Used Fuel Disposition Campaign

Advances in PFLOTRAN Gridding: Octree Refinement and Ghost Node Correction

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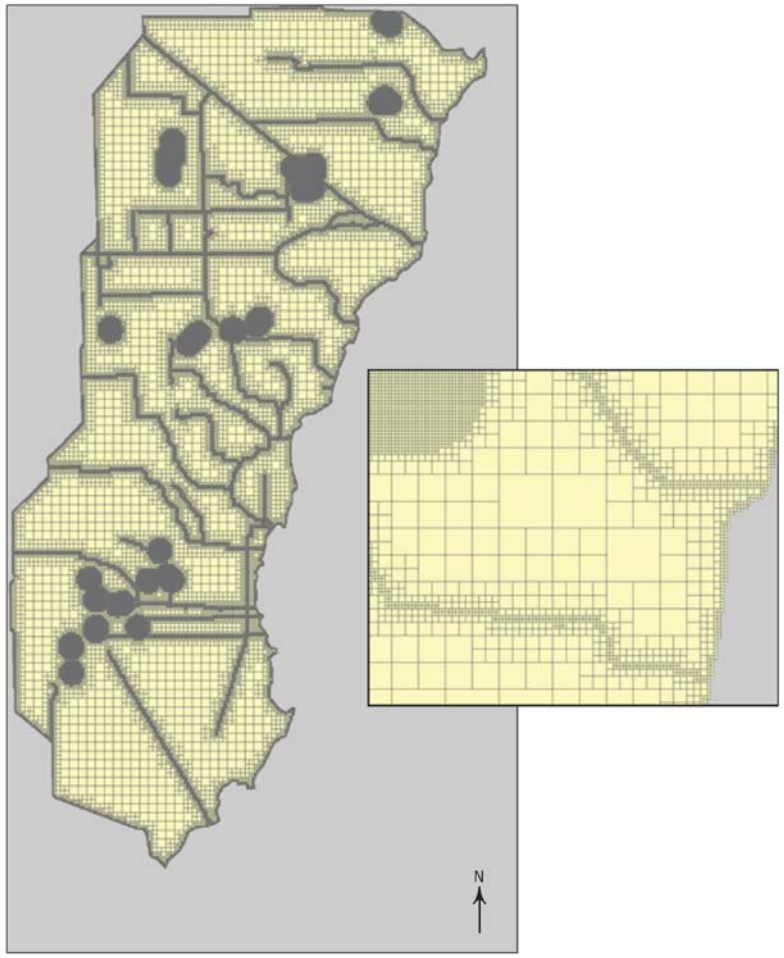
Motivation

- **Why vary grid resolution in space (and/or time)?**
  - Improve accuracy
  - Keep runtimes manageable
- **Why octree grid refinement?**
  - Flexibility
  - Maximize accuracy with a fixed number of degrees of freedom
  - Works within PFLOTRAN's existing unstructured gridding infrastructure
- **Challenges**
  - Data distribution and management
  - Potential load imbalance
  - Development of robust solvers



MODFLOW-USG Manual, Figure 7

Approaches to Gridding in PFLOTRAN

- **Structured**
  - Cartesian
  - Radial
- **Unstructured**
  - Implicit - traditional finite element mesh defined by nodes/elements
  - Explicit - finite volume mesh defined by volumes, areas, distances and connectivity

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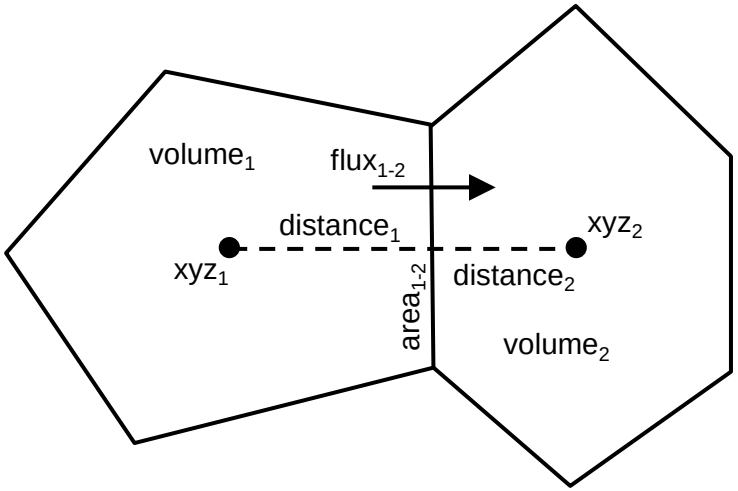
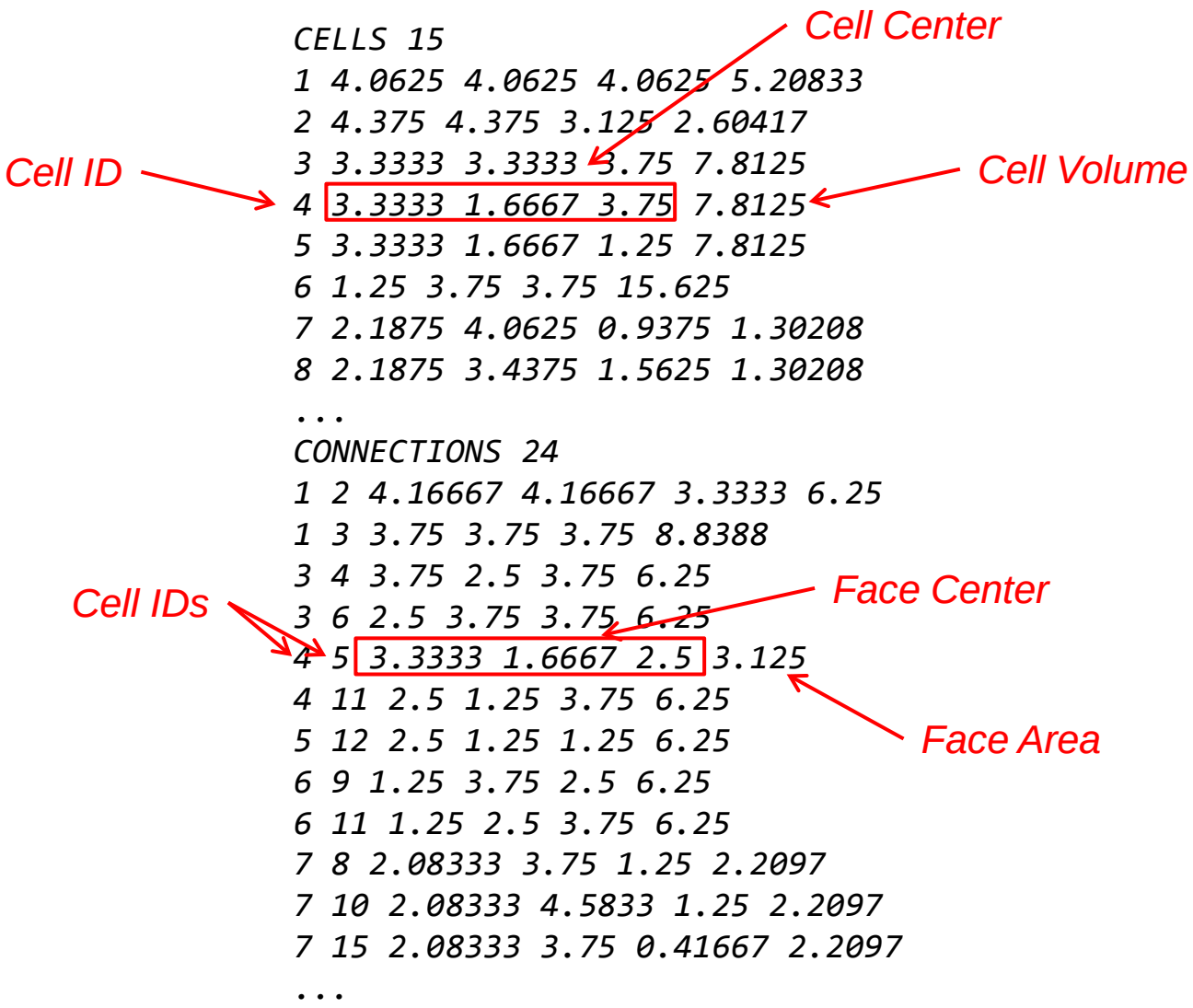


Explicit Unstructured Grid File Format

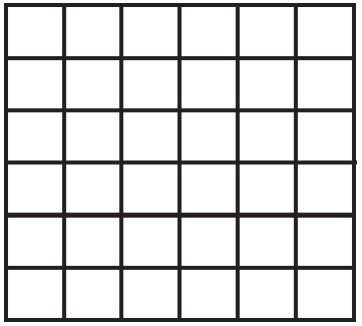



```
CELLS 15
1 4.0625 4.0625 4.0625 5.20833
2 4.375 4.375 3.125 2.60417
3 3.3333 3.3333 3.75 7.8125
4 3.3333 1.6667 3.75 7.8125
5 3.3333 1.6667 1.25 7.8125
6 1.25 3.75 3.75 15.625
7 2.1875 4.0625 0.9375 1.30208
8 2.1875 3.4375 1.5625 1.30208
...
CONNECTIONS 24
1 2 4.16667 4.16667 3.3333 6.25
1 3 3.75 3.75 3.75 8.8388
3 4 3.75 2.5 3.75 6.25
3 6 2.5 3.75 3.75 6.25
4 5 3.3333 1.6667 2.5 3.125
4 11 2.5 1.25 3.75 6.25
5 12 2.5 1.25 1.25 6.25
6 9 1.25 3.75 2.5 6.25
6 11 1.25 2.5 3.75 6.25
7 8 2.08333 3.75 1.25 2.2097
7 10 2.08333 4.5833 1.25 2.2097
7 15 2.08333 3.75 0.41667 2.2097
...
```

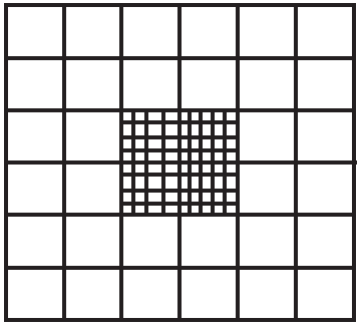
Proofs of Concept Using Explicit Unstructured Grids

- **Explicit unstructured grids provide flexibility for defining many grid configurations in a single format**

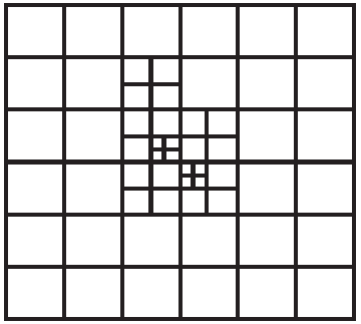
Structured Cartesian



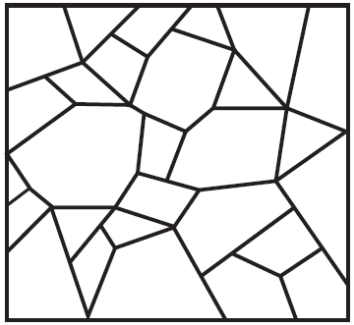
Structured Block Refinement



Unstructured Octree Refinement



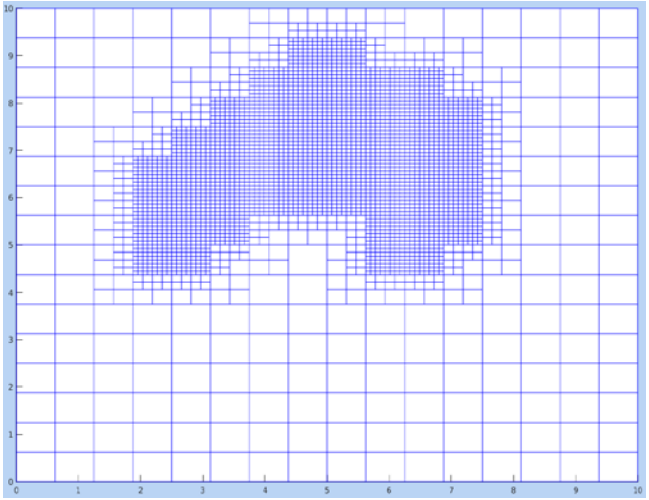
Unstructured



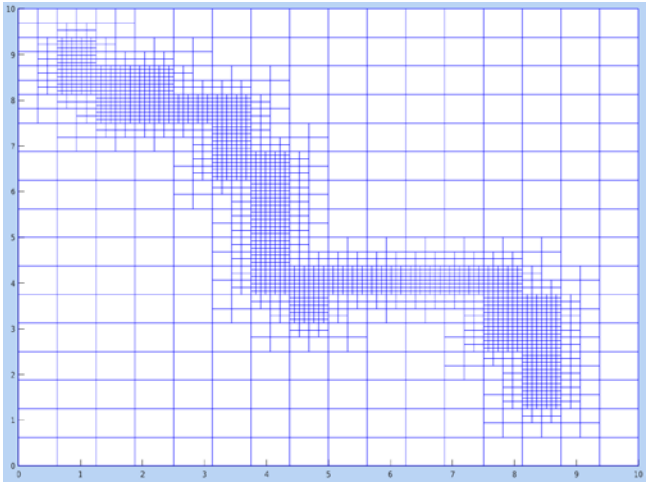
Examples of Octree Grid Refinement

- Each cubic finite volume cell is divided into 8 cells.
- Each rectangular face is divided into 4 faces.
- Levels of refinement can be implemented in PFLOTRAN through the REGION card which is capable of delineating zones based on a point, line, rectangle, polygon, or custom list of points.

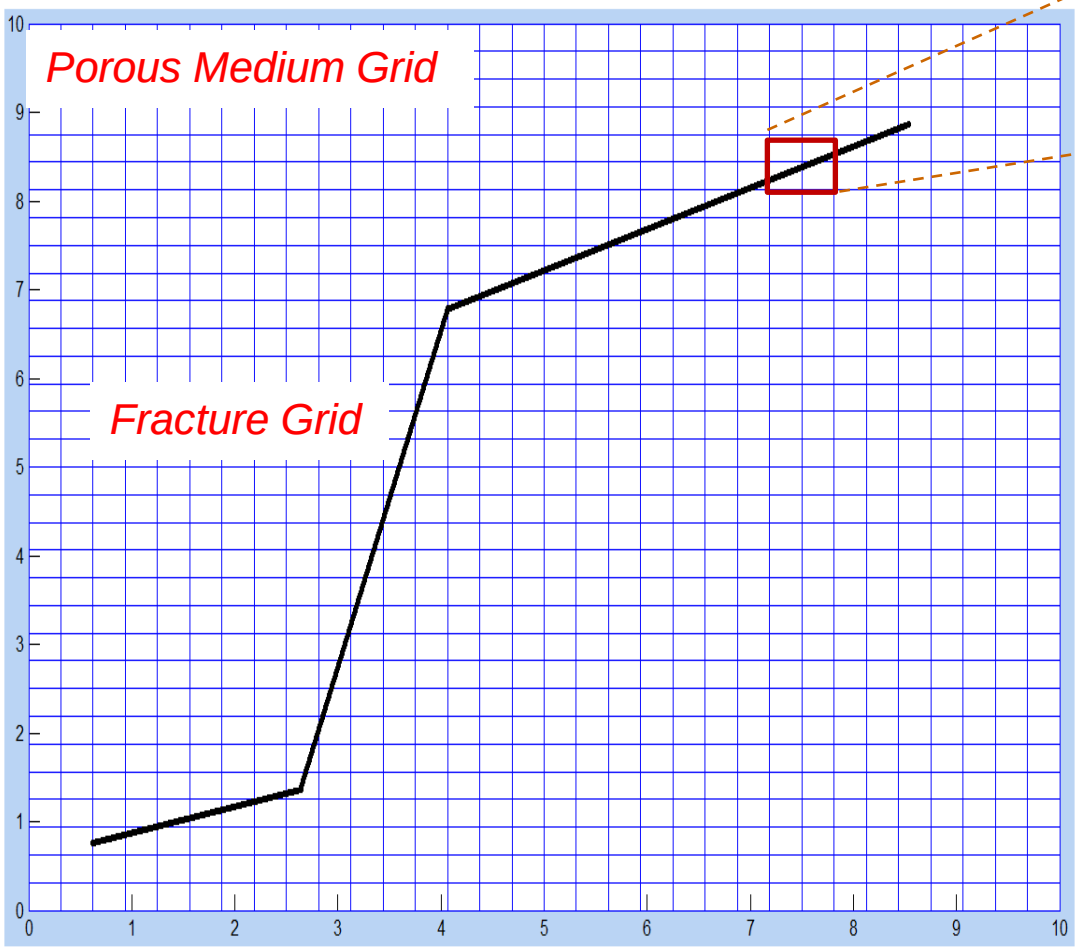
Refine a region defined by a polygon

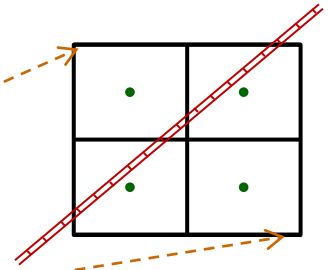


Refine a region defined by a line



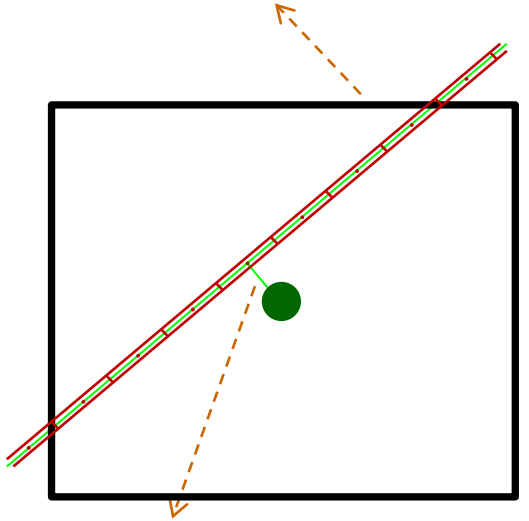
Pseudo Porous Media Approach to Fracture Flow (Capilla et al., 2002)





Connections

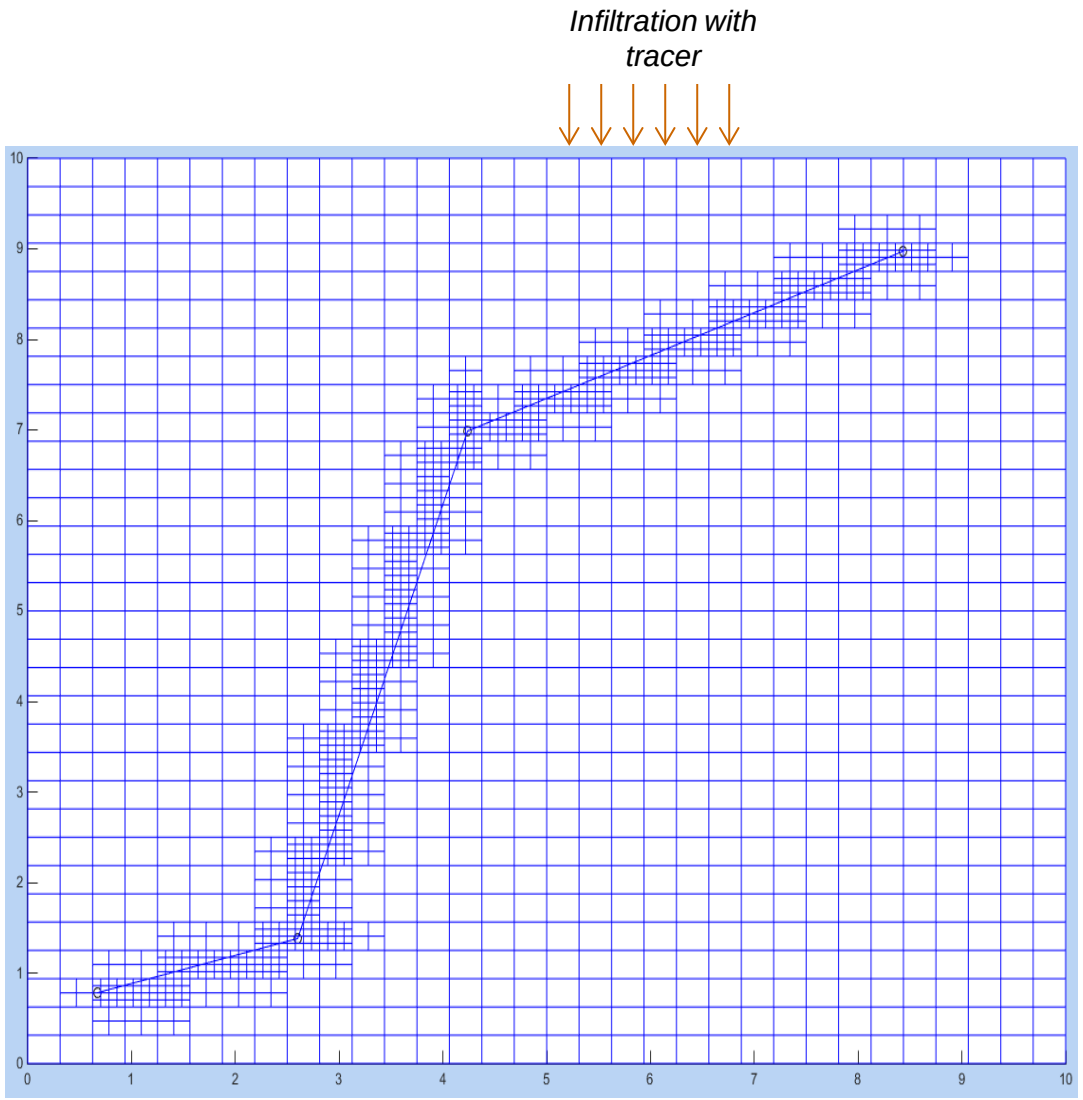
Fracture-Fracture connection



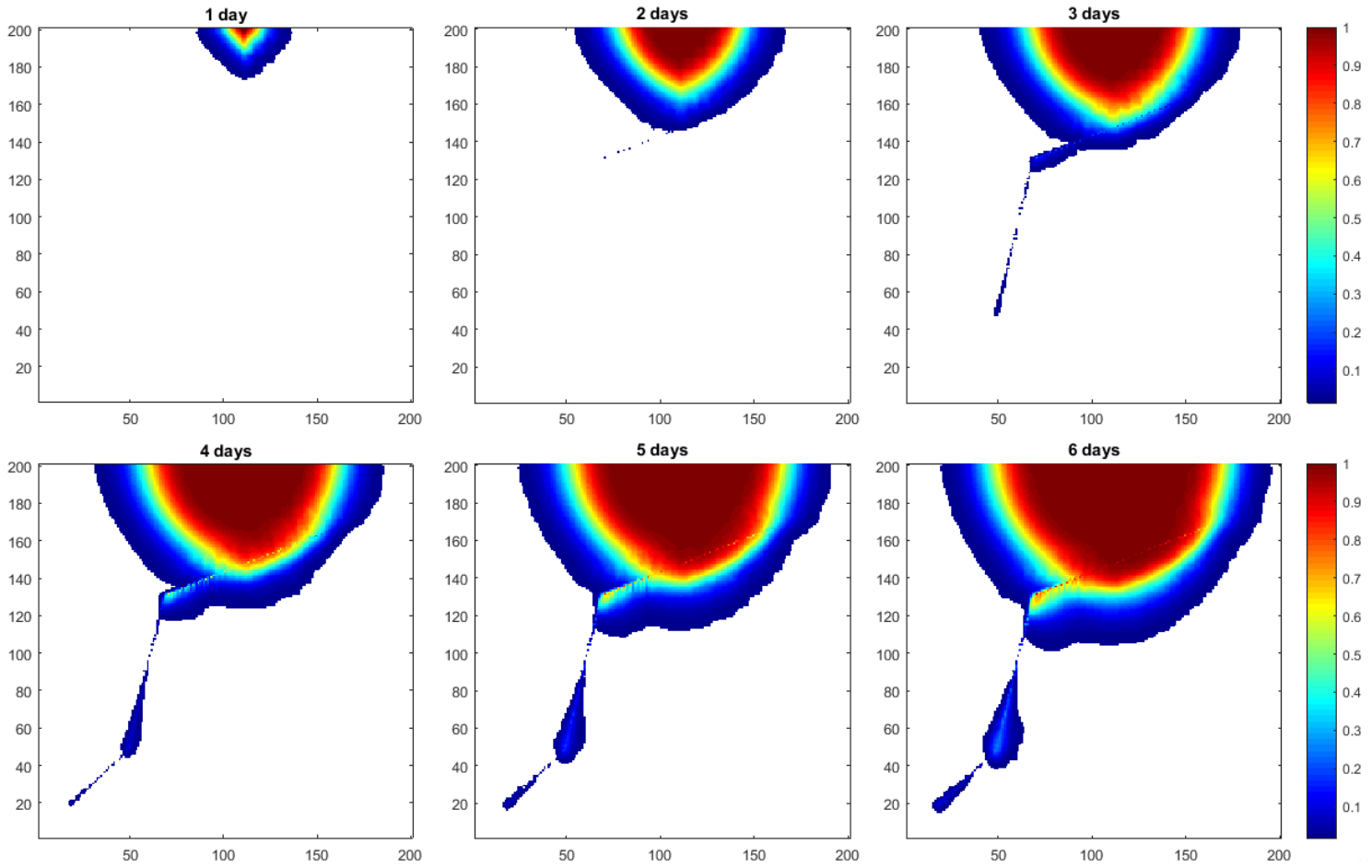
Fracture-Cell connection

Fracture Flow with Octree Refinement

- Octree grid is used to refine the finite volume grid around the fractures.
- Darcy flow is assumed in fractures.



Fracture Flow with Octree Refinement



Network of Fracture on Cartesian Grid

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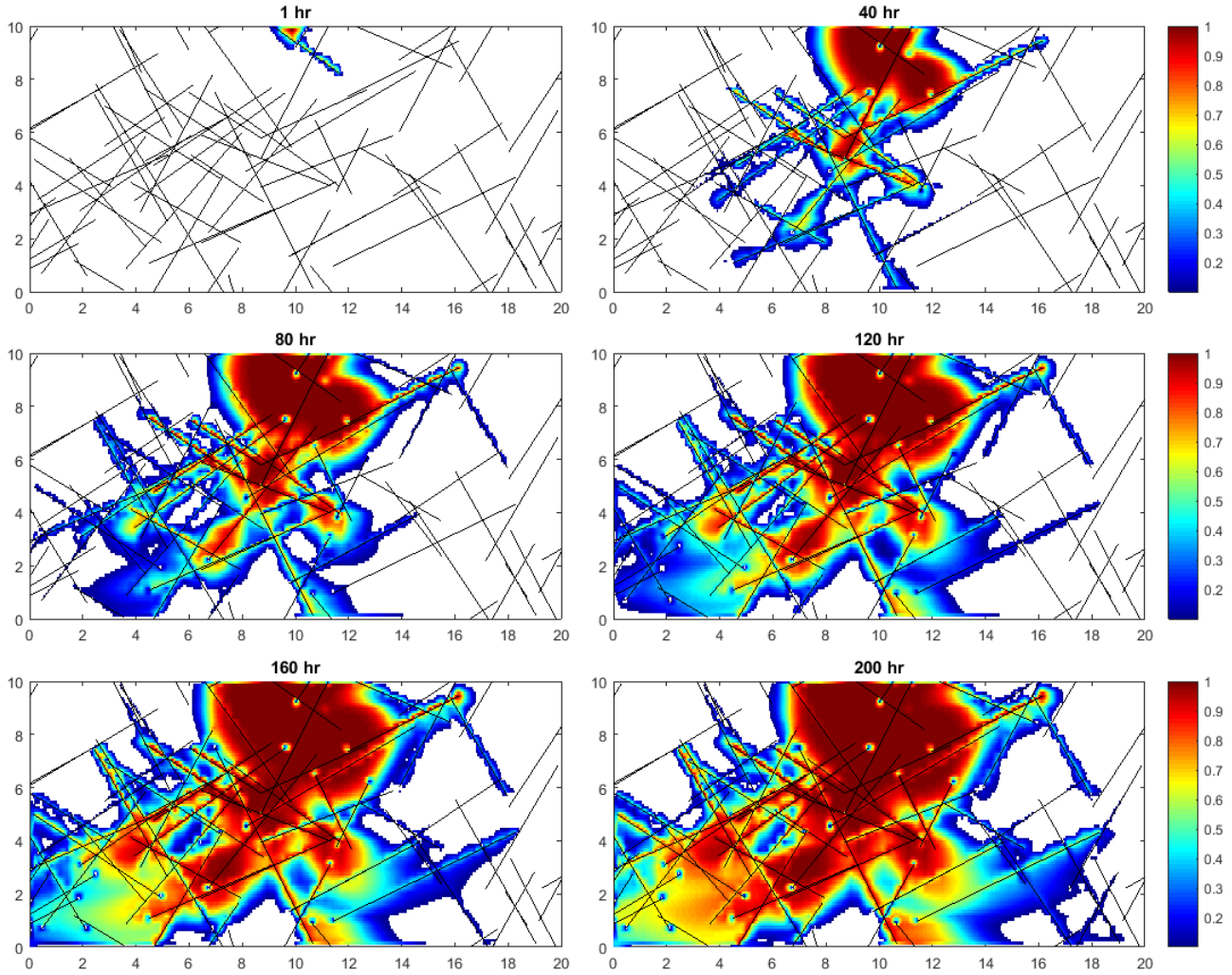
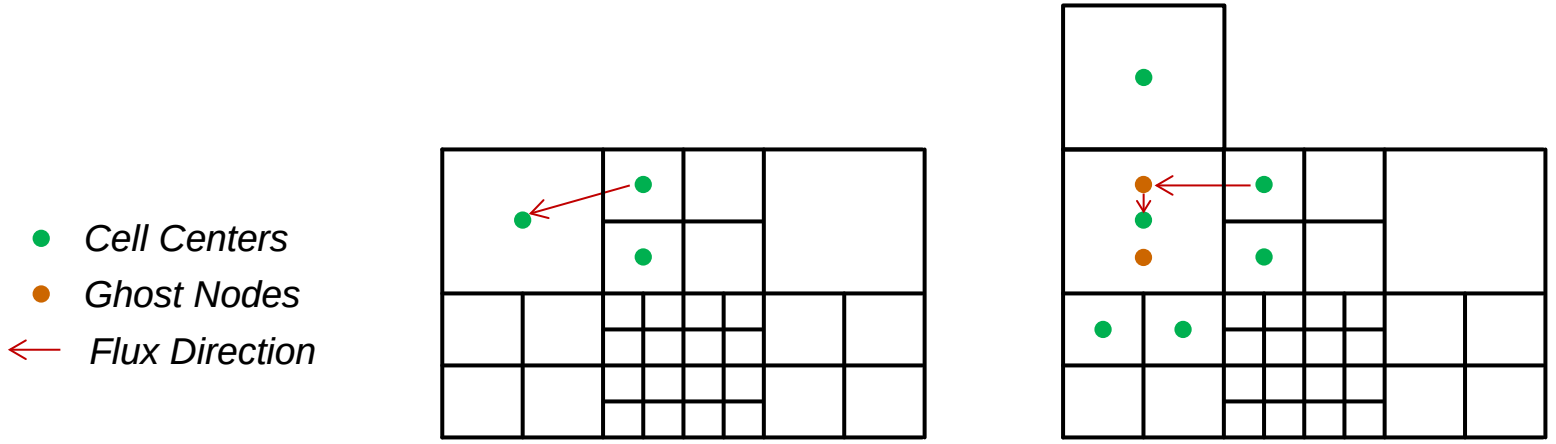


Increasing Accuracy through Ghosting Nodes

- **Fluxes within the finite volume method are more accurate when they are orthogonal to cell interfaces**
- **Ghost node correction can be used to reduce numerical error.**
- **Ghost node approximations are linear interpolations of ordinary cell-centered (non-ghosted) state variables.**
- **Ghost node correction is currently under development in PFLOTRAN.**



Used Fuel Disposition

Proposed Implementation of Ghost Node Correction in PFLOTRAN

Modified GRID card

```
GRID
   TYPE unstructured_explicit ./usgfile.usg
   GRAVITY 0. 0 -9.81
   GHOST_NODE_CORRECTION ./gncorrection.gnc
END
```

Ghost nodes correction file

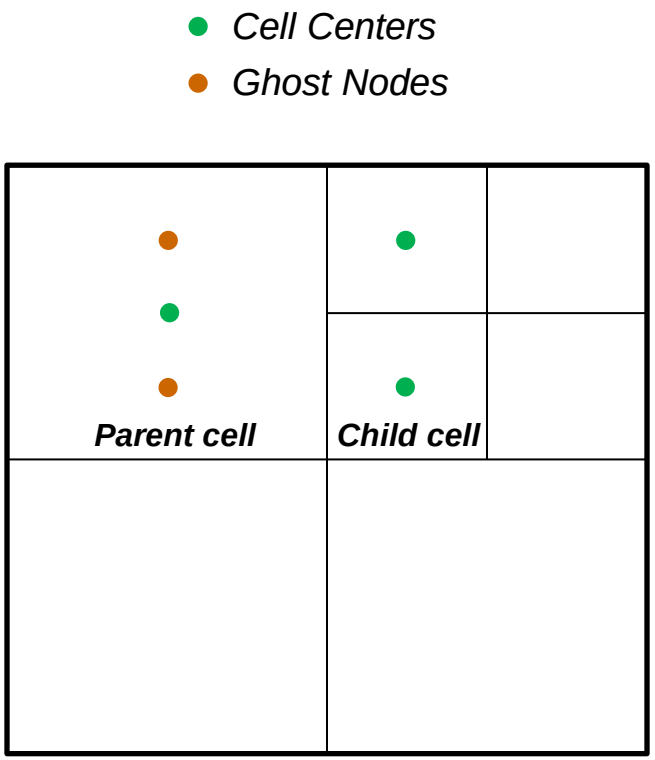
```
1  4
2  35 61 3.125 0.5 5.312
3  28 61 4.0625 0.5 4.375
4  41 71 3.125 0.5 7.1875
5  48 71 4.0625 0.5 8.125
```

Number of ghost nodes

Child cell id

Parent cell id

Coordinates of the ghost nodes



Discrete Fractures Using Unstructured Grids