COMPUTATIONALLY EFFICIENT METHODS FOR UNCERTAINTY QUANTIFICATION IN SEISMIC INVERSION

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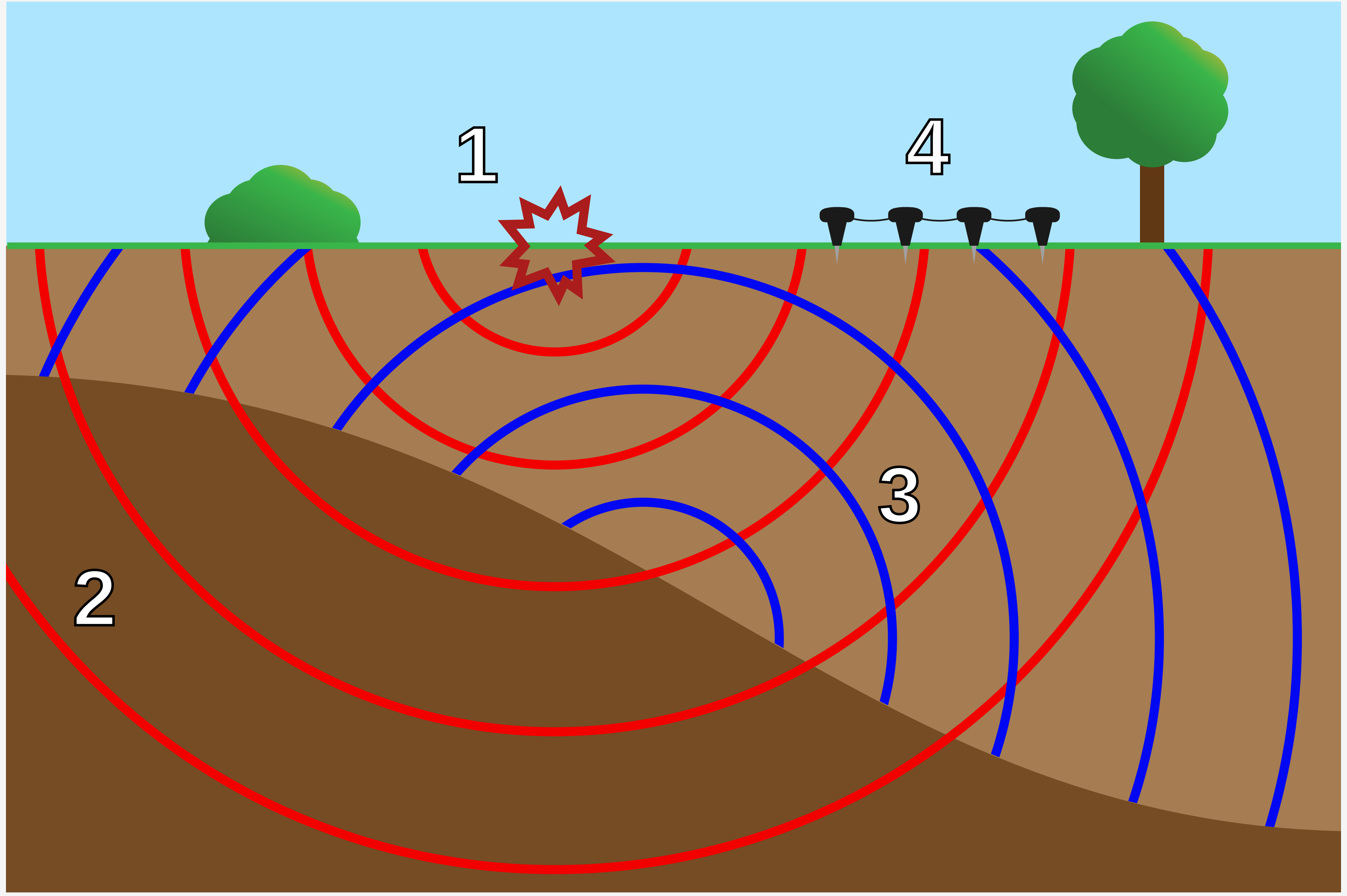
OUTLINE

EXPLORATION SEISMOLOGY



1. A seismic disturbance.
2. Seismic waves propagating through the subsurface.
3. Reflected seismic waves created by the change in material.
4. Geophones that record the direct (red) and reflected (blue) waves.

FULL WAVEFORM INVERSION (FWI)

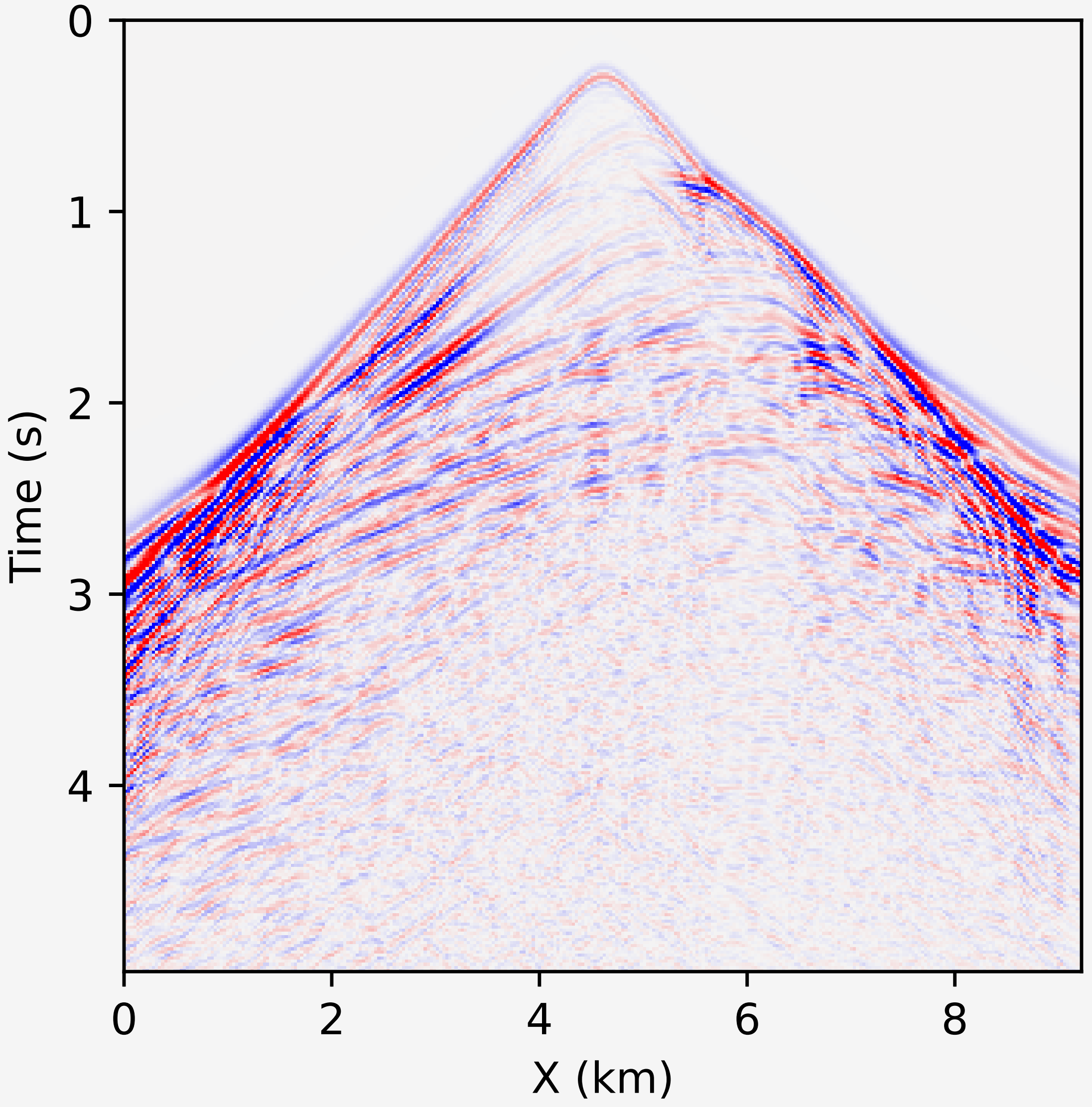


Figure: Synthetic receiver data with a t^2 gain applied to emphasize the later events.

- In Full Waveform Inversion (FWI), the goal is to minimize an objective function, e.g.:

$$\frac{1}{2}\|F(\theta) - D\|^2$$

where θ describes the velocity field, D is the observed seismic data, and $F(\theta)$ is the simulated seismic data.

- We use the 2D constant-density acoustic wave equation:

$$\frac{1}{c^2(x,z)}\frac{\partial^2 p}{\partial t^2} - \Delta p = f$$

WAVE DATA

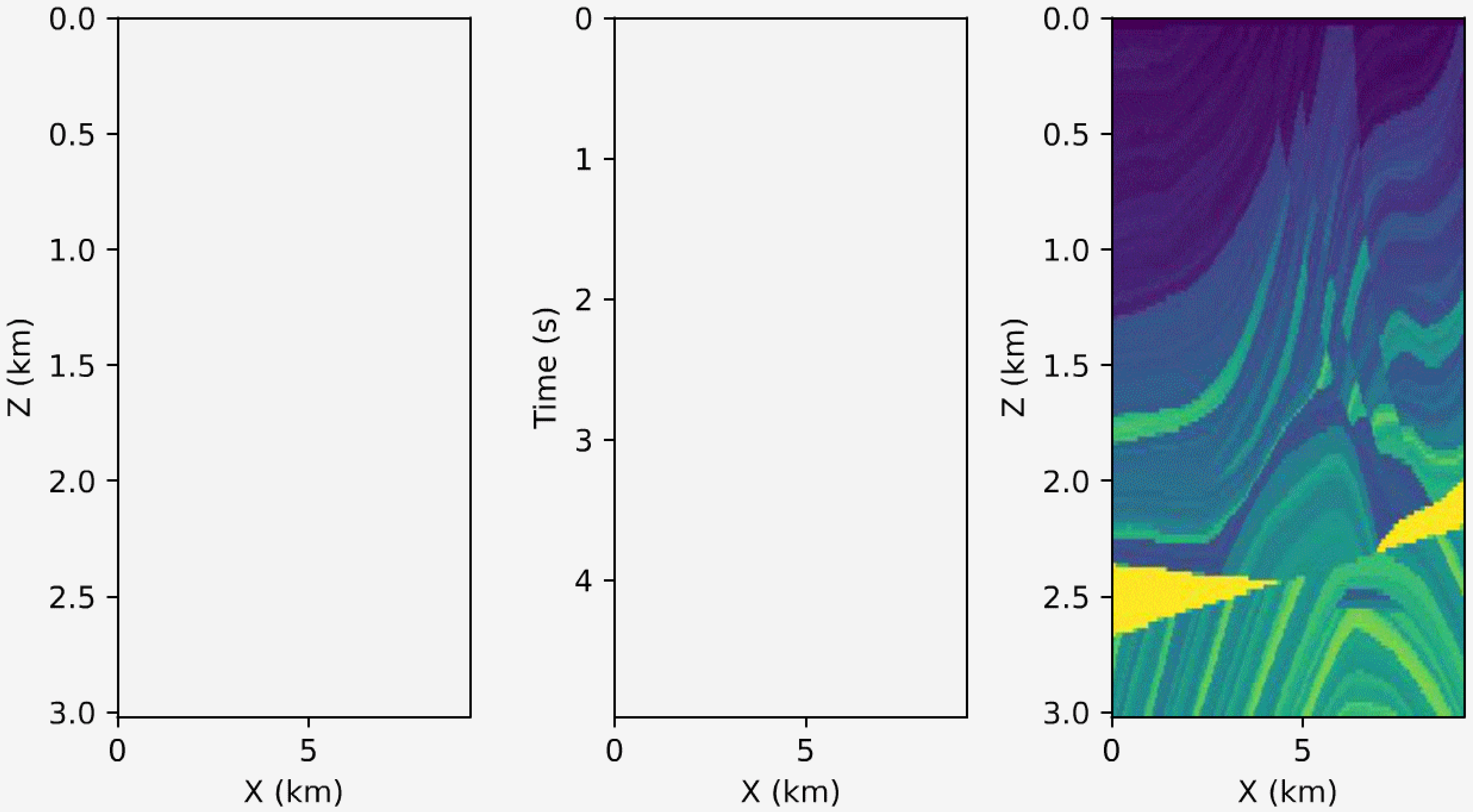
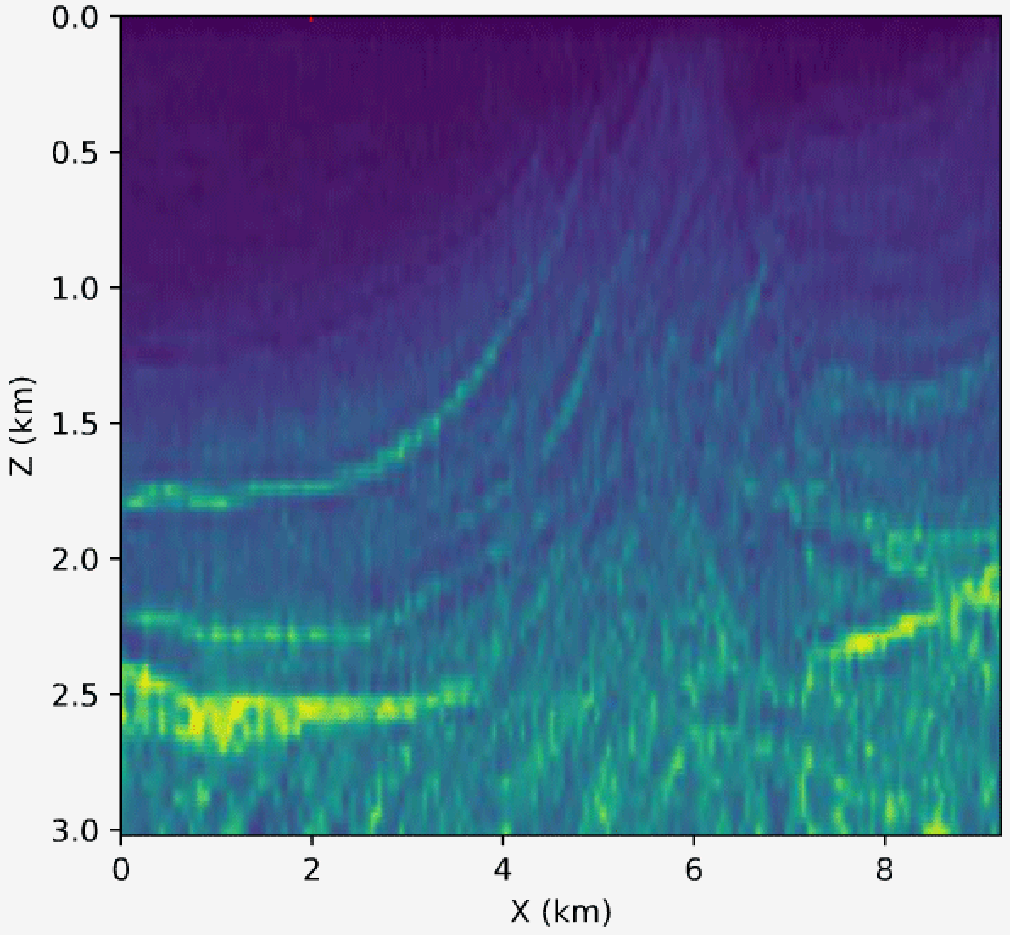


Figure: Left: an acoustic wave propagating through the velocity field on the right. Center: Receiver data by time. Right: the velocity profile.

UNCERTAINTY QUANTIFICATION AND FWI

- Traditional FWI methods result in a single velocity field.
- UQ methods result in distributions of velocity fields.
- UQ indicates where we have more or less certainty about the estimate from FWI.



BAYES' RULE

MARKOV CHAIN MONTE CARLO (MCMC)

- We assume the likelihood function has the form

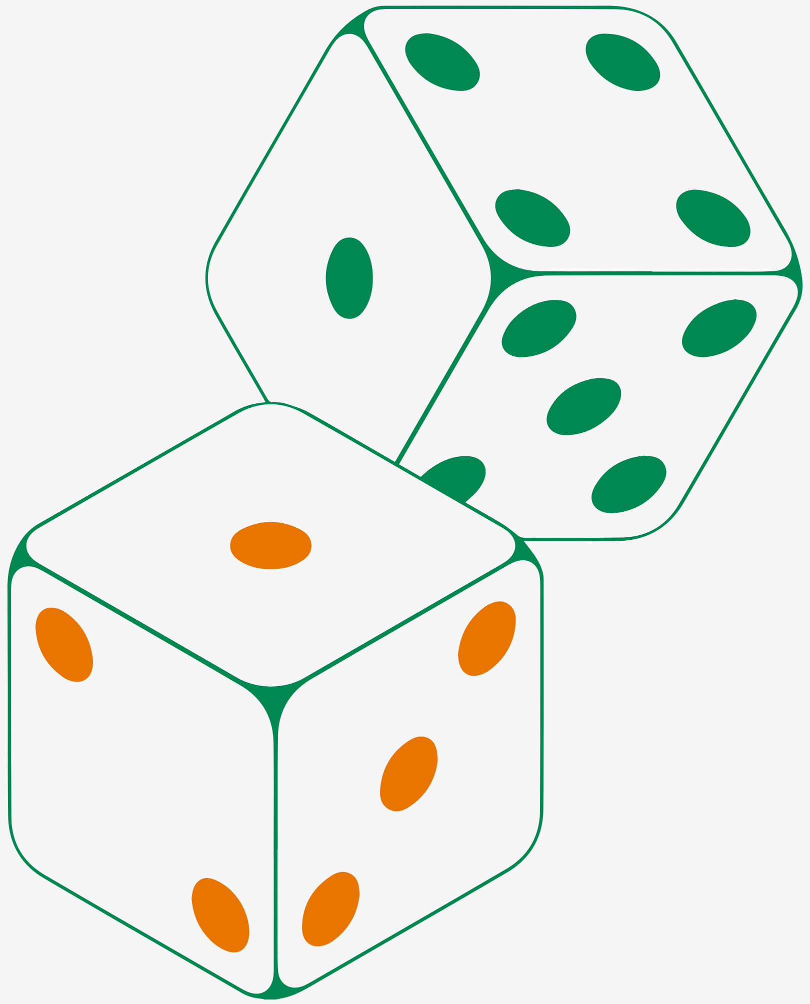
$$\pi(D|\theta) = \exp\left(-\frac{\|F(\theta) - D\|^2}{2\sigma^2}\right)$$

  where $F(\theta)$ is the simulated data, D is the observed data, and σ is the precision parameter.

- The prior distribution can take many forms, e.g. uniform or Gaussian.

- However, the posterior is not necessarily Gaussian.

MARKOV CHAIN MONTE CARLO (MCMC)



- Deterministic approaches to Bayesian FWI require many assumptions.
- Stochastic approaches require fewer assumptions.
- Markov chain Monte Carlo methods sample from the posterior distribution without assumptions on the shape of the distribution.

MARKOV CHAIN MONTE CARLO (MCMC)

START

STOP

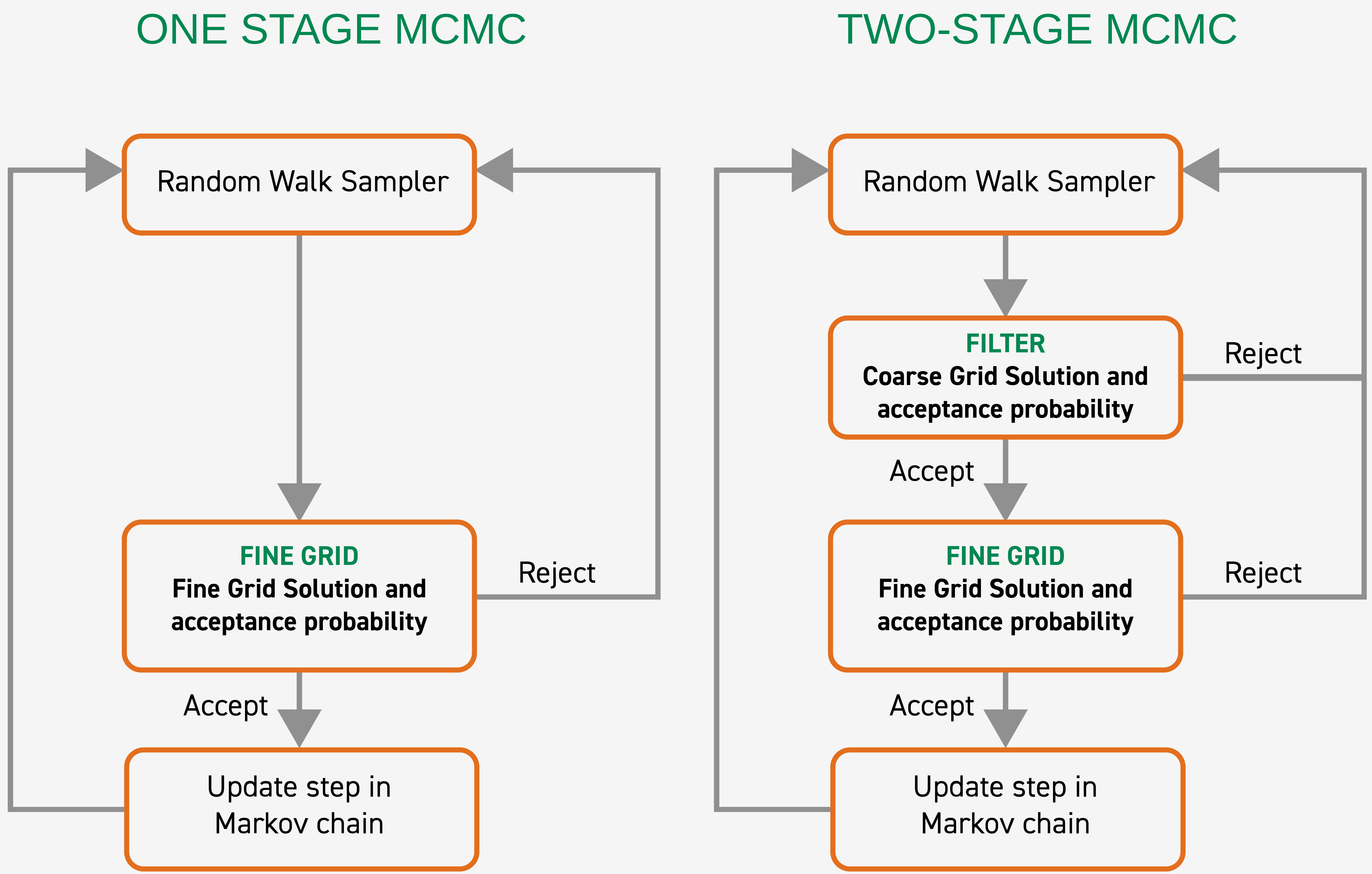
RESET

THE PROBLEM WITH MCMC

- MCMC can take many models (tens of thousands to millions) to converge.
- Each model must be run through a forward simulator (wave equation).
- A single chain can take a week or more on a cluster.
- Often 80% to 90% of the samples are rejected!

HOW CAN WE REDUCE THE COMPUTATIONAL COST OF MCMC METHODS FOR FWI?

TWO-STAGE MARKOV CHAIN MONTE CARLO



Efendiev et al. (2006), Christen and Fox (2005)

OPERATOR UPSCALING

- Modeling wave propagation can be computationally expensive.

- Operator upscaling[1] decomposes the solution into two parts:
  1. Fine grid problem on independent subdomains
  2. Small coarse grid problem over the whole domain

- In this upscaling technique we do NOT upscale the model.

(1) Vdovina et al. (2005), Korostyshevskaya and Minkoff (2006), Vdovina and Minkoff (2008)

OPERATOR UPSCALING

1. Write the acoustic wave equation as a system in space by introducing acceleration, $\vec{v}$

$$\vec{v} = -\nabla p$$
$$\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} = -\nabla \cdot \vec{v} + f$$

2. Solve in parallel for fine grid pressure and acceleration over each independent coarse block. No communication is required at this stage.

3. Solve for coarse grid acceleration over the whole domain.

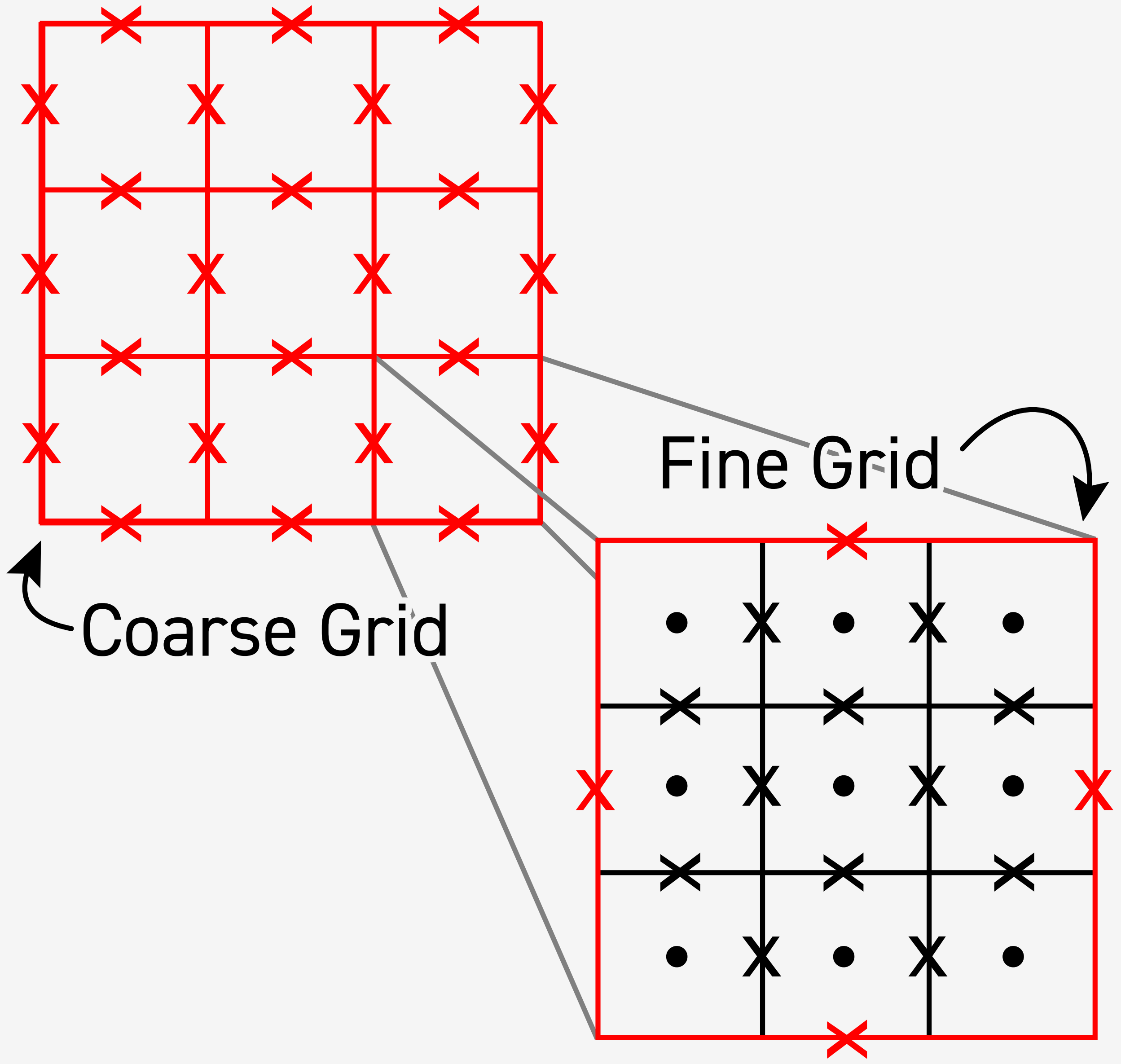
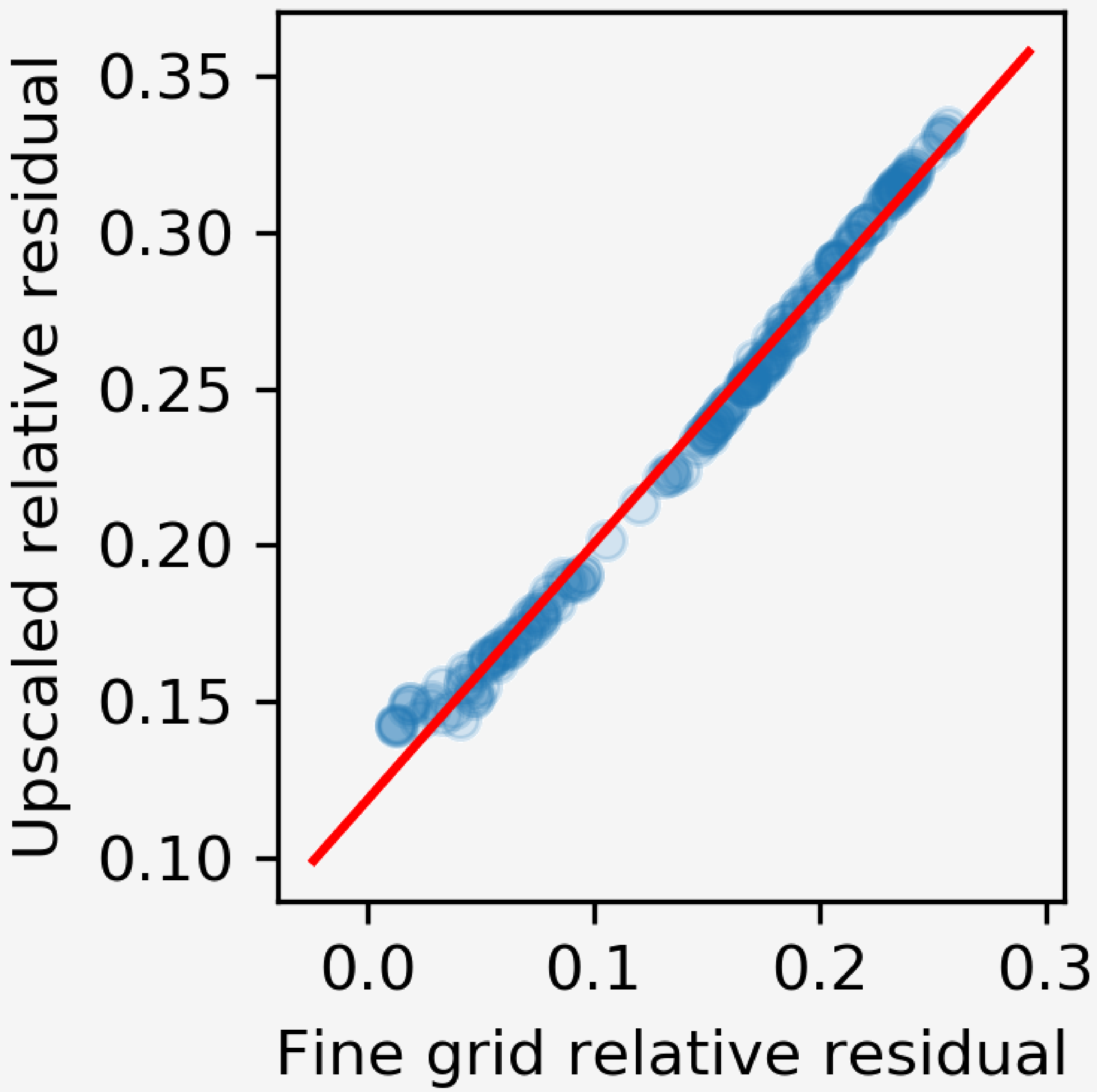


Figure: A picture of the coarse grid (red) and coarse grid acceleration (red X's) and the fine grid (black) and fine grid unknowns (black X's: acceleration, black dots: pressure)

UPSCALING AND FINE GRID CORRELATION



- We see a strong linear relationship between the fine grid relative residuals and the upscaled relative residuals for a layered velocity model.

- This indicates that the upscaling filter is a good surrogate for the fine grid solver.

RESULTS: TWO-STAGE MCMC WITH UPSCALING

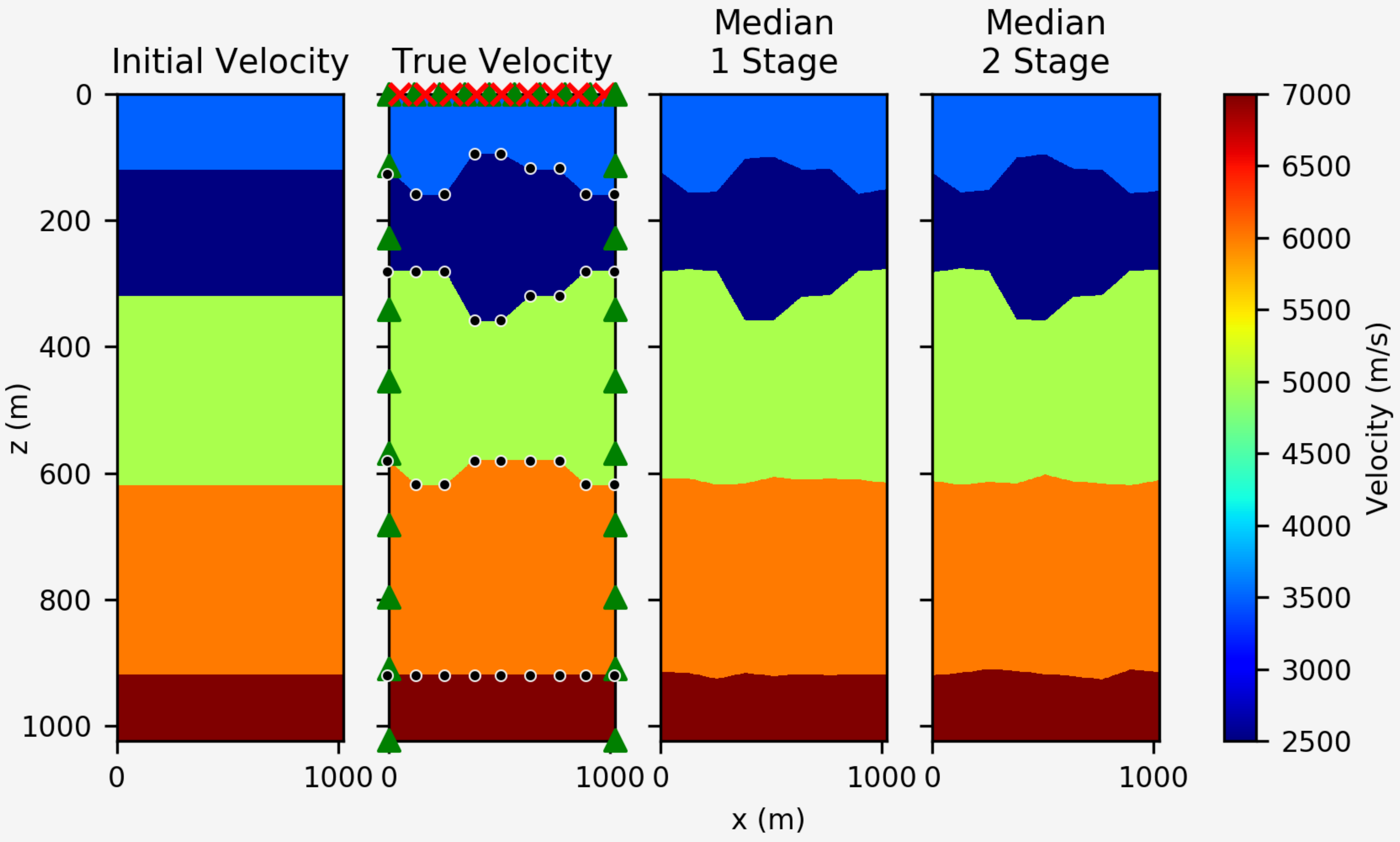


Figure: A comparison of the initial velocity, true velocity, median of the posterior from one-stage MCMC, and the median of the posterior distribution from two-stage MCMC. The true velocity shows the location of a line of sources (red X's), receivers (green triangles), and the unknown nodes that describe the interfaces (black dots). Published in Stuart (2019b).

RESULTS: TWO-STAGE MCMC WITH UPSCALING

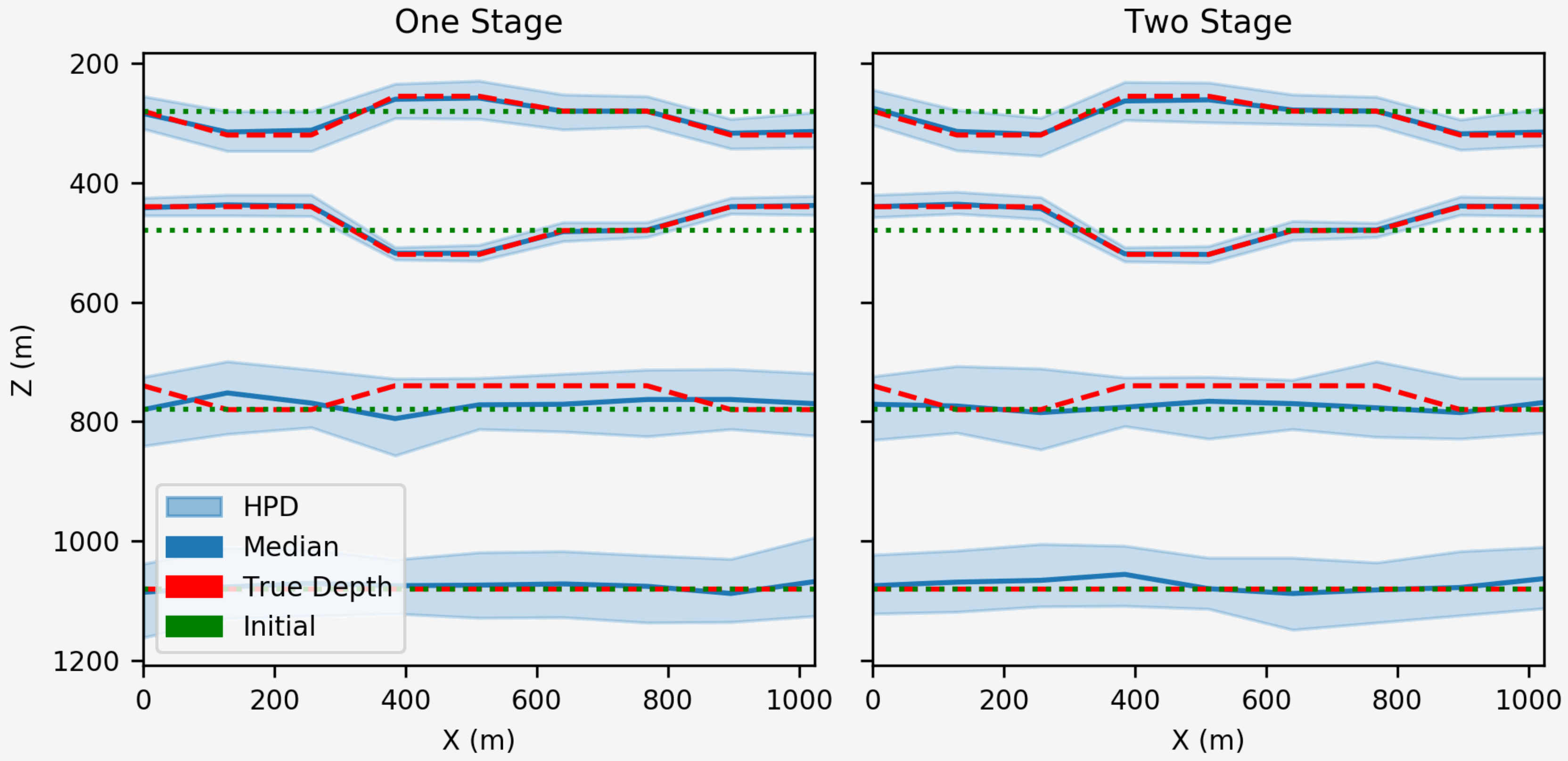
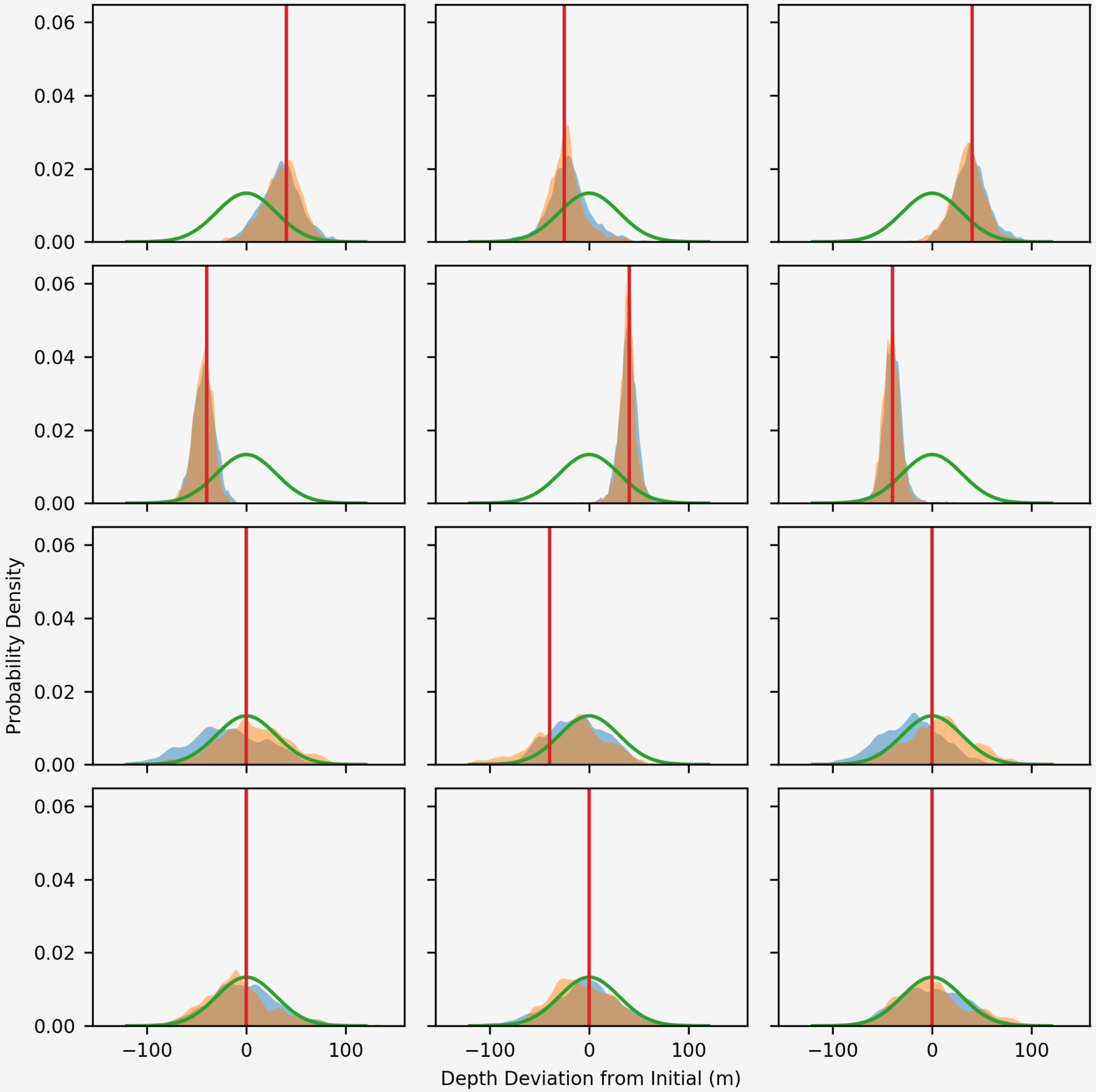


Figure: A comparison between one-stage MCMC highest posterior density (HPD) intervals and two-stage MCMC HPD intervals.

- Acceptance rate increased from 10% to 40%.
- Time per sample decreased by 22% (40% in other experiments).
- Time per rejection decreased by 33%.

RESULTS: TWO-STAGE MCMC WITH UPSCALING



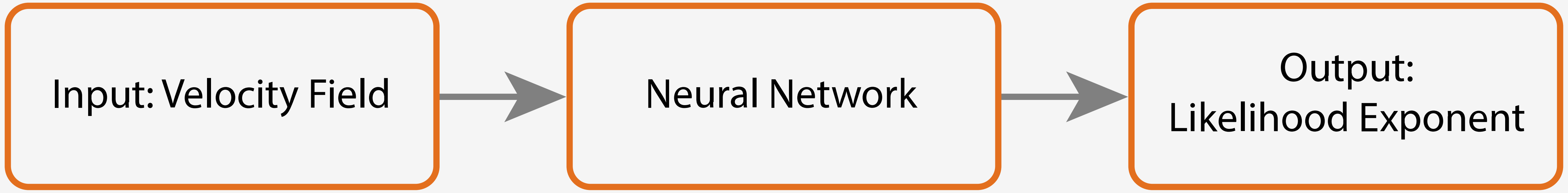
NEURAL NETWORK FILTER

- The likelihood function is:

$$\exp\left(-\frac{\|F(\theta)-D\|^2}{2\sigma^2}\right)$$

where θ is the velocity field, $F(\theta)$ is the simulated data, and D is the observed data.

- Idea: replace the likelihood exponent with a neural network.



PROS AND CONS OF THE NEURAL NETWORK

PROS

- Evaluating a model is extremely fast (< 1 second).
- Neural networks are capable of approximating very complex relationships.
- Data for training can be generated as part of the MCMC process.

CONS

- Where's the physics?
- Training data is expensive to generate
- Predictions are not always very accurate very complex relationships.
- Many knobs to twist in the neural network!

RESULTS: TWO-STAGE MCMC WITH NEURAL NET

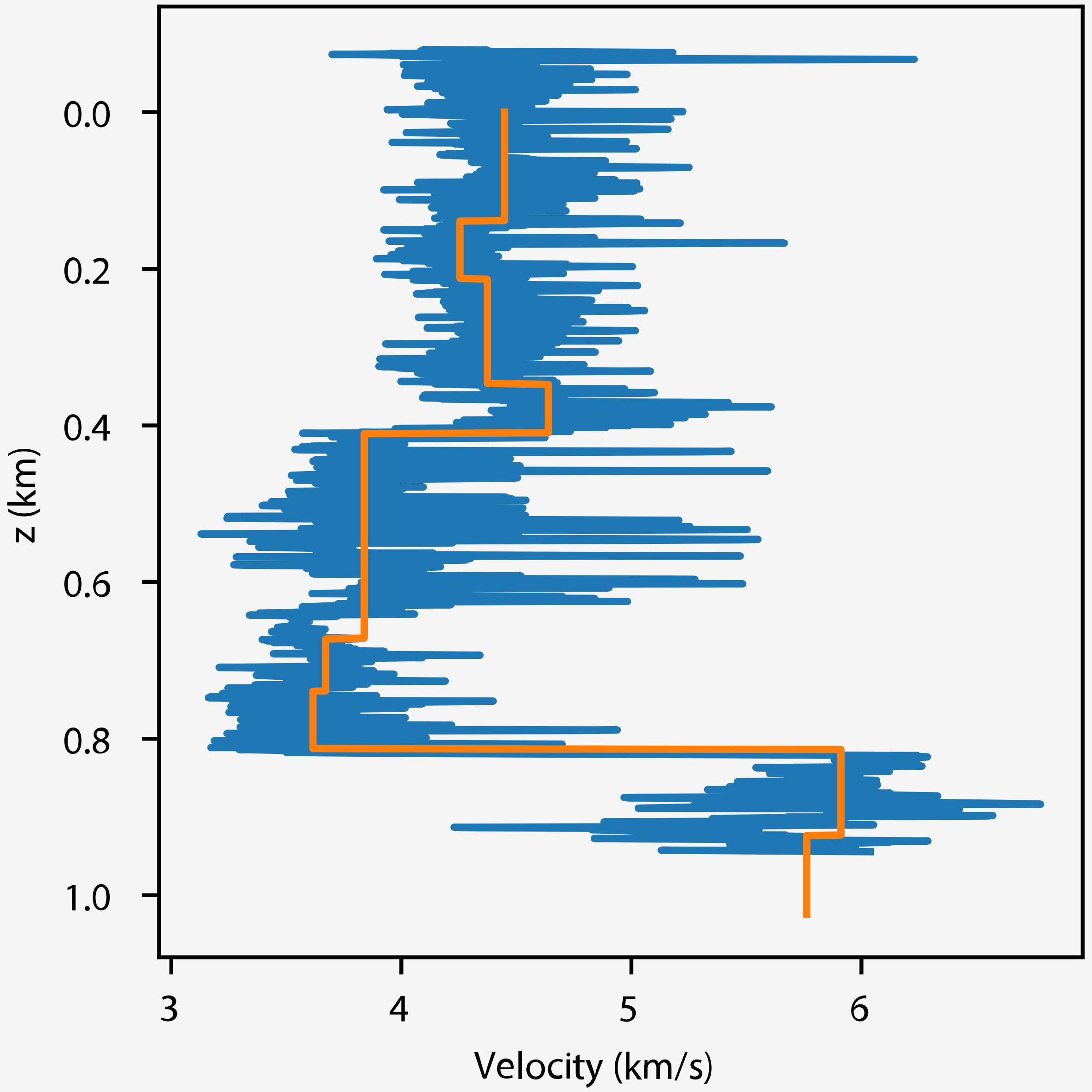


Figure: Well log from the Midland, TX basin (blue, courtesy of Pioneer Natural Resources and 9-layer block (orange).

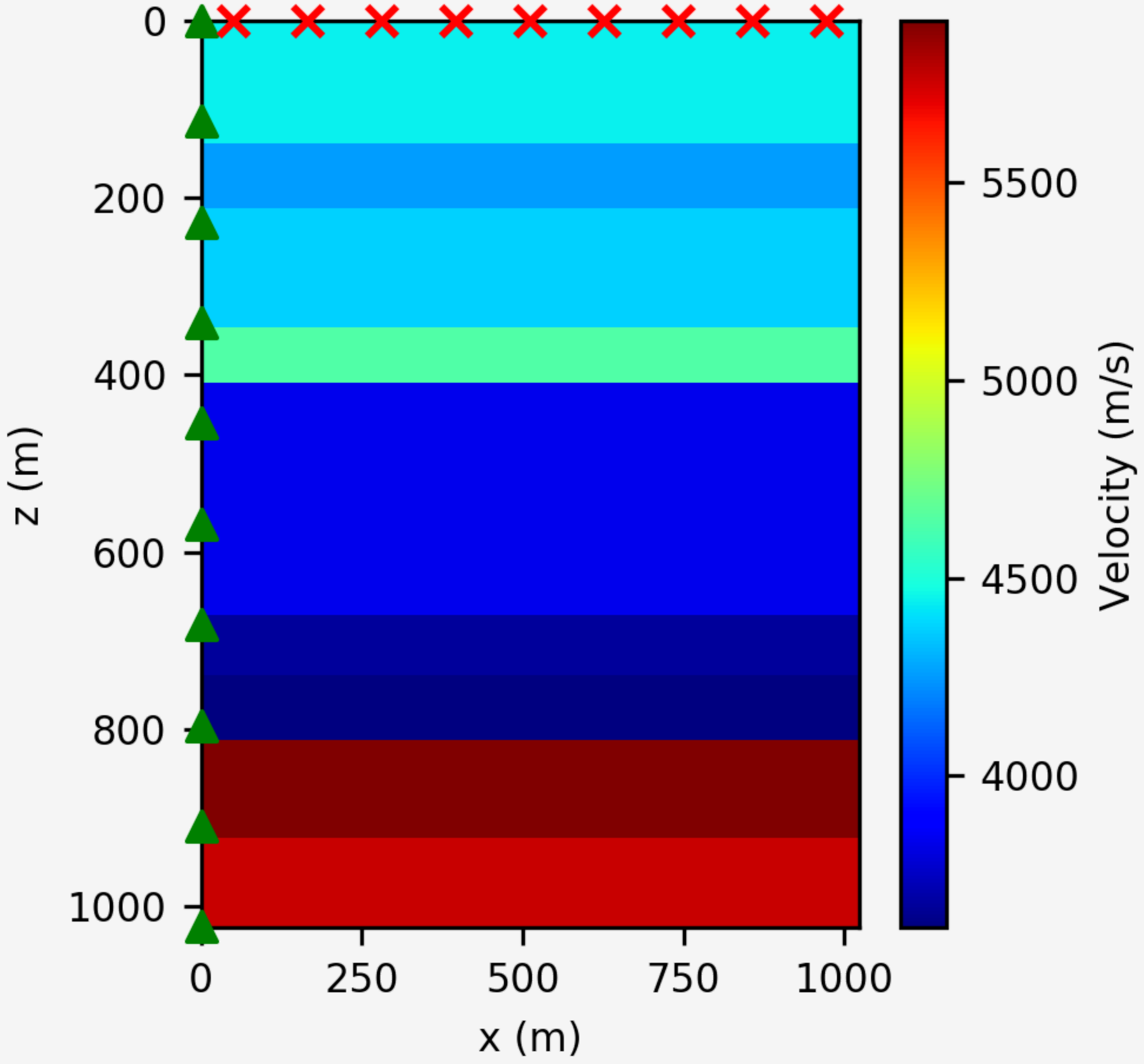


Figure: Flat layered experimental setup with nine unknowns (Stuart et al. 2019a)

RESULTS: TWO-STAGE MCMC WITH NEURAL NET

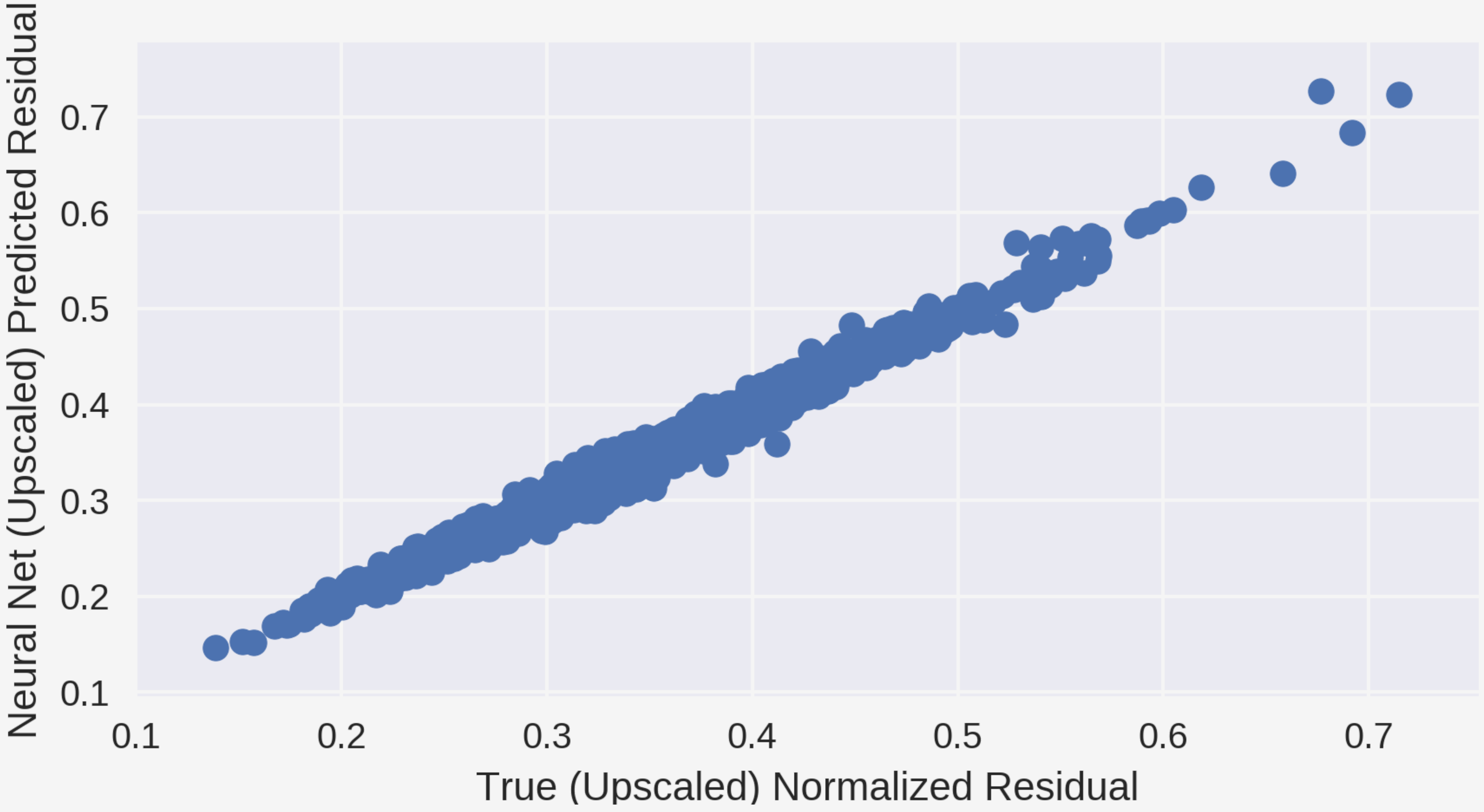
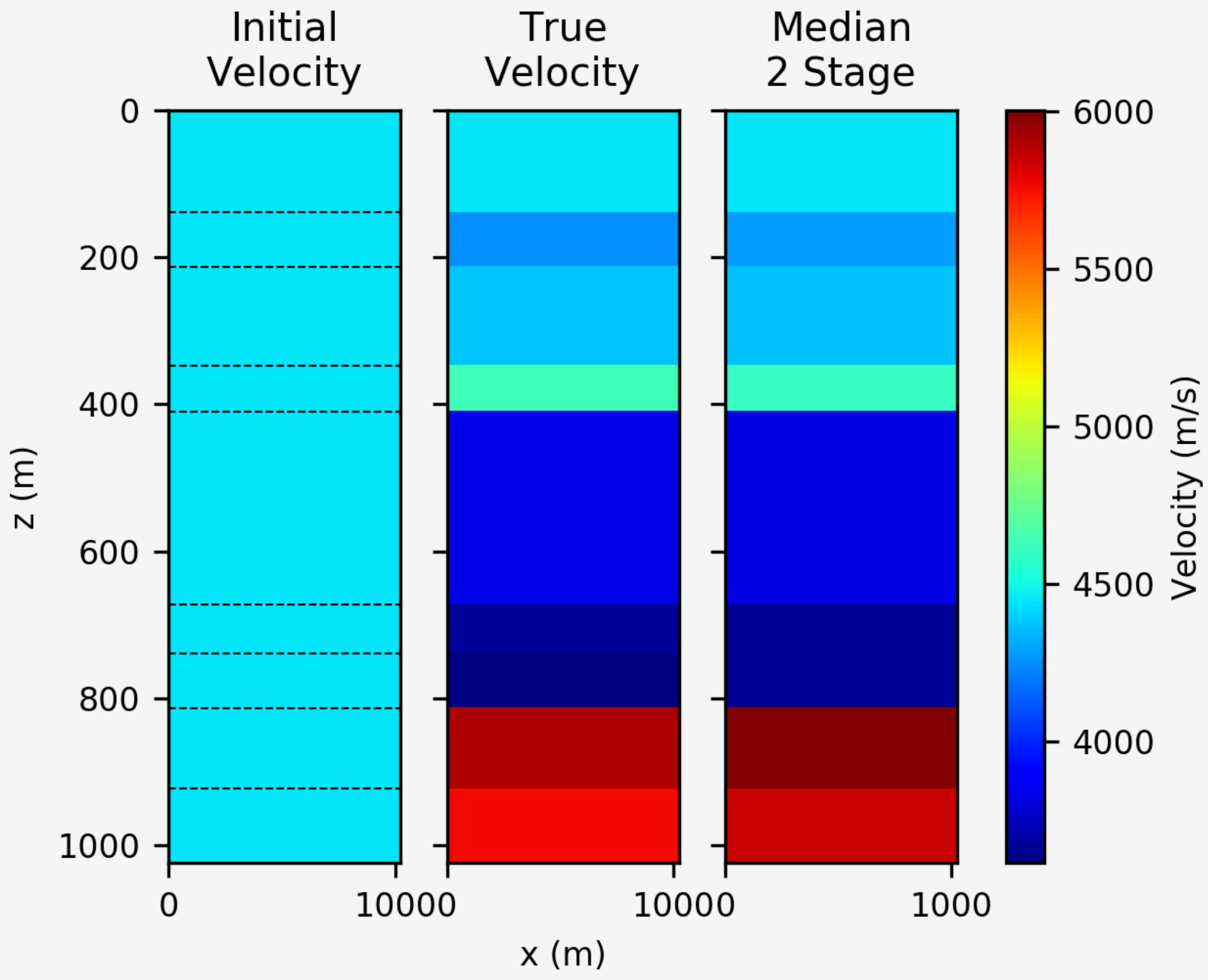


Figure: The fine grid residual norm vs. neural network filter residual norm with continuous learning.

RESULTS: TWO-STAGE MCMC WITH NEURAL NET



- All timings include generating the training set and training the neural network.
- Acceptance rate increased from 29% to 86%.
- Time-per-trial decreased by 65%.
- Time-per-rejection decreased by 84%.

Figure: The initial, true, and median velocity fields for the neural net two-stage MCMC experiment. The dashed lines in the initial velocity field mark the positions of pre-set interfaces.

RESULTS: TWO-STAGE MCMC WITH NEURAL NET

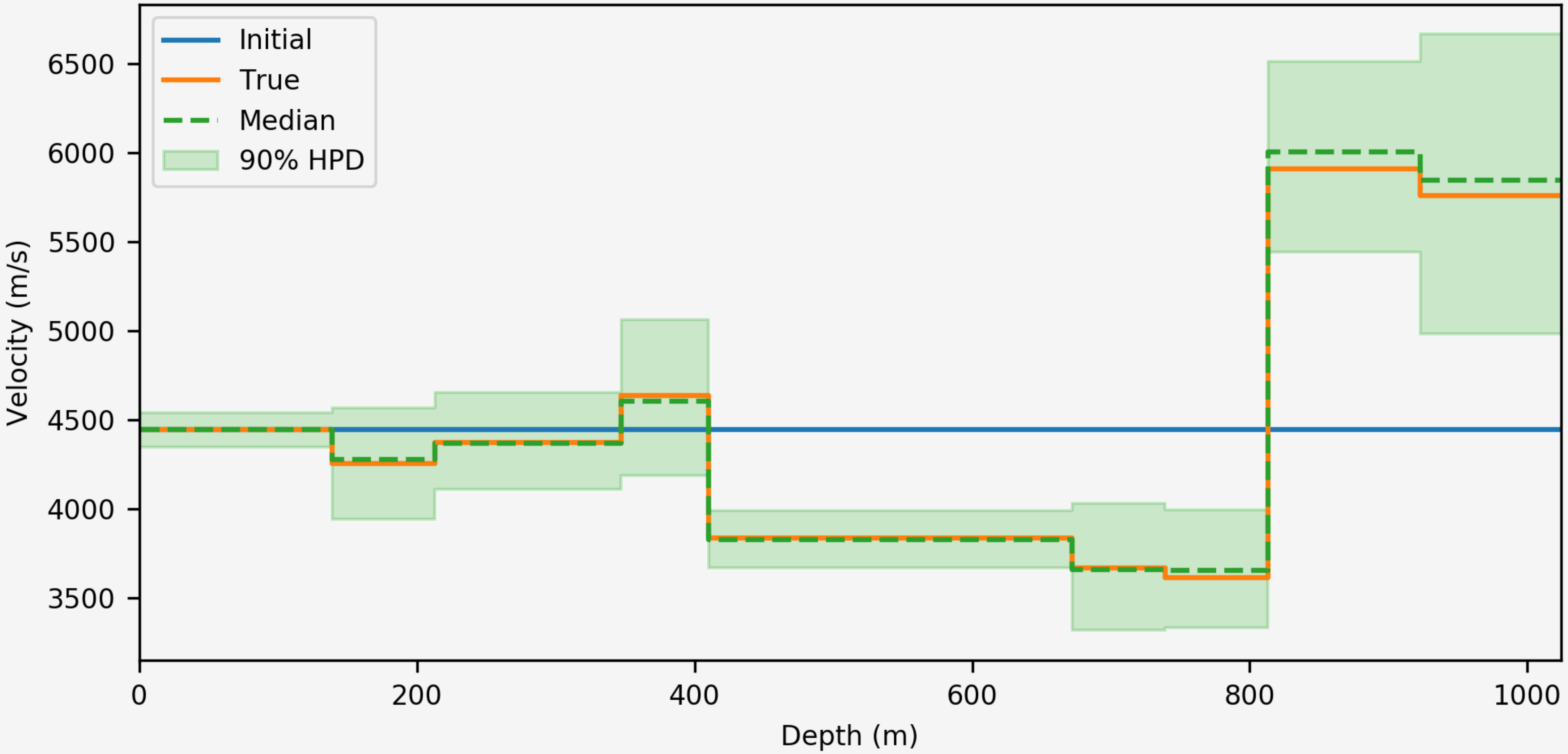


Figure: A vertical slice of the initial (blue), true (orange), and median (green dashed) velocity fields. With 90% highest posterior density intervals.

TROUBLE: THE RANDOM WALK SAMPLER

- In theory, MCMC will converge to the target distribution.
- In practice, methods based on random walk sampling (RWS) can handle a limited number of unknowns ($<$ 100 in our experience)
- RWS produces samples that are highly correlated.[1]

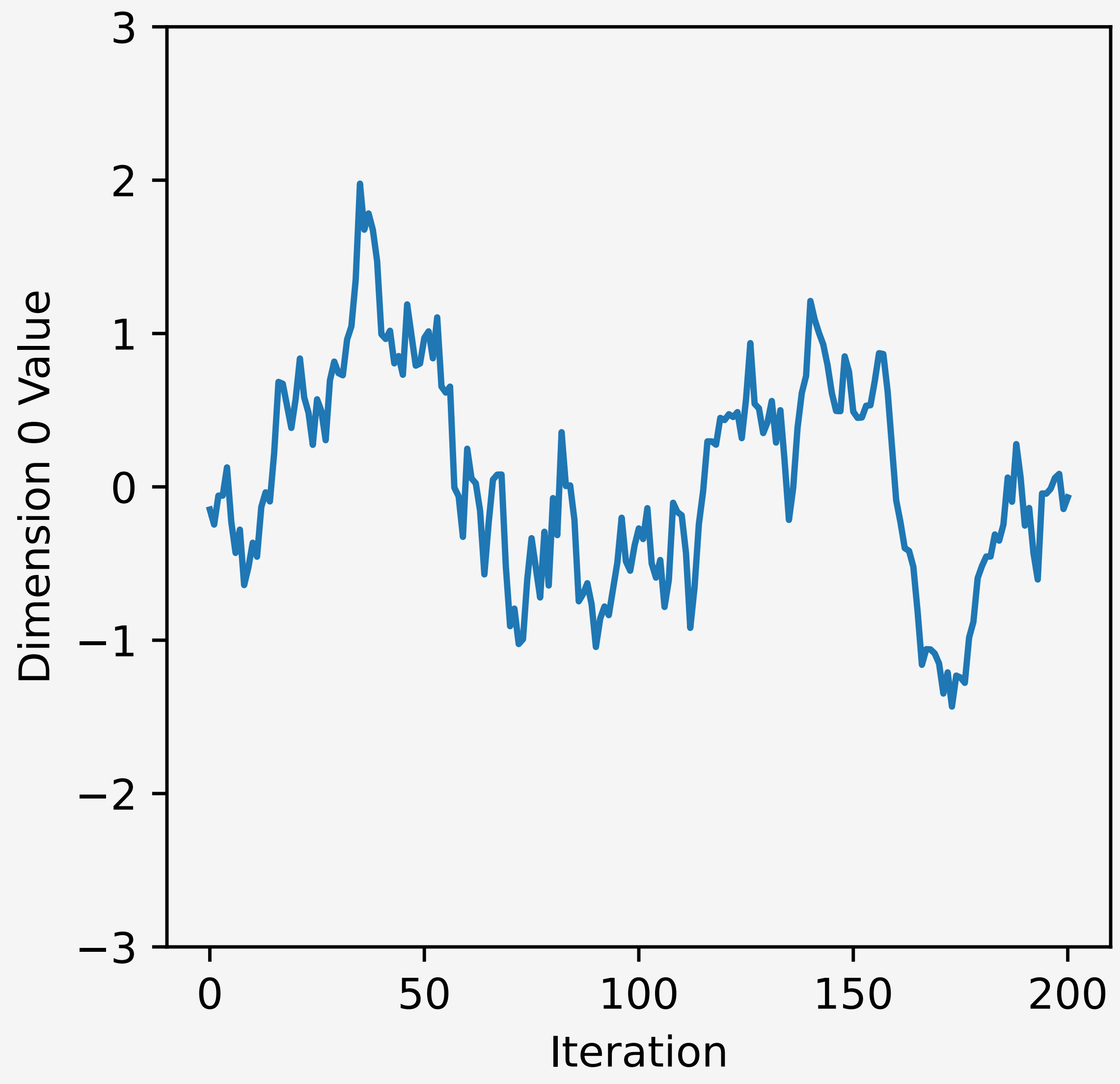


Figure: A view of one dimension of a 100-dimensional Gaussian sampled with Metropolis-Hastings MCMC.

(1) Neal (2011)

THE RANDOM WALK SAMPLER PRACTICALLY LIMITS THE NUMBER OF UNKNOWNS WE CAN USE

HAMILTONIAN MONTE CARLO (HMC)

- HMC uses Hamiltonian Mechanics and gradient information of the posterior distribution to draw samples that are less correlated.

- This results in an algorithm that can handle higher dimensions and converges in fewer samples.

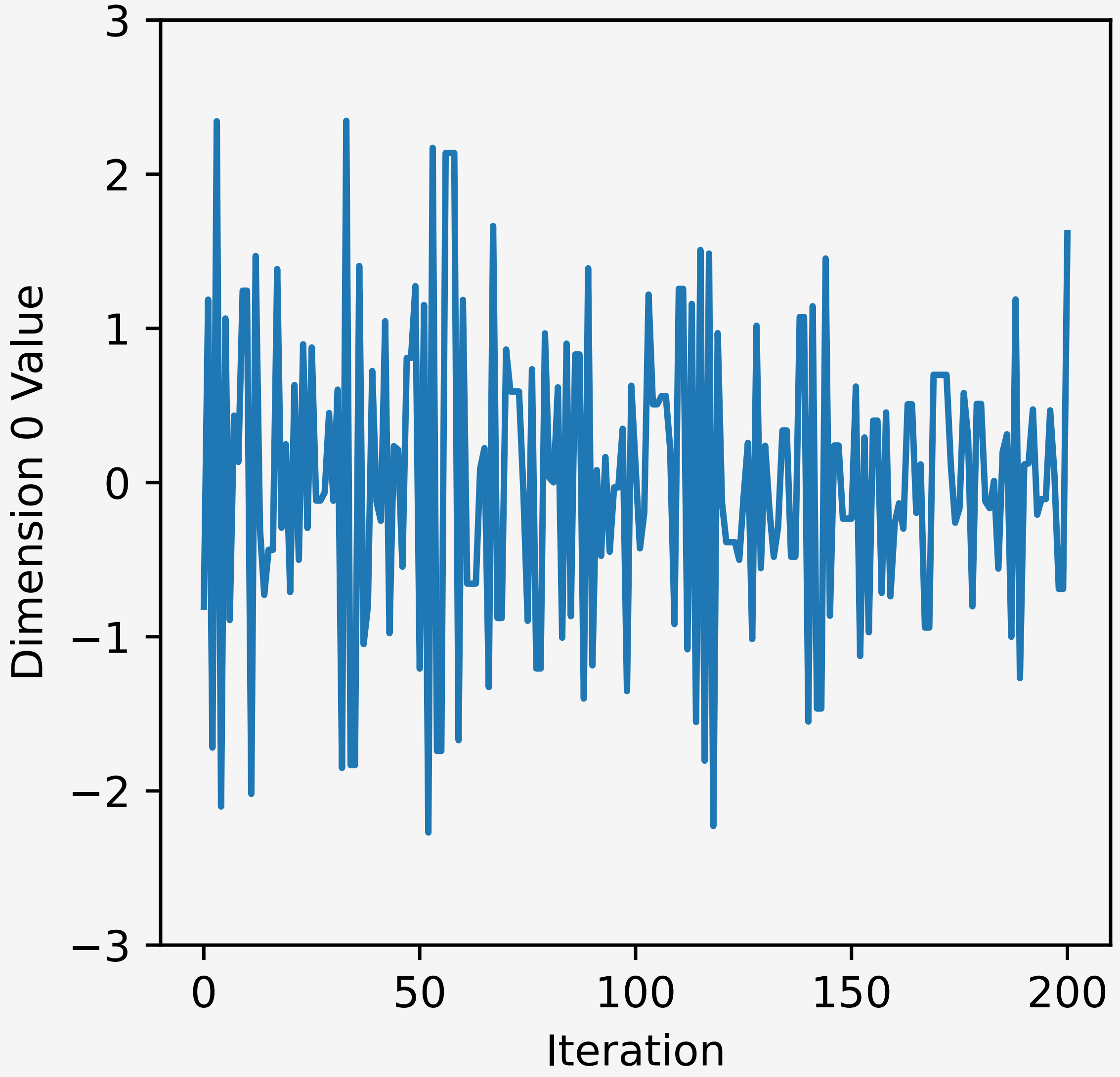


Figure: A view of one dimension of a 100-dimensional Gaussian sampled with HMC.

THE HAMILTONIAN

Potential Energy

Kinetic Energy

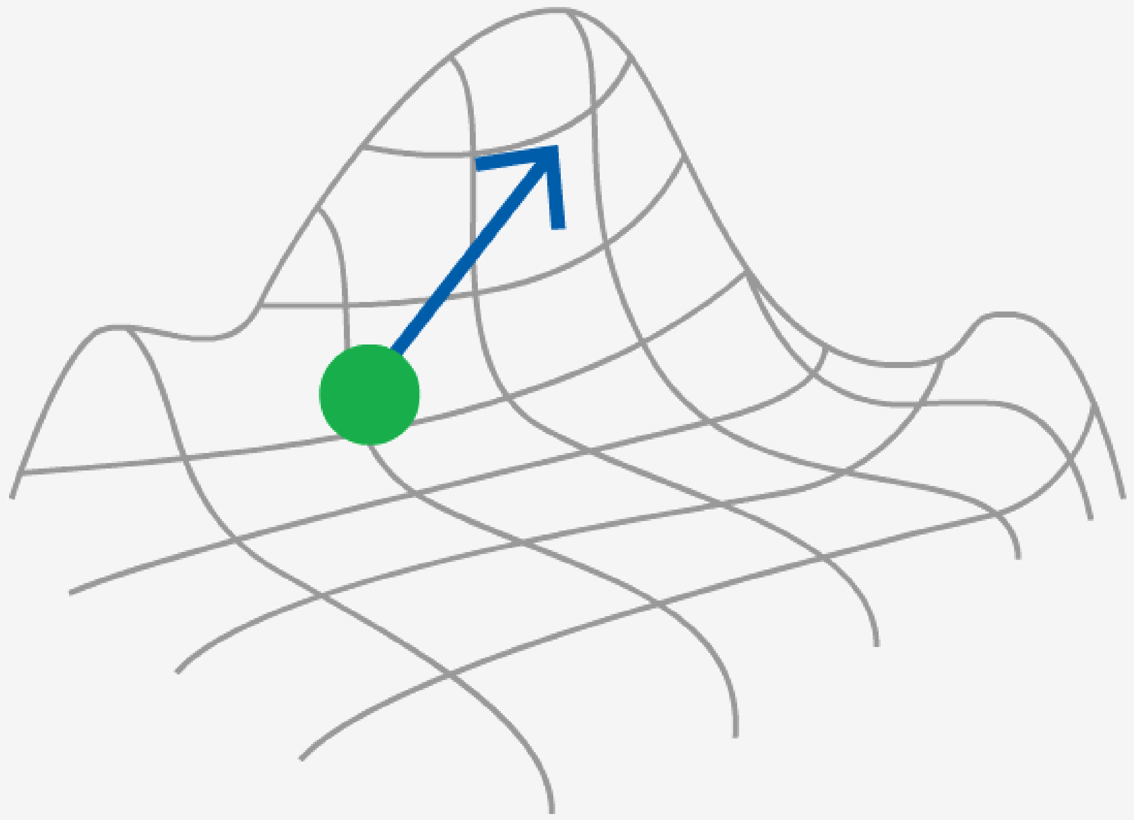
$$H(q, p) = U(q) + K(p)$$

Hamiltonian

Position

Momentum

HAMILTON'S EQUATIONS



HAMILTON'S EQUATIONS AND THE POSTERIOR DISTRIBUTION

- The posterior distribution is embedded in the potential energy by way of the canonical distribution.

$$U(q) = -\log[\pi(q|D)] = -\log[\pi(q)\pi(D|q)]$$

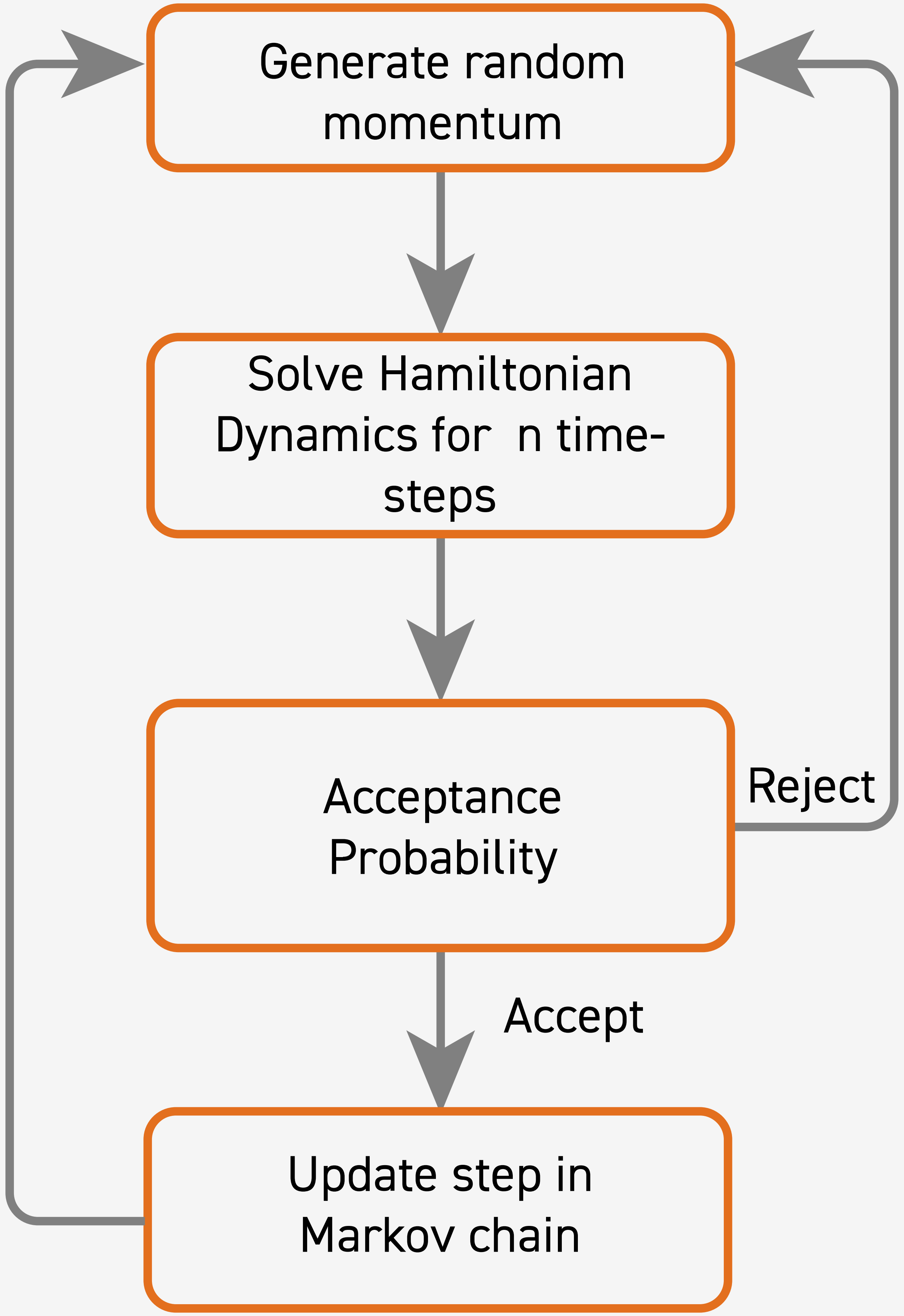
  where $\pi(q|D)$ is the posterior distribution, $\pi(q)$ is the prior distribution, and $\pi(D|q)$ is the likelihood function.

- For Hamilton's equations, we need to take the gradient of the log likelihood.

$$-\nabla \log[\pi(D|q)] = \nabla \frac{\|F(q) - D\|^2}{2\sigma^2}$$

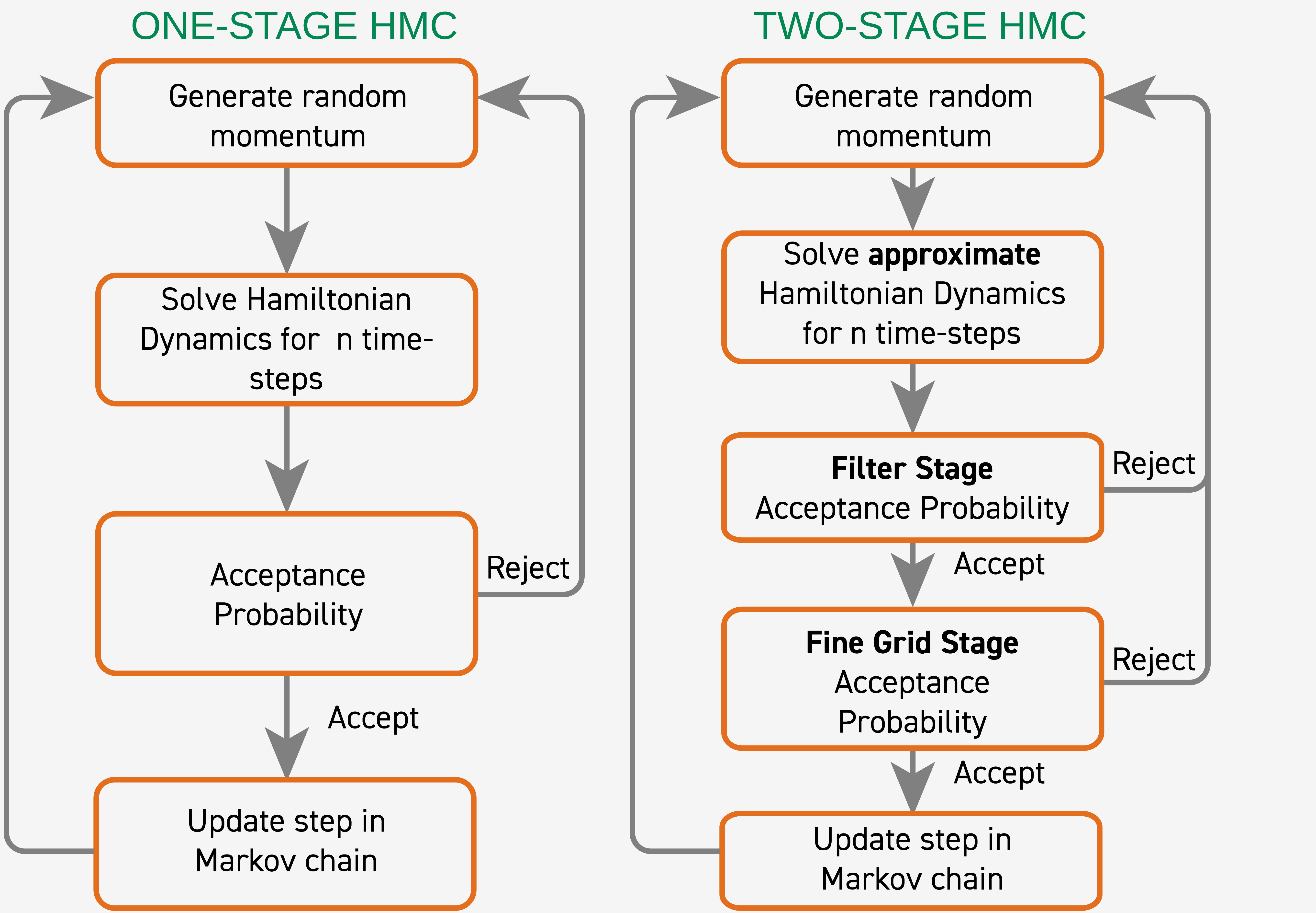
THE LEAPFROG DISCRETIZATION

HMC DEMO AND FLOWCHART

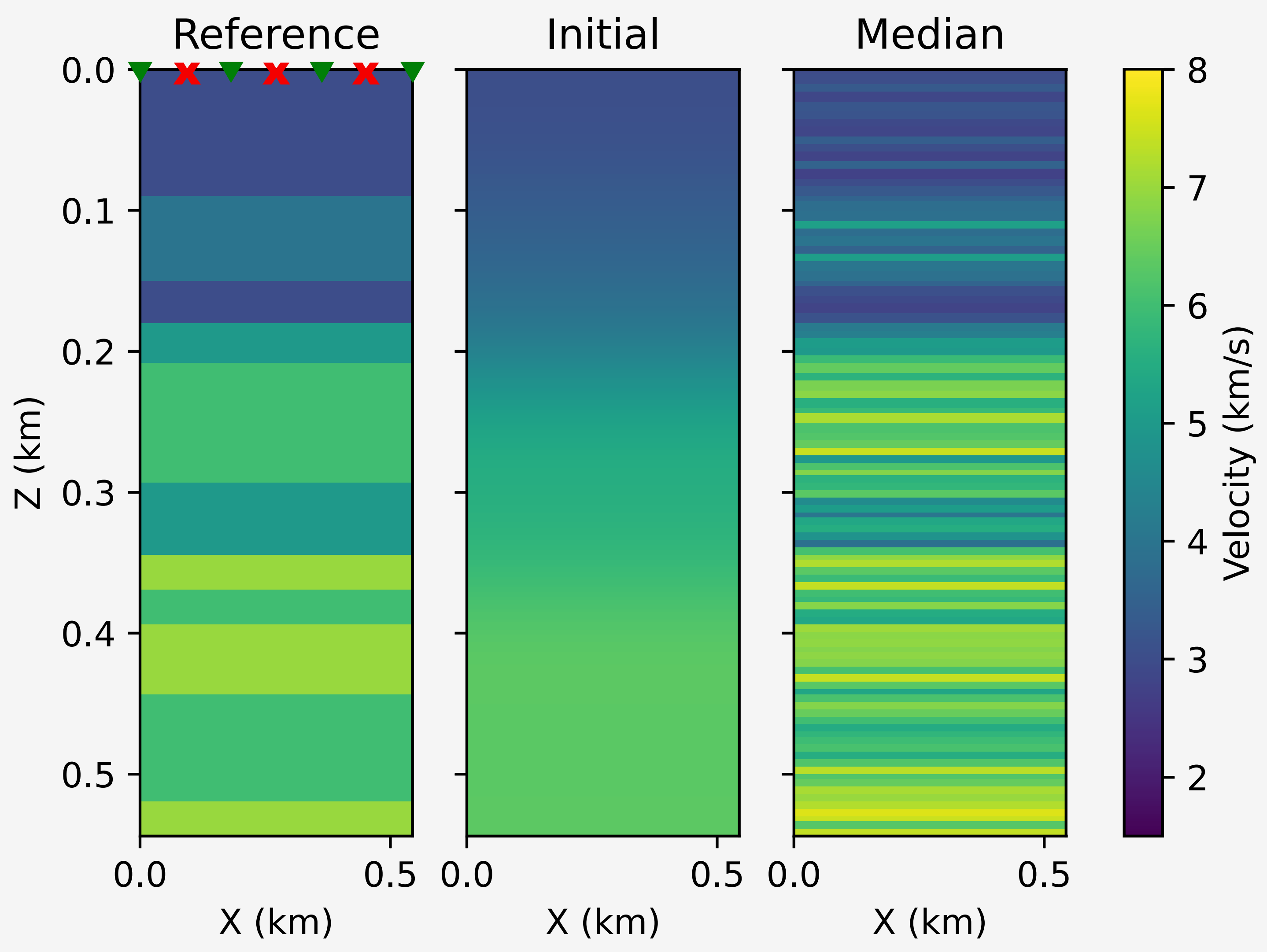


HAMILTONAIN MONTE CARLO REQUIRES NUMEROUS EXPENSIVE GRADIENT CALCULATIONS TO PRODUCE EACH SAMPLE.

TWO-STAGE HMC



RESULTS: NNHMC



- All timings include generating the training set and training the neural network.
- Time-per-trial decreased by 85%.

Figure: The initial (left), true (middle), and median (right) velocity fields for the 100-unknown neural net two-stage HMC experiment. On the left image, red x's represent a line of sources and green triangles represent a line of receivers.

RESULTS: NNHMC

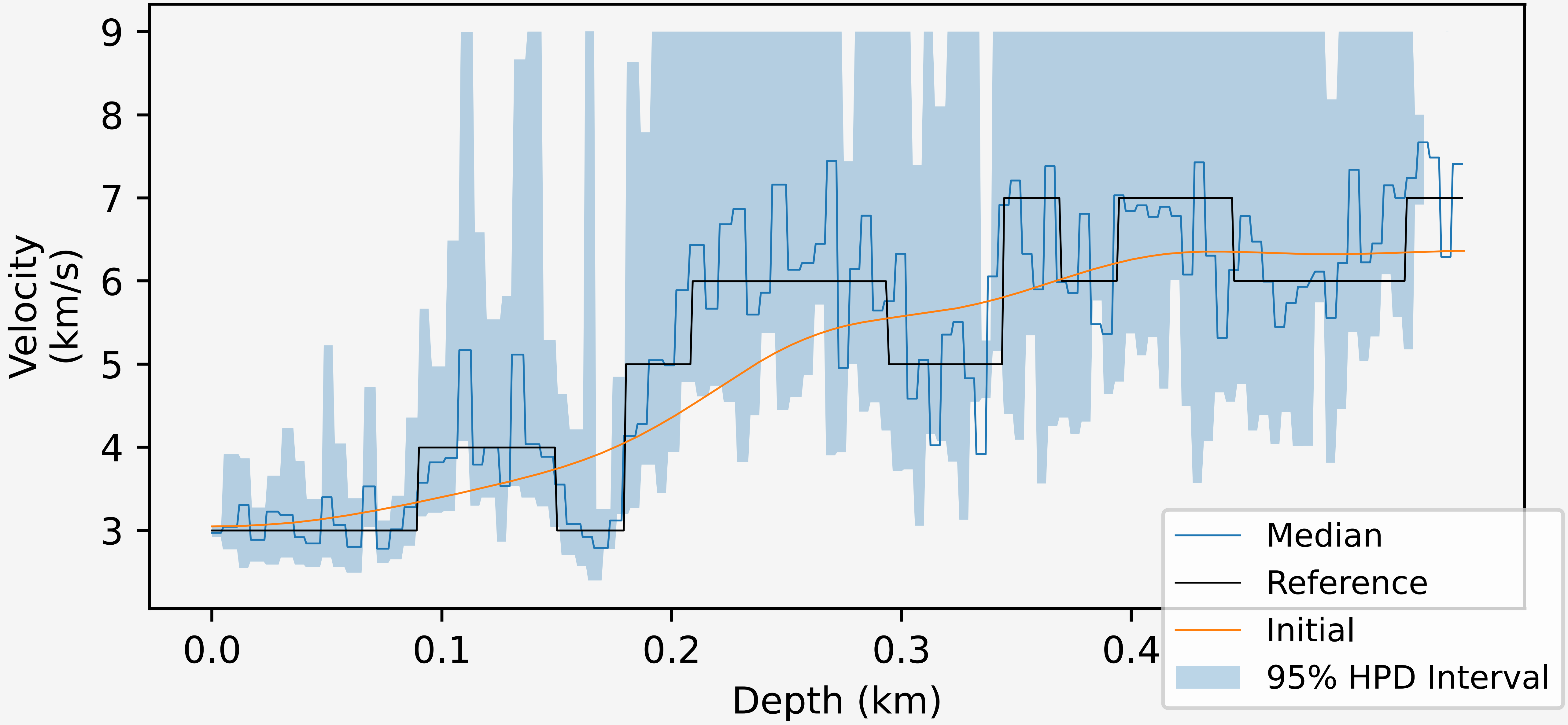


Figure: A one-dimensional slice of the median (blue), reference (black), and initial (orange) velocity fields, with 95% HPD interval shown with blue shading.

RESULTS: NNHMC

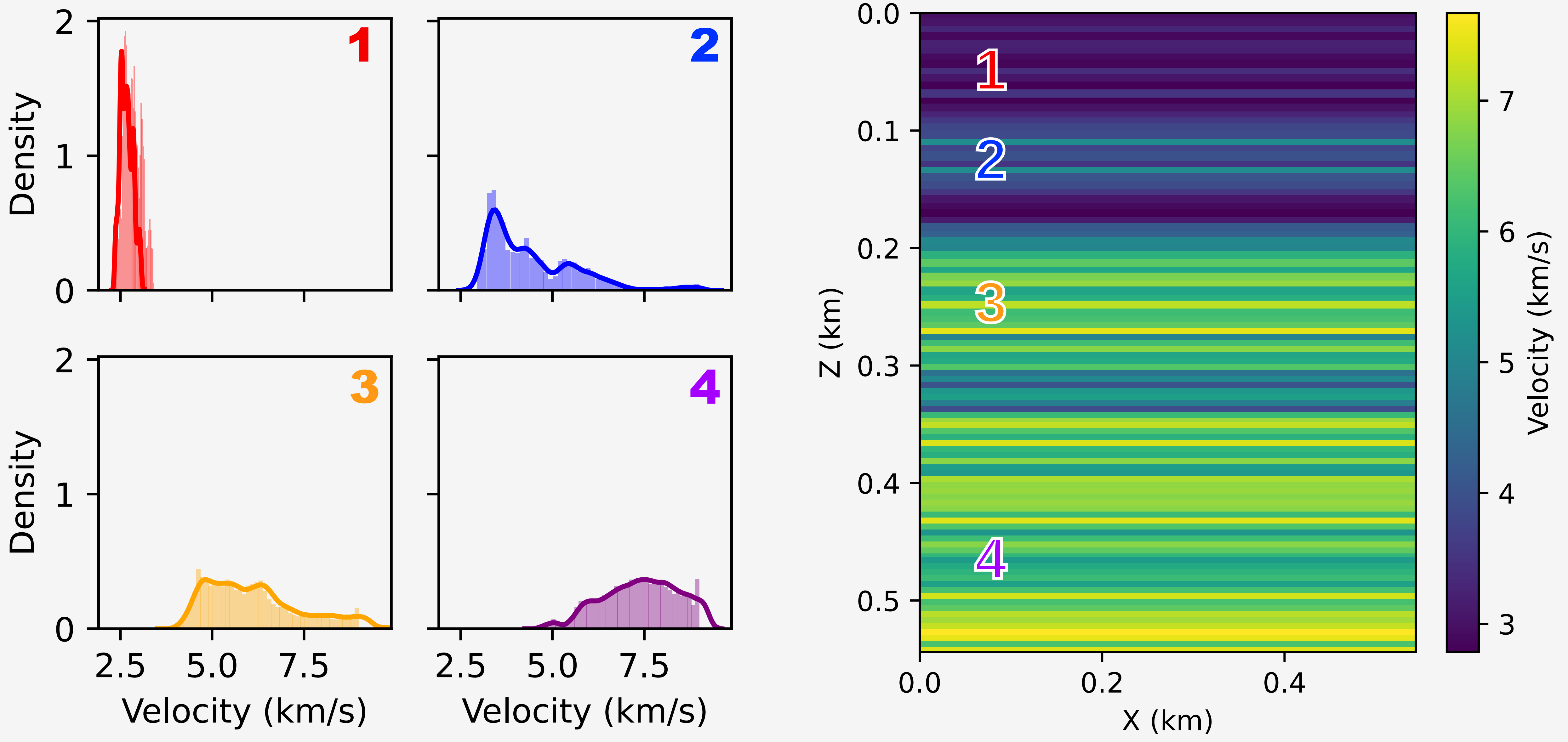
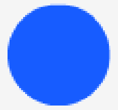


Figure: Four representative posterior distributions (left) from the marked locations (right).

HMC REQUIRES USER-SPECIFIED PARAMETERS TO DISCRETIZE THE HAMILTONIAN DYNAMICS

THE NO-U-TURN SAMPLER (NUTS)

- The No-U-Turn Sampler (NUTS) modifies HMC to have an adaptive trajectory length L.
- Eliminates costly tuning runs for the trajectory length in the leapfrog algorithm.
- From the starting point (blue dot), we we randomly select a forward trajectory (yellow dot) or a backward trajectory (green dots).
- The number of leapfrog steps doubles with each recursive NUTS iteration.



NUMERICAL EXPERIMENT: NUTS

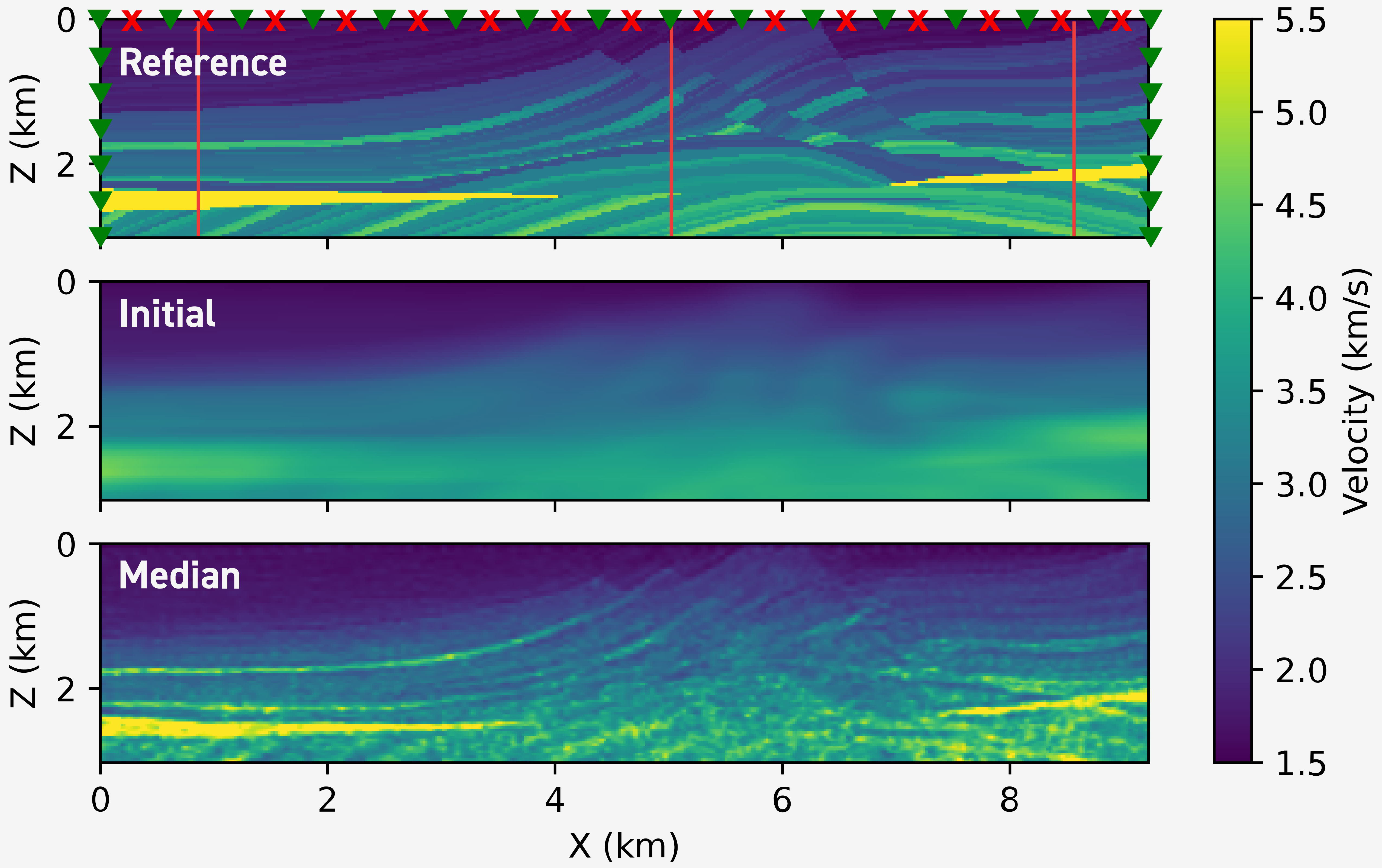


Figure: Top: the reference velocity field with markings for sources (red X's) and receivers (green triangles) and red lines to mark the location of the vertical slices (next slide). Middle: The initial velocity field. Bottom: the median velocity field.

NUMERICAL EXPERIMENT: NUTS

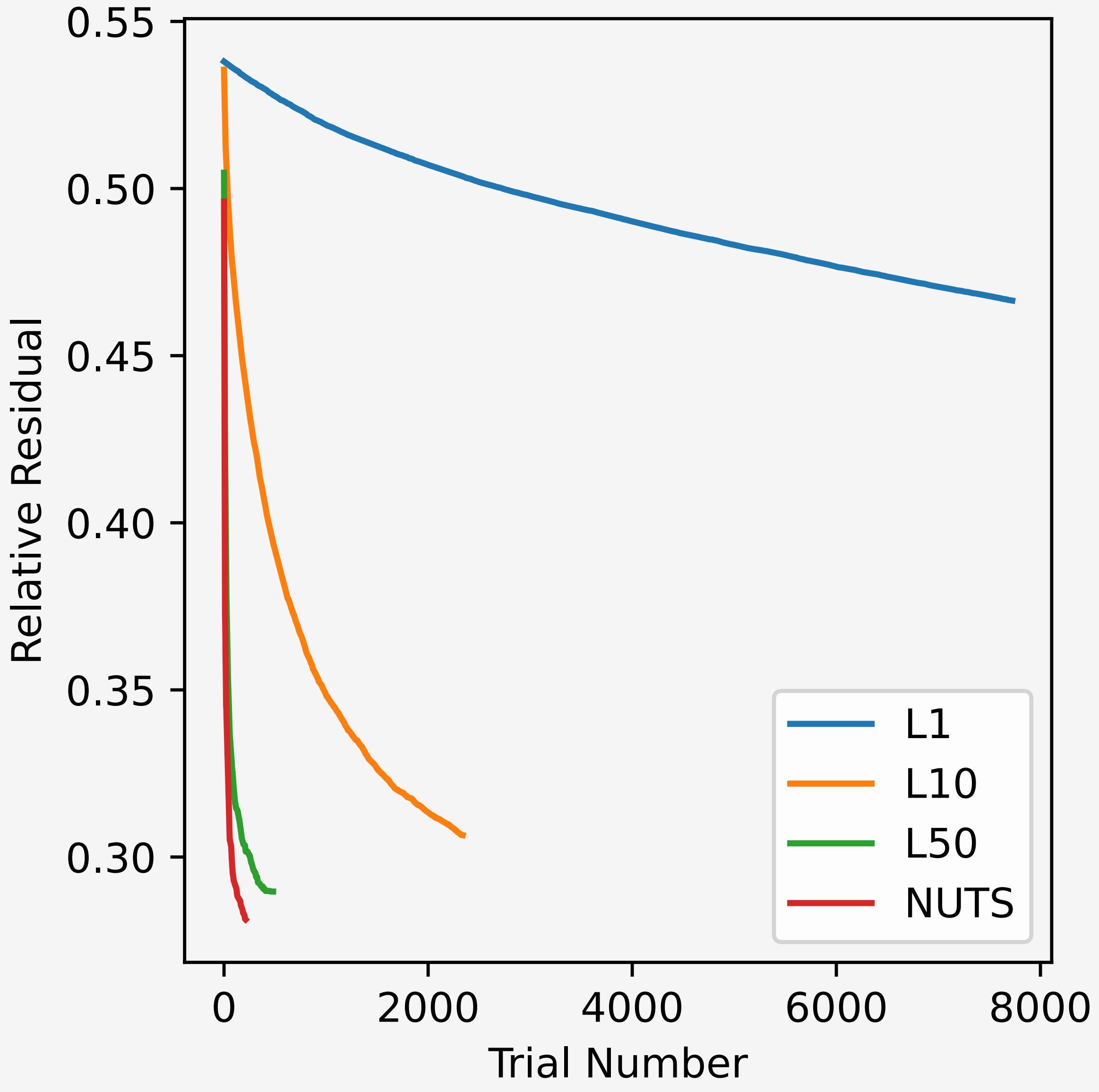


Figure: Relative residual plots for leapfrog step number 1 (blue), 10 (orange), 50 (green), and the NUTS algorithm (red).

- We find that the NUTS algorithm results in superior residual decrease while maintaining a high acceptance rate.

Leapfrog Steps	**Acceptance Rate**
1	0.72
10	0.66
50	0.35
NUTS	0.98

NUMERICAL EXPERIMENT: NUTS

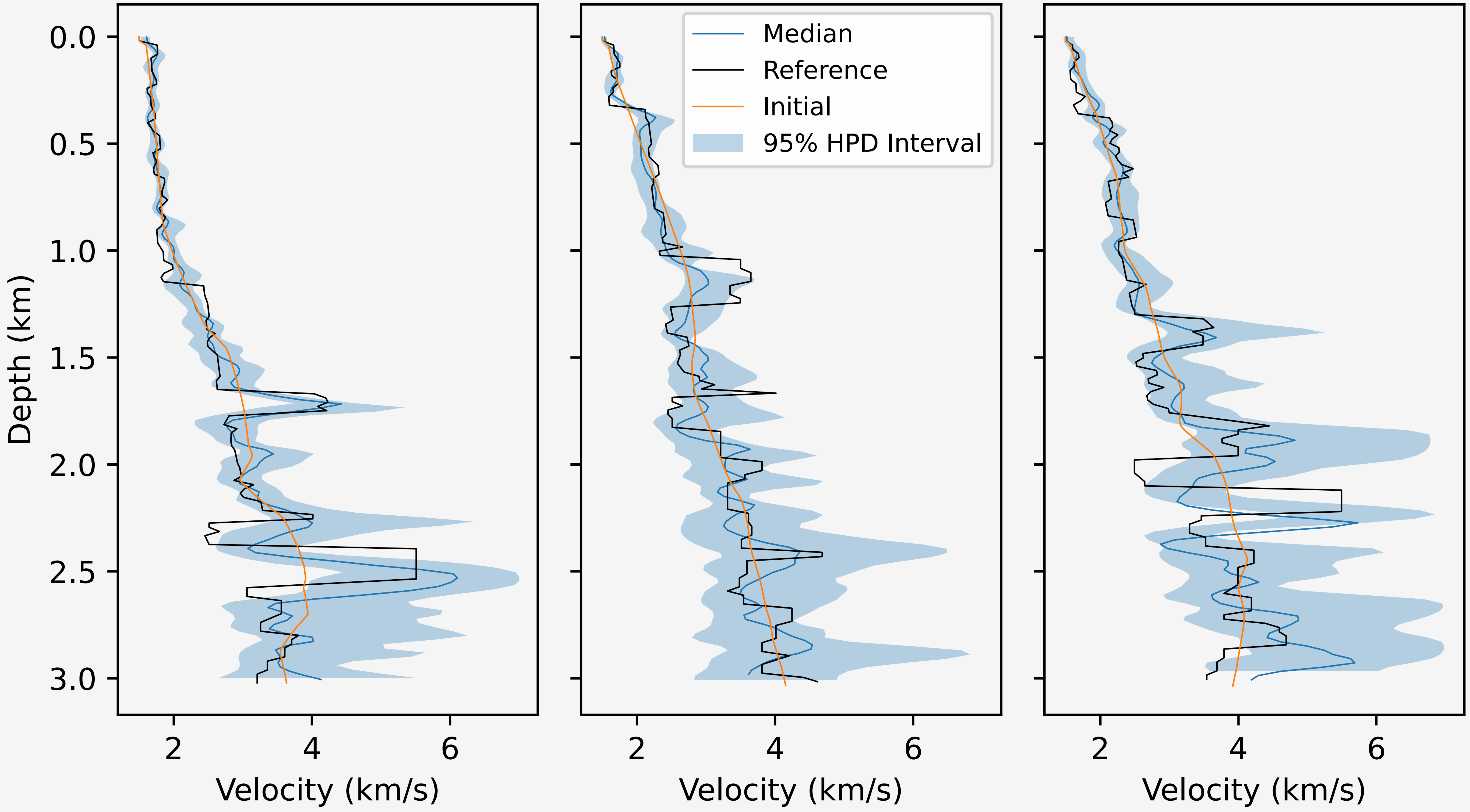


Figure: Vertical slices of the median (blue), reference (black), and initial (orange) velocity fields at locations shown on the previous slide. The blue shaded region marks the 95% HPD intervals

NUMERICAL EXPERIMENT: NUTS

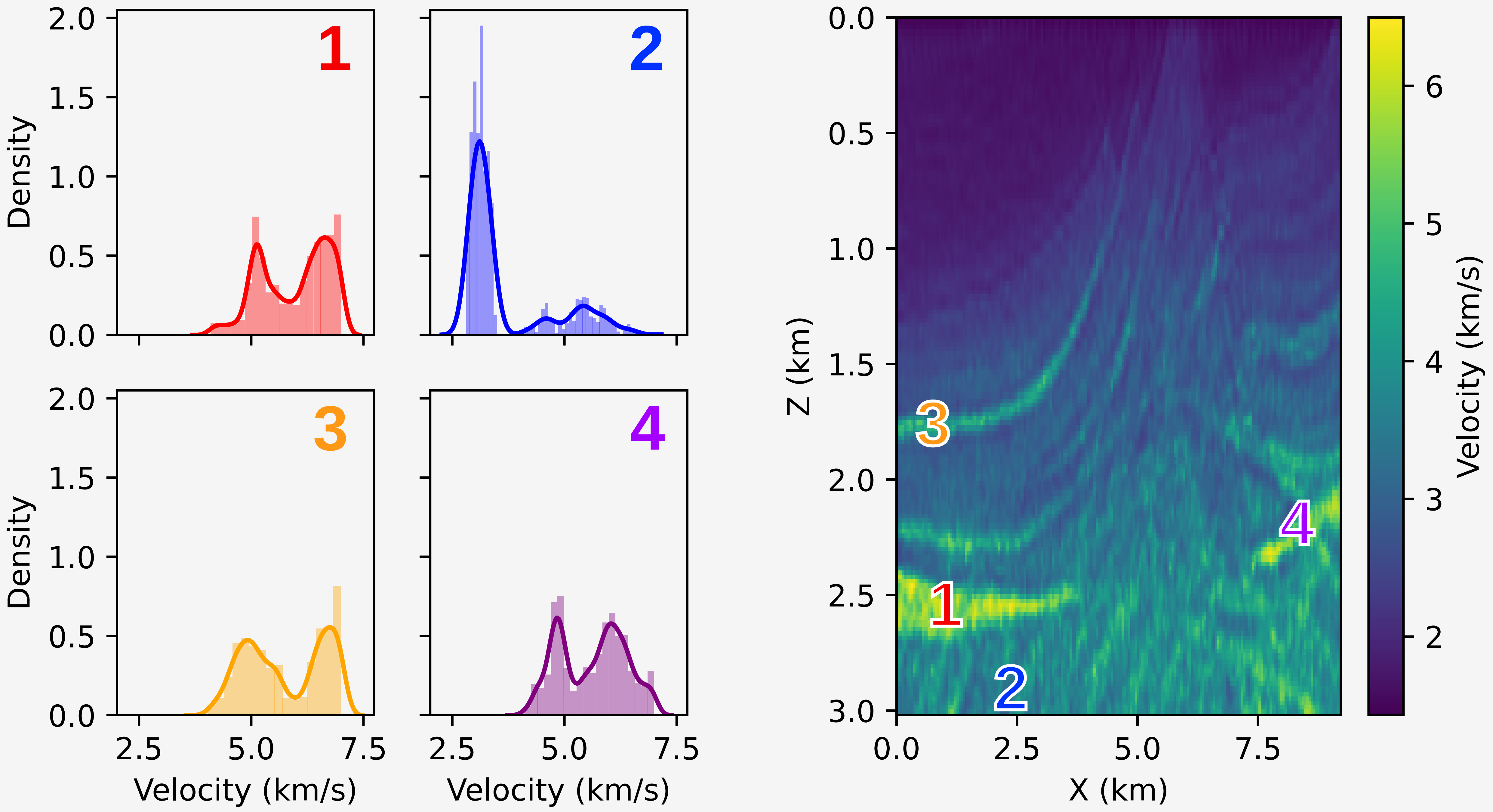


Figure: Four representative posterior distributions (left) at the marked locations shown on the right figure.

CONCLUSIONS

- Two-stage MCMC and HMC is an effective way to quickly reject unacceptable samples and to reduce runtime of the expensive MCMC and HMC procedures.

- Operator upscaling is a highly accurate surrogate that closely replicates the fine-grid receiver data.

- A neural net is an extremely inexpensive surrogate that can do a good job of approximating the exponent of the likelihood function and the likelihood gradient.

- Neural-Net Enhanced HMC reduces the run-time of the HMC algorithm by over 80% for our experiment.

- The No-U-Turn sampler optimizes the leapfrog trajectory length for HMC.

FUTURE WORK

- We recently extended the two-stage HMC framework to the NUTS algorithm.
- Currently in progress: a paper on neural-network enhanced two-stage HMC and NUTS.
- NNHMC/NNNUTS on larger-scale problems with tens of thousands of unknowns.
- Applying our methods to real data.

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CITATIONS

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