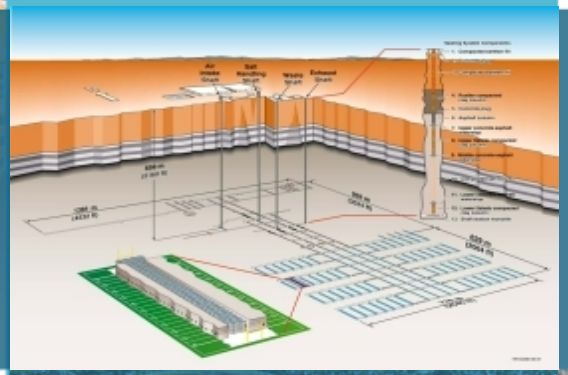
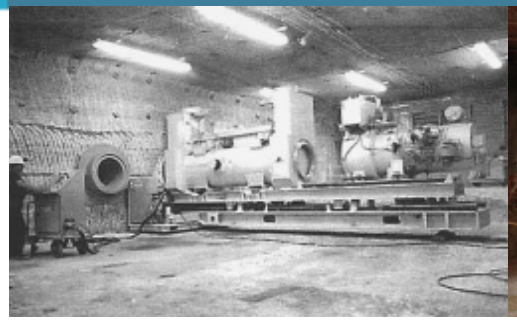
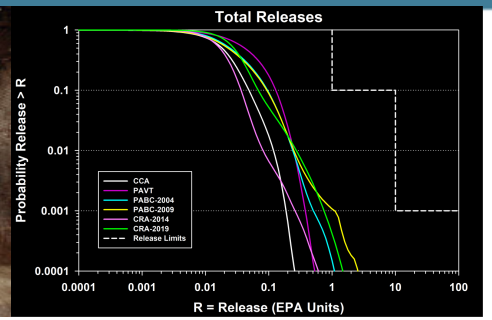
SAND2021-8163PE

Sandia National Laboratories

PFLOTRAN Overview







Michael Nole

Peer Review Orientation Meeting, 07/13/2021

U.S. DEPARTMENT OF ENERGY | NNSA

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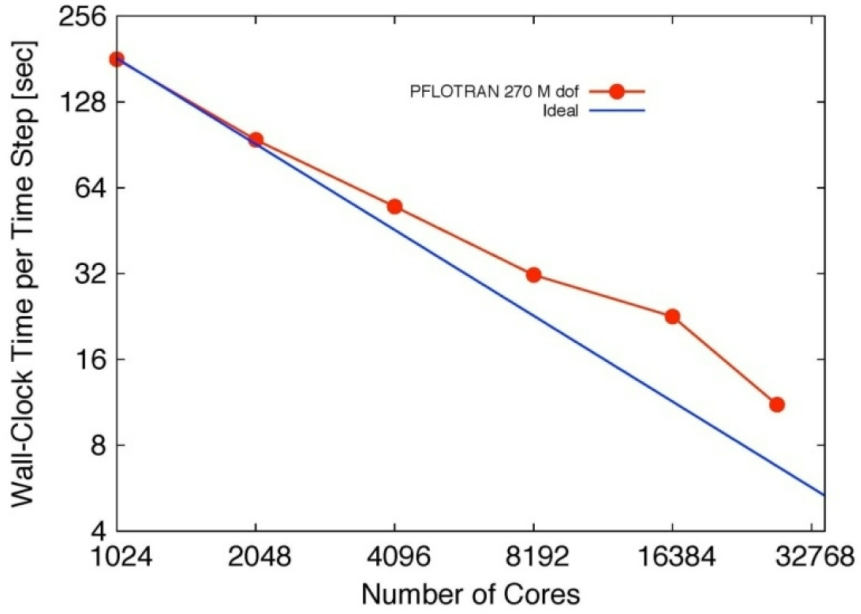
Motivation

- PFLOTRAN is **not yet qualified** for use in PA calculations at WIPP. It is currently only being used here as corroborating evidence of the validity of WIPP 2D 2-phase flow modeling.
- PFLOTRAN is a state-of-the-art, open-source, scalable code for simulating subsurface fluid flow and transport processes
- The code is 3D (can also be run in 1D and 2D), parallel, and capability is being added specifically for future WIPP PA calculations

Overview

- PFLOTRAN is an open-source, massively parallel subsurface fluid flow and transport simulator. The code can be run on supercomputers, single workstations, and laptops
- PFLOTRAN simulates multiphase flow and multicomponent reactive transport in 3D and on both structured and unstructured grids
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)
- Founded upon well-supported open-source libraries
  - MPI, PETSc, HDF5, METIS/ParMETIS/CMAKE
- Demonstrated performance
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom



Applications

Nuclear waste disposal

- Waste Isolation Pilot Plant (WIPP): currently finishing QA on WIPP_FLOW mode
- US DOE NE Spent Fuel and Waste Science and Technology (SFWST) Geologic Disposal Safety Assessment (GDSA) Framework (pictured)

Climate: coupled overland/groundwater flow; CLM

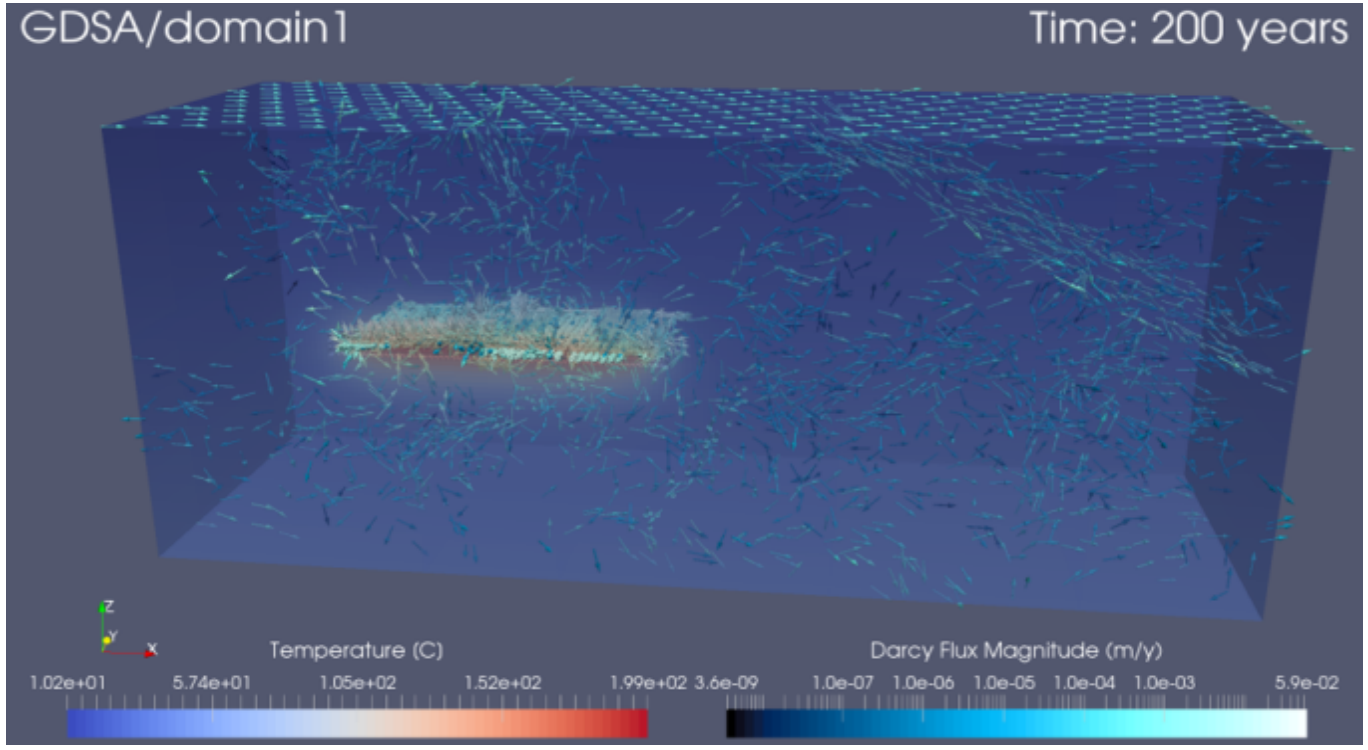
- Next Generation Ecosystem Experiments (NGEE) Arctic
- DOE Earth System Modeling (ESM) Program

Biogeochemical transport modeling

- U(VI) fate and transport at Hanford 300
- Hyporheic zone biogeochemical cycling
  - Columbia River, WA, USA
  - East River, CO, USA

CO_2 sequestration

Enhanced geothermal energy



Applications

Information from a survey of PFLOTRAN users

- 3D near-field models of nuclear waste repositories
- Agriculture
- Apatite reactive barrier
- Behind-casing pressure development in well annulus due to N2 injection
- Biogeochemical hot spots/hot moments
- Biogeochemistry within groundwater-river water exchange zones
- CO2 sequestration
- CO2 storage
- Coupled surface/subsurface land mode
- Geothermal Systems
- Groundwater age
- Groundwater management
- Hydrogeochemical evolution
- Interpretation of in-situ through-diffusion experiments
- Modelling of enhanced oil recovery (using CO2 as solvent)
- Modelling of oil and gas reservoirs
- Mountain block recharge beneath soil mantled hill slopes
- Multicomponent transport of trace gases
- Nuclear waste repository performance assessment
- Permafrost modeling
- pH sweep and water quality data analysis
- Radioactive waste management
- Radionuclide transport
- Redox gradients within hyporheic zones
- Remediation design
- Species specific diffusion and Donnan equilibrium in clays
- Subsurface hydrology and geochemistry
- Surface/hill slope hydrology

Numerical Methods

Spatial discretization
- Finite volume (2-point flux)
- Structured and unstructured grids

Time discretization: fully-implicit backward Euler

Nonlinear solver
- Newton-Raphson
- Line search/damping with custom convergence criteria

Linear solver: direct (LU) or iterative (BiCGStab)

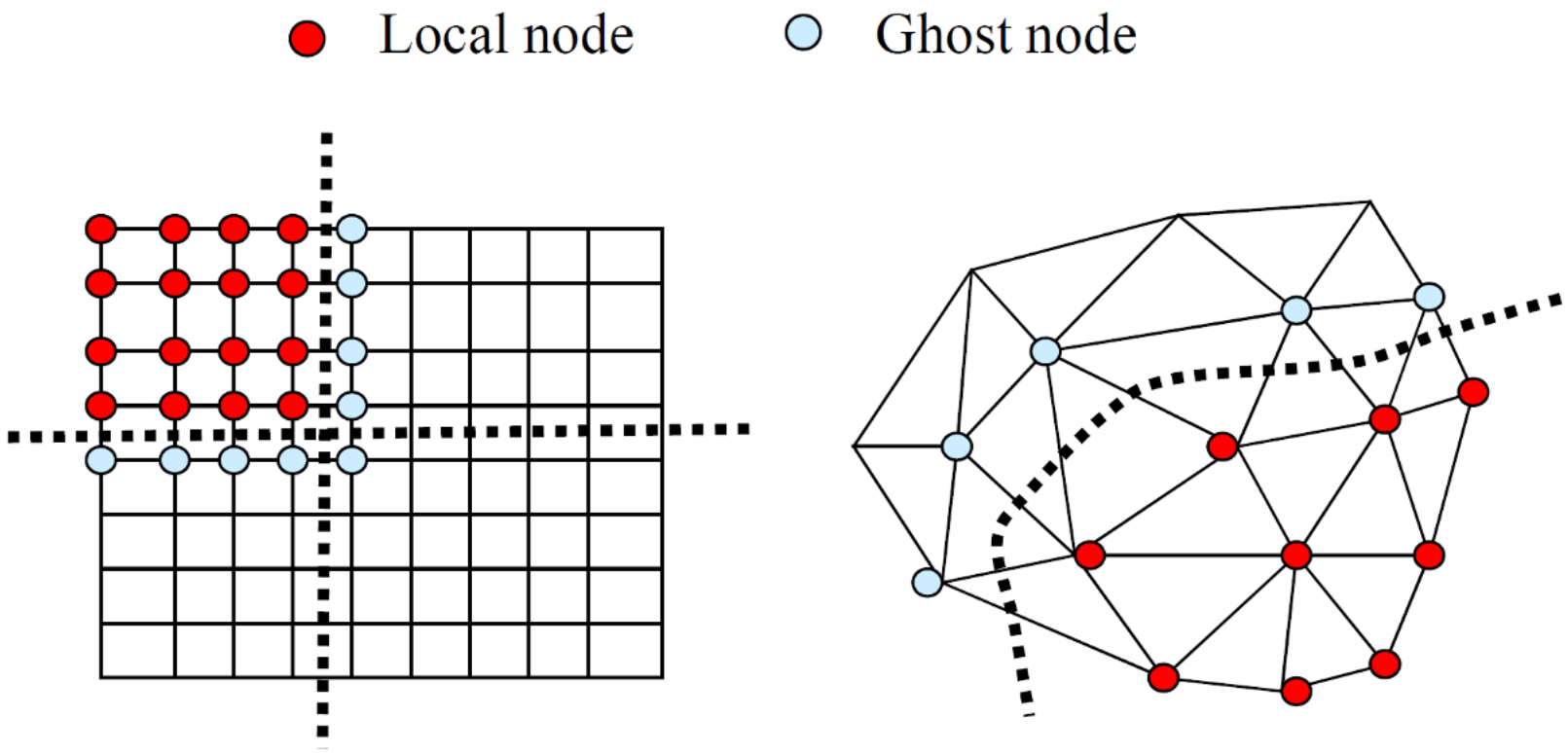
Multi-physics coupling
- Flow and transport/reaction: sequential
- Transport and reaction: global implicit, operator splitting
- Geomechanics and flow/transport: sequential

Deep Borehole Waste Disposal

Emily Stein, SNL, 2015

Parallelization

Domain Decomposition



Ghost node information used only in flux calculations.

PFLOTRAN Flow Modes

- RICHARDS
  - Variably-saturated water
- TH (thermo-hydrologic)
  - Variably-saturated water + energy
- GENERAL
  - multiphase, two-component (air-water) + energy
- WIPP_FLOW
  - Two-phase isothermal and immiscible
- MPHASE
  - Supercritical CO_2-water + energy
- And more experimental flow modes

WIPP_FLOW Mode

Governing Equations:

$$\frac{\partial \phi(s_l \rho_l)}{\partial t} = -\nabla \cdot (\rho_l \boldsymbol{q_l}) + Q_l,$$

$$\frac{\partial \phi(s_g \rho_g)}{\partial t} = -\nabla \cdot (\rho_g \boldsymbol{q_g}) + Q_g,$$

$$\boldsymbol{q_\alpha} = -\frac{k k_\alpha}{\mu_\alpha} \nabla (p_\alpha - \gamma_\alpha \boldsymbol{z}), \quad (\alpha = l,\ g)$$

Constraints:

$$\sum_\alpha s_\alpha = 1$$

$$P_g = P_l + P_c(S_l)$$

WIPP_FLOW Mode Process Models

- WIPP_FLOW mode is in the process of being qualified for use in official WIPP PA calculations (finishing July 2021). Process models QA'd include:
  - Gas and brine generation due to corrosion, microbial degradation, radiolysis, and other rate-controlled chemical reactions
  - Permeability and porosity change due to elastic opening/closing of fractures
  - Porosity evolution due to creep closure
  - WIPP-specific options for liquid and gas equations of state and the Klinkenberg effect on gas permeability
  - WIPP-specific capillary pressure and relative permeability models

- A comparison between PFLOTRAN and BRAGFLO results will be presented at the peer review as corroborative evidence for the validity of the 2D BRAGFLO solution.