SAND2022-15830C

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Advancements in High-Performance Multi-physics Simulation Capabilities for the Geologic Disposal Safety Assessment Framework

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International High Level Radioactive Waste Management Conference, Phoenix, AZ

11/17/2022

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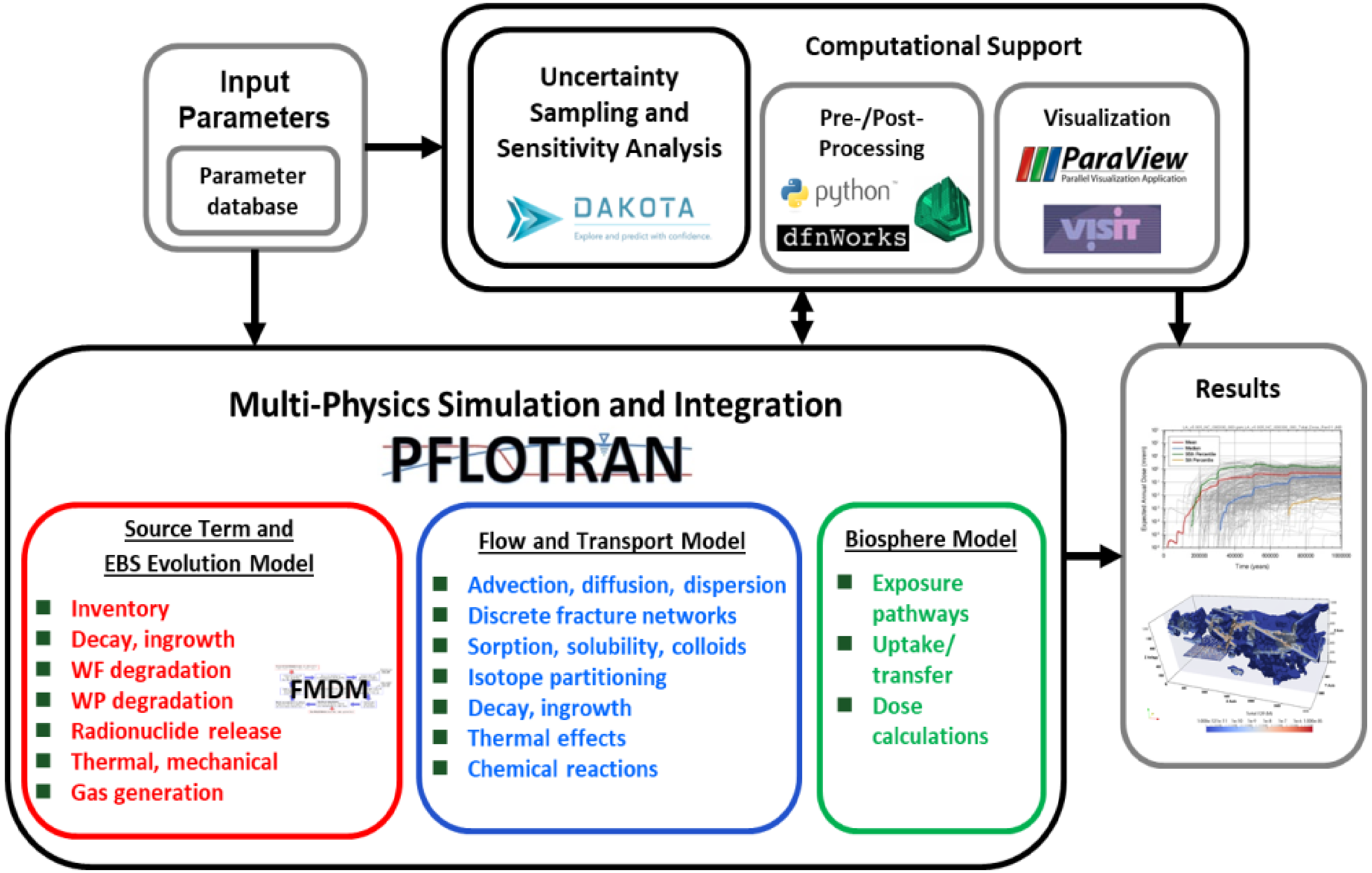
NNSA

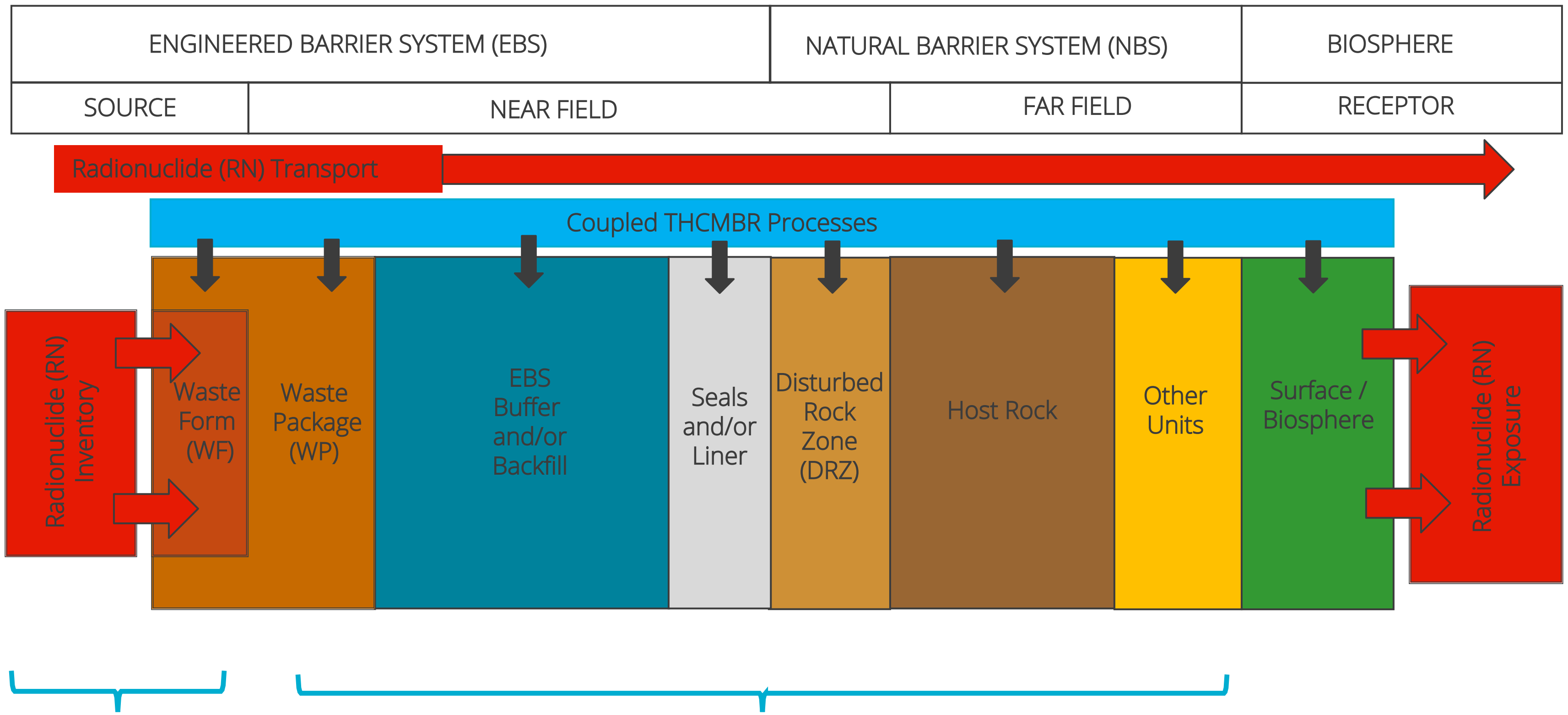
Overview: GDSA Software Framework

- The Geologic Disposal Safety Assessment (GDSA) Framework encompasses a suite of software libraries including the multi-physics simulation engine, PFLOTRAN
- PFLOTRAN simulates evolution of the source term and engineered barrier system (0D models) coupled to flow and radionuclide transport (3D) through the EBS and NBS to the biosphere
- Recent advancements have focused on improving performance and fidelity for high temperature, multiphase, and multi-continuum applications

GDSA Framework



Overview: Conceptual Model in PFLOTRAN



<u>0D Source Term Models</u>

- WF Radionuclide Inventory
- Decay Heat
- Criticality

<u>3D Flow and Transport</u>

- Multiphase flow
- Advective-Diffusive-Dispersive Transport
- Radionuclide SPDI
- Multiple Continuum

Recent PFLOTRAN Advancements

Process modeling

- **Multiple Continuum Transport**
- Thermal Conductivity Anisotropy
- **Material Transform**
- Criticality Module
- Reduced Order Geomechanics Model
- Gas Transport
- Updated EOS including Salinity
- **Fully-coupled Solute Mass Balance**

Software Performance

- **Advanced Linear and Non-linear Solver Options**
- Characteristic Curve Smoothing
- Lookup Table-based Function Evaluations
- 3D Lookup Table Interpolation

Software Infrastructure

- **Agile development process using Jira**
- GDSA QA Test Framework
- GDSA Calculation Archive

PFLOTRAN User Guide

Two sets of documentation:

- Release version (currently v4.0): **documentation.pflotran.org**
- Development version: **doc-dev.pflotran.org**

PFLOTRAN Documentation » PFLOTRAN Documentation

PFLOTRAN

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PFLOTRAN Documentation

PFLOTRAN

This is the development version of the documentation.

PFLOTRAN is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. The code is developed under a GNU LGPL license allowing for third parties to interface proprietary software with the code, however any modifications to the code itself must be documented and remain open source. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. PFLOTRAN's source code repository is on Bitbucket.

Announcements

Documentation

- Developer Guide
- Theory Guide
- User's Guide

Need help beyond the documentation above?

Search topics at or submit a question to the pflotran-users Google Group.
Email user questions to pflotran-users at googlegroups dot com
Email bug reports to pflotran-dev at googlegroups dot com

PFLOTRAN Documentation » User's Guide » MATERIAL_TRANSFORM_GENERAL

PFLOTRAN

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MATERIAL_TRANSFORM_GENERAL

The Material Transform Process Model is documented here.

This option specifies the material transform process model, which is a child of flow and a peer of transport. Under the SIMULATION block, the process model is included by adding the MATERIAL_TRANSFORM block:

```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS
    SUBSURFACE_FLOW flow
      MODE GENERAL
    /
    SUBSURFACE_TRANSPORT transport
      MODE GIRT
    /
    MATERIAL_TRANSFORM <name_string>
    /
  /
END
```

where <name_string> is a user-defined name for the process model. There are currently no additional options for this block. Functionality is currently available for problems utilizing flow modes (such as GENERAL, TH, and RICHARDS) and/or reactive transport with UFD_DECAY.

The details of the process model are included in the MATERIAL_TRANSFORM_GENERAL block, which lists several MATERIAL_TRANSFORM objects that can be associated with a MATERIAL_PROPERTY.

Supported models that can be included in a MATERIAL_TRANSFORM object include the following:

- ILLITIZATION

ILLITIZATION

The illitization function allows for a time- and temperature-dependent change from smectite to illite to be evaluated during the simulation, which in turn can be used to impart a commensurate change in permeability and/or sorption.

Software Infrastructure: Open Source Tools

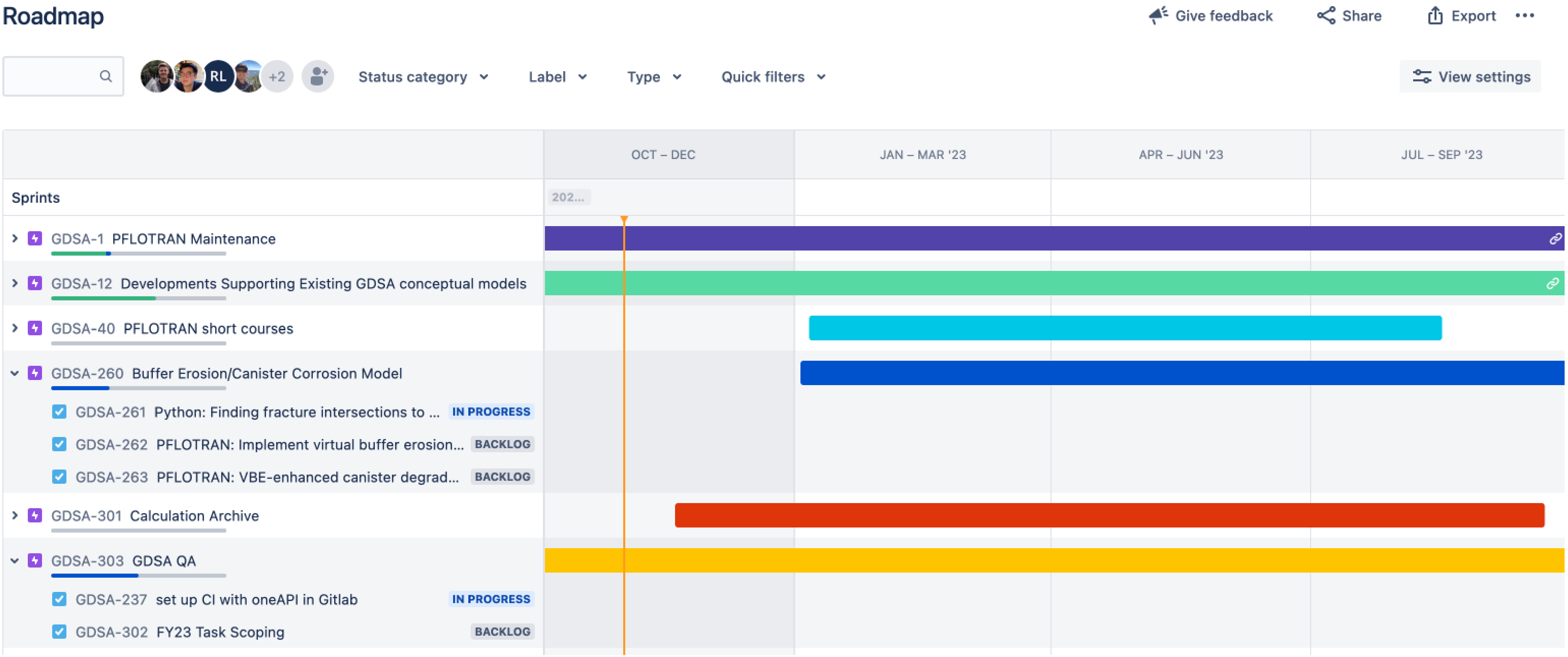
- Public code repository: https://bitbucket.org/pflotran/
  - Version control
  - Development philosophy and coding standards
  - Merge request requirements and mandatory checks
  - Major/minor/patch versioning
- Documentation: https://www.pflotran.org/documentation/
- Continuous integration
  - Regression testing
  - Unit testing
- Task Management
  - Jira
- QA Test Suite: https://www.pflotran.org/qa/
  - Modular design

Jira

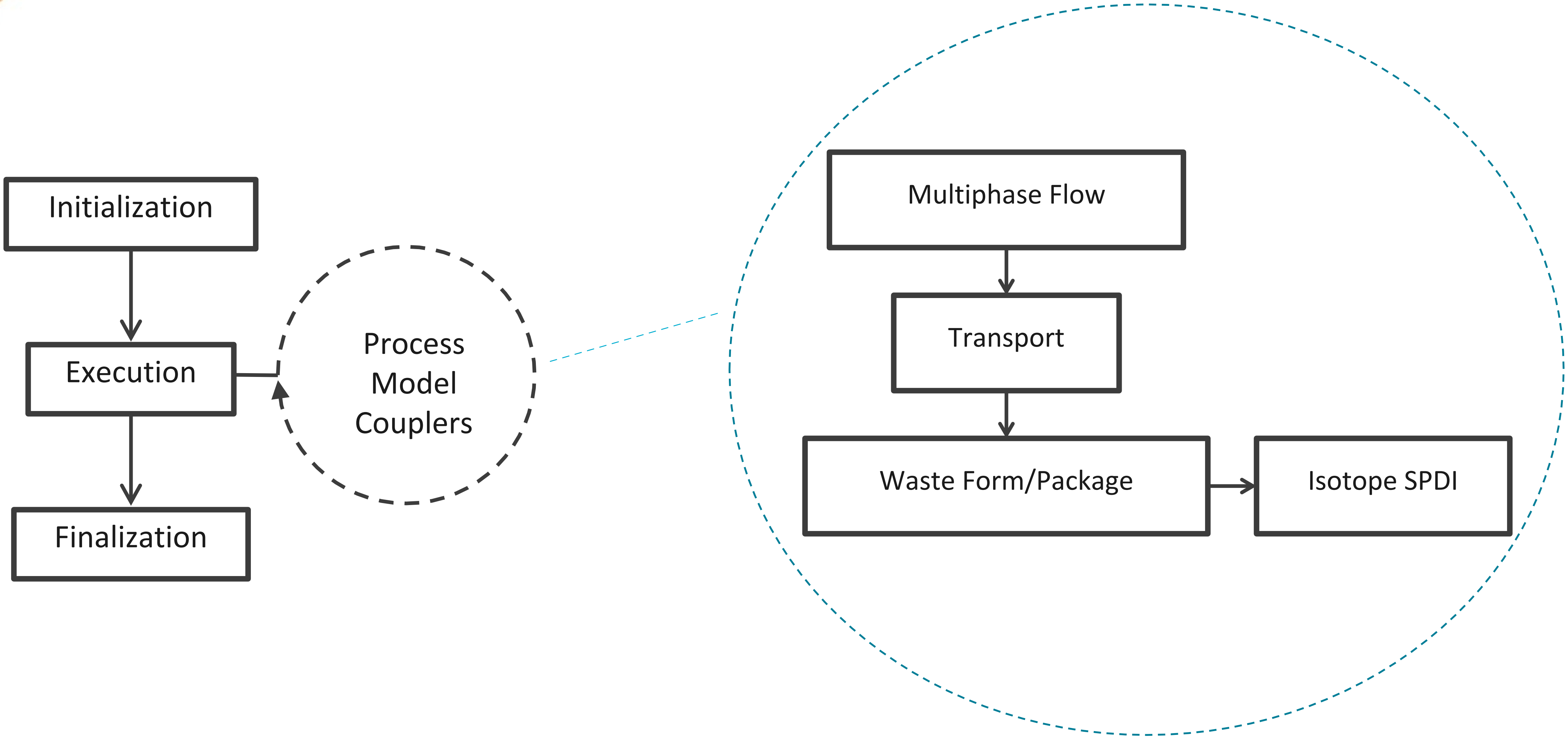
Bitbucket

Gitlab

Software Infrastructure: Jira



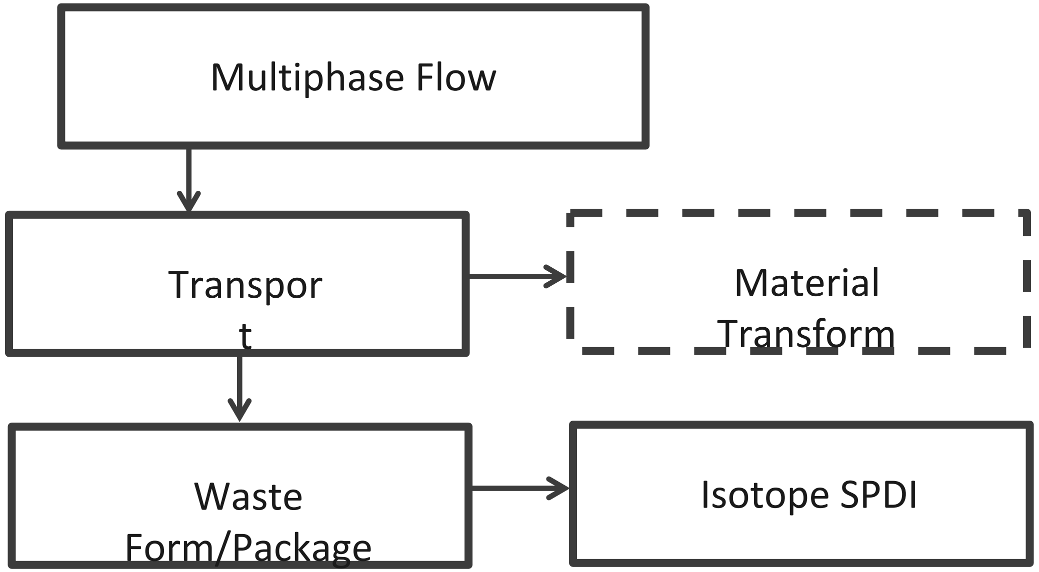
Process Modeling: Process Model Coupling

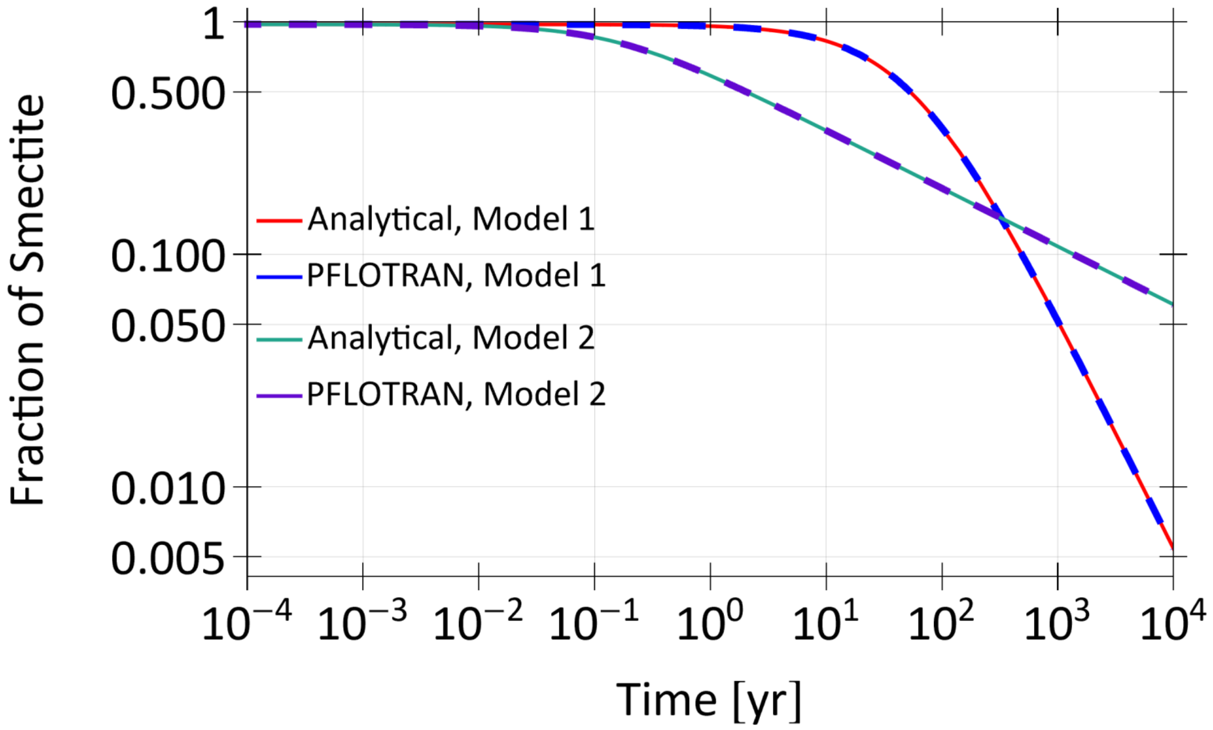


Process Modeling: Material Transformation

Material Transform Module

- Flexible implementation: can modify flow properties (e.g., permeability), transport properties (e.g., k_d), or both

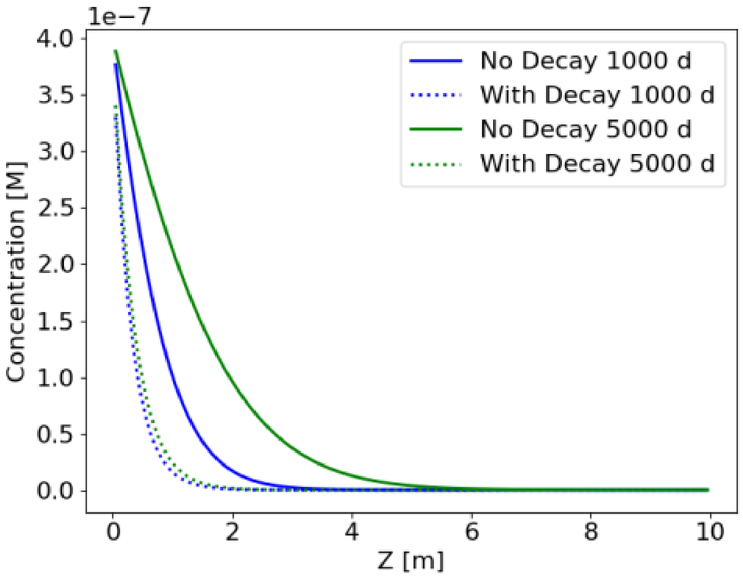




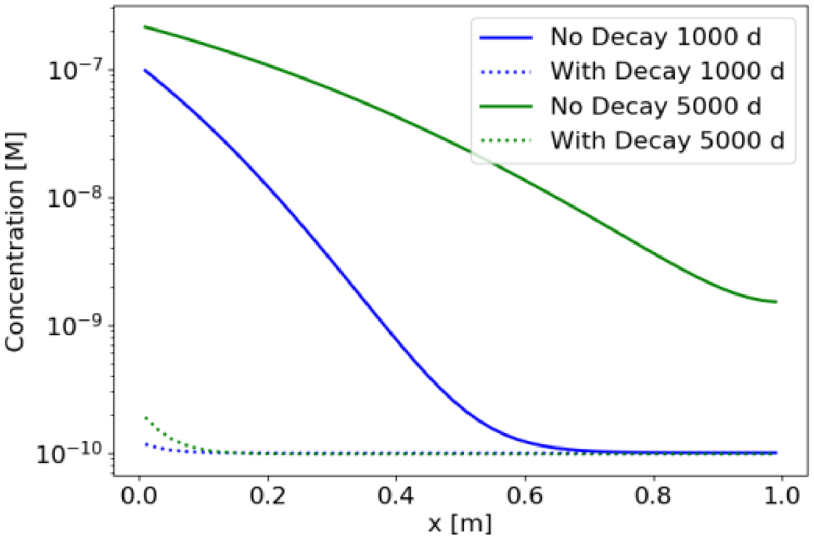
Process Modeling: Multiple Continuum Transport

MULTICONTINUUM transport mode now interfaces with the UFD Decay module

- This allows tracking radioactive decay and ingrowth in both the primary (fracture) and secondary (matrix) continua

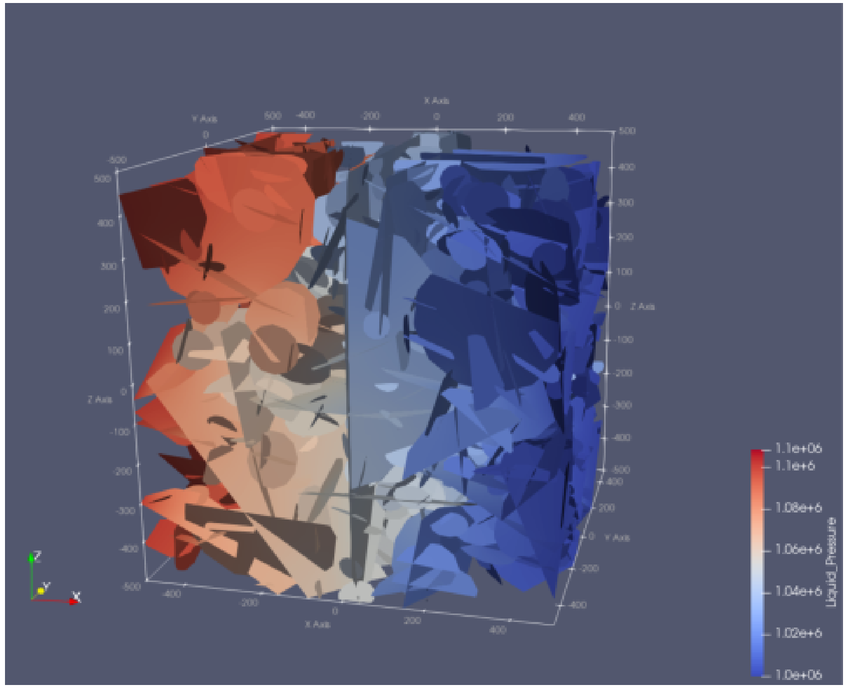


Concentration in Fracture



Concentration in Matrix

Nole et al., 2022



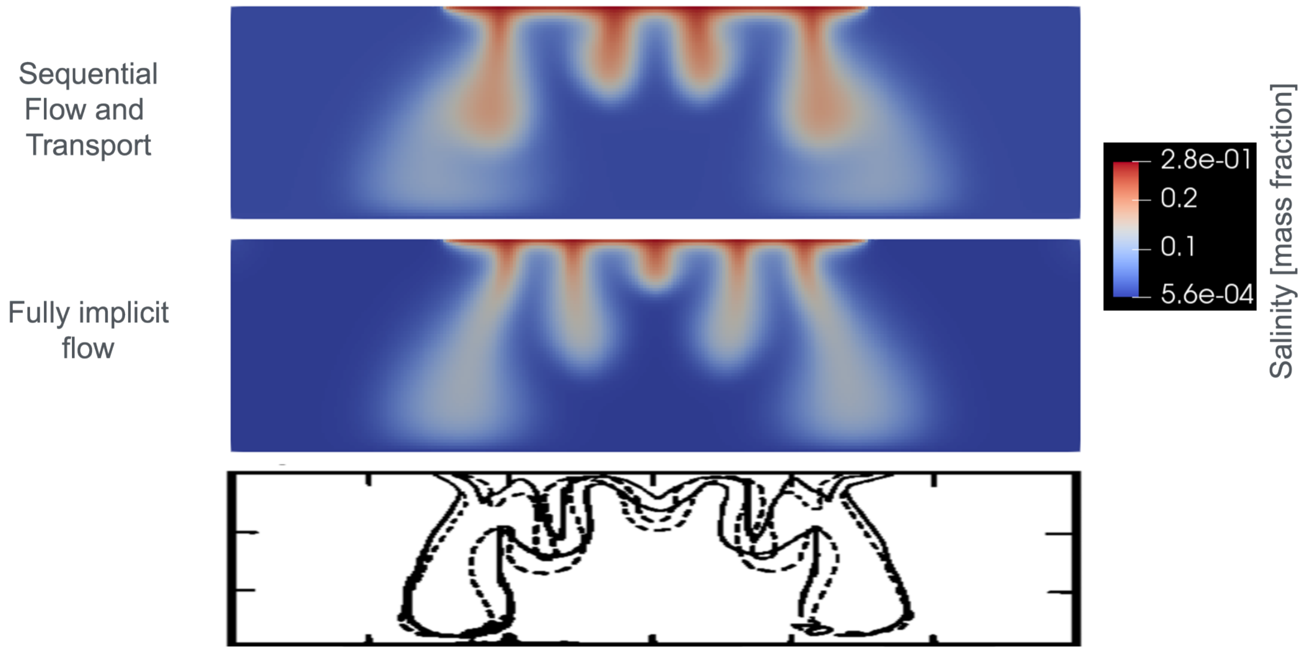
Test case of matrix diffusion in fractured crystalline rock for DECOVALEX Task F

Nole et al., 2021

Process Modeling: Fully-Coupled Solute Mass Balance

GENERAL mode optionally couples a mass balance for a solute

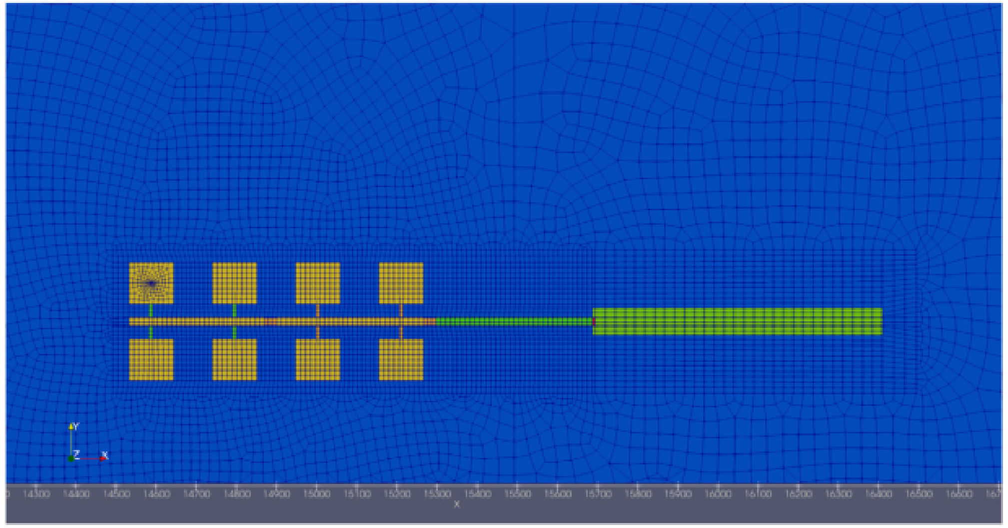
- This should be used when the solute (e.g., salt) appreciably affects flow properties (e.g., density)
- Primary variable switching in GENERAL mode allows for the option to allow for a soluble matrix
- A fully implicit coupling can allow for longer time stepping without inducing oscillation

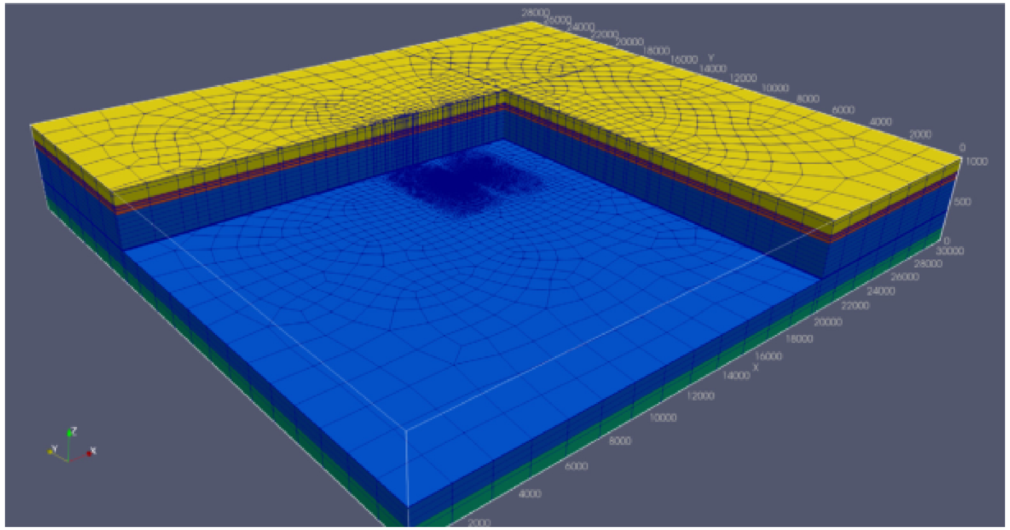


Software Performance

High performance and scalability are foundational to the design of PFLOTRAN

- GDSA runs simulations with massive contrasts in grid resolution, physical properties, and timescales of interest
- Large thermal perturbations and pressure gradients also contribute to a highly nonlinear system of equations
- Efficient numerical solution techniques are important for optimizing performance on these types of problems
- PFLOTRAN now includes options for capillary pressure curve smoothing at the unsaturated limit, and new linear and nonlinear solver options for multiphase flow



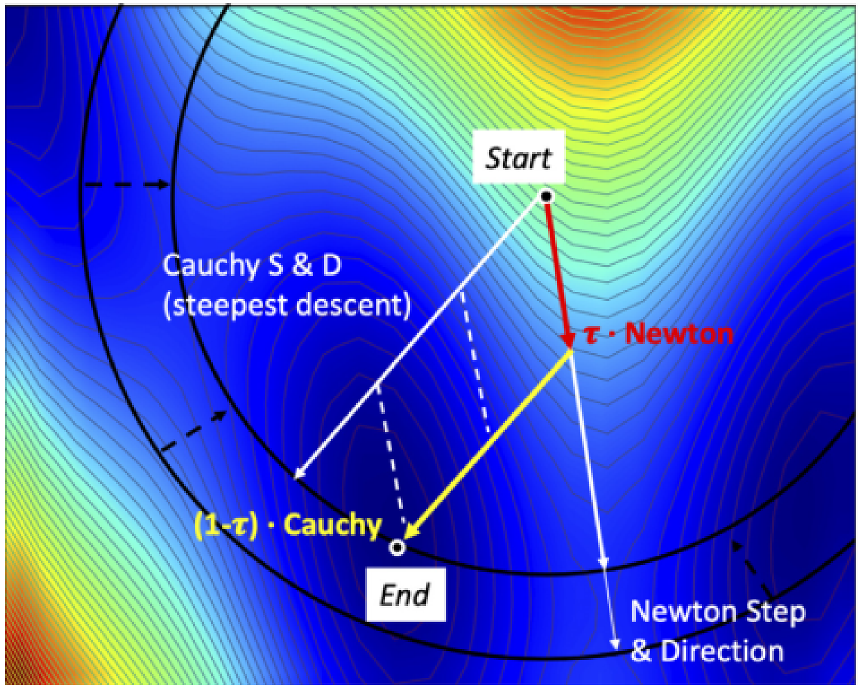


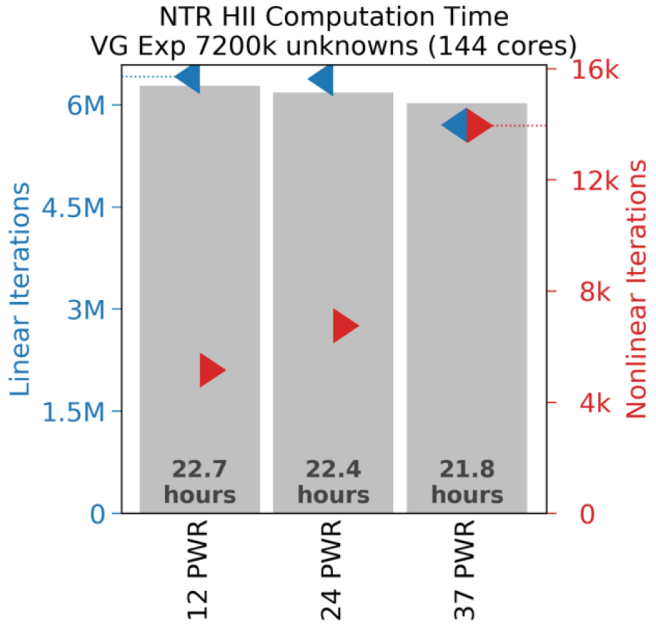
Park et al., 2021

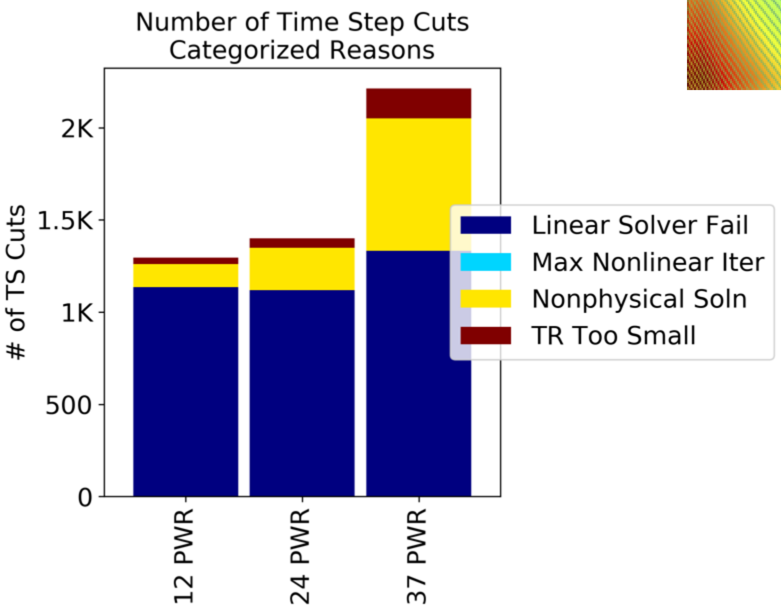
Software Performance: Nonlinear Solvers

New Trust Region-based Solver Options

- Newton-Trust Region-Dogleg-Cauchy (NTRDC)
- Demonstrated performance on large problems with strong nonlinearities, such as:
  - Significant thermal input
  - Competing forces driving phase changes like capillarity, evaporation, condensation, and boiling







Park et al., 2021

Conclusions

Recent software developments have significantly advanced the state of modeling capabilities available in PFLOTRAN to geologic radioactive waste disposal modelers. Developments presented here include:

- New Nonlinear Solvers
  - Great for highly nonlinear, multiphase problems especially when paired with characteristic curve smoothing options
- Material Transform module
  - Model transient 0D material transformations that can affect flow and/or transport properties, like k_d or permeability
- Multicontinuum Transport
  - Efficiently represent fracture-matrix interaction as a dual porosity system, and now with support for radionuclide SPDI
- Fully Implicit Solute
  - Fully couple in a solute (e.g., salt) mass balance for systems where presence of a solute affects flow properties like fluid density

References

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