The Adjoint State Method: Highly Scalable Sensitivity Analysis

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Contributors and coauthors

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Outline

1. Brief theory and overview of the adjoint method
2. Implementation details
3. Some examples

Why sensitivity analysis (again)?!

- Sensitivity analysis is a fundamental aspect of modeling building
- Develop “hydrosense”
- “What inputs are effecting these outputs?”
- “If I change model input X, what does that do?”
- Why not sensitivity analysis?
    - Its computationally expensive…

How?

- Run model at current parameter values
- For each parameter:
  - Change parameter some
  - Run model
  - Process results

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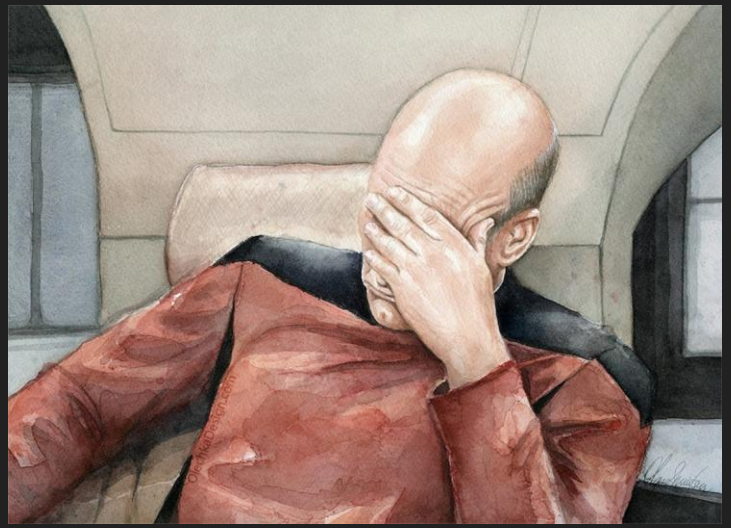


What is an adjoint solver

- An extreme efficient analytical gradient/sensitivity tool
- It’s been done before…
- Problem: its intrusive!
  - Traditionally, someone has to modify the forward model code
  - This leads to long-term maintenance and upkeep issues

Adjoint terminology

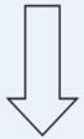
- “Performance measure”: a single or aggregate summary of model outputs of interest
  - Sum of weighted residuals (ie objective function)
  - Heads (single, time series, map)
  - Fluxes (single, time series, map)
- “Parameter”: model input
  - Every node, every stress period

Equation alert!

Modflow-6: Standard Equations for Adjoint Model

Forward model (MF6)
Solving for head (Forward in time)

$$\left[A\left(\vec{\alpha},\vec{h}^{k}\right)\right]\vec{h}^{k}=\vec{b}^{k}\left(\vec{\alpha},\vec{h}^{k-1}\right)$$
$$\vec{h}^{0}=\vec{h}_{i}$$



$$\left(\vec{h}^{1},\vec{h}^{2},\vec{h}^{3},\ldots\vec{h}^{N}\right)$$

Linear/Nonlinear

Performance measure

$$J=\sum_{k=1}^{N}F^{k}\left(\vec{\alpha},\vec{h}^{k}\right)$$

$$\frac{\partial J}{\partial \alpha_{i}}?$$

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$$\vec{h}^0 = \vec{h}_i$$

$$(\vec{h}^1,\vec{h}^2,\vec{h}^3,\dots\vec{h}^N)$$

Linear/Nonlinear

Adjoint model (MF6)
Solving for adjoint states (**Backward** in time)

$$[A(\vec{\alpha},\vec{h}^k)]^T\vec{\lambda}^{k-1} = -\left[\frac{\partial\vec{b}^{k+1}(\vec{\alpha},\vec{h}^k)}{\partial\vec{h}^k}\right]^T\cdot\vec{\lambda}^k - \frac{\partial F^k(\vec{\alpha},\vec{h}^k)}{\partial(\vec{h}^k)^T}$$
$$\vec{\lambda}^N = 0$$

$$(\vec{\lambda}^{N-1},\vec{\lambda}^{N-2},\vec{\lambda}^{N-3},\dots\vec{\lambda}^0)$$

Linear

Performance measure

$$J = \sum_{k=1}^{N} F^k(\vec{\alpha},\vec{h}^k)$$

$$\frac{\partial J}{\partial\alpha_i}?$$

Sensitivity coefficients

$$\frac{\partial J}{\partial\alpha_i} = \sum_{k=1}^{N}\left\{\underbrace{\frac{\partial F^k}{\partial\alpha_i}}_{\text{Direct effect}} + \underbrace{(\vec{\lambda}^{k-1})^T\left(\frac{\partial[A]}{\partial\alpha_i}\vec{h}^k - \frac{\partial\vec{b}^k}{\partial\alpha_i}\right)}_{\text{Indirect effect}}\right\}$$

What is the adjoint state conceptually…

- The sensitivity of a given performance measure to a unit injection of water in each active model cell for each solution time…

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Design goals

- Non-intrusive: easy to maintain as MF6 advances
- Work with *almost* any MF6 GWF model
  - Newton and standard solution schemes
  - Structured and unstructured
- Wide range of performance measures
- Wide range of parameters
- Open source and free!

Approach

- Using the MF6 API
- Forward solve (linear/nonlinear):
  - Only done once
  - Advance thru simulation time, harvesting solution components
- Adjoint solve (always linear!):
  - One per performance measure
  - Solve for adjoint states backwards in time
  - Propagate to parameters via chain rule

Hughes and others (2022). The MODFLOW Application Programming Interface for simulation control and software interoperability

Implementation

- Mf6Adj class
  - Processes .adj file and prepares for forward solve
  - Solves the forward MF6 GWF model
  - Collects solution components
    - Conductance matrix, RHS, head, saturation
  - Writes solution info to HDF5
  - The only place the MF6 shared lib is needed!

Implementation

- PerfMeas class
  - Contains PerfMeasRecord instances
    - One per performance measure entry
    - Spatio-temporal information
    - Residual and weight info
  - Loads forward model HDF5 output file
  - Solves for adjoint state and propagates to parameters
  - Writes to (new) HDF5 file

Currently supported parameters/inputs

- Adjoint state (1 per node per stress period)
  - ~ well flux
- Recharge (1 per node per stress period)
  - area * adj state
- NPF k11,k33 (1 per node)
- STO ss (1 per node)
- GHB bhead,cond (1 per boundary node per stress period)
- DRN elev, cond (1 per boundary node per stress period)
- RIV stage, cond (1 per boundary node per stress period)
- SFR stage, cond (1 per reach per stress period)

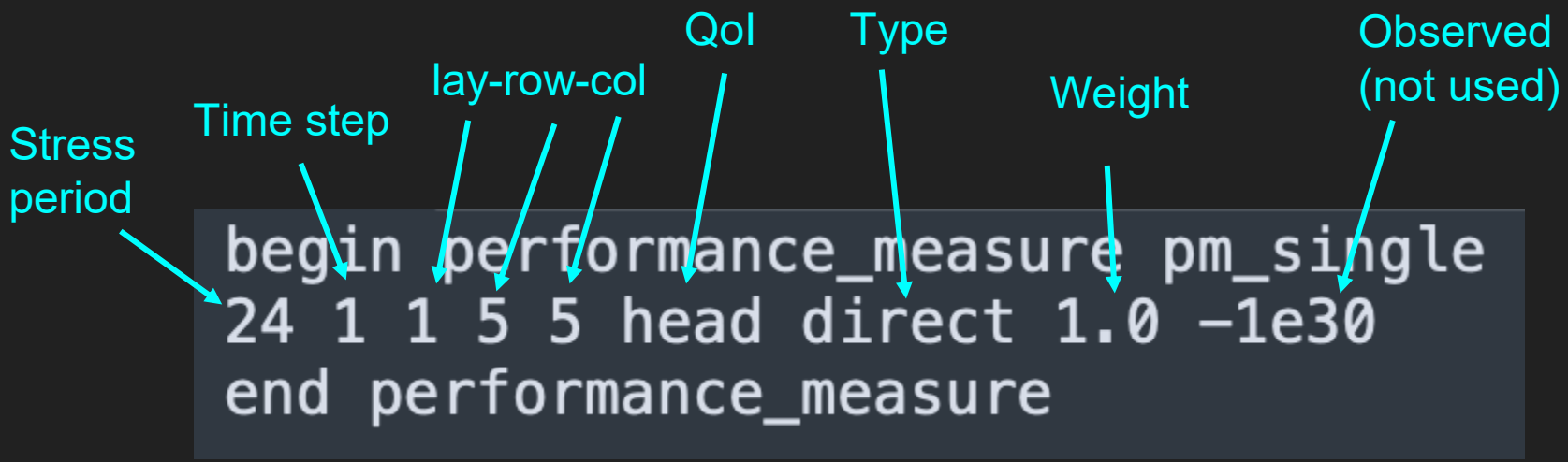
Currently supported performance measures

- Heads
  - At a point in space-time
  - A timeseries at one point in space
  - Aggregate over a region for one time
  - Combinations…
- Boundary fluxes
  - At a point in space-time
  - A timeseries at one point in space
  - Aggregate over a region for one time
  - Combinations…
- Sum of weighted head residuals
  - PEST-style objective function

Example performance measure blocks

```
begin performance_measure pm_single
24 1 1 5 5 head direct 1.0 -1e30
end performance_measure
```

Example performance measure blocks



Example performance measure blocks

```
begin performance_measure pm_single_alltimes
1 1 1 5 5 head direct 1.0 -1e30
2 1 1 5 5 head direct 1.0 -1e30
.
.
.
24 1 1 5 5 head direct 1.0 -1e30
25 1 1 5 5 head direct 1.0 -1e30
end performance_measure
```

Example performance measure blocks

```
begin performance_measure pm_ssr
1 1 3 3 10 head residual 1.0 34.597052432112854
1 1 3 10 2 head residual 1.0 34.61896038291642
.
.
.
11 1 1 27 7 head residual 1.0 36.428347809278l5
11 1 1 34 8 head residual 1.0 34.7015998123468 85
11 1 1 35 11 head residual 1.0 33.959077339551236
end performance_measure
```

Example performance measure blocks

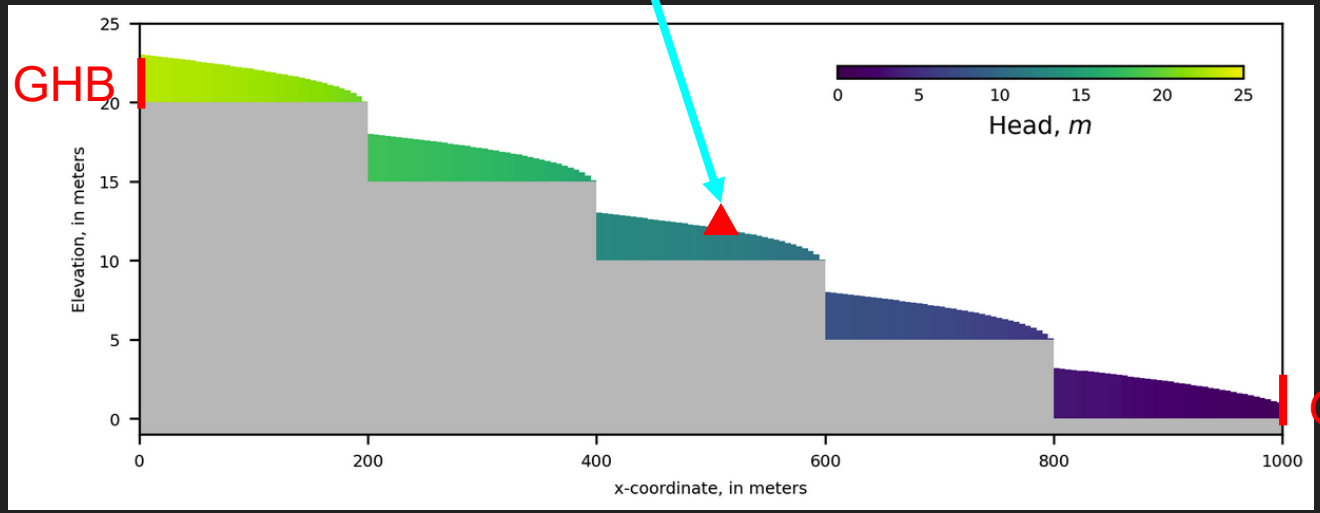
```
begin performance_measure headwater
23 1 1 1 16 sfr_1 direct 1.0 -1.0e+30
23 1 1 2 16 sfr_1 direct 1.0 -1.0e+30
.
.
.
23 1 1 20 16 sfr_1 direct 1.0 -1.0e+30
23 1 1 21 16 sfr_1 direct 1.0 -1.0e+30
end performance_measure
```

Usage

```
adj = mf6adj.Mf6Adj("test.adj",lib_name,verbose_level=1)
adj.solve_gwf()
adj.solve_adjoint()
adj.finalize()
```

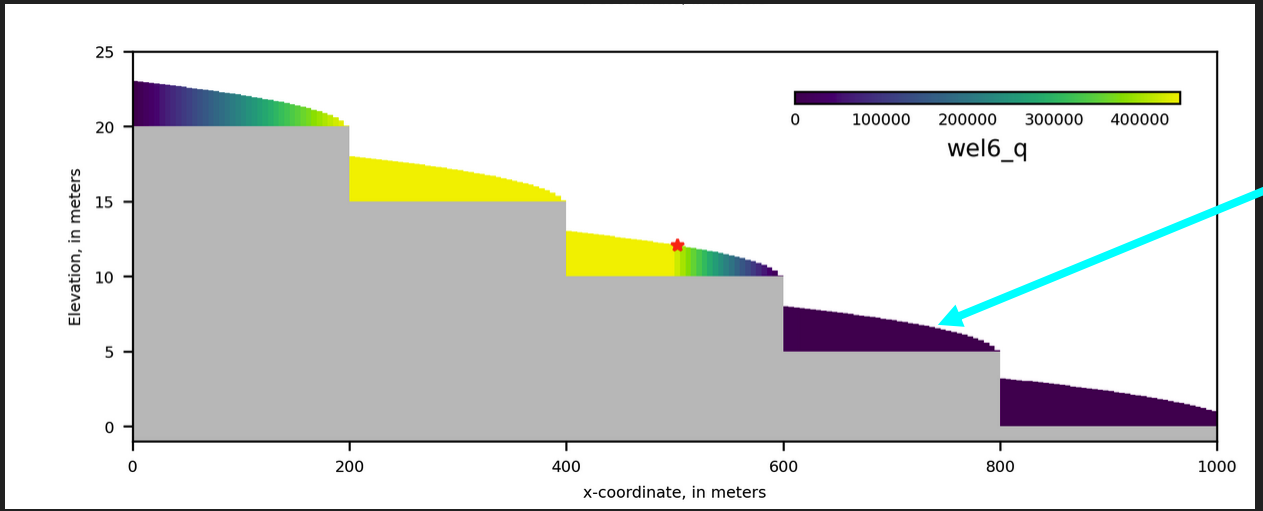
Zaidel problem

- Numerical benchmark for the newton solver
  - Part of the MODFLOW6 examples
- Performance measure: a single groundwater level



Zaidel problem

- Performance measure: a single groundwater level



Insensitive to pumping

Zaidel problem

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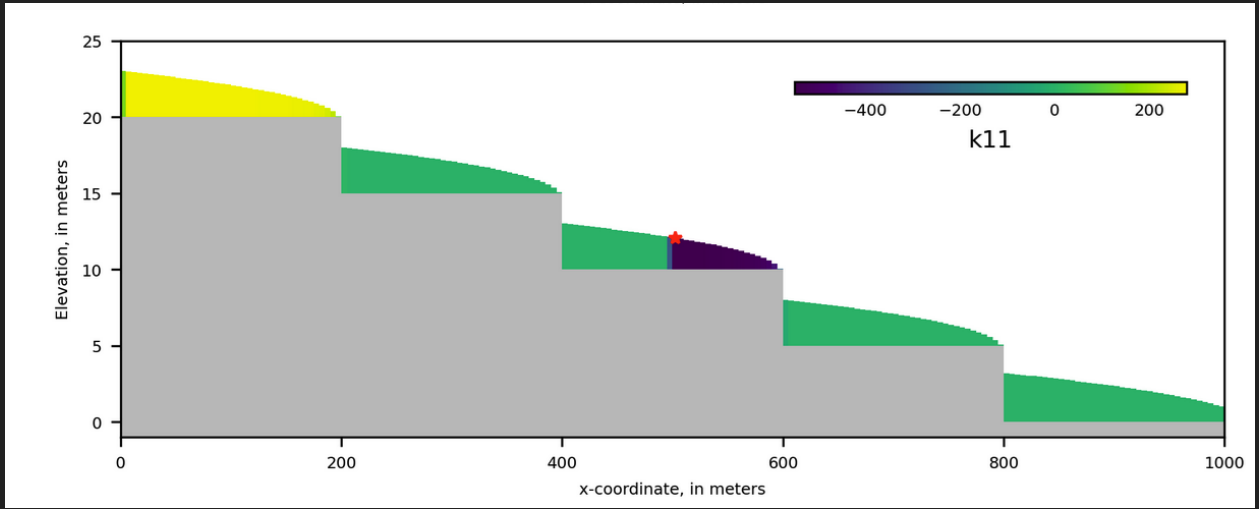

Zaidel problem

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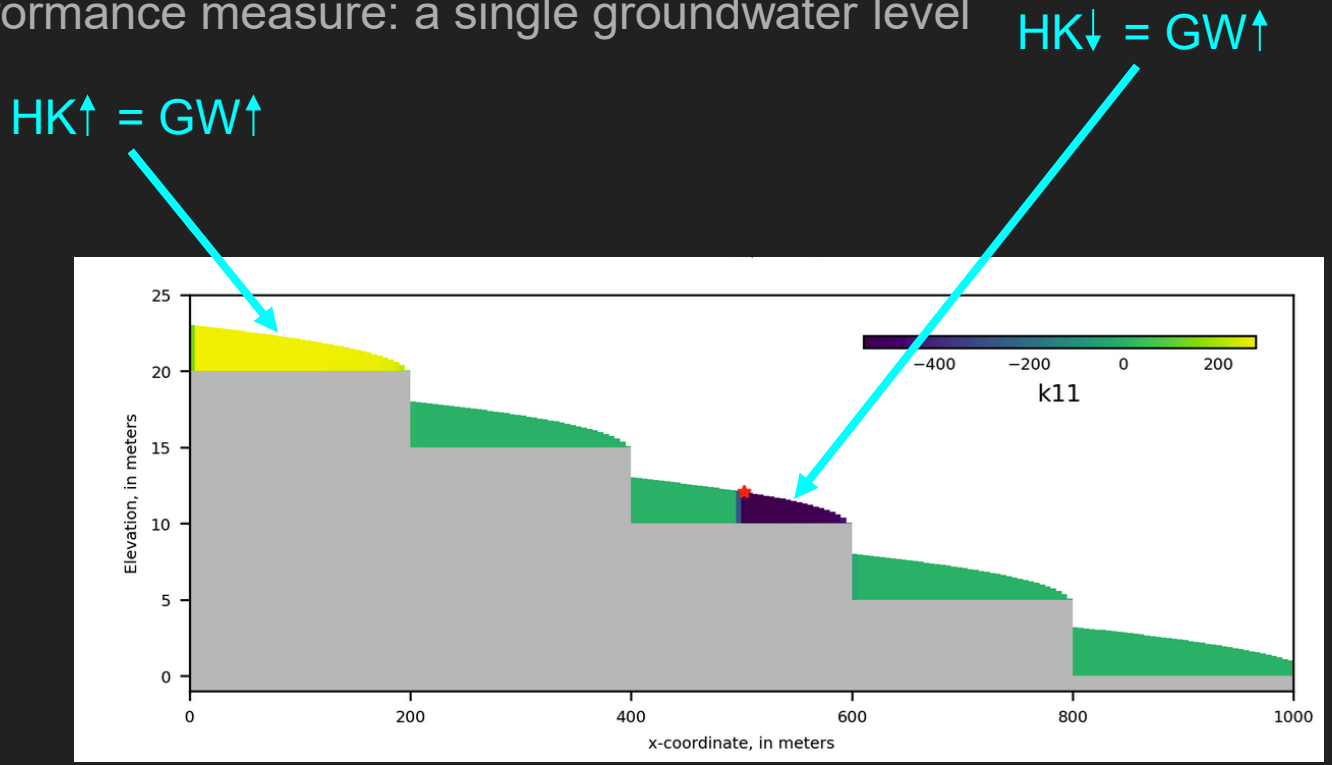


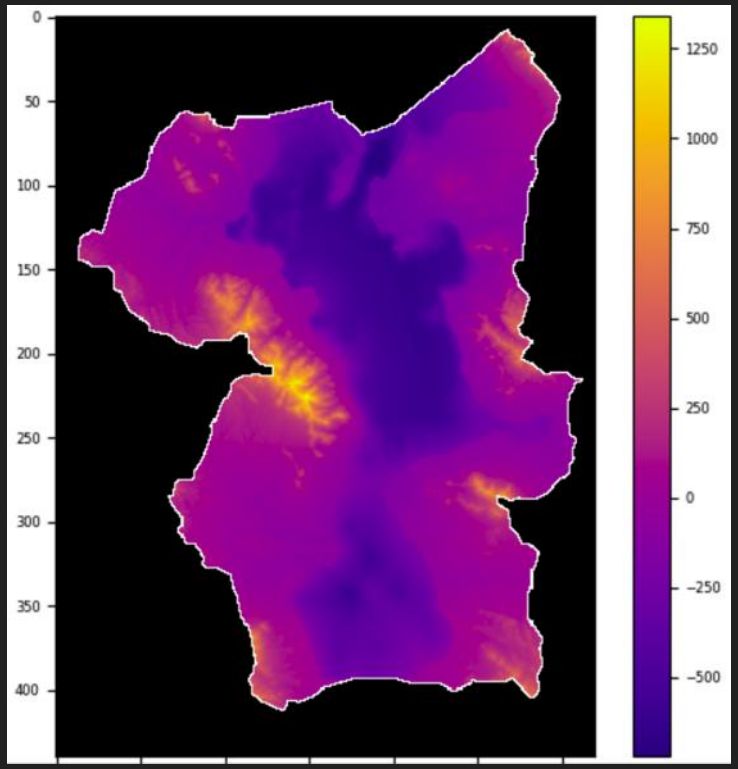
Example: San Pedro

A New Capture Fraction Method to Map How Pumpage Affects Surface Water Flow

Stanley A. Leake, Howard W. Reeves, Jesse E. Dickinson

First published: 19 August 2010 | https://doi.org/10.1111/j.1745-6584.2010.00701.x | Citations: 29

- Originally developed by Stan Leake
- Focus on simulating the relation between gw use and sw flow
- Structured grid, transient
- Thanks to Joe Hughes for porting to MF6!
- An example notebook in the repo…



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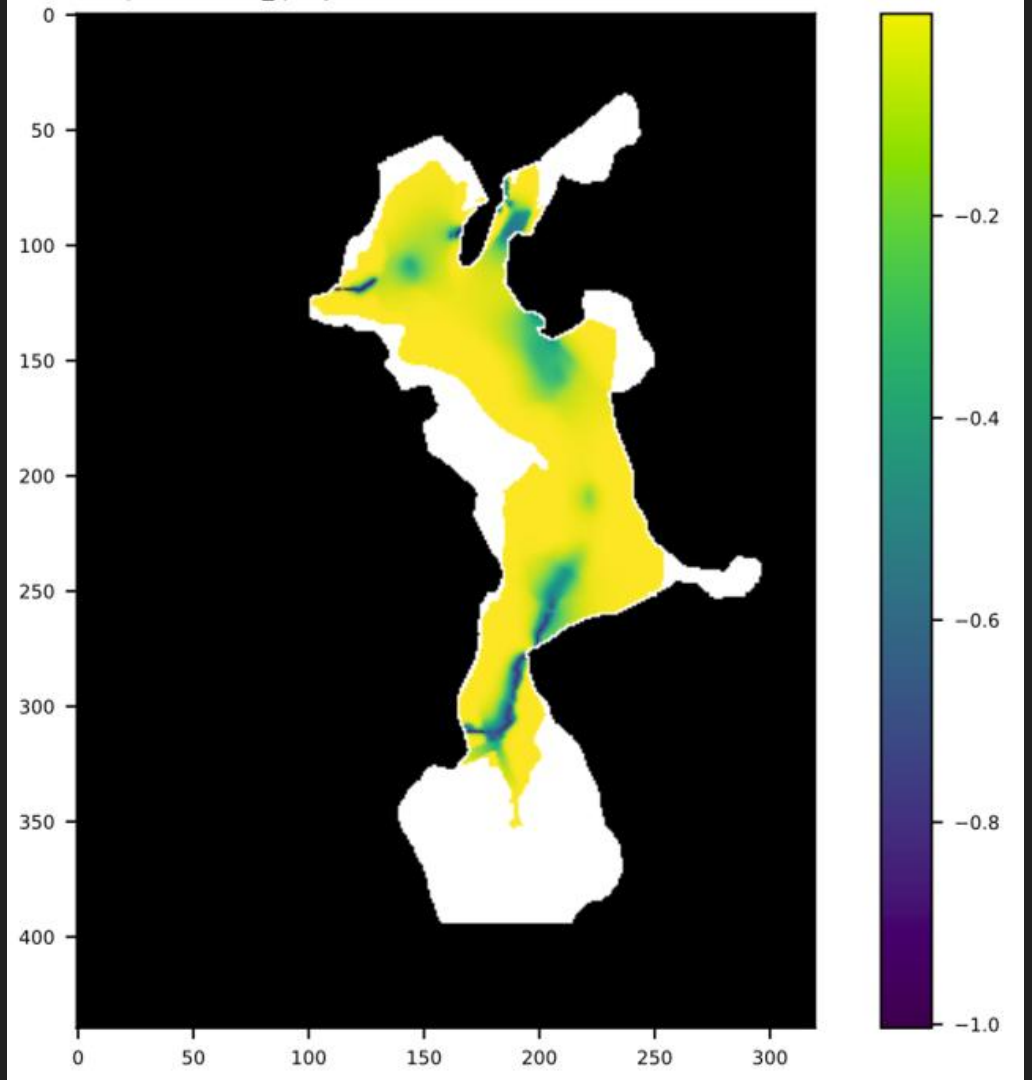
- Performance measure:
  - Sum of SW-GW exchange over all reaches
- 1 forward mf6 run then 1 adjoint run
- ~115K active nodes…~600K model runs required for perturbation sensitivities

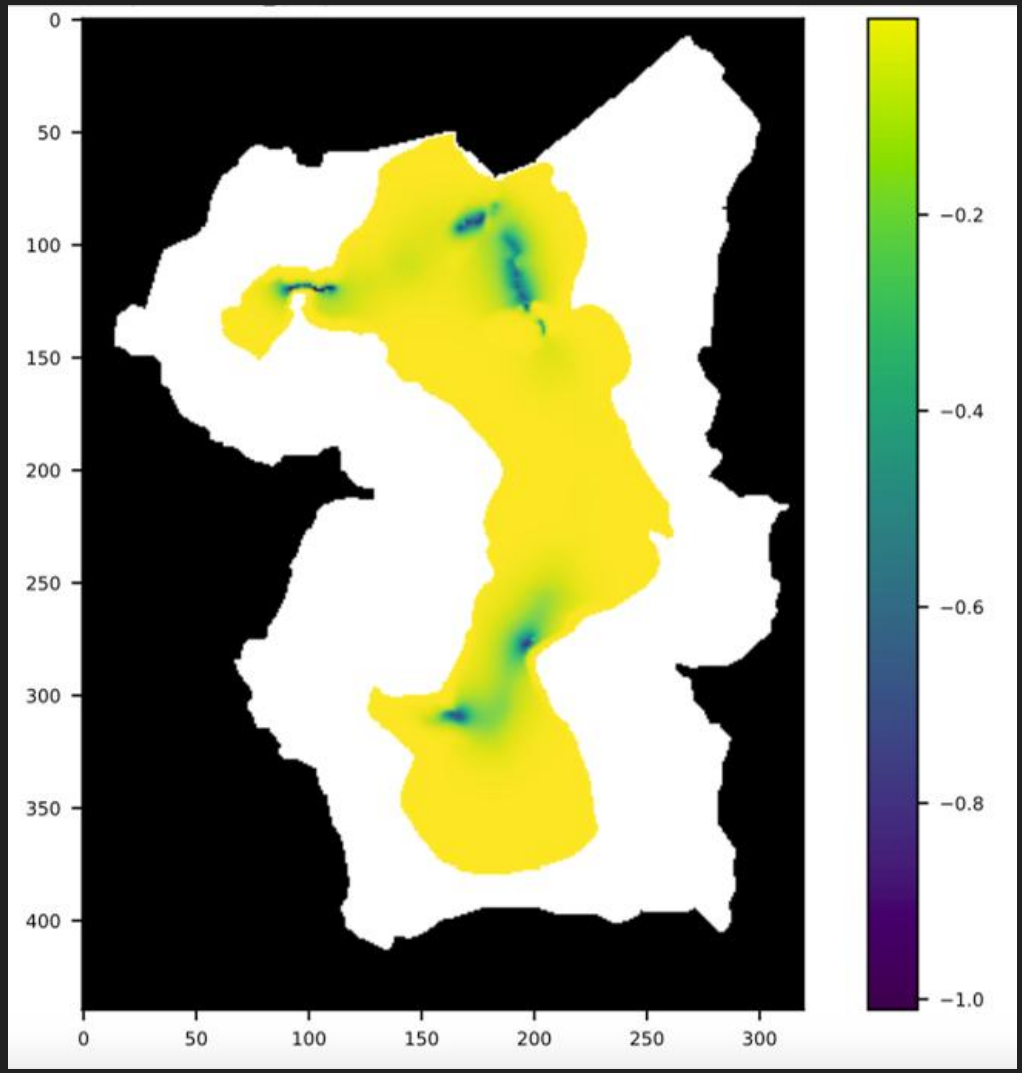
Example: San Pedro

- Capture fraction layer 4
- Higher values = more depletion



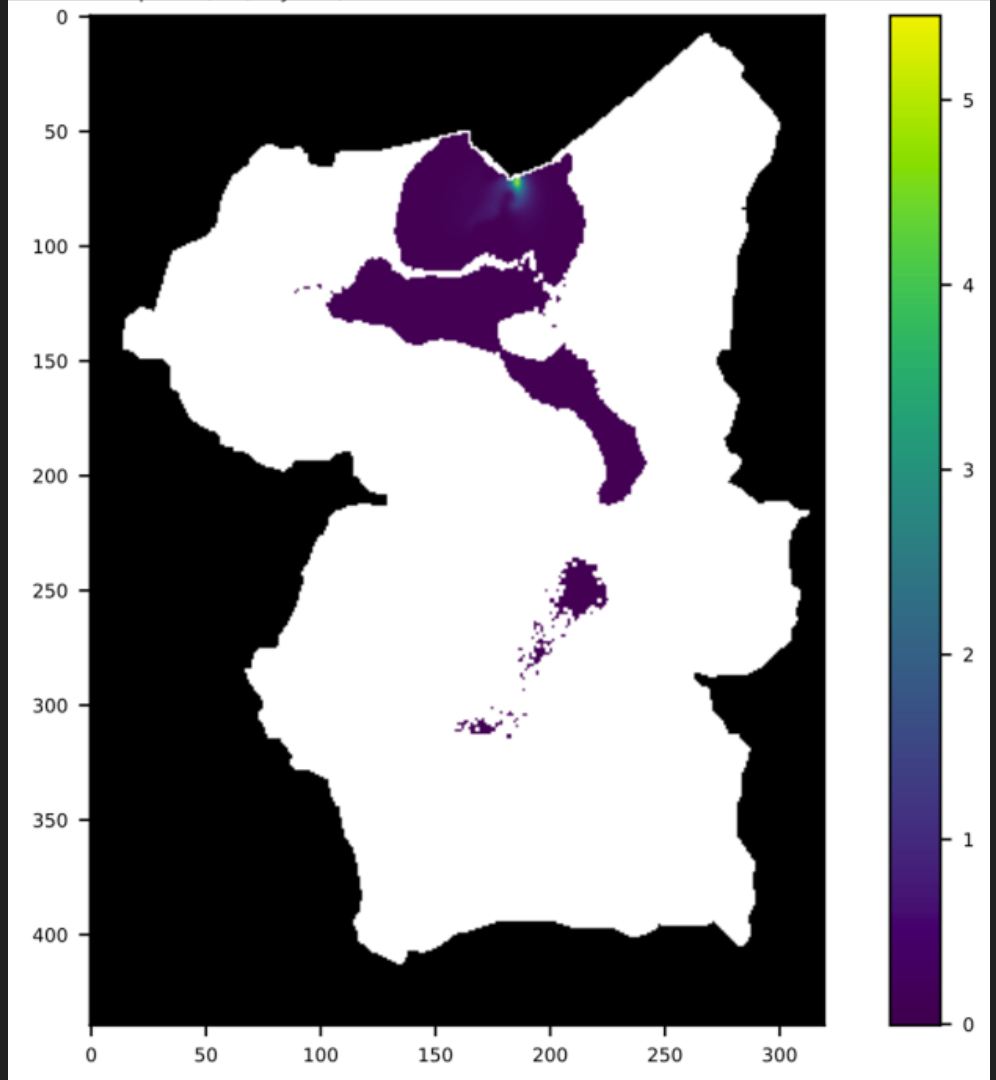
Example: San Pedro

- Capture fraction layer 5
- Higher values = more depletion



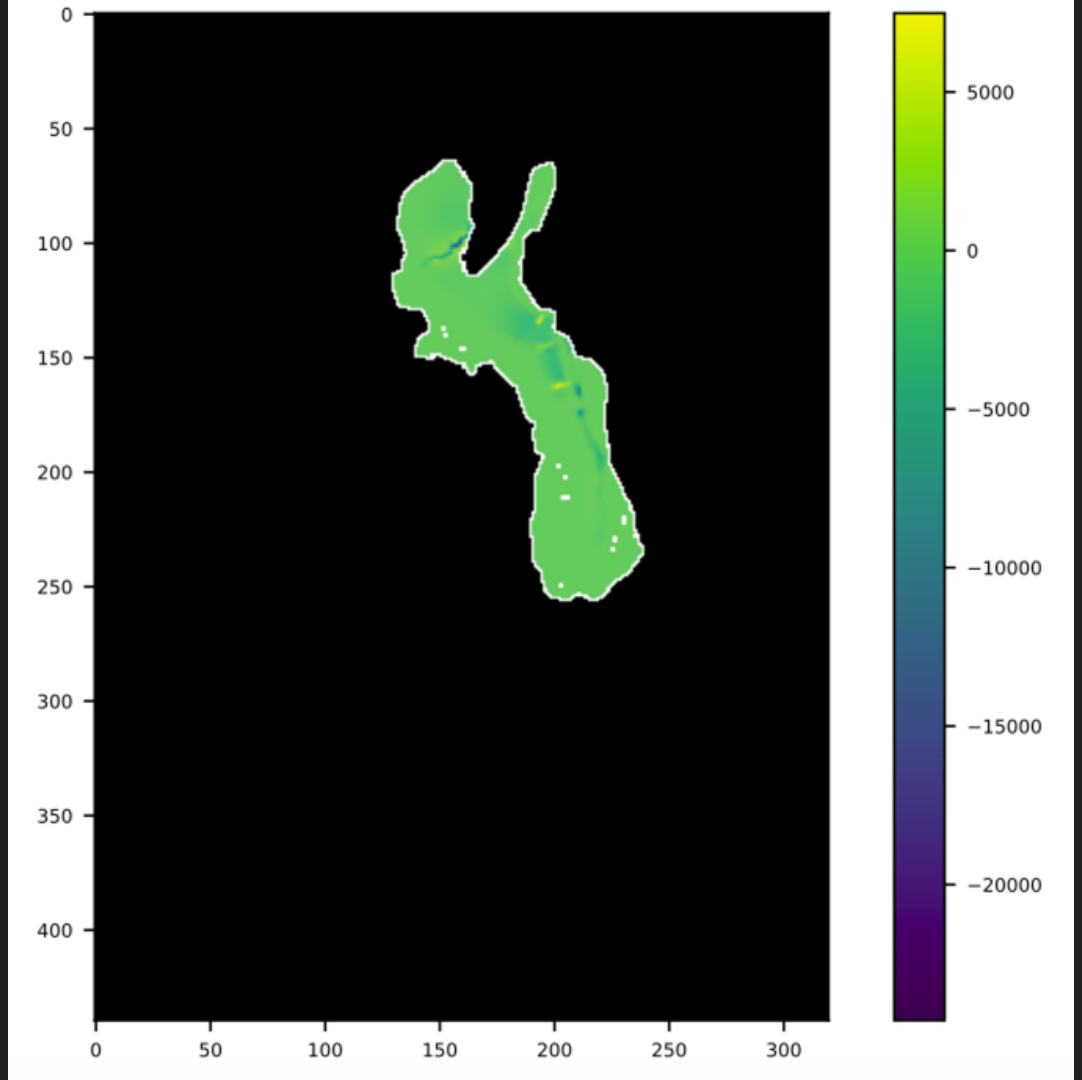
Example: San Pedro

- SS layer 5



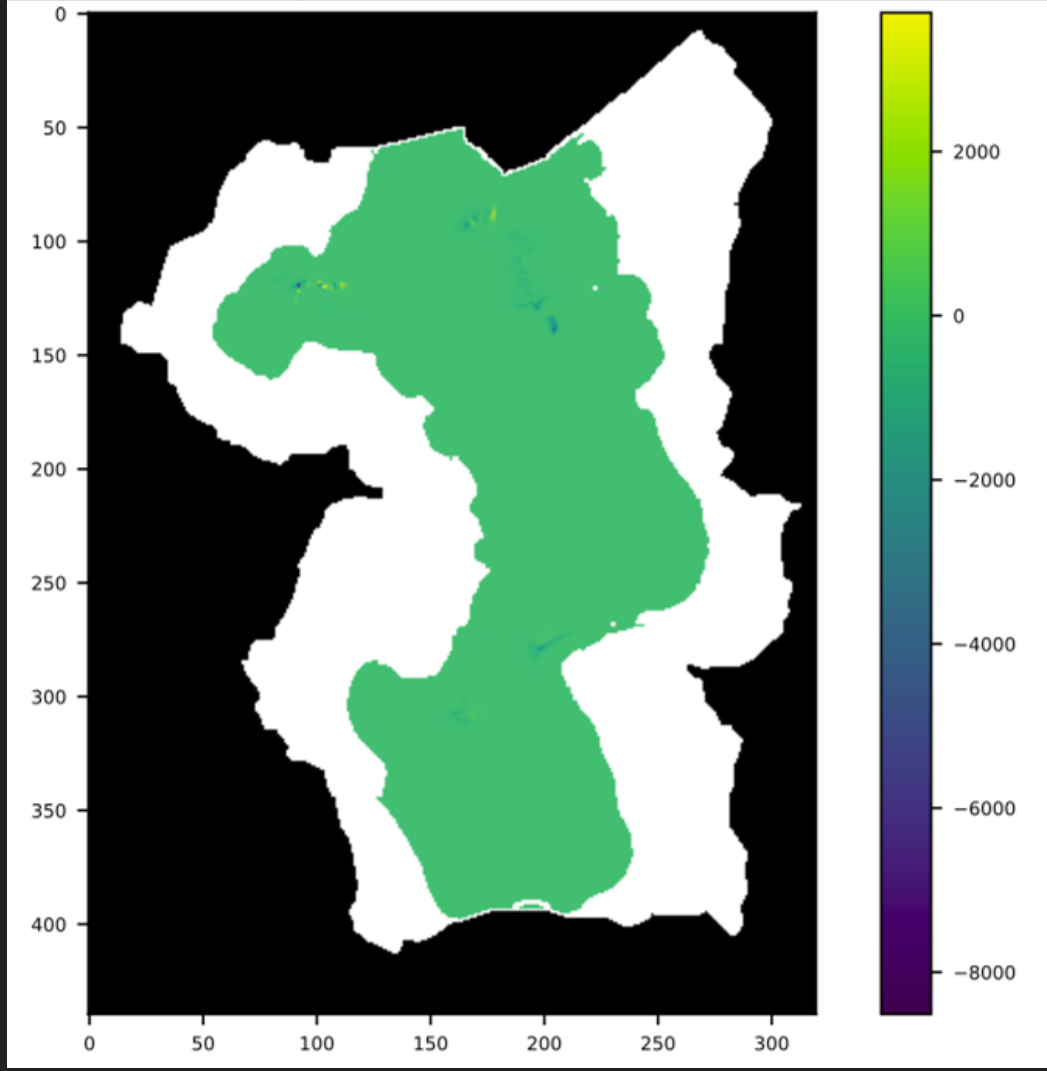
Example: San Pedro

- VK layer 3



Example: San Pedro

- HK layer 5



Future directions

- Quasi-newton optimization
  - Optimization
  - RML
- Hamiltonian Monte Carlo
  - Efficient metropolis sampling - needs gradients
- Model emulator training

Thanks

Contributions welcome!

https://github.com/INTERA-Inc/mf6adj