DUAL STATES ESTIMATION OF A SUBSURFACE FLOW-TRANSPORT COUPLED MODEL USING ENSEMBLE KALMAN FILTERING

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1. SUMMARY

Modeling contaminant evolution in geologic aquifers requires coupling a groundwater flow model with a contaminant transport model. Assuming perfect flow, an ensemble Kalman filter can be directly applied on the transport model but this is very crude assumption as flow models can be subject to many sources of uncertainties. If the flow is not accurately simulated, contaminant predictions will likely be inaccurate even after successive Kalman updates of the contaminant with the data. The problem is better handled when both flow and contaminant states are concurrently estimated using the traditional joint state augmentation approach. In this study, we propose a dual states estimation strategy for this one way coupled system by treating the flow and the contaminant models separately while intertwining a pair of distinct Kalman filters; one on each model. This EnKF-based dual states estimation sxhibits a number of novel features:

{1} it allows for simultaneous estimation of both flow and contaminant states in parallel,

{2} it provides a time consistent sequential updating scheme between the two models,

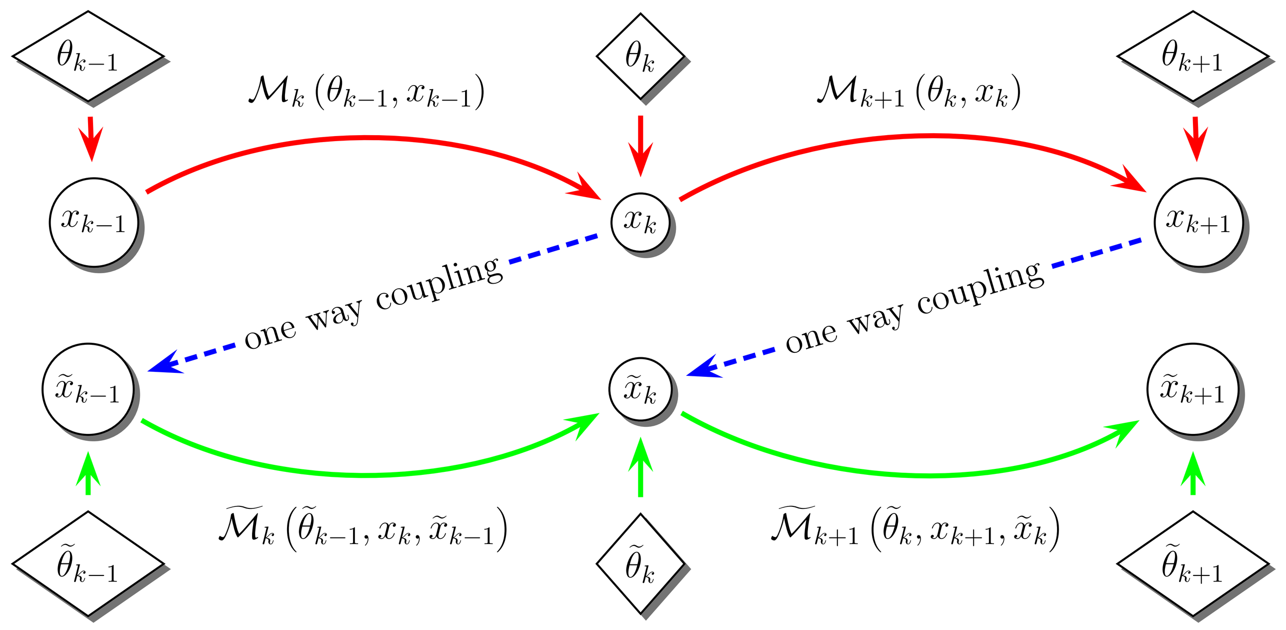
{3} it simplifies the implementation of the filtering system, and

{4} it yields more stable and accurate solutions than the standard joint approach.

2. STATES ESTIMATION FOR ONE-WAY COUPLED MODELS

Consider the following state-space discrete processes for one-way coupled models. Our goal is to estimate the coupled system states x_k and $\widetilde{x}_k$. Assume that observations y_k and $\widetilde{y}_k$ are available from both models at time t_k. From a sequential Bayesian perspective, the Maximum A Posteriori (MAP) estimator of the coupled system is then:

$$\left[x_k^{MAP}, \widetilde{x}_k^{MAP}\right] = \arg\max_{x_k, \widetilde{x}_k} \; p\left(x_k, \widetilde{x}_k | y_{0:k}, \widetilde{y}_{0:k}\right).$$



2.1 *Standard Joint States Sequential Estimation:*

One forms a new joint state, $\mathcal{Z}_k = \left[x_k^T, \widetilde{x}_k^T\right]^T$ and observation, $\mathcal{Y}_k = \left[y_k^T, \widetilde{y}_k^T\right]^T$ vectors. The estimation problem then reduces to:

$$\mathcal{Z}_k^{MAP} = \arg\max_{\mathcal{Z}_k} \; p\left(\mathcal{Z}_k | \mathcal{Y}_{0:k}\right).$$

Pros: Reasonable computational cost requiring $NN_e\left(\mathcal{C}_x + \widetilde{\mathcal{C}}_x\right) + 2NN_e^2N_x + NN_e\left(\mathcal{C}_y + \widetilde{\mathcal{C}}_y\right)$.
Cons: Tractability due to the large degrees of freedom and consistency of the updating scheme between the two models.

2.2 *Dual States Sequential Estimation:*

The joint density of both system states is separated (marginal estimation) and decomposed into two terms:

$$p\left(x_k, \widetilde{x}_k | y_{0:k}, \widetilde{y}_{0:k}\right) = p\left(\widetilde{x}_k | x_k, y_{0:k}, \widetilde{y}_{0:k}\right) \cdot p\left(x_k | y_{0:k}, \widetilde{y}_{0:k}\right).$$

Then, maximization of both densities is simultaneously performed using two parallel filters:

$$x_k^{MAP} = \arg\max_{x_k} \; p\left(x_k | y_{0:k}, \widetilde{y}_{0:k}\right) \qquad \& \qquad \widetilde{x}_k^{MAP} = \arg\max_{\widetilde{x}_k} \; p\left(\widetilde{x}_k | x_k, \widetilde{y}_{0:k}\right)$$

State -1 Filter:

(i) **Forecast ensemble-1:** $x_k^{f,i} = \mathcal{M}_k\left(\theta_k, x_{k-1}^{a,i}\right)$,

(ii) **Forecast ensemble-2:** $\widetilde{x}_k^{f,i} = \widetilde{\mathcal{M}}_k\left(\widetilde{\theta}_k, x_k^{f,i}, \widetilde{x}_{k-1}^{a,i}\right)$,

(iii) **Update with model-1 data:** $x_k^{a,i} = x_k^{f,i} + K_{xx}\left[y_k^i - \mathcal{H}_k\left(x_k^{f,i}\right)\right]$,

(iv) **Update with model-2 data:** $x_k^{a,i} \leftarrow x_k^{a,i} + K_{x\widetilde{x}}\left[\widetilde{y}_k^i - \widetilde{\mathcal{H}}_k\left(\widetilde{x}_k^{f,i}\right)\right]$.

State -2 Filter:

(i) **Forecast ensemble-2:** $\widetilde{x}_k^{f,i} = \widetilde{\mathcal{M}}_k\left(\widetilde{\theta}_k, x_k^{a,i}, \widetilde{x}_{k-1}^{a,i}\right)$,

(ii) **Update with model-2 data:** $\widetilde{x}_k^{a,i} = \widetilde{x}_k^{f,i} + K_{\widetilde{x}\widetilde{x}}\left[\widetilde{y}_k^i - \widetilde{\mathcal{H}}_k\left(\widetilde{x}_k^{f,i}\right)\right]$.

Pros: Ease of implementation, flexible assimilation framework and consistent updating scheme of both model forecasts.
Cons: Computationally intensive requiring $NN_e\left(\mathcal{C}_x + 2\widetilde{\mathcal{C}}_x\right) + 3NN_e^2N_x + NN_e\left(\mathcal{C}_y + 2\widetilde{\mathcal{C}}_y\right)$.

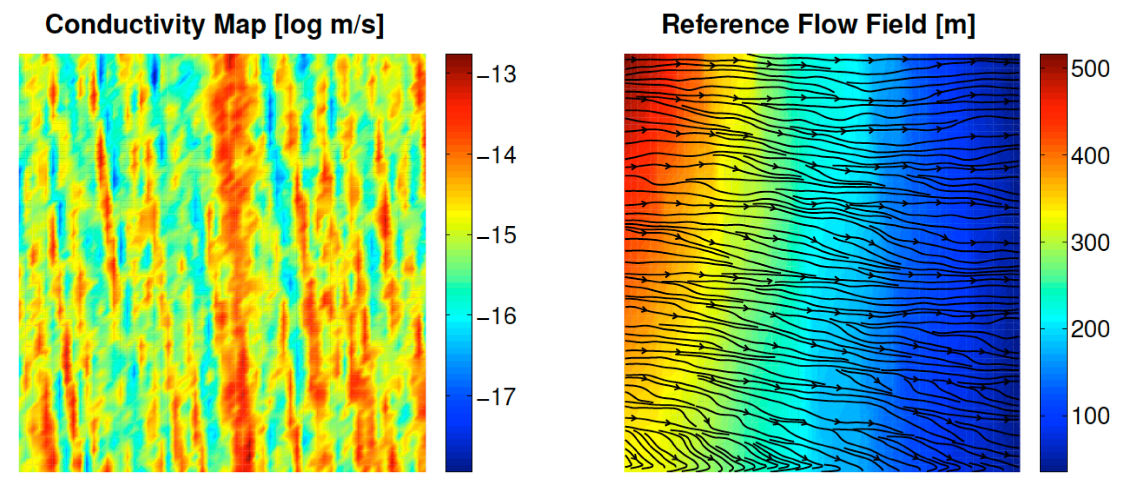
3. FLOW AND CONTAMINANT TRANSPORT EXPERIMENTAL RESULTS

The schemes are tested in a 2D flow and transport system in a confined aquifer. The total modeling time is 17 years.

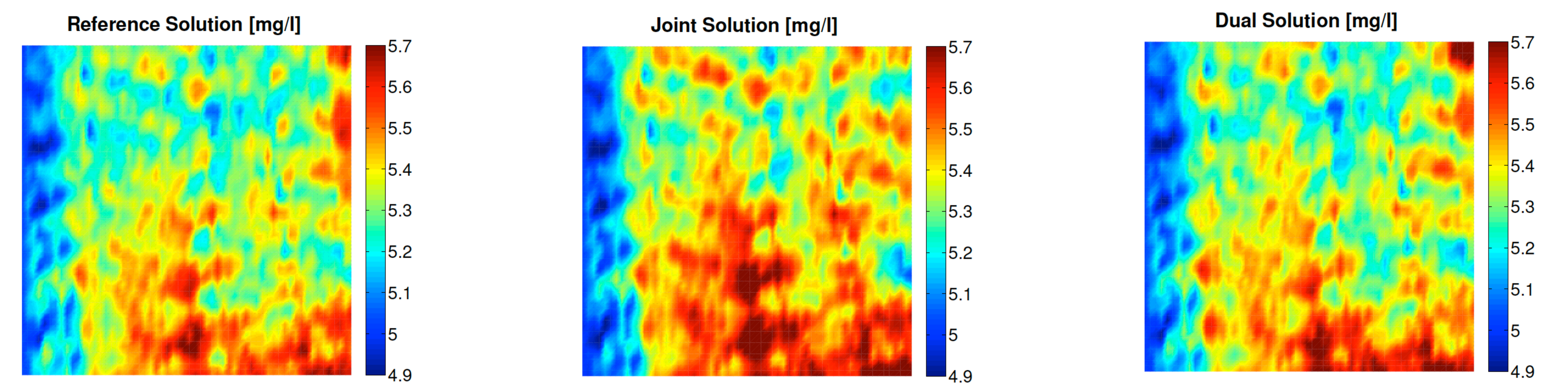
Flow Model (x): $\nabla \cdot (K\nabla\xi) = S_o\dfrac{\partial \xi}{\partial t} + q_\xi, \quad u = -K\nabla\xi,$

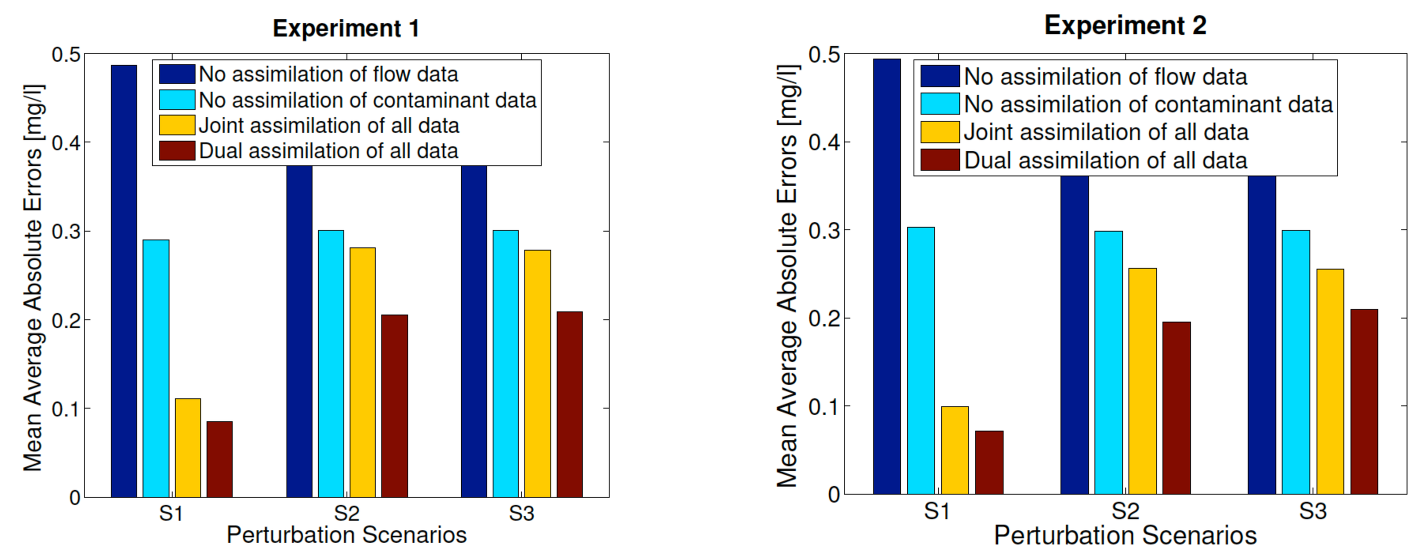
Transport Model ($\widetilde{x}$): $\dfrac{\partial\left(\phi R_d C\right)}{\partial t} + \nabla \cdot \left(uC - D(u)\nabla C\right) = q_C.$

We performed three different experiments with different observation strategies. In each experiment, three perturbation scenarios are conducted.



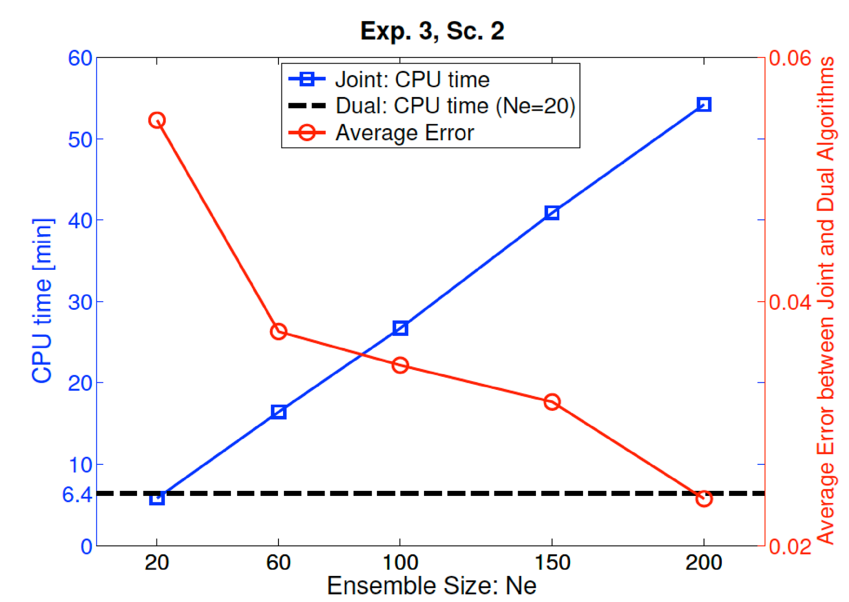
Plotted below are the recovered contaminant fields using joint and dual EnKF schemes (Exp. 1 and Sc. 1), the average absolute error of the estimated contaminant state using both schemes, and comparison of the computational complexity.





4. DISCUSSION

- With perfect forecast flow and transport models, the joint algorithm performs equally well as the dual algorithm.
- Adding modeling errors to the coupled forecast models degrades the accuracy of the joint estimates.
- When large observational errors are imposed on the data, the dual approach provides more accurate results than the joint technique even when fewer observations are assimilated over time.
- The computational cost of using the dual technique, although higher than that of the joint approach, is more beneficial than the joint algorithm with large ensemble sizes.



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