Computational Mechanics for Geosystems Management to Support the Energy and Natural Resources Mission

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Problem

- U.S. energy needs — minimizing climate change, mining and extraction technologies, safe waste disposal — require the ability to simulate, model, and predict the behavior of subsurface systems. We propose development of a coupled thermal, hydrological, mechanical, chemistry (THMC) modeling capability for massively parallel applications that can address these critical needs.

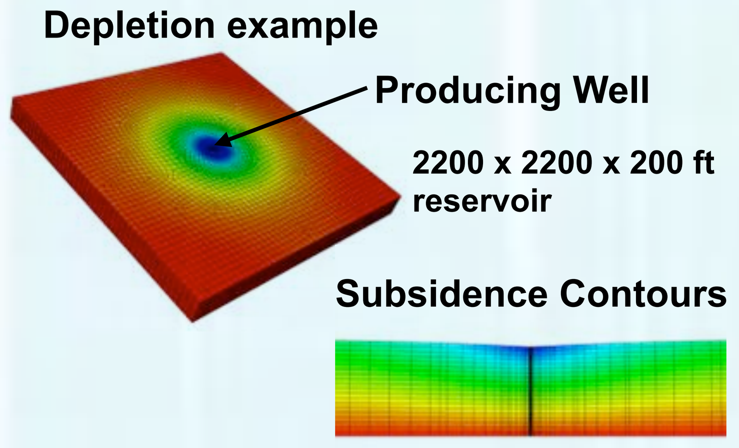
- The goal and expected outcome of this research is a state-of-the-art, extensible, simulation capability, based upon SIERRA Mechanics, to address multiphase, multi-component reactive transport coupled to nonlinear geomechanics in heterogeneous (geologic) porous materials. The THMC code provides a platform for integrating research in numerical mathematics and algorithms for chemically reactive multiphase systems with computer science research in adaptive coupled solution control and framework architecture.

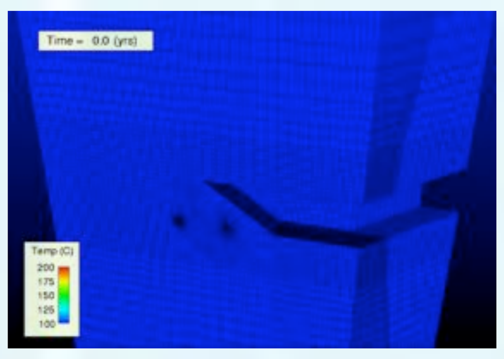
Approach

- Implement a coupled porous flow/mechanics and thermal/mechanical capability in SIERRA Mechanics
- Implement a multiphase flow and reaction-transport capability for heterogeneous porous materials
- Survey existing capability within SIERRA to determine what subcycling and adaptive time-stepping methods can be driven, currently, and what additional functionality is needed.
- Develop adaptive solution controls and robust solvers to enable performance efficiency of the multiphysics simulator

Results

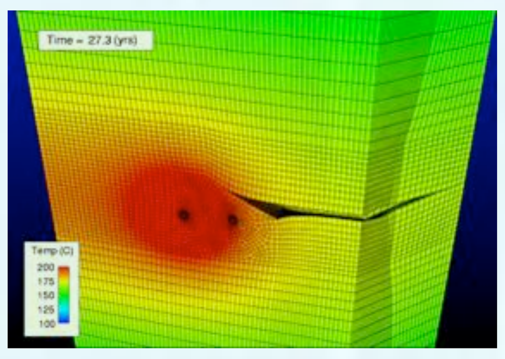
- Demonstrated coupling of porous flow in deforming media (Terzaghi and depletion benchmark examples)
- Benchmarked coupled thermal/geomechanics for waste disposal problems
  - WIPP Heated Benchmark II
  - Heated Reference Parallel Calculation
- Demonstrated ability to adaptively control coupled porous flow/geomechanics and thermal/geomechanics using appropriate metrics





Generic salt repository undeformed mesh

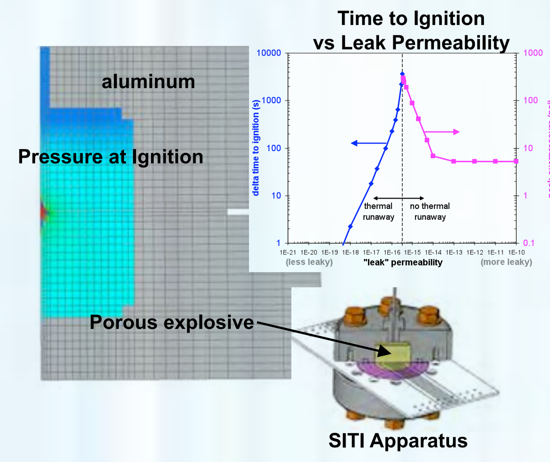
Generic salt repository deformed mesh at final time

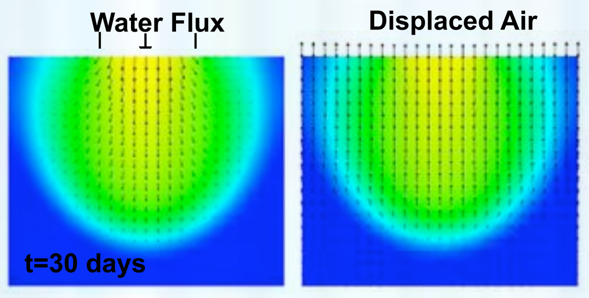


Results (cont.)

- Implemented and verified coupled saturated porous flow/geomechanics
  - Benchmarked against Terzaghi consolidation problem and several reservoir depletion problems (Dean et al. 2006)
- Implemented and verified nonisothermal saturated liquid or gas flow coupled with reactive species transport (applied to cook-off problem)
  - Cook-off problem was extended to include mechanical deformations due to reaction-induced over-pressure (1st cut THMC)
- Implemented and verified two-component, two-phase (EOS for water/air) flow, with capillary pressure and relative permeability

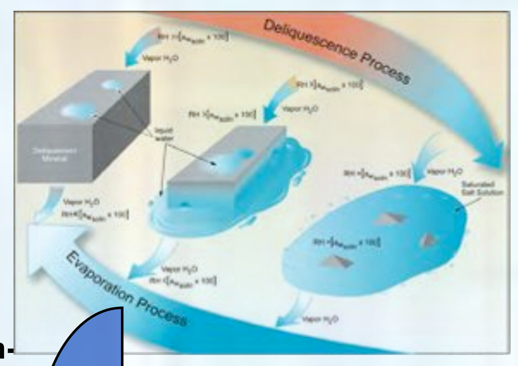
Modeling Cook-Off in Granular Explosives



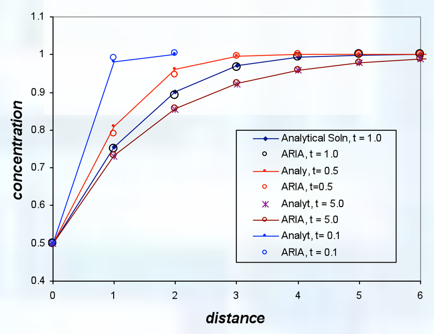


Patch infiltration of water into a dry closed box (6x5 m) with open top. The color depicts liquid saturation. The left figure shows the infiltrating liquid velocity and the right shows the displaced gas velocity.

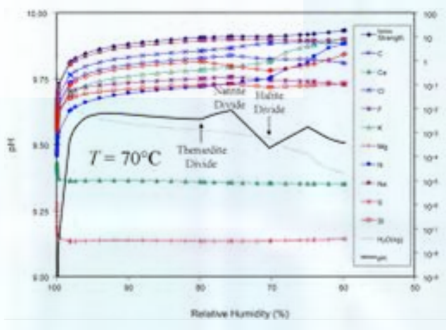
In-drift thermal-chemical processes (after C. Jove-Colon et al.)



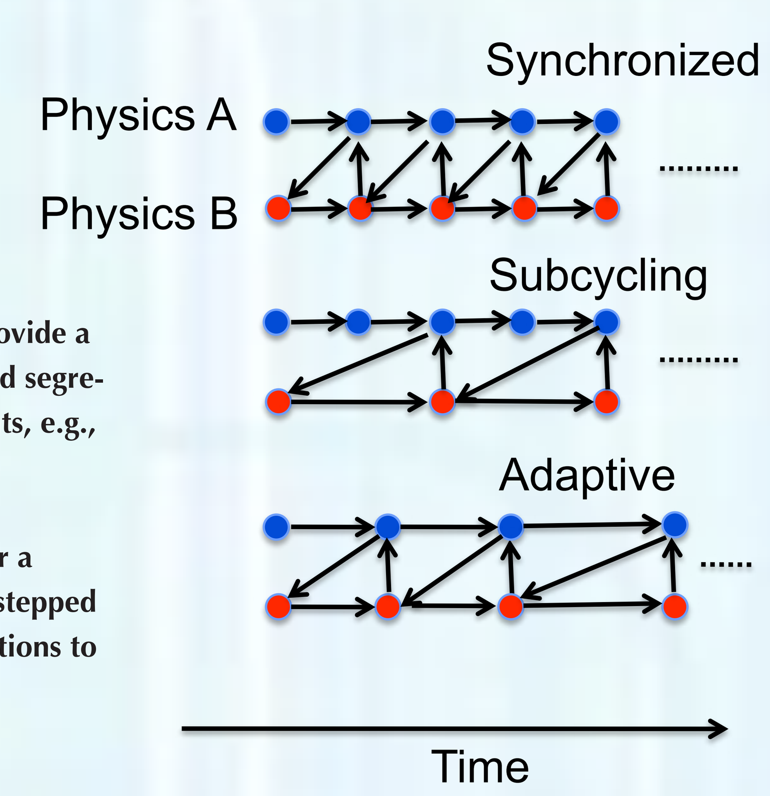
Validation of ARIA reaction-transport scheme



Pitzer (solubility) batch modeling of in-drift chemical evolution of seepage water (after C. Jove-Colon et al., 2004)



- Researched and selected geochemical databases and solubility codes for inclusion (incl. CANTERA, Caltech; EQ3/6, LLNL; PhreeqC, USGS)
- Demonstrated capability in ARIA for fully coupled reaction, advective and diffusive transport



- Solution Control and Encore were found to provide a general capability to drive adaptive explicit and segregated time stepping of multiphysics components, e.g., Aria and Adagio
- Representative approaches were performed for a fully saturated flow in porous media problem stepped adaptively in time using pressure-porosity relations to lag updates to the material deformation

Significance

- Enhance SNL ability to respond to national needs for energy security and solutions to climate change
- Multiphysics modeling capability critical to providing long-term solutions to a host of energy & security problems
- Enhance future business and research collaborations – ICES, NIMS, NETL, FE, CRADAS, WFO, BES, EFRC, NEAMS

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