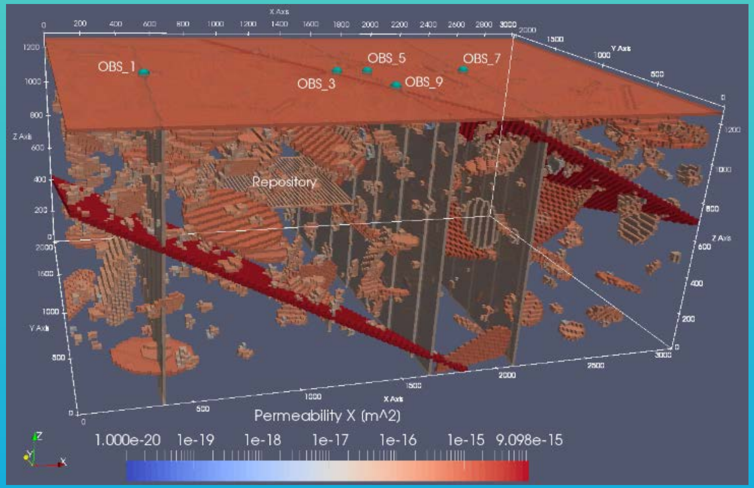
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.



PFLOTRAN Development

U.S. Nuclear Waste Technical Review Board

Fall Workshop

November 3-4, 2021

SAND2021-13690 PE

Michael Nole

Sandia National Laboratories

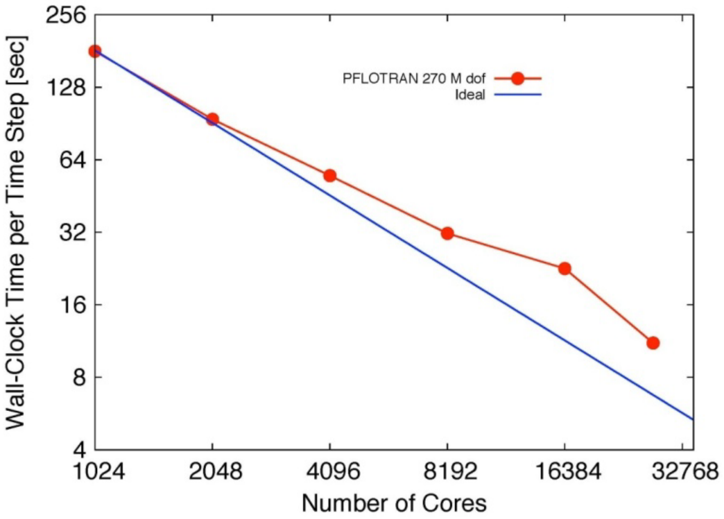
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

- **Introduction**: what is PFLOTRAN, and where is it used?
- **Open Source**: software development and computational framework
  - Version Control
  - Task Management
  - Verification Testing
- **Process Modeling**
  - Where PFLOTRAN fits into Geologic Disposal Safety Assessment (GDSA) Framework
  - Process model coupling
  - Advancements over the original code

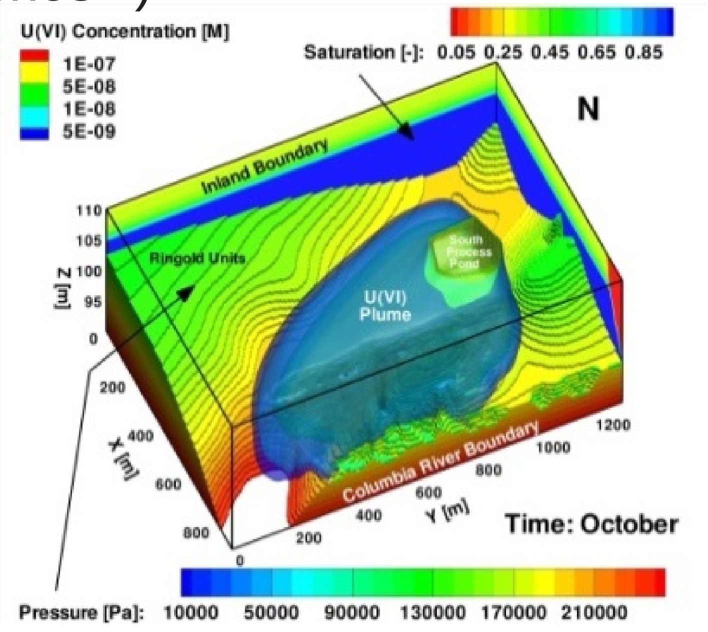
Introduction: What is PFLOTRAN?

- Scalable, finite volume reactive multiphase flow and transport code for simulating subsurface processes
- Open source license (GNU LGPL 2.0)
- 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
  - Scales well to over 10K cores



Introduction: Where is PFLOTRAN used?

- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM: **underwent rigorous Quality Assurance for qualification as an official WIPP PA flow code (July 2021)**
  - US DOE NE Spent Fuel and Waste Science and Technology (SFWST)
  - DEvelopment of COupled models and VALidation against EXperiments (DECOVALEX): international model comparison collaboration
  - Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos[21])
- Climate: coupled overland/groundwater flow
  - Next Generation Ecosystem Experiments Arctic
  - DOE Earth System Modeling Program
- Biogeochemical transport modeling
  - U transport at Hanford 300 Area
  - Hyporheic zone biogeochemical cycling
    - Columbia River, WA, USA
    - East River, CO, USA



Hammond and Lichtner, WRR, 2010

Open Source Framework

- Benefits
  - Collaboration: development, testing, and debugging
  - Transparency: exposes implementation details critical to scientific reproducibility, but excluded by journal publications
  - Lower barrier to entry (none if you have the expertise)
  - Code fitness must be maintained to survive

Open Source Framework

- 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

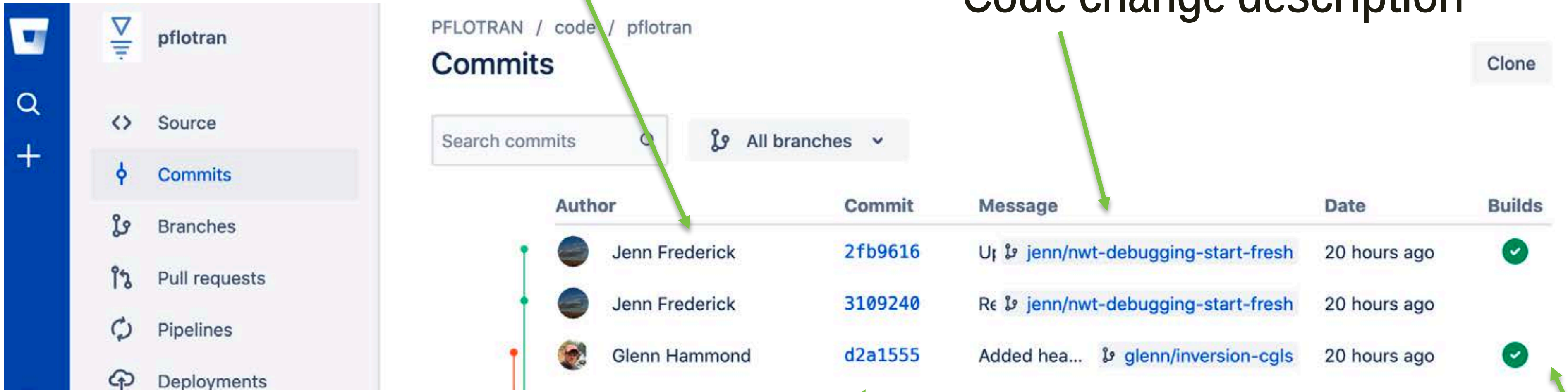
Open Source Framework

- Version Control

Bitbucket

Author

Code change description



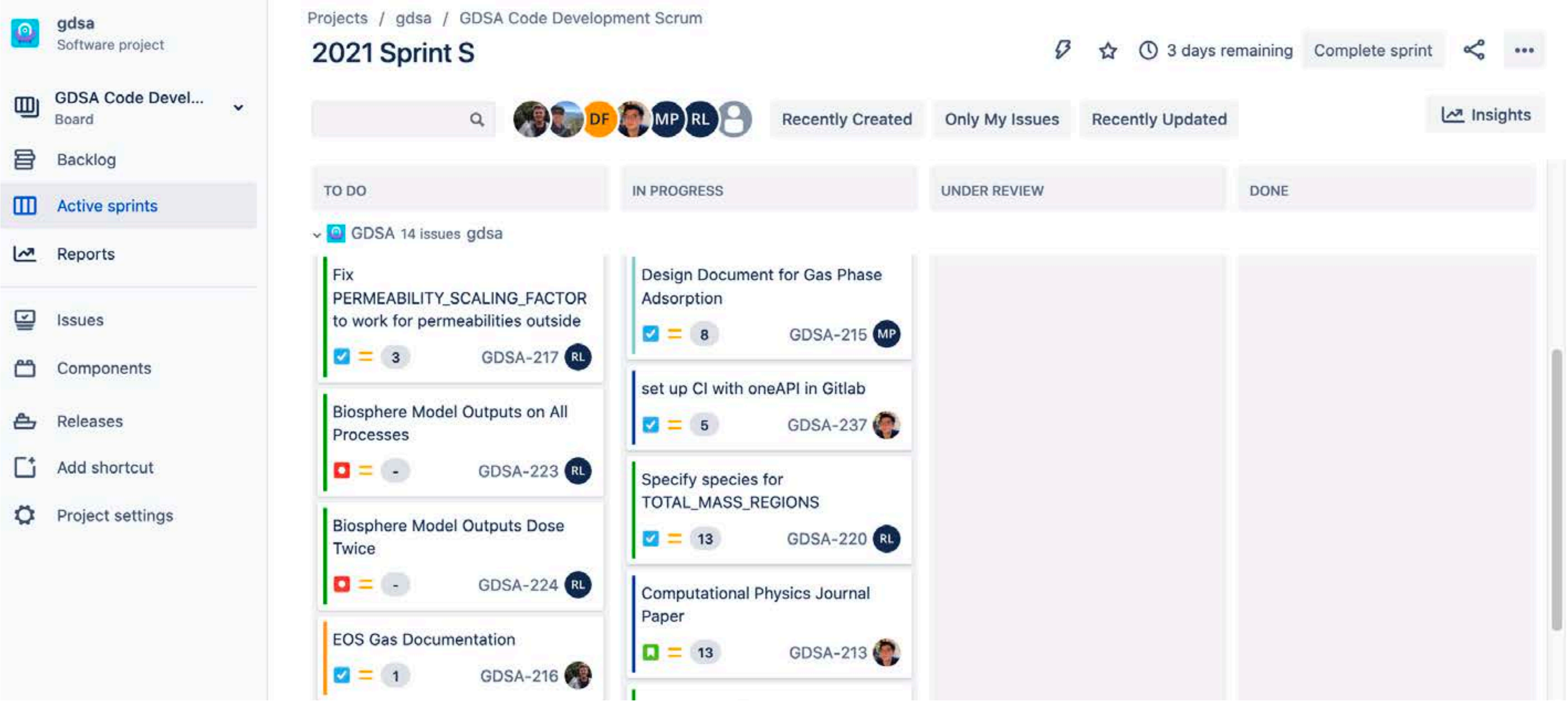
Unique code change identifier

Verification of successful unit/regression testing

Open Source Framework

Jira

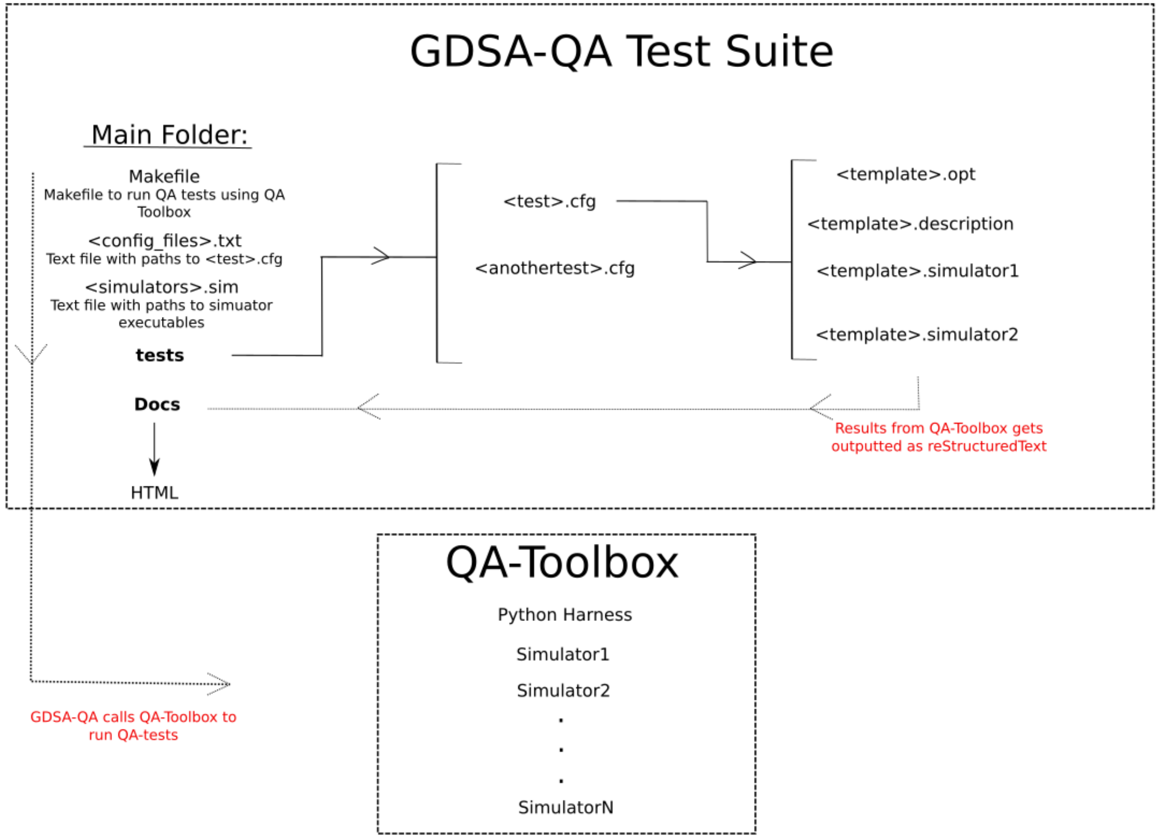
- Task Management
  - Developer assignment
  - Development stage
  - Prioritization
  - Issue type
  - Relative effort
  - Scope re-evaluated bi-weekly

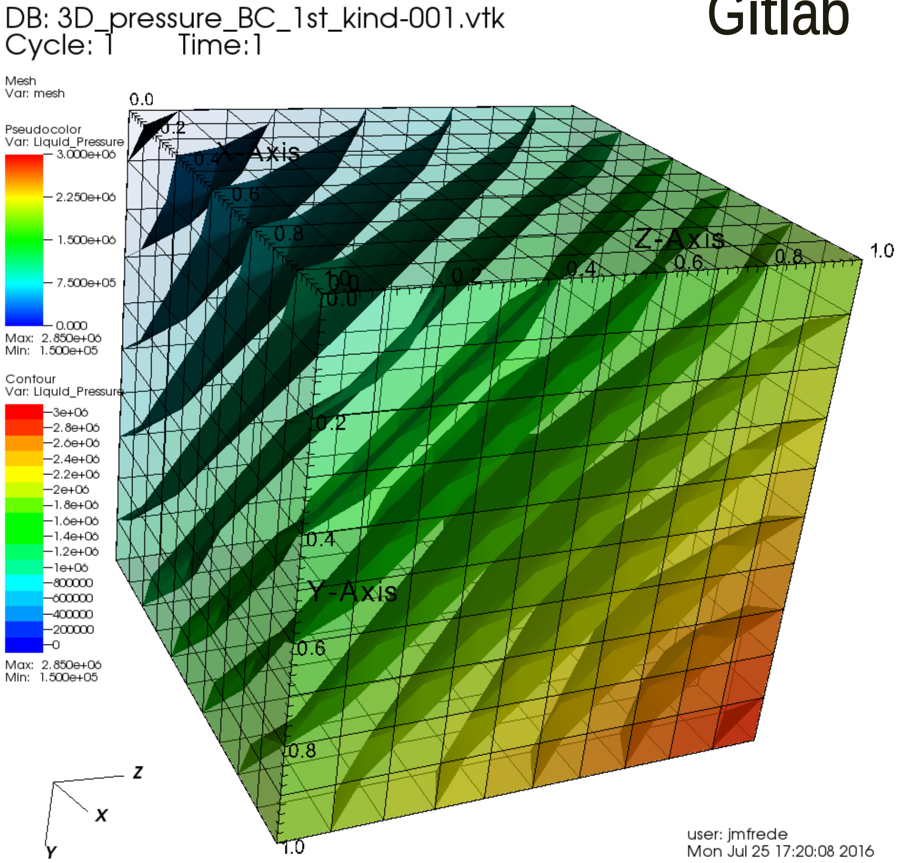


Open Source Framework

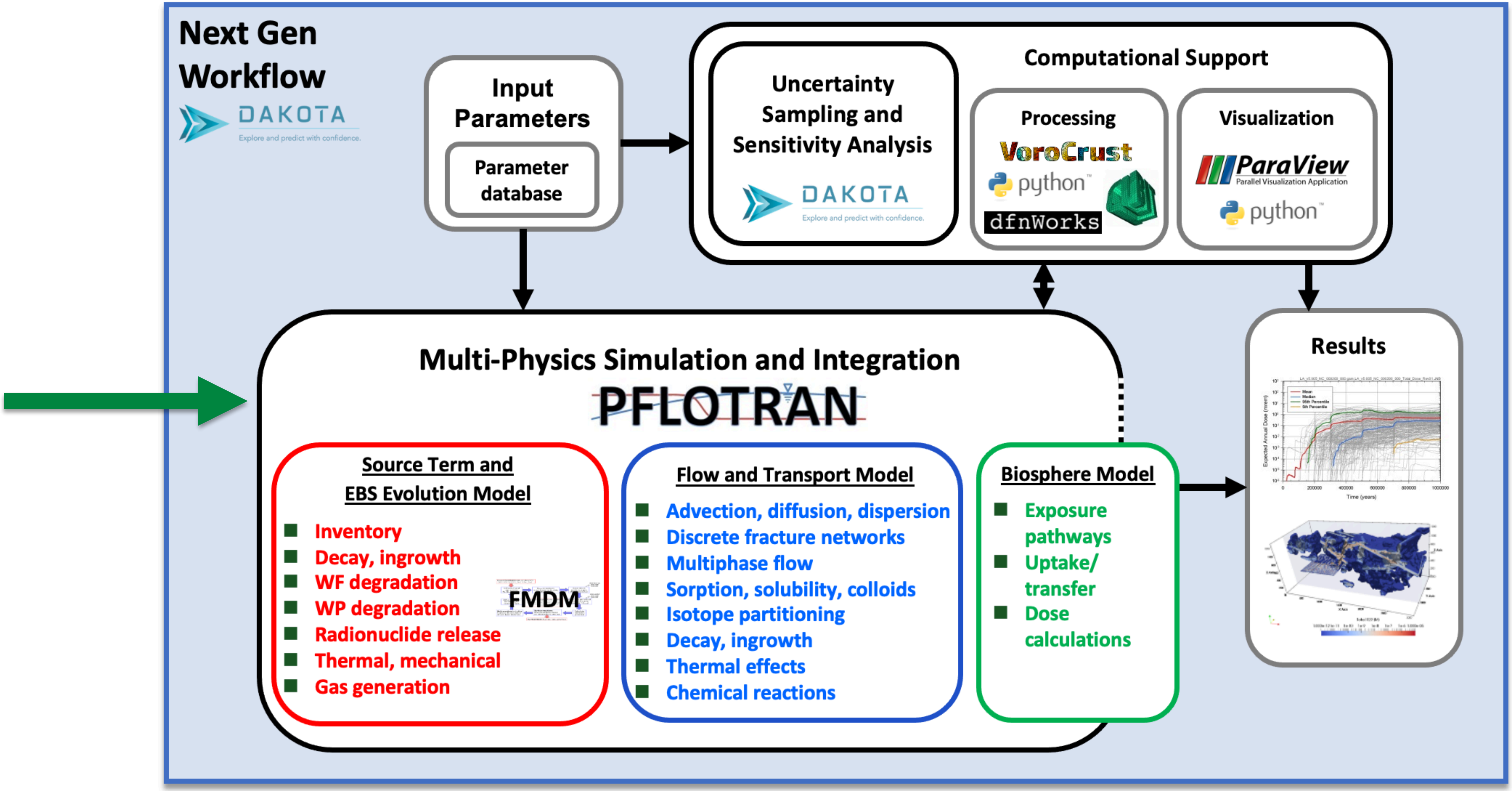
Gitlab

- Code Verification Testing: GDSA Quality Assurance (QA) Test Suite
  - Modular and extendable
  - Tests against analytical solutions and outputs from





Process Modeling: GDSA Framework



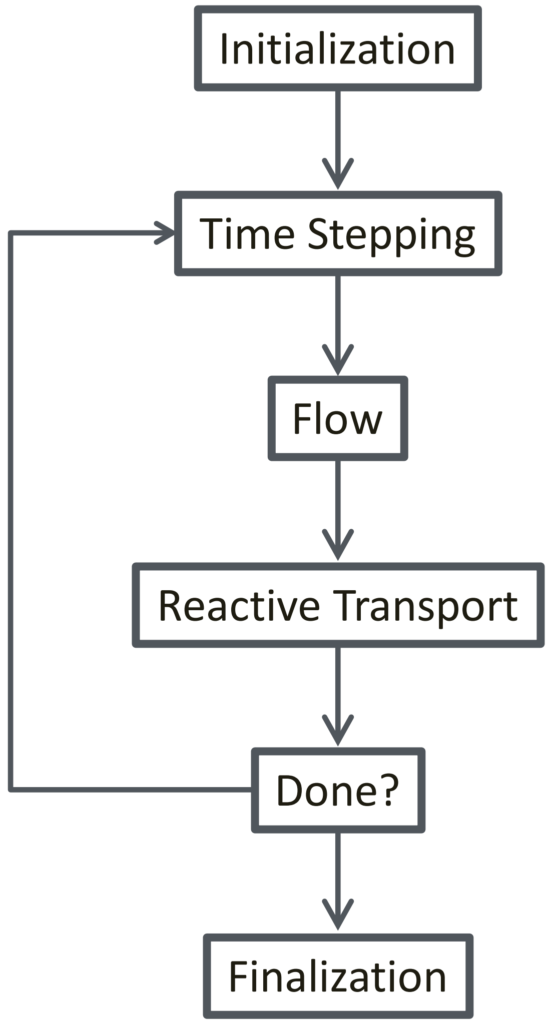
Process Modeling: GDSA Framework

- Fluid “flow” modes:
  - RICHARDS: conservation of water mass, variably saturated flow
  - TH: thermo-hydro; conservation of water mass and conservation of energy
  - GENERAL: conservation of water and air mass and conservation of energy; miscible multiphase flow

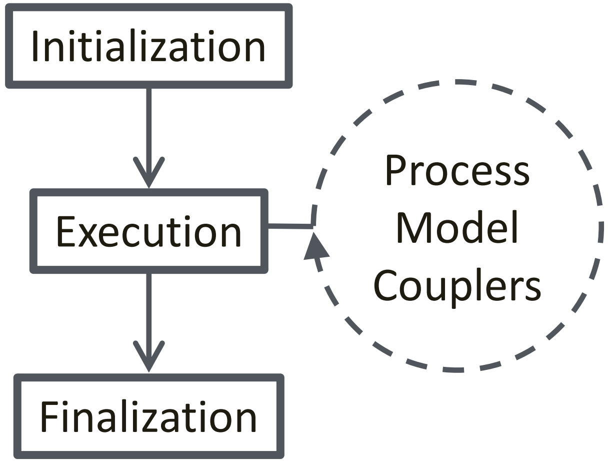
- Solute “transport” modes:
  - GIRT: global implicit reactive transport
  - UFD Decay: radionuclide sorption, partitioning, decay, and ingrowth
  - NWT: nuclear waste transport; different primary independent variables from GIRT or UFD Decay

Process Modeling: Process Model Coupling

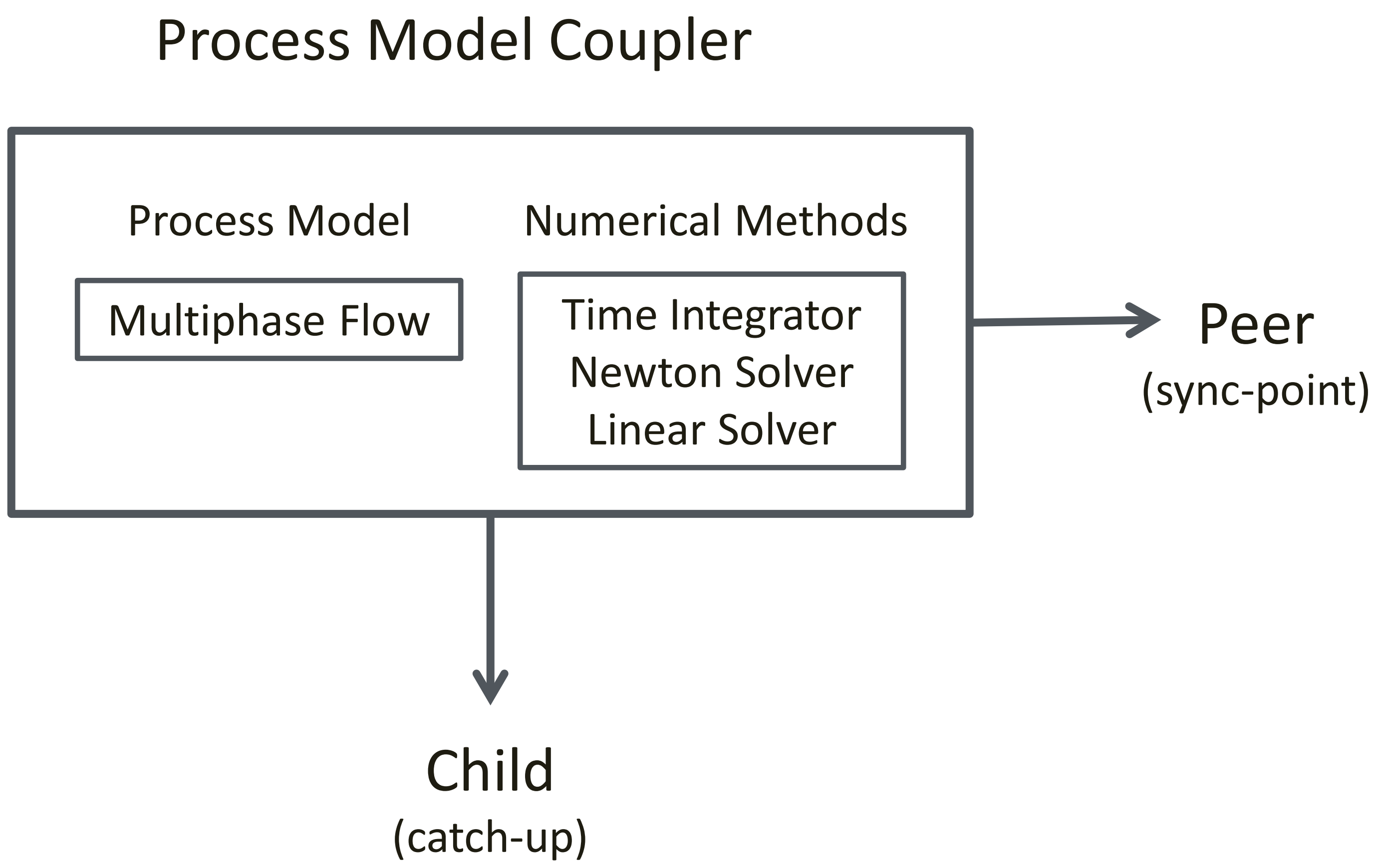
- Traditional Time-stepping Loop



- PFLOTRAN Workflow

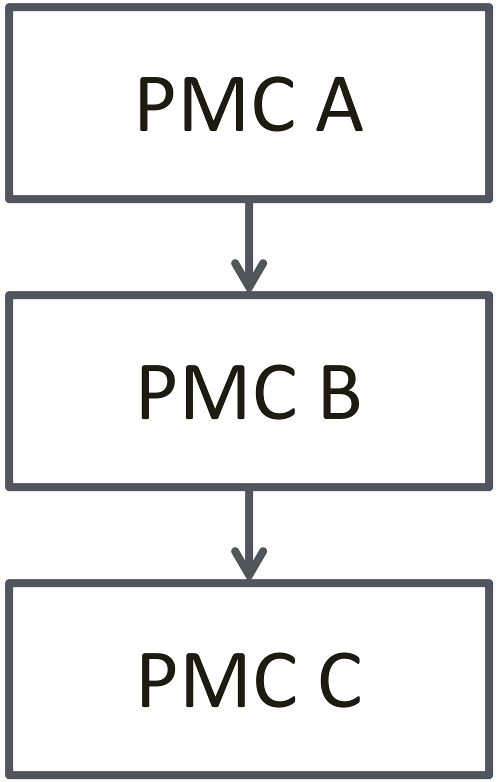


Process Modeling: Process Model Coupling



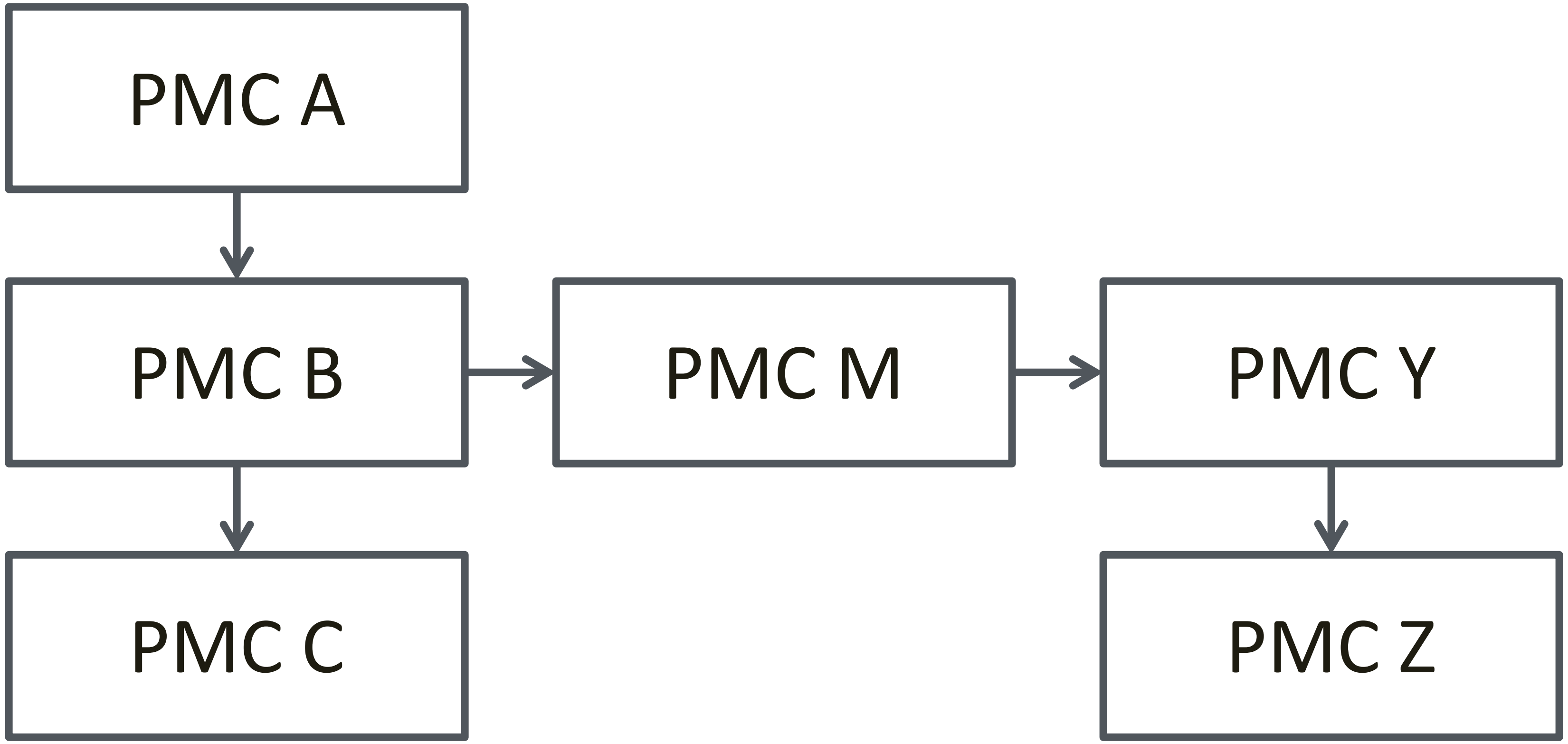
Process Modeling: Process Model Coupling

PMC = Process Model Coupler

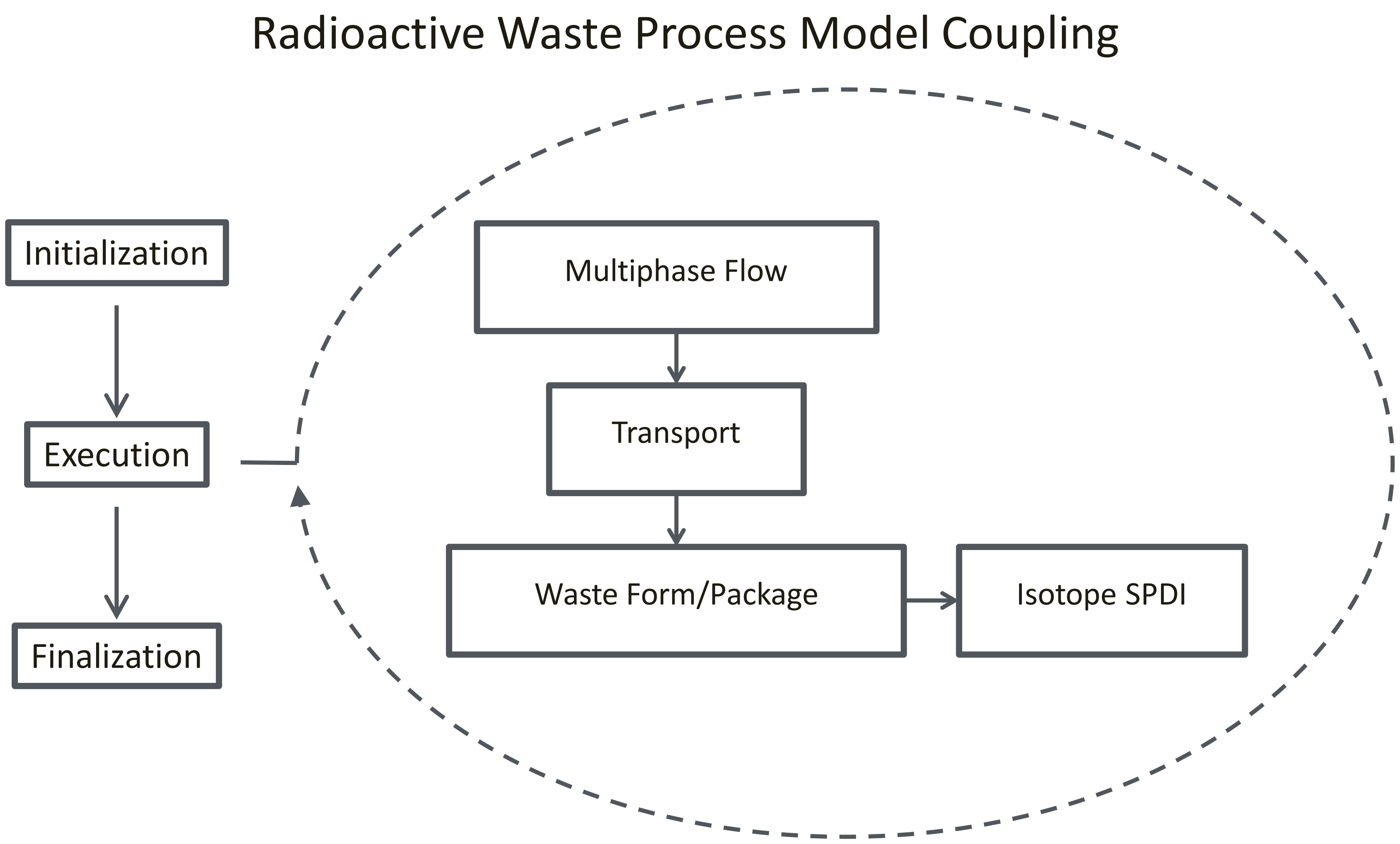


Process Modeling: Process Model Coupling

PMC = Process Model Coupler



Process Modeling: Process Model Coupling

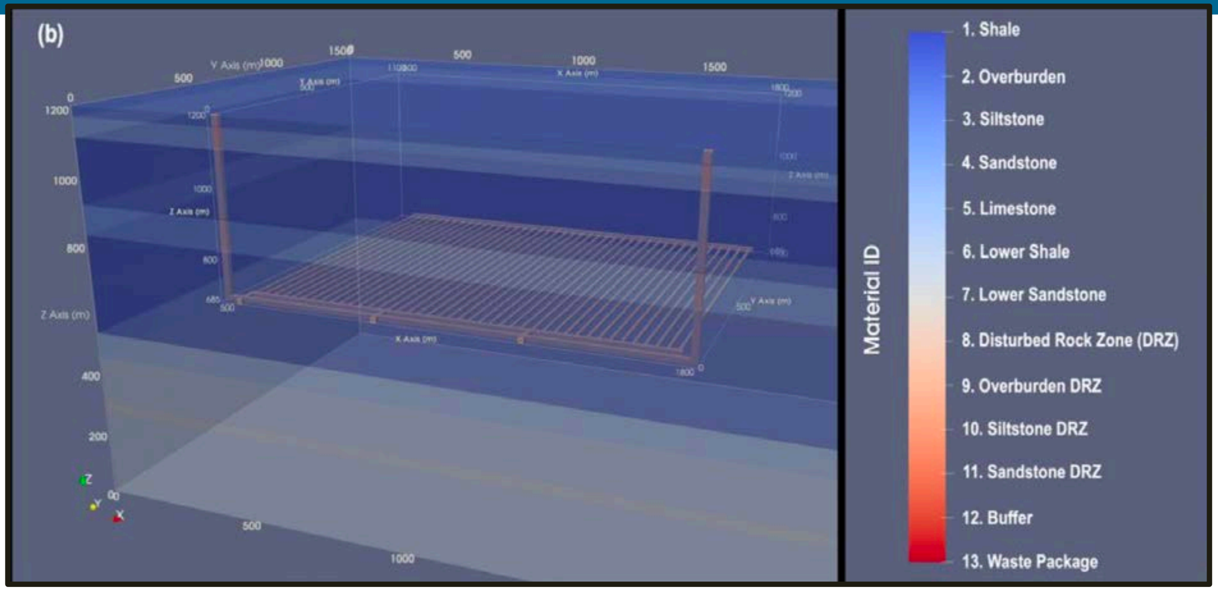


Process Modeling: Process Model Coupling

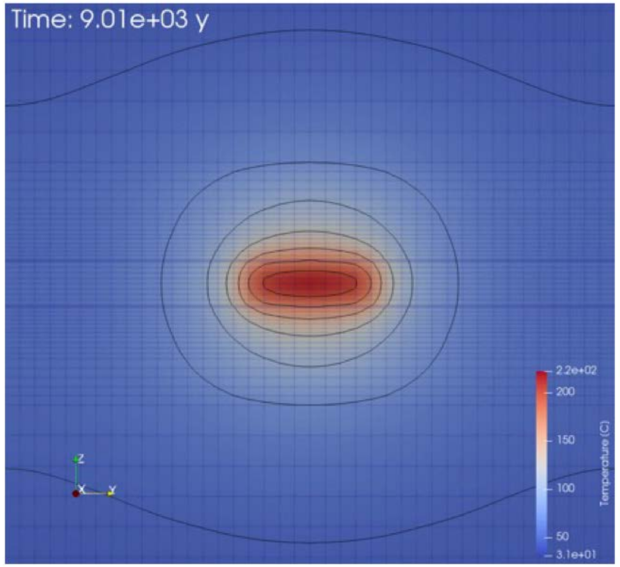
- Benefits
  - Customizable linkage between process models, e.g.
    - Flow
    - Transport
    - Reaction
    - Updates to material properties at select times
  - Flexible time stepping
    - Individual processes may run at their own time scale.
  - Modularity for incorporating new process models
    - Time stepping loops for existing process models are not impacted.

Process Modeling Advancements

- Multiphase fluid and heat flow
- Radioactive sorption/partitioning/decay/ingrowth model (UFD Decay)
- Soil matrix compressibility
- Flexible models for thermal conductivity and anisotropy
- Improved multiphase capabilities during dry-out



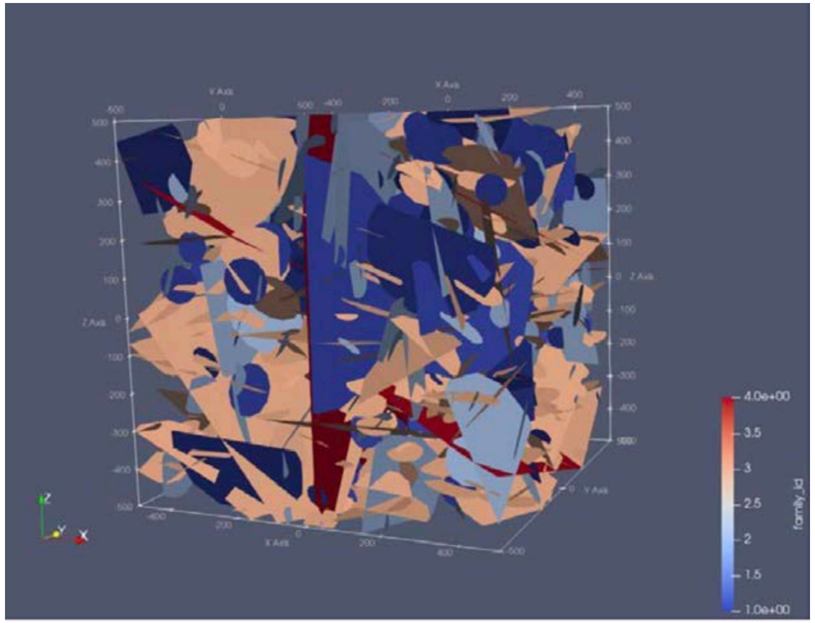
Price et al., 2021



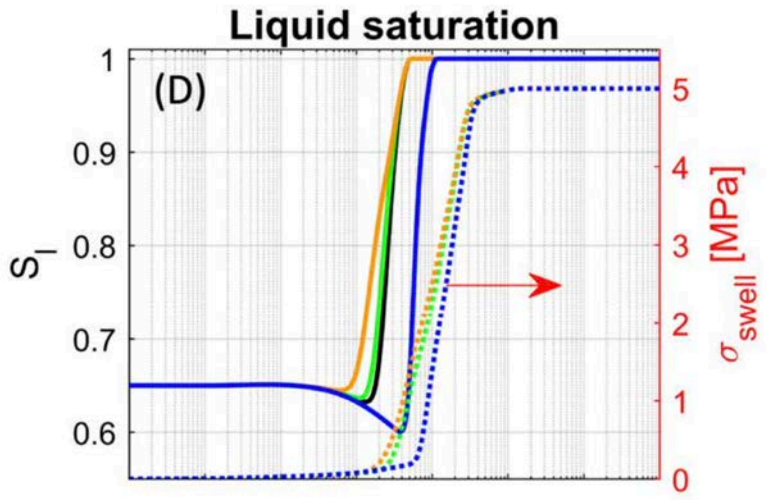
Nole et al., 2021

Process Modeling Advancements

- Sorption isotherm generalization
- Fuel Matrix Degradation Model (FMDM)
- Biosphere well model
- Multi-continuum transport
- Advanced linear and nonlinear solvers
- High temperature equations of state
- Reduced order geomechanics models



LaForce et al., 2021



Chang et al., 2021

References

- Chang, K. W., Nole, M., & Stein, E. R. (2021). Reduced-order modeling of near-field THMC coupled processes for nuclear waste repositories in shale. Computers and Geotechnics, 138, 104326.
- LaForce, T. et al. (2021). *GDSA Repository Systems Analysis Investigations in FY2021*. Sandia National Laboratories. Albuquerque, NM, USA. M2SF-20SN010304062.
- Nole, M. et al. (2021). *PFLOTRAN Development FY2021*. Sandia National Laboratories. Albuquerque, NM, USA. M3SF-21SN010304072.
- Price, L. et al. (2021). *Repository-scale performance assessment incorporating postclosure criticality*. Sandia National Laboratories. Albuquerque, NM, USA. M2SF-21SN010305061.