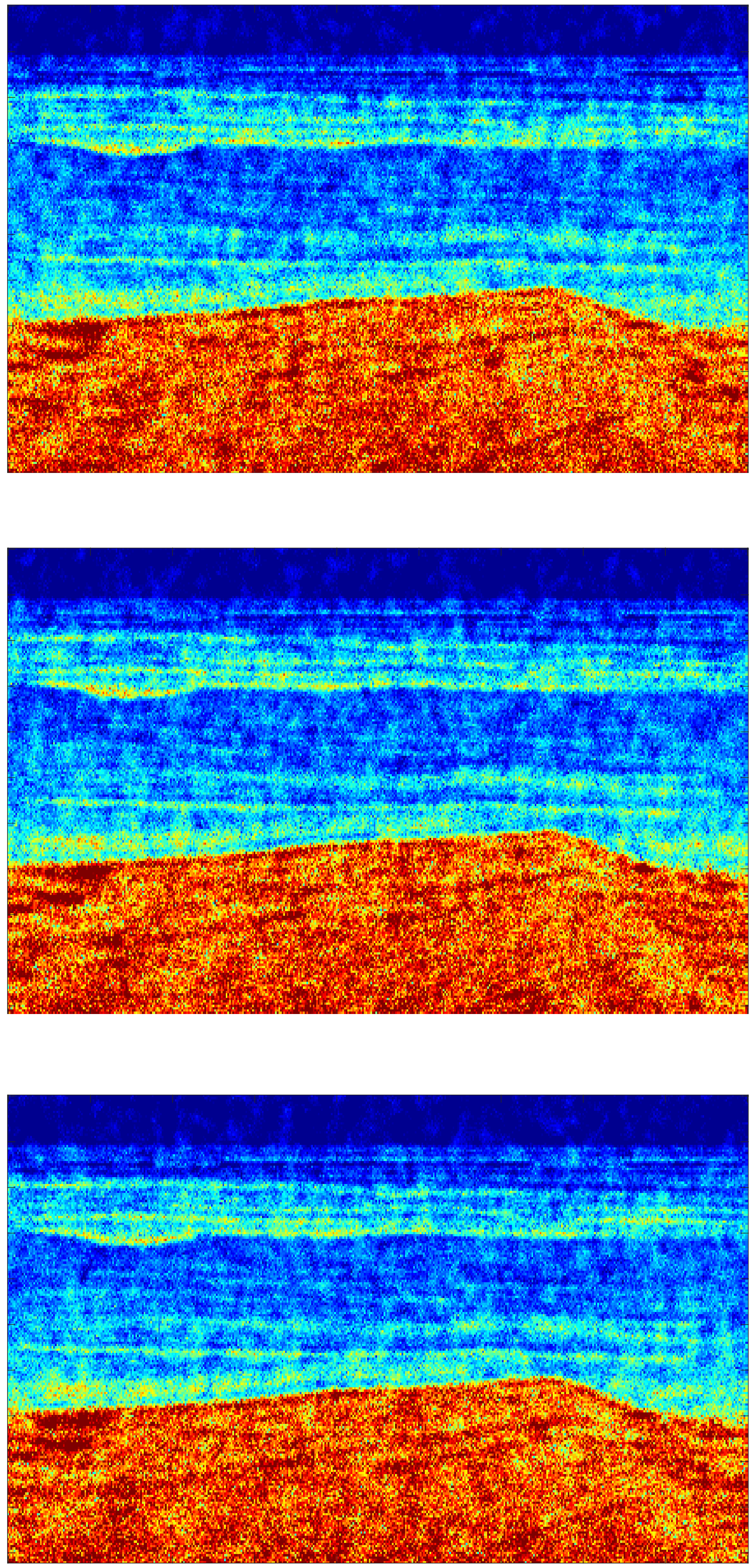



Noisy acquired data

# Motivation



Uncertainty in data

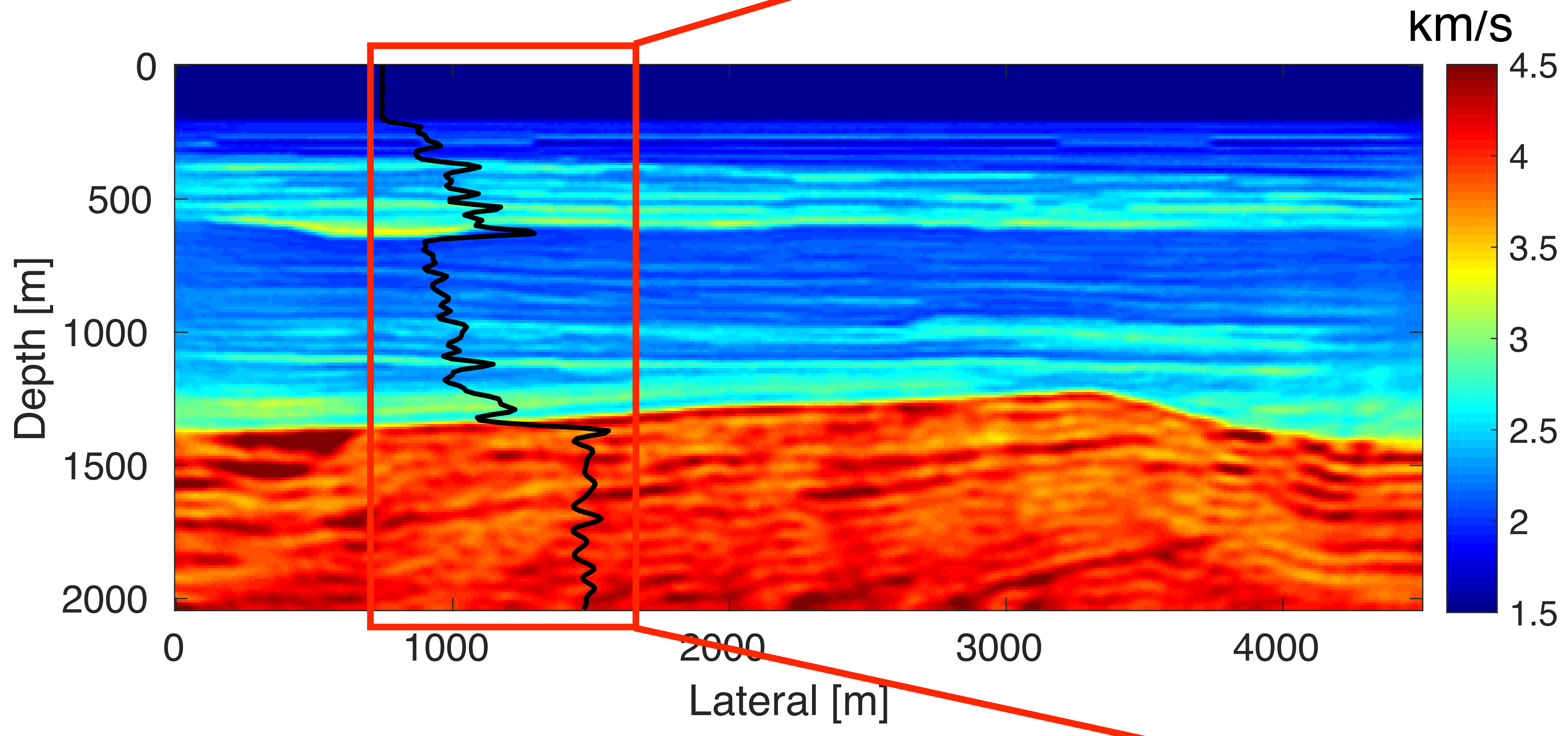


Possible velocity model

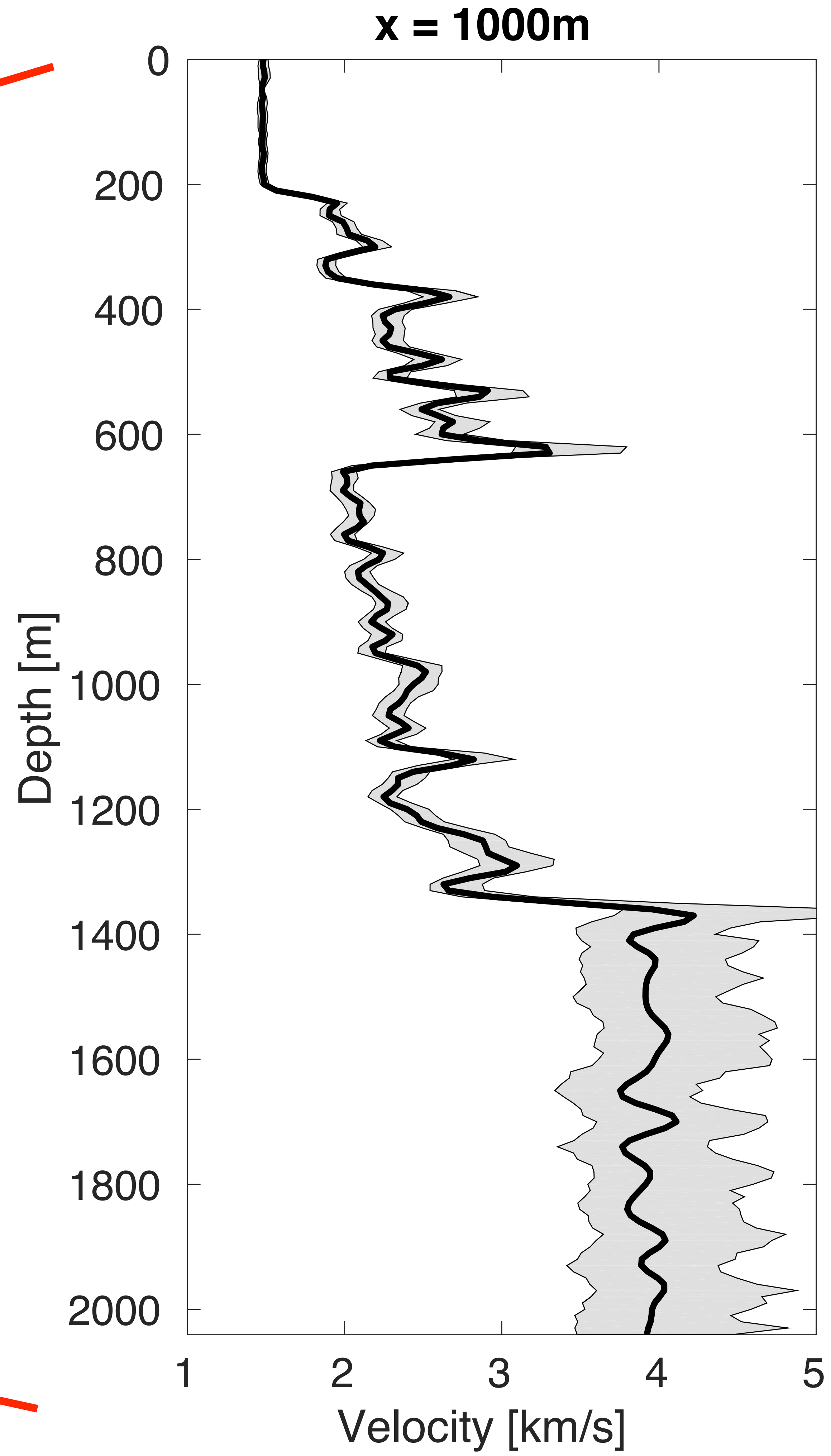
......

Risk in oil and gas volume

# Motivation




**Inversion result**




**Confidence Interval**

[A. Tarantola and B. Valette, 1982]
[J. Kaipio and E. Somersalo, 2004]

# Bayesian inference

Prior probability density function (PDF):

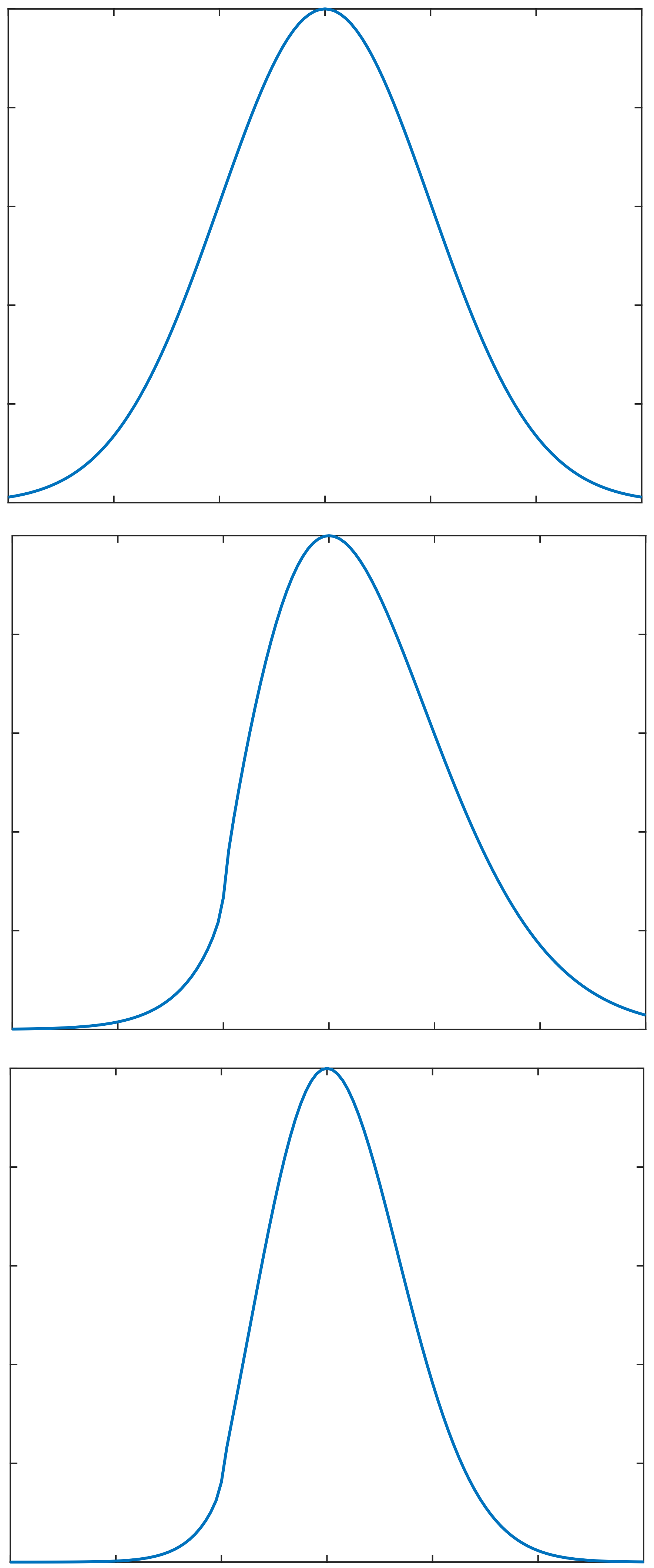
$$\mathbf{m} \longrightarrow \rho_{\text{prior}}(\mathbf{m})$$

Likelihood PDF: given data $\mathbf{d}$

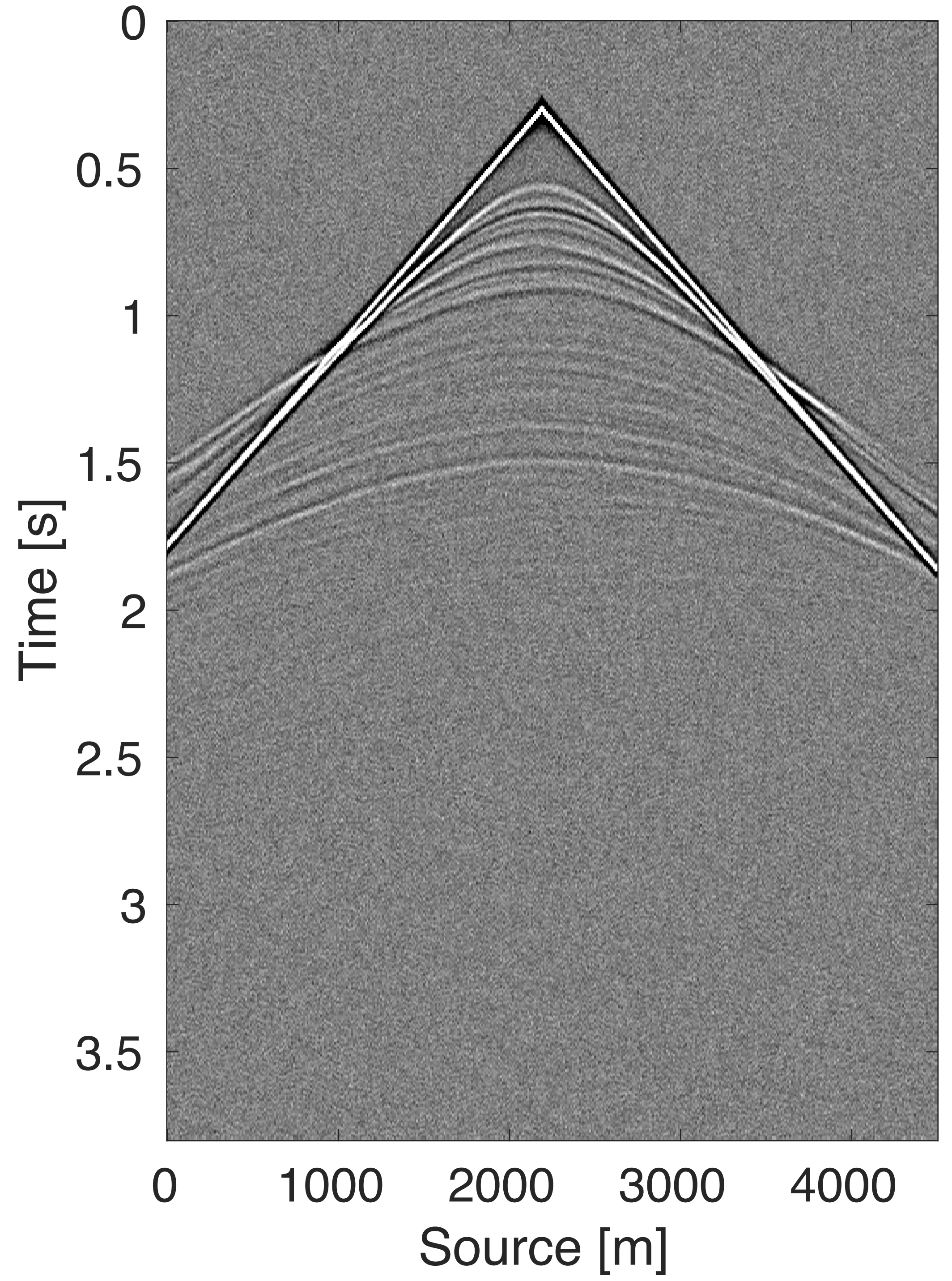
$$\mathbf{m} \longrightarrow \rho_{\text{like}}(\mathbf{d}|\mathbf{m})$$

Posterior PDF (Bayes' rule):

$$\rho_{\text{post}}(\mathbf{m}|\mathbf{d}) = \rho_{\text{like}}(\mathbf{d}|\mathbf{m})\rho_{\text{prior}}(\mathbf{m})$$

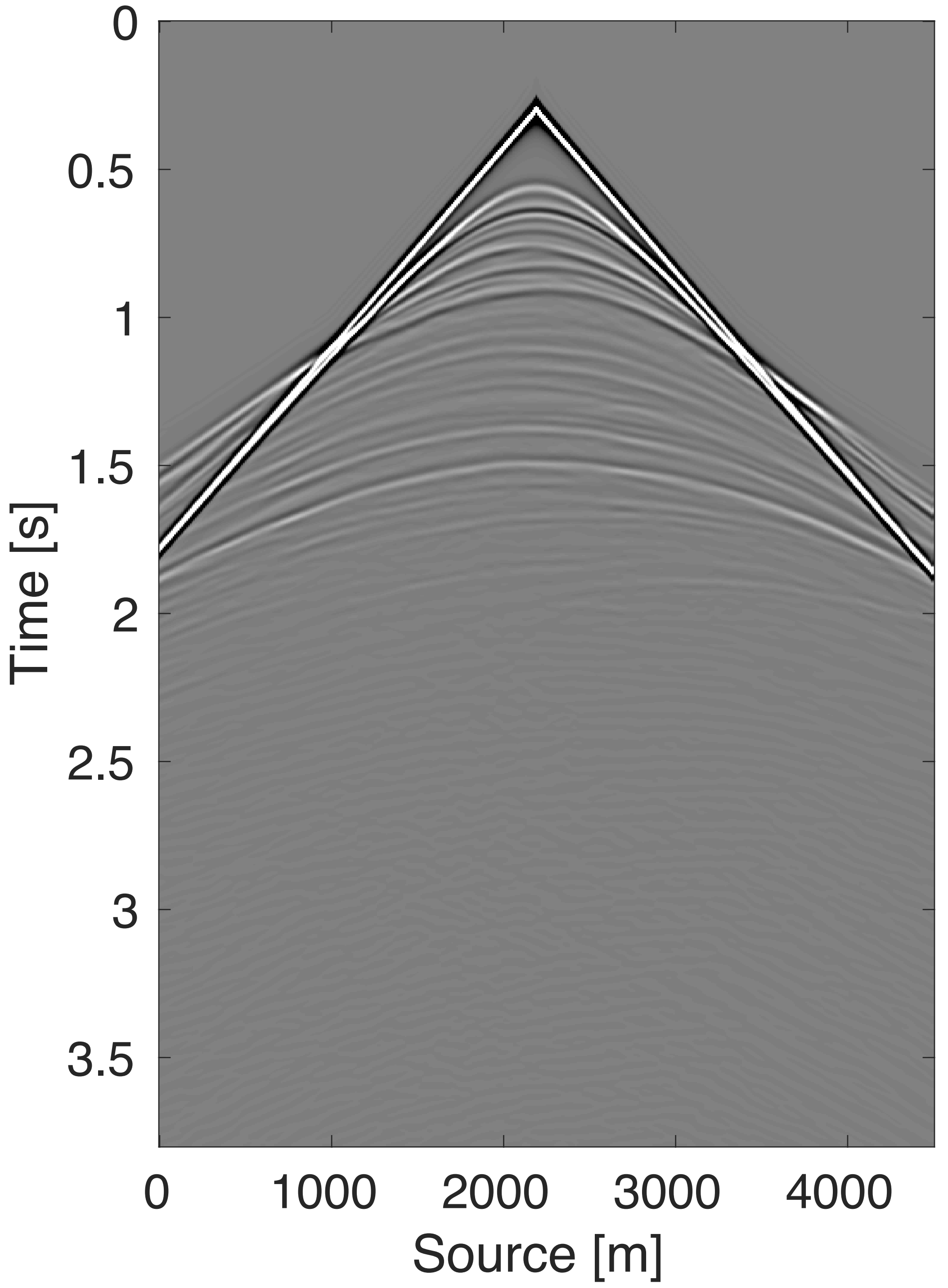


# Bayesian w/ FWI



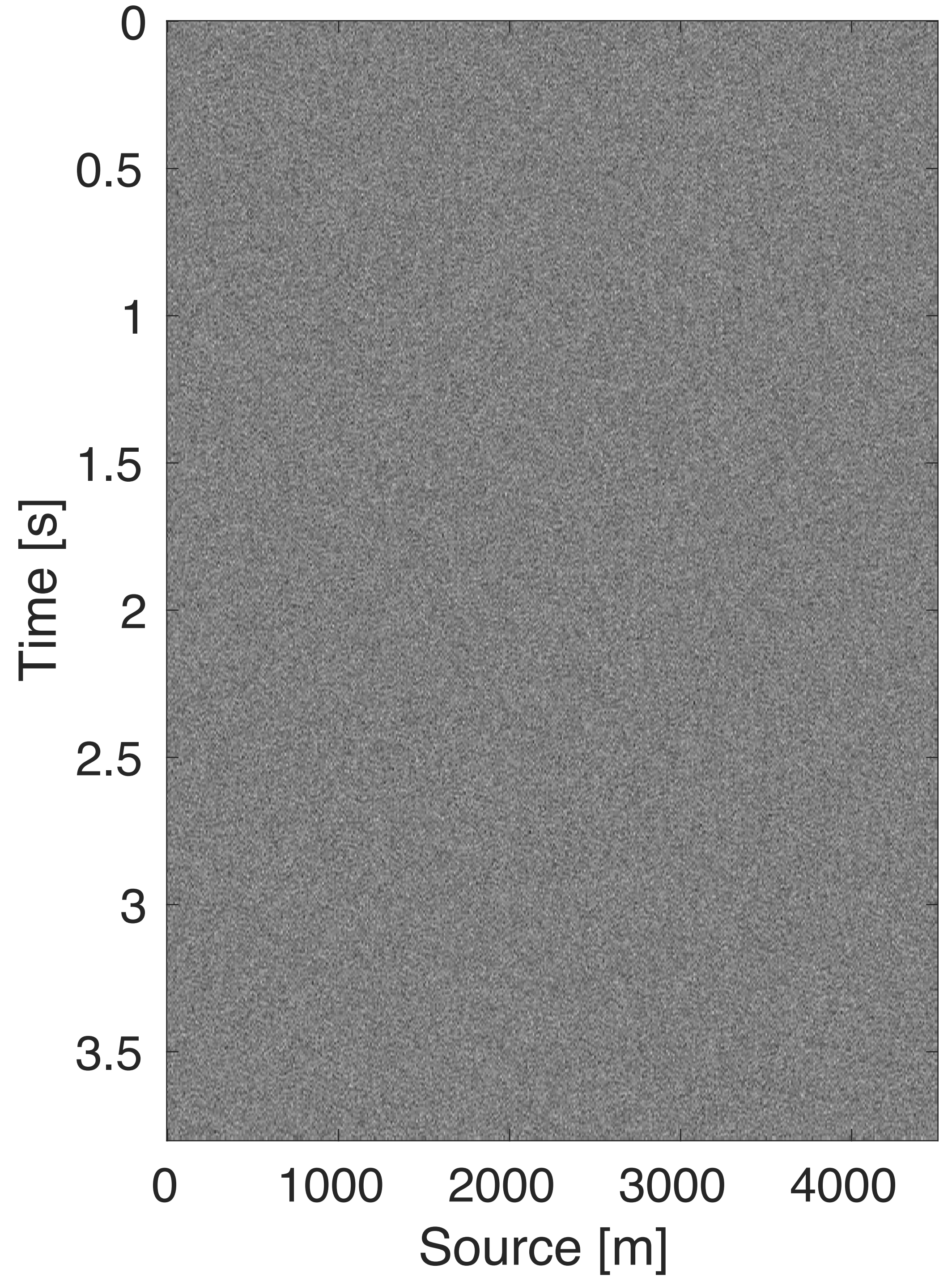

$\mathbf{d}_{\mathrm{obs}}$

$=$




$F(\mathbf{m})$

$+$




$\epsilon \sim \mathcal{N}(0, \Sigma_{\mathrm{noise}})$

# Bayesian w/ FWI

**Reduced formulation in the frequency domain:**

$$F(\mathbf{m}) = \mathbf{P}\mathbf{A}^{-1}\mathbf{q},$$

$$\mathbf{A} = \Delta + \omega^2\mathbf{m}$$

$\mathbf{m}$ : Squared-slowness

$\mathbf{q}$ : Source

$\omega$ : Frequency

$\Delta$ : Laplacian operator

$\mathbf{P}$ : Projection onto receivers

[J. Virieux and S. Operto, 2009]

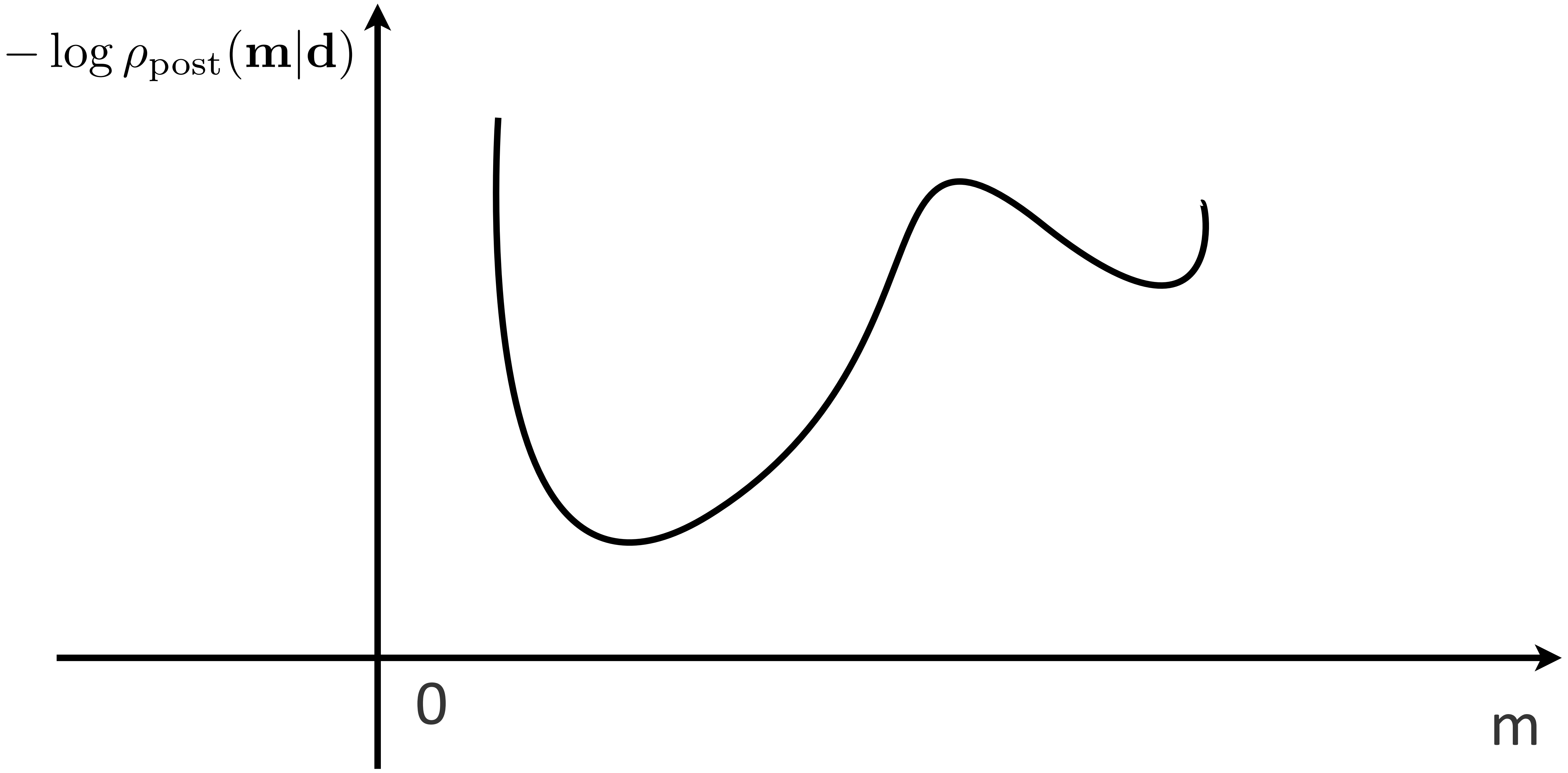
# Bayes w/ FWI

## Posterior PDF of FWI:

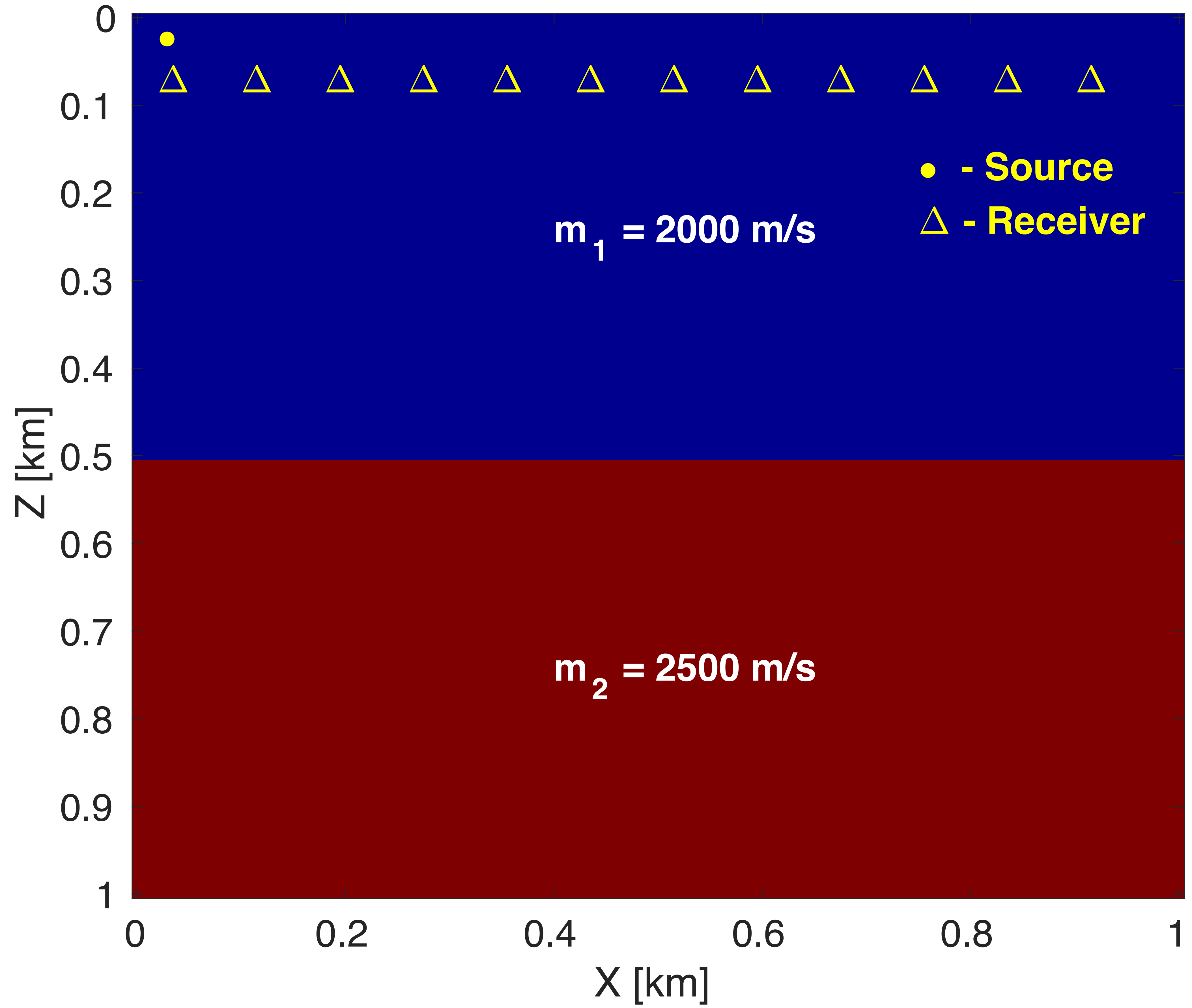
$$\rho_{\text{post}}(\mathbf{m}|\mathbf{d}) \propto \exp\left(-\frac{1}{2}\|\mathbf{P}\mathbf{A}(\mathbf{m})^{-1}\mathbf{q}-\mathbf{d}\|^2_{\mathbf{\Sigma}^{-1}_{\text{noise}}} - \frac{1}{2}\|\mathbf{m}-\mathbf{m}_{\text{prior}}\|^2_{\mathbf{\Sigma}^{-1}_{\text{prior}}}\right)$$

Strong nonlinearity

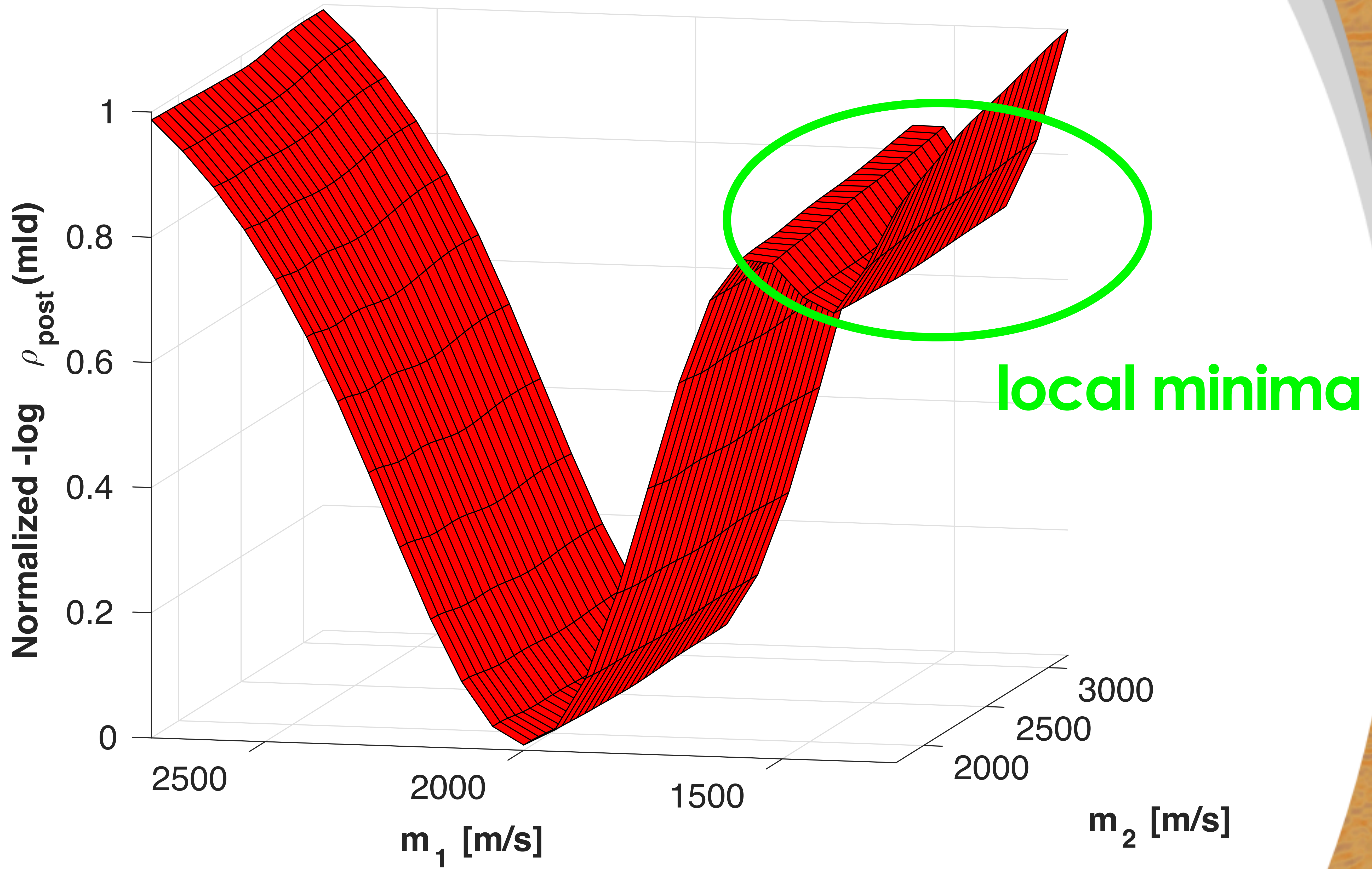
Many local minima



# Two layer example – FWI




**Model**




**FWI** $-\log \rho_{\text{post}}(\mathbf{m}|\mathbf{d})$

# Bayesian w/ FWI

**Local minima:**

- slow down McMC convergence
- render the posterior PDF “less Gaussian“

[T. van Leeuwen and F. J. Herrmann , 2013]
[T. van Leeuwen and F. J. Herrmann , 2015]

# Wavefield Reconstruction Inversion – WRI

## Penalty formulation:

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

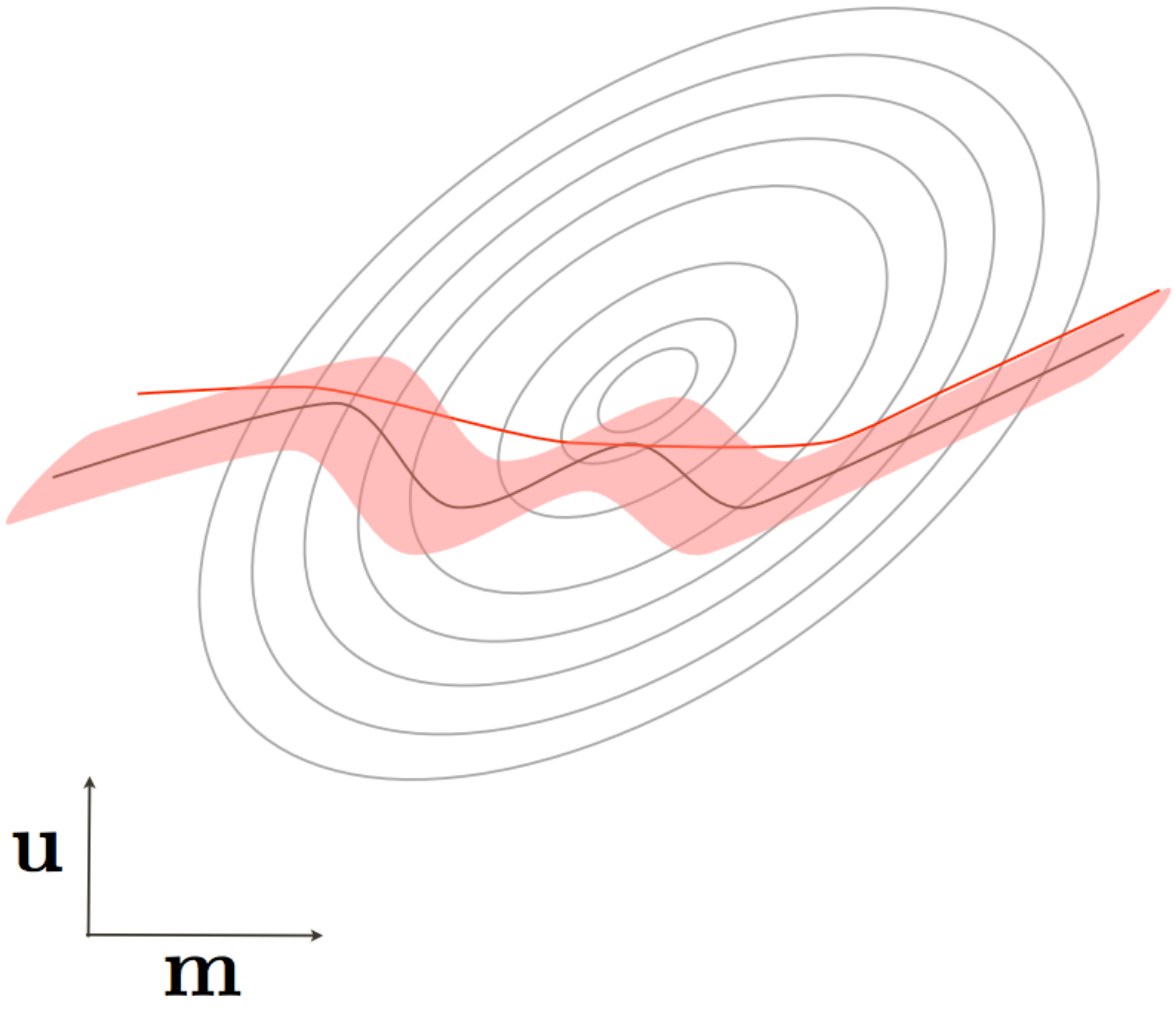
## Properties:

- bi-linear w/ respect to $\mathbf{u}$ and $\mathbf{m}$
- larger searching space

# WRI vs FWI

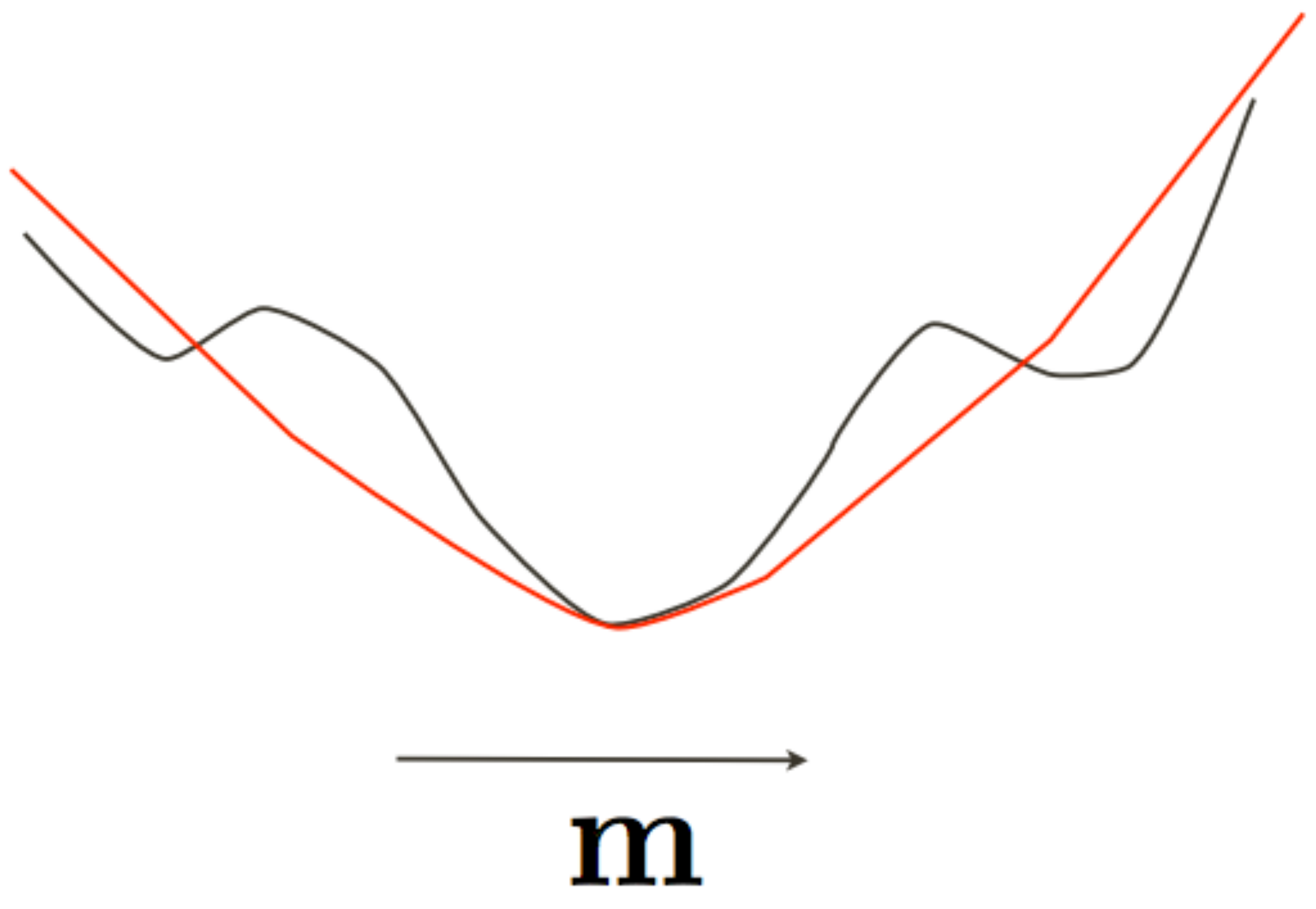
[van Leeuwen, T and Herrmann, F J , 2013]

Larger # of degrees of freedom




“more convex”

less local minima



[T. van Leeuwen and F. J. Herrmann , 2013]
[T. van Leeuwen and F. J. Herrmann , 2015]

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# Solving WRI

**Variable projection:**

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

where

$$\overline{\mathbf{u}}(\mathbf{m}) = \arg\min_{\mathbf{u}} \frac{1}{2}\|\mathbf{P}\mathbf{u} - \mathbf{d}\|_2^2 + \frac{\lambda^2}{2}\|\mathbf{A}(\mathbf{m})\mathbf{u} - \mathbf{q}\|_2^2$$

[Z. Fang *et al*, 2015]

# Bayes w/ WRI

**Posterior PDF of WRI:**

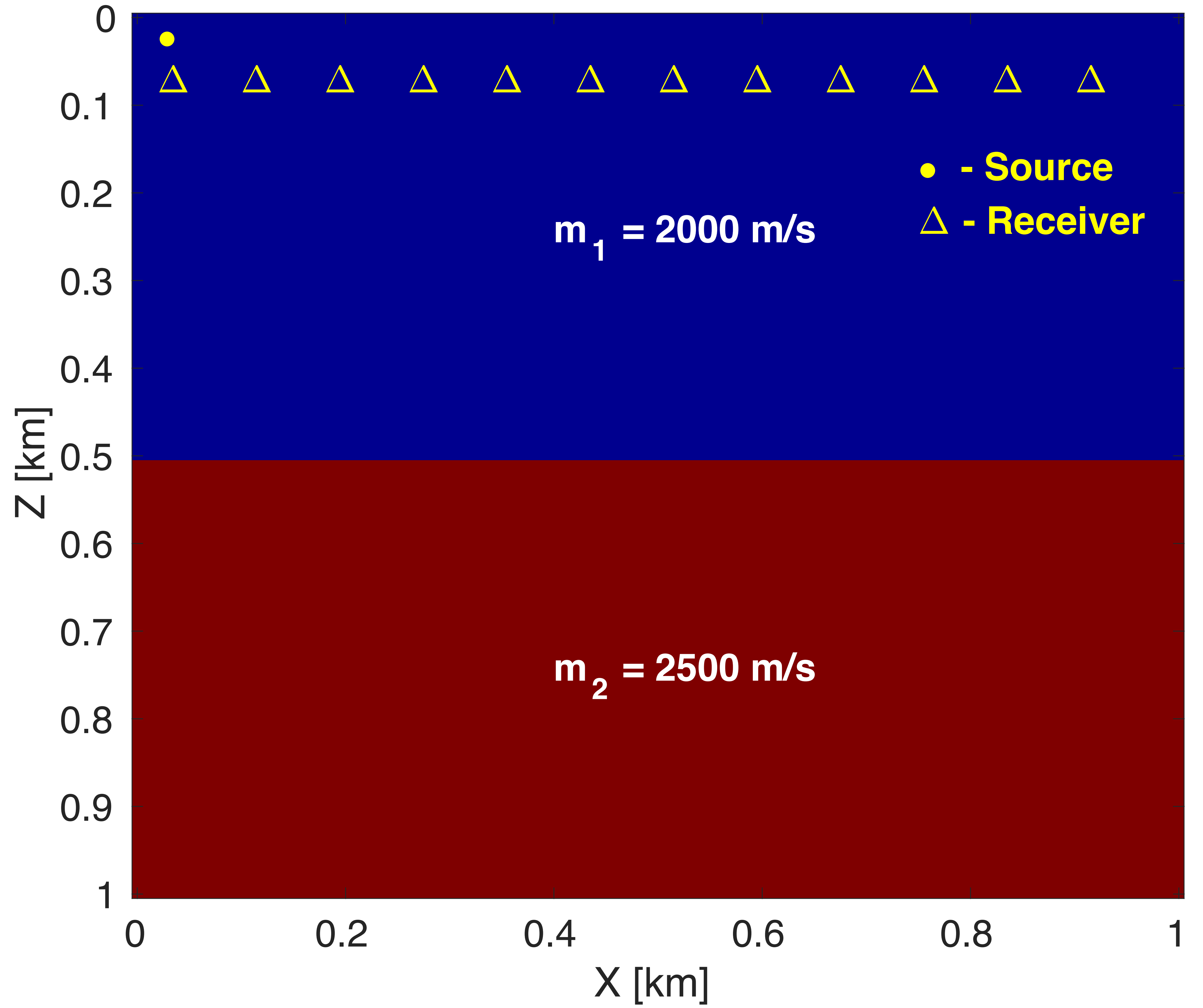
$$\rho_{\text{post}}(\mathbf{m}|\mathbf{d}) \propto$$

$$\exp\left(\underbrace{-\frac{1}{2}\|\mathbf{P}\bar{\mathbf{u}}(\mathbf{m})-\mathbf{d}\|^2_{\mathbf{\Sigma}^{-1}_{\text{noise}}} - \frac{\lambda^2}{2}\|\mathbf{A}(\mathbf{m})\bar{\mathbf{u}}(\mathbf{m})-\mathbf{q}\|^2}_{\text{Likelihood}} \underbrace{- \frac{1}{2}\|\mathbf{m}-\mathbf{m}_p\|^2_{\mathbf{\Sigma}^{-1}_{\text{prior}}}}_{\text{Prior}}\right),$$

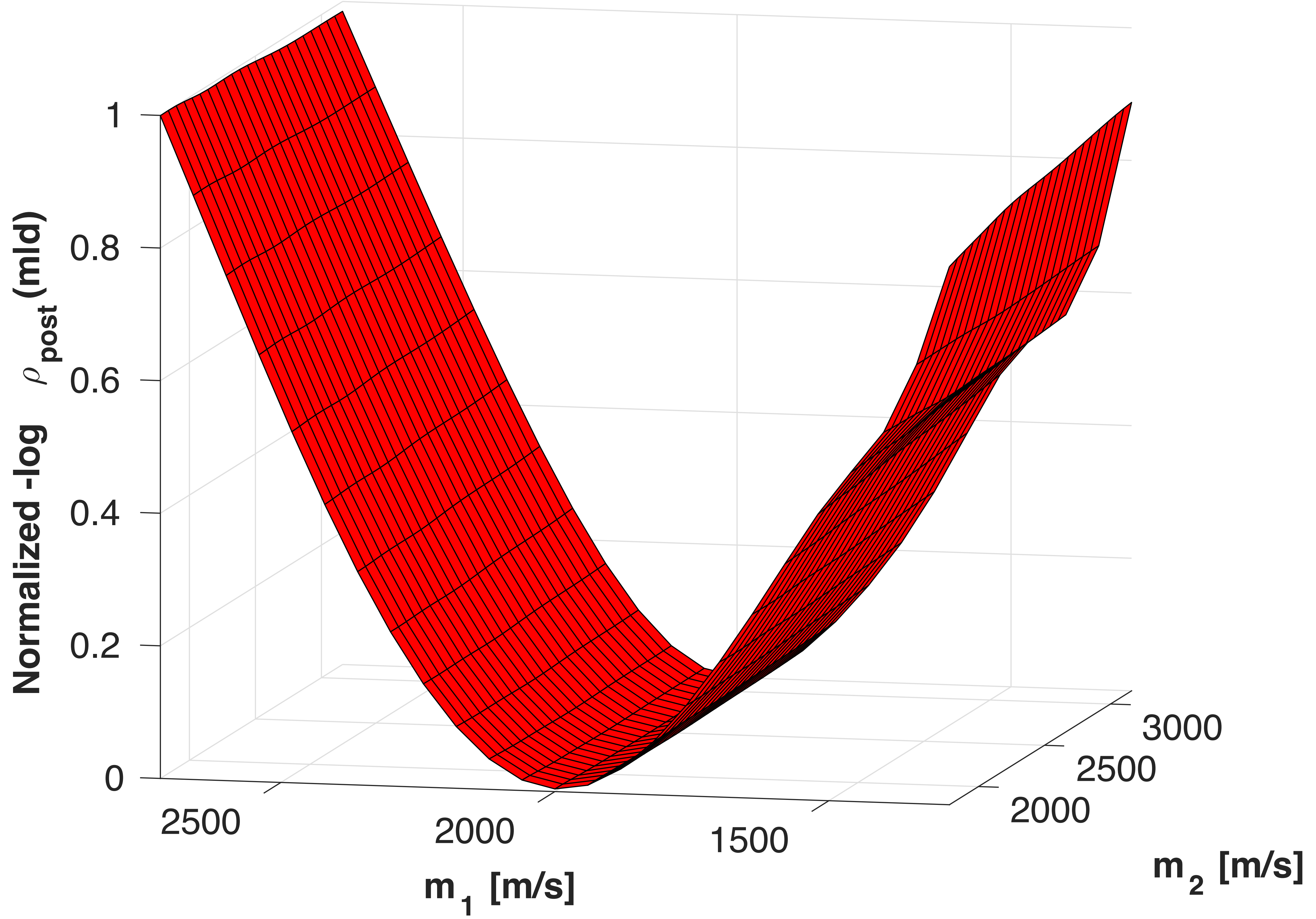
where

$$\bar{\mathbf{u}}(\mathbf{m}) = \arg\min_{\mathbf{m}} \frac{1}{2}\|\mathbf{P}\mathbf{u}-\mathbf{d}\|^2_{\mathbf{\Sigma}^{-1}_{\text{noise}}} + \frac{\lambda^2}{2}\|\mathbf{A}(\mathbf{m})\mathbf{u}-\mathbf{q}\|^2.$$

# Two layer example – WRI




**Model**




WRI $-\log \rho_{\text{post}}(\mathbf{m}|\mathbf{d})$

## Challenges for large-scale UQ

Evaluations of the posterior PDF

- many PDE solves to evaluate PDF
- expensive PDE solves

High-dimensional space to explore

- numerical integration to expensive
- McMC based methods are impractical
  - too many iterations
  - converge too slow

# UQ for large-scale problems

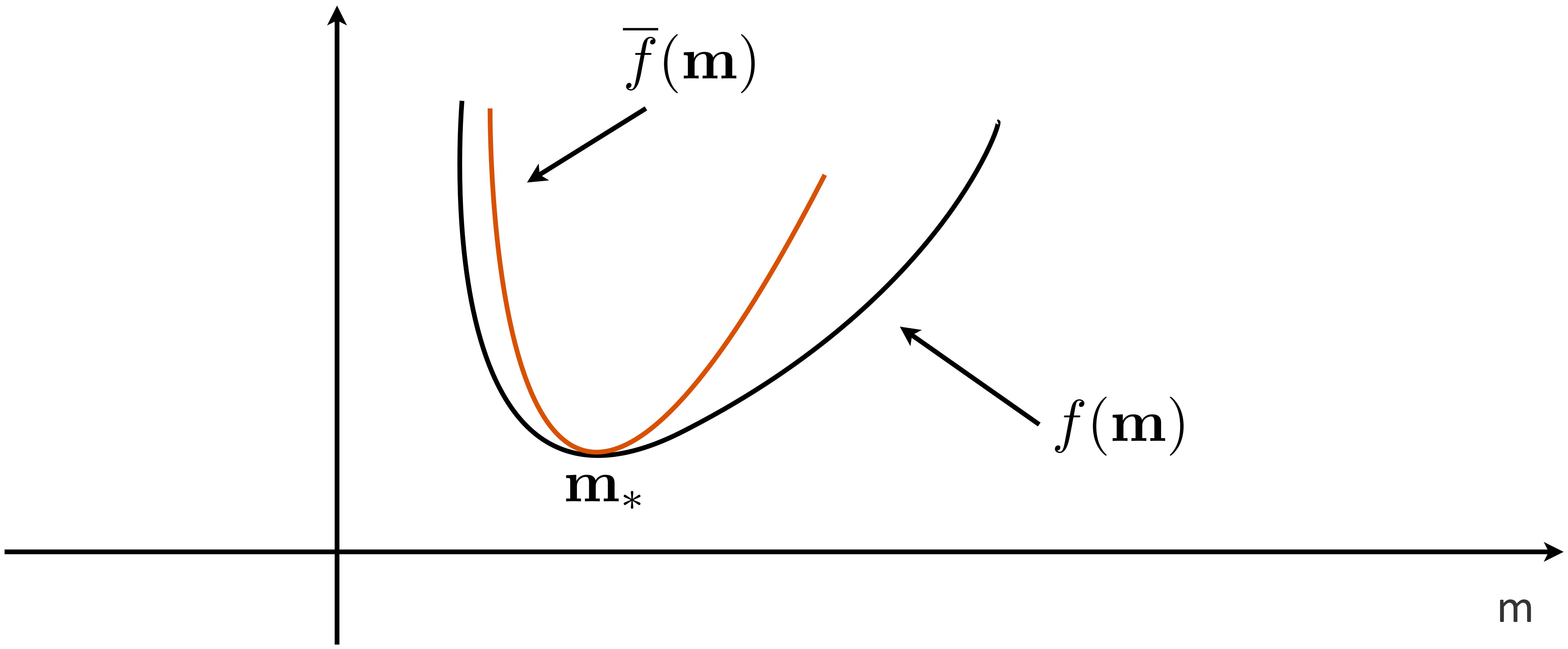
Approximate posterior PDF by Gaussians

Sample the Gaussians w/ randomize then optimize (RTO) method

# Quadratic approximation of $-\log \rho_{\text{post}}(\mathbf{m})$

$$
\begin{aligned}
-\log \rho_{\text{post}}(\mathbf{m}) &= f(\mathbf{m}) \\
&\approx f(\mathbf{m}_*) + \frac{1}{2}(\mathbf{m} - \mathbf{m}_*)^\top \mathbf{H}(\mathbf{m} - \mathbf{m}_*) := \overline{f}(\mathbf{m})
\end{aligned}
$$

where $\mathbf{H} = \dfrac{\partial^2 f}{\partial \mathbf{m}^2}$.



# Approximate posterior PDF

**Gaussian approximation:**

$$\rho_{\text{post}}(\mathbf{m}) \approx \rho_{\text{Gauss}}(\mathbf{m}) = \mathcal{N}(\mathbf{m}_*, \mathbf{H}^{-1})$$

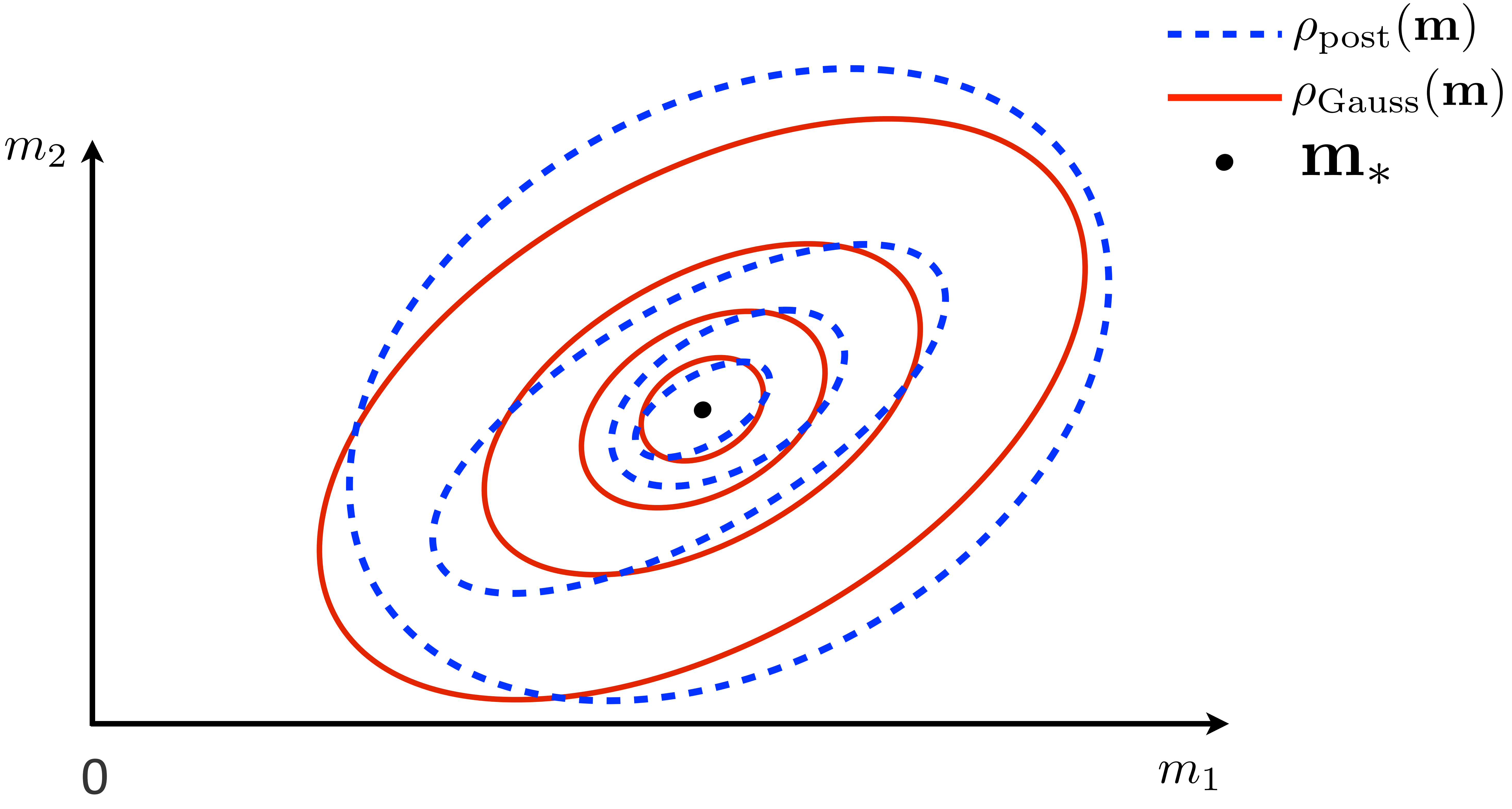
where

$$\mathbf{H} = \mathbf{H}_{\text{l}} + \mathbf{H}_{\text{p}},$$

$$\mathbf{H}_{\text{l}} = \frac{\partial^2 f_{\text{l}}(\mathbf{m})}{\partial \mathbf{m}^2}, \quad f_{\text{l}}(\mathbf{m}) = \text{-log}\rho_{\text{like}}(\mathbf{d}|\mathbf{m}),$$

$$\mathbf{H}_{\text{p}} = \frac{\partial^2 f_{\text{p}}(\mathbf{m})}{\partial \mathbf{m}^2}, \quad f_{\text{p}}(\mathbf{m}) = \text{-log}\rho_{\text{prior}}(\mathbf{m}).$$

# Approximate posterior PDF



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# Form Hessian

## Gauss-Newton Hessian:

$$\mathbf{H}_{\mathrm{l}} = \mathbf{G}^{\top}\mathbf{A}^{-\top}\mathbf{P}^{\top}(\mathbf{I} + \frac{1}{\lambda^2\sigma^2}\mathbf{P}\mathbf{A}^{-1}\mathbf{A}^{-\top}\mathbf{P}^{\top})^{-1}\mathbf{P}\mathbf{A}^{-1}\mathbf{G},$$

where $\Sigma_{\mathrm{noise}} = \sigma^2\mathbf{I}$ and $\mathbf{G} = \dfrac{\partial\mathbf{A}\bar{\mathbf{u}}}{\partial\mathbf{m}}$ .

[T. van Leeuwen and F. J. Herrmann , 2015]

# Form Hessian

## Gauss-Newton Hessian:

$$\mathbf{H}_{\mathrm{l}} = \underbrace{\boxed{\mathbf{G}^\top}\boxed{\mathbf{A}^{-\top}\mathbf{P}^\top}}_{\mathbf{W}^\top}\underbrace{\left(\mathbf{I} + \frac{1}{\lambda^2\sigma^2}\mathbf{P}\mathbf{A}^{-1}\mathbf{A}^{-\top}\mathbf{P}^\top\right)^{-1}}_{\mathbf{S}}\mathbf{P}\mathbf{A}^{-1}\mathbf{G},$$

where $\Sigma_{\mathrm{noise}} = \sigma^2\mathbf{I}$ and $\mathbf{G} = \dfrac{\partial \mathbf{A}\bar{\mathbf{u}}}{\partial \mathbf{m}}$ .

# GN Hessian of WRI

$$\mathbf{H}_{\mathrm{l}} = \mathbf{W}^\top \mathbf{S} \mathbf{W}$$

**Computational cost:**

$n_{\mathrm{freq}} \times (n_{\mathrm{src}} + n_{\mathrm{rcv}})$

**storage cost:**

$n_{\mathrm{freq}} \times n_{\mathrm{grid}} \times (n_{\mathrm{src}} + n_{\mathrm{rcv}})$

**in parallel !!**

## UQ for large-scale problems

Approximate posterior PDF by Gaussians

Sample the Gaussians w/ randomize then optimize (RTO) method

[Rue, 2001]

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# Conventional method

## Sample Gaussian distribution:

$$\rho_{\text{Gauss}}(\mathbf{m}) \propto \exp(-\frac{1}{2}(\mathbf{m}-\mathbf{m}_*)^\top \mathbf{H}(\mathbf{m}-\mathbf{m}_*)).$$

## Cholesky factorization:

$$\mathbf{H} = \mathbf{L}^\top \mathbf{L},$$

$$\mathbf{m}_{\text{s}} = \mathbf{m}_* + \mathbf{L}^{-1}\mathbf{r}, \mathbf{r} \sim \mathcal{N}(0, \mathcal{I}_{n_{\text{grid}} \times n_{\text{grid}}}).$$

$\mathbf{H}$ should be an explicit matrix,

Computational cost is $\mathcal{O}(n_{\text{grid}}^3)$.

# RTO method

Re-formulate the posterior distribution with:

$$\mathbf{H} = \mathbf{H}_{\mathrm{l}} + \mathbf{H}_{\mathrm{p}}, \ \mathbf{H}_{\mathrm{l}} = \mathbf{L}_{\mathrm{l}}^{\top}\mathbf{L}_{\mathrm{l}}, \text{ and } \ \mathbf{H}_{\mathrm{p}} = \mathbf{L}_{\mathrm{p}}^{\top}\mathbf{L}_{\mathrm{p}},$$

then

$$\begin{aligned}\rho_{\text{Gauss}}(\mathbf{m}) \propto \exp(&-\frac{1}{2}(\mathbf{L}_{\mathrm{l}}\mathbf{m} - \mathbf{L}_{\mathrm{l}}\mathbf{m}_*)^{\top}(\mathbf{L}_{\mathrm{l}}\mathbf{m} - \mathbf{L}_{\mathrm{l}}\mathbf{m}_*) \\ &-\frac{1}{2}(\mathbf{L}_{\mathrm{p}}\mathbf{m} - \mathbf{L}_{\mathrm{p}}\mathbf{m}_*)^{\top}(\mathbf{L}_{\mathrm{p}}\mathbf{m} - \mathbf{L}_{\mathrm{p}}\mathbf{m}_*))\end{aligned}$$

[J. M. Bardsley *et al*, 2014]

## RTO method

Generate a sample by solving the optimization problem:

$$\mathbf{m}_{\mathrm{s}} = \arg\min_{\mathbf{m}} \left\| \mathbf{L}_{\mathrm{l}}\mathbf{m} - (\mathbf{L}_{\mathrm{l}}\mathbf{m}_* + \mathbf{r}_{\mathrm{l}}) \right\|^2 + \left\| \mathbf{L}_{\mathrm{p}}\mathbf{m} - (\mathbf{L}_{\mathrm{p}}\mathbf{m}_* + \mathbf{r}_{\mathrm{p}}) \right\|^2,$$

where

$$\mathbf{r}_{\mathrm{l}} \sim \mathcal{N}(0, \mathcal{I}_{n_{\mathrm{rcv}} \times n_{\mathrm{rcv}}}),$$

$$\mathbf{r}_{\mathrm{p}} \sim \mathcal{N}(0, \mathcal{I}_{n_{\mathrm{grid}} \times n_{\mathrm{grid}}}).$$

## RTO method

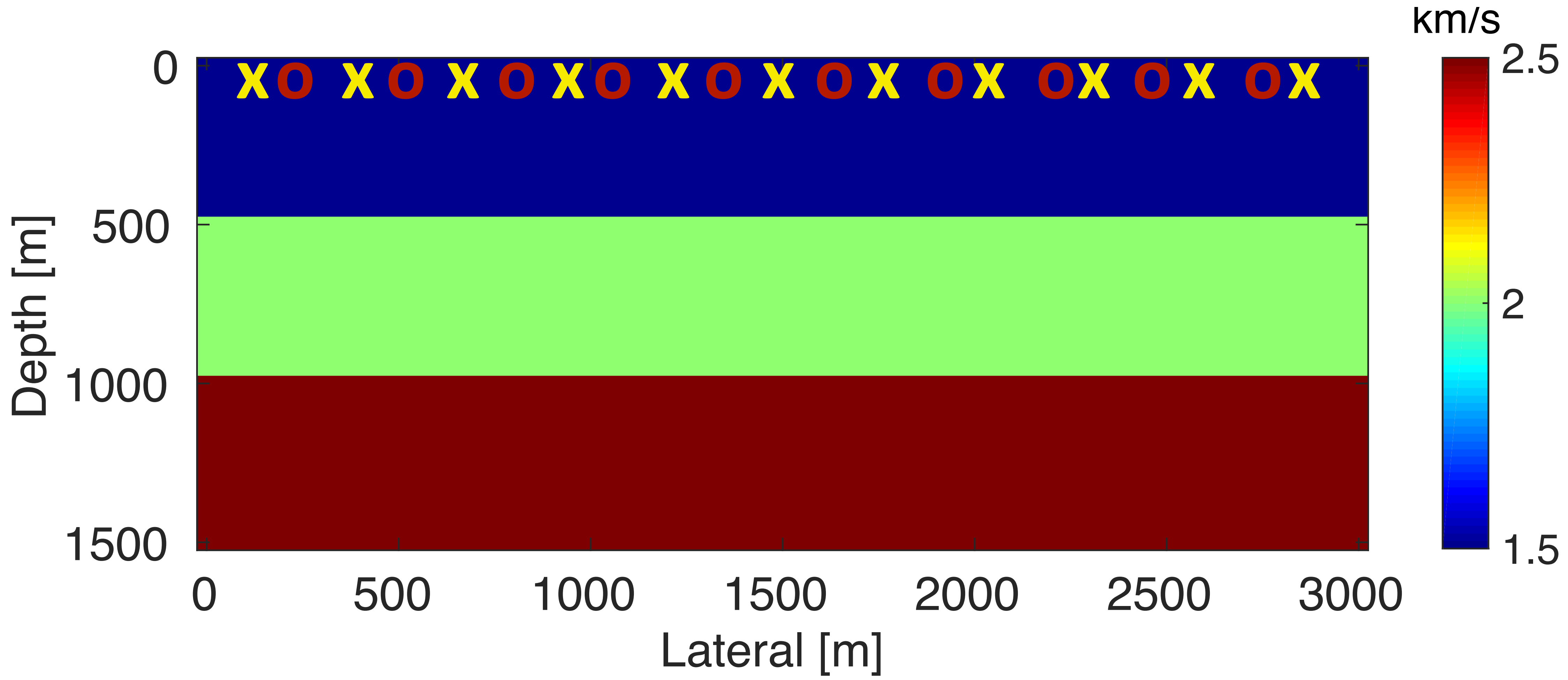
Factorization of $\mathbf{H}_{\mathrm{l}}$:

$$\mathbf{H}_{\mathrm{l}} = \mathbf{L}_{\mathrm{l}}^{\top}\mathbf{L}_{\mathrm{l}},$$

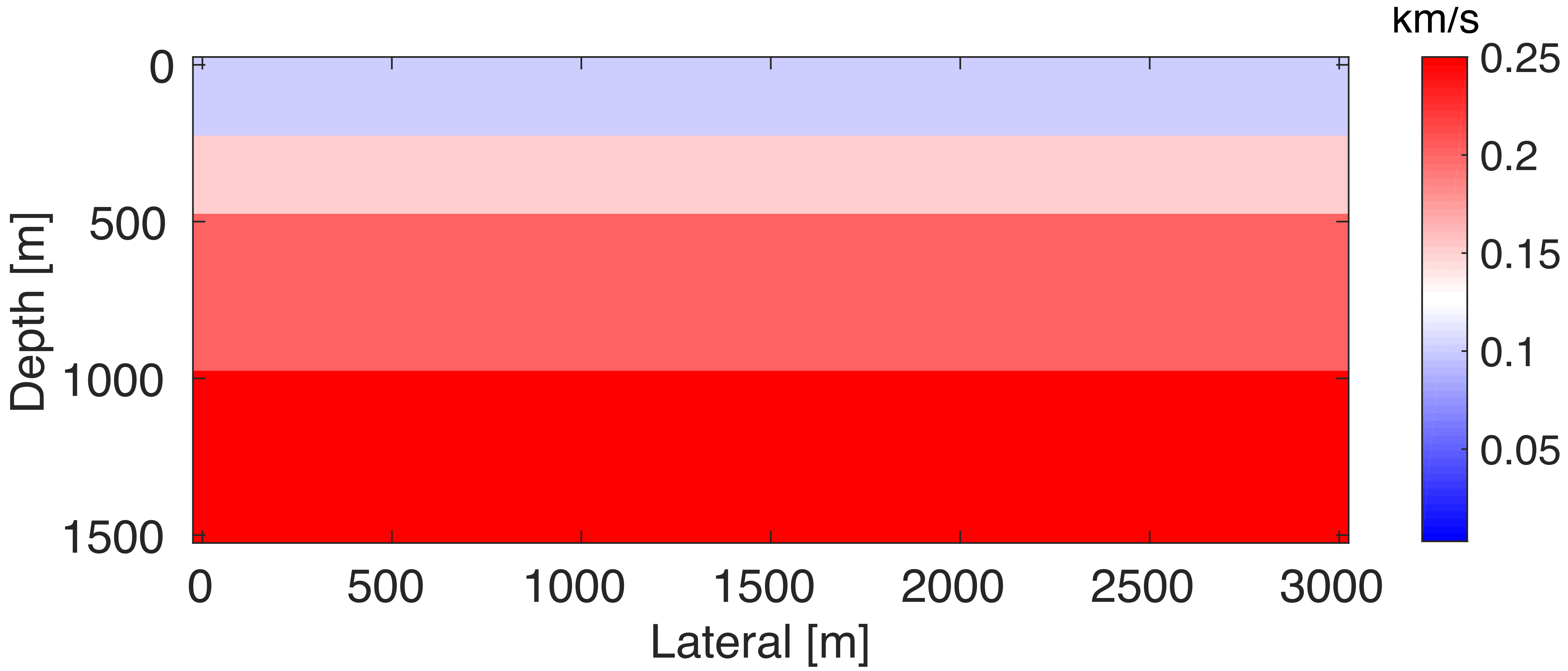
$$\mathbf{L}_{\mathrm{l}} = \underbrace{(\mathbf{I} + \frac{1}{\lambda^2\sigma^2}\mathbf{P}\mathbf{A}^{-1}\mathbf{A}^{-\top}\mathbf{P}^{\top})^{-\frac{1}{2}}}_{n_{\mathrm{rcv}} \times n_{\mathrm{rcv}}}\mathbf{P}\mathbf{A}^{-1}\mathbf{G}.$$

# Numerical Experiment – Layer model

Depth of sources and receivers: 50 m
Number of sources and receivers: 61
Frequency: 2,3 and 4 Hz
Lambda: 4e4
sigma: 10




(a) True model and prior model




(b) STD of the prior distribution

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# Randomized Maximum Likelihood - RML

Generate independent samples from $\rho_{\text{post}}(\mathbf{m})$ by solving:

$$\min_{\mathbf{m}} \frac{1}{2}(\sigma^{-2}\|\mathbf{P}\overline{\mathbf{u}}(\mathbf{m}) - \mathbf{d} - \mathbf{r}_{\text{d}}\|^2 + \lambda^2\|\mathbf{A}(\mathbf{m})\overline{\mathbf{u}}(\mathbf{m}) - \mathbf{q} - \mathbf{r}_{\text{s}}\|^2) + \frac{1}{2}\|\mathbf{m} - \mathbf{m}_{\text{p}} - \mathbf{r}_{\text{p}}\|^2_{\Sigma^{-1}_{\text{prior}}},$$

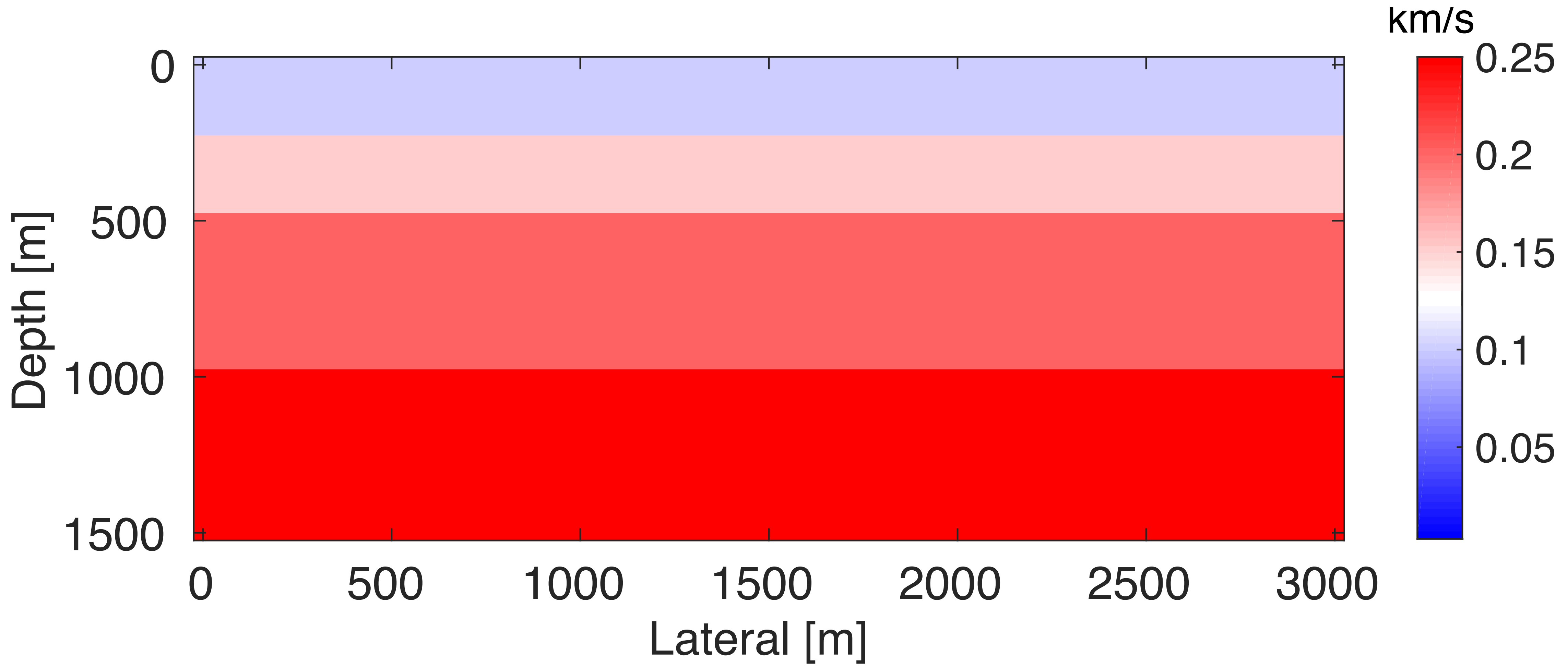
where

$$\mathbf{r}_{\text{d}} \sim \mathcal{N}(0, \sigma^2 \mathcal{I}_{n_{\text{rcv}} \times n_{\text{rcv}}}),$$

$$\mathbf{r}_{\text{s}} \sim \mathcal{N}(0, \lambda^{-2} \mathcal{I}_{n_{\text{grid}} \times n_{\text{grid}}}),$$

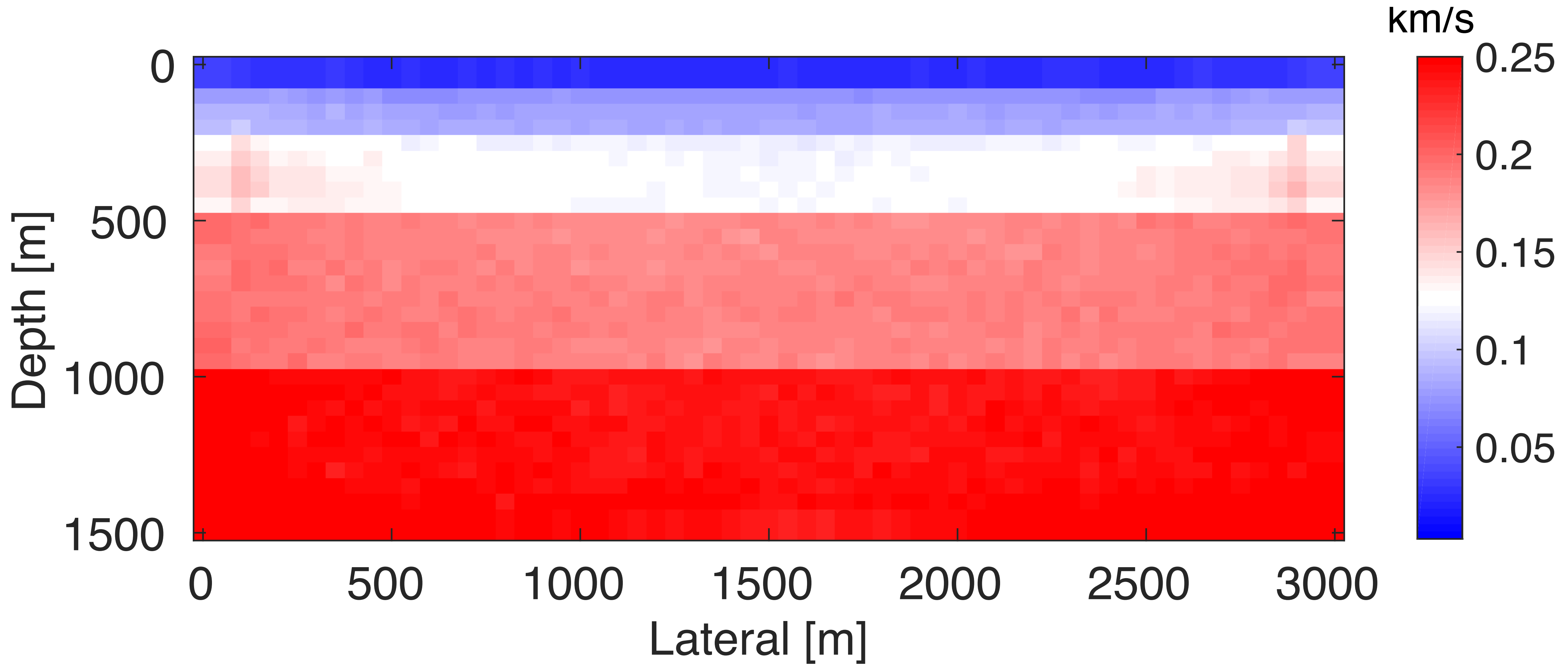
$$\mathbf{r}_{\text{p}} \sim \mathcal{N}(0, \Sigma_{\text{prior}}).$$

# STD result comparison
## – 2-4 Hz

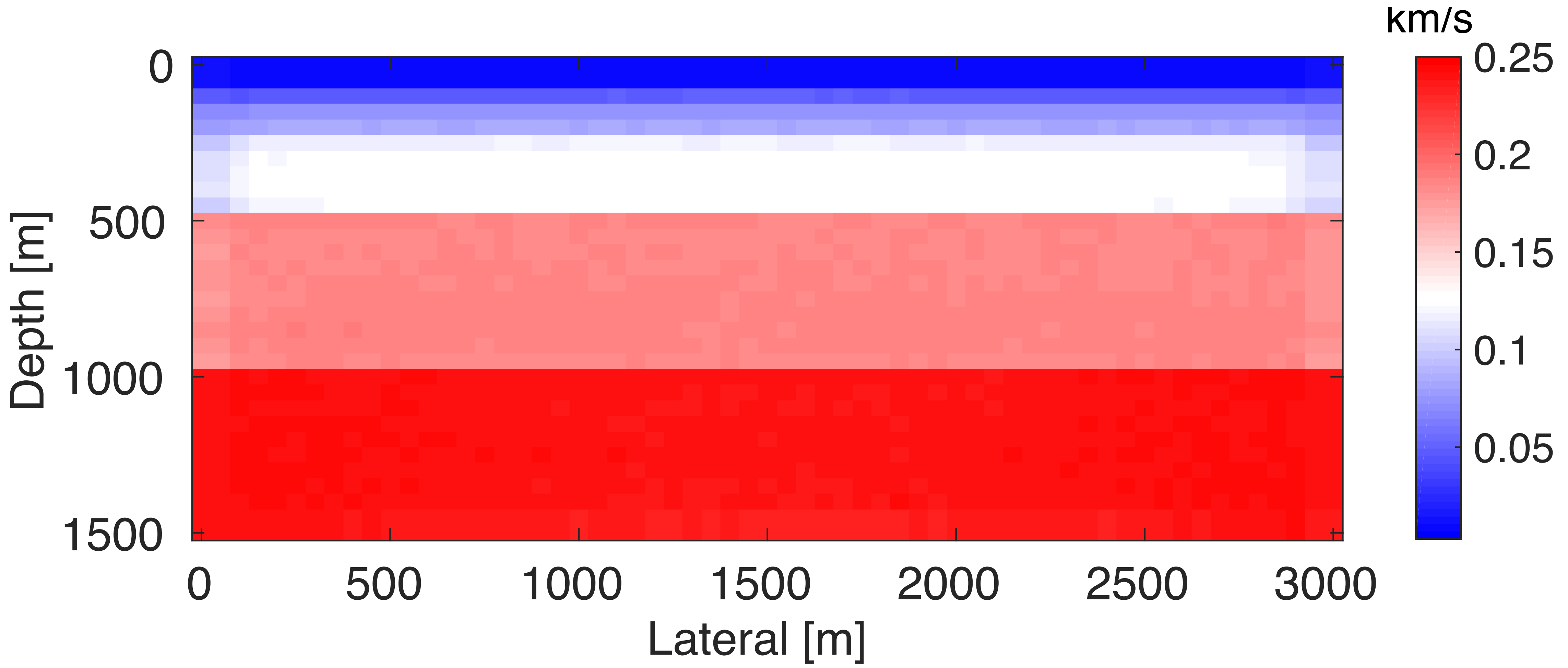



(a) STD of prior distribution

10000 realizations for both methods

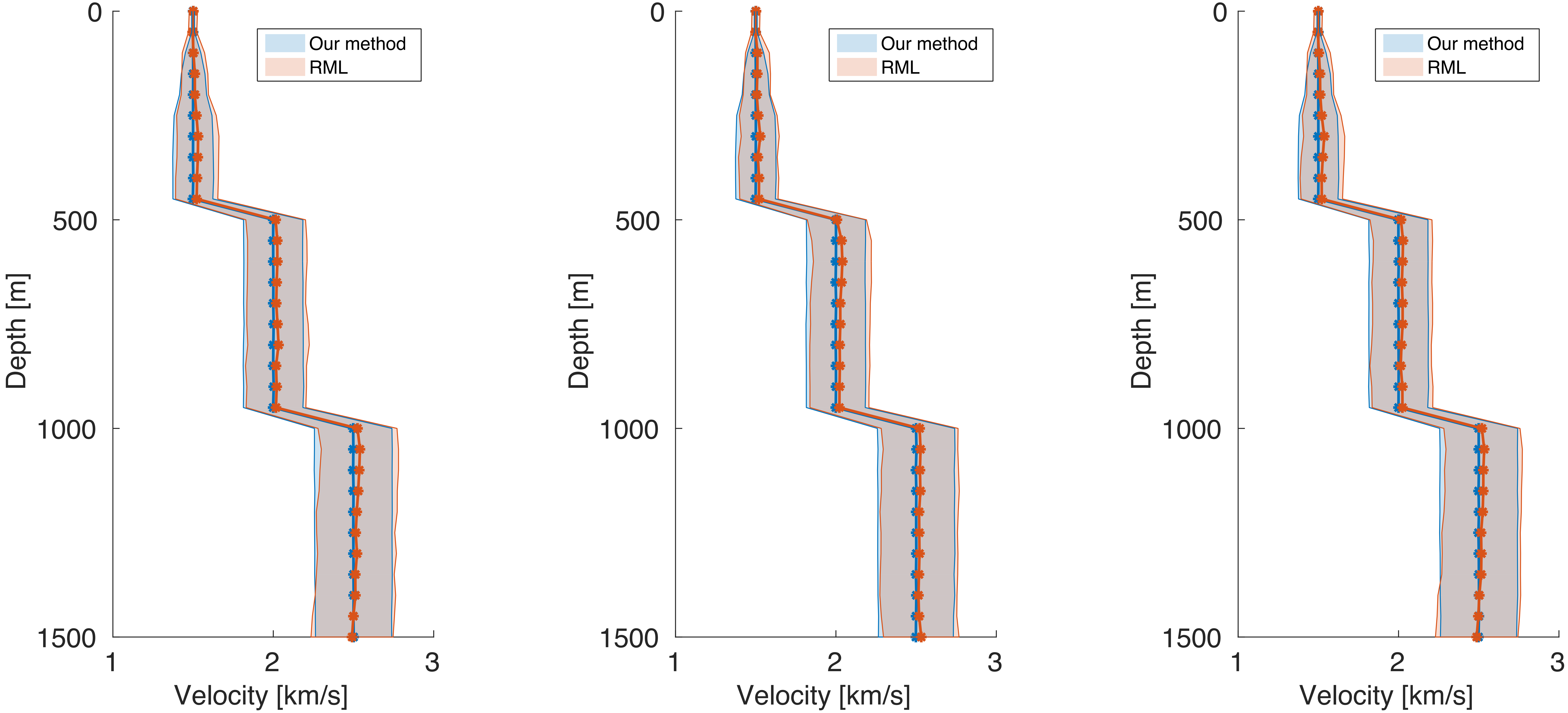



(b) STD obtained by RML



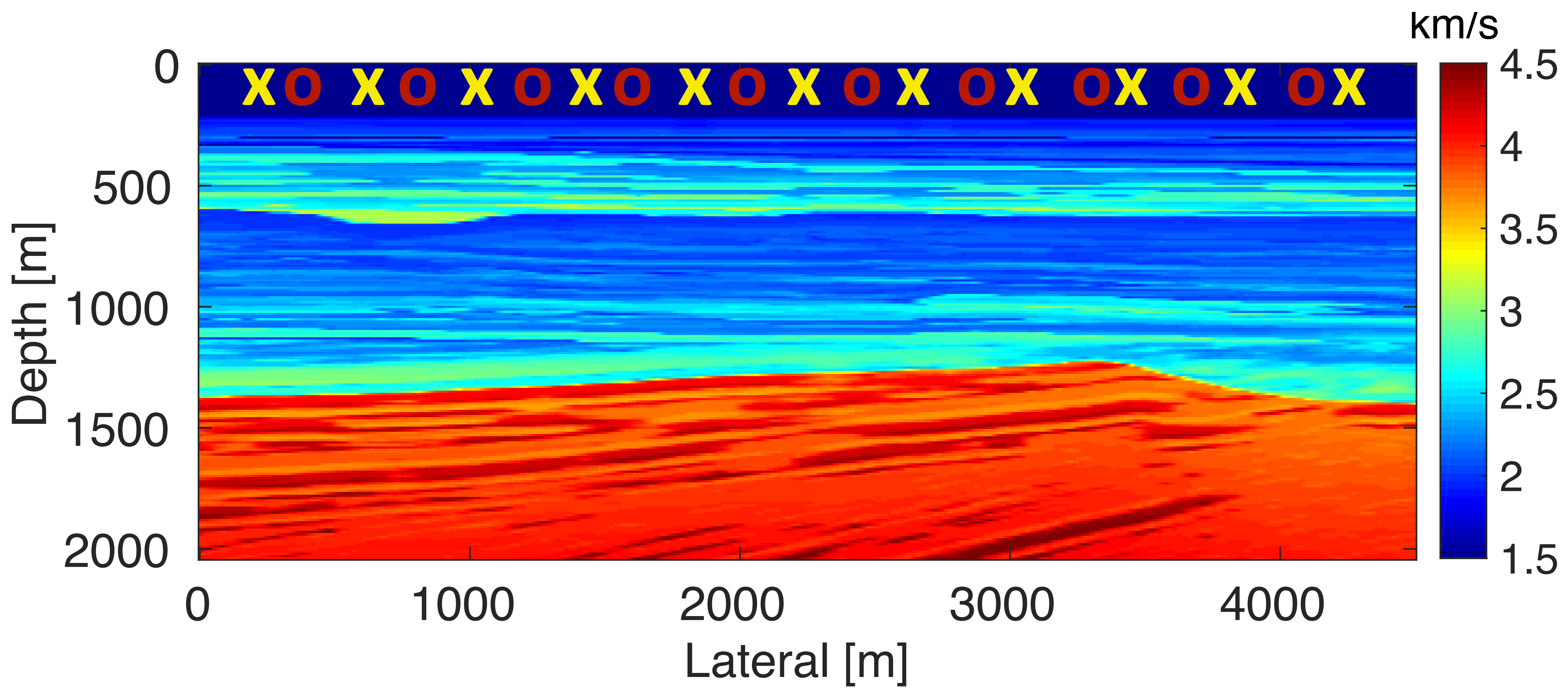

(c) STD of our method

# Cross section comparison



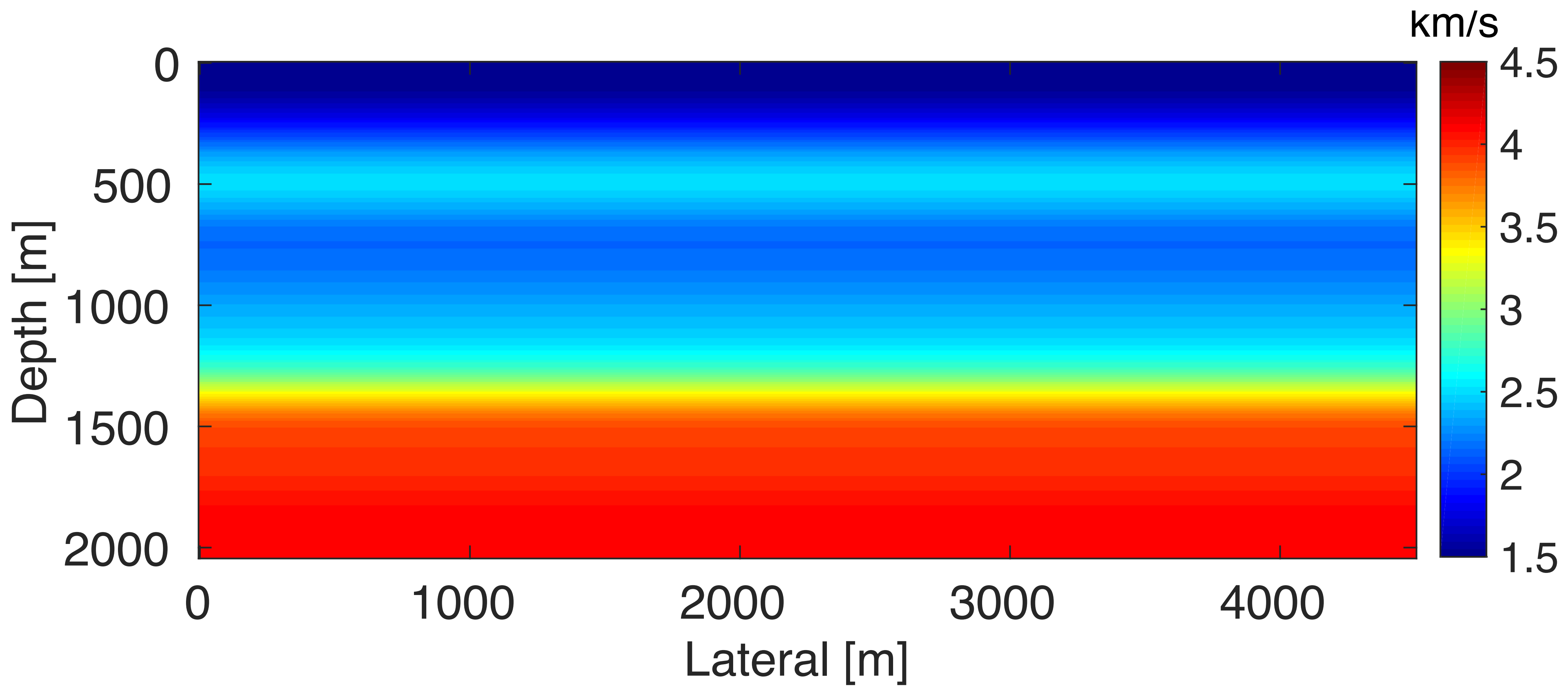

(a) x = 500 m (b) x = 1500 m (c) x = 2500 m

# BG Compass model

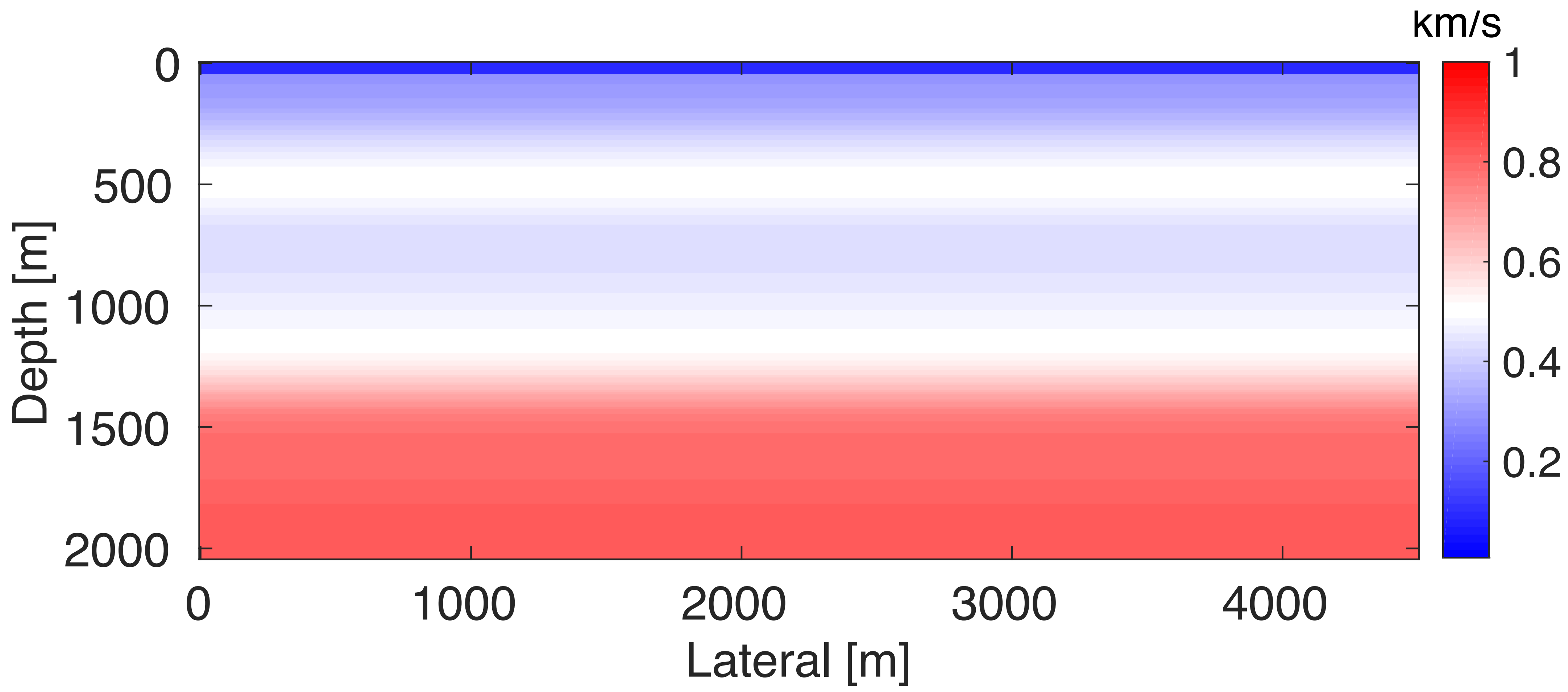



(a) True model

**Depth of sources and receivers: 50**
**Number of sources and receivers: 91 / 451**
**Central frequency: 15 Hz**
**Frequency: 2-31 Hz**
**Lambda: 1e4**



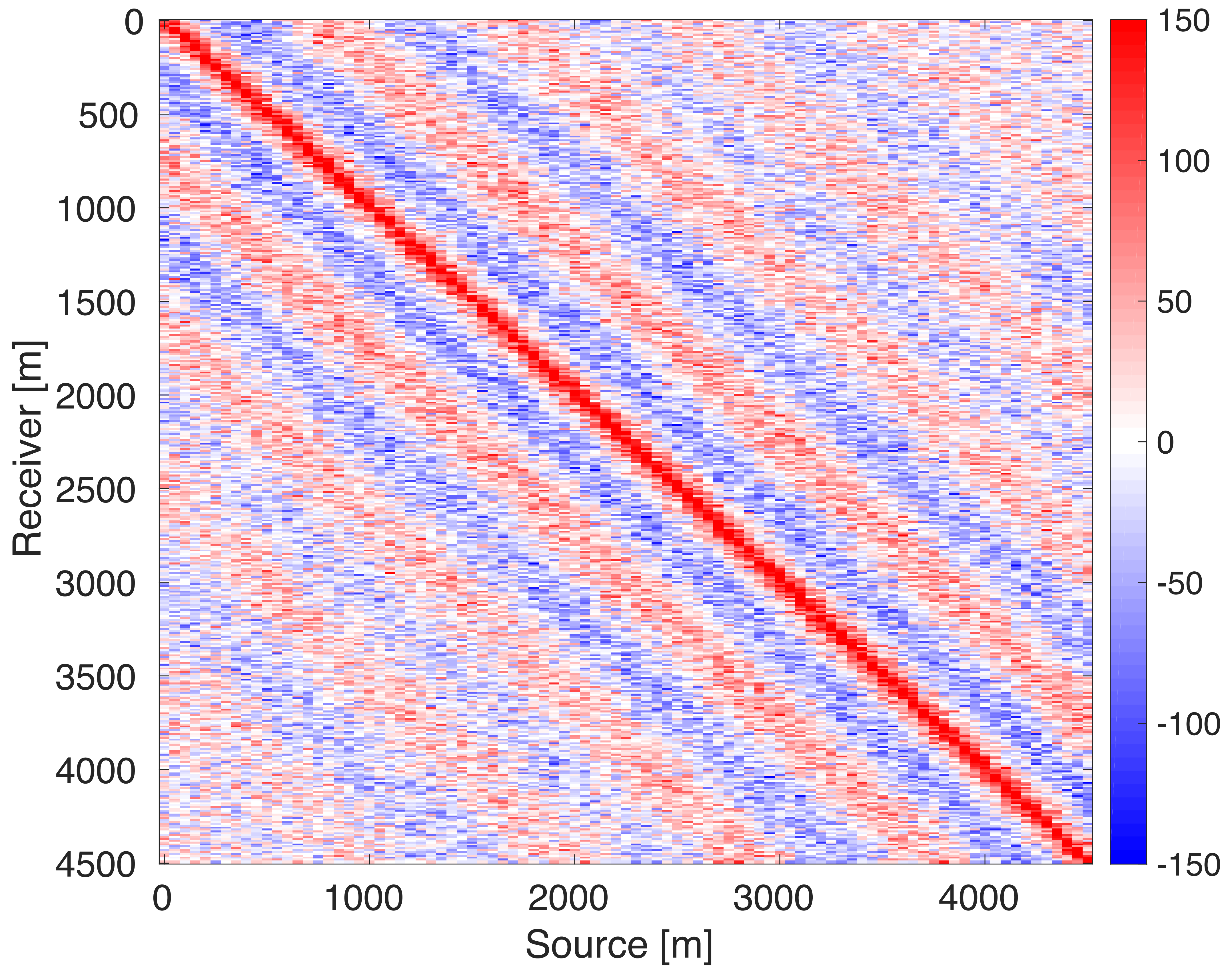

(b) Prior model



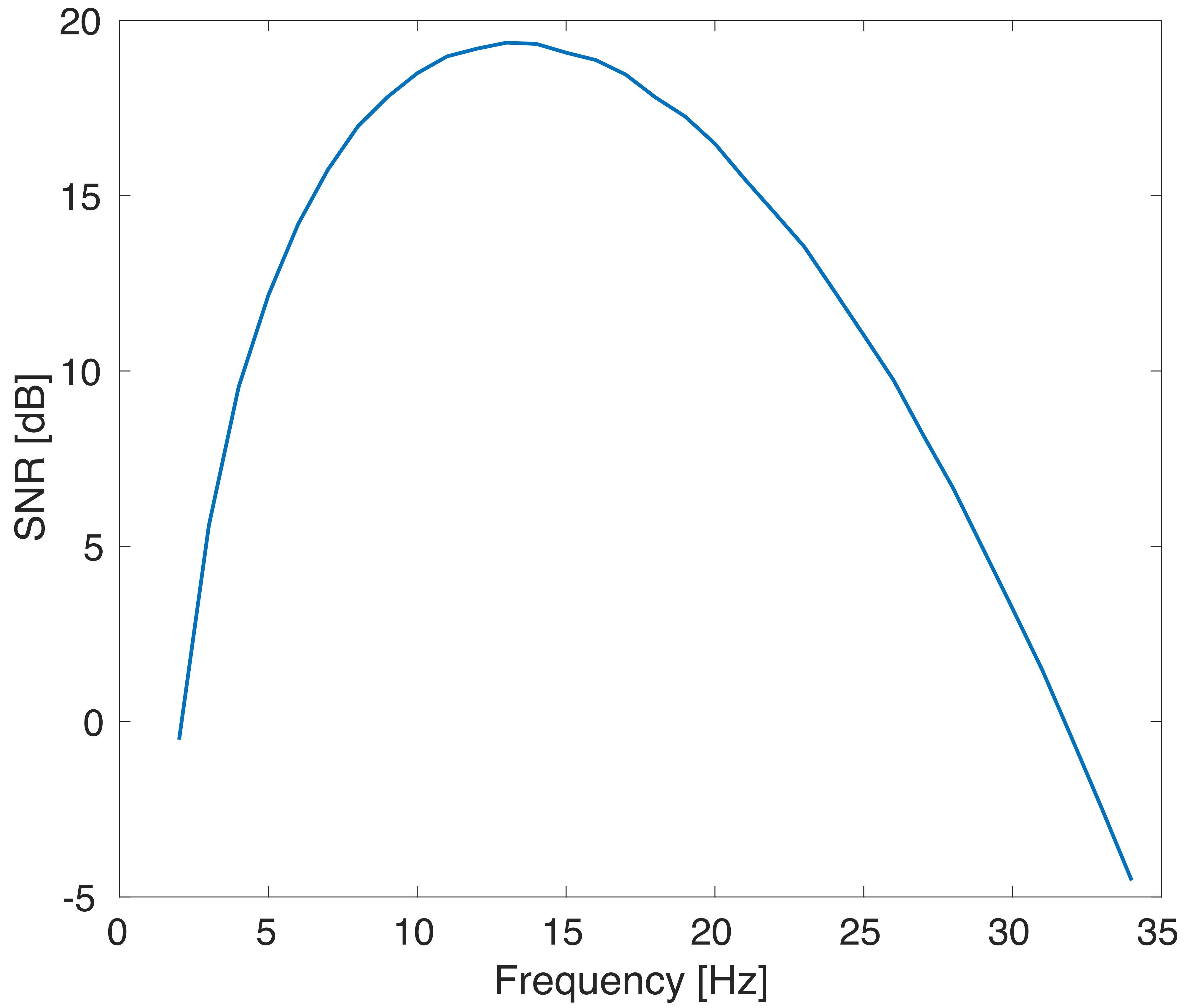

(c) STD of prior distribution

# Data

$\sigma = 34$

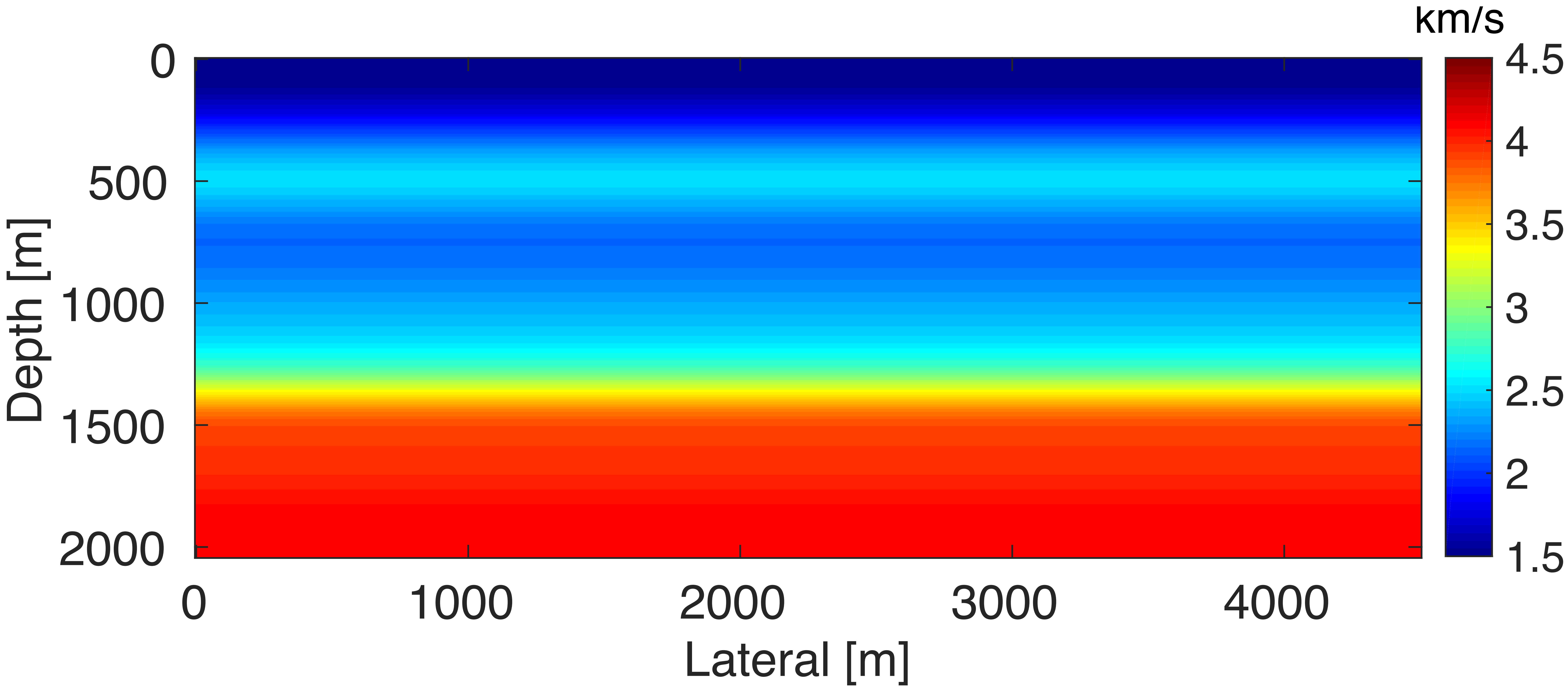



(a) Data at 2Hz

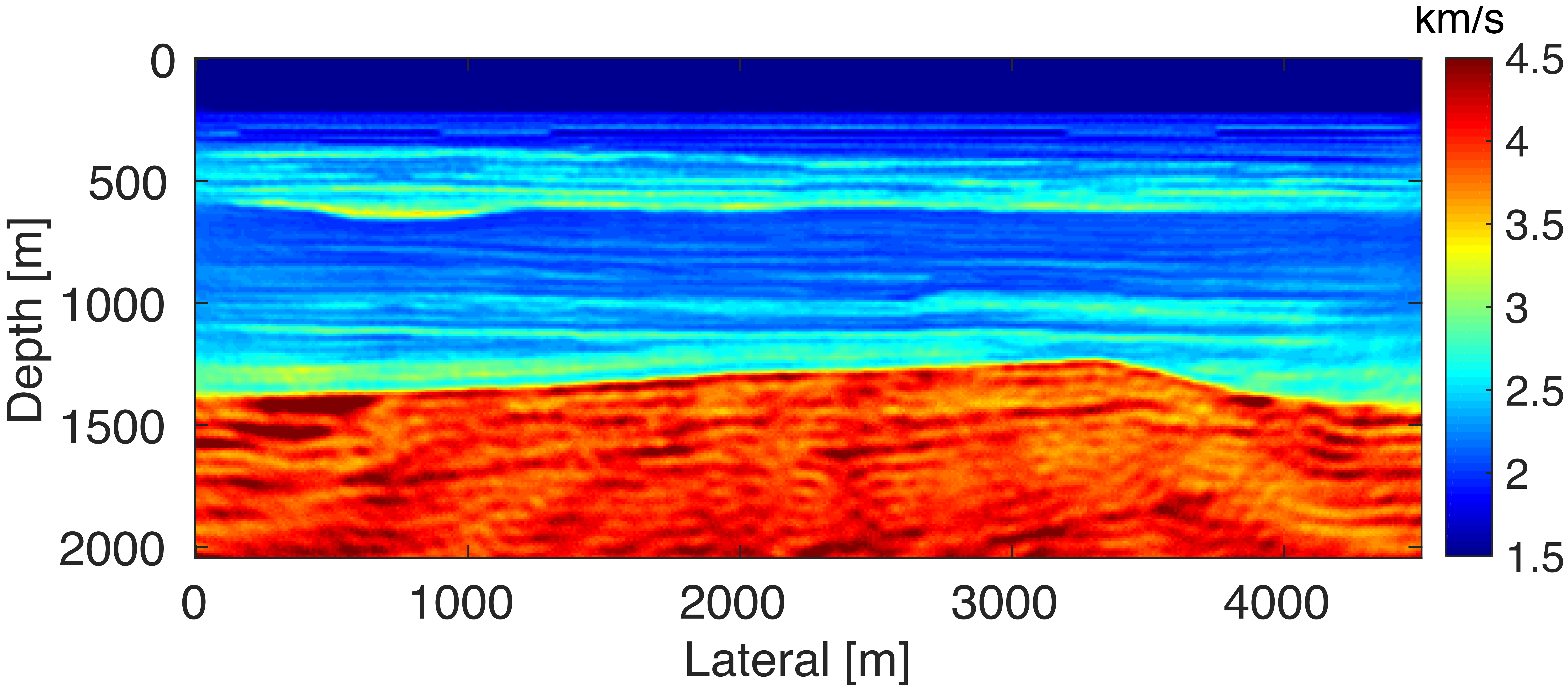



(b) Signal to noise ratio

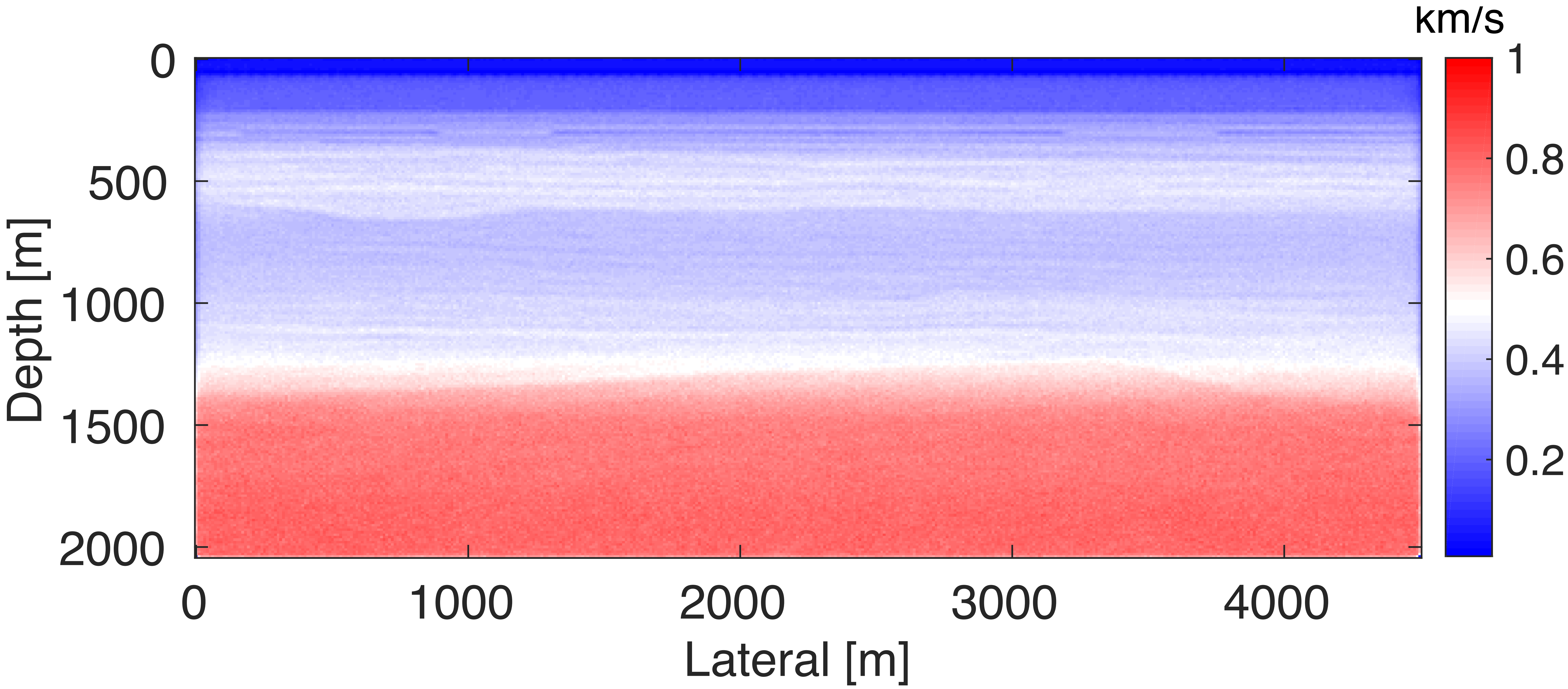
# Prior and initial model



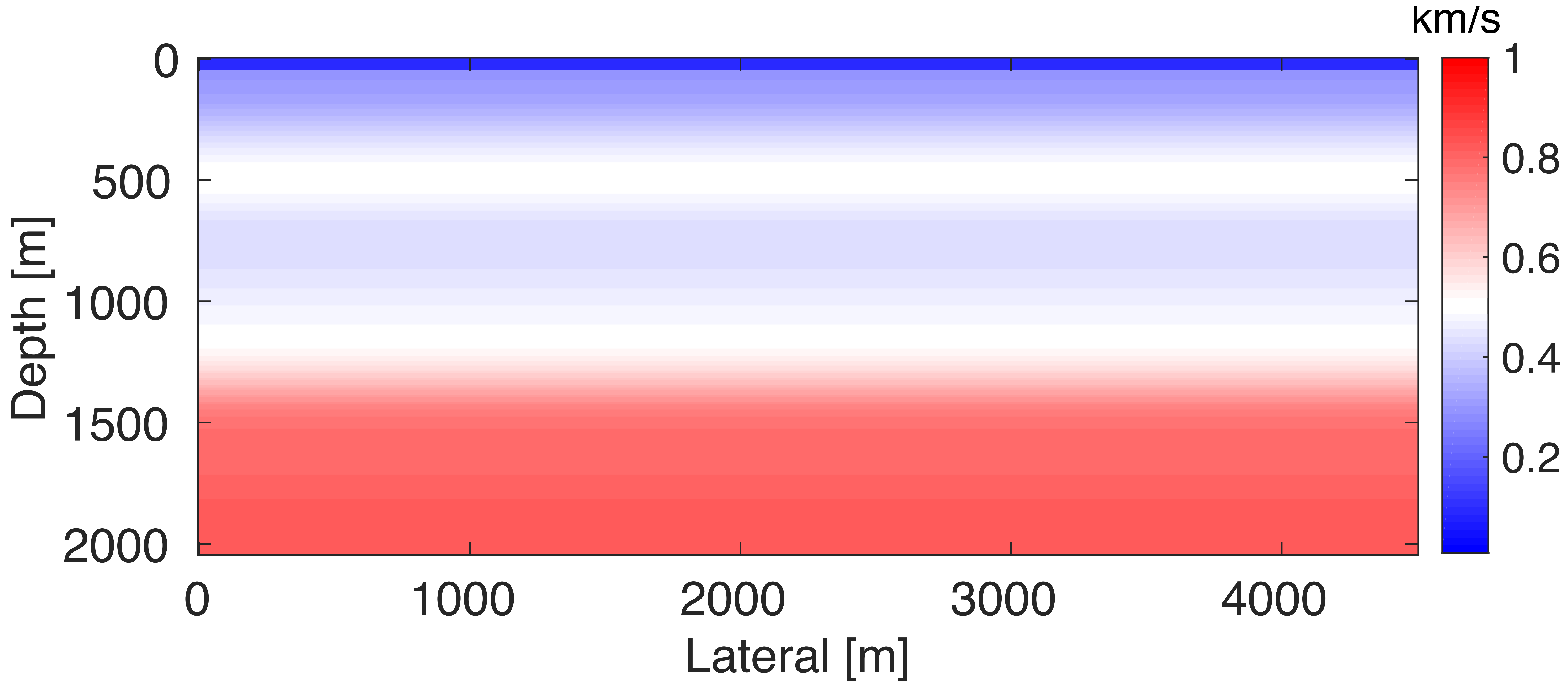
# MAP estimate



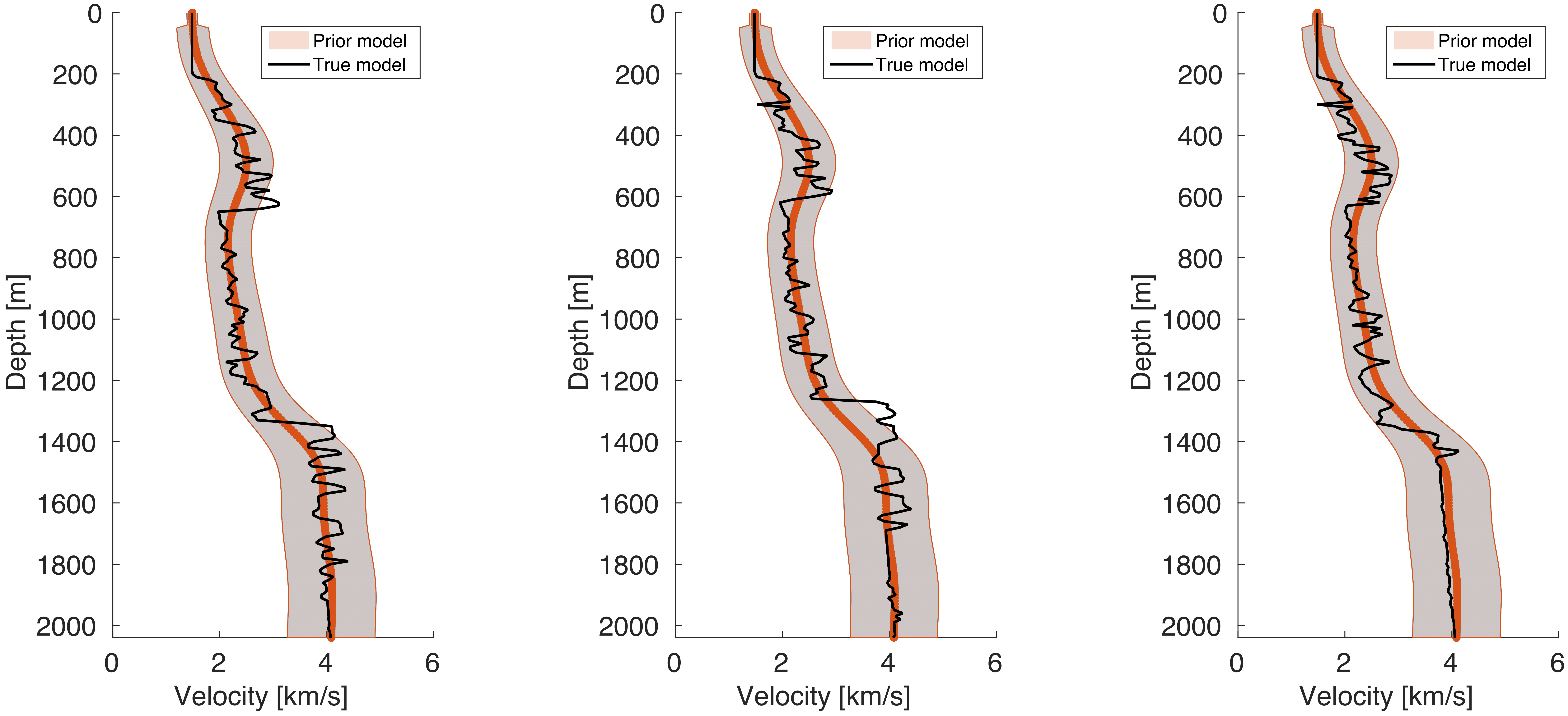
# Posterior STD



# Prior STD


km/s
1
0.8
0.6
0.4
0.2
0
500
1000
1500
2000
Depth [m]
0
1000
2000
3000
4000
Lateral [m]

# Cross section comparison
## – prior

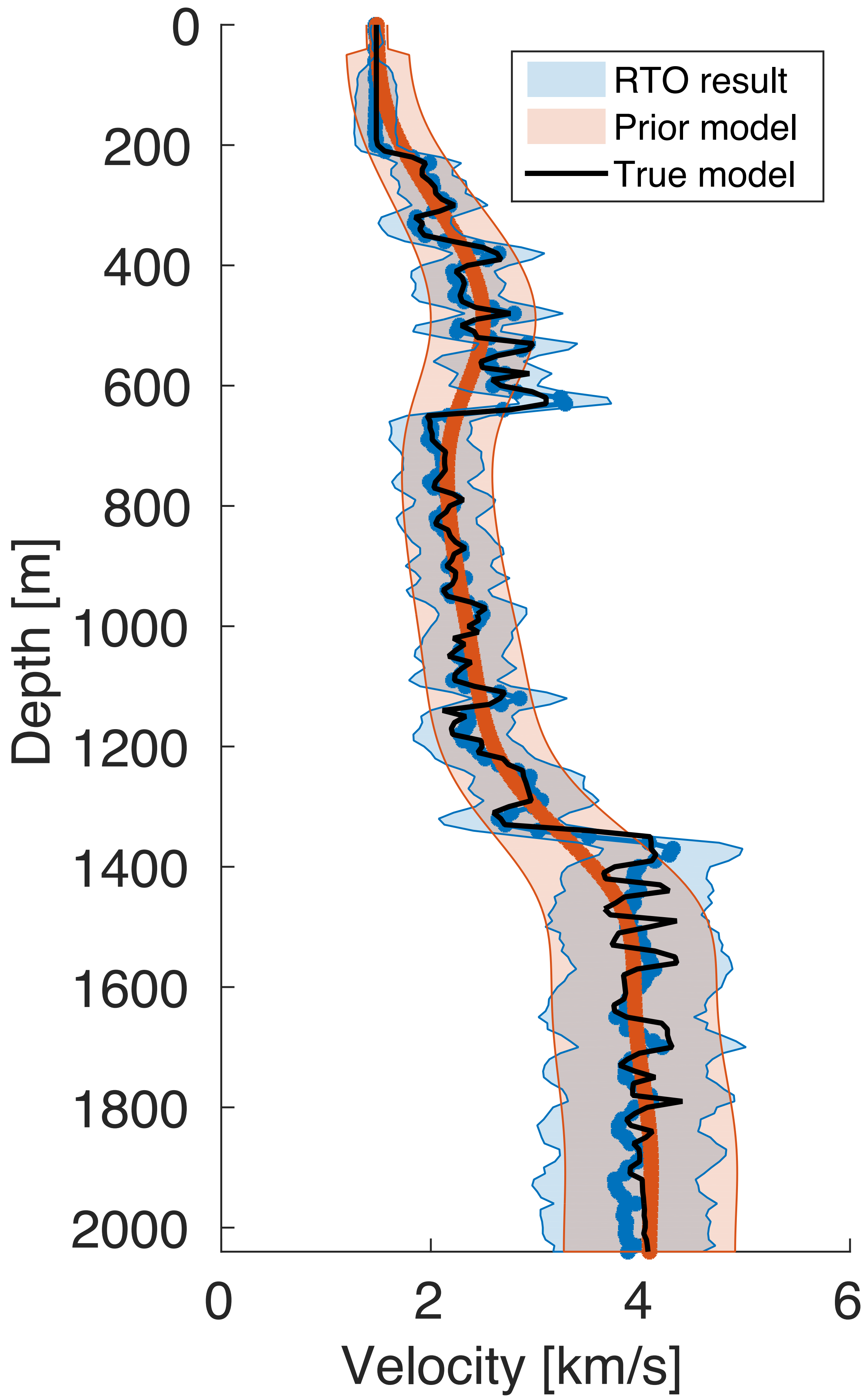



(a) x = 1000 m

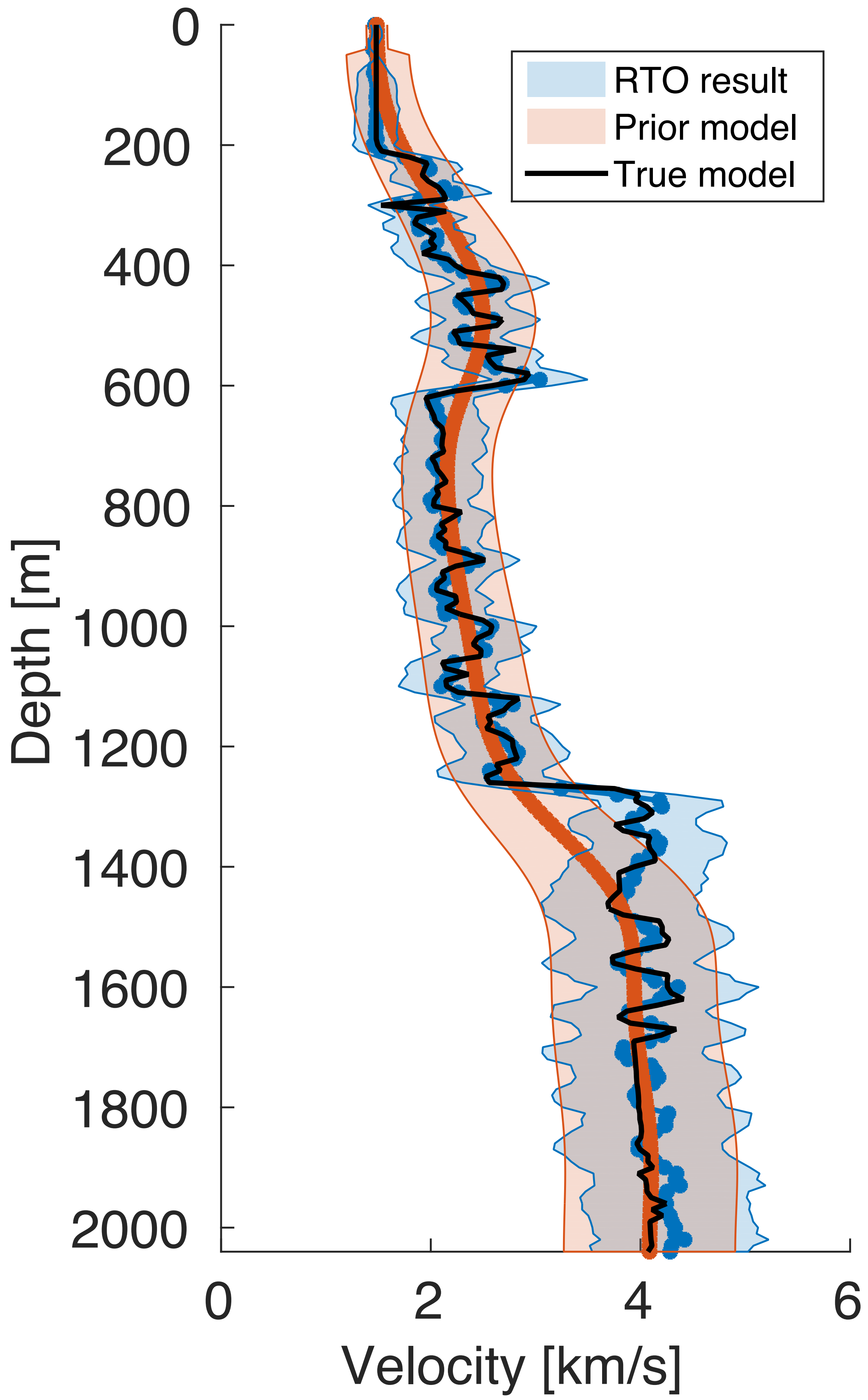
(b) x = 2500 m

(c) x = 4000 m

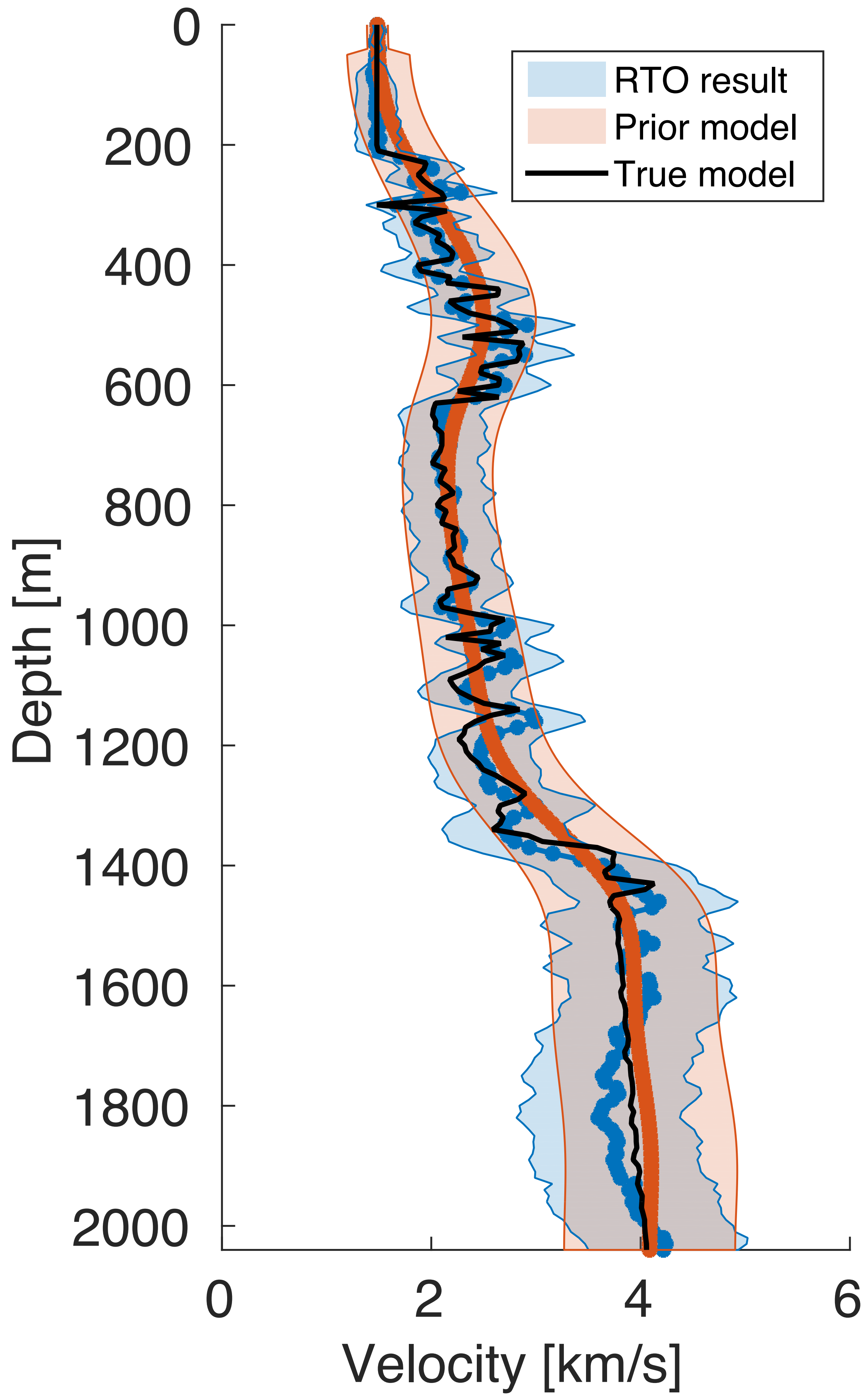
# Cross section comparison
## – posterior vs prior




(a) x = 1000 m

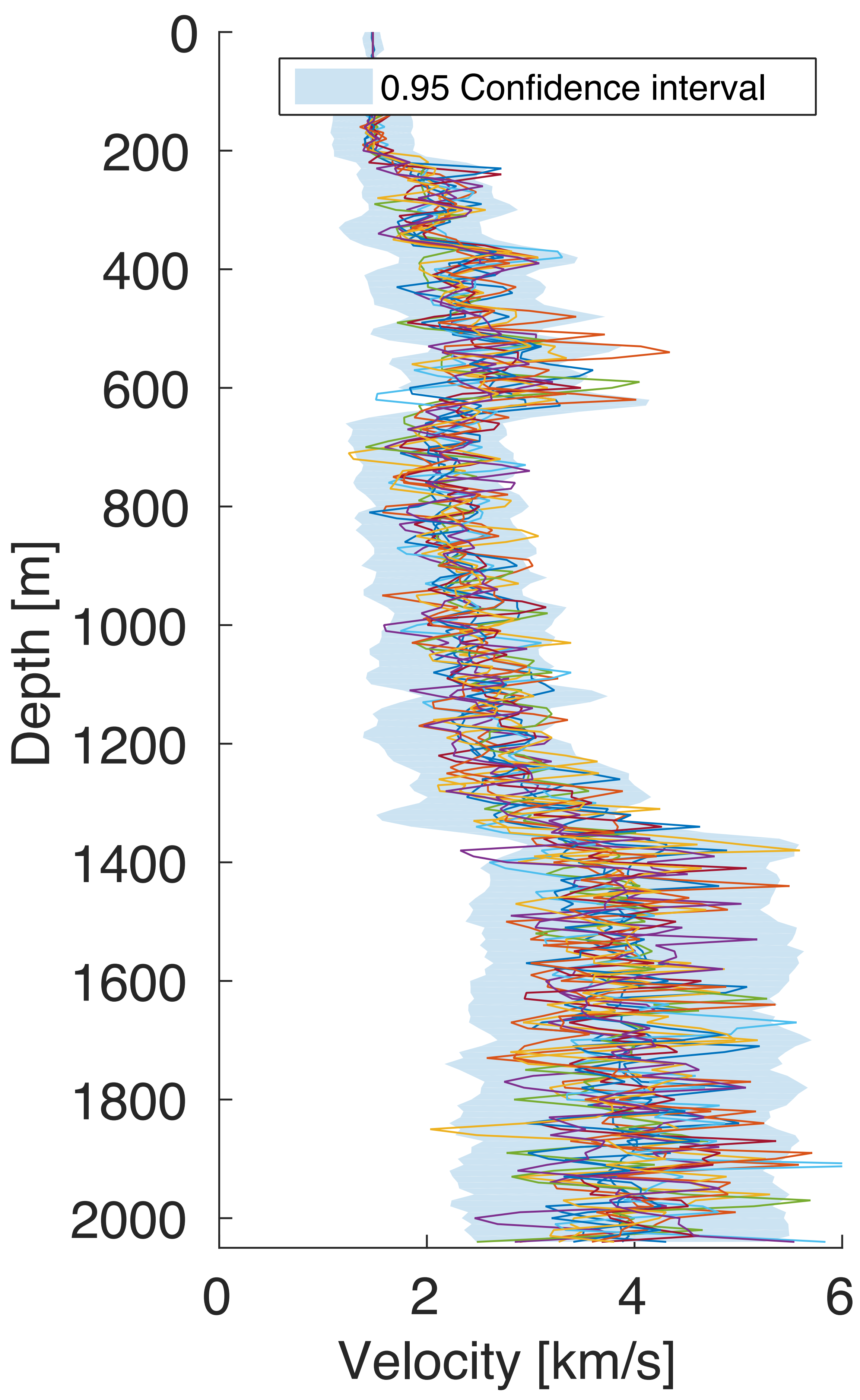



(b) x = 2500 m

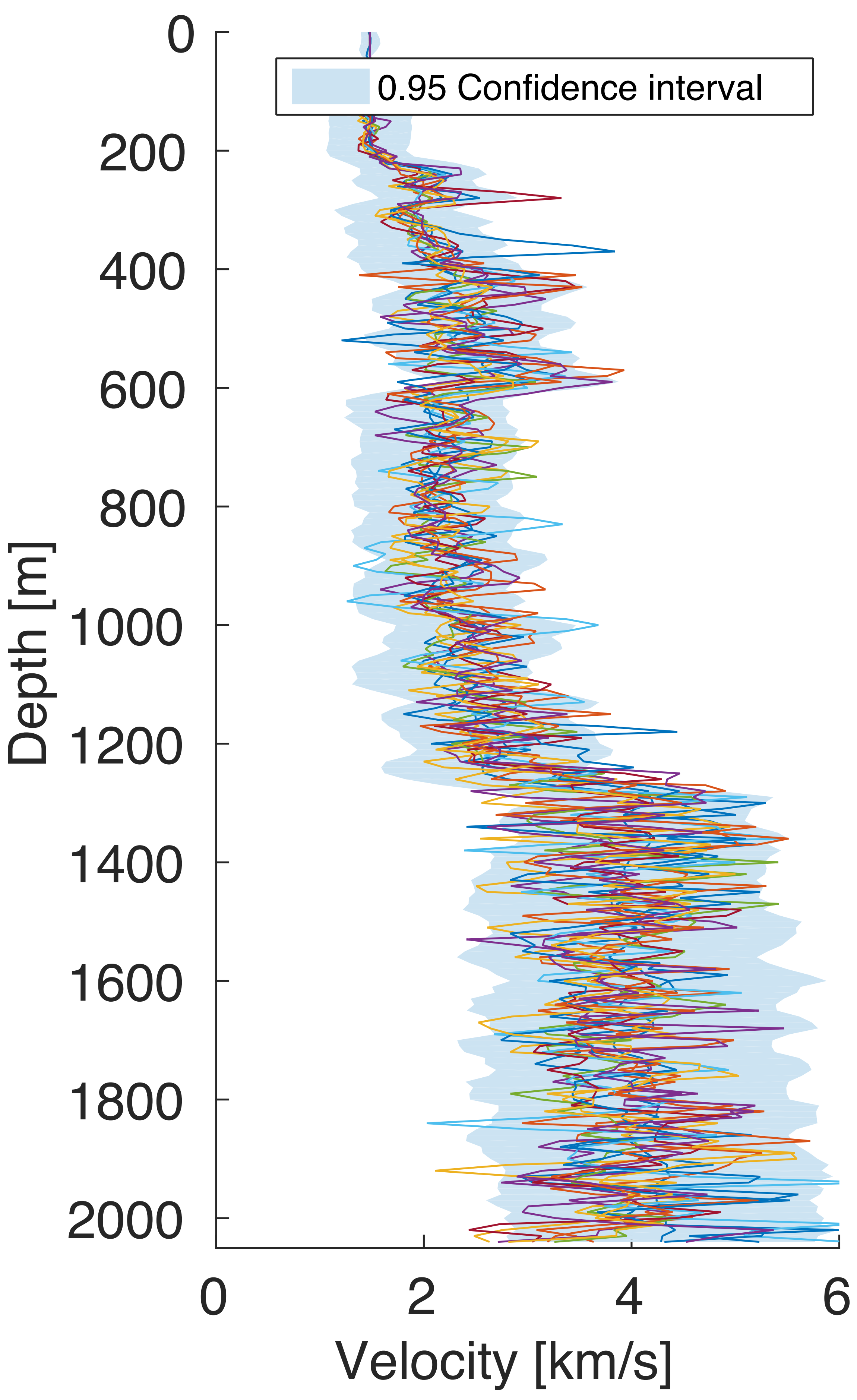



(c) x = 4000 m

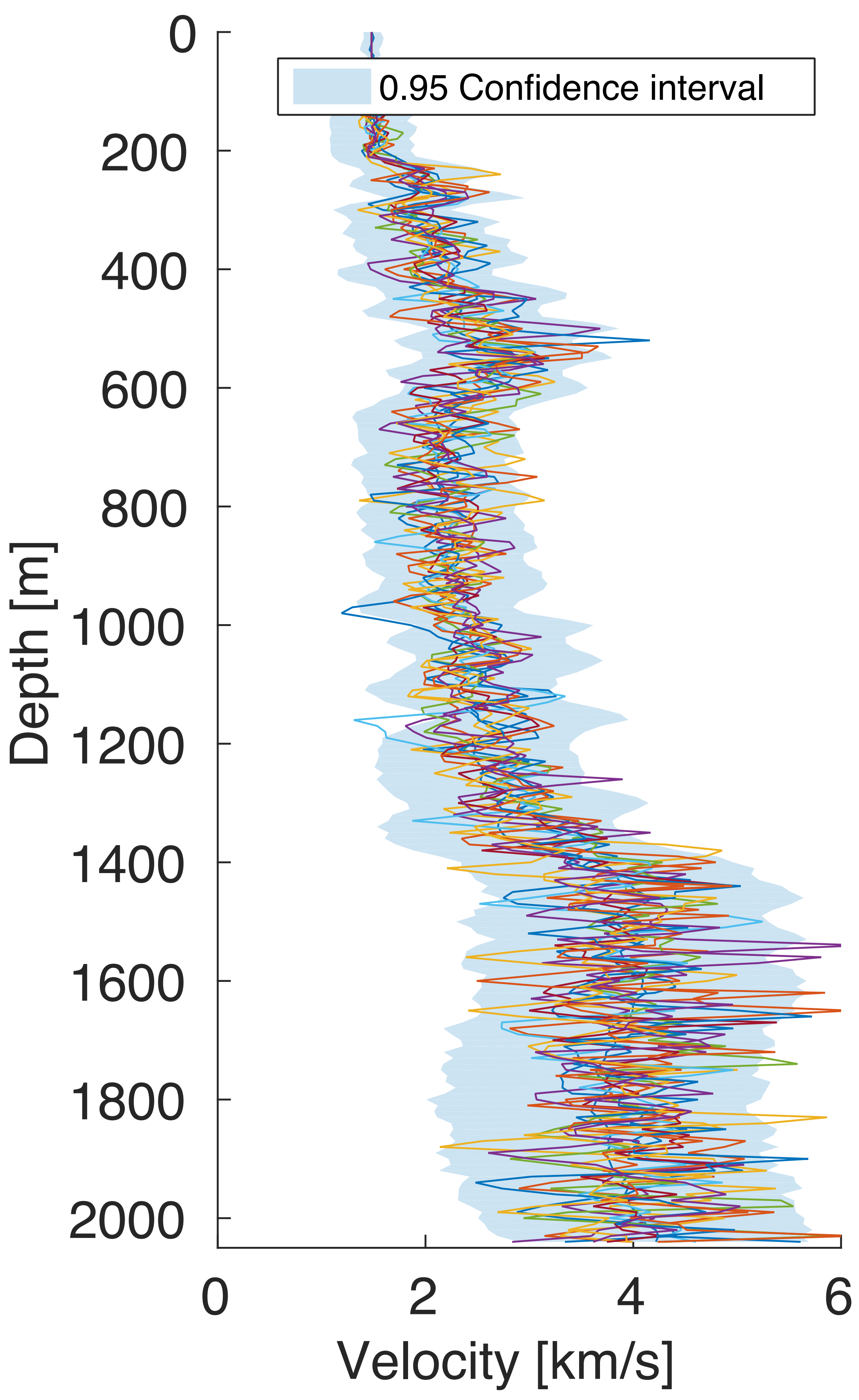
# Cross section comparison
## – 95% confidence interval vs 10 realizations by RML




**(a) x = 1000 m**




**(b) x = 2500 m**




**(c) x = 4000 m**

# Conclusion

The penalty method provides a formulation of posterior PDF with less local maxima, which has a better Gaussian approximation than the reduced formulation.

The implicit formulation of the Gauss-Newton Hessian for WRI provides an efficient way to compute the matrix-vector products.

The RTO method can sample the Gaussian PDF efficiently without the requirement of the explicit Hessian matrix. Numerical experiments show the effectiveness of our method.

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