Modelleichung und Schätzung der Unsicherheiten In Modellprognosen mit inversen Methoden

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Why do we calibrate models ?
Theoretical frameworks
Parametrization approach
Real case example

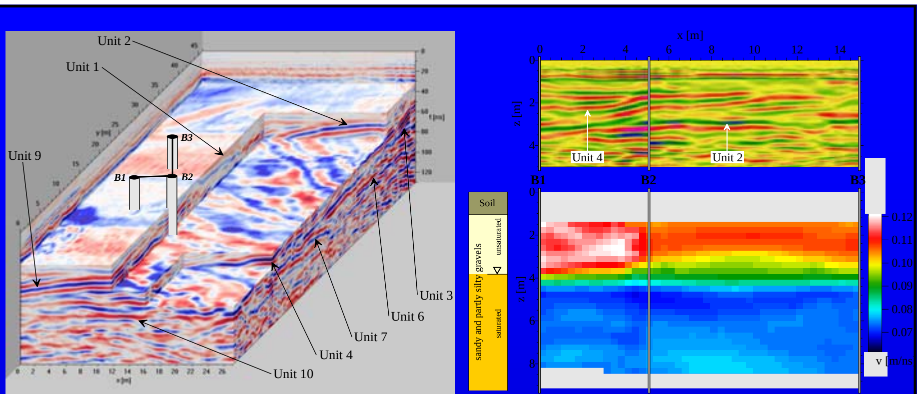
Groundwater Model

Mathematical model
Modeling of the processes
Numerical solutions

Geological model
Heterogeneity
Parameters

Interesting for
– Interpolation
– Scenarios
– Sampling strategy
– Sensitivity analysis

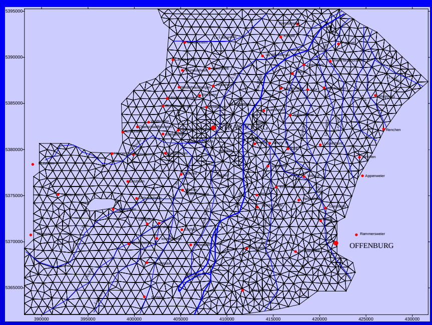
Many scales are involved



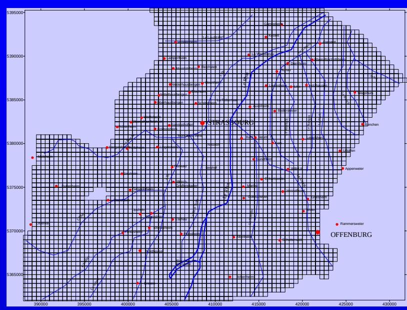
	Grain size	Micro-moulinet	Pumping test
	K (m/s)	K(m/s)	T/e (m/s)
Nbre of meas.	318	207	20
Minimum	$1.5\ 10^{-5}$	$3.4\ 10^{-5}$	$8.7\ 10^{-4}$
Maximum	0.21	$1.9\ 10^{-2}$	$3.9\ 10^{-3}$
Average (geo.)	$1.5\ 10^{-3}$	$1.9\ 10^{-3}$	$2.5\ 10^{-3}$
Variance (LnK)	2.56	1.43	0.264

From Ptak & Teutsch, 1994

Comparisons of two calibrated models



HPP



MODFLOW

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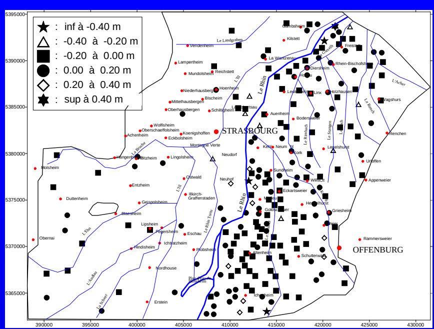

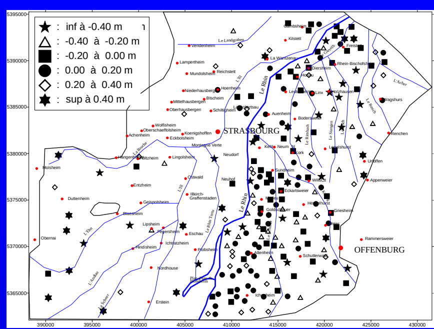

Match between computed and measured heads

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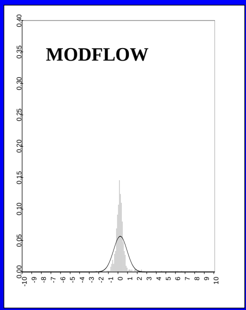
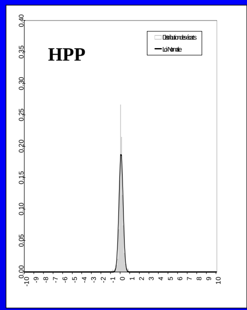
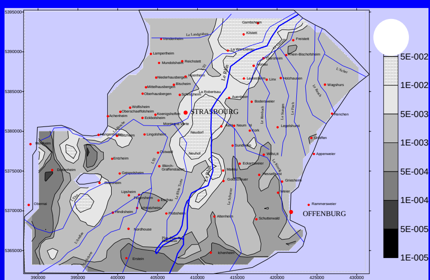
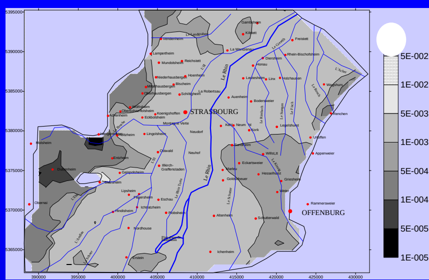
Analysis of the residuals

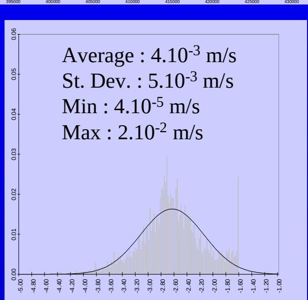


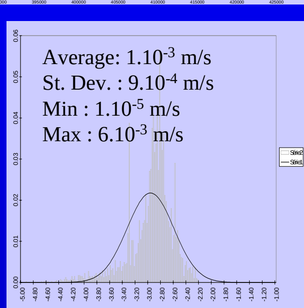


		Average (m)	St. Dev. (m)	Min. (m)	Max.(m)
Low water	HPP-INV	-0.06	0.21	-0.91	0.54
	MODFLOW	0.02	0.37	-2.31	1.03
Average water	HPP-INV	-0.01	0.15	-0.87	0.66
	MODFLOW	-0.01	0.40	-1.16	2.34
High water	HPP-INV	0.06	0.23	-0.65	0.77
	MODFLOW	0.39	1.04	-0.76	8.06
All	HPP-INV	0.00	0.20	-0.91	0.77
	MODFLOW	0.14	0.70	-2.31	8.06

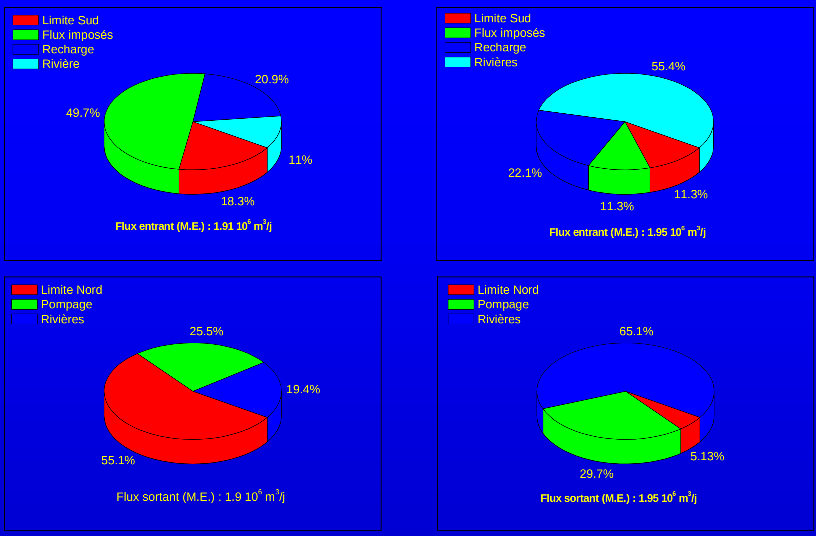








Hydraulic conductivity distribution



WATER BALANCES HPP WATER BAL. MODFLOW

Main difficulties of model calibration by trial and error

- Very time consuming
- Difficulty in handling large data sets
- Simplified parameterization (zonation)
- All possible solutions cannot be analyzed

Inverse approach

Objectives :
Differences between observations and simulations should be as small as possible

Differences between observations and simulations ….

$$J(p)=\sum_{i=1}^{nm}\sigma_i(h_{mi}-\hat{h}(p)_i)^2$$

$$J(p)=\sum_{i=1}^{nm}\sigma_i(h_{mi}-\hat{h}(p)_i)^2+\sum_{j=1}^{nn}\lambda_j(h_{u,j}-\hat{h}(p)_i)^2+\lambda_p\sum_{k=1}^{np}\left[\left(\frac{\partial p_k}{\partial x}\right)^2+\left(\frac{\partial p_k}{\partial y}\right)^2\right]$$

…. should be as small as possible.

$$\frac{\partial J(p)}{\partial p_k}=\sum_i^n\frac{1}{\sigma_{hi}^2}(h_i^{n+1}(p)-h_{obs,i}{}^{n+1})\frac{\partial h_i^{n+1}(p)}{\partial p_k}=0$$

Results interpretation

Analysis of the residuals $\varepsilon_i=\left(h(p)-h_m\right)_i$

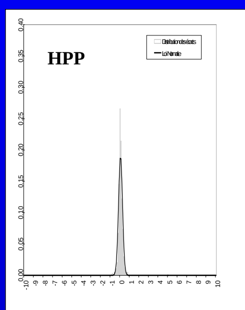
⇨ Graphical representation of the results

⇨ Histogram of the residuals

⇨ Objective function value

If the results are consistent with the theory, the residuals have a gaussian distribution with zero mean and standard deviation of 1

$$\frac{J(p)}{nm-np}\approx 1$$



First order analysis: Parameter confidence interval

$$[J_{ac}]_{(n\times np)} = \begin{bmatrix} \frac{\partial h_1}{\partial p_1} & \frac{\partial h_1}{\partial p_2} & .. & \frac{\partial h_1}{\partial p_k} & .. & \frac{\partial h_1}{\partial p_{np}} \\ .. & .. & .. & .. & .. & .. \\ .. & . & .. & . & .. & . \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ \frac{\partial h_n}{\partial p_1} & \frac{\partial h_n}{\partial p_2} & .. & \frac{\partial h_n}{\partial p_k} & .. & \frac{\partial h_n}{\partial p_{np}} \end{bmatrix}$$

Sensitivity matrix

Covariance matrix

$$C = \left(J^T W^{-1} J\right)^{-1}$$

Uncertainty

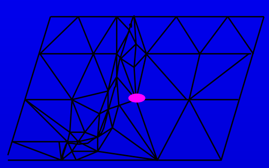
$$\Delta p_k = \pm \sqrt{J(p)}\,\sqrt{C_{kk}}$$

Correlation matrix

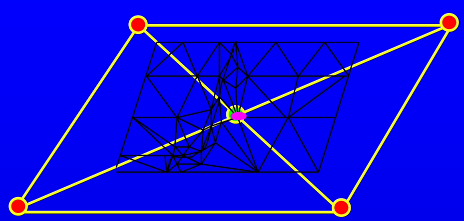
$$CR_{ij} = \frac{C_{ij}}{\sqrt{C_{ii}\,C_{jj}}}$$

Parametrization by interpolation and downscaling

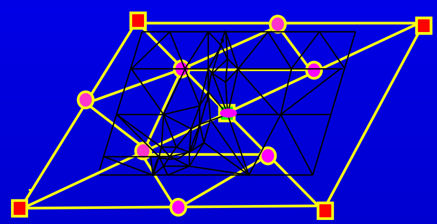
$$p(X) = \sum_{i=1}^{N_p} \hat{p}_i \Phi_i(X)$$



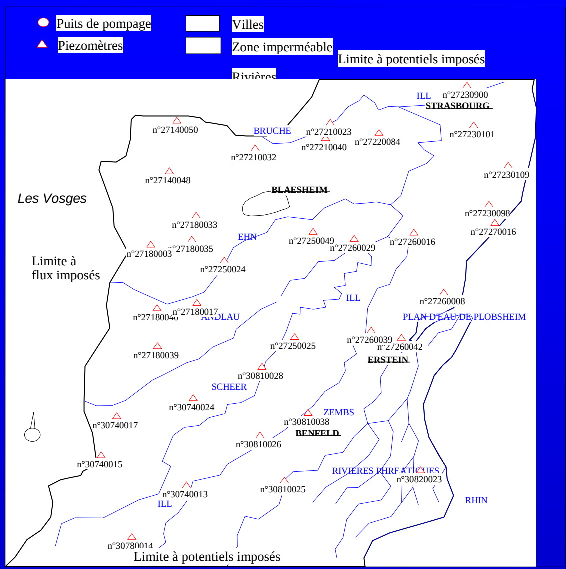
GW model mesh



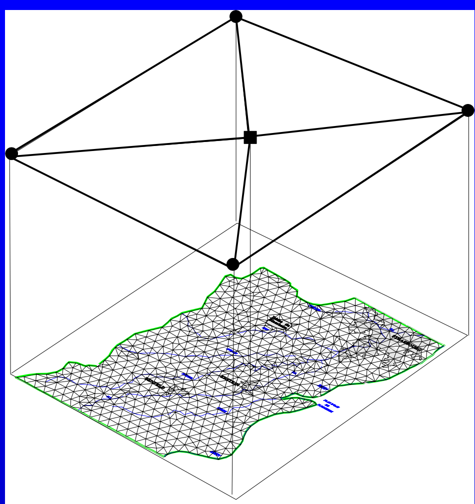
First scale



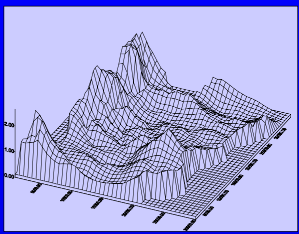
Second scale



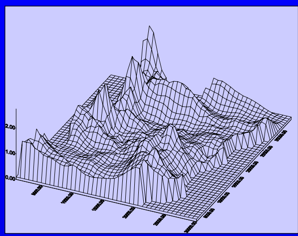
Initial parameterization



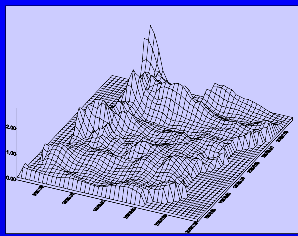
Distribution of $\sigma_K/\bar{K}$



$J(p) = J_h$



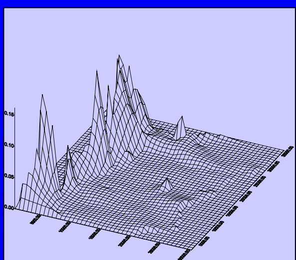
$J(p) = J_h + J_u$



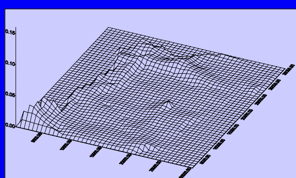
$J(p) = J_h + J_u + J_r$

Function	Average	St. Dev.	Min	Max
Jh	0.790	0.473	0.099	2.823
Jh+Ju	0.758	0.400	0.071	3.115
Jh+Jrp+Ju	0.563	0.318	0.101	2.985

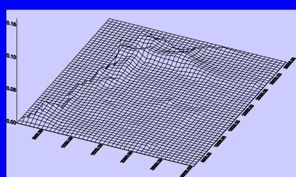
Distribution of $\sigma_h/\bar{h}$



$J(p) = J_h$

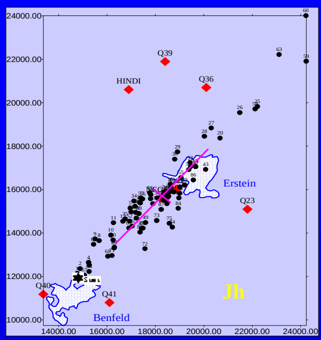


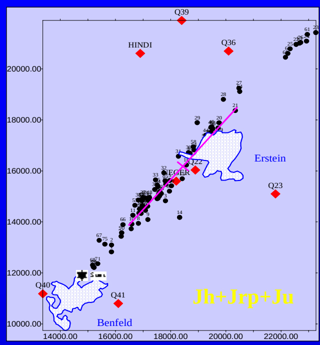
$J(p) = J_h + J_u$



$J(p) = J_h + J_u + J_r$

Function	Average	St. Dev.	Min	Max
Jh	0.10	0.024	0.000	0.17
Jh+Ju	0.04	0.004	0.000	0.16
Jh+Jrp+Ju	0.02	0.003	0.000	0.01





J(p)	Mx (m)	My (m)	σ_L(m)	σ_T(m)	θ (°)
Jh	18483.	15852.	3201.	569.77	48.70
Jh+Ju	18066.	15712.	3393.	502.68	51.38
Jh+Jrp+Ju	18444.	16180.	3020.	249.43	49.58

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Parameter estimation by inverse methods requires

An accurate objective function with an estimate of measurements errors

A consistent parameterization

Fast and robust numerical solutions (model, minimization)

Advantages of Model calibration by inverse methods

More time to think about the concepts

Theoretical framework for results analyses

Exploration of possible solutions

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