3D local-scale SRVM based Elastic FWI & Uncertainty Quantification on a Supercomputing platform Shaheen II

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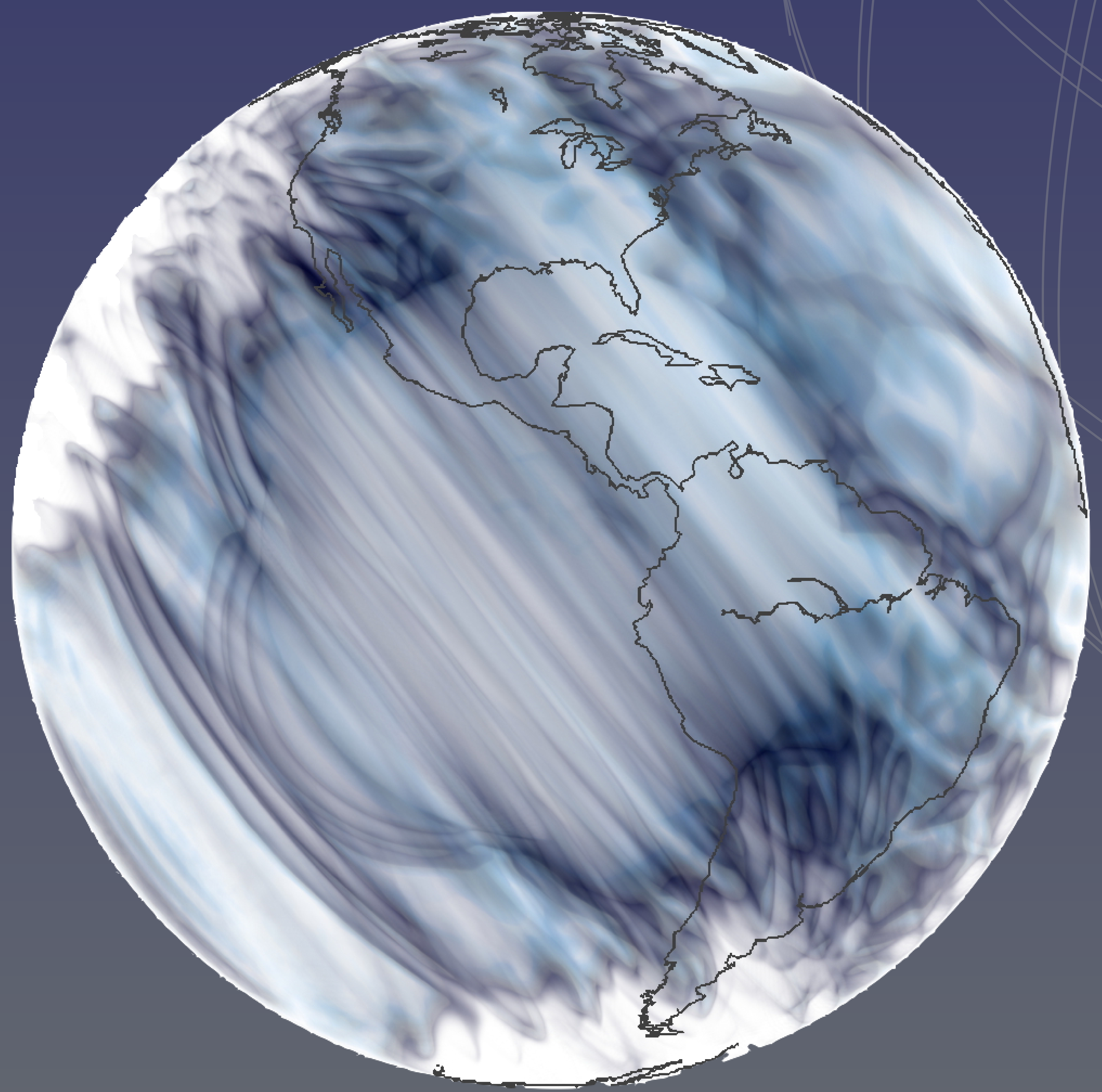

Summary

In full-waveform inversion (**FWI**), the Hessian-related **Uncertainty Quantification** is very crucial but very challenging to **large-scale 3D problems**. Herein, we develop a **vector-version Square-Root Variable Metric (SRVM)** algorithm, which is applicable to 3D large-scale elastic FWI because only one SRVM vector of the model size is stored per iteration.

After the SRVM-based elastic FWI is done, we have access to the **posterior covariance** by sampling the inverse data-misfit Hessian from the stored SRVM vectors and scalars. To facilitate the posterior analysis and samplings, we probe the stored SRVM vectors and scalars with a **randomised singular value decomposition (SVD)** method. Due to that **millions of parameters are involved**, the 3D local-scale SRVM based elastic FWI & Uncertainty Quantification run on the Shaheen II supercomputing platform.

SRVM Theory & Method

The derivation of the vector-version SRVM is based on the DFP algorithm:

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k \Delta\mathbf{g}_k \Delta\mathbf{g}_k^T \mathbf{B}_k}{\Delta\mathbf{g}_k^T \mathbf{B}_k \Delta\mathbf{g}_k} + \frac{\Delta\mathbf{m}_k \Delta\mathbf{m}_k^T}{\Delta\mathbf{g}_k^T \Delta\mathbf{m}_k}, \tag{1}$$

with $\mathbf{B} = \mathbf{H}^{-1}$ the inverse Hessian, $\Delta\mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ and $\Delta\mathbf{m}_k = \mathbf{m}_{k+1} - \mathbf{m}_k$. To ensure the positive-definite property of $\mathbf{B}$, SRVM reads:

$$\mathbf{S}_{k+1}\mathbf{S}_{k+1}^T = \mathbf{S}_k \left(\mathbf{I} - (1/P_k)\mathbf{S}_k^T \mathbf{y}_k \mathbf{y}_k^T \mathbf{S}_k \right) \mathbf{S}_k^T, \tag{2}$$

with $\mathbf{B}_k = \mathbf{S}_k \mathbf{S}_k^T$.To make Eq. (2) matrix-free, we express a vector-verion SRVM workflow as

Algorithm 1 SRVM vector-version workflow

for $k \leftarrow 0$ to n **do**
- $\Delta\mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ ▷ Gradient update
- $\mathbf{y}_k = \mu_k \mathbf{g}_k + \Delta\mathbf{g}_k$
- $\mathbf{w}_k = \mathbf{S}_k^T \mathbf{y}_k$ ▷ Vectors
- $\boldsymbol{\beta}_k = \mathbf{S}_k^T \Delta\mathbf{g}_k$
- $P_k = \mathbf{w}_k^T \boldsymbol{\beta}_k$ ▷ Scaling factors
- $Q_k = \mathbf{w}_k^T \mathbf{w}_k$
- $\nu_k = \frac{1-\sqrt{1-Q_k/P_k}}{Q_k/P_k}$
- $\mathbf{S}_{k+1} = \mathbf{S}_k \left(\mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)$ ▷ Matrix update
- $\mathbf{B}_{k+1} = \mathbf{S}_{k+1}\mathbf{S}_{k+1}^T = \mathbf{S}_k \left(\mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right) \left(\mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)^T \mathbf{S}_k^T$

end for

The vector-version SRVM can be easily extend to 3D cases. To facilitate the uncertainty quantification a posteriori we put randomised SVD into SRVM.

Software & Supercomputing platforms

In this research, we use **SPECFEM3D** (*Peter et al., 2011*) for the forward and adjoint modelings and **Seisflows** (*Modrak and Tromp, 2016*) for the inversion workflow management.

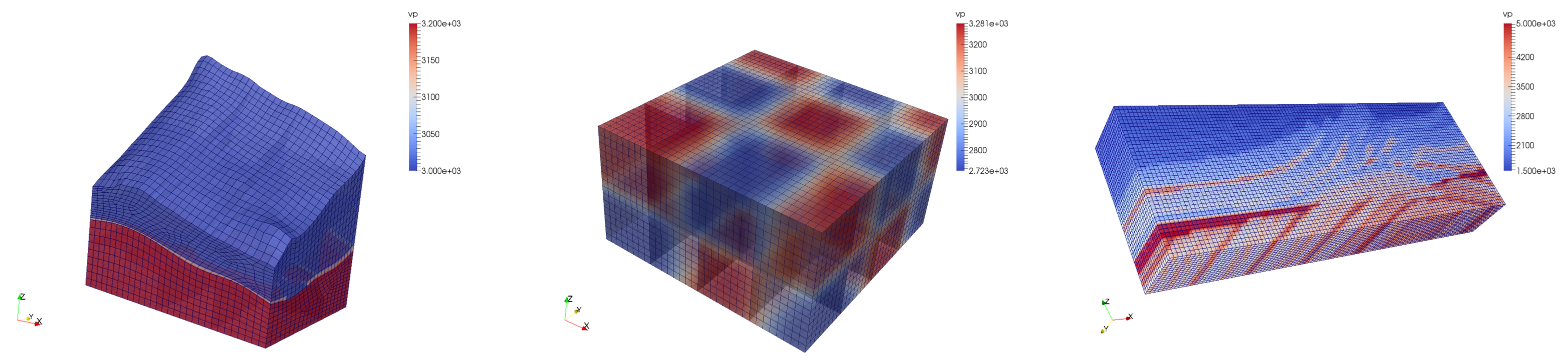

Figure 1: 3D velocity models together with the meshes by the in-house mesher of SPECFEM3D. The Marmousi one will be used in this study. The sources and receivers are deployed on the top and bottom of the model to provide an observation system mainly for transmission waves.

3D local-scale Marmousi on Shaheen II

1. Parameterisation:	**Vp & Vs**
2. Model size in X-Y-Z:	**8400-1200-3000** (m)
in NX-NY-NZ:	**112-16-40** with dX=dY=dZ=**75** (m)
3. Observation system:	**Shots@Top** and **Sensors@Bottom**
4. Numbers of Shots & Sensors:	**64** & **3841**
5. Slices & MPI processes:	**16** & **16**
6. Total Vp/Vs elastic elements:	**71680 × 2 = 143360**
7. Total GLL elements:	**71680 × 2 × 125 = 17920000**
8. Time steps & dT (s):	**6000** & **1.25e-3** (s)
9. Aver-runtime Forward & Adjoint:	**04** (m) **36** (s) & **11** (m) **52** (s)
10.Total iteration number:	**43**
11. Number of SRVM vectors & scalars:	**43** & **43**
12.Total CPU/hours:	**50176**

Figure 2: Supercomputer Shaheen II and the 3D Marmousi FWI specifications. **The SRVM vectors, each is of the model size, are stored on the disk**, with the main **data storage solution being a Lustre Parallel file system** a storage capacity of 17.2 PB delivering around 500 GB/s of I/O throughput.

FWI Results

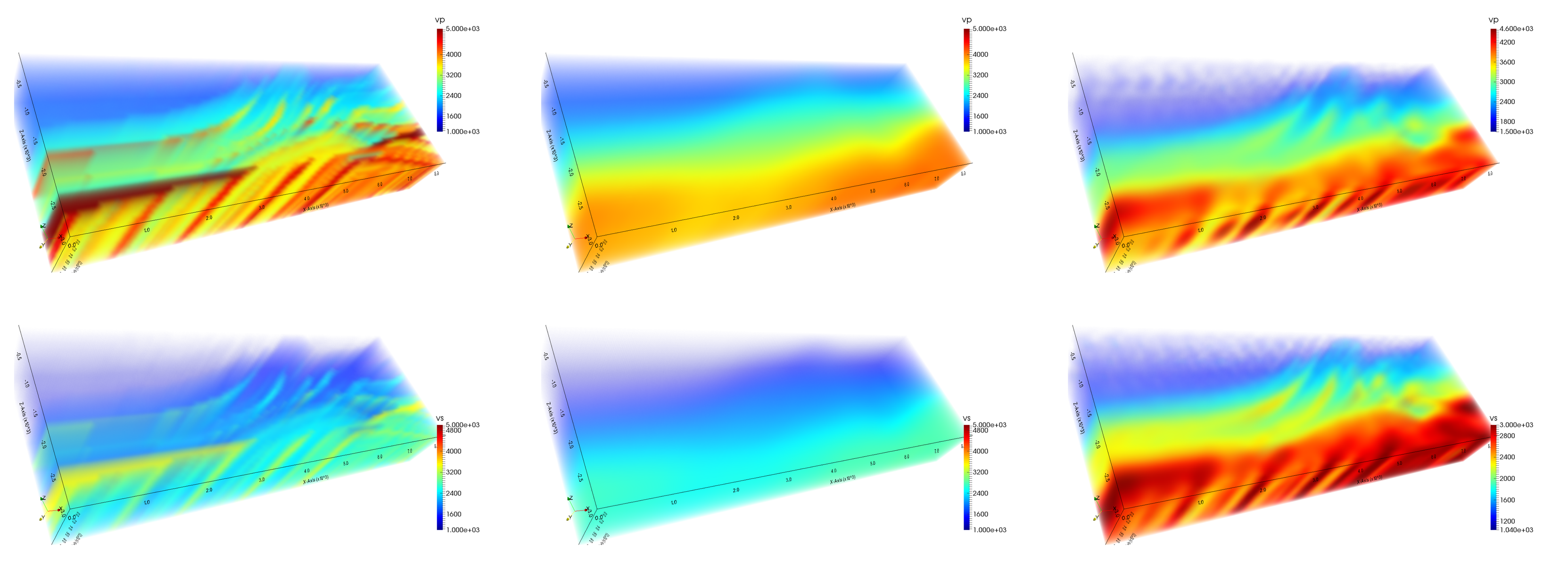

Figure 3: 3D Marmousi examples (from left to right): true, initial, and inverted models. Note that we set the same colouring style to the inverted results for comparison of the inverted Vp and Vs models.

Uncertainty Quantification

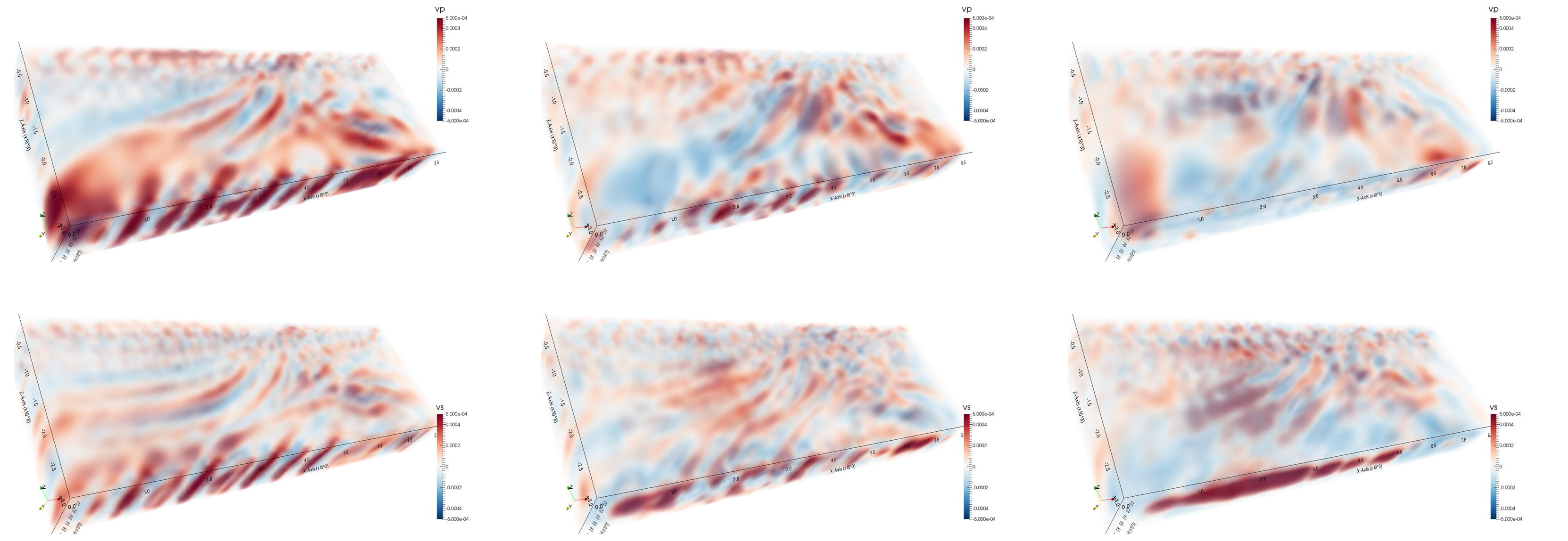

Figure 4: Examples of contributing *1st, 3rd, 5th* eigenvectors of the inverse Hessian, by randomised SVD.

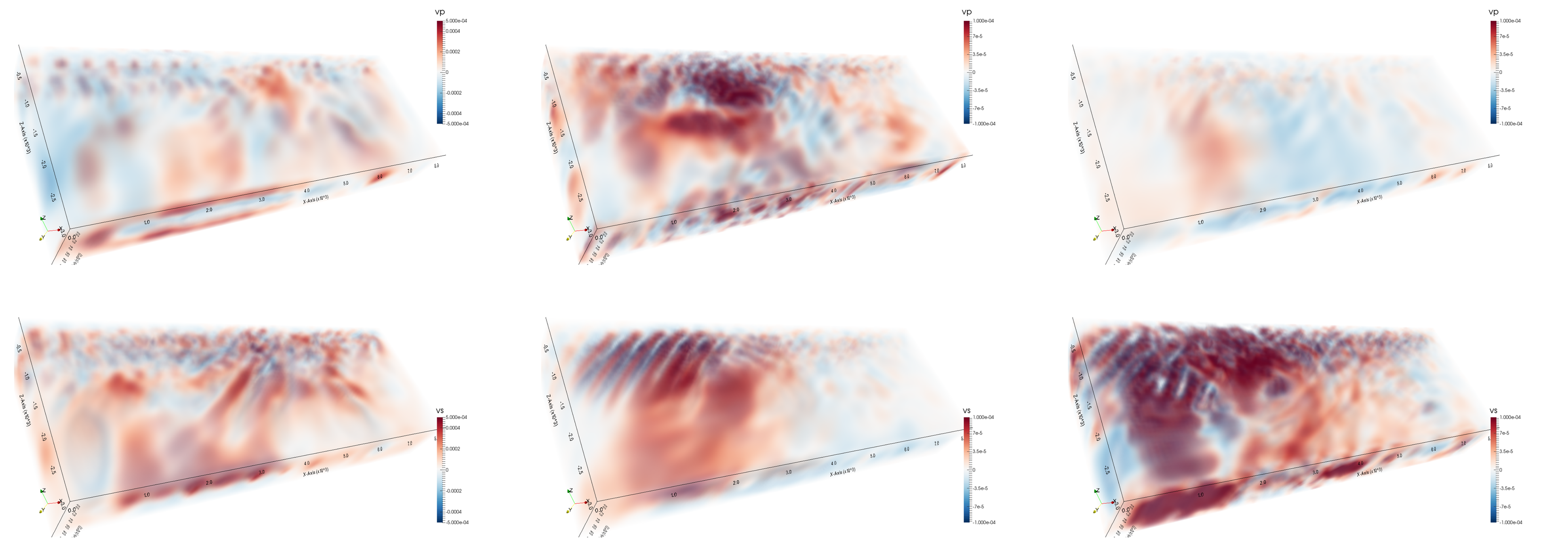

Figure 5: Examples of contributing *10th, 20th, 40th* eigenvectors of the inverse Hessian, by randomised SVD. Note that the last two groups of figures are using displaying scales five times smaller than the others.

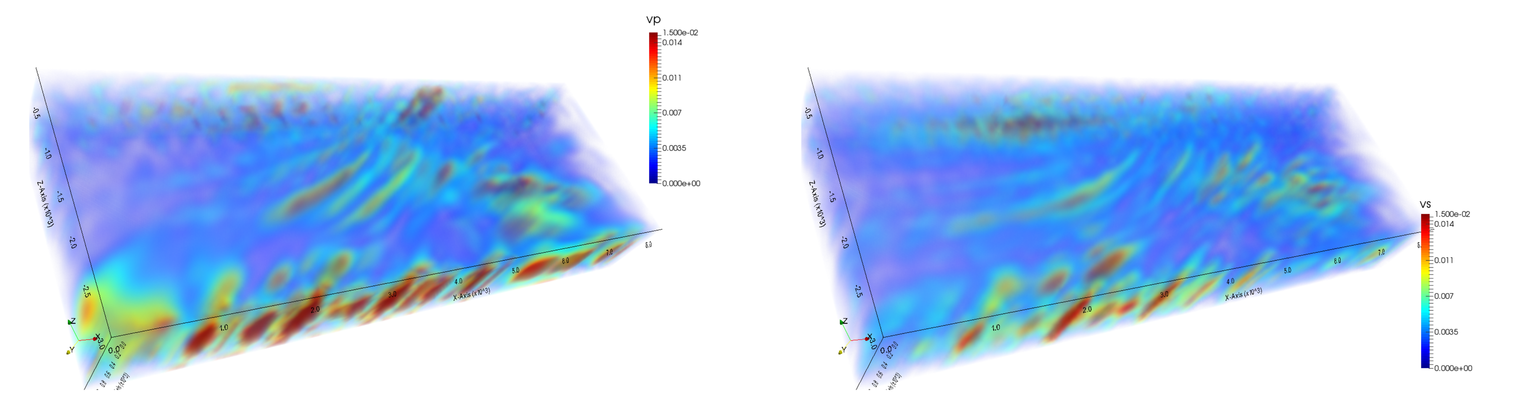

Figure 6: Uncertainty maps (from the diagonals of posterior covariance).

Conclusions

We run 3D local-scale SRVM-based elastic FWI on the Shaheen II supercomputer. The vector-version SRVM algorithm allows for **large-scale applications even with millions of parameters**. This algorithm together with randomise SVD allows **efficiently accessing the posterior covariance** by reconstructing the inverse Hessian with **memory-affordable vector series**. Based upon this 3D local-scale application, our next move will be towards **3D regional-scale applications** with synthetic & **real data** using the theories & methods reported here.

Acknowledgments & References

Peter, D., et al. (2011), *Forward and adjoint simulations of seismic wave propagation on fully unstructured hexahedral meshes*, Geophys. J. Int., **186**, 721-739.

Modrak, R., and J. Tromp (2016), *Seismic waveform inversion best practices: regional, global and exploration test cases*, Geophys. J. Int., **206**, 1864-1889.