Goal

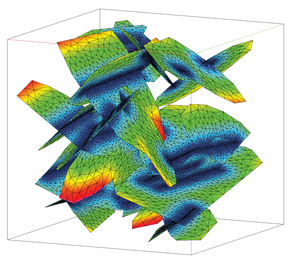
Optimizing the computations of geometric coefficients for discrete fracture networks (DFN) of high density: loosing the bottleneck

1. overhead memory usage
2. CPU runtime

What are DFN?

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

(a) Fractured rock



(b) Example of simple DFN

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

dfnWorks a HPC computational suite for modeling flow and transport in large DFN developed by the Subsurface Flow and Transport team (EES-16) at the Los Alamos National Laboratory.

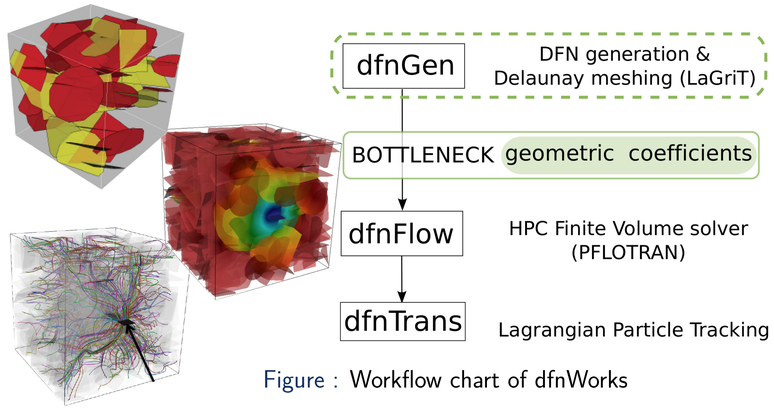
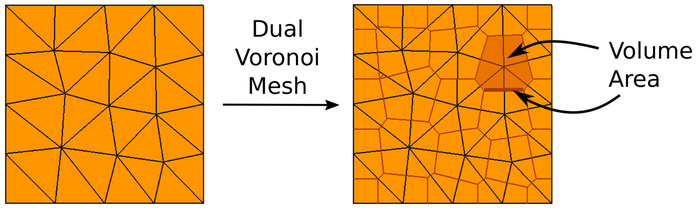


Figure : Workflow chart of dfnWorks

Numerical Challenges

Geometric Coefficients (GC) Coefficients that characterize the dual Voronoi mesh: volume and area

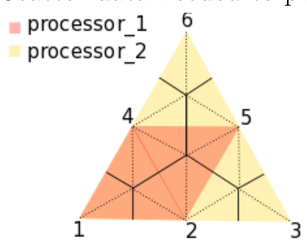


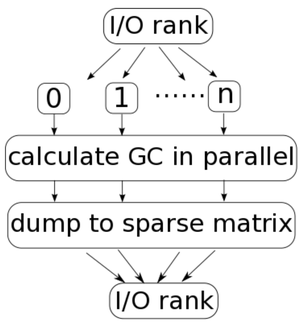
Parallel Programming in PETSc

PETSc Portable, Extensible Toolkit for Scientific Computation, is a suite of data structures and routines for the scalable (parallel) solution of scientific applications (Argonne National Laboratory)

- Parallel vectors and matrices
- Sparse matrices data structure and operations
- Support scatter/gather (MPI)
- Intensive error checking
- Profiling feature
- Complete and friendly documentation
- Portable to UNIX and Windows
- Being actively supported for many years

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

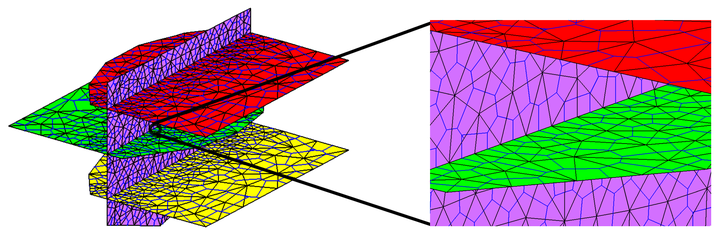




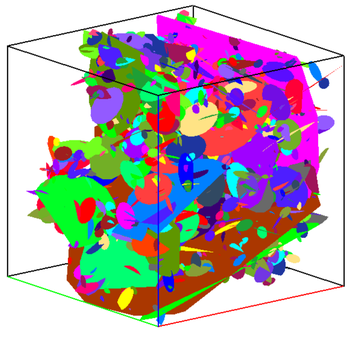
3. Volume → diagonal entry; Area → off-diagonal entry
4. Gather data and write into various formats: FEHM, TOUGH2, PFLOTRAN.

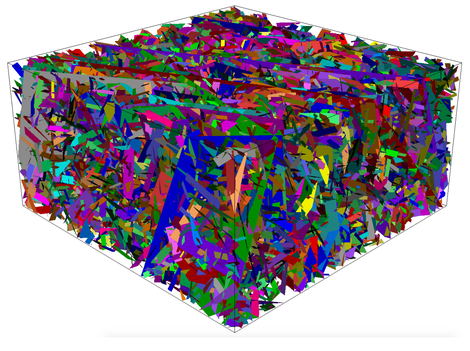
Test Problems

- Simple Network (4 fractures/1161 cells)



- Large Networks (1475 fractures/1,320,282 cells & 17237 fractures/14,480,540 cells)





Loosing the Bottleneck

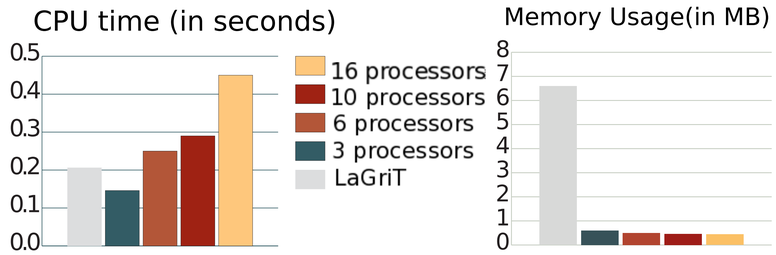


Figure : CPU time and memory usage comparison for four fractures DFN.

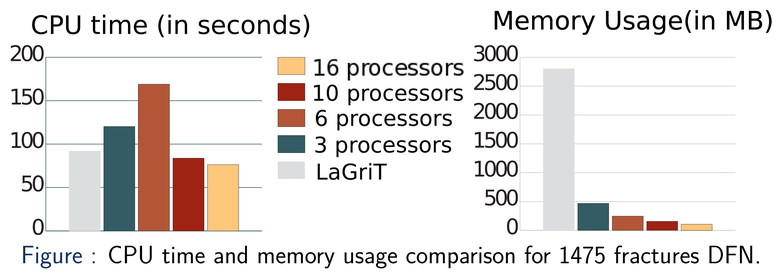


Figure : CPU time and memory usage comparison for 1475 fractures DFN.

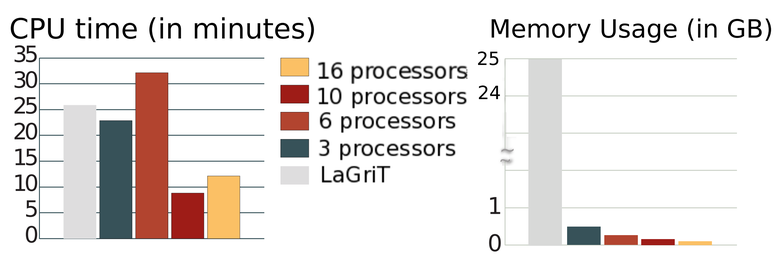


Figure : CPU time and memory usage comparison for 17237 fractures DFN.

References

[1] 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.

[2] Los Alamos National Laboratory. Los alamos grid toolbox, (lagrit). `http://lagrit.lanl.gov`, 2013.

[3] P. C. Lichtner, G. E. Hammond, C. Lu, S. Karra, G. Bisht, B. Andre, R. T. Mills, and J. Kumar. Pflotran user manual: A massively parallel reactive flow and transport model for describing surface and subsurface processes. Technical report, Los Alamos National Laboratory, 2015.

[4] N. Makedonska, S. L. Painter, Q. M. Bui, C. W. Gable, and S. Karra. Particle tracking approach for transport in three-dimensional discrete fracture networks. *Computation Geosciences*, under review.

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