Development of a reliable hydraulic conductivity upscaling tool for high dimensional groundwater flow models

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1. Overview

Porous media in nature exhibit complex and irregular geometry and structure at different scales. Understanding of the underlying heterogeneity is key to the accurate description of groundwater flow and transport processes. Specifically, the appropriate representation of hydraulic conductivity at different scales is the first step for constructing a numerical groundwater model for use in field applications. In this presentation, we revisit the hydraulic conductivity upscaling approach of Kitanids [1990], which is valid **under the assumption of gradually varying flow**, and develop **an efficient open-source computational tool** to provide researchers and field practitioners **upscaled hydraulic conductivity fields**, in a tensor form that accounts for anisotropy, of any arbitrary size from fine resolution ones. We test our tool with high dimensional 2D fine-scale model upscaling examples and compare fine-scale head fluctuations with coarse-scale counterparts. We also investigate how robust our proposed tool can work for cases with different degrees of variability, anisotropy, and scales.

2. Theoretical Backgrounds

1) From fine-scale hydraulic conductivity field K, we would like to find the equivalent effective conductivity tensor K^e at any larger continuum scale:

$$\nabla\cdot\left[K\nabla\phi\right] \approx \nabla\cdot\left[K^e\nabla\phi^e\right] = q \qquad K^e = \begin{vmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{xy} \end{vmatrix} \qquad (1)$$

where K^e [L/T] is the effective conductivity tensor and Φ and Φ^e [L] are the fine-scale and upscaled hydraulic heads, respectively.

2) With the method of moments under the assumption of gradually vary flow (Kitanids, 1990):

$$\nabla\cdot\left[K(x)\nabla g^i(x)\right] = \nabla\cdot k_i(x) \qquad i = 1,\ \cdots,\ n \quad (n\le 3) \qquad (2)$$

$$K_{ij}^e = -\frac{1}{2V}\int_V \left(k_i\cdot\nabla g^j + k_j\cdot\nabla g^i\right)\,dx + \bar{K}_{ij} \qquad (3)$$

where $g^i(x)$ is the unknown auxiliary function, n is the dimension of the flow domain, k_i is the i^{th} column of K.

3) Then, the effective conductivity on the discretized domain can be computed as:

$$\sum_{p=1}^{n}\frac{\partial}{\partial x_p}\left(K\frac{\partial g^i}{\partial x_p}\right) = \frac{\partial K}{\partial x_i} \qquad i = 1,\ \cdots,\ n \quad (n\le 3) \qquad (4)$$

$$K_{ij}^e = -\frac{1}{2V}\int_v K\left(\frac{\partial g^j}{\partial x_i} + \frac{\partial g^i}{\partial x_j}\right)dx + \bar{K}\delta_{ij} \qquad (5)$$

3. Numerical Implementation in Python

3.1. Fourier Galerkin Method

The Fourier Galerkin method is used to solve Eq. (4) and (5). Applying this methodology, first expand K and g^i in their respective truncated Fourier series:

$$K(x) \approx \sum_{|k|\le k^c}\hat{K}_k e^{i2\pi x\cdot f} \qquad g^i(x) \approx \sum_{|k|\le k^c}\hat{g}_k^i e^{i2\pi x\cdot f}$$

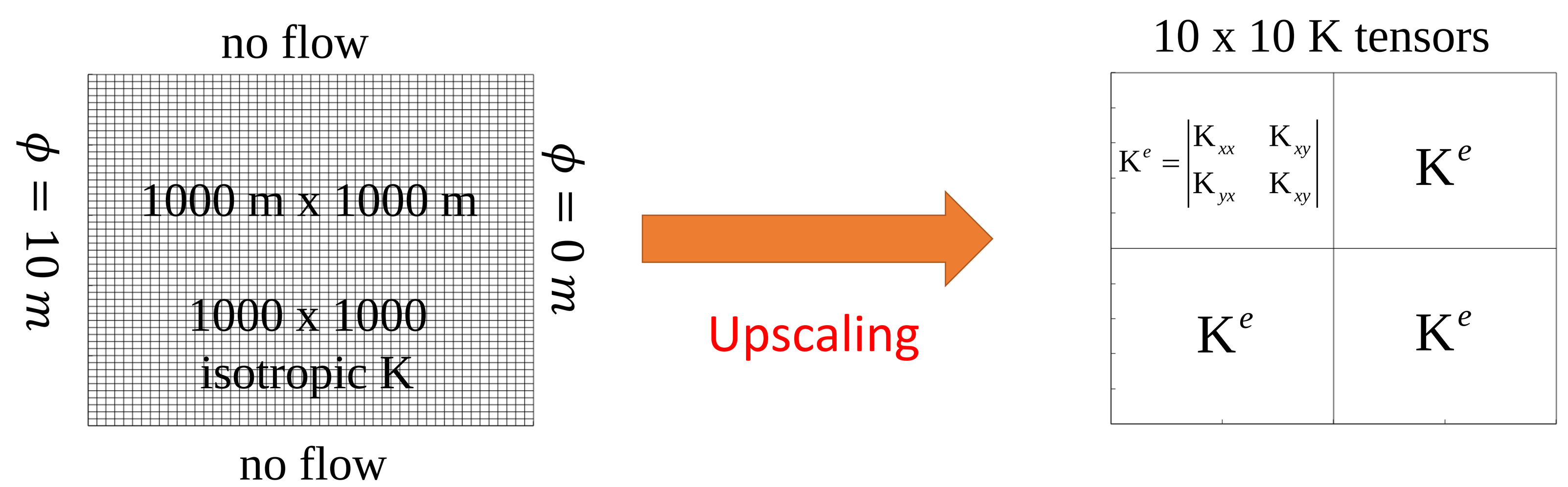
Then, Eq. (4) becomes a linear system using a spectral approach:

$$A\hat{g}^i = i\,\bar{m}_i \circ \hat{K} \qquad A = -\sum_{i=1}^{2} D_{m_i}\left(F\otimes F\right)D_K\left(F^*\otimes F^*\right)D_{m_i}$$

where F and F* are DFT and IDFT matrix, and D_m and D_k are a diagonal matrix with the entries of the vector **m** and **K** as the diagonal entries, respectively.

3.2. Groundwater Flow in MODFLOW6 with USGS Flopy

- 2D flow simulations with MODFLOW6 on a domain (1000 m x 1000 m) with constant head boundary/no-flow conditions.
- We compute **10 x 10 2D K tensors from 1000 x 1000 isotropic K.**



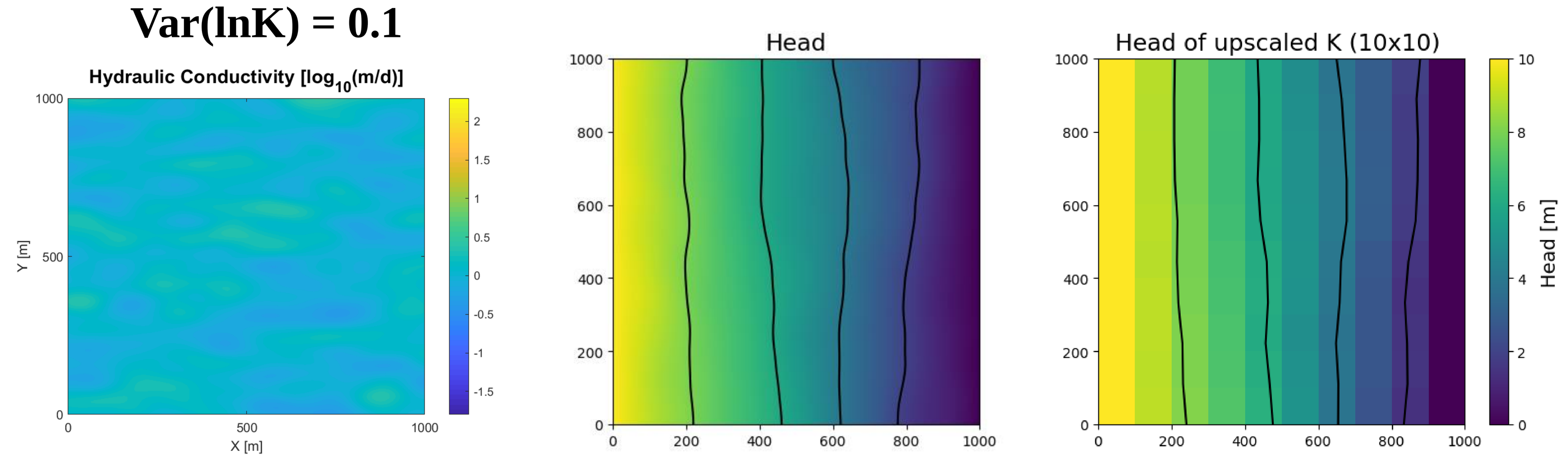
- Using use the "XT3D" option for simulation with K tensor
- **Took only 3 mins** to compute 10 x 10 2D K tensors from 1000 x 1000 K grid on a laptop

4. Results

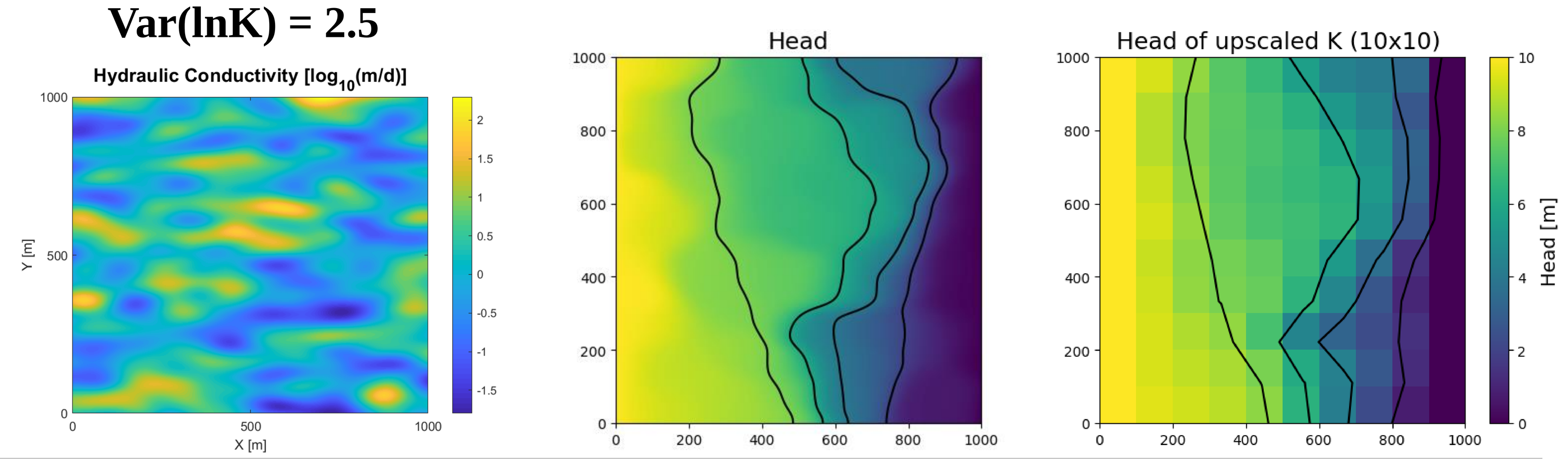
We illustrate the results exploring (1) the impact of K variability, (2) rotation angle in K anisotropy, and (3) the effects of high-K inclusions.

(1) Anisotropic K with different variability (Gaussian w/ 250, 50 m)

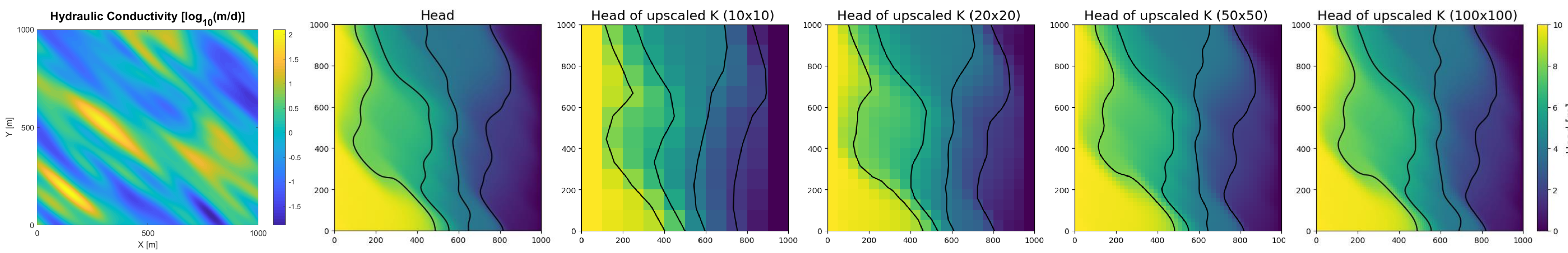
Var(lnK) = 0.1

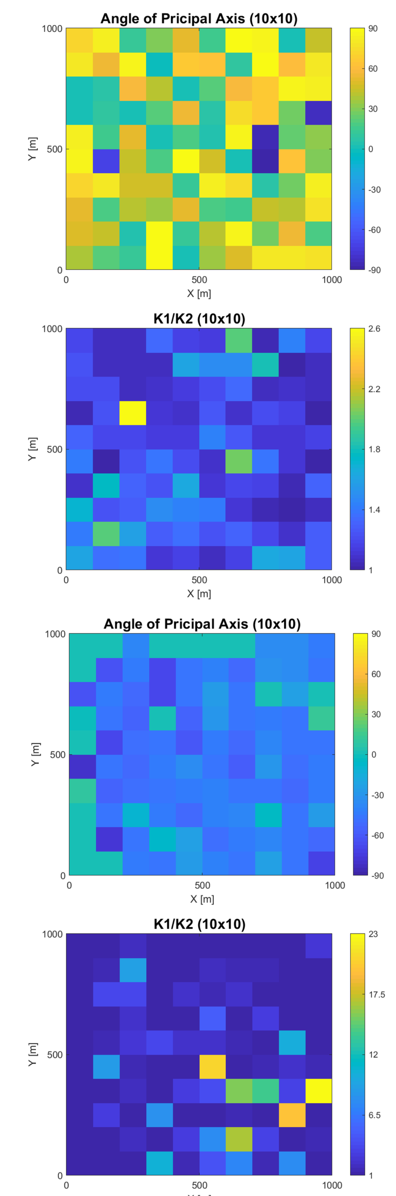


Var(lnK) = 2.5



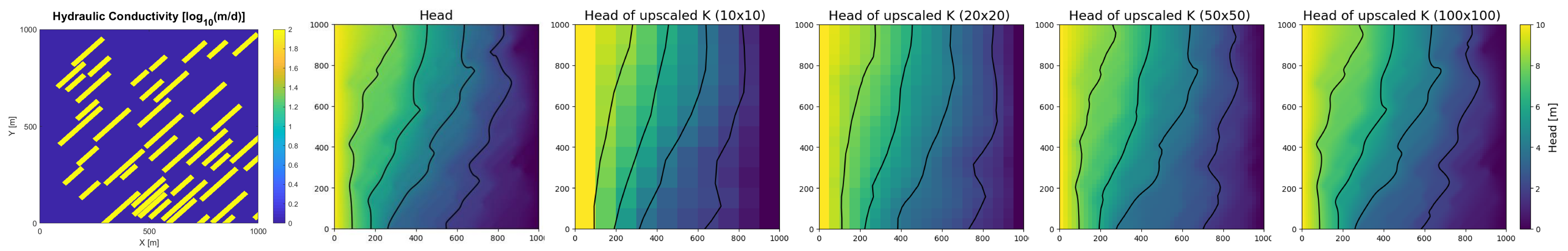
(2) 45 degree rotated anisotropic K with var(lnK) = 1.6, Gaussian covariance kernel with correlation length = [250 m, 50 m]





(3) High K inclusions

Original (1000x1000 grid) **Upscaled (10x10 grid)** **Upscaled (100x100 grid)**



5. Concluding Remarks and Future Works

- We develop a computationally efficient K upscaling tool to obtain K tensors at any continuum scale.
- Numerical tests show that our proposed method produces upscaled K tensors accurately.
- Our software package is in a Github repository (https://github.com/jonghyunharrylee)
- The developed K upscaling approach will be extended to dispersion tensor computation.

6. References

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