UNIVERSITÀ DEGLI STUDI DI PADOVA

AFM project

Topology Optimization inside a fluid region

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Outline

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

$$
\begin{cases}
\min\limits_{\gamma} J(\mathbf{u}, p, \gamma) & \\
\text{subject to} \quad : \displaystyle\int_{\Omega} \gamma(\mathbf{r}) d\mathbf{r} - \beta|\Omega| \leq 0, & \text{Volume constraint,} \\
\qquad\qquad\quad : 0 \leq \gamma(\mathbf{r}) \leq 1, & \text{Design variable bounds} \\
\qquad\qquad\quad : \text{Governing equations} &
\end{cases}
\tag{1}
$$

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

1. T1 (6,0.5,0.9);
2. T2 (3,0.5,0.9);
3. T3 (0.2,0.5,0.9);
4. 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($\sim$ 84days) $\implies$ Time unit: hours (days);
Length unit: meter.

- Pressure head $[\psi] = m$;
- Hydraulic conductivity $[K] = mhours^{-1}$;
- 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 m/hour $\div$ 2.53 m/hour;
- S_s = 1E-5 $m^{-1} \div$ 0.01 m^{-1};
- η = 50% $\div$ 57%.

The first values used are: images/first.JPG

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: MSE $= 0.0133\ m^2$; NSE $=$ 0.3144; 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 and 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 $= 2\alpha r - \alpha^2 - \beta_n^2$
    $\alpha = \frac{\sigma_s}{\sigma_o}$, $\beta_n = (\mu_s - \mu_o)/\sigma_o$.

KGE

- Ideas:
  - Corrected formulations;
  - Multi-objective perspective (KGE).
- Klinga-Gupta efficiency (KGE) = 1- ED
- ED = $\sqrt{(r-1)^2 + (\alpha-1)^2 + (\beta-1)^2}$
- $\beta = \mu_s/\mu_o$

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 Geneucthen.

images/T1VGN1.jpg

images/T2VGN1.jpg

Change one parameter's value: *VGN*2

Change theta parameter of Van Geneucthen.

images/T1VGN2.jpg

images/T2VGN2.jpg

Change one parameter's value: *VGN3*

Change inverse alpha parameter of Van Geneucthen.

images/T1VGN3.jpg

images/T2VGN3.jpg

Calibration with KGE

Calibration with KGE and first approach for drain boundary conditions.

images/KGEimprT1.jpg

Figure: Best: MSE = 0.0097 m^2; NSE = 0.4122; KGE = 0.450

images/KGEimprT2.jpg

Figure: Best: MSE = 0.0056 m^2; NSE = -0.2154; KGE = 0.6803

Calibration with KGE

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

images/KGEimprT3.jpg

Figure: Best: MSE = 0.0293 m^2; NSE = -0.512; KGE = -0.083

images/regressionKGE.jpg

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: MSE $= 0.0058\ m^2$; NSE $= 0.65$; KGE $= 0.52$

images/calibNSE2.jpg

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

Calibration with NSE

images/calibNSE3.jpg

Figure: Best: MSE = 0.0041 m^2; NSE = -1.10; KGE = -0.29

images/scatterNSE.jpg

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

KGE validation

images/finalKGE.jpg

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

images/finalKGE2.jpg

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

KGE validation

images/finalKGE3.jpg

Figure: Best: MSE = 0.0250 m^2; NSE = -0.3285; KGE = 0.23

images/finalregressionKGE.jpg

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

NSE validation

images/finalNSE.jpg

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

images/finalNSE2.jpg

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

NSE validation

images/finalNSE3.jpg

Figure: Best: MSE = 0.0268 m^2; NSE = -0.43; 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 paramters:
  - ELSTOR = 0.65 is not so realistic for KGE;
  - PORSO = 0.7 is not so realistic for NSE.

images/ultimo.JPG

images/WTcomparison.jpg