H31F-1462
LA-UR-16-29323

Identifying Aquifer Heterogeneities using the Level Set Method

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ABSTRACT

Material interfaces between hydrostatigraphic units (HSU) with contrasting aquifer parameters (e.g., strata and facies with different hydraulic conductivity) have a great impact on flow and contaminant transport in subsurface. However, the identification of HSU shape in the subsurface is challenging and typically relies on tomographic approaches where a series of steady-state/transient head measurements at spatially distributed observation locations are analyzed using inverse models. In this study, we developed a mathematically rigorous approach for identifying material interfaces among any arbitrary number of HSUs using the level set method. The approach has been tested first with several synthetic cases, where the true spatial distribution of HSUs was assumed to be known and the head measurements were taken from the flow simulation with the true parameter fields. These synthetic inversion examples demonstrate that the level set method is capable of characterizing the spatial distribution of the heterogeneity. We then applied the methodology to a large-scale problem in which the spatial distribution of pumping wells and observation well screens is consistent with the actual aquifer contamination (chromium) site at the Los Alamos National Laboratory (LANL). In this way, we test the applicability of the methodology at an actual site. We also present preliminary results using the actual LANL site data. We also investigated the impact of the number of pumping/observation wells and the drawdown observation frequencies/intervals on the quality of the inversion results. We also examined the uncertainties associated with the estimated HSU shapes, and the accuracy of the results under different hydraulic-conductivity contrasts between the HSU's.

Motivations

Traditionally, model calibration involves two major steps:

- A geological conceptual model (e.g. interfaces between stratigraphic/faulted units) is created based on geological information (borehole logs, out-crops, etc.).
- The parameter values (e.g. permeability) associated with the geological units are calibrated using measurements of state variables (drawdowns/pressure head, saturation, solute concentration).

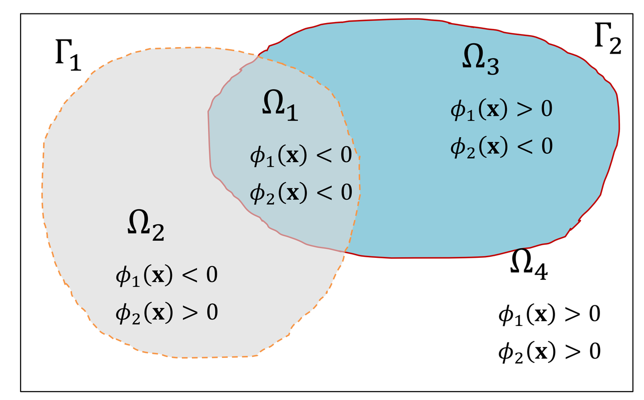
Certainly there is a gap between building a geological conceptual model and calibrating the model: In building a conceptual model, measurements on state variables are not used, while in calibrating the model, the interfaces between stratigraphic/faulted zones cannot be modified (unless manually).

- ✓ If the simulated state variables do not fit the observed data, one may need to modify the conceptual model and run inverse modeling again, which is very tedious because there may be a large number of alternative conceptual models.
- ✓ Estimation of parameter zonation is probably one of the most difficult inversion problems.
- ✓ A major difficulty for automatic modification of the conceptual model lies in parameterization of complex interfaces between stratigraphic units.

The level-set method provides an effective way to characterize complex shapes, and the shapes (or their interfaces) evolve from an initial guess to fit the observed data.

Methodology

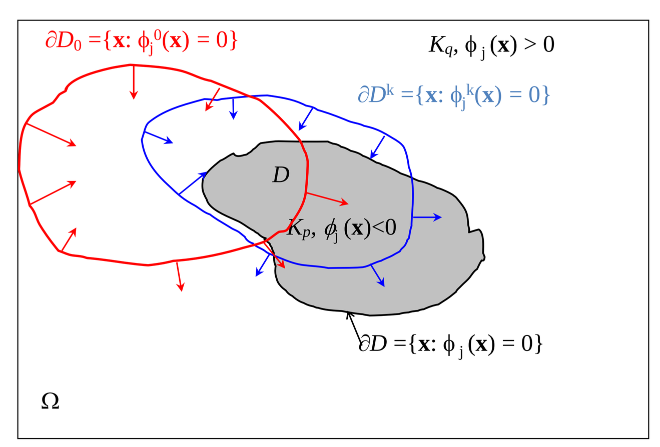
- Zonal heterogeneity is represented by a set of level-set functions (LSFs):



- These LSFs are initialized with an initial guess zonation;
- LSFs are updated by solving level-set equations:

$$\frac{\partial \phi_j(\mathbf{x},t)}{\partial t} + \alpha_{pq}(\mathbf{x},t)\left|\nabla \phi_j(\mathbf{x},t)\right| = 0$$

where $\alpha_{pq}(\mathbf{x},t)$ is the propagation velocity at the interface between materials p and q..



- We need to minimize the objective function

$$F(K) = \frac{1}{2}\|\boldsymbol{h}(K) - \boldsymbol{h}_m\|$$

where $\boldsymbol{h}_m$ is measured head and $\boldsymbol{h}(K)$ is simulated head. If we assume that the parameter (permeability/specific storage) values are known but the locations of the material interfaces are unknown, one chooses [1,2]

$$\alpha_{pq}(\mathbf{x},t) = sign(K_q - K_p)\boldsymbol{J}^T(K)(\boldsymbol{h}(K) - \boldsymbol{h}_m)$$

where $\boldsymbol{J} = (\mathrm{d}\boldsymbol{h}/\mathrm{d}K)$ is the Jacobian matrix, which can be calculated using the adjoint method[3]. This selection of $\alpha_{pq}(\mathbf{x},t)$ensures that the variation of the objective function is negative:

$$\delta F(K) = -\sum_{p,q}\int_{\Omega_{pq}}\left[\alpha_{pq}(\mathbf{x},t)\right]^2 d\mathbf{x} < 0$$

- We may also update piece-wise parameter values (for given interfaces)

$$\delta K_i = -|\Omega_i| J^T(K_i)[\mathbf{h}(K) - \mathbf{h}_m]$$

which leads to

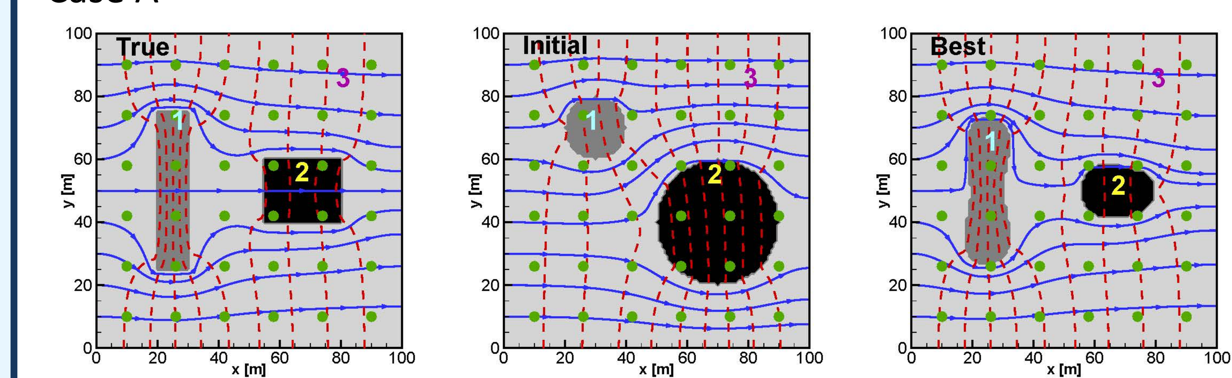
$$\delta F(K) = \sum_{i=1}^{M}\delta K_i \int_{\Omega_i} J^T(K_i)[\mathbf{h}(K) - \mathbf{h}_m] < 0$$

The interface locations and parameter values may be updated alternately.

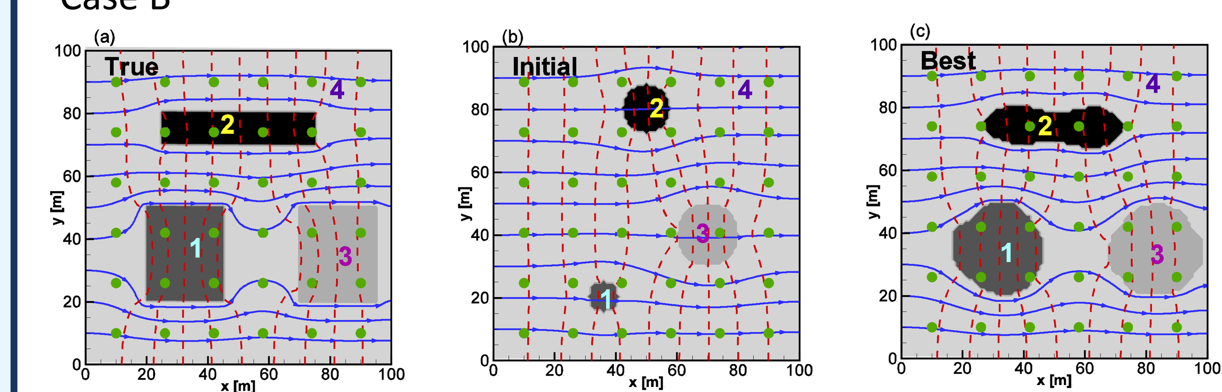
Illustrative Examples

1. We consider two-dimensional inverse problems with a number of materials to be identified, using steady-state head "measurements" simulated with the "true" parameter zonation.

Case A



Case B

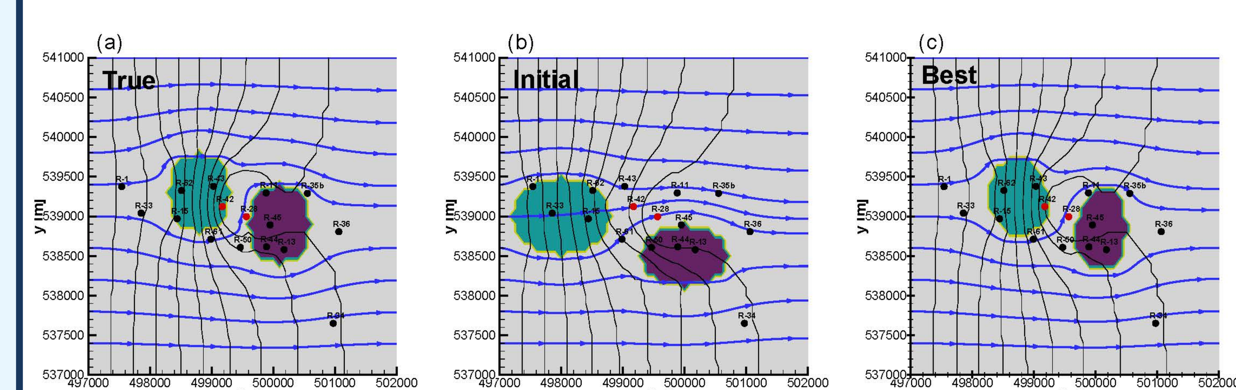


"True" field | Initial guess | The best solution out of 400 iterations

2.LANL Chromium site.

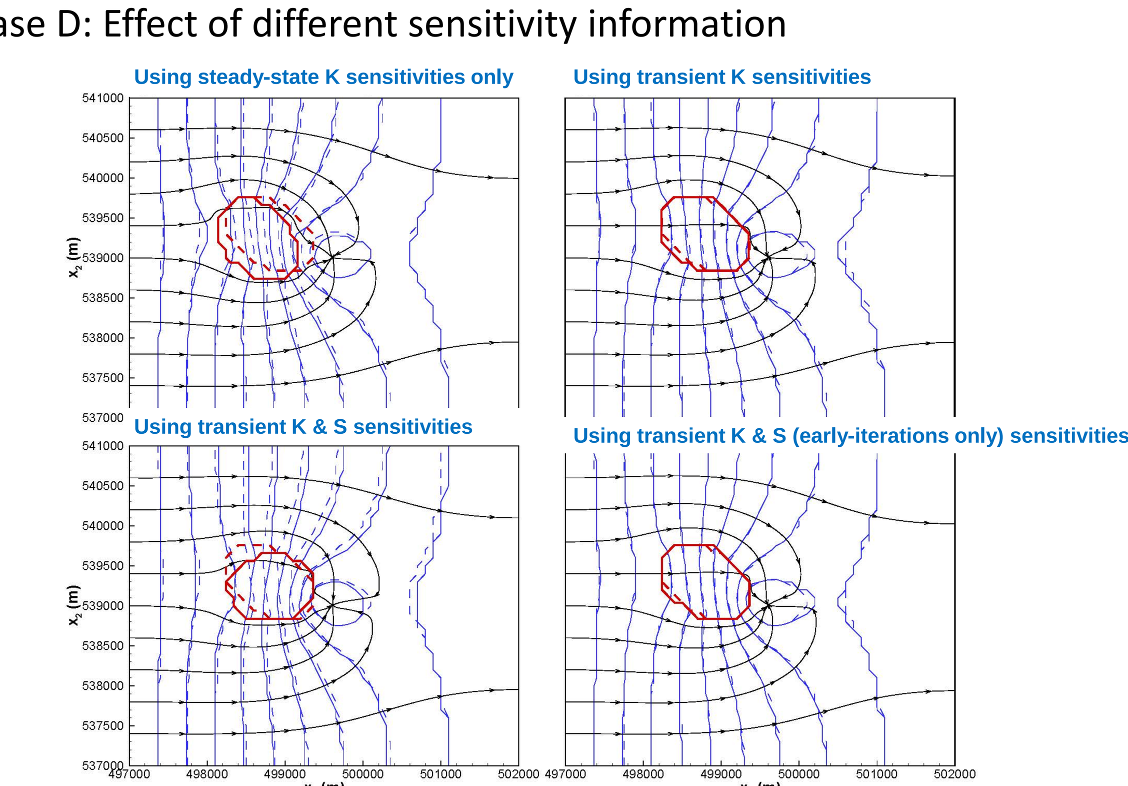
- 2D domain, as the flow in the regional aquafer is nearly horizontal;
- 2 pumping wells (red dots) with variable pumping rates;
- 22 transient drawdowns at each of 14 observation wells/screens (black dots);

Case C: Three materials; transient drawdown at 14 wells



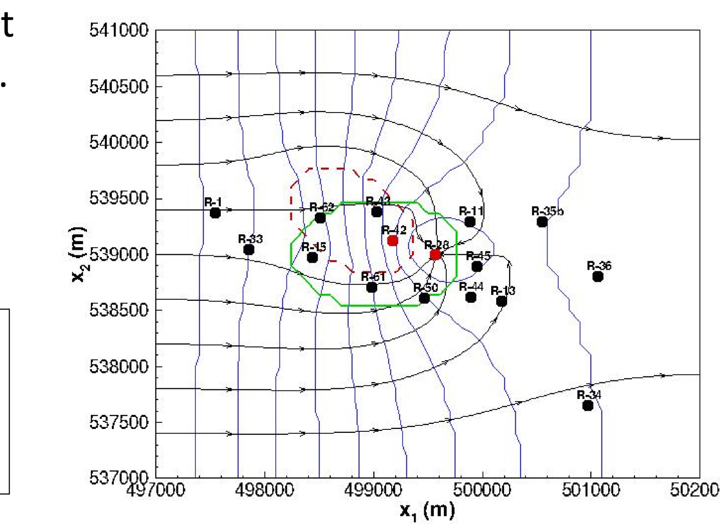
Note: This is again a test case, because the pumping rates are arbitrary chosen and the drawdown at the observation wells are simulated from a selected "true" parameter zonation.

Case D: Effect of different sensitivity information

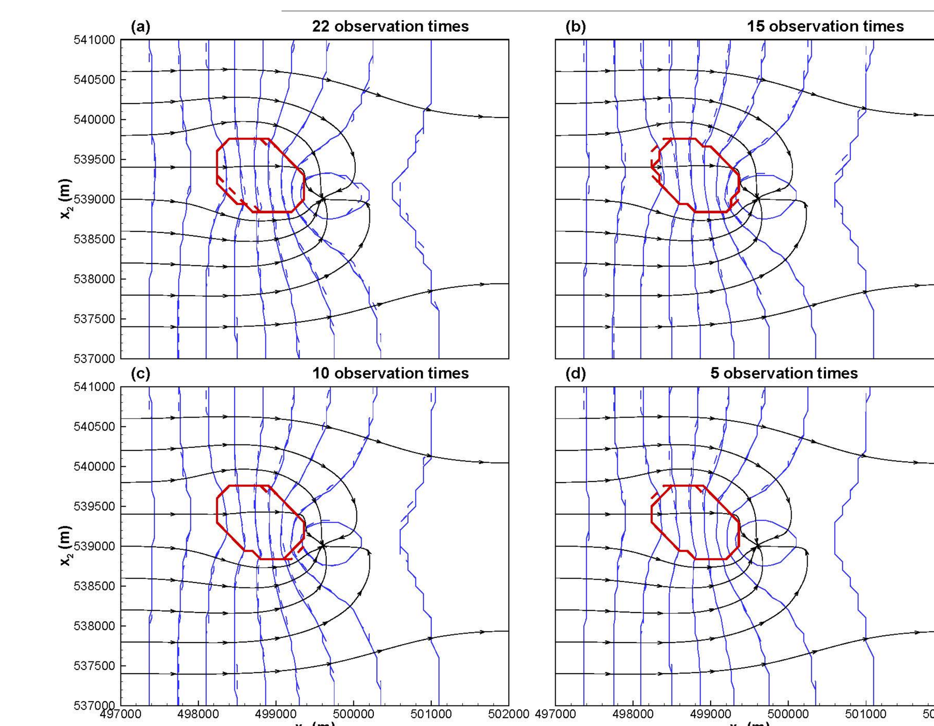


Dashed: **"True" low-perm zone**
Solid: **Inversion result**

Case E: Effect of different observation frequencies.



Green: **Initial guess**
Dashed: **"True"**
Solid: **Inversion result**



Conclusions

1. Through mathematically rigorous derivations, we extended the level-set method for identifying zonation in a binary system [4,5] to an arbitrary number of materials.
2. The propagation speed at points on any material interface is proportional to the parameter contrast between materials on the two sides of the interface.
3. Including transient data, especially at earlier times, improves the inversion results.
4. This approach ensures that the residual always decreases, which means that the solution converges to a local minimum. In other words, the solution is highly dependent on the initial guess field. To overcome this, one may start a set of inverse model runs with various initial guesses.

References

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