









Loop 'Flow'

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6ias 3D modelling and Loop workshop

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What is LoopFlow?



- A Python package authored by Mark Jessell and Guillaume Pirot, to:
 - Generate graphs from Loop models
 - Calculate flow parameters based on those graphs
- Available on GitHub:
 - https://github.com/Loop3D/LoopFlow
- With some example Python notebooks:
 - one derived from 'Draw your own model' example (6ias map2loop workshop)
 - the other hardwired to loading van der Wielen et al. Emmie Bluff Gocad surfaces



Motivations – part 1



- Understanding and Targeting Mineral Systems
 - Source
 - Path
 - Host
- Testing different scenarios
 - Source locations
 - Potential path or barriers
 - Potential hosts



Motivations – part 2



Groundwater management

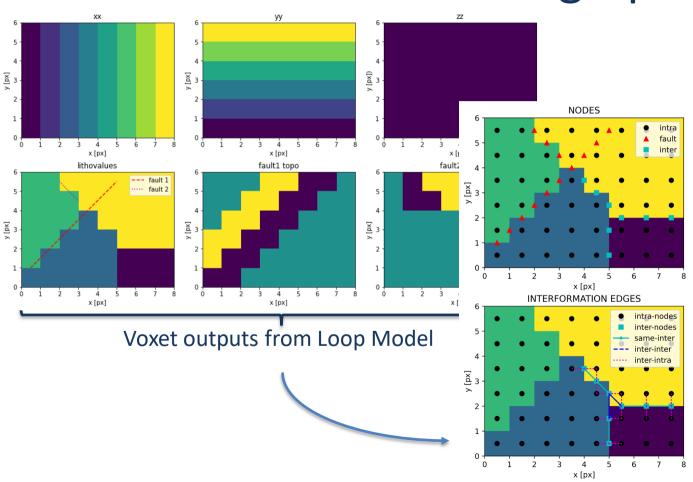
Subsurface characterization

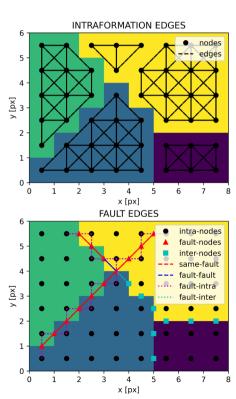
- Inverse problem
 - ➤ Challenging computing costs of flow and transport simulations with finite element or finite difference solvers



From voxet to graph







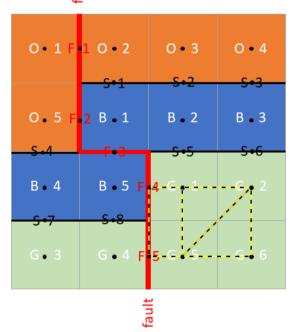


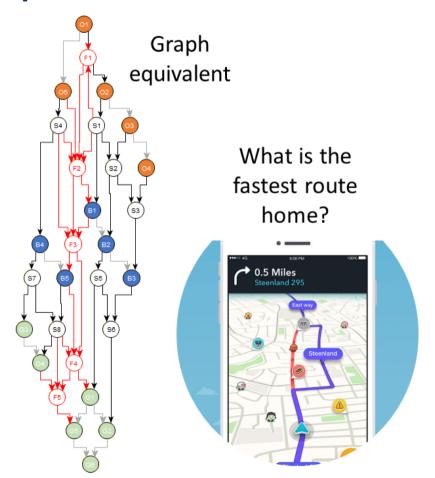
Graphs



Small slice through voxel model





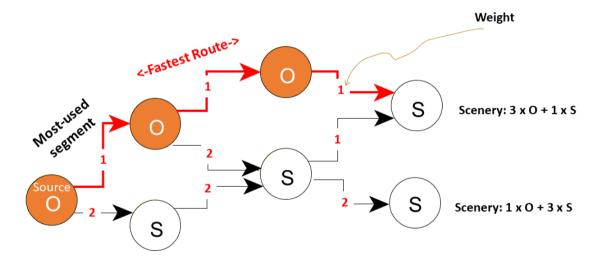




Possibilities



Distance, pathways, scenery...

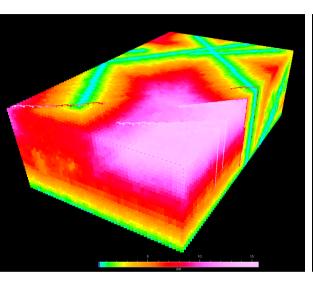


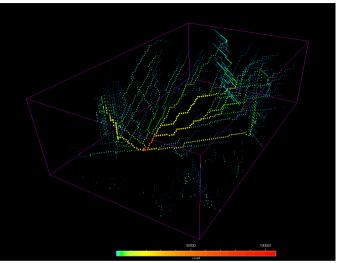
Does it work to approximate flow and transport in aquifers with complex structures?

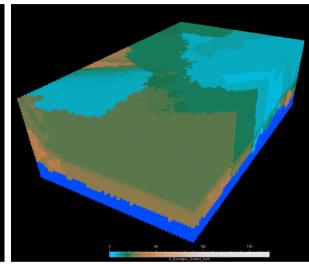


WESTERN Mineral resources perspectives LOOP









Distance from source

Preferred pathways

Path scenery

- Mineralization halo
- Contaminant remobilization
- Chemical reaction paths

Python notebook: https://github.com/Loop3D/6IAS/blob/main/LoopFlow/2 m2l wa flow.ipynb



A groundwater application



- Can we approximate flow and transport simulations by computations through graph representations of subsurface models?
- Darcy's law

$$\vec{q} = -K\nabla h$$

Advection dispersion equation (ADE)

$$\frac{\partial c}{\partial t} = -\vec{q}\nabla c + D_m\nabla^2 c$$
advection diffusion

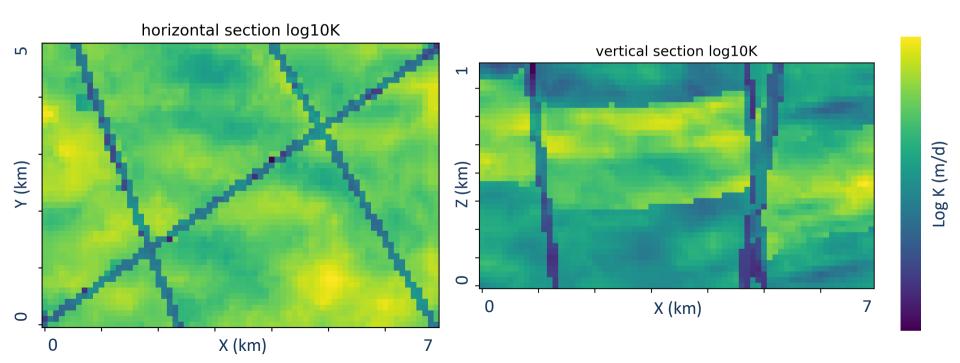


Experimental setting



- 7km x 5km x 1km (x-axis,y-axis,z-axis)
- 70 x 50 x 40 cells

- 3 heterogeneous stratigraphic units
- 3 faults (fixed geometry)



Scenarios & boundary conditions

3 faults paths or barriers

 $2^3 = 8$ possibilities

- path $log_{10}K + 2$

barrier log₁₀K -2

▲injection well

Scenario 0

Scenario 1

Scenario 2

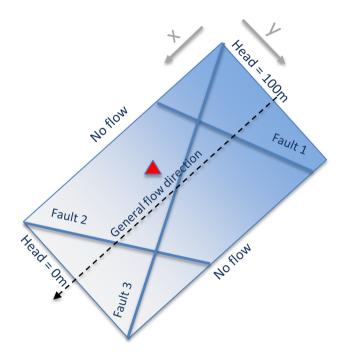
Scenario 3

Scenario 4

Scenario 5

Scenario 6

Scenario 7

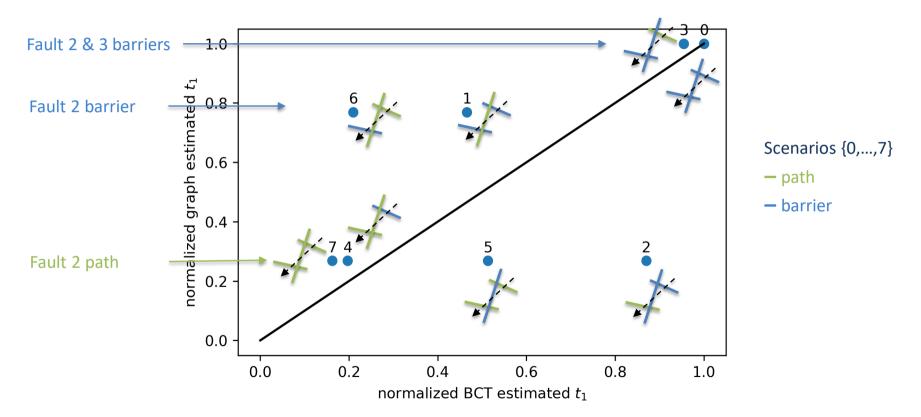


Steady state flow Transient transport, advection and diffusion 10 years of simulation (timestep = 1 month)



First arrival travel times



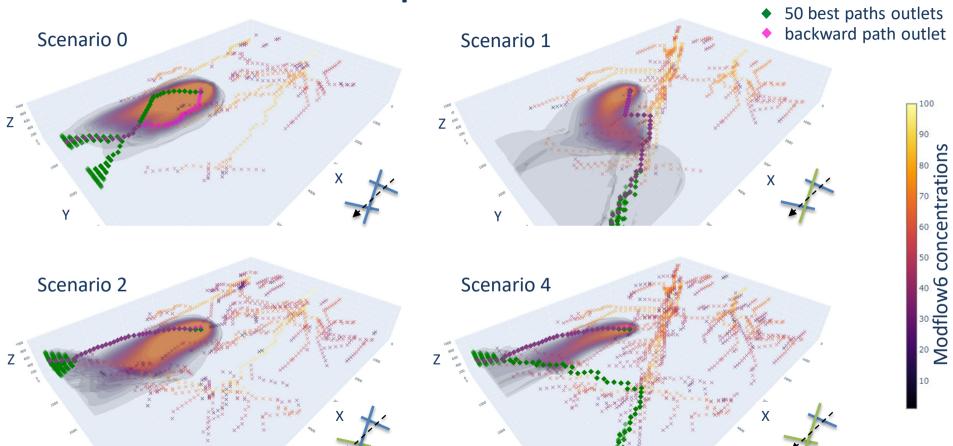


Fault 3 most influential, then Fault 2 then Fault 1



Transport results

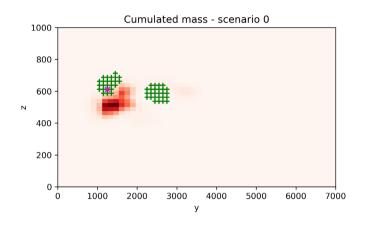


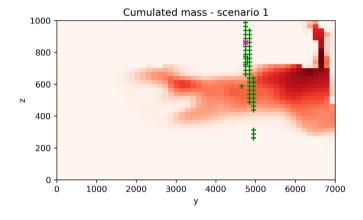


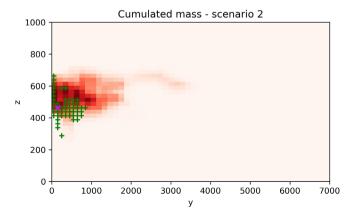


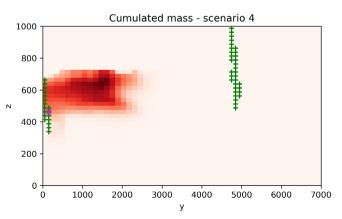
Transport results











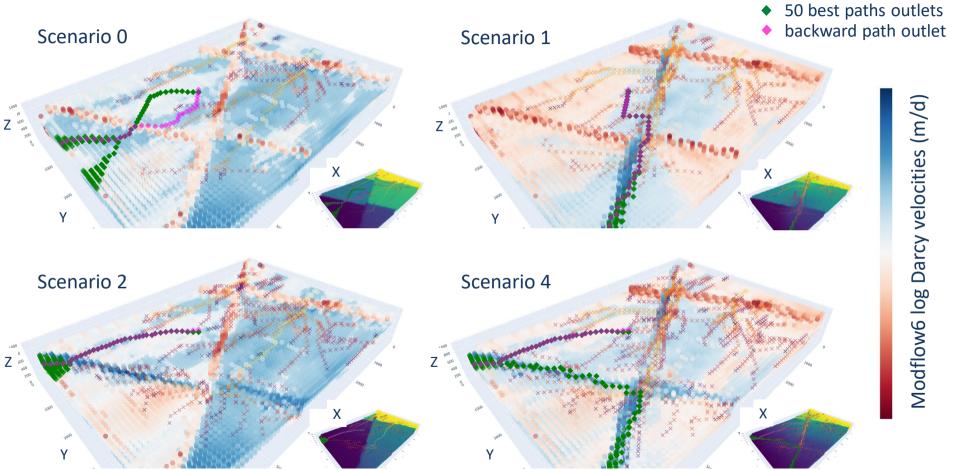
- 50 best paths outlets
- x backward path outlet

cumulated mass from Modflow6



Flow results







Computing requirements



From an existing voxet model (140k cells)

- Using Python libraries networkx and flopy
- Graph generation: ~30 seconds per graph
- Backward or forward distances from graphs: ~ 3 seconds per computation
- Modflow6 simulation (1 steady state + 120 timesteps for a total of 10 years): ~ 5 minutes per simulation

Groundwater application summary

- Graph approximations are blind to upstream flow conditions
- Backward path approximation seems more accurate
- Cumulative mass outlet locations are relatively coherent
- Least resistant paths are consistent with the field of Darcy velocity magnitudes



Future work



- Graph weight tuning
- First arrival time calibration
- Find alternative paths to see if we can approximate the plume shape
- What if we used the velocity field rather than the K field to build a graph
- Comparison with particle tracking simulations
- Unstructured mesh to better explore fault effects
- Ideas for other applications and collaboration?

THANK YOU



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Detailed parameters



- Upper hydro stratigraphic unit log₁₀K
 - $\mu = -4.45 \text{ m/s}$
 - $\sigma = 0.4 \text{ m/s}$
- Middle hydro stratigraphic unit log₁₀K
 - $\mu = -3.10 \text{ m/s}$
 - $\sigma = 0.5 \text{ m/s}$
- Lower hydro stratigraphic unit log₁₀K
 - $\mu = -4.69 \text{ m/s}$
 - $\sigma = 0.6 \text{ m/s}$
- $K_{xx} = K_{yy} = 10K_{zz}$

Porosity: 25%

$$Q_{well} = 50 \cdot 10^3 \, \text{m}^3 / \text{d}$$

- $\alpha_L = 1$ m (longitudinal dispersivity)
- $\alpha_T = 0.1 \text{ m (transvers dispersivity)}$



Estimation of first arrival travel **LOOP** time from breakthrough curves

