Hamiltonian Monte Carlo methods for uncertainty quantification in waveform inversion

Jinji Li and Kris Innanen

2023/12/08

NSERC CRSNG
UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
Department of Earth, Energy, and Environment

- Motivation
- Hamiltonian dynamics
- Numerical experiments
- Discussion & future work
- Conclusion

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HMC: a step towards affordable and more efficient MC

- Full waveform inversion (FWI): expensive.
- Uncertainty in FWI?
- Monte Carlo (MC) searches the model space, but...
- **HMC**: a guided MC variant.

https://www.youtube.com/watch?v=iXLEfsecGNs

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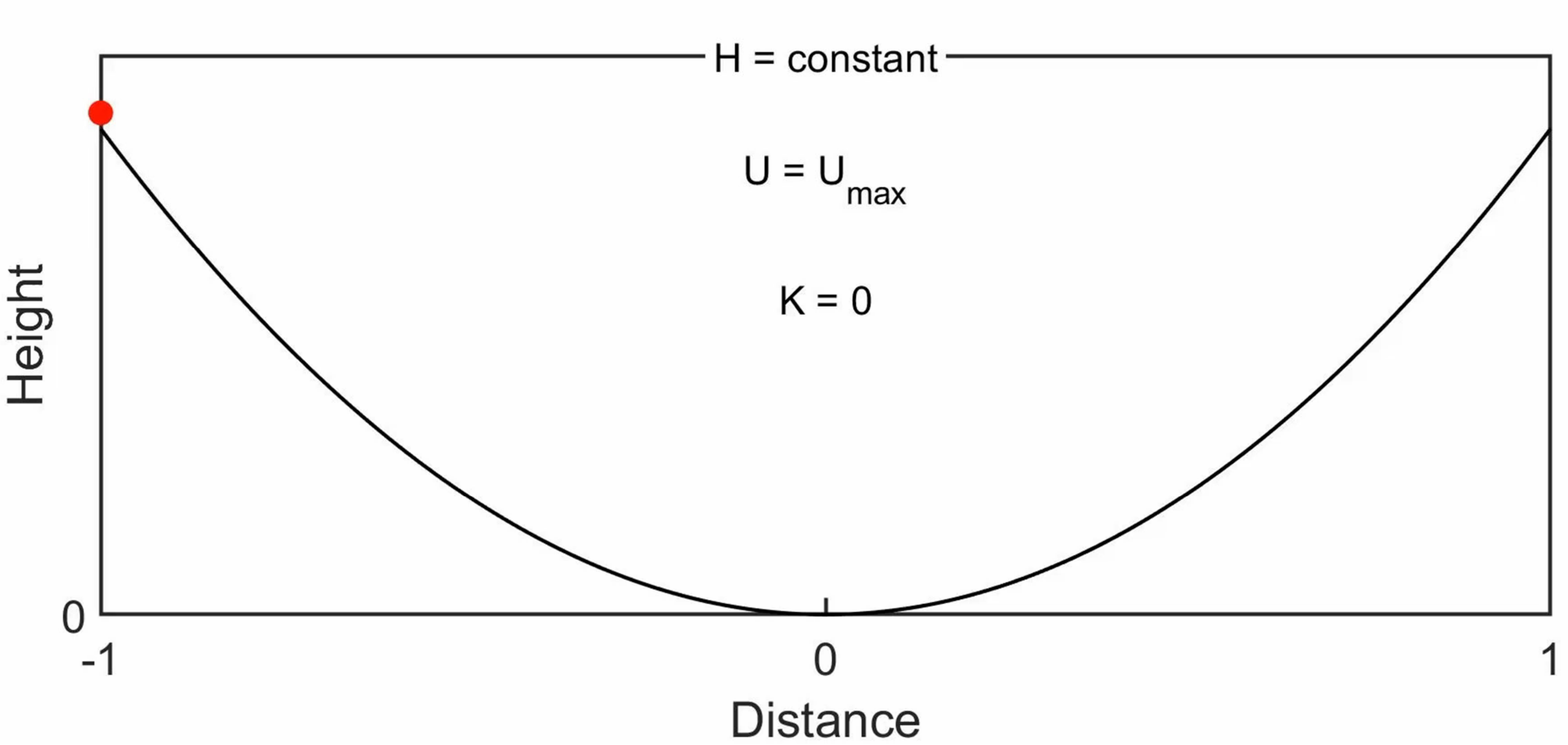
Position and momentum describe the state in Hamiltonian dynamics



U: potential energy

$$U = U(\boldsymbol{q})$$

K: kinetic energy

$$K = {}^{1}\!/_{2}\, \boldsymbol{p}^{T}\mathbf{M}^{-1}\boldsymbol{p}$$

H: total energy

$$H = U + K$$

(Hamilton, 1833)

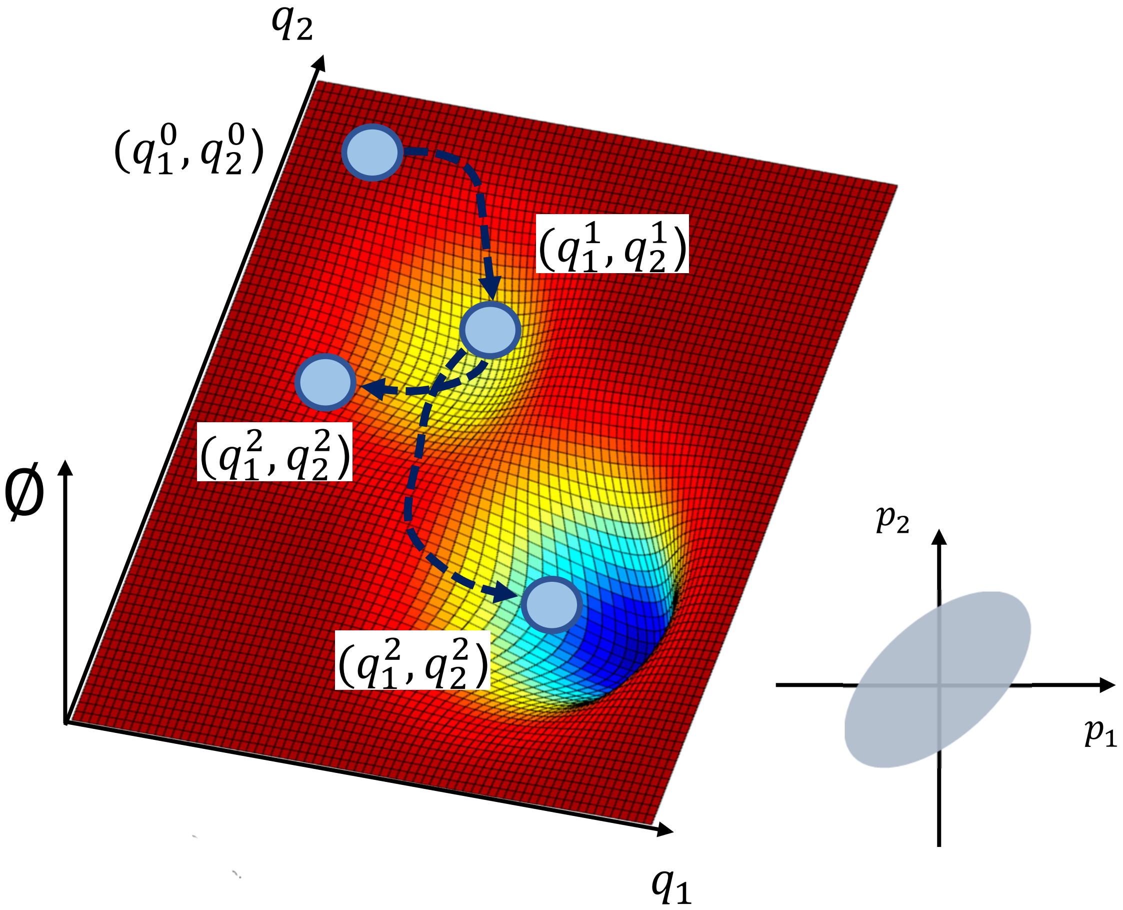
a. Start from somewhere $\boldsymbol{q}_0$.

b. Draw $\boldsymbol{p} \sim \mathcal{N}(0, \mathbf{M})$.

c. Simulate Hamiltonian dynamics for L steps with Δt (leapfrog method, Iserles, 1986).
   - $\Delta t\ \nabla U$ -> $\boldsymbol{p}_{new}$
   - $\Delta t\ \nabla K$ -> $\boldsymbol{q}_{new}$

d. Accept or not (energy)
   - Yes -> $\boldsymbol{q}_1 = \boldsymbol{q}_{new}$
   - No -> $\boldsymbol{q}_1 = \boldsymbol{q}_0$

e. Back to b.



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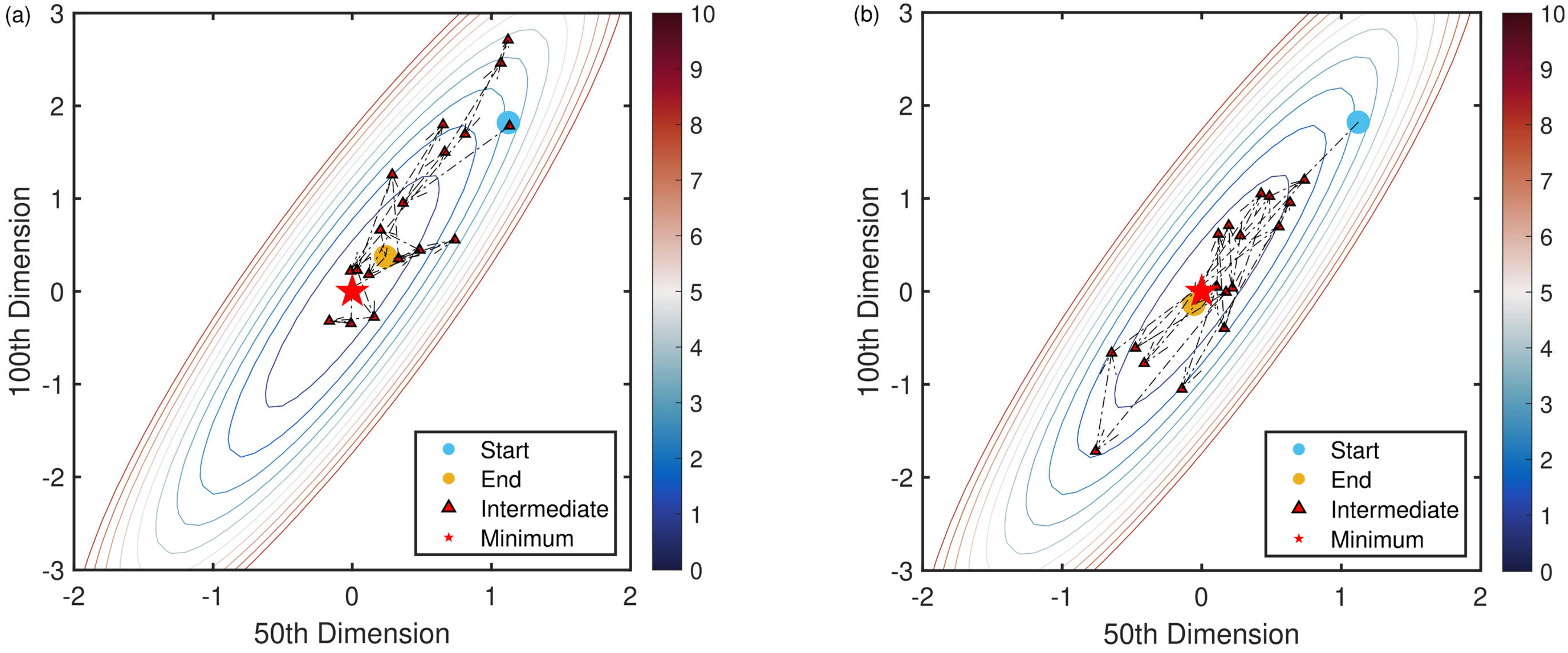
100-D example with 0.45 correlation in the 50th and 100th dimension

$$U(\boldsymbol{m}) = \frac{1}{2}\boldsymbol{m}^T C_M^{-1}\boldsymbol{m} \qquad C_M = \begin{bmatrix} 0.01^2 & 0 & \cdots & 0 \\ 0 & 0.02^2 & 0 & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & 1^2 \end{bmatrix}$$

- 0.45 correlation in the 50th and 100th dimensions
- MCMC: 1.5e+5
- HMC: 1e+3 samples, with $L = 150$, and $\Delta t \sim \mathcal{U}(0.0104, 0.0156)$ (Brooks et al., 2011)
- **Not a fair game!**

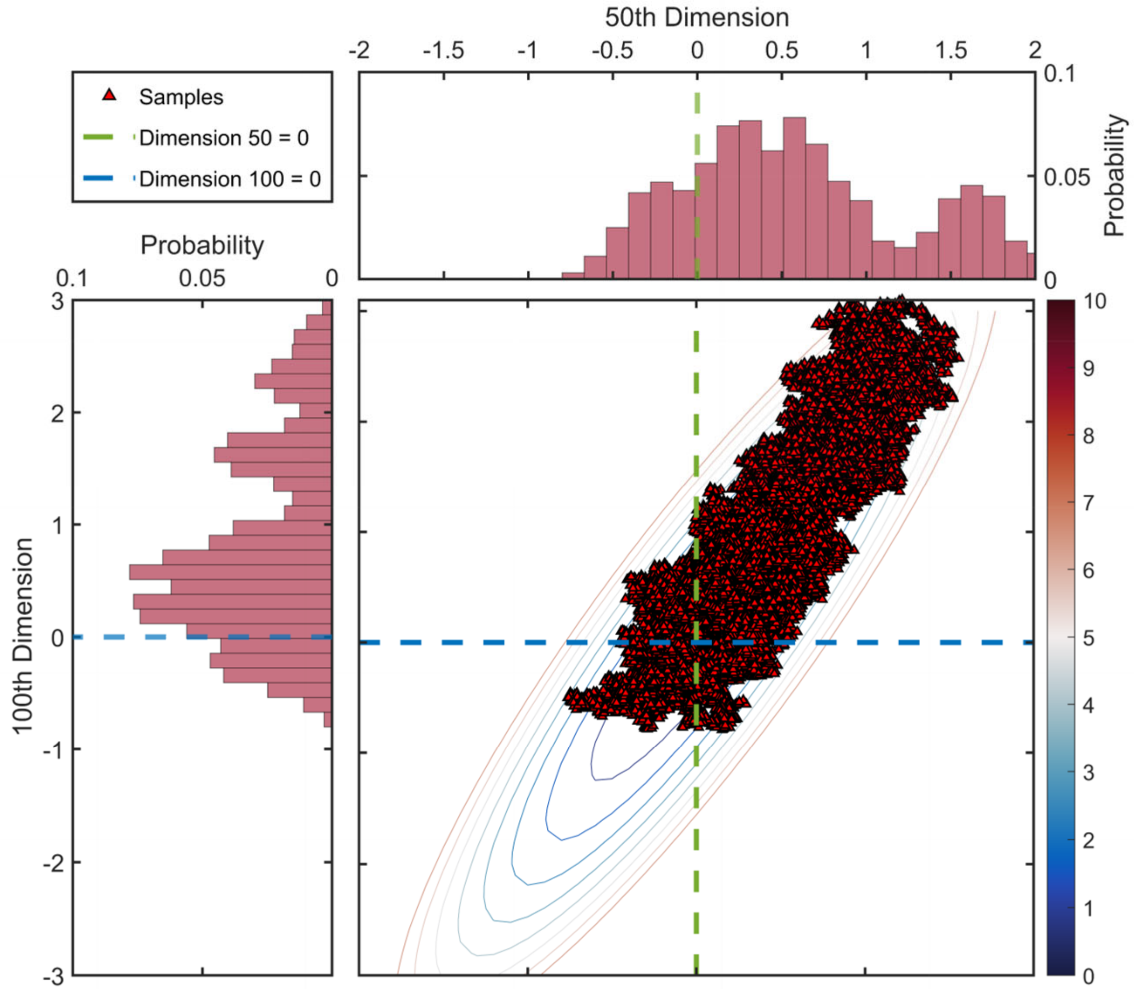
Initial 20 walks show that HMC takes larger steps



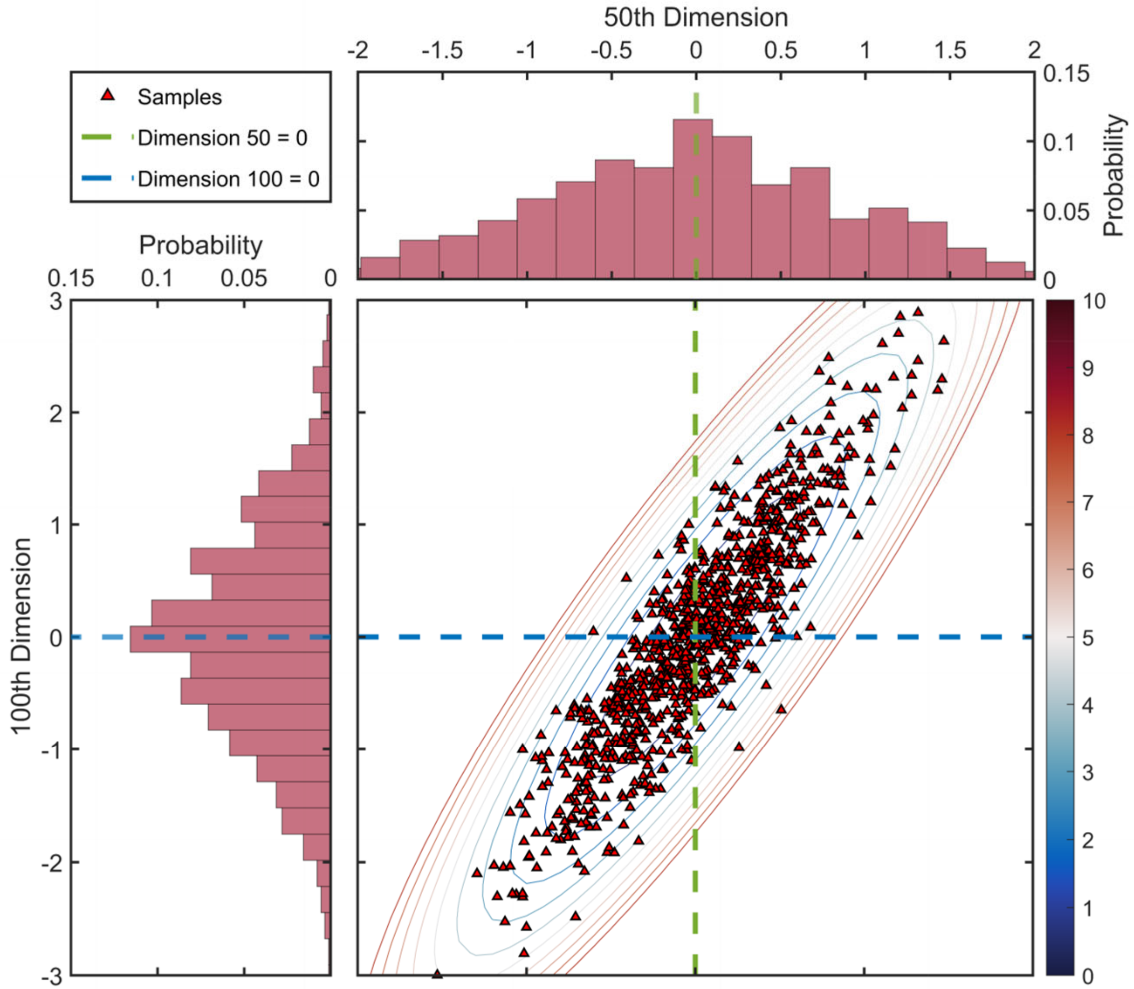
MCMC

HMC

HMC gives more plausible marginal distributions



MCMC



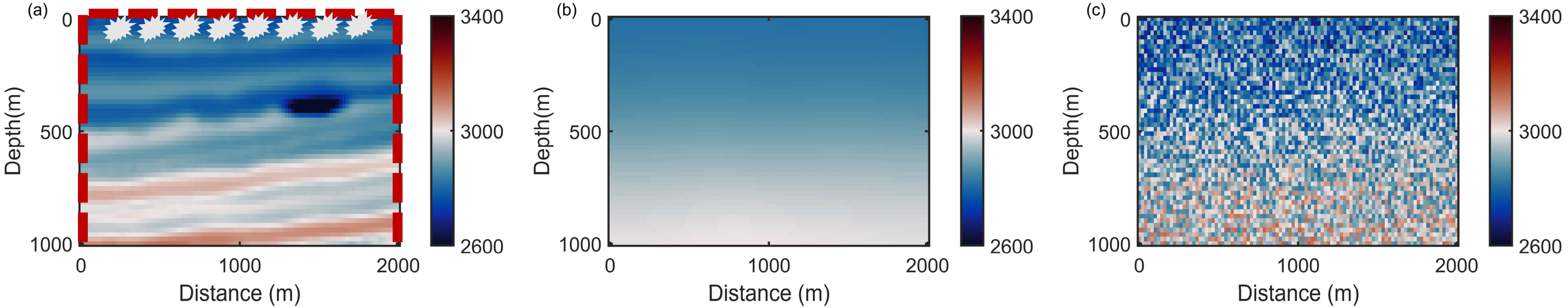
HMC

HMC-FWI test on acoustic model

$$U(\boldsymbol{m}) = \frac{1}{2}\left(\boldsymbol{d}_{syn} - \boldsymbol{d}_{obs}\right)^T C_D^{-1}\left(\boldsymbol{d}_{syn} - \boldsymbol{d}_{obs}\right)$$

N samples: 30,000

Adaptive tuning: Li and Innanen (2023)



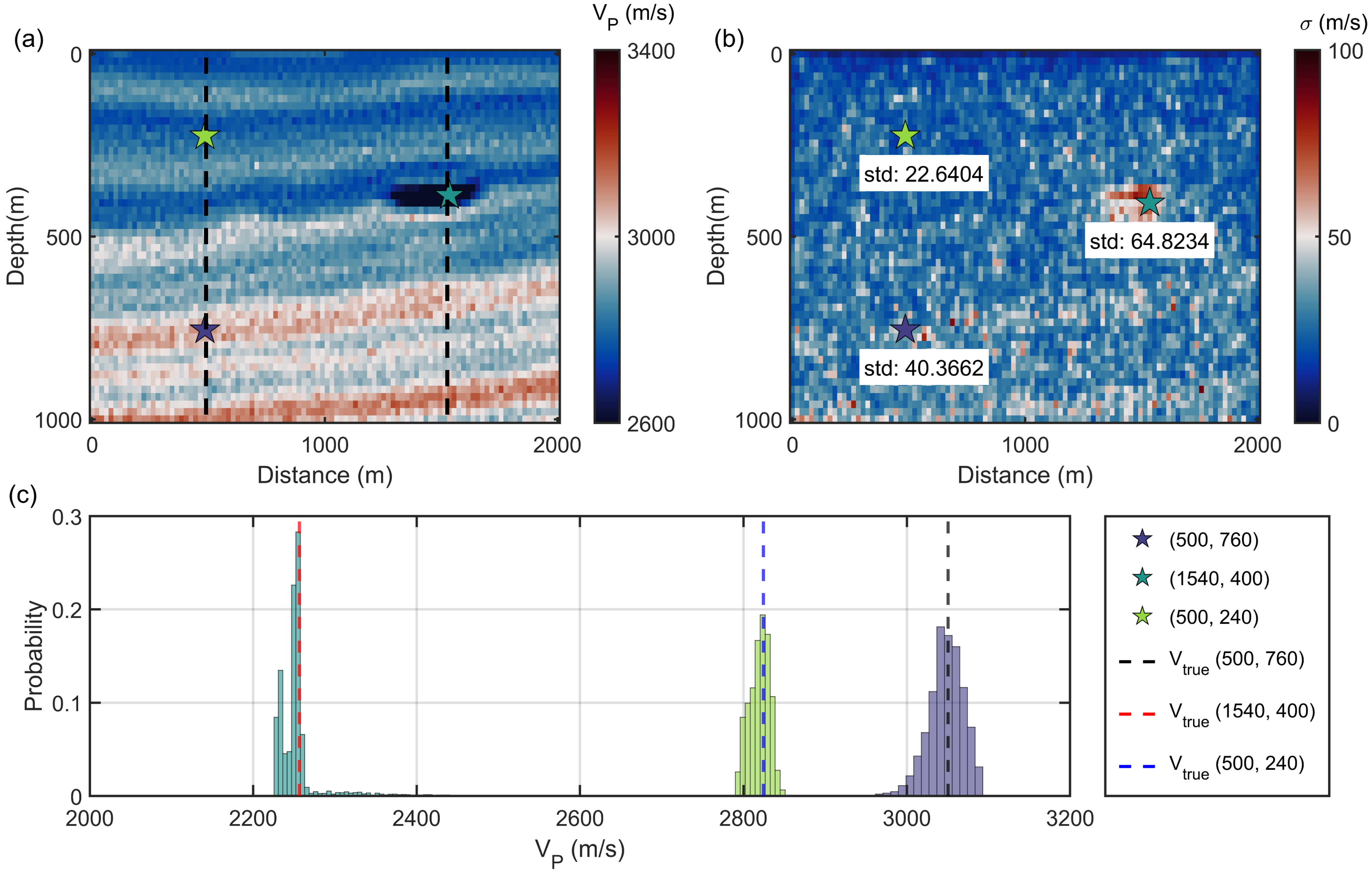
True model

Smoothed model

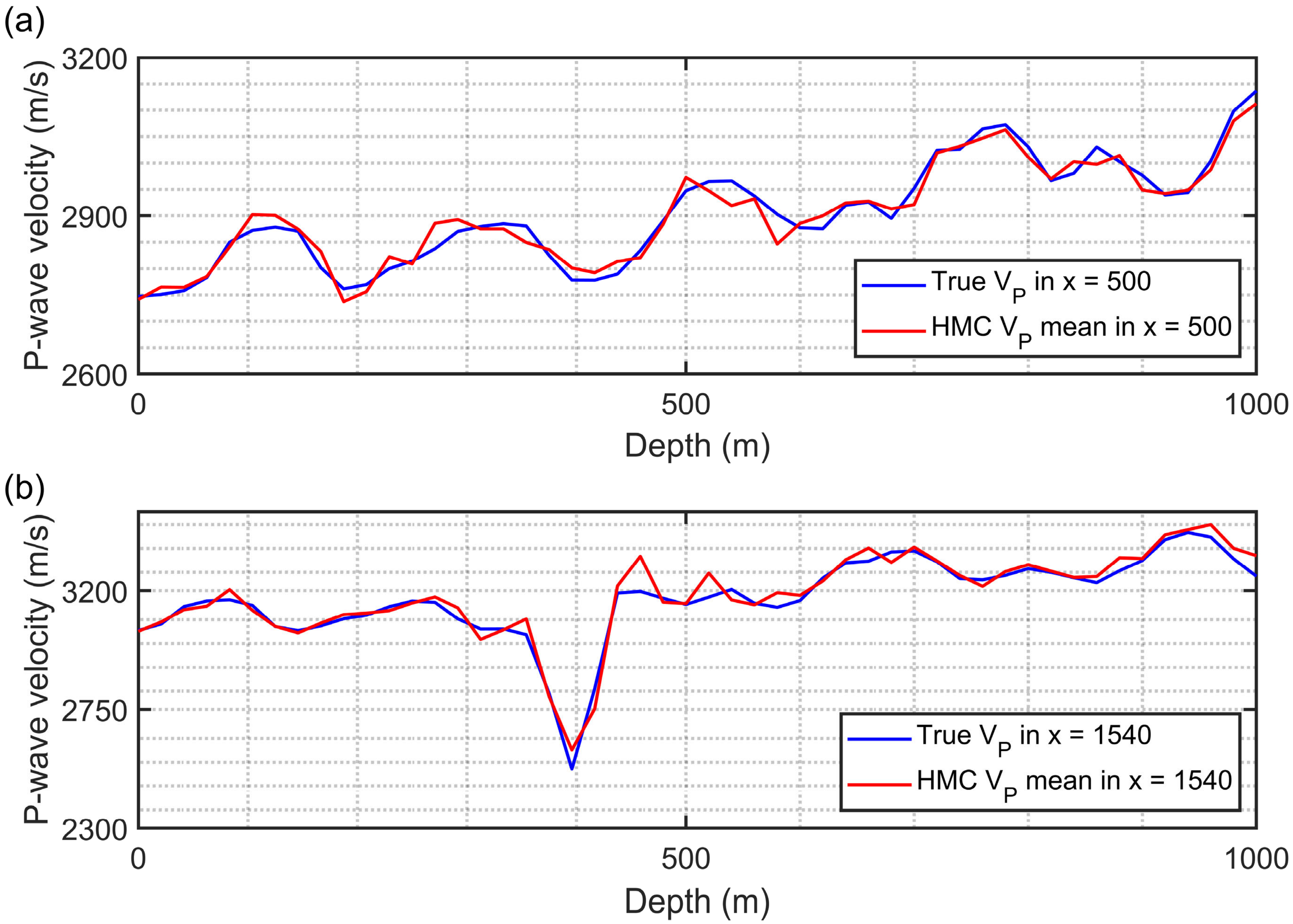
Actual initial model

$U(\boldsymbol{m}_{smooth} \pm 150)$

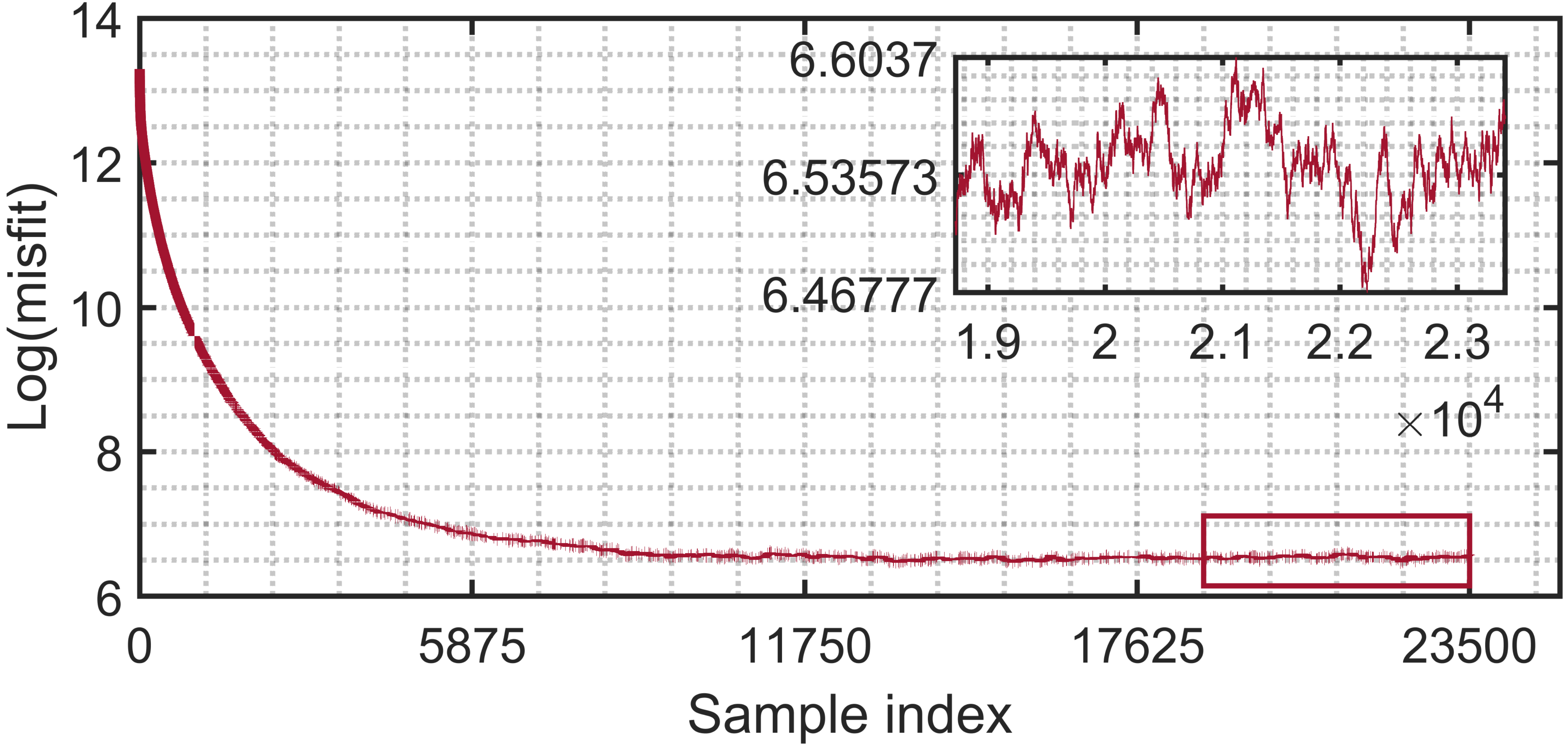
HMC gives descent results, and depicts uncertainties of FWI



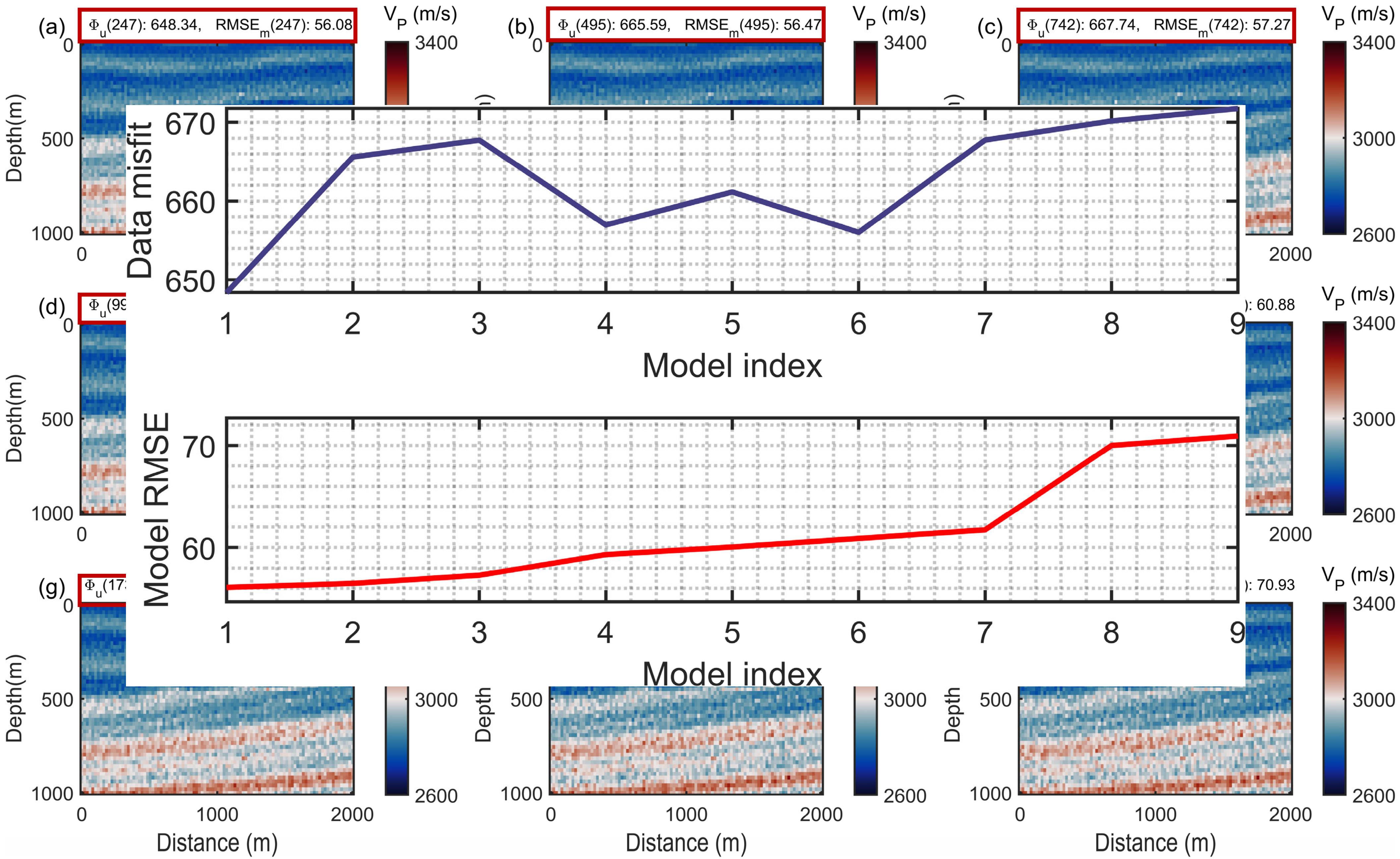
Profiles are close, although HMC is not fully converged



Misfit information: perspective to inversion nullspace



9 models in the "inversion nullspace" when setting tolerance to 0.11%



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Discussion & future work

- Ensemble chain adaptation (ECA).
- Quantum-inspired HMC.
- Accessing inversion nullspace (Fichtner et al., 2021)?
- Tunable parameters (L, Δt, $\mathbf{M}$) need more comprehension (Li and Innanen, 2023).
- Time-lapse.

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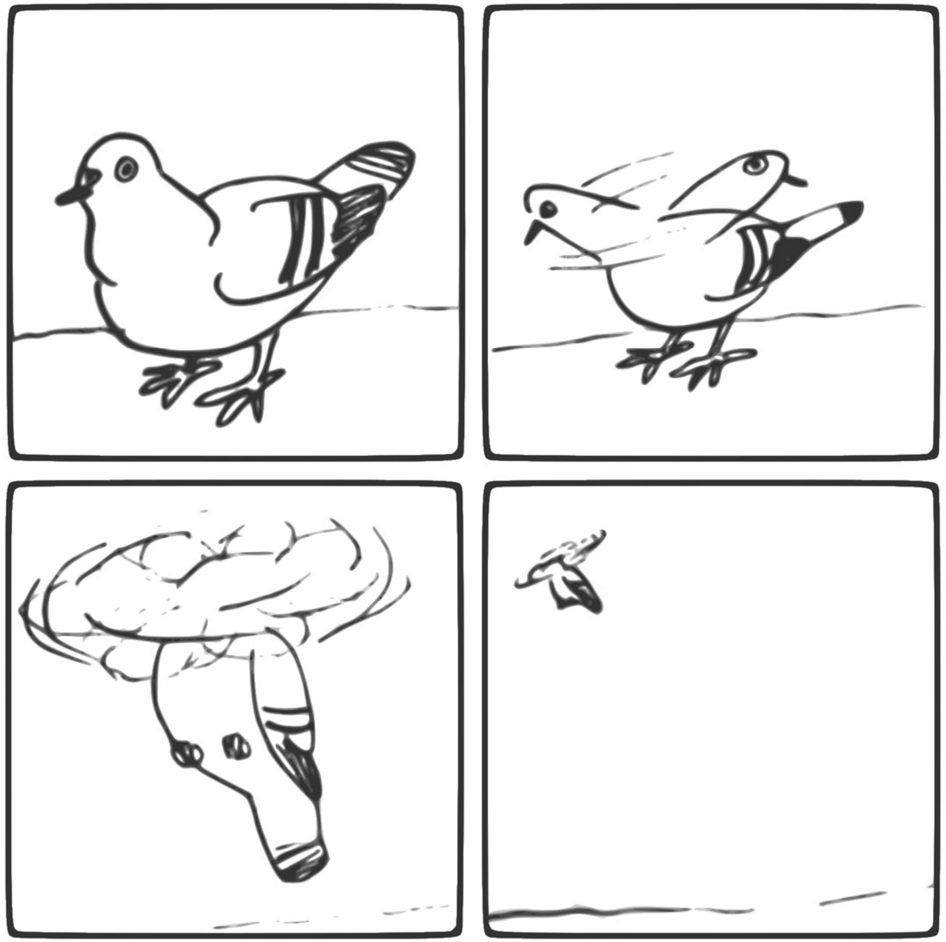
Conclusion

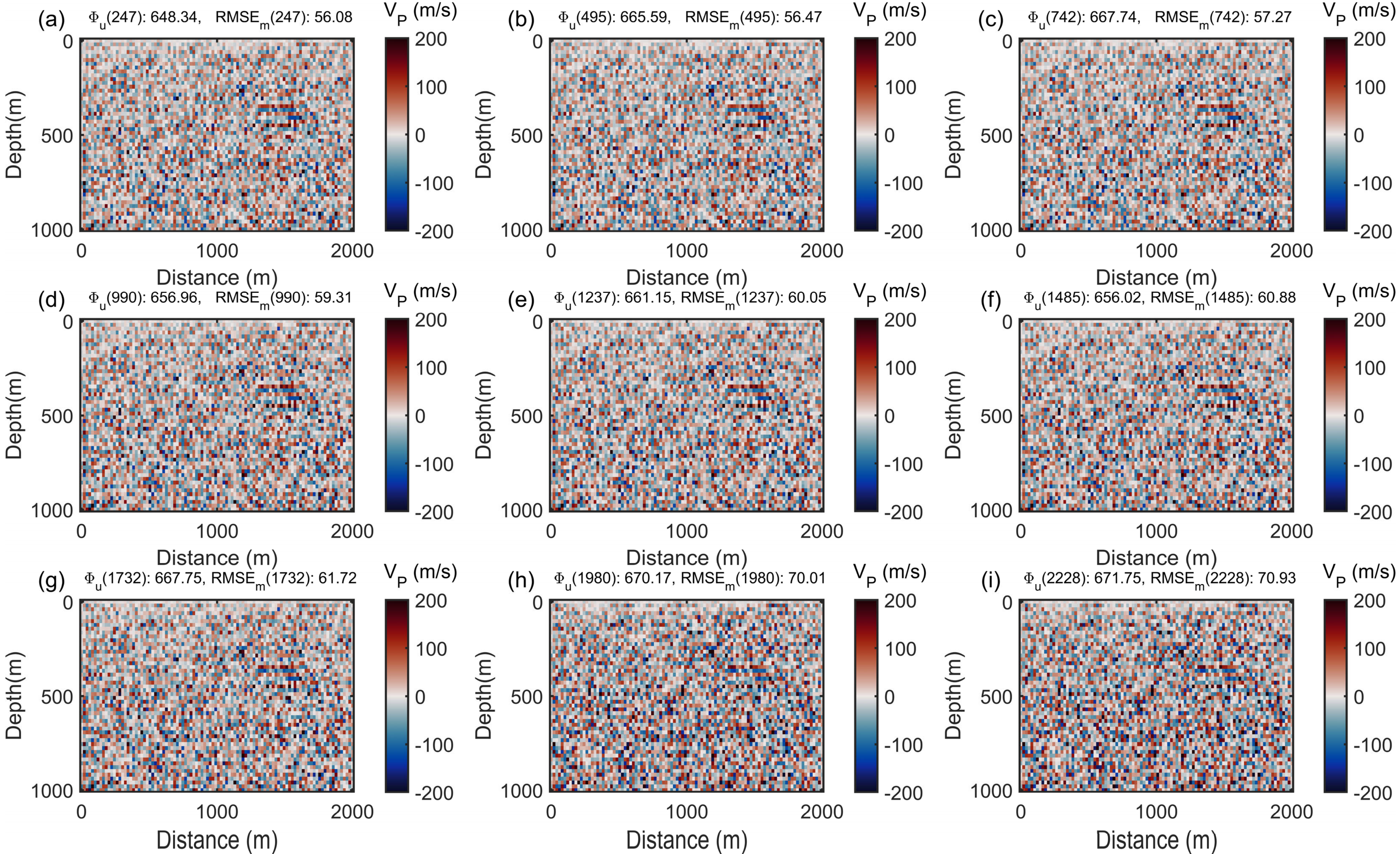
- HMC better explores the model space in MC variants.
- Needs to be tailored and tuned.
- Uncertainty quantification in FWI with HMC is feasible.
- Potential to extend to various topics.

Acknowledgements

- CREWES sponsors & colleagues
- NSERC
- CSEGF

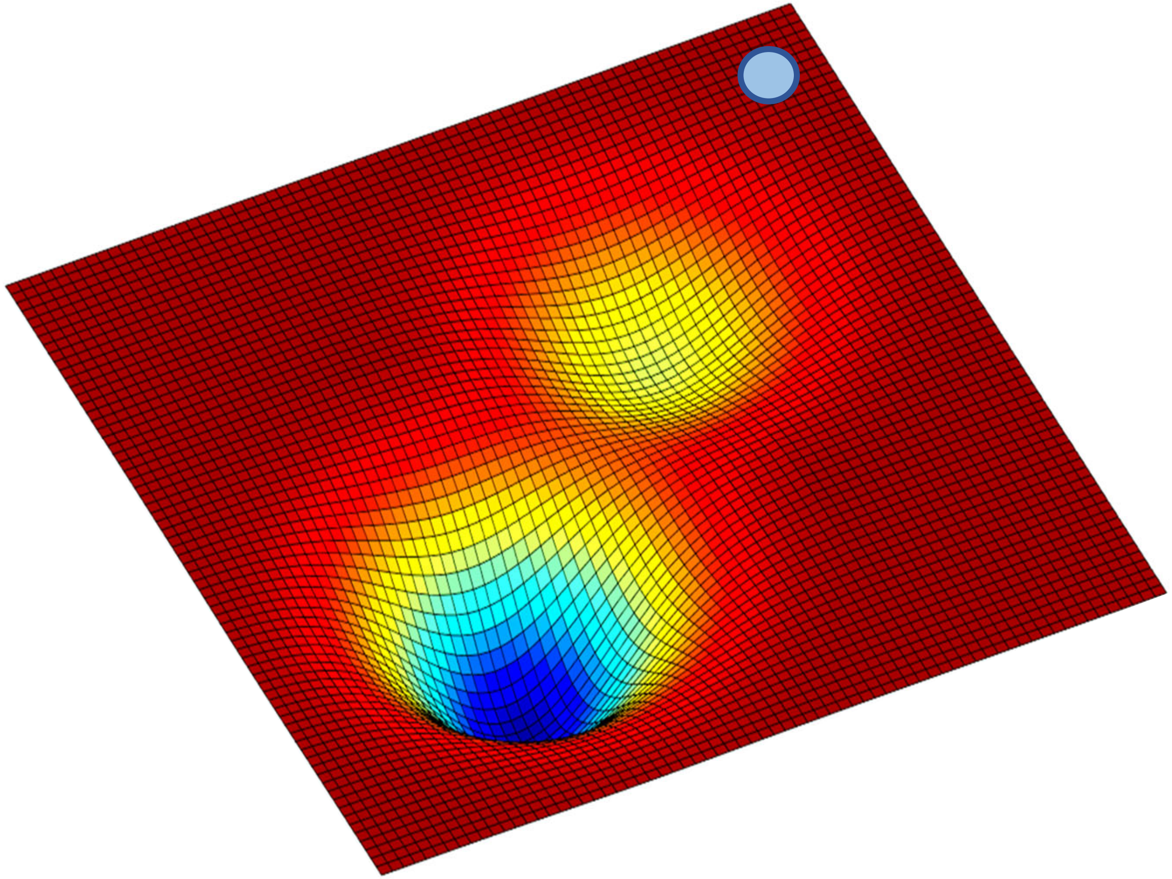
When your program
is a complete mess,
but it does its job



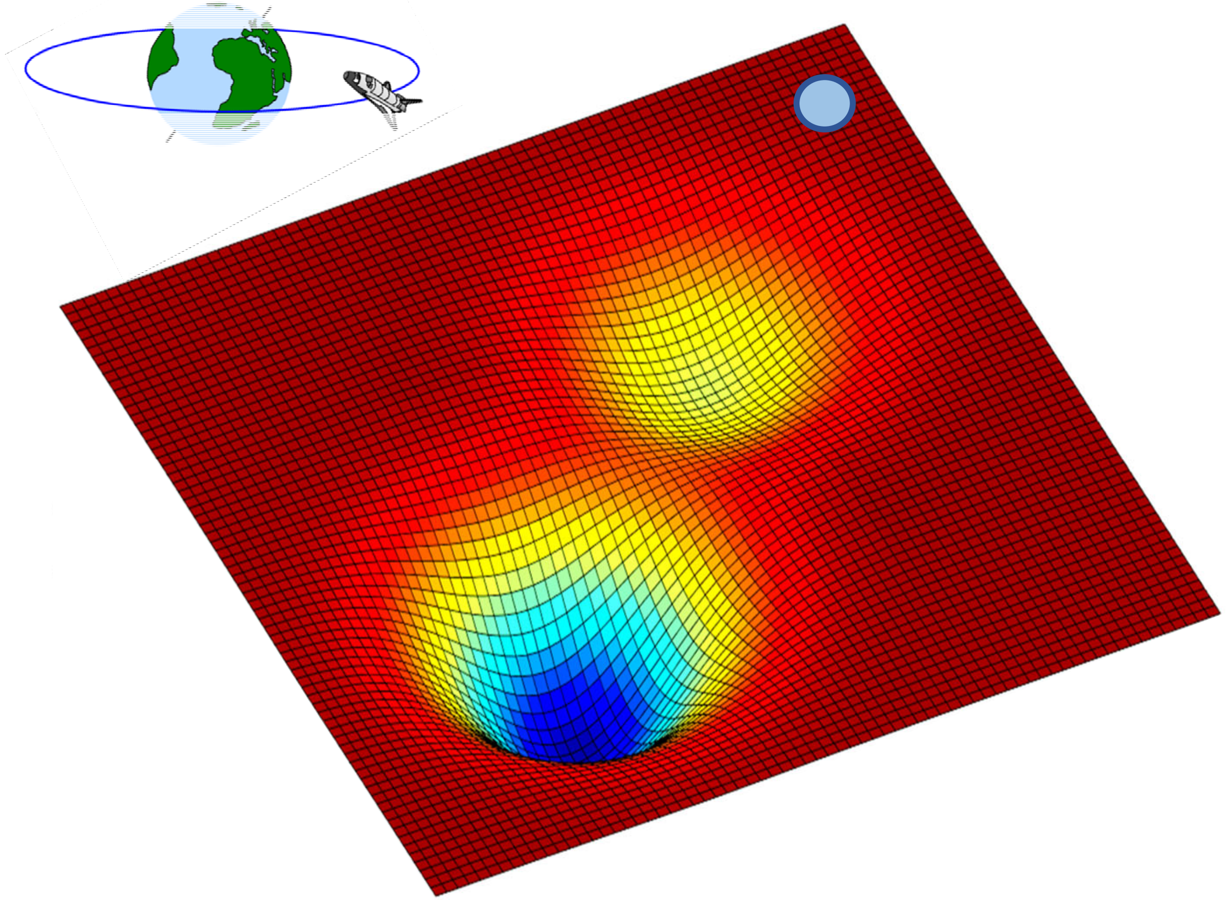


(a) Φ_u(247): 648.34, RMSE$_m$(247): 56.08
(b) Φ_u(495): 665.59, RMSE$_m$(495): 56.47
(c) Φ_u(742): 667.74, RMSE$_m$(742): 57.27
(d) Φ_u(990): 656.96, RMSE$_m$(990): 59.31
(e) Φ_u(1237): 661.15, RMSE$_m$(1237): 60.05
(f) Φ_u(1485): 656.02, RMSE$_m$(1485): 60.88
(g) Φ_u(1732): 667.75, RMSE$_m$(1732): 61.72
(h) Φ_u(1980): 670.17, RMSE$_m$(1980): 70.01
(i) Φ_u(2228): 671.75, RMSE$_m$(2228): 70.93
V_P (m/s)
200
100
0
-100
-200
Depth(m)
0
500
1000
Distance (m)
0
1000
2000

Informed paths access certain model subsets

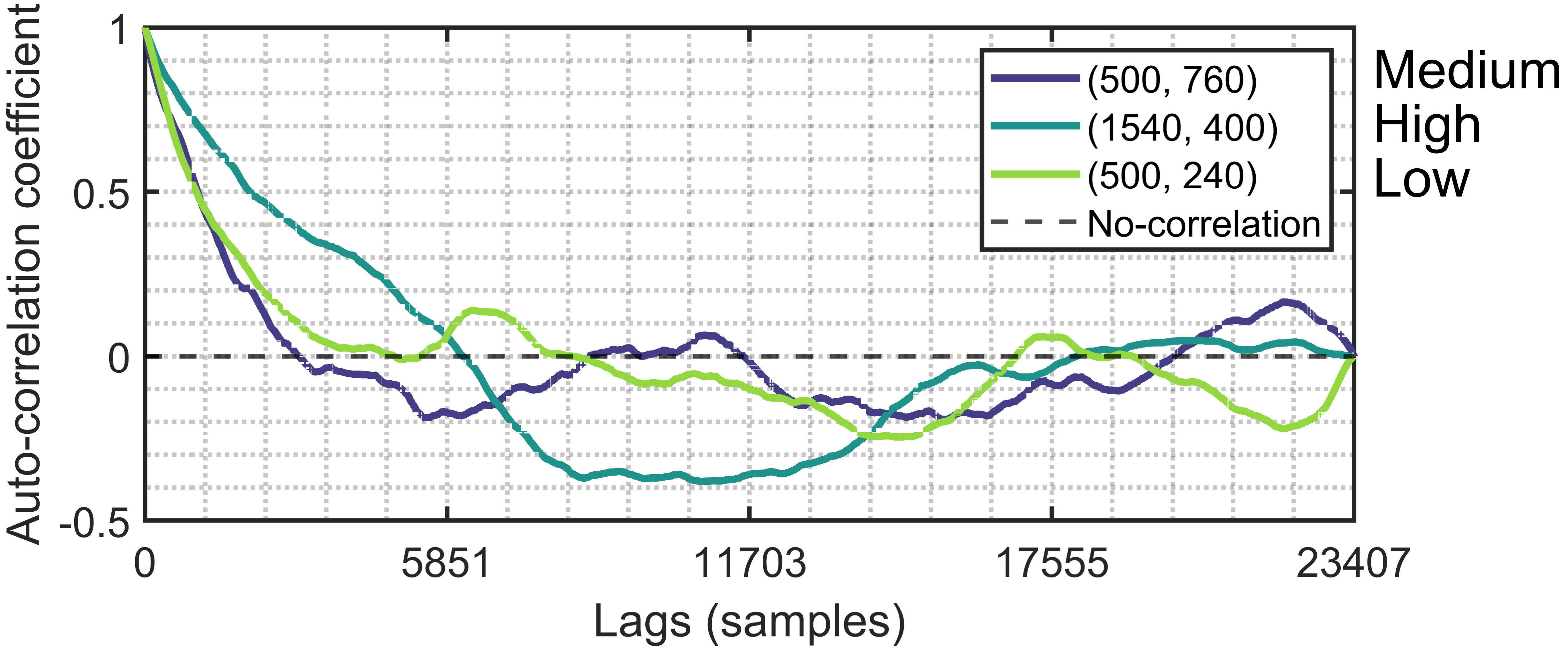


Random walk: Not allowable searches cause a waste of resources.

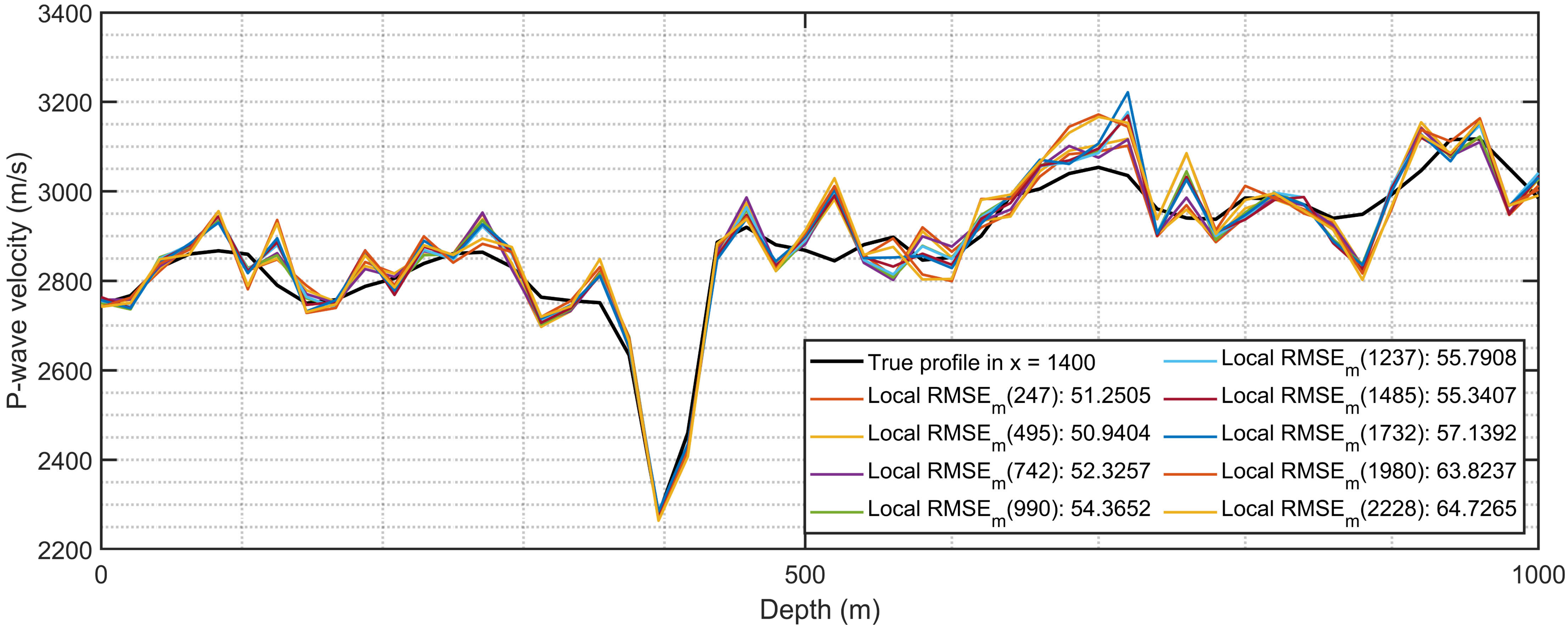


Guided path: certain trajectories, fewer dependent proposals.

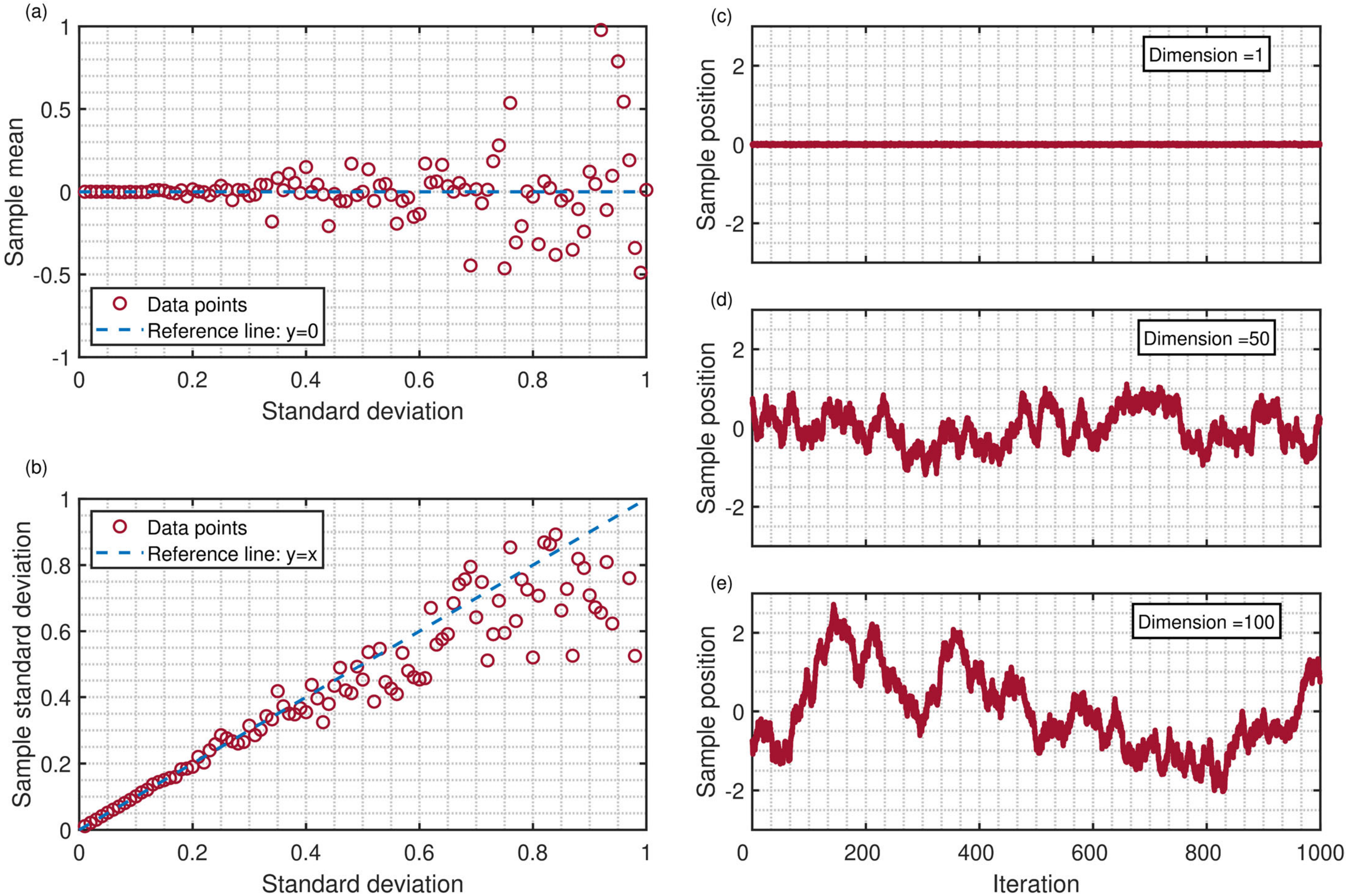
Model correlation drops to reasonably small after ~5k samples



Essential features are captured by all the models in the subset



100D-MCMC: strong correlation while searching (25% acceptance)



100D-HMC: relatively independent samples (87% acceptance)