Worst-case scenario tools for Verification and Validation

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Outline

- **Problem setting: elliptic equations with uncertain input parameters**
- **Worst-Case Scenario approach: mathematical formulation and some examples**
- **On the Validation of a WCS model**
- **Solution strategy based on perturbation techniques: application to uncertainty in coeffs, forcing terms and boundary conds**
- **Verification issues**
- **Conclusions**

Model problem – linear elliptic equation

$$\begin{cases} -\operatorname{div}(\mathrm{A}\nabla u) + \mathrm{b}\cdot\nabla u + \sigma u = f & \textbf{in } D \\ u = g & \textbf{on } \Gamma_D \\ \Phi(u) := (\mathrm{A}\nabla u)\cdot \mathrm{n} = h & \textbf{on } \Gamma_N \end{cases}$$

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- **The solution u depends on**
  - **model's coefficients** $\beta = [A_{ij},\ b_i,\ \sigma]$
  - **forcing terms** $\mathcal{L} = [f,\ h]$
  - **Dirichlet boundary conditions** g

$$\boxed{\Longrightarrow \quad u = u(\beta, \mathcal{L}, g)}$$

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- **All the parameters** $\eta = (\beta, \mathcal{L}, g)$ **are supposed to be uncertain.**

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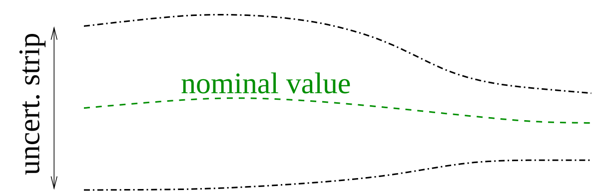

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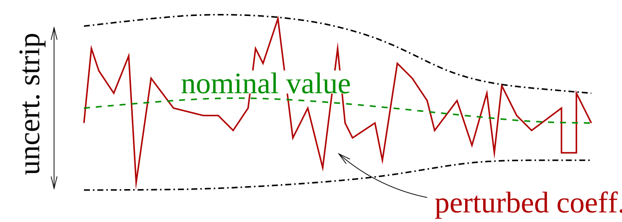

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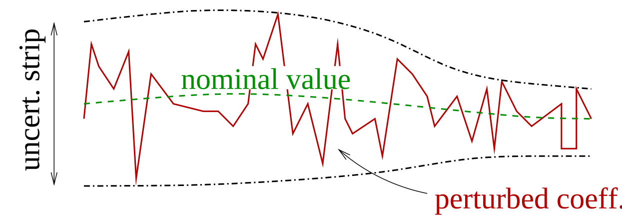

$$\mathcal{A}_\eta \equiv \{\eta = \eta_0 + \delta\eta, \quad |\delta\eta(x)| \leq \varepsilon_\eta(x), \ \forall x\}$$

- **Other parameter sets could be considered as well, with e.g. smoother perturbations. Computations get more involved.**

Goal of the analysis

- We focus on a specific feature of the solution: Quantity of interest

Examples :

$$\begin{cases} \text{local average of the solution} & Q = \displaystyle\int_{\omega \subset D} u \\ \text{local average of the flux} & Q = \displaystyle\int_{\omega \subset D} A \nabla u \cdot e_i \\ \text{boundary flux} & Q = \displaystyle\int_{\Gamma_D} \Phi(u) \end{cases}$$

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General form for the Q.o.I. $Q(\eta, u, \Phi) = Q_1(\eta, u) + Q_2(\Phi)$.

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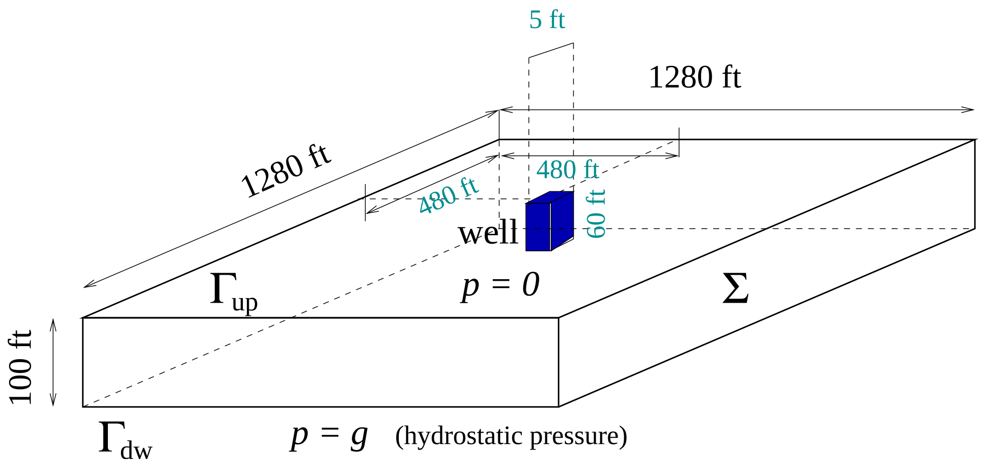
Worst scenario analysis
- compute $Q_0 = \psi(\eta_0)$ (nominal value)
- estimate $\Delta Q = \sup_{\eta\in\mathcal{A}_\eta} |\psi(\eta) - \psi(\eta_0)|$

Example: groundwater flow problem



- $\Gamma = \Gamma_{up} \cup \Gamma_{dw}$: **upper and lower surf.**
- Σ : **lateral surf.**
- β : **permeability**

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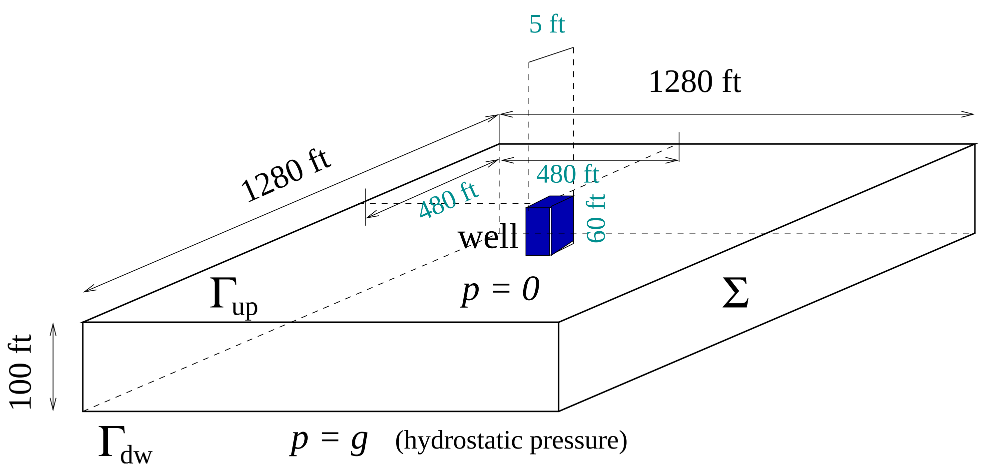

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Mathematical Model

$$\begin{cases} \mathrm{div}(\beta \nabla p) = 0 & \text{in } D \\ p = 0 & \text{on } \Gamma_{up} \\ p = g & \text{on } \Gamma_{dw} \\ \beta \partial_n p = 0 & \text{on } \Sigma \end{cases}$$

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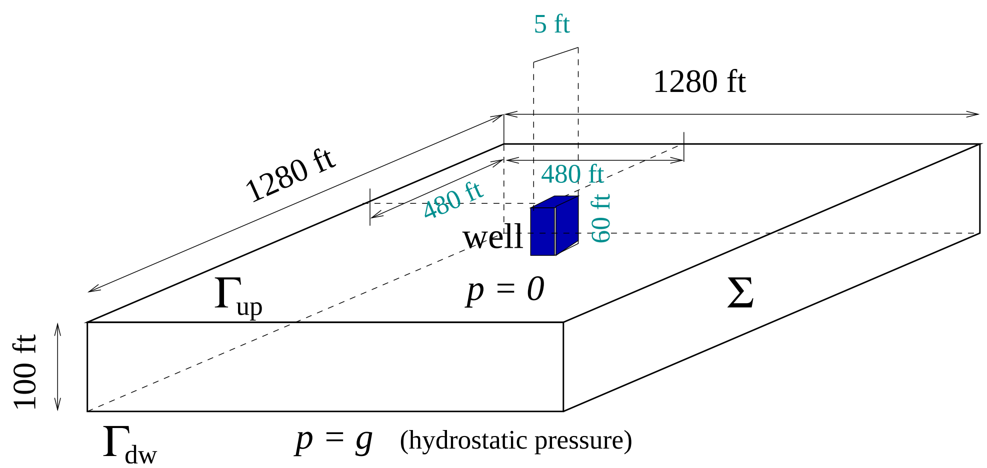

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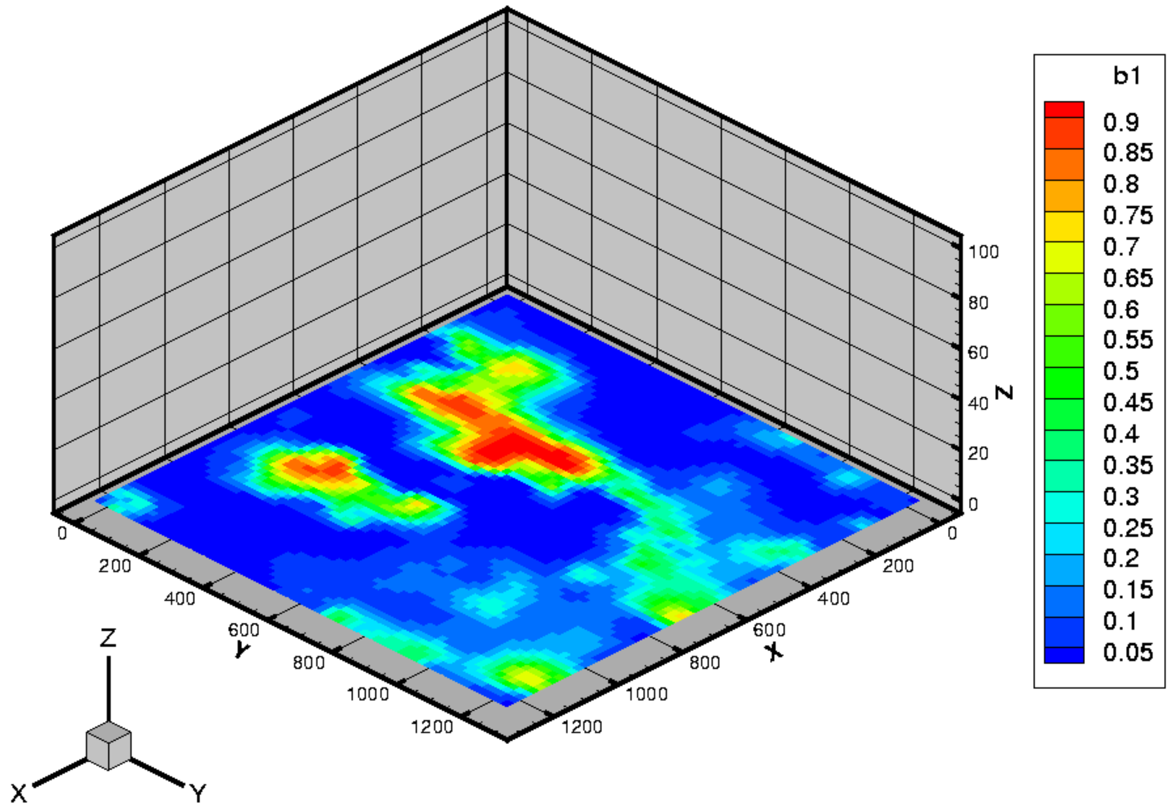
- **Q.o.I. extraction rate from the well:** $Q(p) = \int_{well} \beta \nabla p \cdot n$
- **uncertainty in permeability and bottom pressure.**

Permeability (real data)



depth $H = 100ft$

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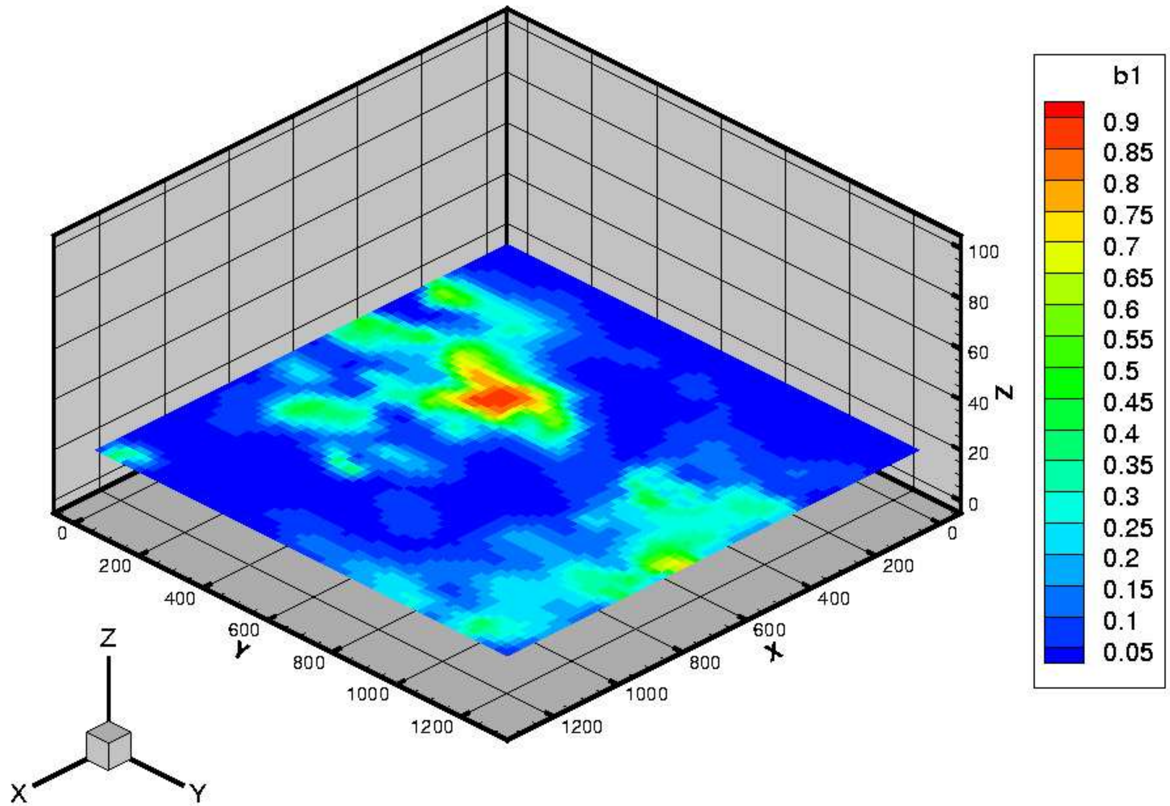

depth $H = 80ft$

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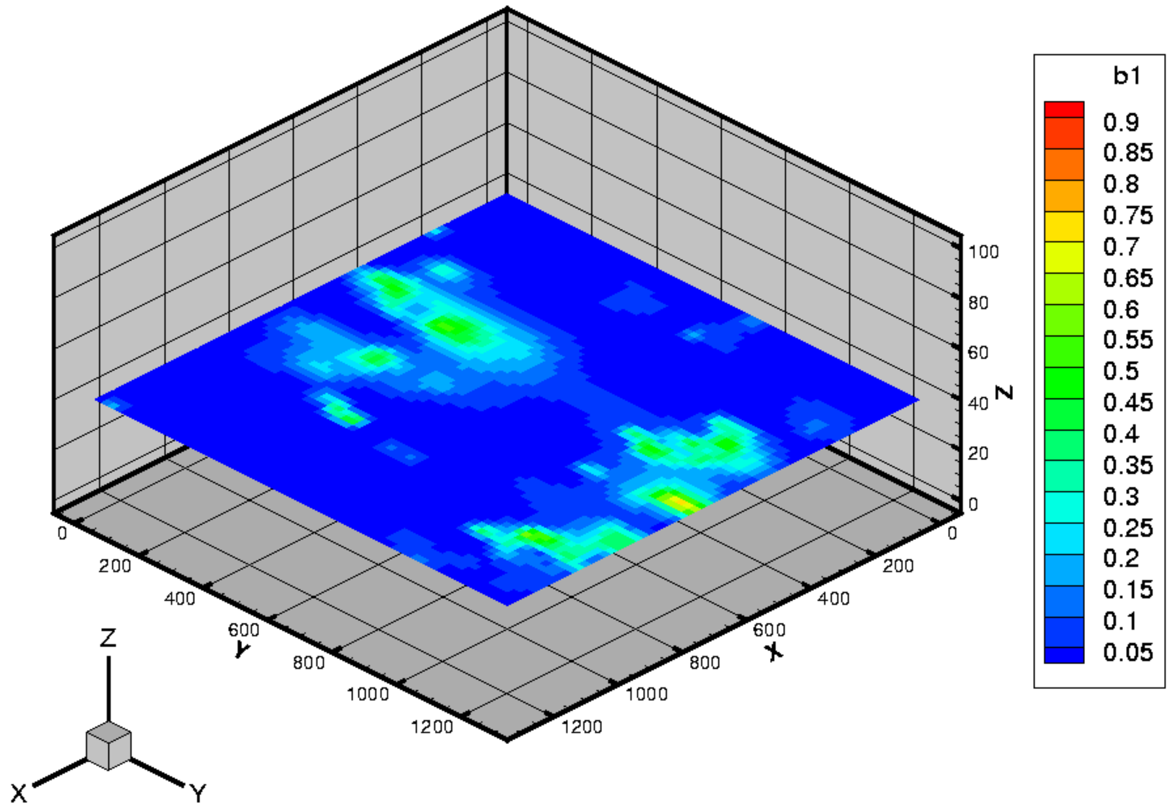
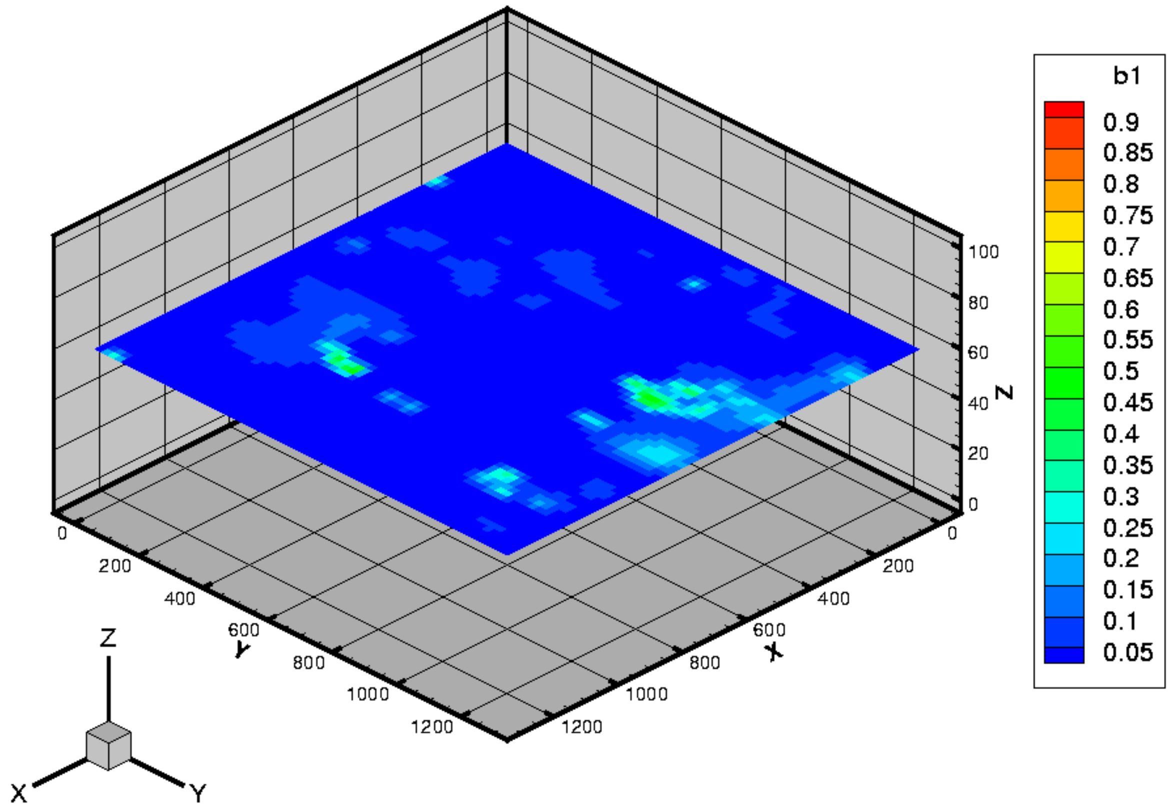


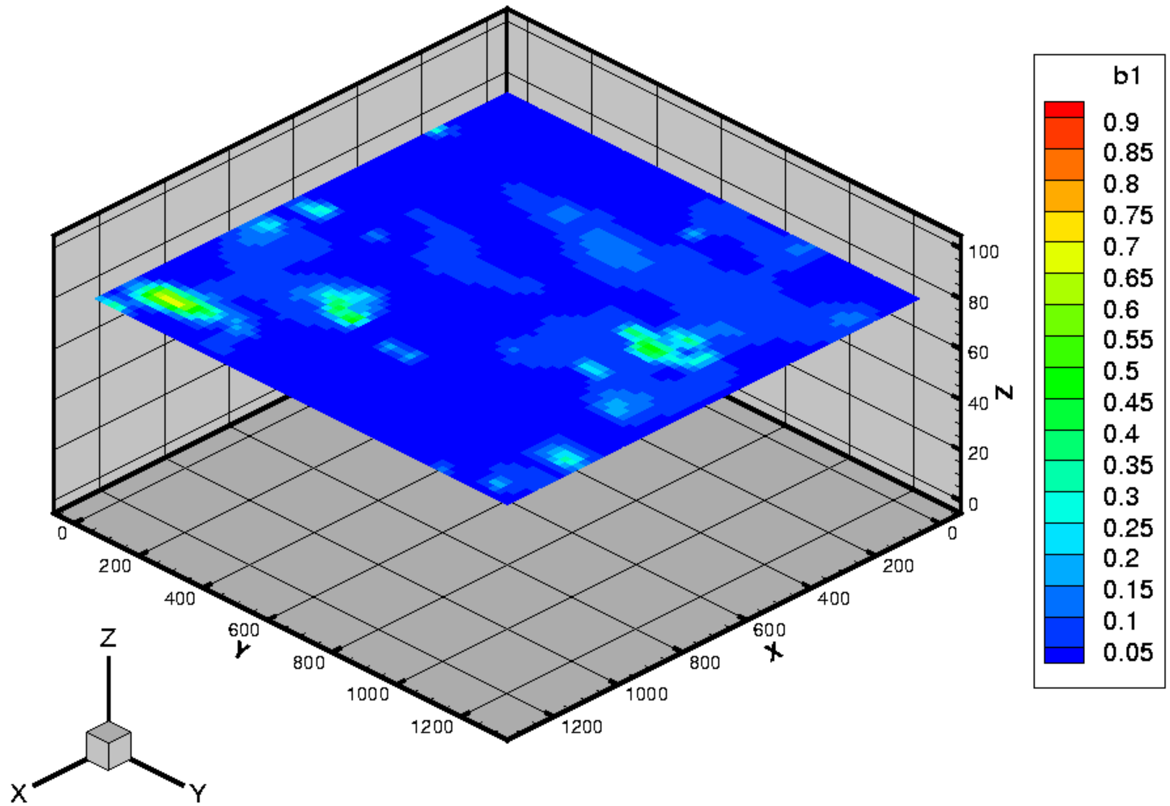
depth $H = 60ft$

Permeability (real data)



depth $H = 40ft$

Permeability (real data)



depth $H = 20ft$

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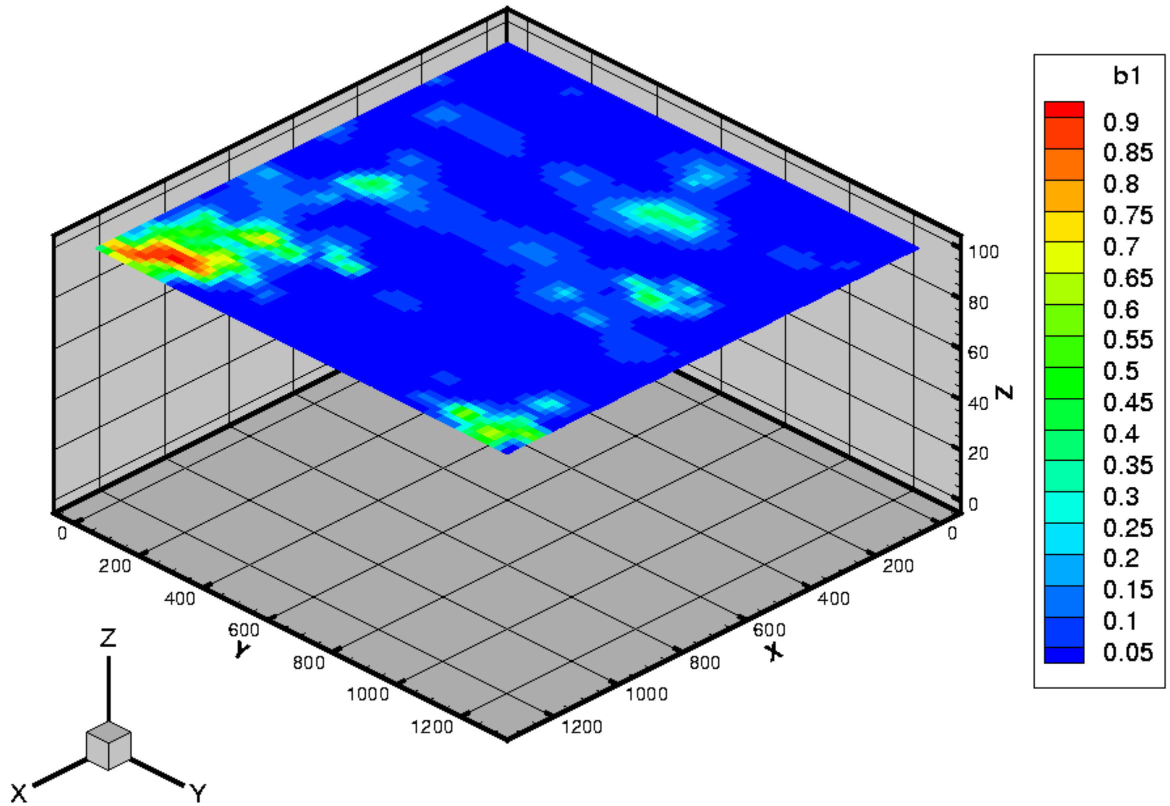
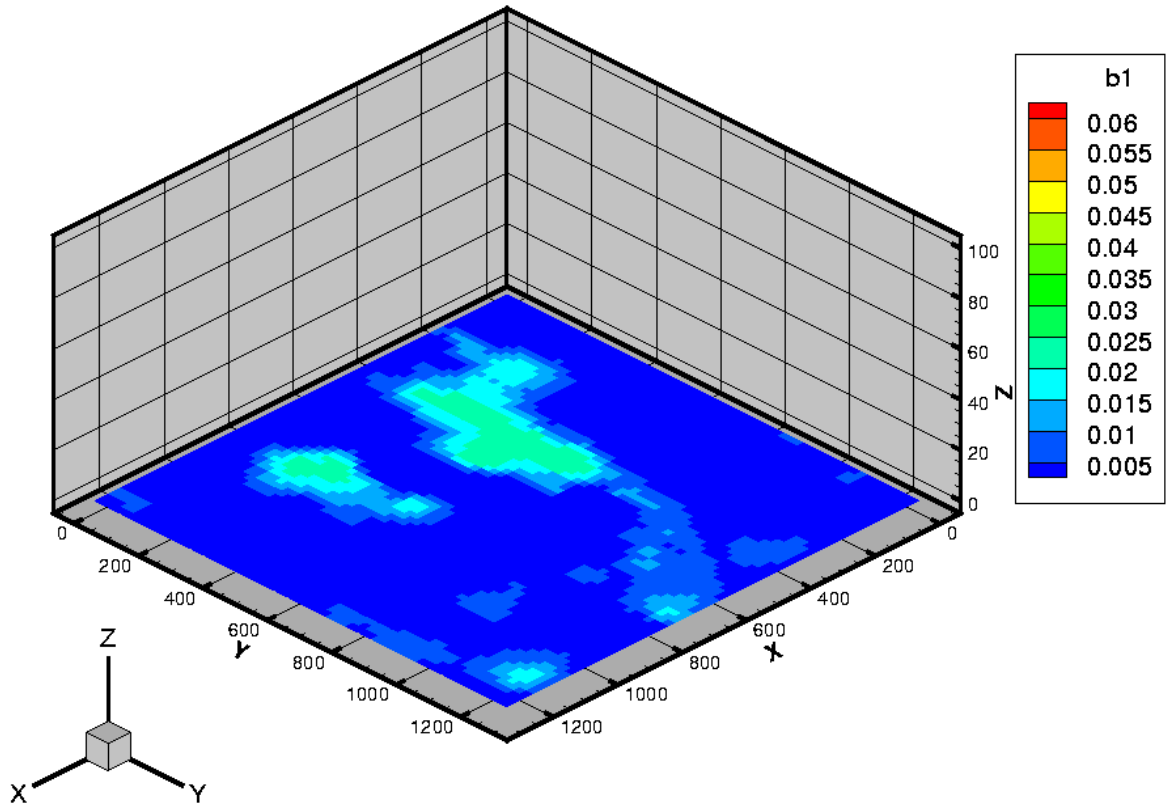


depth $H = 0ft$

Uncertainty bounds for the permeability



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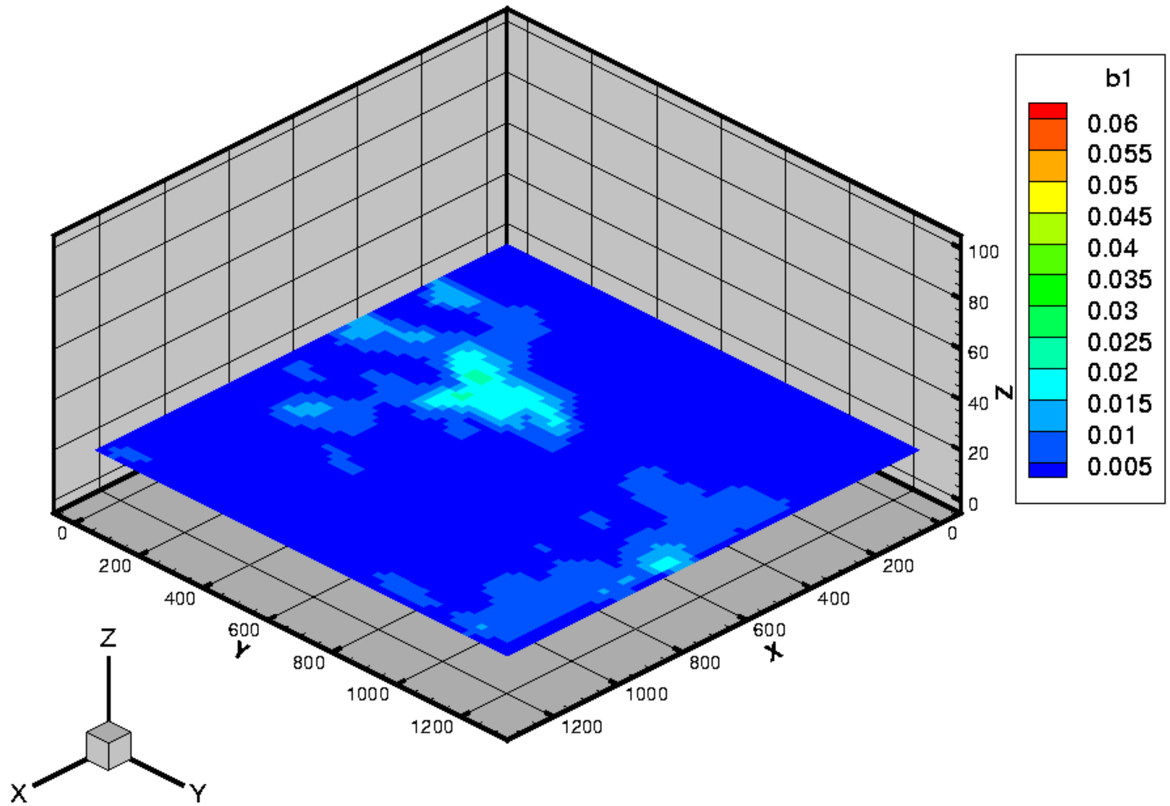

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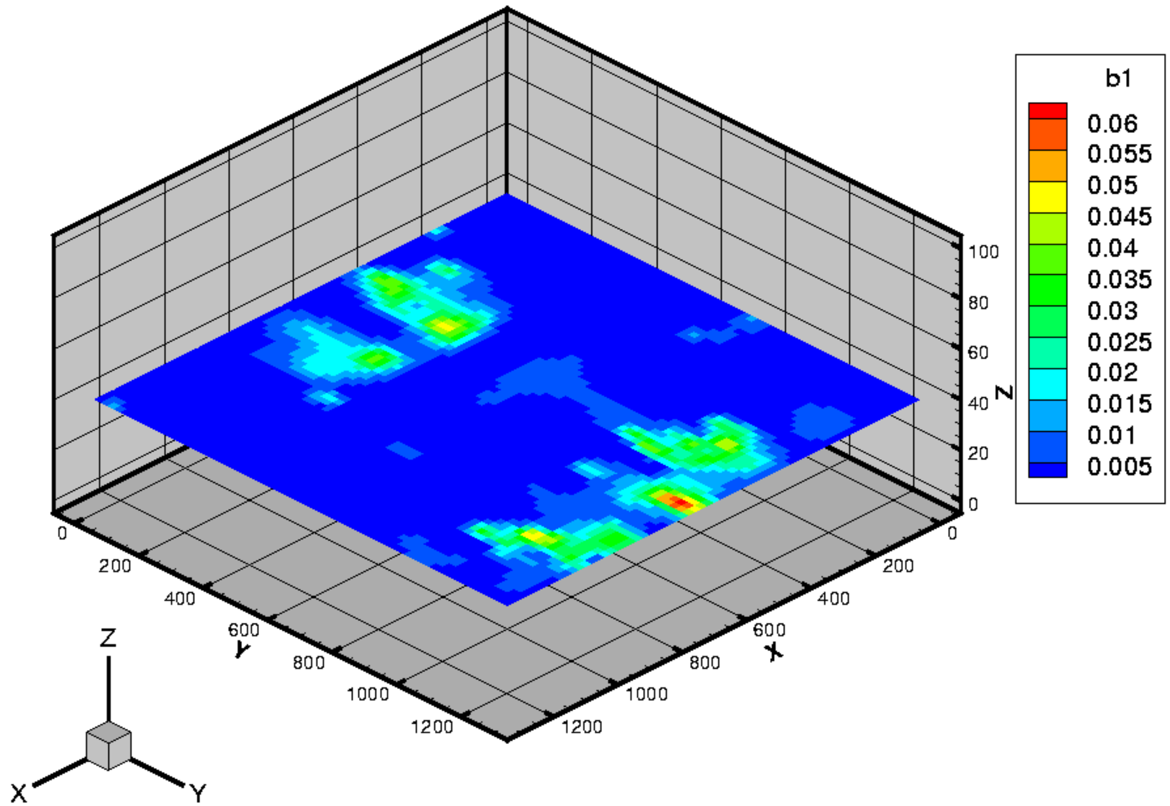

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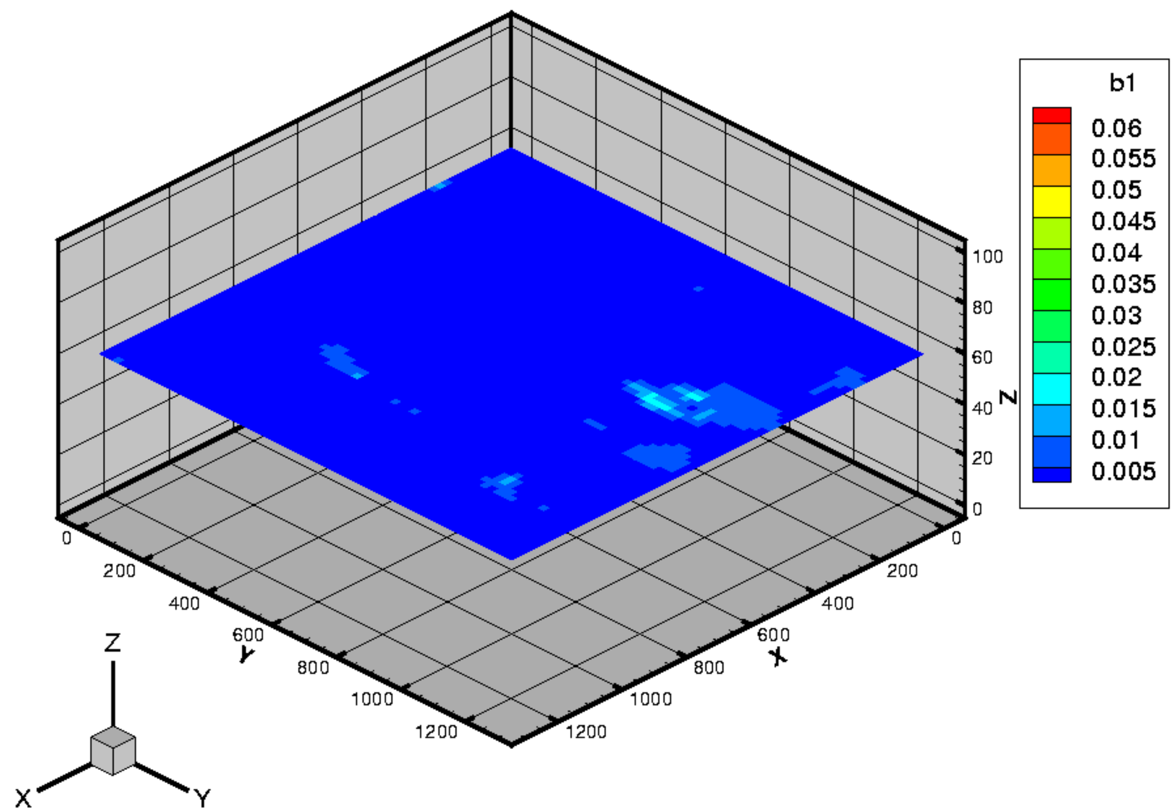

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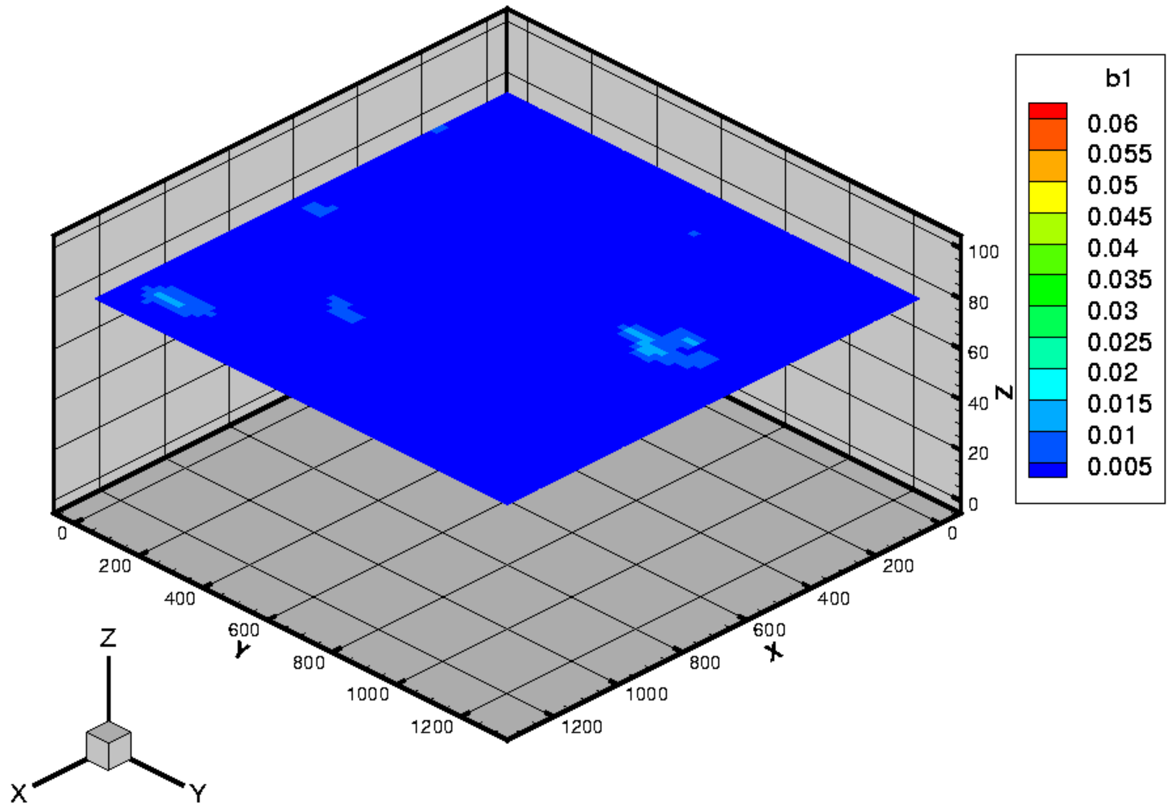

depth $H = 20ft$

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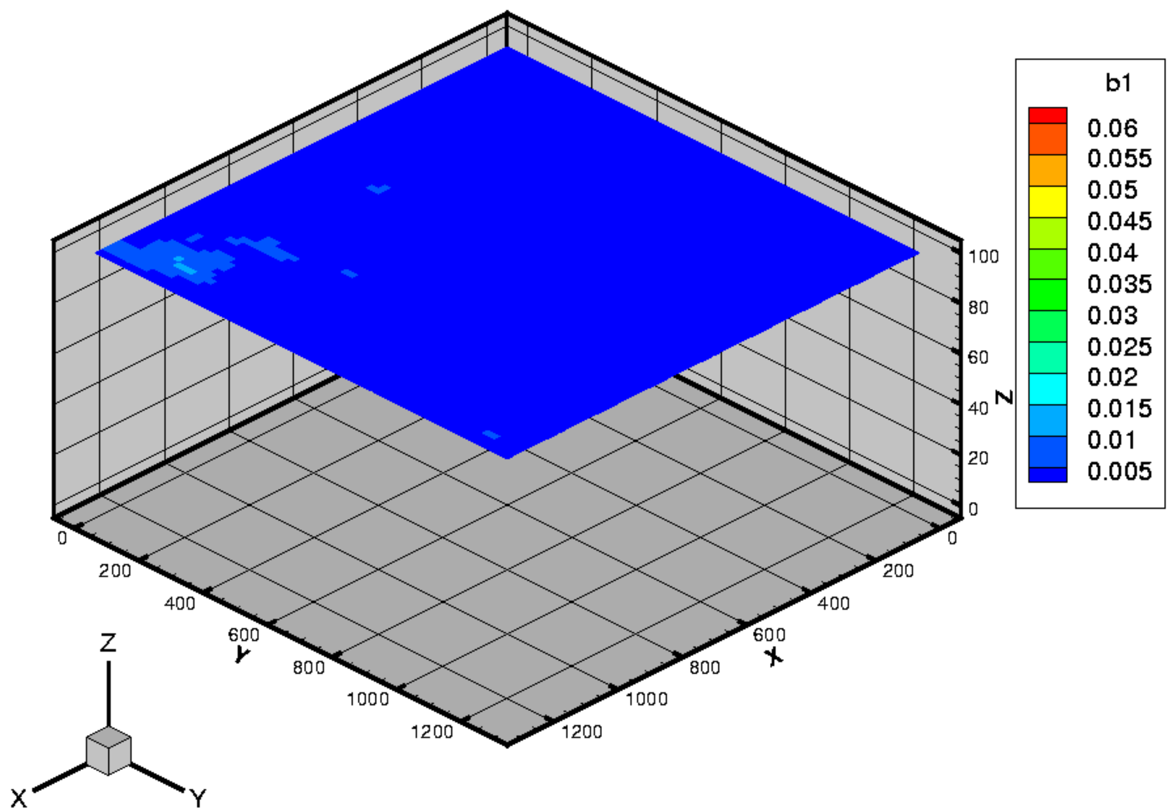

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Validation of a worst-case scenario model

Worst-case scenario model:

- **input**: nominal value + uncertainty band $(\eta_0, \varepsilon(x))$
- **output**: uncertainty interval $\mathcal{I}Q = [Q_0 \pm \Delta Q]$

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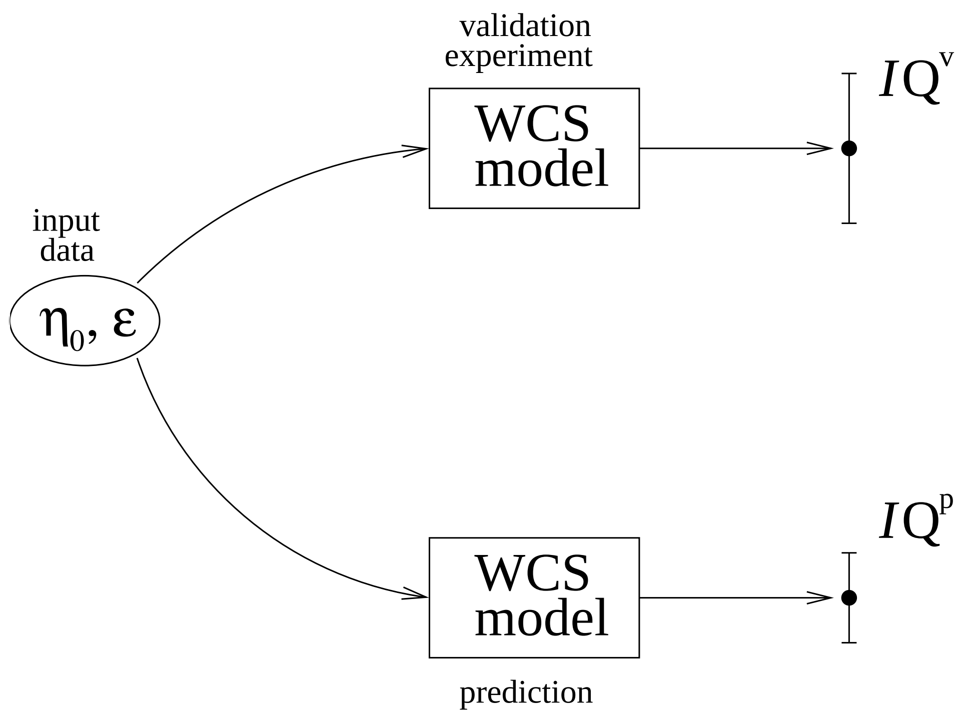

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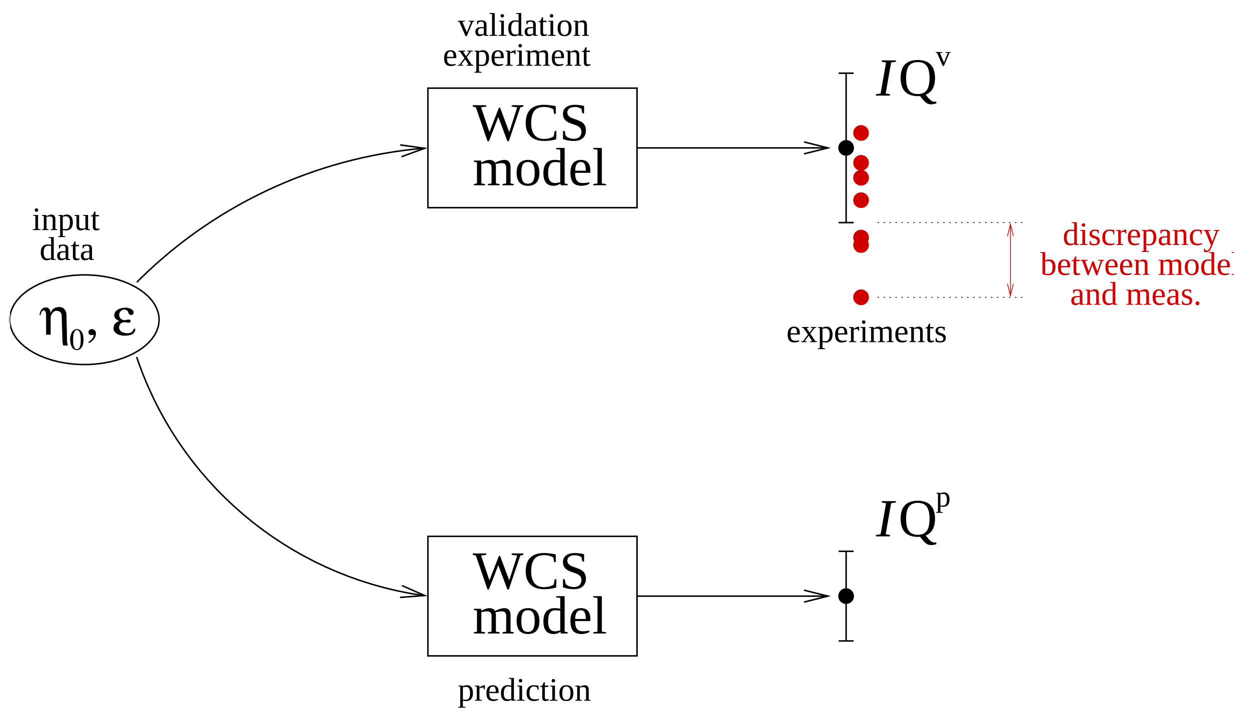

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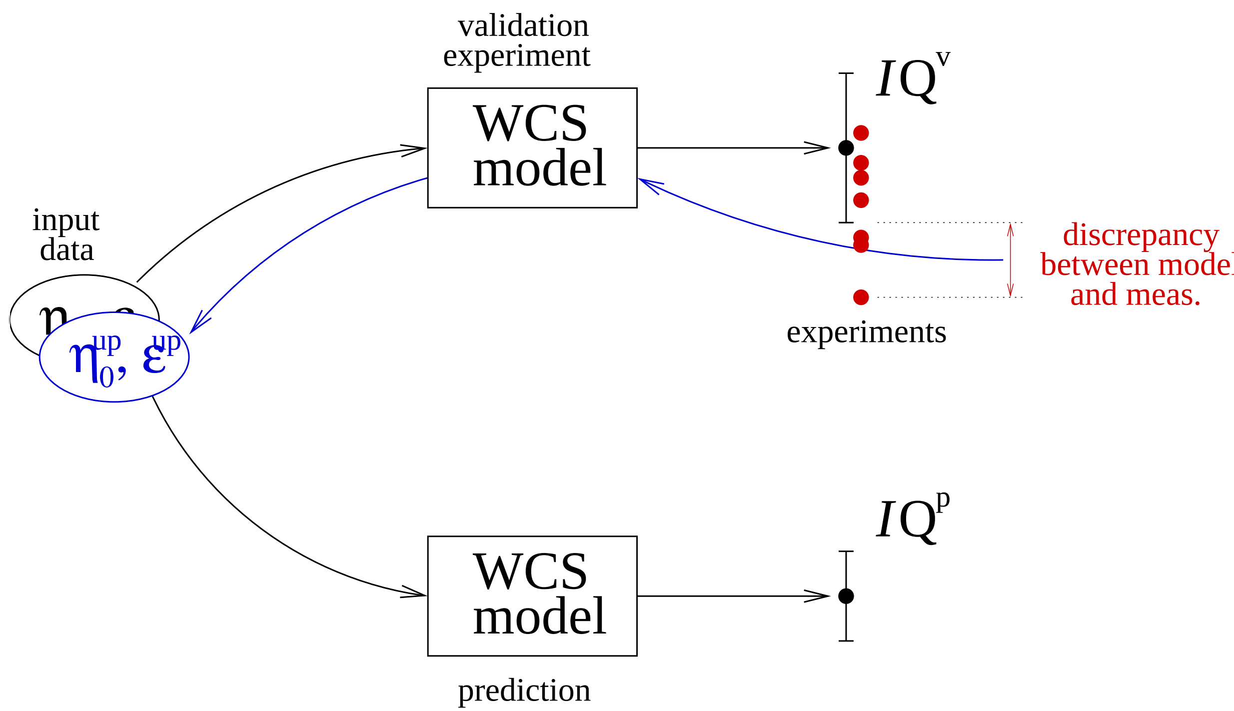

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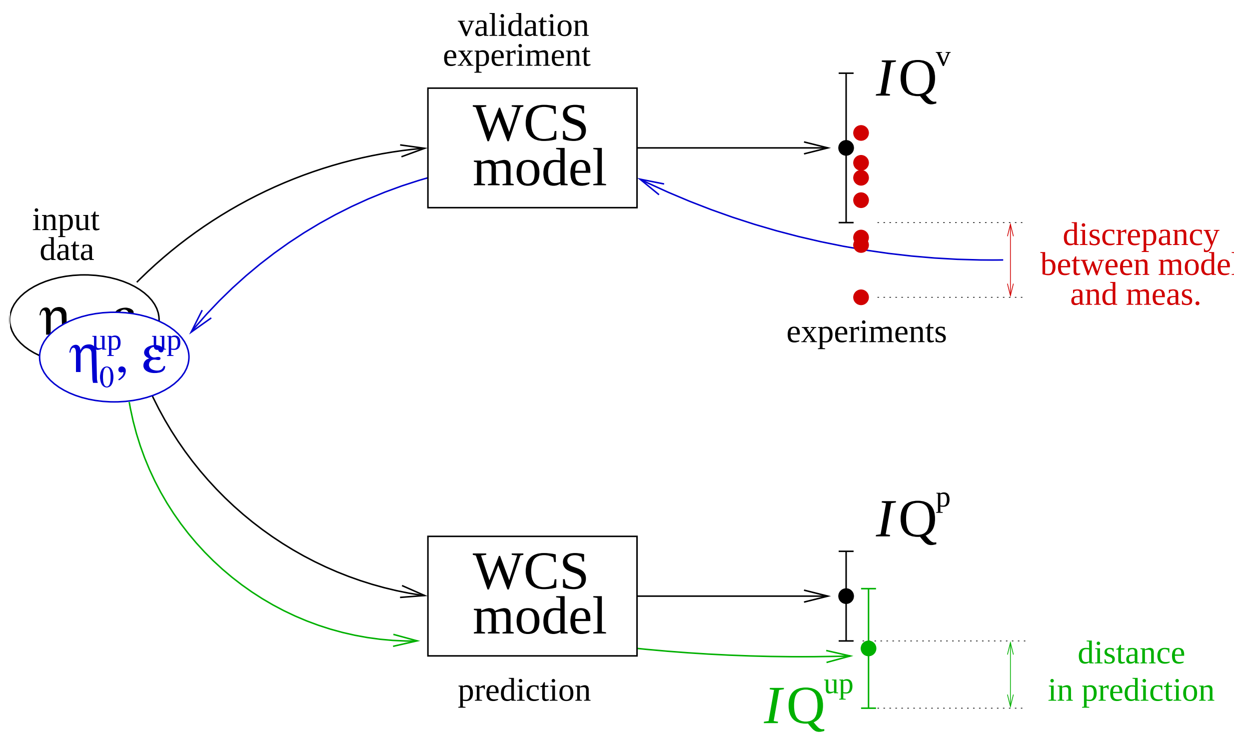

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- **Model update** based on N validation data Q_i^v, $i = 1, \ldots, N$.

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Idea: interpret it as a uniform random variable $Q^v \sim \mathcal{U}(\mathcal{I}Q^v)$. This allows us to write a **likelihood**

$$L(\eta_0, \varepsilon | Q_i^v) = \begin{cases} \dfrac{1}{|\mathcal{I}Q^v(\eta_0, \varepsilon)|^N} & \text{if all } Q_i^v \in \mathcal{I}Q^v(\eta_0, \varepsilon) \\ 0 & \text{otherwise} \end{cases}$$

and perform a **Bayesian update** of the input data (η_0, ε).

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and perform a **Bayesian update** of the input data (η_0, ε). Take for instance **maximum likelihood estimator**

$$(\eta_0^{up}, \varepsilon^{up}) = \arg\max \; L(\eta_0, \varepsilon | Q_i^v) \pi_{prior}(\eta_0, \varepsilon)$$

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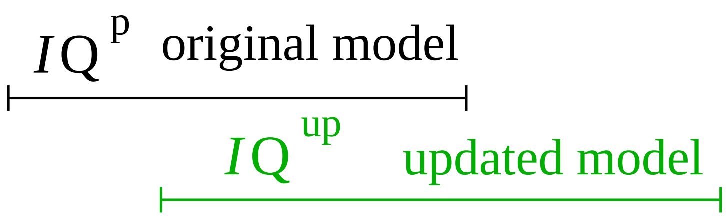
- **Distance in the prediction (validation metric):**

In the prediction level we measure the distance between the original model and the updated one: distance among intervals



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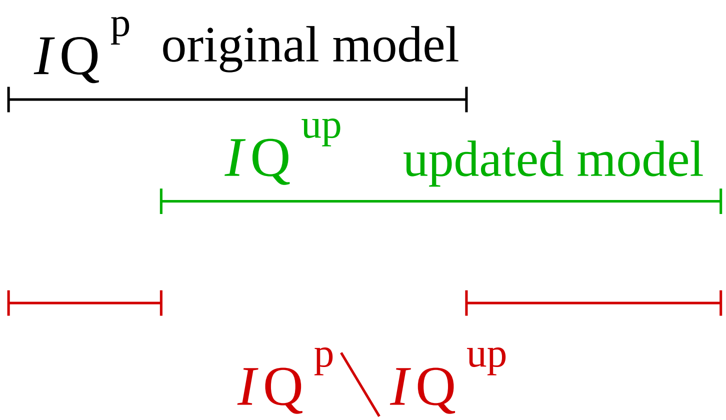

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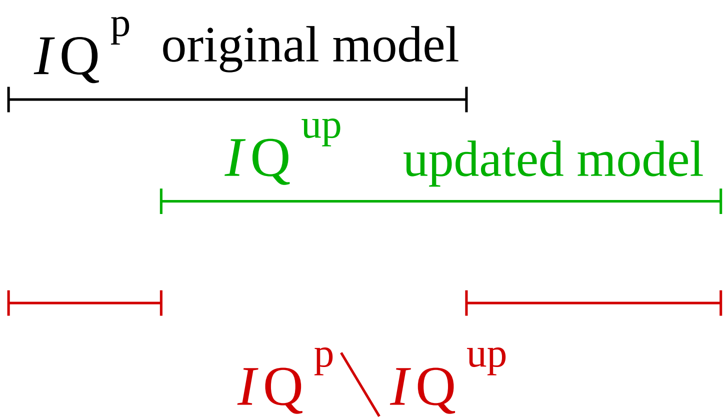

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- **Rejection criterion: for a given tolerance** $tol > 0$

model rejected if $\quad |\mathcal{I}Q^p \setminus \mathcal{I}Q^{up}| > tol$

Solution Technique

The computation of the Worst-Case Scenario bound

$$\Delta Q = \sup_{\eta \in \mathcal{A}_\eta} |\psi(\eta) - \psi(\eta_0)|$$

is a constrained optimization problem

- **non convex in general**
- **may have many local maxima**

$\Longrightarrow$ **Very difficult to solve**

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- **We have followed a simpler approach based on perturbation techniques**

Perturbation method

Taylor expansion of $\psi(\eta)$ around η_0: $\exists \theta \in (0,1)$ **s.t.**

$$\psi(\eta) - \psi(\eta_0) = < D_\eta \psi(\eta_0), \delta\eta > + \frac{1}{2} D^2_\eta \psi(\eta_0 + \theta\delta\eta)(\delta\eta, \delta\eta).$$

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Then

$$\Delta Q \leq \underbrace{\sup_{\delta\eta \in \mathcal{A}_\eta - \eta_0} | < D_\eta \psi(\eta_0), \delta\eta > |}_{\text{Linear term } (\Delta Q^{lin})}$$

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- **Remark:** Q **depends linearly on the boundary conditions** g **and forcing terms** $\mathcal{L}$**. In this case** $\mathcal{R} = 0$**.**

Duality method

We first rewrite the primal problem in the following weak form: *find* $u \in H^1(D)$ *and* $\lambda \in H^{-\frac{1}{2}}(\Gamma_D)$ *s.t.*

$$\begin{cases} B(\beta; u, v) + \int_{\Gamma_D} \lambda v = \mathcal{L}(v) & \forall v \in H^1(D) \\ \int_{\Gamma_D} u\mu = \int_{\Gamma_D} g\mu & \forall \mu \in H^{-\frac{1}{2}}(\Gamma_D) \end{cases}$$

where we use a Lagrange multiplier to impose boundary conds. and

$$B(\beta; u, v) = \int_D \left[(\mathrm{A}\nabla u) \cdot \nabla v + \mathrm{b} \cdot (\nabla u)\, v + \sigma u v \right] \, d\mathrm{x}$$

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- The Lagrange multiplier λ corresponds to the outgoing normal flux $\quad \lambda = -\Phi(u)$
- A Q.o.I. associated to the normal flux can be written in the form

$$\boxed{Q = Q(\lambda)}$$

Duality method (cont'd)

We also introduce a dual problem: *find* $\varphi \in H^1(D)$ *and* $\xi \in H^{-\frac{1}{2}}(\Gamma_D)$ *s.t.*

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- **The dual problem has non homogeneous Dirichlet boundary cond.**
- **The following representation of the quantity of interest holds**

$$\boxed{Q(u, \lambda) = B(\beta; u, \varphi) + \int_{\Gamma_D} \xi u + \int_{\Gamma_D} \varphi \lambda}$$

Duality method (cont'd)

We also introduce a dual problem: *find* $\varphi \in H^1(D)$ *and* $\xi \in H^{-\frac{1}{2}}(\Gamma_D)$ *s.t.*

$$\begin{cases} B(\beta; v, \varphi) + \int_{\Gamma_D} \xi v = Q_1(\beta, v) & \forall v \in H^1(D) \\ \int_{\Gamma_D} \varphi \mu = Q_2(\mu) & \forall \mu \in H^{-\frac{1}{2}}(\Gamma_D) \end{cases}$$

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We typically have $\begin{cases} B(\beta; u, v) = \int_D G(\beta; u, v)\, dx & \text{with } G \in L^1(D) \\ Q_1(\beta; v) = \int_D F(\beta; v)\, dx + \int_{\Gamma_N} H(v)\, dS & \text{with } F, H \in L^1 \end{cases}$

Uncertainty in the coefficients $\beta = [\beta_1, \ldots, \beta_m]$

By a duality argument, the Fréchet derivative of ψ wrt β is

$$< D_{\boldsymbol{\beta}}\psi(\boldsymbol{\beta_0}), \delta\boldsymbol{\beta} >= \int_{D} \nabla_{\boldsymbol{\beta}} \left(F - G \right) \left(\boldsymbol{\beta_0}, \boldsymbol{u_0}, \boldsymbol{\varphi_0} \right) \cdot \delta\boldsymbol{\beta} \, d\boldsymbol{x}$$

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We consider the set of coefficients (pointwise uncorr. perturbations):

$$\mathcal{A}_{\boldsymbol{\beta}} = \{\boldsymbol{\beta} = \boldsymbol{\beta_0} + \delta\boldsymbol{\beta} : D \rightarrow \mathbb{R}^m, \quad |\delta\beta_i(x)| \leq \varepsilon_i(x), \ \forall x \in D\}$$

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Linear worst scenario analysis: [Babuška-N-Tempone, 2005]

a) $$\Delta Q^{lin} = \sum_{i=1}^{m} \int_D \left| \frac{\partial(F - G)}{\partial \beta_i} (\boldsymbol{\beta}_0; u_0, \varphi_0) \right| \varepsilon_i \, dx,$$

b) **worst perturbation:** $$\delta\beta_i^* = \varepsilon_i \operatorname{sign}\left(\frac{\partial(F - G)}{\partial \beta_i}\right)$$

- To compute ΔQ^{lin} we need only to
  - solve the primal and dual problems for $\beta = \beta_0$
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- Other types of perturbation sets could be considered as well. For instance, correlated coefficients or smoother perturbations. In this case the postprocess is more involved but still relatively cheap.

Bounds for the reminder

Not easy in general !

Bounds for the reminder

- **Reminder** $$\mathcal{R} \equiv \frac{1}{2} \sup_{\delta\beta \in \mathcal{A}-\beta_0} \sup_{\theta \in (0,1)} |D^2_\beta \psi(\beta_0 + \theta\delta\beta)(\delta\beta, \delta\beta)|.$$
- **Second order Gâteaux derivative (case $Q = Q(u(\beta))$)**

$$D^2_\beta \psi(\beta)(\delta\beta, \delta\beta) = - D^2_\beta B(\beta; u(\beta), \varphi(\beta))(\delta\beta, \delta\beta)$$
$$- 2 < D_\beta B(\beta; D_\beta u(\beta)(\delta\beta), \varphi(\beta)), \delta\beta >$$

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- **For symmetric problems: combine a priori and a posteriori estimates to get a bound of the form**

$$\mathcal{R} \leq \frac{1}{2} |u_0|_{E,\beta_0} |\varphi_0|_{E,\beta_0} \sup_{\beta \in \mathcal{A}_\beta} \left\{ \sum_{i,j} C_{ij}(\beta) \bar{\varepsilon}_i \bar{\varepsilon}_j \right\}$$

where $\bar{\varepsilon}_i = \sup_{x \in D} \varepsilon_i(x)$: maximum perturbation for the i-th coefficient.

The constants $C_{ij}(\beta)$ can be estimated in simple cases.

Other estimates for the reminder

- If computable a priori bounds are impossible to obtain or the previous estimate is too pessimistic, then we can take as an estimate for the reminder the second derivative of $\psi(\beta)$ computed in the worst-direction $\delta\beta^*$: $\mathcal{R} \approx \frac{1}{2} D^2_{\beta}\psi(\beta_0)(\delta\beta^*, \delta\beta^*)$

Implies the computation of $w = D_{\beta}u(\beta_0)(\delta\beta^*)$ which satisfies

$$B(\beta, w, v) = -\int_D \nabla_{\beta} G(\beta, u_0, v) \cdot \delta\beta^* \, dx, \qquad \forall v \in V_0$$

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- Alternatively: sample at random some perturbations $\delta\beta^{(j)}$, $j = 1, \ldots, M$ and compute $\mathcal{R} \approx \max_{j=1,\ldots,M} \frac{1}{2} D^2_\beta \psi(\beta_0)(\delta\beta^{(j)}, \delta\beta^{(j)})$.
Implies the solution of M additional problems.

Uncertainty in load and boundary cond.s

It can be done in a similar way as for the coefficients. Observe that for a linear problem and linear Q.o.I, the reminder $\mathcal{R}$ vanishes.

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Uncertainty in the load [Babuška-N-Tempone, 2005]:

uncertainty set $\mathcal{A}_f \equiv \{f = f_0 + \delta f : \ \|\delta f\|_{L^2(D)} \leq \varepsilon\}$

uncertainty bound $\Delta Q = \varepsilon \|\varphi_0\|_{L^2(D)}$.

worst perturbation $\delta f^* = \varepsilon \varphi_0 / \|\varphi_0\|_{L^2(D)}$

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Uncertainty in Dirichlet boundary conditions [Babuška-N-Tempone, 07]:

uncertainty set	$\mathcal{A}_g \equiv \{g = g_0 + \delta g : \quad \lvert\delta g(x)\rvert \leq \varepsilon_g(x)\}$
uncertainty bound	$\Delta Q = \int_{\Gamma_D} \lvert\xi_0\rvert\, \varepsilon_g(x)\, dx$
worst perturbation	$\delta g^* = \mathrm{sign}(\xi_0)\varepsilon_g(x).$

Verification issues

Assume we compute primal and dual finite element solutions u_{0h} and φ_{0h}.

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a) The computation of the quantity of interest Q_{0h} based on the FE solution. We used Dual Weighted Residual error estimators.

b) The computation of the linear uncertainty bound ΔQ_h^{lin} based on the FE solution. Need both a priori and a posteriori error bounds.

In [Babuška-N-Tempone '05] we proved that

$$\boxed{|\Delta Q^{lin} - \Delta Q_h^{lin}| \leq C \left(\|u_0 - u_{0h}\|_{H^1} + \|\varphi_0 - \varphi_{0h}\|_{H^1} \right)}$$

Verification issues

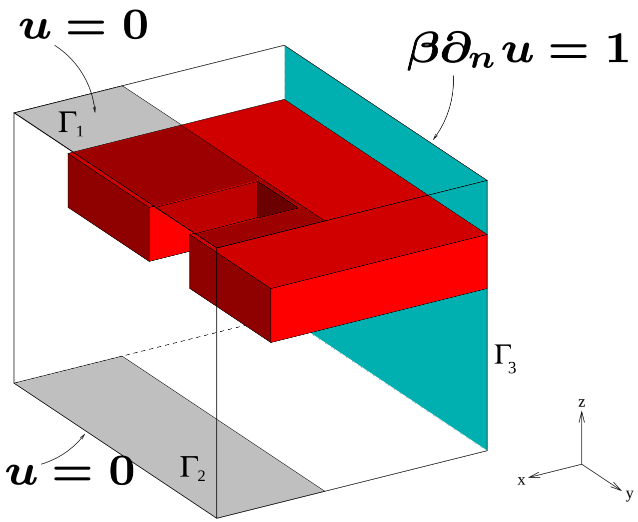
c) A posteriori control on the accuracy in the computation of

$$\Delta Q_h^{lin} = \sum_{i=1}^{m} \int_D \left| \frac{\partial(F-G)}{\partial \beta_i}(\beta_0; u_{0h}, \varphi_{0h}) \right| \varepsilon_i \, dx.$$

The function $\left|\frac{\partial(F-G)}{\partial\beta_i}\right| \varepsilon_i$ is not regular, in general (has surfaces of non differentiability). We have used adaptive integration. FromSlide2

d) Check the accuracy of the estimate for the reminder. How to do it properly is an open question.

Numerical Results – Heat transfer

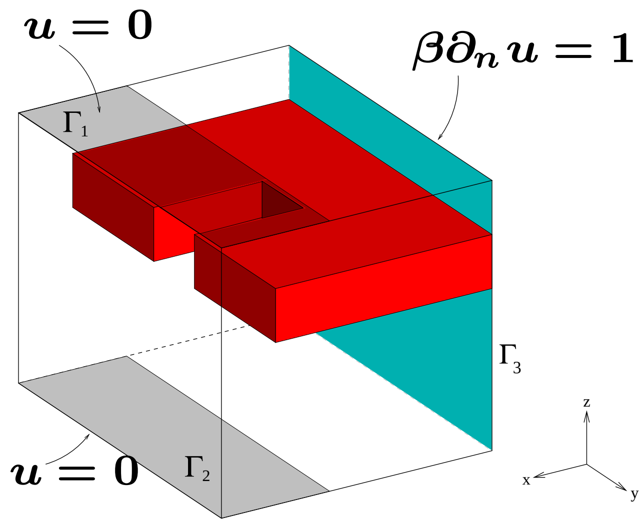


$$\begin{cases} -\operatorname{div}(\beta \nabla u) = 0, & \text{in } D \subset \mathbb{R}^3 \\ u = 0, & \text{on } \Gamma_1 \cup \Gamma_2 \\ \beta\, \partial_n u = 1 & \text{on } \Gamma_3 \\ \beta\, \partial_n u = 0 & \partial D \setminus \Gamma_{1,2,3} \end{cases}$$

u: temperature; β: conductivity;

$$\beta_{inclusion} = 50 * \beta_{material}$$

Numerical Results – Heat transfer



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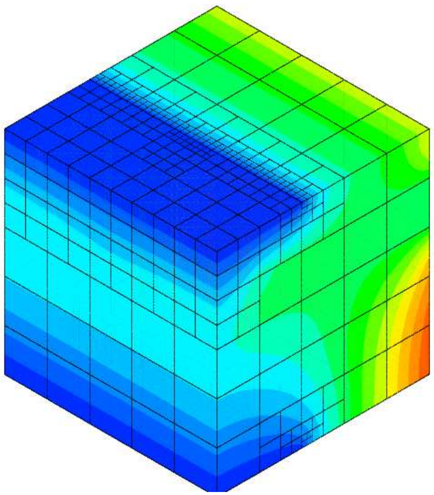
u: temperature; β: conductivity;

$$\beta_{inclusion} = 50 * \beta_{material}$$

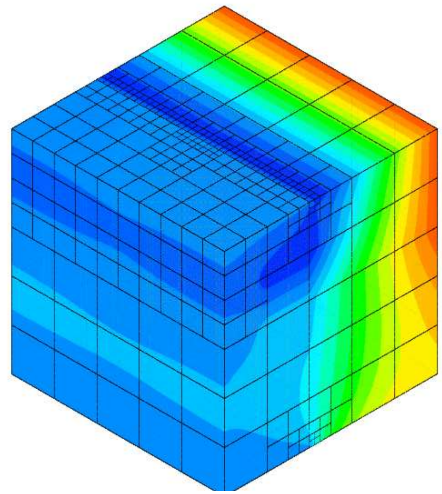
- **Q.o.I: outward flux on Γ_1.** $Q(\beta, u(\beta)) = -\int_{\Gamma_1} \beta \partial_n u(\beta)\, dS$.
- **Uncertainty characterization:**

$$\beta \in \mathcal{A}_\beta \equiv \{\beta \in L^\infty(D),\ |\beta(x) - \beta_0(x)| \leq \varepsilon_\beta(x),\ \ \forall x \in D\}$$

Numerical Results – heat transfer



primal solution



dual solution

$Q(\beta_0) = 0.597 \pm 1\%$

Mesh adapted w.r.t. a goal-oriented error estimator;
7535 $\mathbb{Q}^2$ FE.

Numerical Results – heat transfer

Uncertainty in conductivity coefficient: $\frac{|\beta(x)-\beta_0(x)|}{\beta_0(x)} \leq 10\%$.

$$\Delta Q_h^{lin} = 0.0446 = 7.47\%\, Q(\beta_0, u(\beta_0))$$

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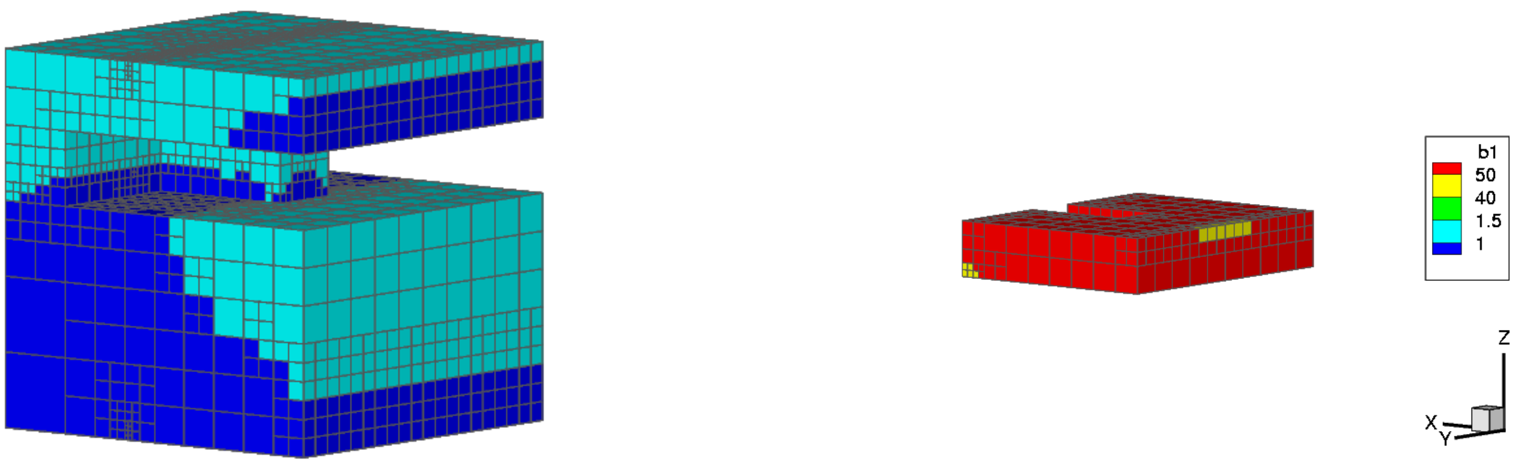
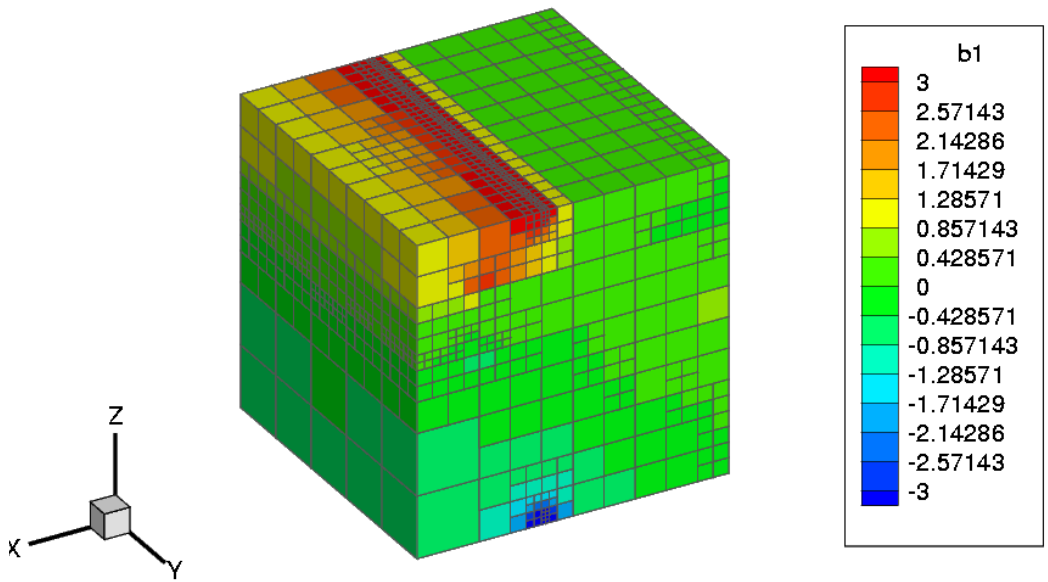


Worst distribution β^* of the conductivity coefficient in the material (left) and the inclusion (right).

Numerical Results – heat transfer

Sensitivity function



Numerical Results – heat transfer

The following computable bound can be obtained

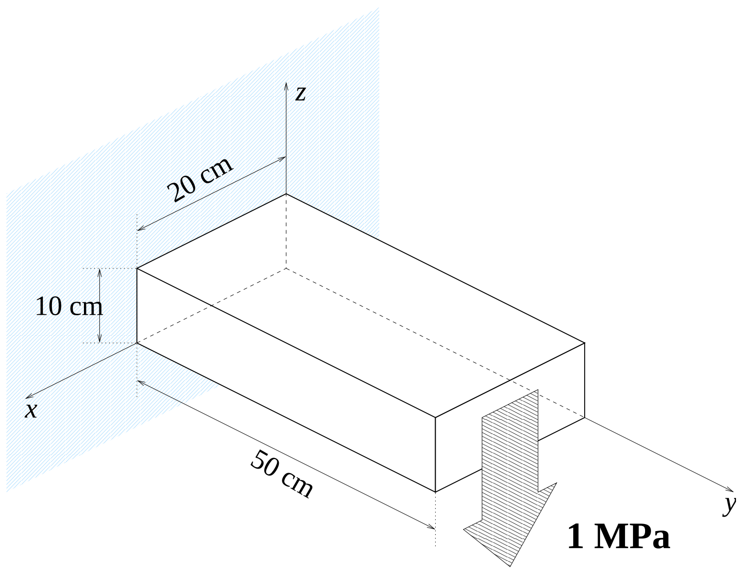
$$|\mathcal{R}| \leq |u_0|_{E,\beta_0} |\varphi_0|_{E,\beta_0} \left(1 + \left\| \frac{\beta_0}{\beta_{min}} \right\|_{L^\infty}^{\frac{1}{2}} \varepsilon\right) \left\| \frac{\beta_0}{\beta_{min}} \right\|_{L^\infty}^{\frac{5}{2}} \varepsilon^2.$$

where ε is the relative maximum perturbation: $\varepsilon = \sup_{\delta\beta} \|\delta\beta/\beta_0\|_{L^\infty(D)}$.

$$\Delta Q_h^{lin} = 0.0446 = 7.47\% \, Q(\beta_0, u(\beta_0))$$

$$\mathcal{R} < 6.5\varepsilon^2 + O(\varepsilon^3) \approx 0.065, \quad \textbf{for } \varepsilon = 0.1$$

Numerical results – Linear elasticity



Isotropic material: $\boldsymbol{\beta_0 = [E_0, \nu_0]}$

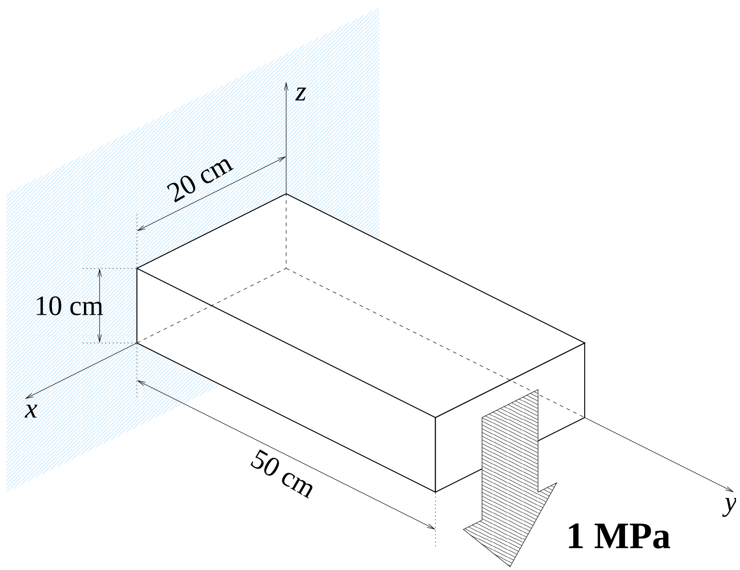
load: $\mathbf{g}_0 = [0,0,1]^T\, MPa$ **on** S**.**

Quantities of interest:

$$Q_1(\mathbf{u}) = \frac{1}{|S|}\int_S u_z\, dS$$

$$Q_2(\mathbf{u}) = \frac{1}{|S/2|}\int_{S/2} u_y\, dS$$

Numerical results – Linear elasticity



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Uncertainty:

coefficients: $\mathcal{A}_\beta \equiv \{|E(x) - E_0| \leq \varepsilon_E; \quad |\nu(x) - \nu_0| \leq \varepsilon_\nu, \quad \forall x \in D\}$

load: $\mathcal{A}_\mathcal{L} \equiv \{g \in [L^2(S)]^3 \; s.t. \; \|g_i - g_{0i}\|_{L^2(S)} \leq \varepsilon_{g_i}, \quad i = 1,2$ **or** $3\}$

we can also impose constraints such as $\int_S (g_i - g_{0i}) = 0$**.**

Numerical results – linear elasticity

Uncertainty characterization of material properties:

$$|E(x) - E_0| \leq 1\% E_0 \qquad |\nu(x) - \nu_0| \leq 8\% \nu_0$$

Quantity of Interest	$\Delta Q^{lin}/Q$	$\mathcal{R}/Q$	$1/2 D^2_\beta \psi / Q$
$Q_1 = -7.36135\,10^{-4}$	1.536%	$> 15\%$	0.027%
$Q_2 = 5.3964\,10^{-5}$	1.594%	$> 27.6\%$	0.016%

Numerical results – linear elasticity, Q_1

Worst distribution of E (left) and ν (right).

Sensitivity functions α^E (left) and α^ν (right).

Numerical results – linear elasticity, Q_2

Worst distribution of E (left) and ν (right).

Sensitivity functions α^E (left) and α^ν (right).

Numerical results – linear elasticity

Uncertainty characterization of the load g: let

$$\varepsilon_x = \varepsilon_y = 1\% \|g_z\|_{L^2(S)}, \qquad \varepsilon_z = 5\% \|g_z\|_{L^2(S)}$$

set $\tilde{\mathrm{g}} = [\frac{g_x}{\varepsilon_x}, \frac{g_y}{\varepsilon_y}, \frac{g_z}{\varepsilon_z}]^T$. Perturbation set:

first case: $$\mathcal{A}^1_{\mathcal{L}} \equiv \{\mathrm{g} = \mathrm{g}_0 + \delta\mathrm{g} : \ \|\widetilde{\delta\mathrm{g}}\|_{[L^2(S)]^3} \leq 1\}$$

second case: $$\mathcal{A}^2_{\mathcal{L}} \equiv \{\mathrm{g} \in \mathcal{A}^1_{\mathcal{L}}, \ \int_S \delta\mathrm{g} = 0\}$$

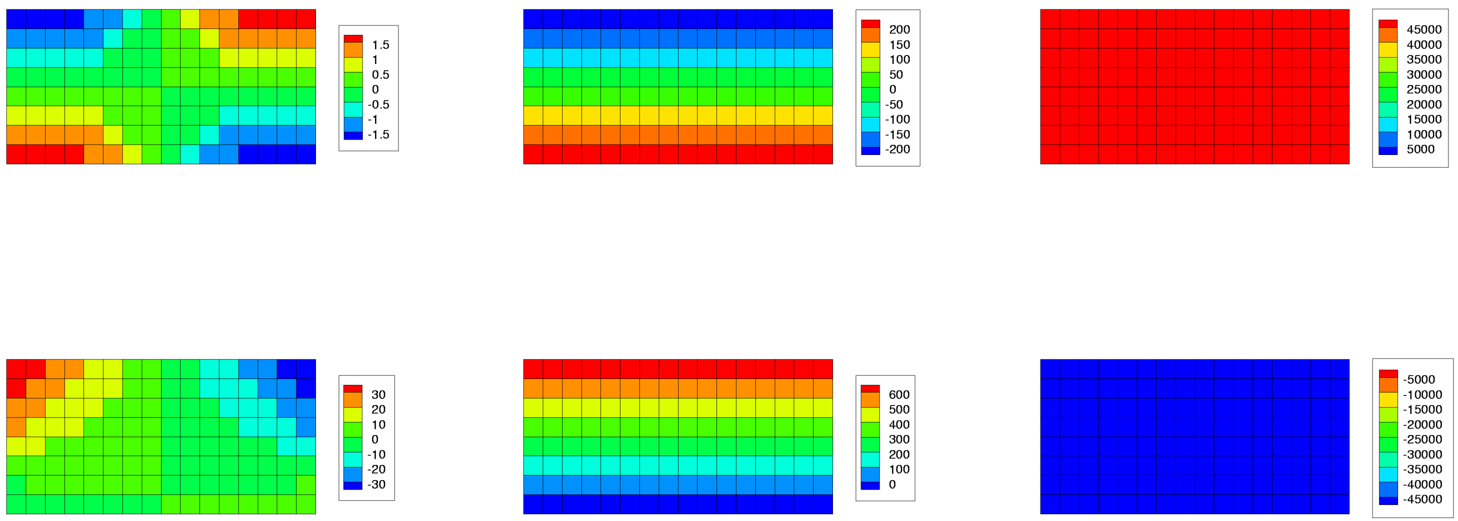
	$\Delta Q_1/Q_1$	$\Delta Q_2/Q_2$
$\mathcal{A}^1_{\mathcal{L}}$	5.007%	5.003%
$\mathcal{A}^2_{\mathcal{L}}$	0.085%	0.12%

Numerical results – linear elasticity

δg_x^* δg_y^* δg_z^*

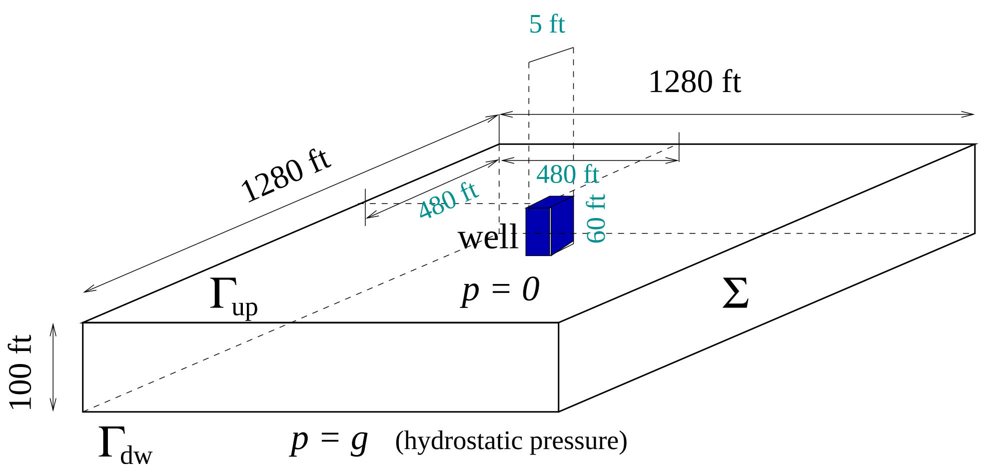
Q_1

Q_2



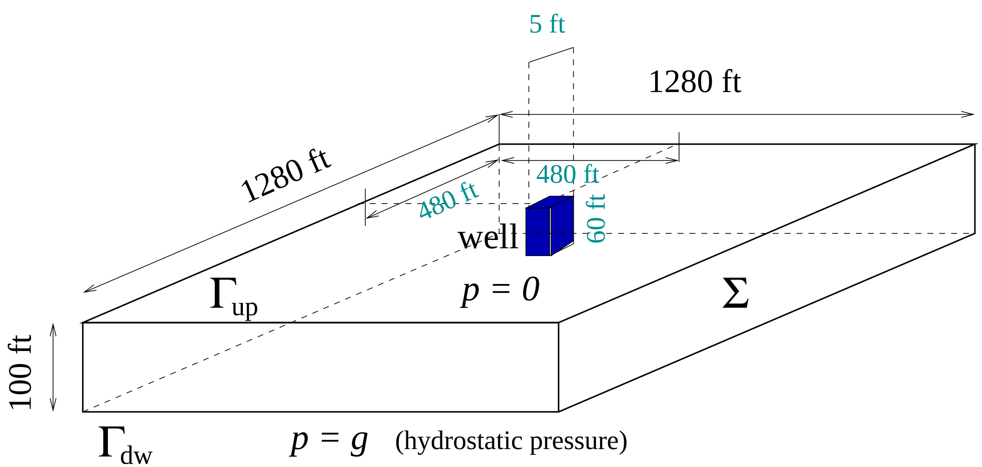
Worst distribution of the load for the set $\mathcal{A}_{\mathcal{L}}^1$

Numerical Results – groundwater flow problem



- $\Gamma = \Gamma_{up} \cup \Gamma_{dw}$: **upper and lower surf.**
- Σ **: lateral surf.**
- β **: permeability**

Numerical Results – groundwater flow problem



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Mathematical Model

$$\begin{cases} \mathrm{div}(\beta \nabla p) = 0 & \text{in } D \\ p = 0 & \text{on } \Gamma_{up} \\ p = g & \text{on } \Gamma_{dw} \\ \beta \partial_n p = 0 & \text{on } \Sigma \end{cases}$$

Numerical results – groundwater flow

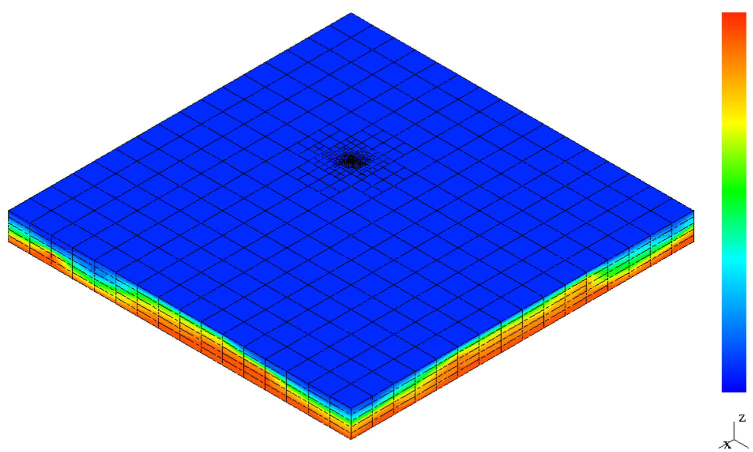
- well model: $5ft$ diameter hole with permeability 20 times larger.

  - Q.o.I: extraction rate from the well: $Q(p) = \int_{well} \beta \nabla p \cdot n$

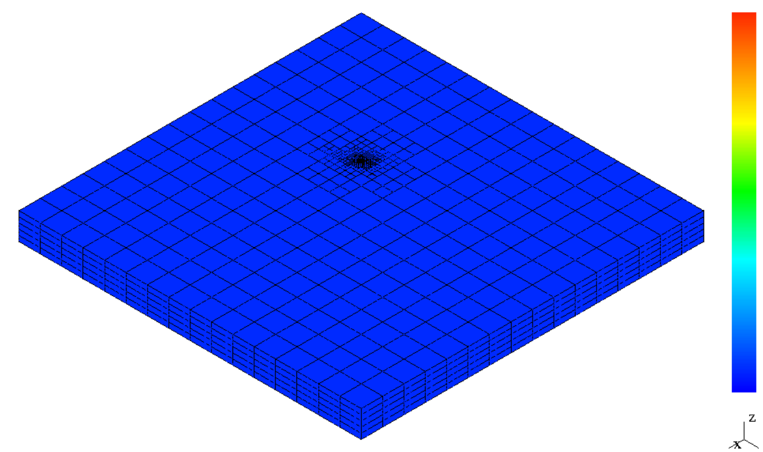
- Primal and dual solutions computed with $\mathbb{Q}_1$ finite elements, 14K dofs on a goal oriented mesh. $Q(p) = 497.4$ with a discretization error smaller than 5%
- Perturbation in permeability coeff: max. 10% pointwise
- Perturbation in boundary pressure on the bottom: 10% pointwise

Numerical results – groundwater flow

primal and dual solutions



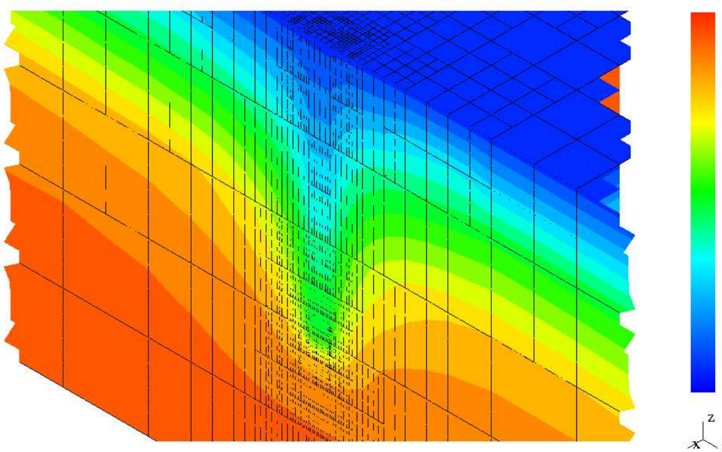
Pressure in the domain



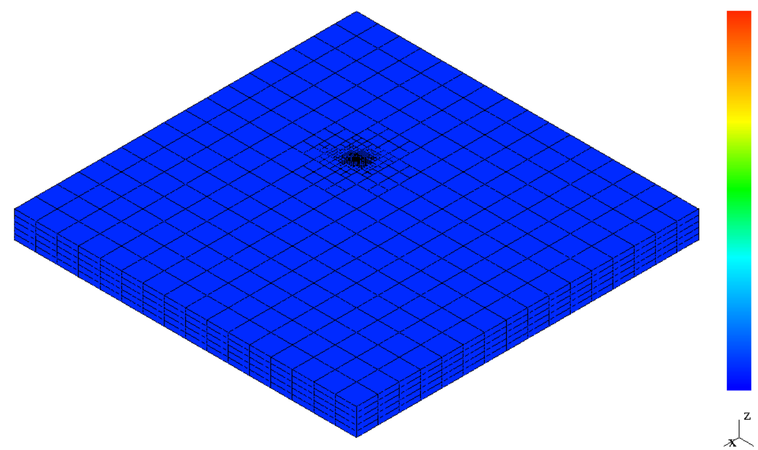
Dual solution

Numerical results – groundwater flow

primal and dual solutions



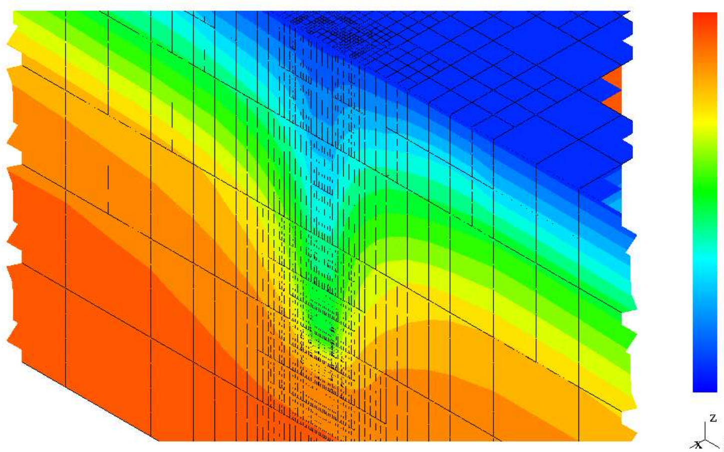
Enlargement around the well (zoom x 16)



Dual solution

Numerical results – groundwater flow

primal and dual solutions



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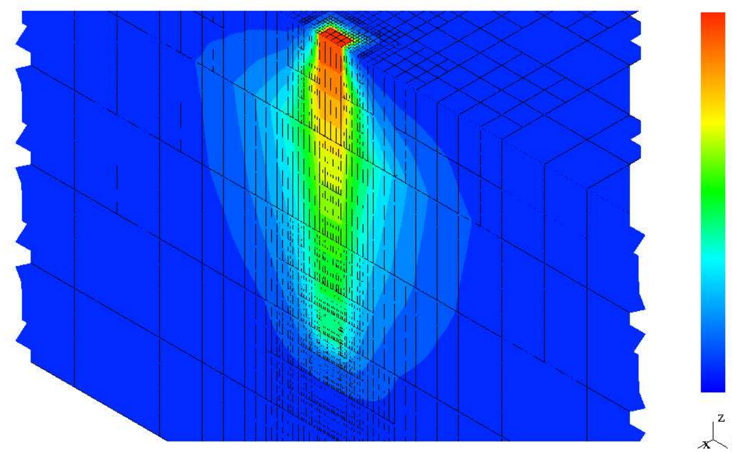
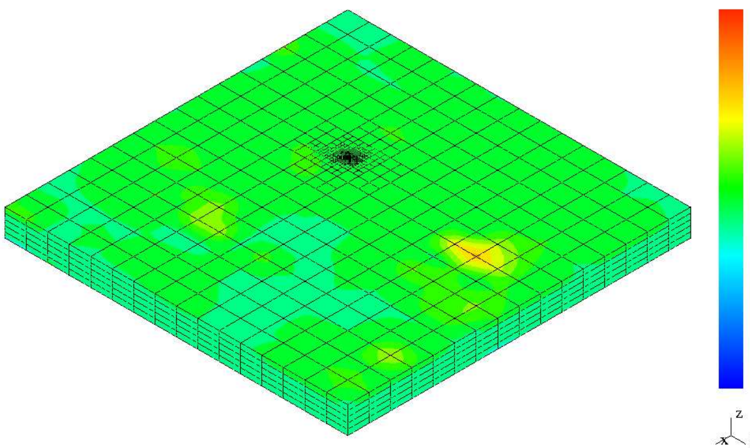


Enlargement around the well (zoom x 16)

Numerical results – groundwater flow

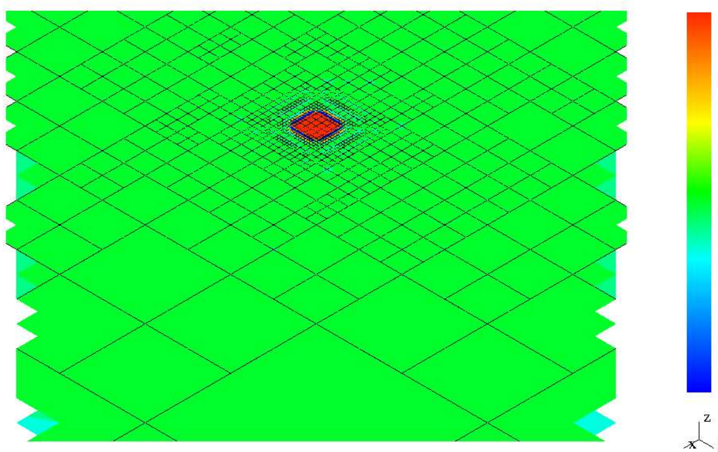
flux on the bottom and top surfaces



Top

Numerical results – groundwater flow

flux on the bottom and top surfaces



Top: enlargement x16

Numerical results – groundwater flow

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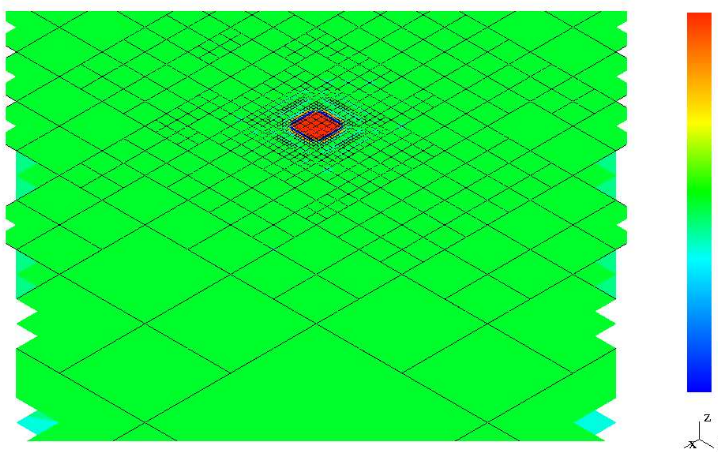

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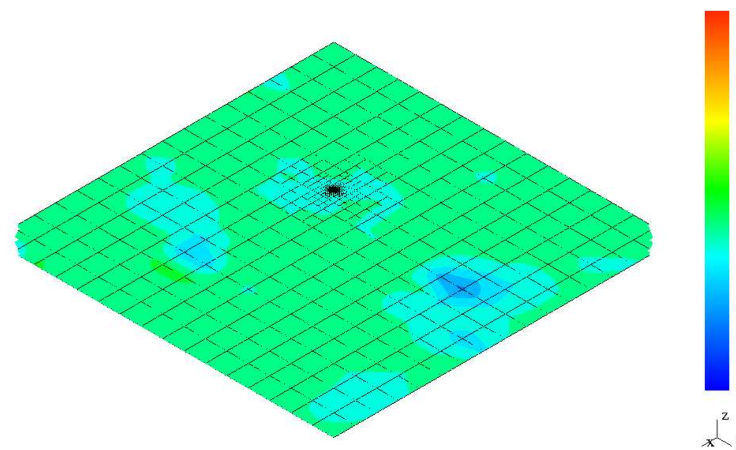


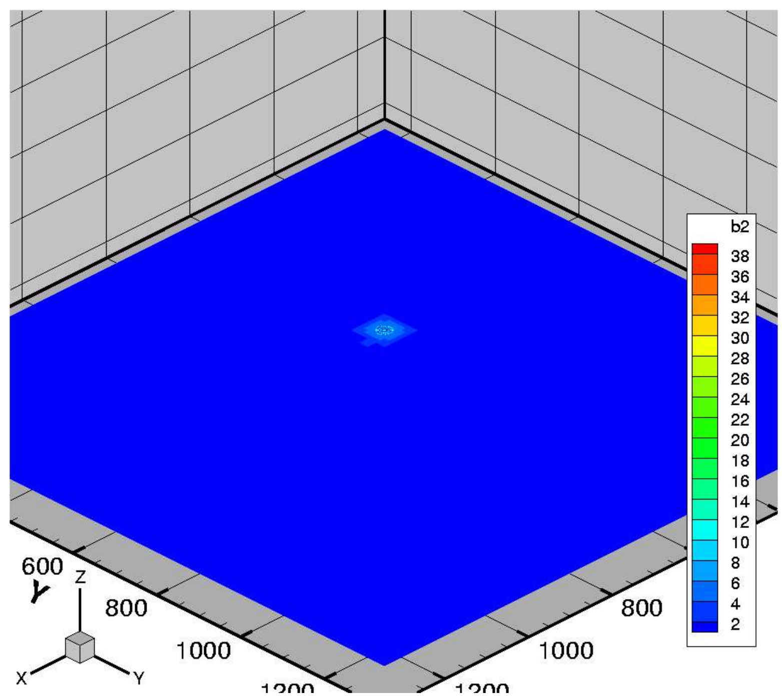
Bottom

Numerical Results – groundwater flow

Uncertainty analysis

- **Pert. in permeability**: $\Delta Q^{lin} = 4.83\ (\ 1\%Q)$ **(error in quadrature formula < 1%). The estimate for the Reminder is too pessimistic in this case.**
- **Pert. in boundary pressure**: $\Delta Q = 51\ (10\%Q)$ **(no error in quadrature formula)**

Sensitivity function



Conclusions

- The Worst-Case Scenario can be easily computed, for certain classes of infinite dimensional perturbations in coefficients and loads, by postprocessing the solutions of the primal and dual problems computed for the nominal values of the parameters
- The WCS analysis can be set at the continuous level. Allows for rigorous convergence results of the finite element solution to the theoretical bounds.
- We have shown how the WCS approach fits nicely in a Verification and Validation framework.
- We have proposed an effective way to compute the worst-case scenario for perturbations in Dirichlet boundary conditions, by the use of Lagrange multipliers.
- How to obtain good (guaranteed) bounds for the reminder is still an open question in many applications.

References

- [BNT-Numer.Math.05] Worst-case scenario analysis for elliptic problems with uncertainty, Numer. Math., 101(2005), pp. 185–219.
- [BNT-Eurodyn 05] Worst-case scenario analysis for elliptic PDE's with uncertainty, Proceeding of EURODYN 2005
- [BNT-07] Propagating uncertainty from boundary conditions in elliptic equations via a worst scenario analysis, in preparation.

Other types of perturbation sets (I)

a) Correlated coefficients

$$\mathcal{A}_{\boldsymbol{\beta}} = \{\delta\beta \in [L^\infty(D)]^m, \;\; (\beta)(x) \in \boldsymbol{\Sigma}(x) \subset \mathbb{R}^m, \, \forall x \in D\}$$

where $\Sigma(x)$ is a convex polygon, piecewise smooth w.r.t. x.

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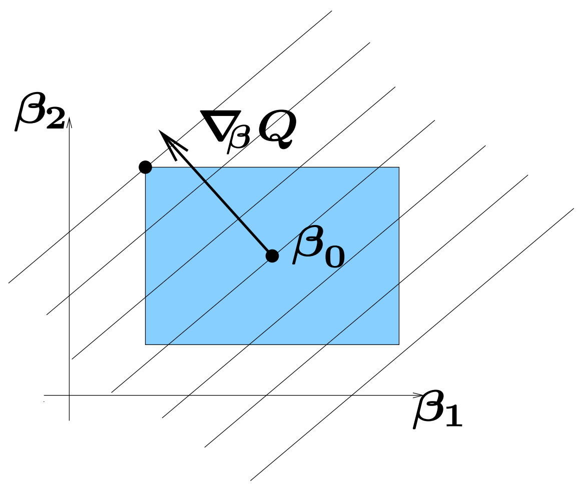

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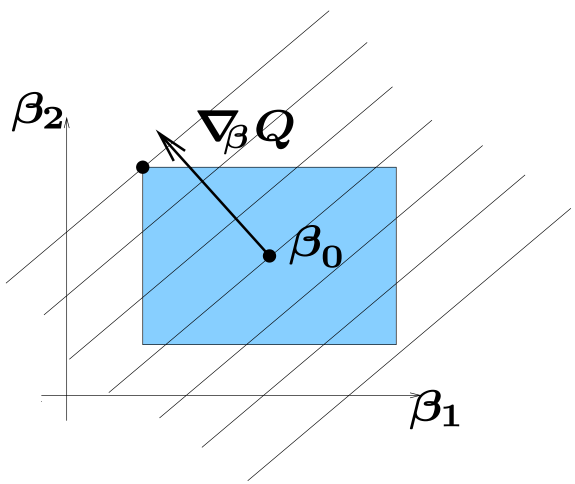
$\Longrightarrow$ in each element K of the mesh we have to solve a linear constrained optimization problem to find the maximum over the set Σ.



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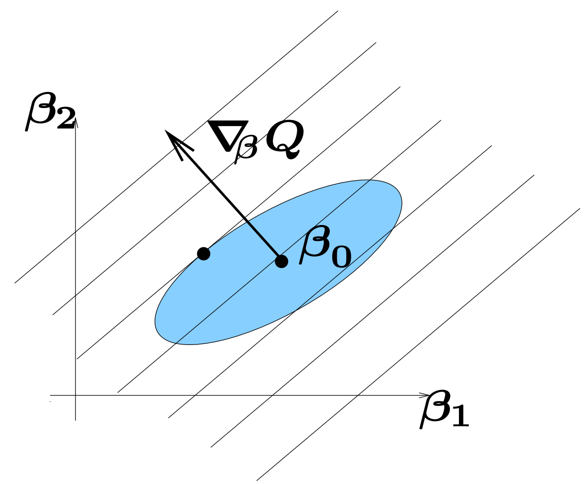

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Other types of perturbation sets (II)

b) Smoother perturbations

We could use a penalization approach: find the worst perturbation $\delta\beta^*$ s.t.

$$\delta\boldsymbol{\beta}^* = \underset{\delta\boldsymbol{\beta}\in\boldsymbol{\mathcal{A}}-\boldsymbol{\beta}_0}{\arg\max}\left\{ < D_{\boldsymbol{\beta}}\psi(\boldsymbol{\beta}_0), \delta\boldsymbol{\beta} > -\frac{1}{2}\sum_{i=1}^{m}\rho_i \|\delta\boldsymbol{\beta}_i\|^2_{H^1(D)} \right\}.$$

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$\Longrightarrow$ this problem is no longer separable in x. Implies a greater computational effort.

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$$\mathcal{A}_{\mathcal{L}} \equiv \{\mathcal{L} = \mathcal{L}_0 + \delta\mathcal{L} : \ \ \delta\mathcal{L} \in W', \qquad \|\delta\mathcal{L}\|_{W'} \leq \varepsilon\}$$

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Theorem [BNT 05]:

a) $$\Delta Q = \sup_{\mathcal{L}\in\mathcal{A}_{\mathcal{L}}} |\psi(\mathcal{L}) - \psi(\mathcal{L}_0)| = \varepsilon\|\varphi\|_W.$$

b) There exists a worst perturbation $\delta\mathcal{L}^*$.

Uncertainty in the Dirichlet boundary cond.

The first Fréchet derivative of ψ w.r.t. the boundary datum g is

$$< \boldsymbol{D_\beta \psi(g_0), \delta g} >= \int_{\boldsymbol{\Gamma_D}} \boldsymbol{\xi_0 \, \delta g}$$

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Worst Scenario bound [BNT 07]: if the dual flux is at least in $L^1(\Gamma_D)$.

a) $\Delta Q = \sup_{g \in \mathcal{A}_g} |\psi(g) - \psi(g_0)| \leq \int_{\Gamma_D} |\xi_0| \, \varepsilon_g(x) \, dx$

b) worst perturbation $\delta g^* = \mathrm{sign}(\xi_0) \varepsilon_g(x)$.

Details on adaptive integration

Build a sequence of adapted meshes $h_q[k],\ k = 1, 2, \ldots$.

for each element $n = 1, 2, \ldots, N[k]$,

- **compute the integral $I_n = \int_{K_n} \left| \frac{\partial(F-G)}{\partial \beta_i} \right| \varepsilon_i$**
- **uniformly h-refine the element, recompute the integral and use the difference as error indicator $r_n[k]$**
- **if $r_n[k] > \frac{TOL}{N[k]}$ then**
  mark the element for refinement
- **end if**

end for

refine the marked elements

(Convergence proof in "Moon-Von Schwerin-Szepessy-Tempone '04")

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The final mesh is well suited to represent the worst perturbation $\delta\beta^*$ (as a piecewise constant function).

Numerical computation of the dual flux

If one computes the finite element dual solution $\varphi_0^h \in V_h$ with strong imposition of the boundary conds., the dual flux can be reconstructed as: *find* $\xi_0^h \in V_h(\Gamma_D)$ *s.t.*

$$\boxed{\int_{\Gamma_D} \xi_0^h \, \mu_h = Q_1(\beta, E(\mu_h)) - B(\beta; E(\mu_h), \varphi_h), \quad \forall \mu_h \in V_h(\Gamma_D)}$$

where $E(\mu_h)$ is an arbitrary extension of μ_h inside the domain.

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- To compute ξ_h^0 we need only to invert a mass matrix on Γ_D.
- For a quasi-uniform mesh and $\xi \in L^2(\Gamma_D)$, one has sub-optimal rate of convergence [BNT - 05]

$$\|\xi_0 - \xi_0^h\|_{L^2(\Gamma_D)} \leq C_1 h^{-\frac{1}{2}} \inf_{v_h \in V_h(D)} \|\varphi_0 - v_h\|_{H^1(D)} + C_2 \inf_{\mu_h \in V_h(\Gamma_D)} \|\xi_0 - \mu_h\|_{L^2(\Gamma_D)}$$