Nonisothermal Multiphase Multicomponent Reactive Transport in a Deforming Fractured Porous Media

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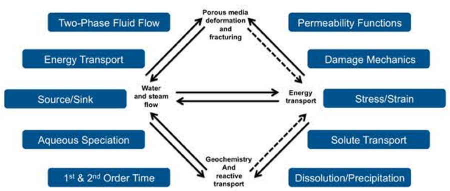
Introduction

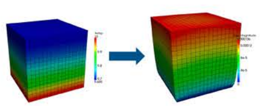
Numerical modeling of nonisothermal, multiphase, multicomponent reactive transport in a geomechanically active subsurface, at a relevant scale such as that for evaluating the impacts of hydraulic fracturing on drinking water resources, typically requires solving problems with a large amount of unknowns. This is particularly challenging because the systems of governing partial differential algebraic equations (PDAEs) are highly nonlinear and tightly coupled. Here we present a simulation code/methodology to solve the governing PDAEs in a fully coupled, fully implicit manner using a Jacobian-Free Newton-Krylov approach.



Coupling and Solution Approach

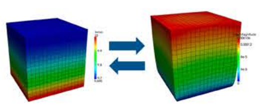
Loose Coupling / Operator Split

1. Solve PDE1
2. Pass Data
3. Solve PDE2
4. Move To Next Timestep



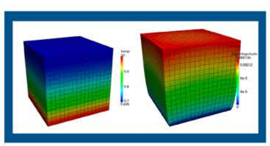
Sequential Coupling w/Iteration

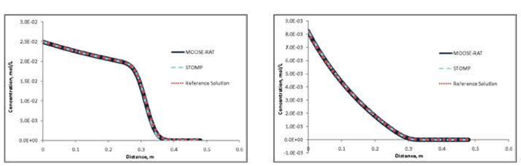
1. Solve PDE1
2. Pass Data
3. Solve PDE2
4. Pass Data
5. Return to 1 Until Convergence
6. Move To Next Timestep



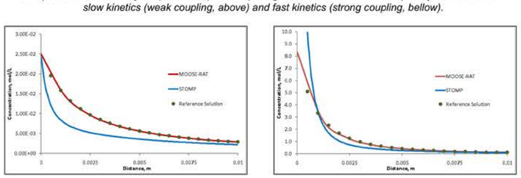
Fully Coupled

1. Solve PDE1 and PDE2 simultaneously in <u>one</u> system
2. Move To Next Timestep



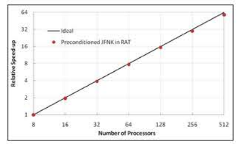


Comparison between fully-coupled and operator-splitting solutions for reactive transport systems that have slow kinetics (weak coupling, above) and fast kinetics (strong coupling, bellow).

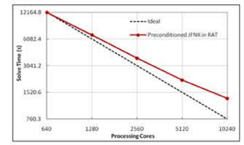


Advanced Computing Capabilities

Parallel Scalability - scales almost ideally on both workstation and large-scale computer clusters



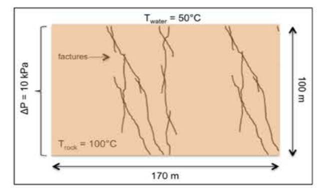
- Strong scaling tests
- Heterogeneous medium
- 5 primary variables
- ~200,000 grid cells
- ~1,024,000 DoFs
- CPU # range: 8 - 512



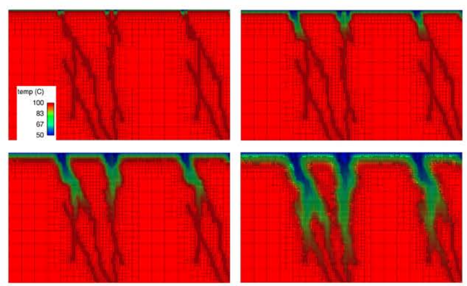
- Strong scaling tests
- Heterogeneous medium
- 5 primary variables
- ~32 million grid cells
- ~170,000,000 DoFs
- CPU # range: 640 - 10,240

1. Fluid Flow through a Discrete Fractured Medium with Mesh Adaptivity

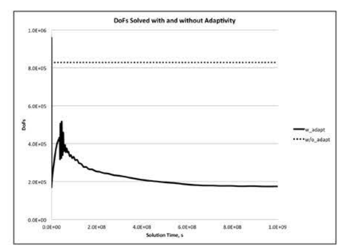
- Initial mesh adaptivity utilized to capture a predefined intersecting, aperture-varying fracture distribution
- During simulation, regions of high pressure/temperature gradient jumps are refined for additional detail and regions of little activity, far field rock domain, is coarsened
- Reduces computation time by saving >70% of DoFs calculated in comparison to uniform mesh



Input fracture distribution



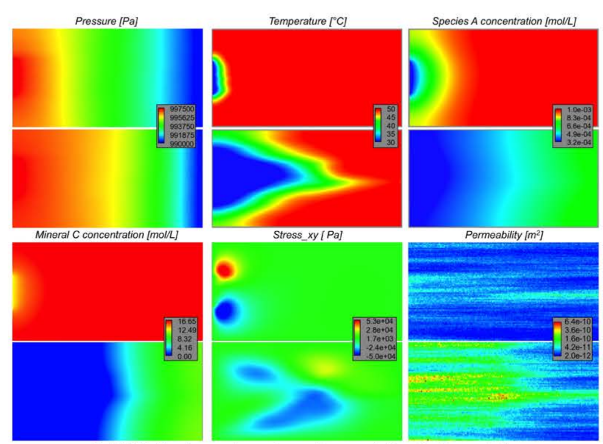
Adaptive mesh overlaid upon temperature field



Comparison of DoFs between a uniform mesh and an adaptive mesh.

2. Coupled THMC Simulation in a Heterogeneous Medium

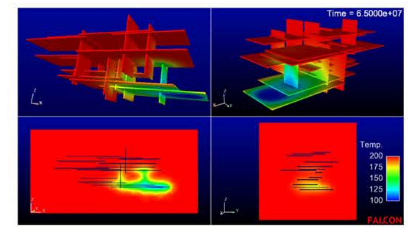
- Preferential flow paths (high perm layers)
- Dissolution of in situ mineral, c, by injecting undersaturated solution
- Thermal and pressure induced stress
- Torsional/non-uniform stress caused by heterogeneous flow paths



Spatial distribution of pressure, temperature, species a concentration, mineral c concentration, xy component of stress, and permeability for an earlier time (upper) and later time (lower).

Conclusion

- A fully-coupled fully-implicit solution approach has been developed and applied to solve coupled hydro-thermo-mechanical-chemical systems.
- Advanced computing capabilities, such as massive parallelism and mesh adaptivity, have enhanced the efficiency and effectiveness of the solution approach.
- Applications of simulators to THMC problems have provided insights into understanding the nonlinear coupling effects among various processes that take place during hydraulic fracturing operations and it's potential impacts on drinking aquifers.



Future Work

- Explore better ways to describe the discrete fracture initiation/propagation process. Previous approaches to this problem such as smeared crack and damage mechanics methods have produced unsatisfactory results. Current work includes looking at the xFEM method.
- Implementing finite volume capability which enables better mass and energy conservation.
- Developing an interface with the FracMan© fracture network code in order to create fracture domains that include non-planar, stochastic, and field realistic distributions.

Acknowledgments

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