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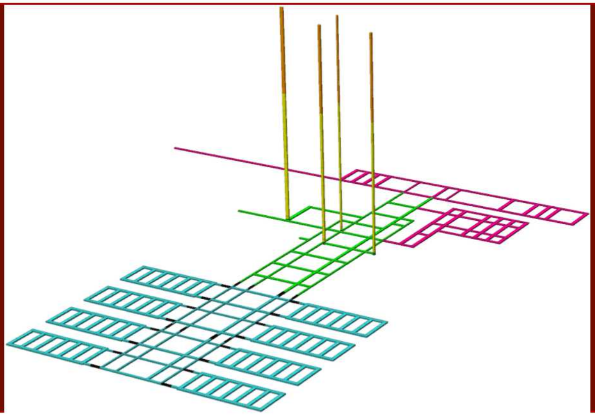

Culebra Hydrologic Model in WIPP Performance Assessment

Presented by Amelia Hayes

8800 Energy and Earth Systems Symposium 2019

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Outline

- Culebra Performance Assessment (PA) Flow Model
  - Motivation for Culebra Hydrology Model
  - Current Representation of Culebra Brine Aquifer Flow
- MODFLOW & SECOTP2D Replacement with PFLOTRAN
- Culebra Flow Model Conversion to PFLOTRAN Progress
  - Input File Conversion
  - Comparison Between MODFLOW and PFLOTRAN
- Summary

WIPP Performance Assessment

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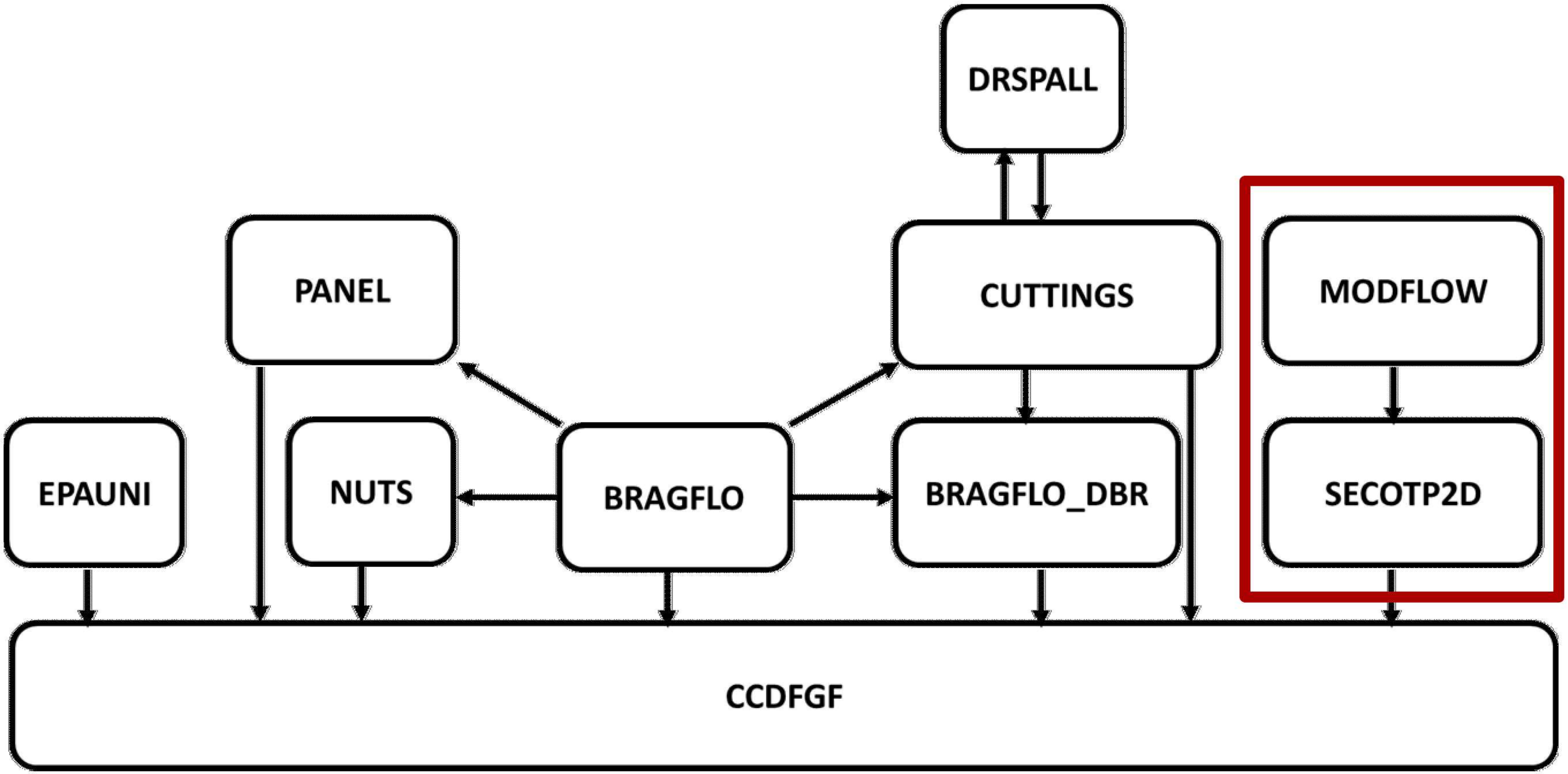


Current generalized code map and run control configuration

Release Pathways in WIPP PA

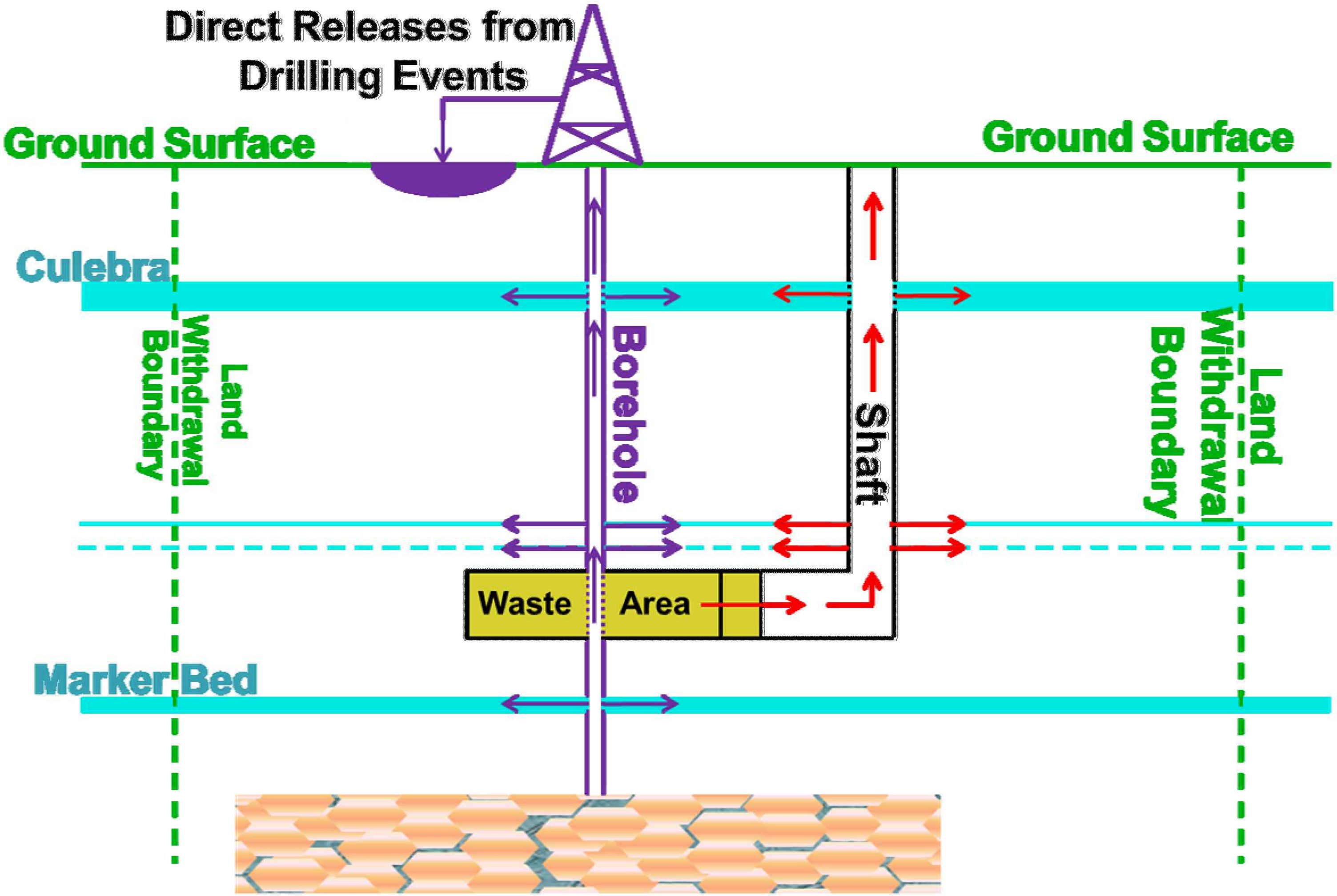
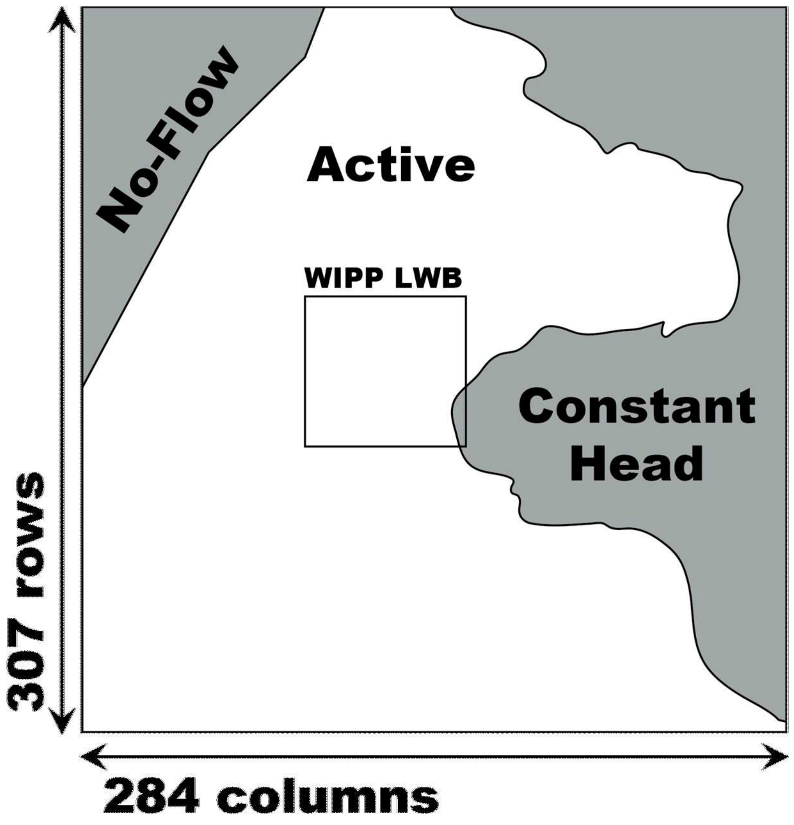


Figure from SAND2017-11103C (Dunagan, 2017)

Culebra PA Flow Model - MODFLOW

Overview:

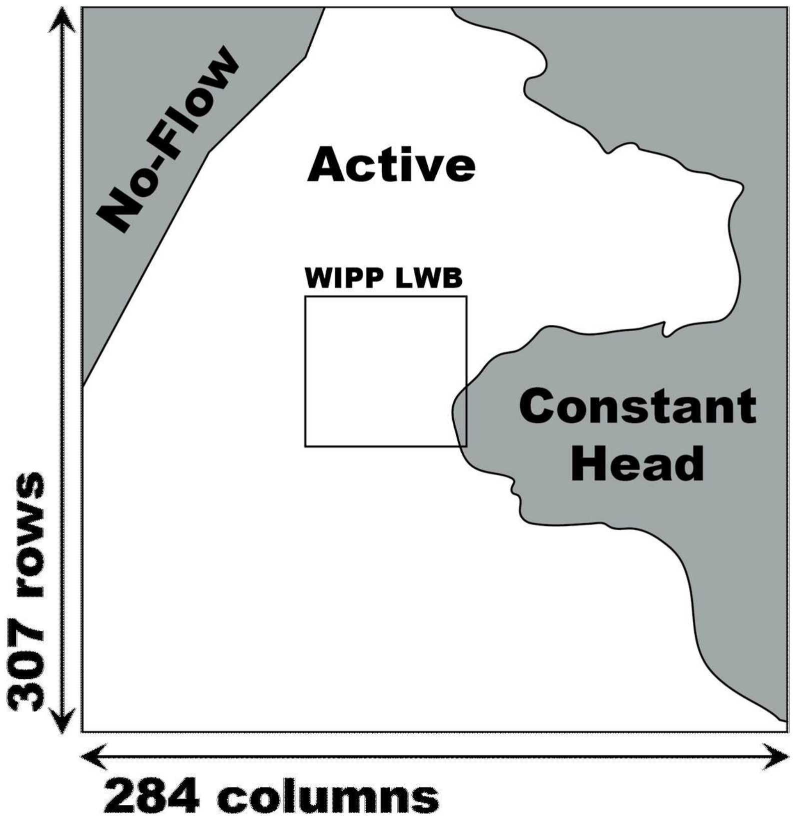
- MODFLOW-2000
- Steady state, 2D, confined
- Uniform thickness, 7.75 m
- Model cells
  - 87,188
  - 100 m × 100 m
  - Active (67%)
  - No-flow (8%)
  - Constant head (CH) (25%)
- Eastern CH: land surface elevation
- Northern, southern, and western CH: extrapolated from parametric surface equation



Culebra PA Flow Model - MODFLOW

MODFLOW realizations

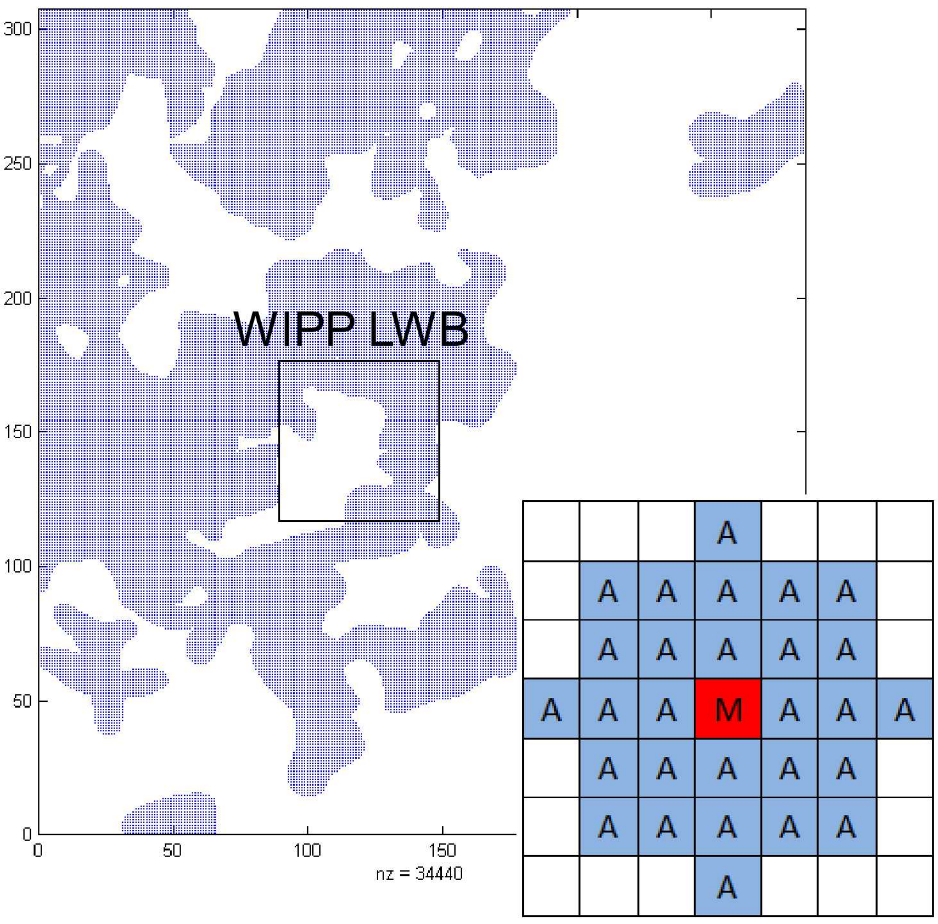
- **Start:** 1000 base realizations
- "T-FIELDS"
  - [T] Transmissivity
  - [A] Anisotropy
  - [R] Recharge
  - [S] Specific storage
- [T] Calibration
  - 200 of 1000 realizations
  - Snapshot observations
  - Transient observations
- **Finish:** 100 realizations best matched to well observations



Culebra PA Flow Model - MODFLOW

Commercial Mining Modifications

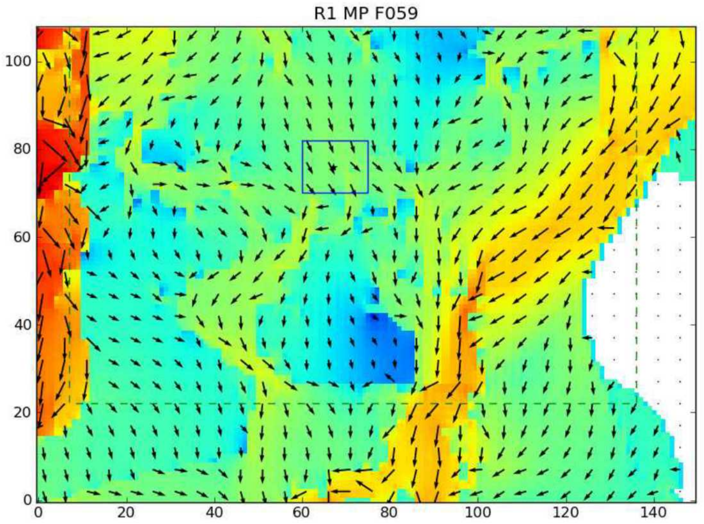
- **Start:** 100 calibrated MODFLOW realizations
- Identify cells influenced by mining
  - Partial mining = inside LWB
  - Full mining = inside & outside LWB
- T scaled by random mining factor in affected cells
  - Three replicates per mining process, 600 realizations total
- Modify boundary conditions according to mining shape definition.
- Conduct 600 (mining-modified) + 100 (unmodified) MODFLOW simulations.

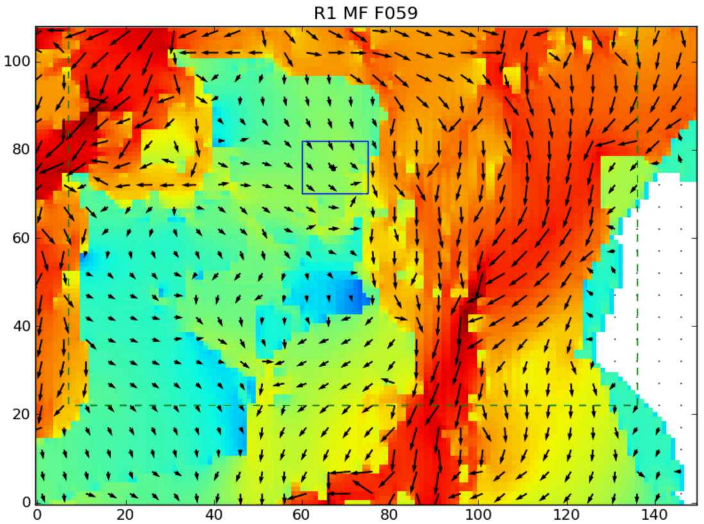


Culebra PA Flow Model - MODFLOW

Mining Modifications (continued)

- Conduct 700 particle tracking simulations with DTRKMF.
- Convert 600 (mining-modified) MODFLOW input files from 100 x 100m cell size to 50 x 50m cell size.
- Conduct 600 (mining-modified) MODFLOW and DTRKMF simulations.
- **Finish:** 600 MODFLOW (mining-modified) solutions at 50 x 50m resolution.
- Velocity fields from MODFLOW simulations later used for solute transport modeling with SECOTP2D.





MODFLOW & SECOTP2D to PFLOTRAN

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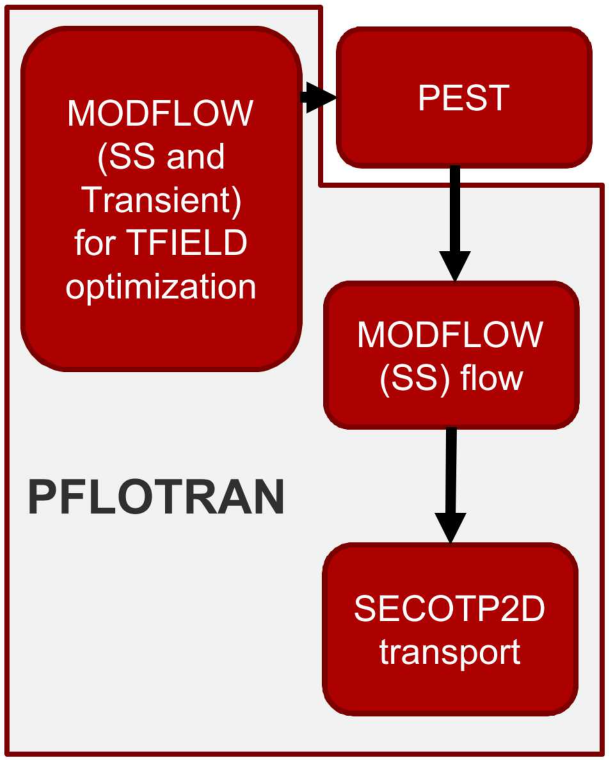
Hydrology PA Workflow



- Streamlined hydrology PA workflow
  - Flow and transport calculations done with a single code (coupled)
  - Flow and transport calculations done potentially over a single grid
- TFIELDS can potentially be recalculated with PFLOTRAN rather than MODFLOW2000 if needed.
- Other non-PA applications (ASER contour maps & COMPs) will also benefit from updated/streamlined process.

Code	PA Role	PFLOTRAN Replacement Capabilities
MODFLOW2000	Culebra flow	Provides similar fully saturated, 2-D transient flow solutions (steady state is just transient run out to long time)
SECOTP2D	Culebra transport	Has existing transport capability comparable to SECOTP2D. Some aspects (e.g., dual domain mass transport) will require modification and testing.

MODFLOW vs. PFLOTRAN

MODFLOW-2000

- Total head
- Hydraulic conductivity
- Specific storage
- Finite difference
  - Origin: upper left
- Boundary conditions assigned to cell-center
  - Specified total head

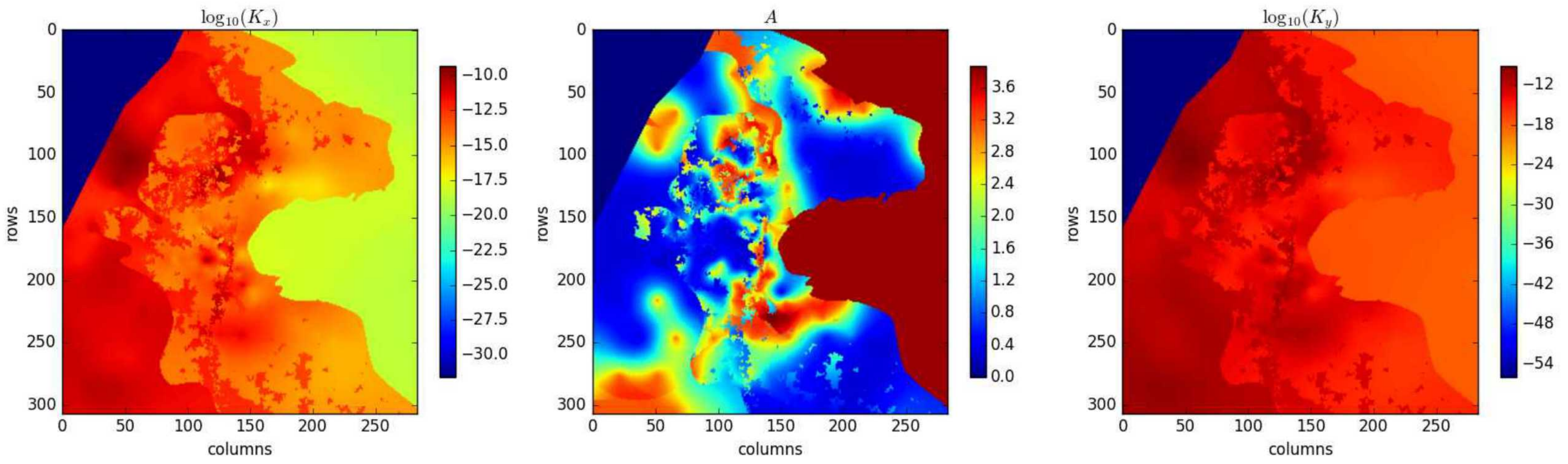
PFLOTRAN

- Fluid pressure
- Permeability
- Compressibility
- Finite volume
  - Origin: lower left
- Boundary conditions assigned to cell-edge
  - Specified pressure

Culebra PA Flow Model - PFLOTRAN

convert_MODFLOW_inputs_to_PFLOTRAN.py

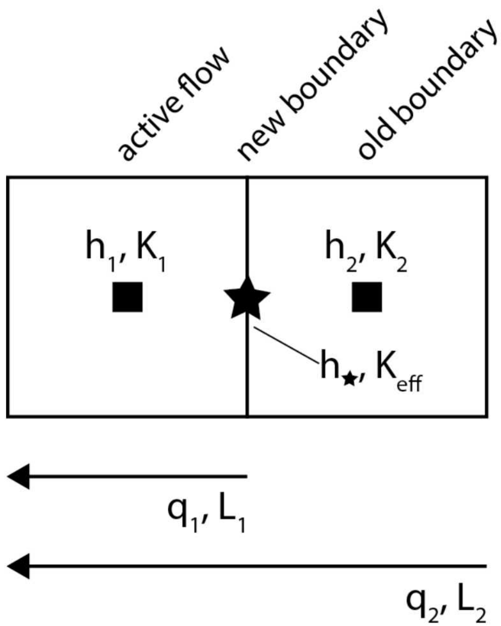
- Import *modeled_{T,A,R,S,}_field.mod* (MODFLOW input files).
- Convert saturated hydraulic conductivity to permeability.
- Calculate horizontal (y-direction) anisotropy.
- Convert specific storage to compressibility.
- Reshape spatially-variable parameters to match the PFLOTRAN coordinate convention.



Culebra PA Flow Model - PFLOTRAN

convert_MODFLOW_inputs_to_PFLOTRAN.py (continued)

- Apply recharge boundary conditions.
- Apply specified pressure boundary conditions.
  - MODFLOW (cell-centered), PFLOTRAN (cell-edge)
  - Getting specified pressure at a cell edge requires calculating the effective conductivity (harmonic average) and equivalent discharge:



$$q_1 = K_1 ((h_1 - h_\star)/L_1))$$

$$q_2 = K_{eff}((h_1 - h_2)/L_2))$$

$$K_{eff} = (2/((1/K_1)+(1/K_2)))$$

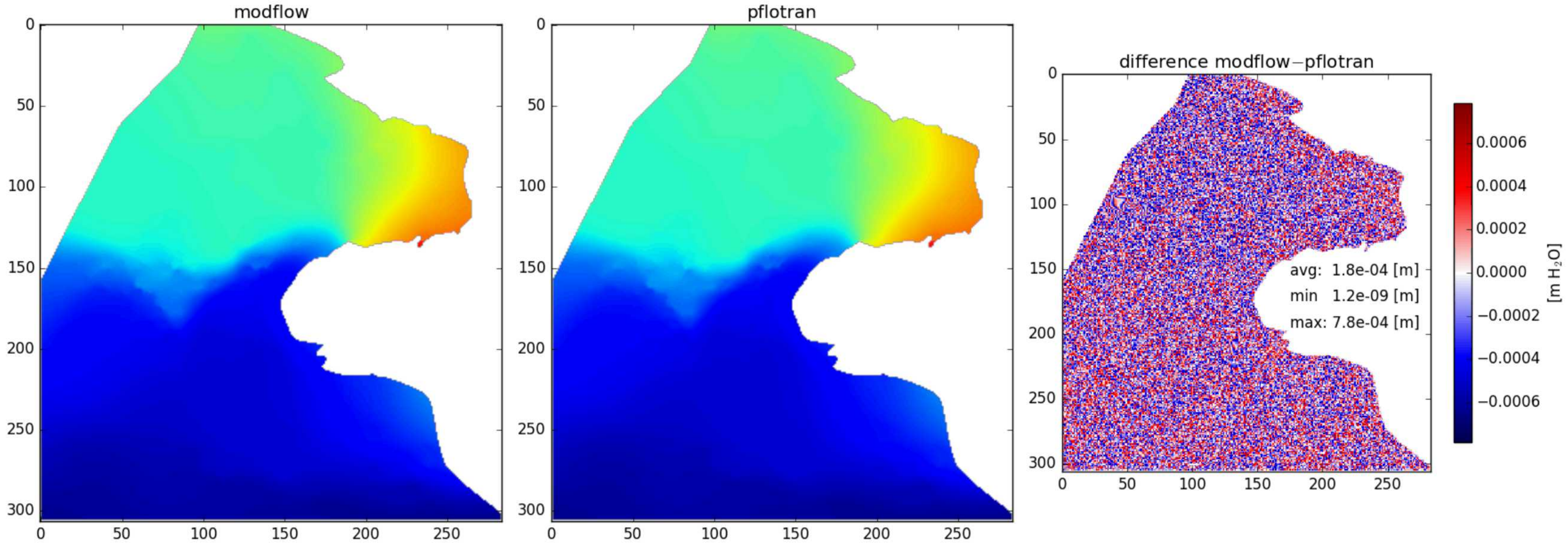
$$q_1 = q_2$$

Solve for $h_\star$

Culebra PA Flow Model - PFLOTRAN

compare-MODFLOW-pflotran-output.py

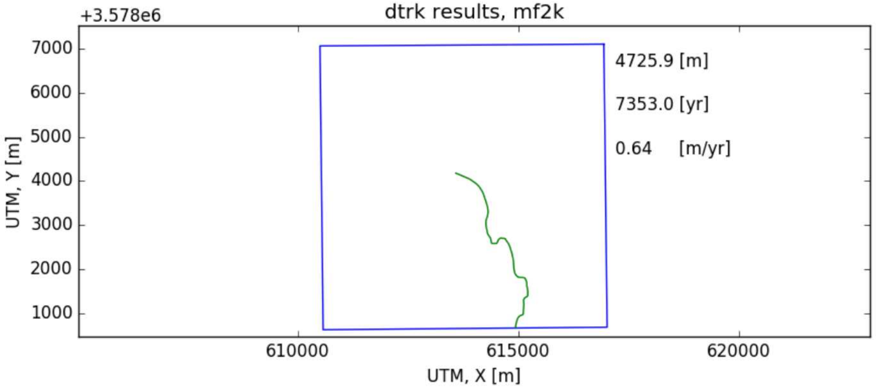
- Import original MODFLOW results for the 100 realizations.
- Import PFLOTRAN results for the 100 realizations.
- Plot and compare.
- Very good agreement for all 100 cases; average difference is approximately 2.E-04 m; this within the solution "noise" space.

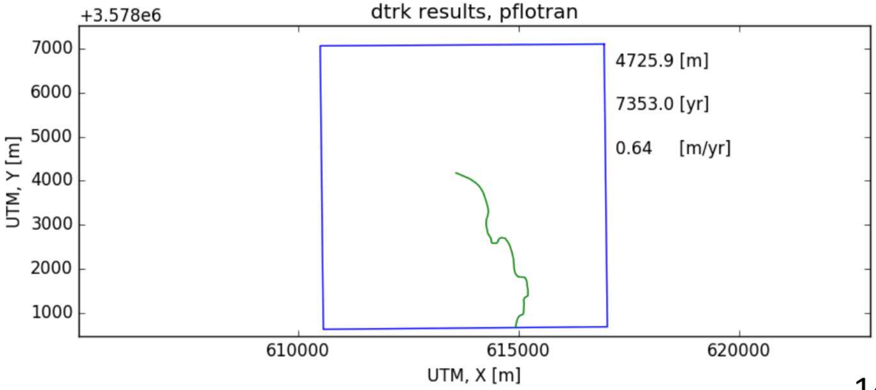


Culebra PA Flow Model - PFLOTRAN

convert-pflotran-to-mf2k-cbc.sh

- DTRKMF (part of Mining Modifications protocol)
  - Qualfied code that calculates particle tracks with groundwater flow velocity data.
  - Originally designed to accept MODFLOW-2000 binary output files as inputs.
  - PFLOTRAN outputs can be written to look like MODFLOW-2000 binary output files.
- Shell scripts runs five python scripts to…
  - Writes PFLOTRAN cell-by-cell flow budget file.
  - Compares MODFLOW- and PFLOTRAN-based cell-by-cell flow budget files.
- Very good agreement for all 100 cases.





Summary

- Conversion of the WIPP Culebra hydrology model is part of the larger integration of PFLOTRAN into WIPP PA
  - Potential to combine flow and transport calculations on a single grid
- Comparison between MODFLOW and PFLOTRAN has very good agreement
  - Average difference is about 2.E-04 m for all 100 base cases
  - Particle track distance, travel time, and rate calculated agreement for all 100 cases
- Next steps are converting Culebra transport code to PFLOTRAN

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Questions?