Efficient, Scalable, and Parallelized Computation of Geometric Coefficients for HPC Finite Volume Based Subsurface Flows and Transport Solvers

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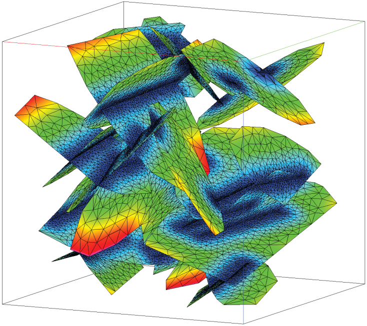
Outlines

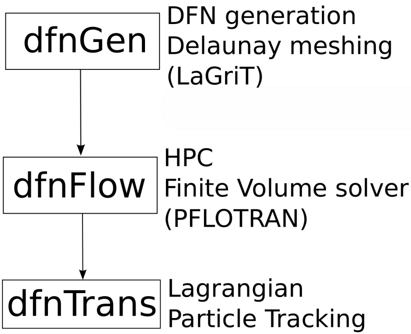
Discrete Fracture Network (DFN)

Interconnected networks of fractures act as the principal pathways for transport in relatively impermeable rocks.



DFN model explicitly represents these fractures and therein resolves flow and transport of solutes through the subsurface.

Subsurface Simulations – *dfnWorks*



Subsurface Simulations – *dfnWorks*

dfnGen — DFN generation
Delaunay meshing
(LaGriT)

↓

dfnFlow — HPC
Finite Volume solver
(PFLOTRAN)

↓

dfnTrans — Lagrangian
Particle Tracking

Bottleneck for Large DFN of High Density

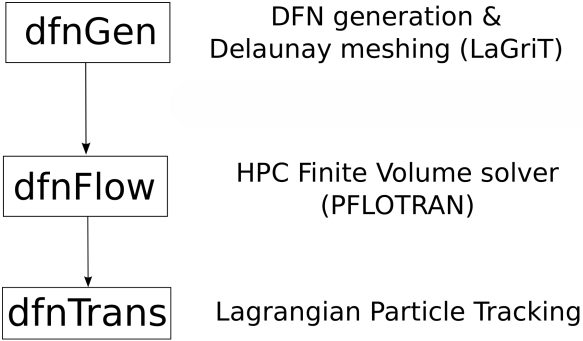
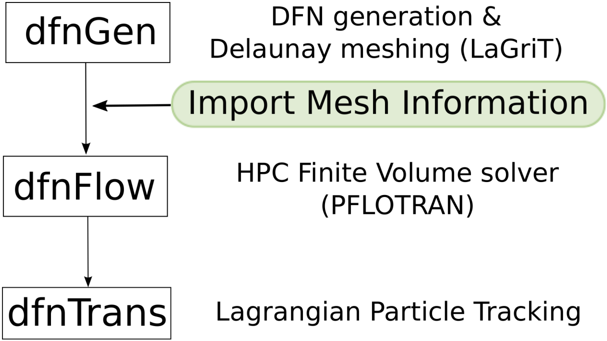


Figure: Workflow chart of *dfnWorks*

Bottleneck for Large DFN of High Density



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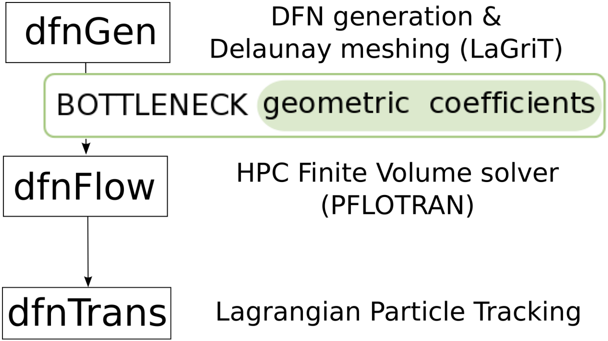

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Geometric Coefficients

Coefficients that characterize the geometric feature of the dual Voronoi mesh, including

- Control Volume (of Voronoi cell)
- Area (of the cell interface)

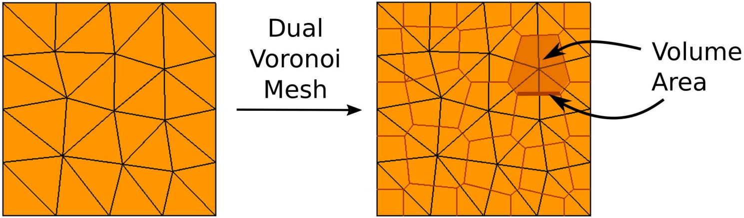
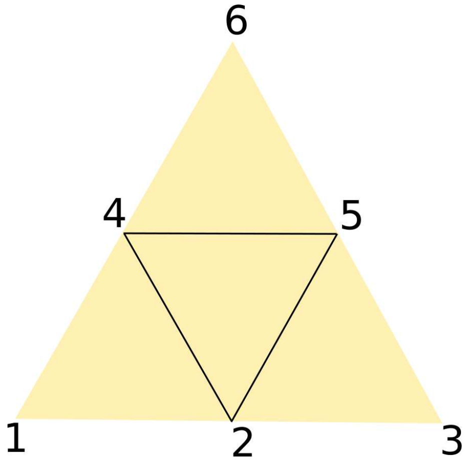


Figure: Geometric Coefficients: Volumes and Areas

Outlines

Calculations of Control Volumes Ex: V_4



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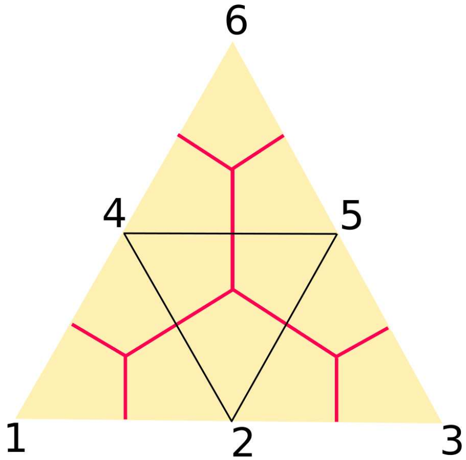

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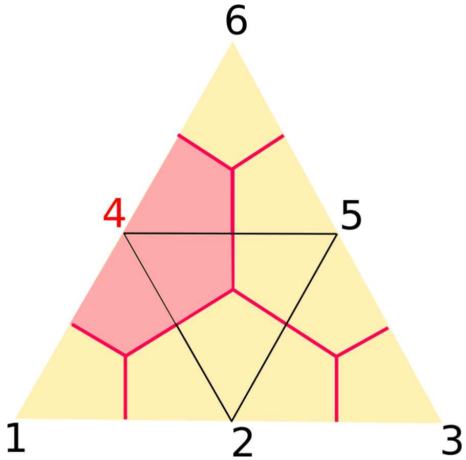

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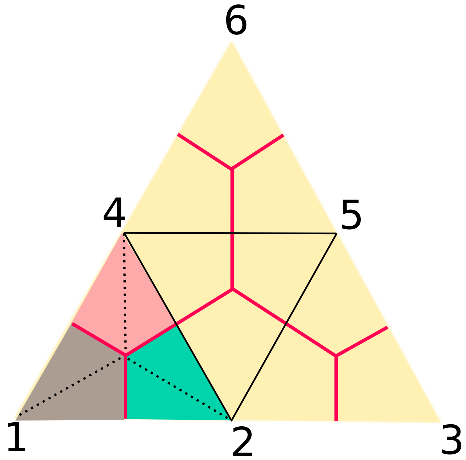

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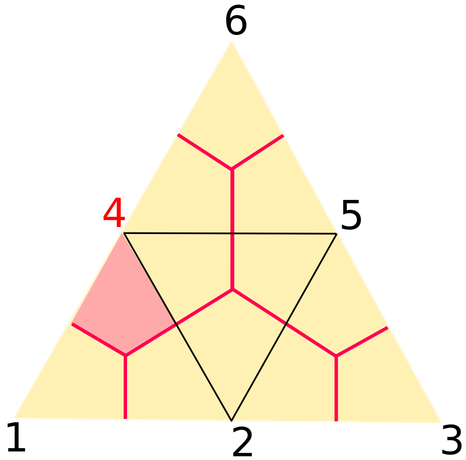

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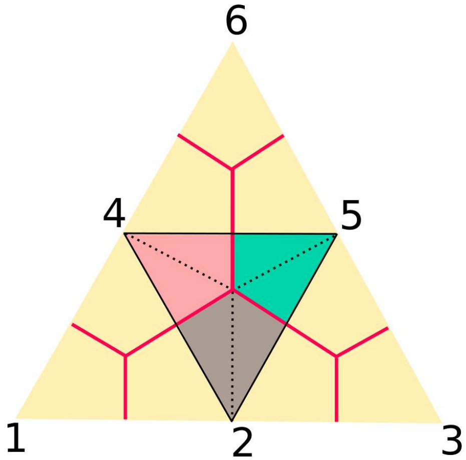

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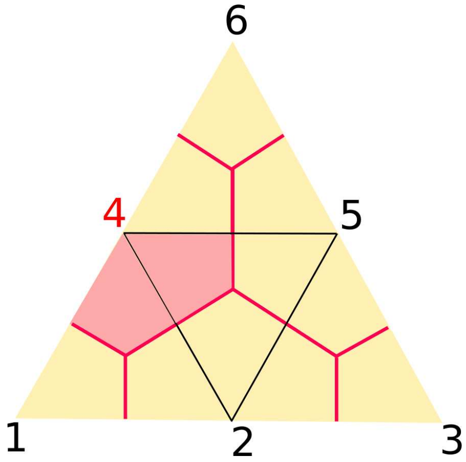

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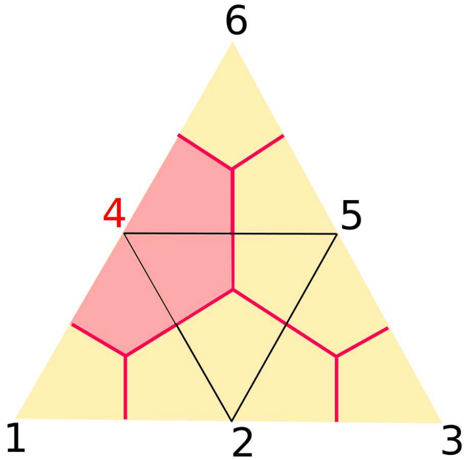
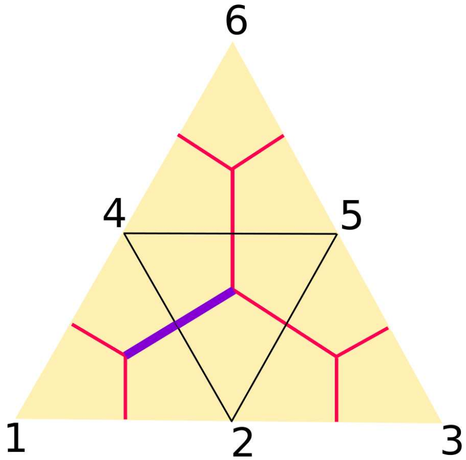


Calculations of Areas Ex: $A_{2,4}$



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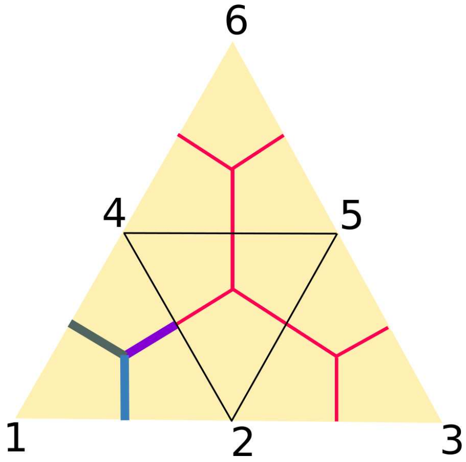

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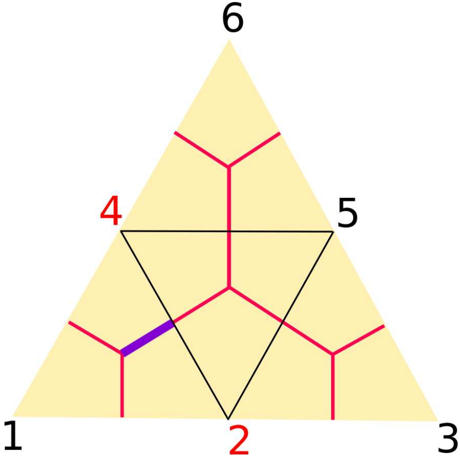

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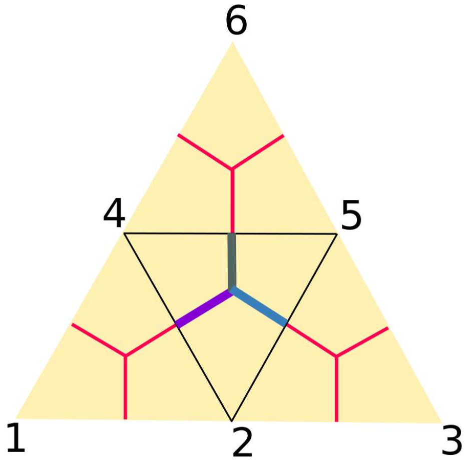

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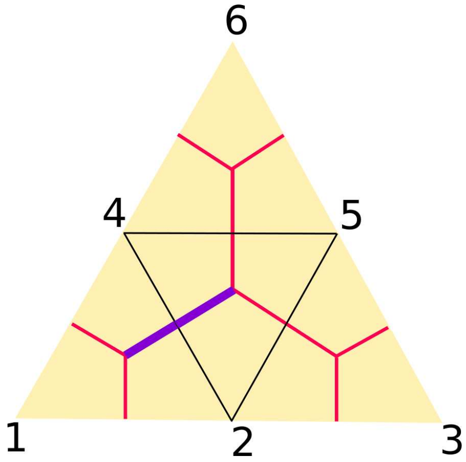

Upper Diagonal and Sparse Matrix

- Volumes $\rightarrow$ diagonal entry
- Areas $\rightarrow$ upper-diagonal entry

$$\begin{pmatrix} V_1 & A_{1,2} & \cdots & A_{1,n} \\ & V_2 & \cdots & A_{2,n} \\ & & \ddots & \vdots \\ & & & V_n \end{pmatrix}$$

- Upper triangular matrix
- Sparse matrix: entry = connection

No full dense matrix with lots of 0's $\Rightarrow$ Save memory usage!

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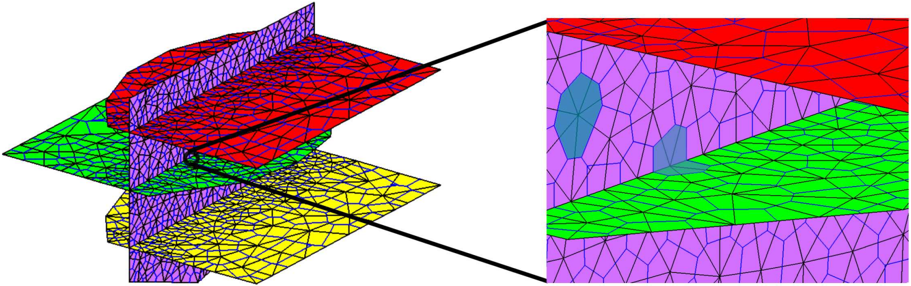
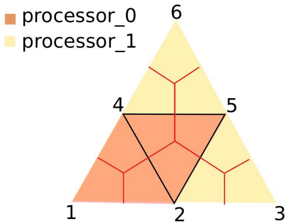
Same Algorithm for DFN



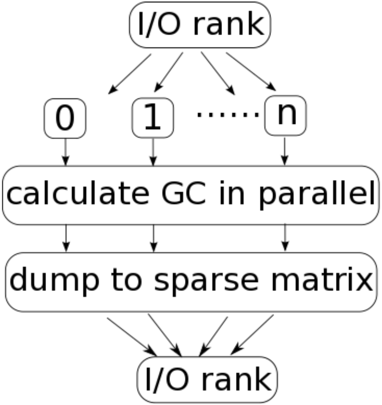
Outlines

Parallelization: Distribute the Workload

1. Read the mesh information through I/O rank.
2. Scatter data needed to processors.



3. Volume $\rightarrow$ diagonal entry;
   Area $\rightarrow$ upper-diagonal entry
4. Gather data to I/O rank and dump to files.



Tool – PETSc

- Portable, Extensible Toolkit for Scientific Computation
- a suite of data structures and routines for the scalable (parallel) solution of scientific applications
- Argonne National Laboratory
- `http://www.mcs.anl.gov/petsc/`

Why PETSc?

- Parallel vectors and matrices
- Sparse matrices data structure and operations
- Support scatter/gather in Message Passing Interface (MPI)
- Intensive error checking (error handler for functions)
- Profiling feature
- Complete and friendly documentation
- Portable to UNIX and Windows
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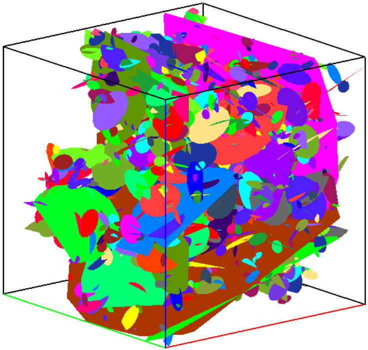
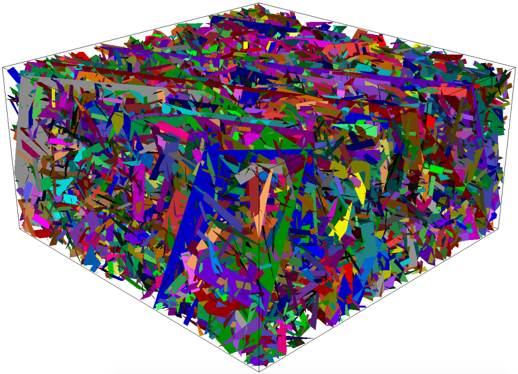
Large Networks

- 1475 fractures / 1,320,282 cells (left)
- 17237 fractures / 14,480,540 cells (right)





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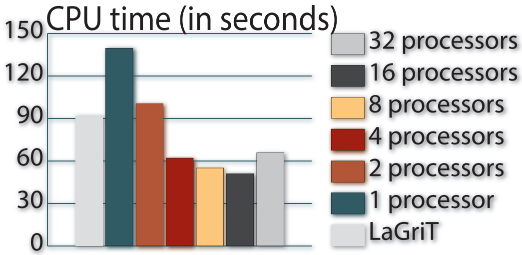

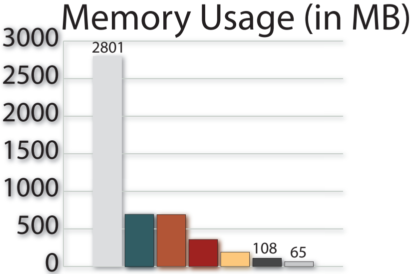

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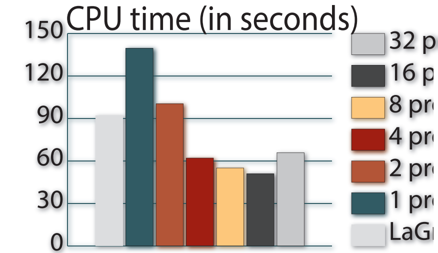

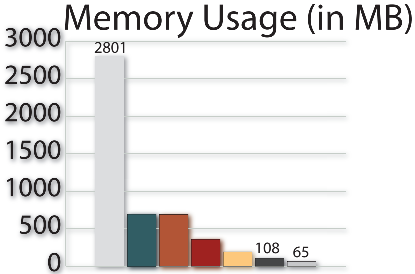

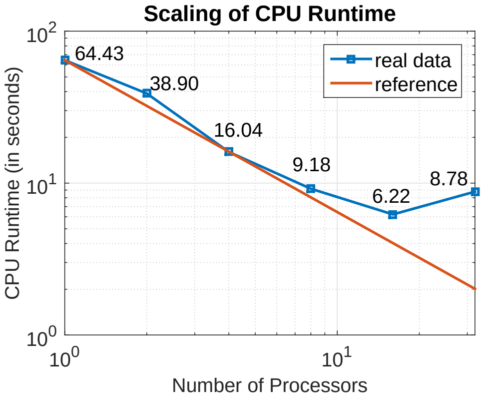

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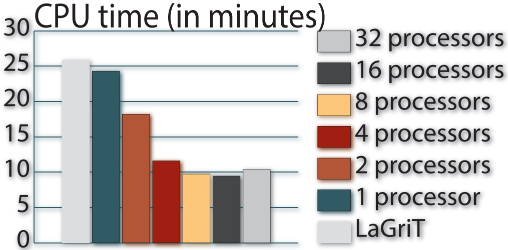

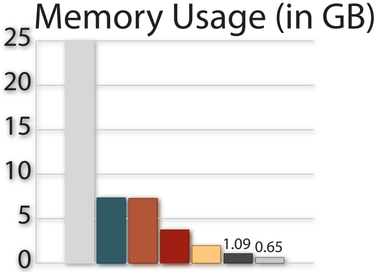

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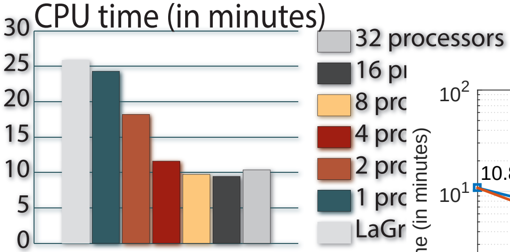

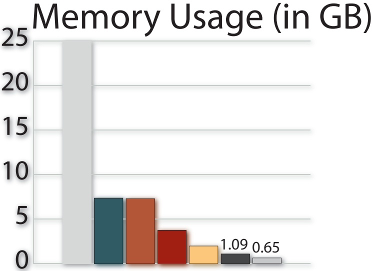

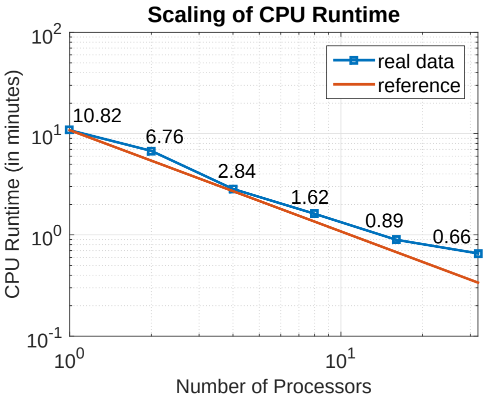

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Conclusion

- Optimizing the computations of geometric coefficients:
  reduce the overhead memory usage significantly
  reduce the CPU runtime
- Approach:
  dynamic data structure and sparse matrix
  parallel programming
- Test Problems:
  structured/unstructured Delaunay triangle mesh
  scaling from 10 to 10^7 cells
  small/large discrete fracture network mesh
- Outputs:
  output coefficients in FEHM STOR file
  direct PFLOTRAN output
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Future Work

- Instructive diagnostic output (like LaGriT)
- Add *scalar*/*area_scalar* option for 2-D in LaGriT (3-D; TOUGH2)
- PFLOTRAN output with triangular control volumes
- Extension: Voronoi $\Rightarrow$ median mesh/hybrid mesh
- Generalization: 2-D triangle mesh $\Rightarrow$ 3-D tetrahedron mesh

Reference

J. D. Hyman, C. W. Gable, S. L. Painter, and N. Makedonska. Conforming delaunay triangulation of stochastically generated three dimensional discrete fracture networks: a feature rejection algorithm for meshing strategy. *SIAM Journal on Scientific Computing*, 36(4):A1871–A1894, 2014.

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