### SIMULATION ERROR IN GROUNDWATER MODELS WITH RECTANGULAR AND NON RECTANGULAR DISCRETIZATION

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Session HW2004: Towards Improved Evaluation of Hydrological Models: The Need to Understand and Characterize Uncertainties in the Modelling Process E. Rozos and D. Koutsoyiannis, Department of Water Resources, National Technical University of Athens

#### 1. Abstract

The error of groundwater numerical models depends on the boundary conditions, the hydraulic conditions-properties of the aquifer, the geometry of the flow field, the parameterization used to describe the heterogeneity of hydraulic field, the measurements and the discretization. In this study we focus on the dependence of the error to the type and resolution of the spatial discretization. Using a 2D stochastic model, we produced a synthetic field of 100×100 hydraulic transmissivities and then we used a finite differences model (MODFLOW) to obtain synthetic measurements of hydraulic head. Hereupon we used 4 grids (100×100, 50×50, 20×20, 12×12) and a simple parameterization (6 zones of homogeneous conductivity), common for all grids, along with a parameter estimation algorithm based on a modified Gauss-Newton method. Moreover we used 3dkflow, a model based on finite volumes method with simplified integration that uses a non rectangular sparse discretization (43 cells) in conjunction with the Shuffled Complex Evolution optimization algorithm. By assessing the simulations of the 4 rectangular grids and the sparse non rectangular discretization we concluded that to keep the model error low a reliable parameterization along with a rectangular grid of high resolution should be used. Alternatively a sparse non rectangular spatial discretization can keep the error small and is more advantageous in the applications that require simulation speed.

### 2. Synthetic data

A 2D stochastic model is used to produce 100×100 synthetic transmissivity values (Theodoratos, 2004).



Uniform intermittent recharge is applied to the aquifer along with a rank of drains at the middle section of the top side and a rank of intermittent injecting wells at the left section of the bottom side.





# 3. Discretization-ParametYrrization with 3dkflow



The concept of the 3dkflow model is described by Rozos and Koutsoyiannis (2005) and by Rozos and Koutsoyiannis (2006). The 3dkflow cells design was based on the most representative contours map for the whole simulation of the hypothetic aquifer.



# 4. Discretization-Parameterization with MODFLOW







## 5. Comparison of 4 MODFLOW models and 3dkflow model results

Scatter diagram of estimated parameters with the 5 models versus reference values.

- Estimated parameters using MODFLOW with a 100×100 grid are almost identical with reference values.
- Parameters estimation using 3dkflow with 43 cells is as good as those using MODFLOW with a 12×12 grid.

Models RMS error of simulated hydraulic heads with respect of the number of grid points.

- With the help of the trend line it is estimated that the RMS of 3dkflow is almost as low as the RMS of the 50×50 grid.
- The MODFLOW with a discretization of only 43 cells would result in an RMS of 19.12 m.

#### References

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•Rozos, E., and D. Koutsoyiannis, Application of the Integrated Finite Difference Method in groundwater flow, 2nd General Assembly of the European Geosciences Union, Geophysical Research Abstracts, Vol. 7, Vienna, 00579, European Geosciences Union, 2005.

 Theodoratos, N., Stochastic simulation of two-dimensional random fields with preservation of persistence, Diploma thesis, 69 pages, Department of Water Resources, Hydraulic and Maritime Engineering -National Technical University of Athens, Athens, July 2004.

### 6. Conclusions

- MODFLOW combined with a optimization algorithm can estimate reliably the hydraulic parameters and can simulate very accurately an aquifer provided that a dense discretization is used.
- If a sparse discretization is imposed either by the lack of data and/or the need for fast calculations, models with non rectangular discretization, like the 3dkflow, can achieve more reliable parameters estimation and better simulation accuracy.
- The derivative based (Gauss-Newton) algorithm converggu much faster than Shuffled Complex Evolution.
  For problems with very few parameters, the derivative based algorithms may be the indicated choice. Nevertheless for complex problems, a global optimization algorithm is imperative since it is not trapped easily at local minimums.