



UNIVERSITÀ DEGLI STUDI DI PADOVA

AFM project

Topology Optimization inside a fluid region

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Outline

1 Introduction: Model Description

- Layout Optimization
- Governing equations
- Problem Formulation
- Chosen Functional
- Adjoint approach

2 Model Implementation

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- FEM derivation
- Boundary conditions

3 Results

- Solver validation
- Some Results
- Conclusions

4 First Part: Model setting in Cathy

- Creation of the geometry
- Initial and Boundary conditions
- Atmospheric conditions/ soil parameters

Layout Optimization

Motivations:

- Incredible tool for design projects
- Growing interest in last decades
- Used in various fields

Three mayor types:

- Size Optimization
- Shape Optimization
- Topology optimization

Problem Formulation

$$\left\{ \begin{array}{l} \min_{\gamma} J(\mathbf{u}, p, \gamma) \\ \text{subject to} \quad : \int_{\Omega} \gamma(\mathbf{r}) d\mathbf{r} - \beta |\Omega| \leq 0, \\ \quad : 0 \leq \gamma(\mathbf{r}) \leq 1, \\ \quad : \text{Governing equations} \end{array} \right.$$

Volume constraint,

Design variable bounds

(1)

Creation of the geometry

Exploit main features of the assignment.

`images/assignment.JPG`

Creation of the geometry

Idea: z -axis horizontal plane 1 meter below surface. z discretization with parallel planes. Drain at $x = 0$ as a long monodimensional tube in the y -direction.

Mesh to have exact points at

- I T1 (6,0.5,0.9);
- II T2 (3,0.5,0.9);
- III T3 (0.2,0.5,0.9);
- IV Drain (0,0:1,0);

Surface definition: hap.in

Domain extension in $x = 6$, $\frac{6}{0.2} = 30 \implies 30$ cells in x .

Problem y -symmetric \implies Consider sufficient 2 cells in y .

images/hap.JPG

Surface definition: dem13.val

File with 30 columns and 2 rows of "1.0".

Last value equal to 0.99999 to ensure possibility of outflow.

images/dtm13mat.JPG

Mesh creation: dem_parameters

Exact points at T1 (6,0.5,0.9), T2 (3,0.5,0.9), T3 (0.2,0.5,0.9), Drain (0,0:1,0).

Layer at 0.1 (5% of 2) from the top (not necessarily the first layer);

Layer at 1 (50% of 2) from the top.

Finer discretization near surface and near drain?

images/dem.JPG

Mesh creation: Parm file

Set $IPRT1 = 3$ and obtain the mesh.

Adapt some convergence parameter (DELTAT, DTMIN, DTMAGM).

One VTK file for each hour.

Set maximum time equal to 500 for calibration (see next).

images/parm.JPG

Units of measure

Data for 2018 hours(~ 84 days) \implies Time unit: hours (days);
Length unit: meter.

- Pressure head $[\psi] = m$;
- Hydraulic conductivity $[K] = m\text{hours}^{-1}$;
- Specific storage $[S] = 1/m$.

Mesh Results

images/mesh1.JPG

Mesh Results

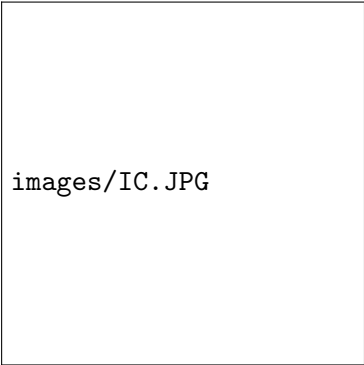
images/mesh2.JPG

Initial condition: IC file

Unsaturated zone \implies partially saturated vertical hydrostatic equilibrium as IC.

WTPOSITION in depth from the surface.

First trial: initial water table depth of 0.4 meters (will be calibrated).



images/IC.JPG

Boundary Conditions: drain

Three possibilities:

- $\psi = 0$ at the drain;
- $\psi = 0$ at drain + hydrostatic pressure in the vertical;
- $\psi = 0$ at the points in N3 (variable condition in time).

images/Freeze.JPG

Dirichlet BC

images/Dir.JPG

images/Dir2.JPG

Dirichlet BC: class Nodes

images/findNode.JPG

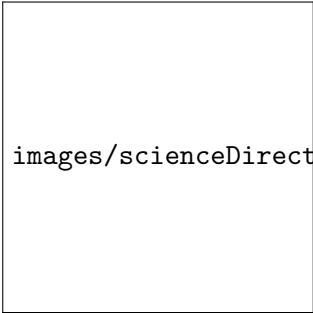
Atmospheric BC: rain+evapotranspiration

Compute NET flow : $drain - ET$ for each time step and adjust the dimensions.


images/atmbc.JPG

Soil parameters

Assume medium-textured soil (50-70% sand, 25-40% silt, 5-15% clay).



images/scienceDirect.JPG



images/article.JPG

Soil: Range of parameters

Obtain an approximate range of variability of the parameters

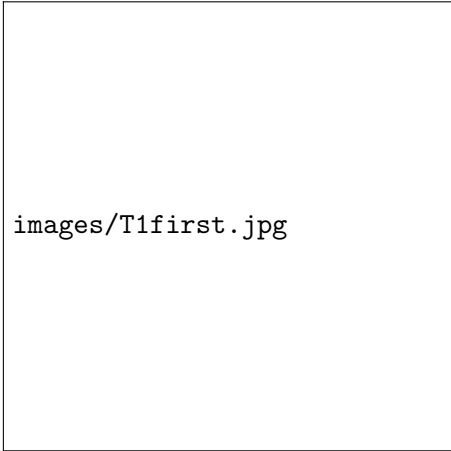
- $K = 0.02 \text{ m/hour} \div 2.53 \text{ m/hour}$;
- $S_s = 1\text{E-}5 \text{ m}^{-1} \div 0.01 \text{ m}^{-1}$;
- $\eta = 50\% \div 57\%$.

images/first.JPG

The first values used are:

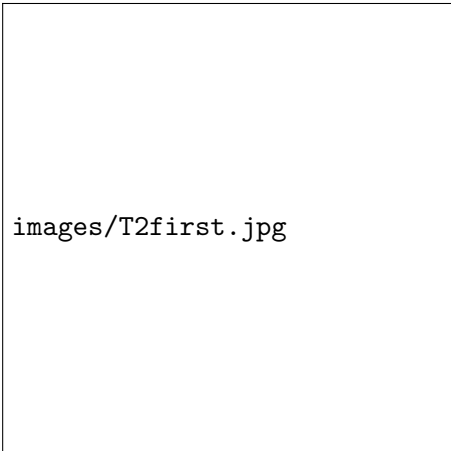
First Result

Drain applied with second approach.



images/T1first.jpg

Figure: MSE = 0.033 m^2 ; NSE = -0.999; KGE = 0.173



images/T2first.jpg

Figure: MSE = 0.027 m^2 ; NSE = -4.87; KGE = 0.357

First Result

images/T3first.jpg

images/regressionfirst.jpg

Figure: $\text{MSE} = 0.0133 \text{ m}^2$; $\text{NSE} = 0.3144$; $\text{KGE} = 0.233$

Scatter plots depicting simulated and observed head pressures. $k_s = 2.31$.

First Result

Pressure "Pseudocolor" result in Visit at time 1.12 hours.

images/firstVTK.JPG

CALIBRATION

Introduction


- Test on 1/4 of total data (approximately 500 hours). Remaining used for validation.
- Choose an objective function to minimize (MSE) or maximize (NSE or KGE).
- Various possible heuristic models to find "good" values of parameters.
- Just some:
 - ▶ First improvement local search;
 - ▶ Best improvement local search;
 - ▶ Genetic algorithm (?).
- Need to discretize the search space (finite number of possible values combinations).
- Define a "move". Idea: Firstly great steps, find local optima, then reduce steps.

Local Search

`images/calibration.jpg`

Code hints


- Increase first parameter (horizontal permeability).
- Build dynamically IC, parm and soil files.
- Launch the cathy_ft.
- Get the pressure values and the interested nodes.
- Compute KGE (NSE) errors and check for improvements.
 - ▶ If improvement restart the cycle and increase horizontal permeability
 - ▶ else decrease permeability to previous value and increment the new one.
- Finally, "change move" and check convergence.



images/dynamicIc.jpg

Objective function

- From results: parameters that increase fit at T1 or T2 decrease it in T3.
- Possible motivations:
 - ▶ Drain might not be ideal;
 - ▶ Observed data near drain can be affected by errors;
 - ▶ Richard's equation is not enough near the drain.
- Idea: Penalize the error in T3 in the objective function.



images/objfunc.jpg

First Improvement Local Search

`images/firstImpr.JPG`

First Improvement Local Search

images/firstImpr2.JPG

images/output0.jpg

MSE and NSE

- MSE (mean squared error) $[0, +inf]$; $MSE = \frac{\sum_{t=1}^n (x_{s,t} - x_{o,t})^2}{n}$
- NSE (Nash–Sutcliffe efficiency) $[-inf, 1]$;
 - ▶ $NSE = 1 - \frac{MSE}{\sigma_o^2}$;
 - ▶ Classic skill score. If $NSE \leq 0$ observed mean is a better predictor;
 - ▶ Likely underestimates of the variability in the flows;
 - ▶ May lead to a Pareto set of optimal solutions
- Decomposition:
 - ▶ $MSE = 2\sigma_s\sigma_o(1 - r) + (\sigma_s - \sigma_o)^2 + (\mu_s - \mu_o)^2$;
 - ▶ $NSE = 2\alpha r - \alpha^2 - \beta_n^2$
 $\alpha = \frac{\sigma_s}{\sigma_o}, \beta_n = (\mu_s - \mu_o)/\sigma_o$.

- Ideas:
 - ▶ Corrected formulations;
 - ▶ Multi-objective perspective (KGE).

- Klinga-Gupta efficiency (KGE)
= 1- ED

- ED =
$$\frac{1}{\sqrt{(r-1)^2 + (\alpha-1)^2 + (\beta-1)^2}}$$

- $\beta = \mu_s / \mu_o$

images/theory.jpg

Move: change one parameter's value

- Useful to understand parameters effects on the solution.
- Not so effective if parameters effects are dependent to each other.

images/T1WT.jpg

images/T2WT.jpg

Effects of initial conditions decrease in time and vanish at approximately 350 hours.

Change one parameter's value: K_x/K_y

Change the horizontal conductivity.

images/T1PERMX.jpg

images/T2PERMX.jpg

Change one parameter's value: K_z

Change the vertical conductivity.

images/T1PERMZ.jpg

images/T2PERMZ.jpg

Change one parameter's value: *ELSTOR*

Change the specific storage value.

images/T1ELSTOR.jpg

images/T2ELSTOR.jpg

S_s proportional to volume water released per surface area per head drop.
High $S_s \implies \psi$ less sensible to atmospheric conditions.

Change one parameter's value: *POROS*

Change the porosity.

images/T1POROS.jpg

images/T2POROS.jpg

Porosity decrease $\implies S_y$ decrease. More sensible to atmospheric conditions.

Change one parameter's value: *VGN1*

Change N parameter of Van Geneuchten.

images/T1VGN1.jpg

images/T2VGN1.jpg

Change one parameter's value: *VGN2*

Change theta parameter of Van Geneuchten.

images/T1VGN2.jpg

images/T2VGN2.jpg

Change one parameter's value: *VGN3*

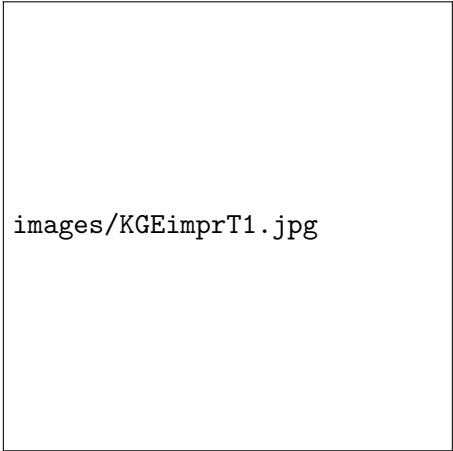
Change inverse alpha parameter of Van Geneuchten.

images/T1VGN3.jpg

images/T2VGN3.jpg

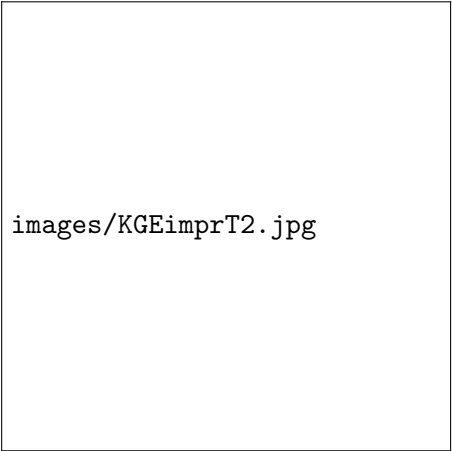
Calibration with KGE

Calibration with KGE and first approach for drain boundary conditions.



images/KGEimprT1.jpg

Figure: Best: $\text{MSE} = 0.0097 \text{ m}^2$; $\text{NSE} = 0.4122$; $\text{KGE} = 0.450$

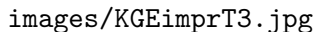


images/KGEimprT2.jpg

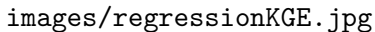
Figure: Best: $\text{MSE} = 0.0056 \text{ m}^2$; $\text{NSE} = -0.2154$; $\text{KGE} = 0.6803$

Calibration with KGE

See how the best approximation for T1 and T2 is almost the worst for T3.

A scatter plot showing simulated versus observed head pressures for the KGEimprT3 model. The plot area is currently blank, with only the filename visible.

images/KGEimprT3.jpg

A scatter plot showing simulated versus observed head pressures for the regressionKGE model. The plot area is currently blank, with only the filename visible.

images/regressionKGE.jpg

Figure: Best: $\text{MSE} = 0.0293 \text{ m}^2$; $\text{NSE} = -0.512$; $\text{KGE} = -0.083$

Figure: Scatter plots depicting simulated and observed head pressures. $k_s = 1.63$.

Calibration with KGE: Comparison

images/compKGE1.jpg

images/compareKGE2.jpg

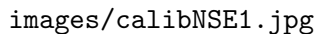
Calibration with KGE: Comparison

images/compKGE3.jpg

images/scatterKGE.jpg

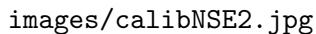
Figure: Scatter plots depicting simulated and observed head pressures. $k_s = 1.49$.

NSE calibration



images/calibNSE1.jpg

Figure: Best: $\text{MSE} = 0.0058 \text{ m}^2$; $\text{NSE} = 0.65$; $\text{KGE} = 0.52$



images/calibNSE2.jpg

Figure: Best: $\text{MSE} = 0.0020 \text{ m}^2$; $\text{NSE} = 0.57$; $\text{KGE} = 0.81$

Calibration with NSE

images/calibNSE3.jpg

images/scatterNSE.jpg

Figure: Best: $\text{MSE} = 0.0041 \text{ m}^2$; $\text{NSE} = -1.10$; $\text{KGE} = -0.29$

Figure: Scatter plots depicting simulated and observed head pressures. $k_s = 1.65$.

KGE validation

images/finalKGE.jpg

Figure: Best: $\text{MSE} = 0.0101 \text{ m}^2$; $\text{NSE} = 0.3315$; $\text{KGE} = 0.49$

images/finalKGE2.jpg

Figure: Best: $\text{MSE} = 0.0056 \text{ m}^2$; $\text{NSE} = 0.1503$; $\text{KGE} = 0.61$

KGE validation

images/finalKGE3.jpg

images/finalregressionKGE.jpg

Figure: Best: $\text{MSE} = 0.0250 \text{ m}^2$; $\text{NSE} = -0.3285$; $\text{KGE} = 0.23$

Figure: Scatter plots depicting simulated and observed head pressures. $k_s = 1.12$.

NSE validation

images/finalNSE.jpg

Figure: Best: $\text{MSE} = 0.0099 \text{ m}^2$; $\text{NSE} = 0.3324$; $\text{KGE} = 0.48$

images/finalNSE2.jpg

Figure: Best: $\text{MSE} = 0.0054 \text{ m}^2$; $\text{NSE} = 0.18$; $\text{KGE} = 0.61$

NSE validation

images/finalNSE3.jpg

Figure: Best: $\text{MSE} = 0.0268 \text{ m}^2$; $\text{NSE} = -0.43$; $\text{KGE} = 0.20$

images/finalregressionNSE.jpg

Figure: Scatter plots depicting simulated and observed head pressures. $k_s = 1.099$.

Conclusions

- Better accuracy with second approach for drain, but worst fit in T3;
- Better fit in T3 with third approach, but worst fit overall;
- Calibration on NSE and KGE provides similar results overall of fit, but extremely different parameters:
 - ▶ $ELSTOR = 0.65$ is not so realistic for KGE;
 - ▶ $PORSO = 0.7$ is not so realistic for NSE.

images/ultimo.JPG

images/WTcomparison.jpg