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Quantifying Uncertainties in Monitoring Megatonne-Scale CO_2 Injection: A Synthetic Seismic Study in the Appalachian Basin

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Summary

Seismic surveys are a key method for monitoring CO_2 storage. Seismic Full Waveform Inversion (FWI) is an advanced approach that reconstructs a detailed subsurface model using seismic data. Due to its ill-posed and non-unique nature, quantifying uncertainty is essential for evaluating model confidence and guiding decision-making. Bayesian inference techniques, such as the Metropolis-Hastings algorithm, are commonly applied to quantify uncertainty in geophysical inversion by generating a set of samples to estimate the posterior probability distribution. However, MCMC methods can be computationally demanding particularly for complex problems. This makes choosing the parameterization of the model critical (Kotsi and Malcolm, 2020; Wei et al., 2024).

This study proposes a novel approach for uncertainty quantification in seismic monitoring surveys in a synthetic large-scale Carbon Capture and Storage (CCS) scenario in the Oriskany sandstone within the Appalachian basin. By simplifying the model to only two parameters—eastern and western edges of the CO_2 plume, vertically constrained by upper and lower horizons—we reduce the number of model parameters. Consequently, the required sample size for convergence decreases, providing a more efficient method to estimate uncertainties in the geometry of the CO_2 plume.

Method

FWI aims to estimate the subsurface model parameters $\boldsymbol{\theta} \in \mathbb{R}^m$ from observed seismic data $\boldsymbol{d}^{obs} \in \mathbb{R}^n$ where m and n represent the dimensions of the model parameters and observed data, respectively. Within the Bayesian inference framework, the posterior probability density of the model parameters, $p_{post}(\boldsymbol{\theta} \mid \boldsymbol{d}^{obs})$ is obtained by combining prior information with observed data, expressed as

$$p_{post}(\boldsymbol{\theta} \mid \boldsymbol{d}^{obs}) \propto p_{like}(\boldsymbol{d}^{obs} \mid \boldsymbol{\theta})\, p_{prior}(\boldsymbol{\theta}), \qquad (1)$$

where p denotes a probability density function. Here, $p_{like}(\boldsymbol{d}^{obs} \mid \boldsymbol{\theta})$ is the likelihood function describing the probability of observing data $\boldsymbol{d}^{obs}$ given the model $\boldsymbol{\theta}$ and $p_{prior}(\boldsymbol{\theta})$ represents the prior distribution which we choose to be a uniform distribution. The likelihood function, $p_{like}(\boldsymbol{d}^{obs} \mid \boldsymbol{\theta})$ we use is

$$p_{like}(\boldsymbol{d}^{obs} \mid \boldsymbol{\theta}) = \frac{1}{(2\pi)^{n/2}\sqrt{det(C)}} exp(-\frac{1}{2}\boldsymbol{r}^{\top} C^{-1}\boldsymbol{r}), \qquad (2)$$

where C is the covariance matrix and $\boldsymbol{r} = \boldsymbol{d}^{obs} - f(\boldsymbol{\theta})$ is the residual vector between the observed data $\boldsymbol{d}^{obs}$ and the simulated data $f(\boldsymbol{\theta})$. Here f represents the forward modelling operator that predicts seismic data based on the model parameters $\boldsymbol{\theta}$.

To accept or reject a candidate sample, we use the Metropolis-Hastings acceptance criteria

$$\alpha = min\left(1, \frac{p_{like}\left(\boldsymbol{d}^{obs}|\boldsymbol{\theta}_i\right)}{p_{like}\left(\boldsymbol{d}^{obs}|\boldsymbol{\theta}_j\right)}\right), \quad (3)$$

where i and j indicate the proposed and current models, respectively (Mosegaard and Tarantola, 1995).

Result & Discussion

Oriskany Sandstone: The target reservoir in this study is the Oriskany sandstone within the Appalachian Basin located in southwestern Virginia. This specific location features a doubly plunging synclinal structure with a potential reservoir-seal system in the fault footwall (Bartholomew, 1987). The Oriskany sandstone has a thickness of 50 to 100 m with a varying depth of approximately 500 to 3000 m. The formation has an average permeability of 1.45×10^{-14} m^2 with a varying porosity of 10.9% to 12.2% (Carr, 2024). Previous studies show promising results for the injection and trapping of megatonnes of CO_2 (Kohen et al., 2023).

Assuming homogeneous saturation patterns in the Oriskany sandstone, we apply Gassmann's equation to establish the relationship between reservoir parameters and seismic velocities, including the impact of water saturation (Gassmann, 1951). Figure 1 illustrates the change in P-wave velocity as water saturation decreases, corresponding to an increase in CO_2 saturation for the target reservoir. Beyond approximately 15% CO_2 saturation levels, the changes in P-wave velocity for this specific reservoir become negligible. This observation allows us to assume constant velocities within the plume.

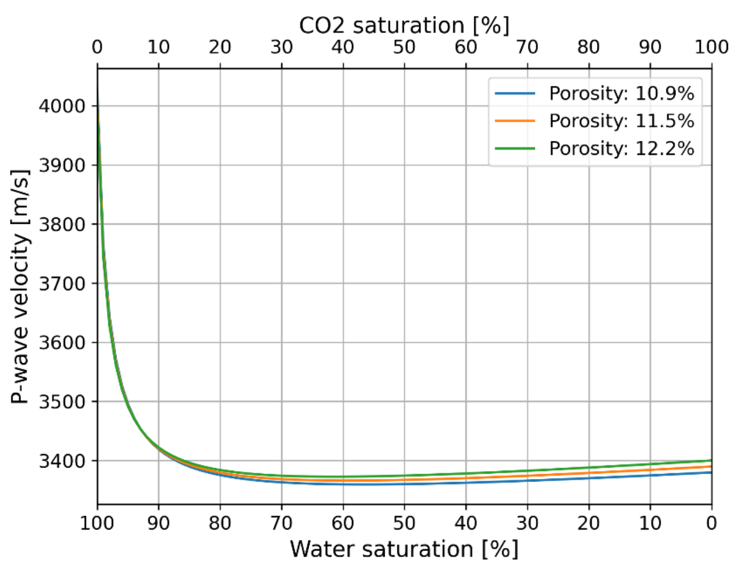
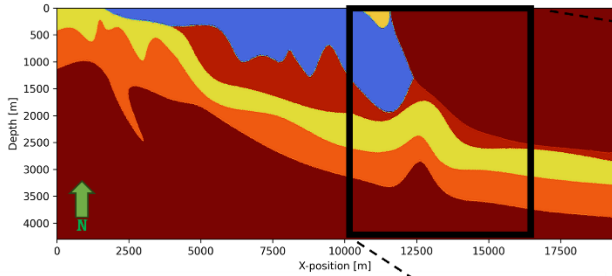


Figure 1. Changes in P-wave velocity for different water saturation levels in different porosities.

To test our algorithm, we use a slight modification of the geological model from Kohen et al., (2023) in a surface seismic scenario. Figure 2 shows the target model and the region of interest.



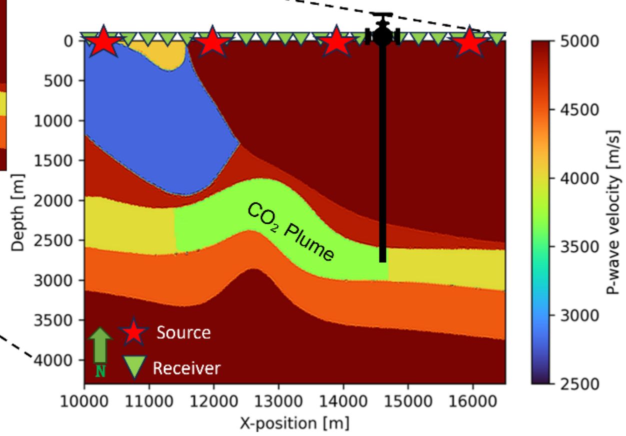
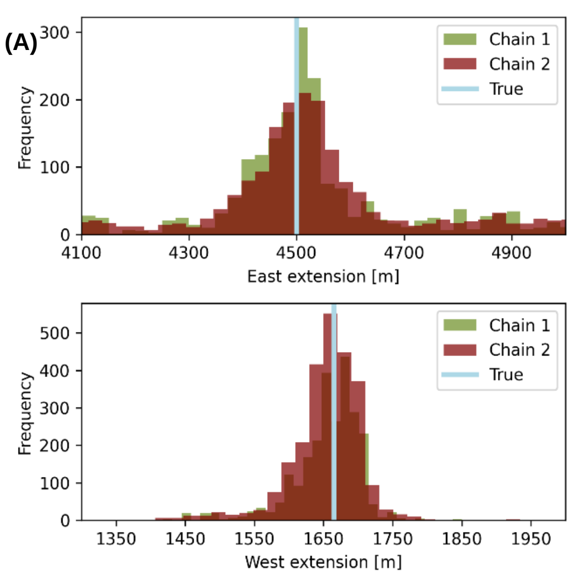


Figure 2. Target model, the region of interest (illustrated with the black rectangle), and injection well. Seismic sources are depicted as red stars and receivers are green triangles.

Parametrization: Assuming well-defined top and bottom horizons of the reservoir and a constant P-wave velocity for the CO_2 plume, the geometry of the target model is characterized using two key parameters: one representing the east-side extent of the plume and the other its west-side extent. Based on these parameters, two-dimensional models of elastic properties were then generated using Coreform Cubit 2024.3 and the corresponding seismic data was calculated using SPECFEM2D (Peter et al., 2011). We use the same approach for generating models of elastic properties during MCMC simulations for each candidate sample in an automated manner to exploit the full capacity of unstructured meshing and spectral element method.

Uncertainty Quantification: We conduct three independent MCMC simulations with identical setups but different initial models. We run each simulation for 5000 iterations. In our method, through trial and error, we set the temperature before simulations to maintain an acceptance rate between 15% and 20%. We also used a burn-in period of 2500 samples during MCMC simulations, meaning that we ignored the first 2500 samples in the chain when computing the final histograms of the results. Figure 3-A shows the recovered posteriori distributions for each parameter in the two of the three chains while Figure 3-B shows the average over the last 25% of the samples in one of the chains.



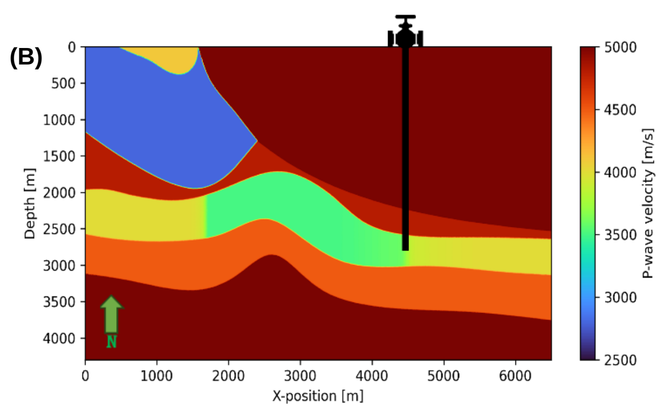


Figure 3. (A) Histogram of the final 50% of the samples for chains 1 and 2. The true value is shown with a light blue line. (B) Average of the last 25% of models in the second chain.

To evaluate convergence between the three MCMC chains, we calculated the Gelman-Rubin ($\hat{R}$) metric which is considered optimal within the range of 1.0 to 1.1 (Gelman and Rubin, 1992). The average $\hat{R}$ value across all three chains for two parameters (east & west extensions) is 1.002. This value suggests that all three chains have statistically converged to the same distributions.

Conclusion

This study demonstrates a sparse re-parametrization method for CO_2 plume geometry that significantly reduces the number of samples needed for uncertainty quantification using MCMC methods, particularly in the context of large-scale CCS projects. By combining this method with automated meshing, we have fully used the potential of unstructured meshes and spectral element methods in FWI, improving both the efficiency and accuracy of seismic modeling during sampling. Future work will focus on extending this sparse re-parametrization approach to more complex geological settings with more degrees of freedom and integrating it with advanced machine learning techniques to further enhance computational efficiency in uncertainty quantification for CCS projects.

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