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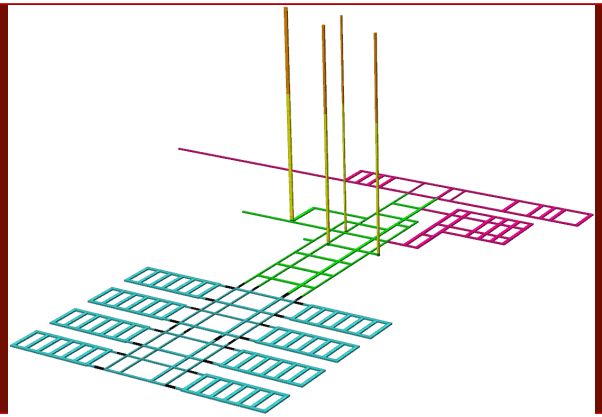
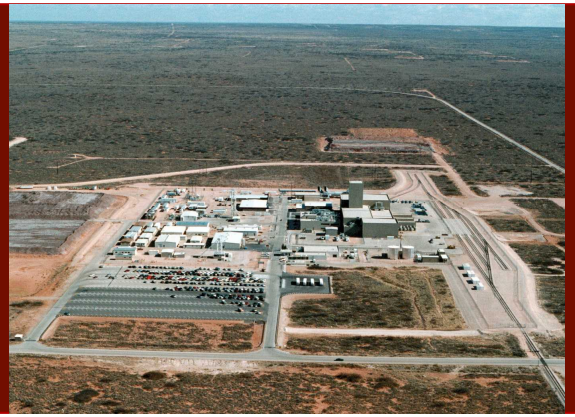
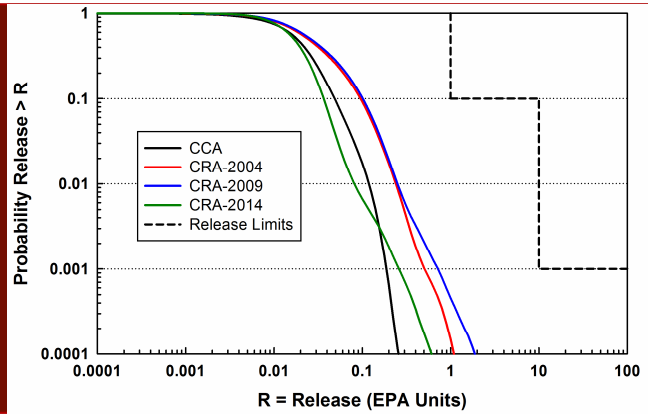




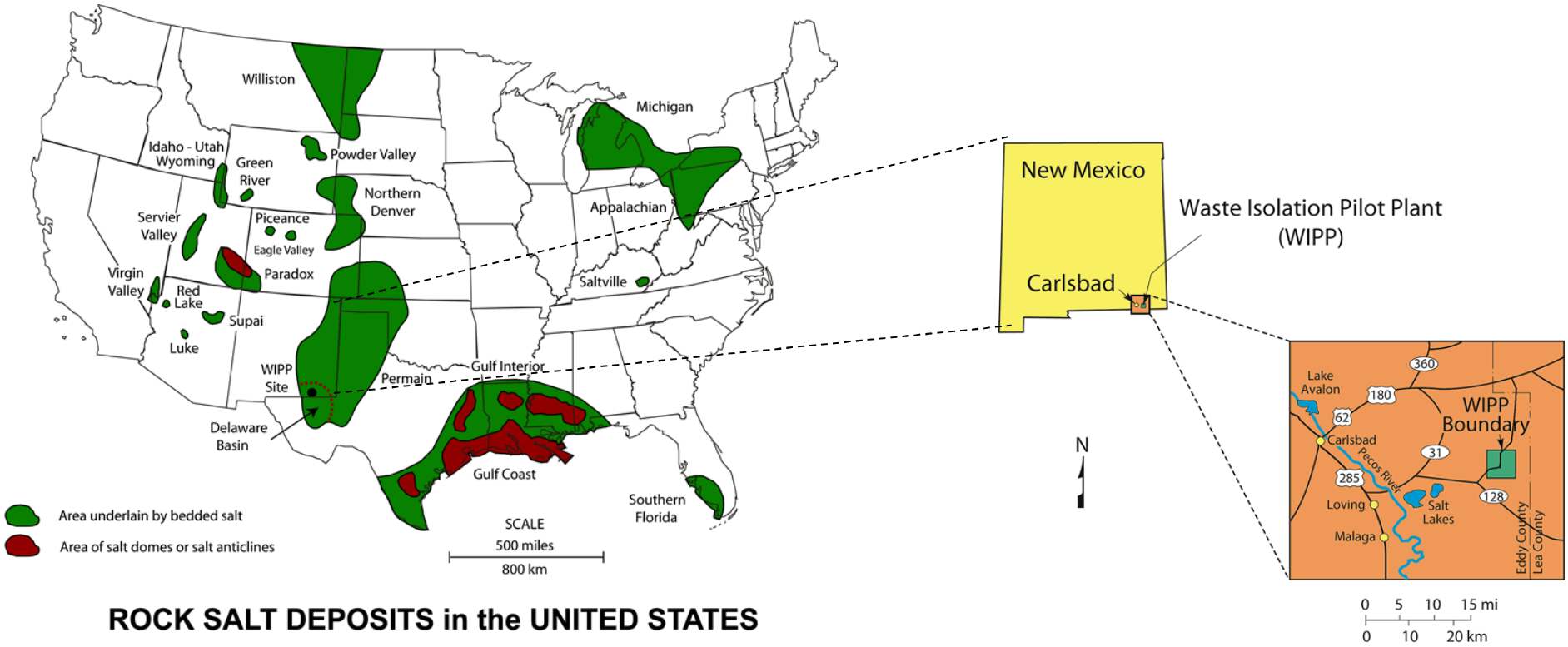


PFLOTRAN Code Development for Waste Isolation Pilot Plant Performance Assessment

Glenn Hammond, Todd R. Zeitler

2017 P&RA CoP Annual Technical Exchange Meeting
Albuquerque, NM October 18-19, 2017

Waste Isolation Pilot Plant Location



ROCK SALT DEPOSITS in the UNITED STATES

About The WIPP

Sandia National Laboratories

The WIPP is a permanent disposal facility for transuranic waste

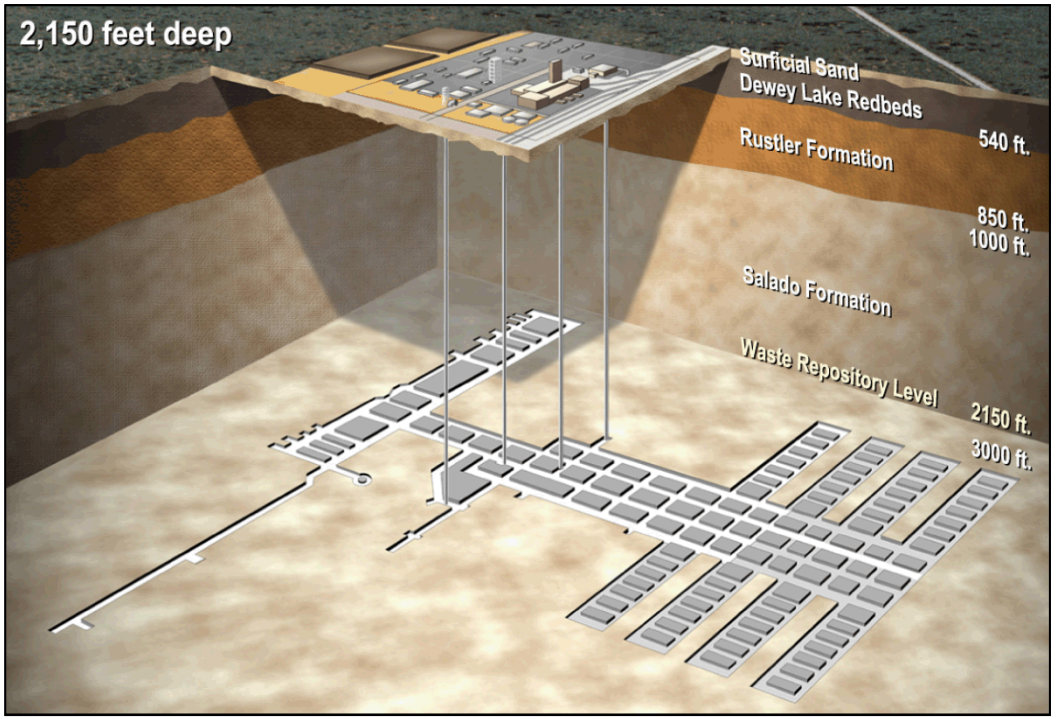
- The nation's only licensed deep geologic repository for nuclear waste

- Operated by U.S. Department of Energy (DOE)

- Long-term performance regulated by U.S. Environmental Protection Agency (EPA)

- Waste is emplaced in a **salt formation** deep underground

- Long-term regulatory compliance is demonstrated via Performance Assessment (PA) undertaken by SNL Carlsbad

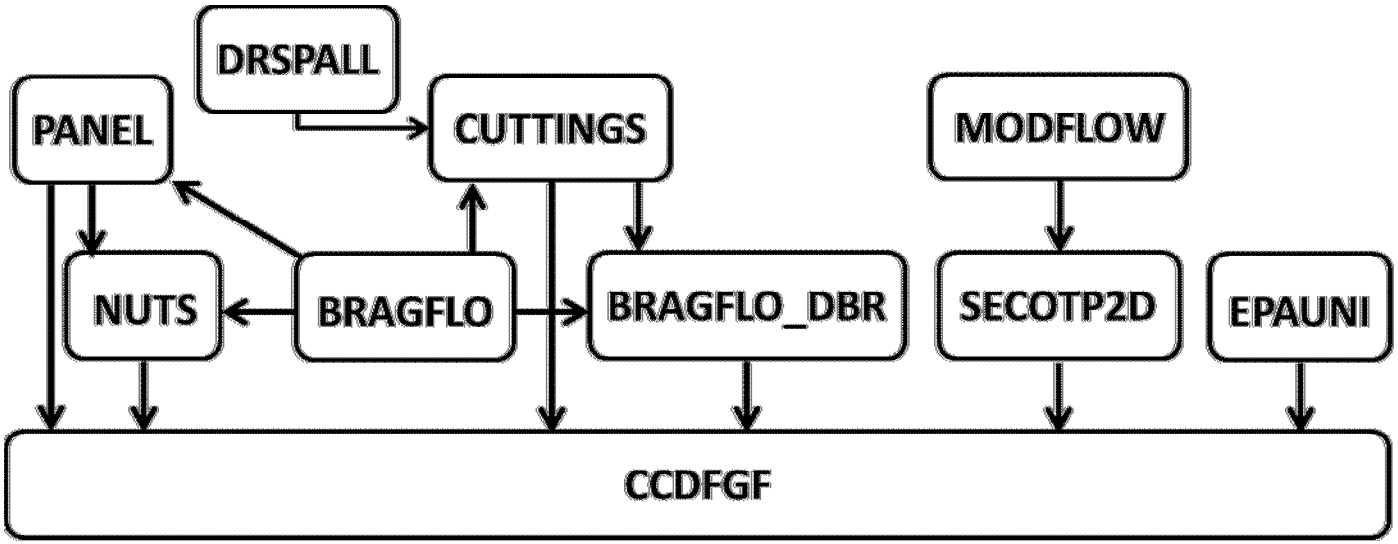


Outline

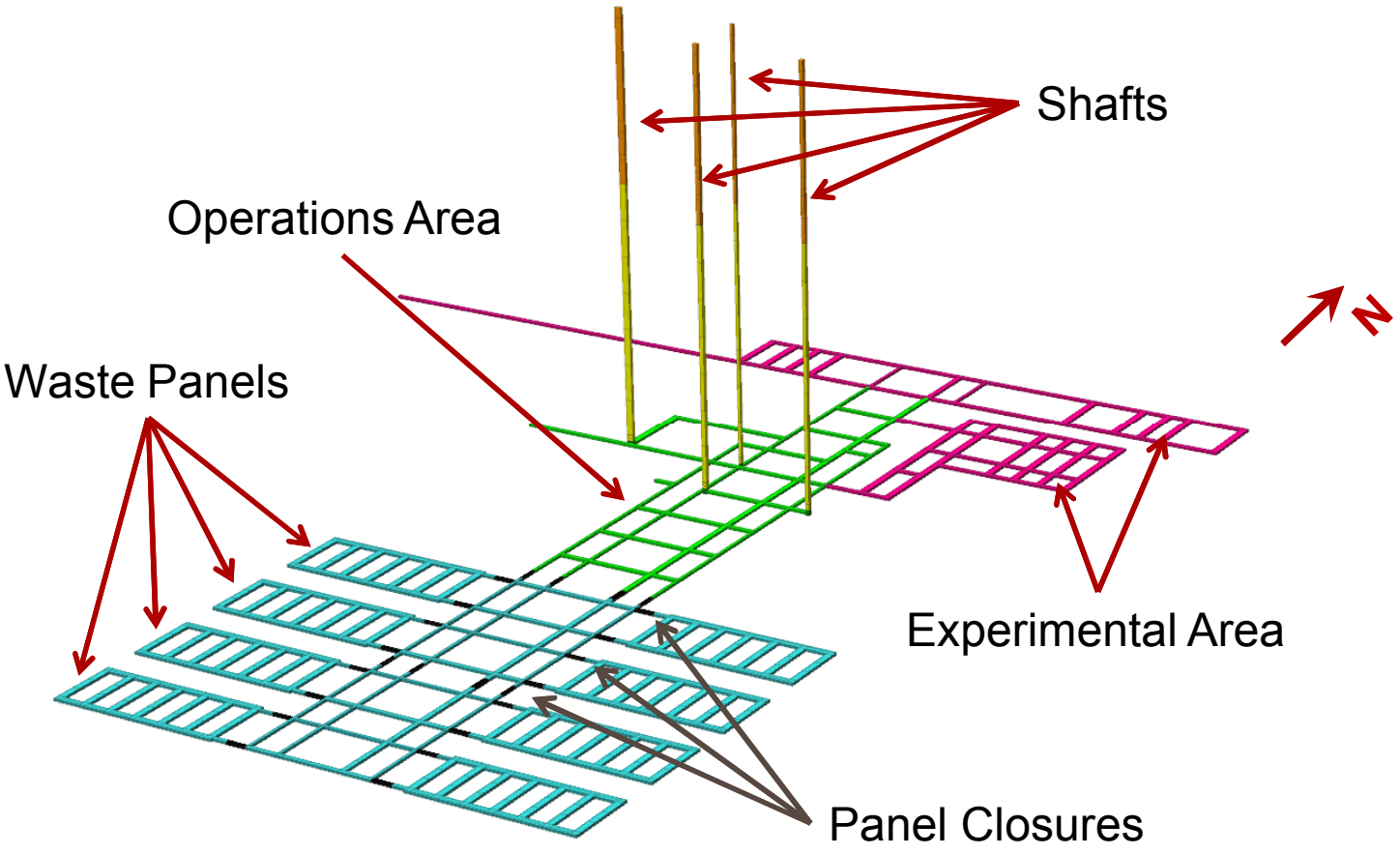
- Current Representation of WIPP Repository in WIPP PA
  - Challenges of potential layout changes
- PFLOTRAN Development for WIPP PA
  - Long-term integration plan
  - Process model workflow
  - Code testing
- Summary

WIPP Performance Assessment

- PA calculations cover 24 peer-reviewed conceptual models
- PA codes include 10 principal codes and many utility codes



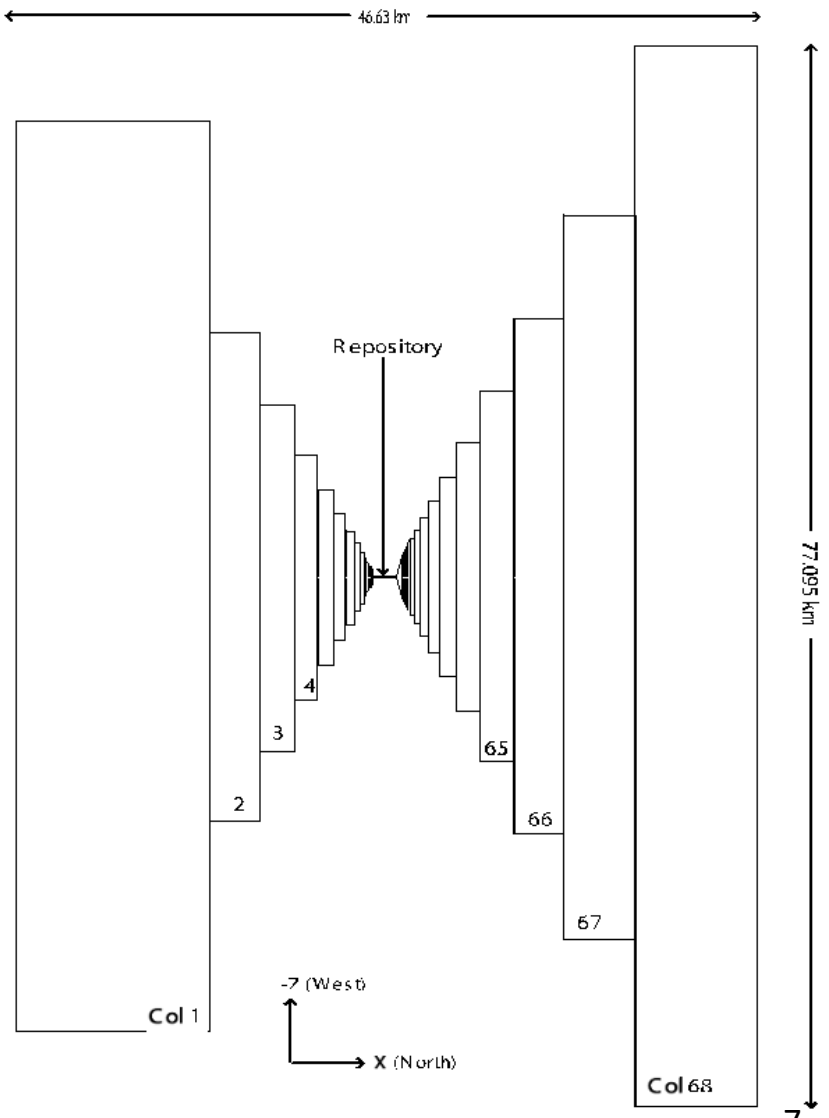
WIPP Repository Layout



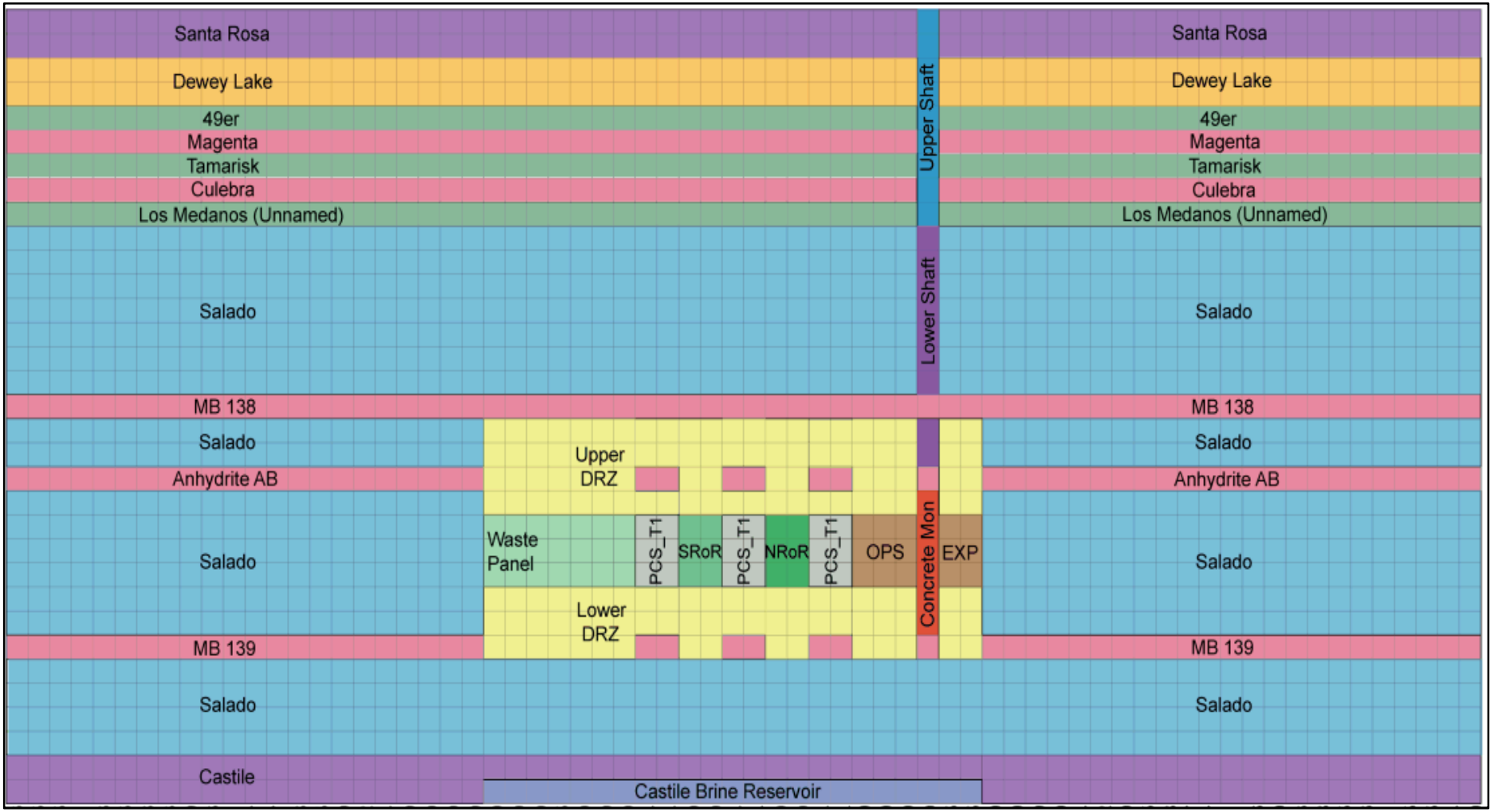
2D Representation of Repository

Current 2-D "Flared" Grid (plan view)

- One cell in thickness
- Thickness of each cell varies
- Approved for use in Compliance Certification Application (CCA)
- Shown to give similar results to a 3-D representation using BRAGFLO
- Radial concentric flow
  - No lateral flow
- Relies on (approximately) symmetric repository layout



2D Representation of Repository



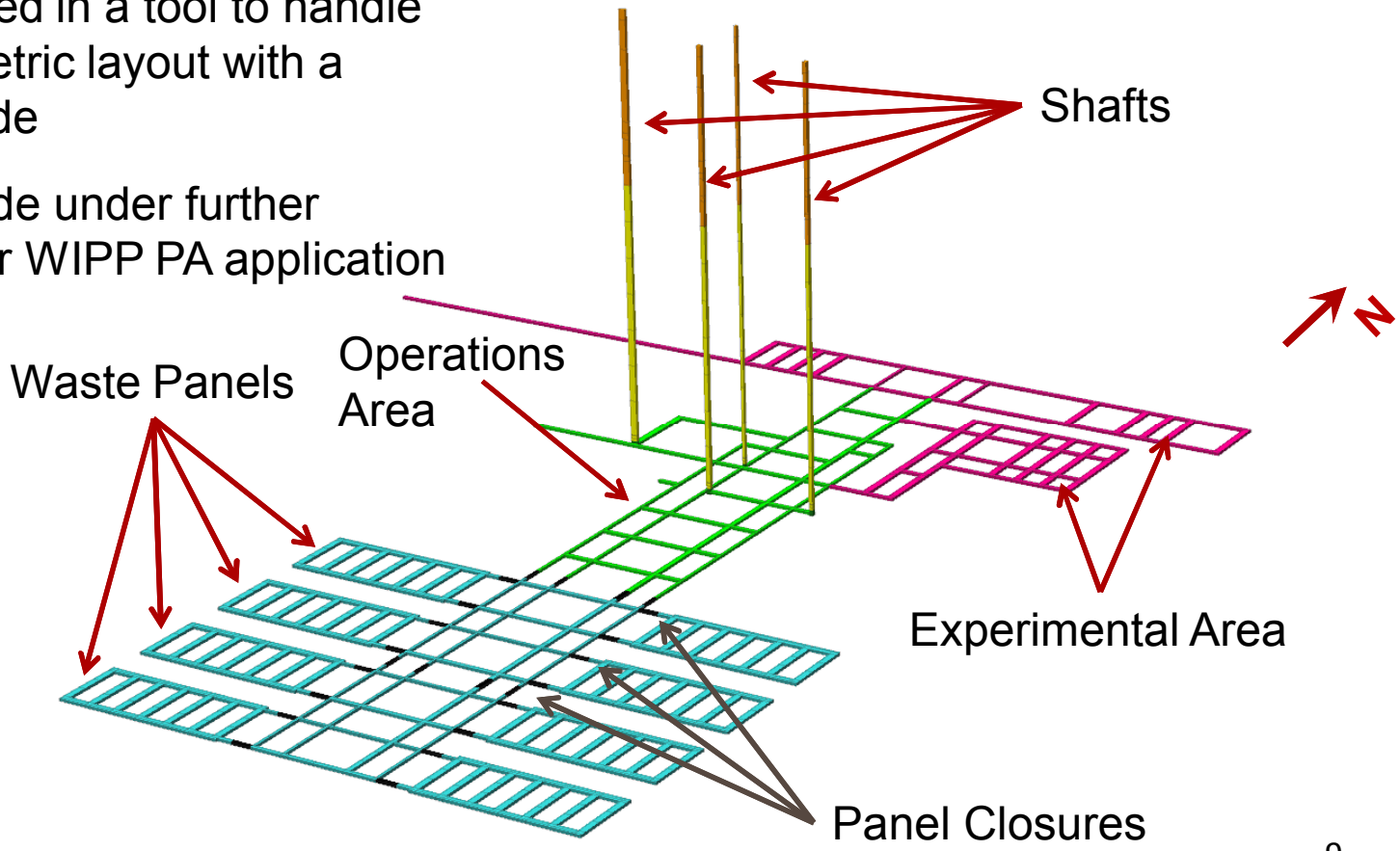
Current 2-D Grid
(cross-sectional view)

- Used by BRAGFLO
- Two-phase flow (brine and gas)

N

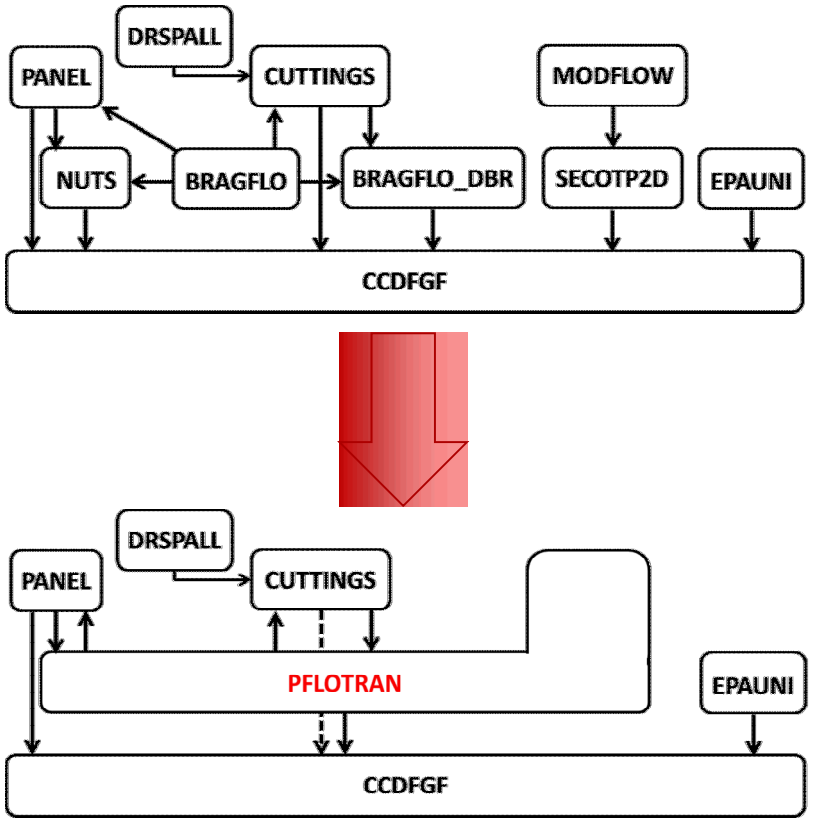
Potential for Asymmetric Layout

- Potential for additional waste panels challenges the radial concentric flow assumption
- DOE is interested in a tool to handle a more asymmetric layout with a modern 3-D code
- PFLOTRAN code under further development for WIPP PA application



Long-term Approach to Integration

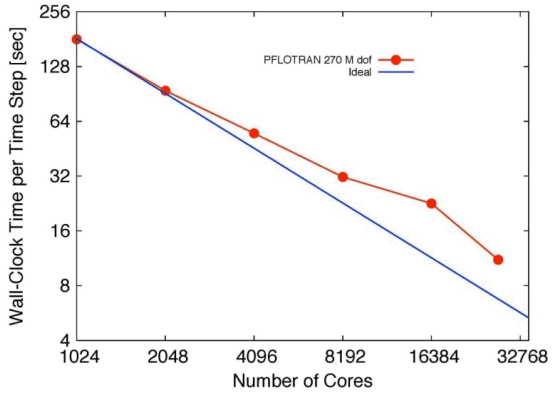
- Implementation of WIPP-specific process models
  - Gas generation, creep closure, etc.
- Comparison of PFLOTRAN against BRAGFLO/NUTS for 2-D flared grid
  - Validates flow and transport
- Comparison of PFLOTRAN w/3-D representation against 2-D flared grid
  - Quantifies impact of 2-D→3-D
- Development of 3-D grid
  - Resolution
  - Run-time
- Formal reviews
  - EPA review
  - Peer review
- Use in Compliance Recertification 2024 PA (CRA-2024 PA) (and beyond…)



PFLOTRAN

Sandia National Laboratories

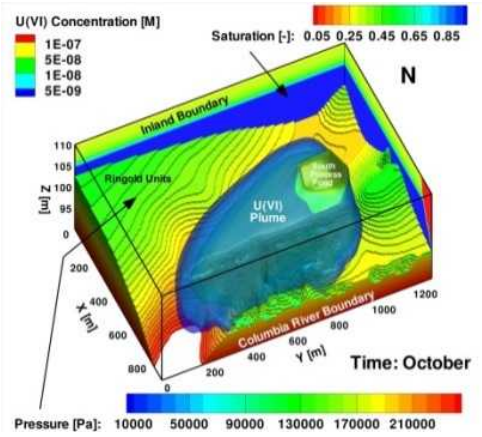
- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)



- Founded upon well-known (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

Application of PFLOTRAN

- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - DOE Used Fuel Disposition Program
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos^{21})
- 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 Area
  - Hyporheic zone biogeochemical cycling
    - Columbia River, WA, USA
    - East River, CO, USA
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers
- Colloid-facilitated transport

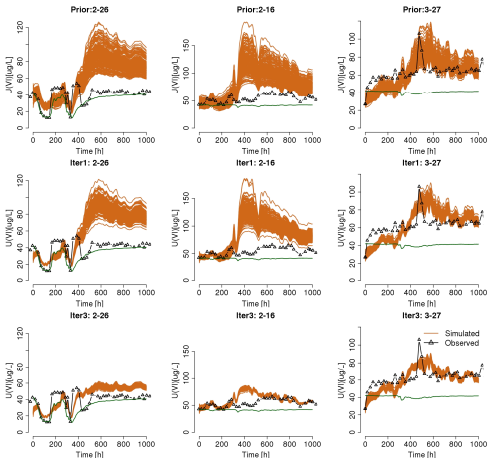


Hammond and Lichtner, WRR, 2010

PFLOTRAN Computing Capability

- High-Performance Computing (HPC)
  - Increasingly mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- Open Source Collaboration
  - Leverages a diverse scientific community
  - Sharing among subject matter experts and stakeholders from labs/universities
- Modern Fortran (2003/2008)
  - Domain scientists remain engaged
  - Modular framework for customization
- Leverages Existing Capabilities
  - Meshing, visualization, HPC solvers, etc.
  - Configuration management, testing, and QA

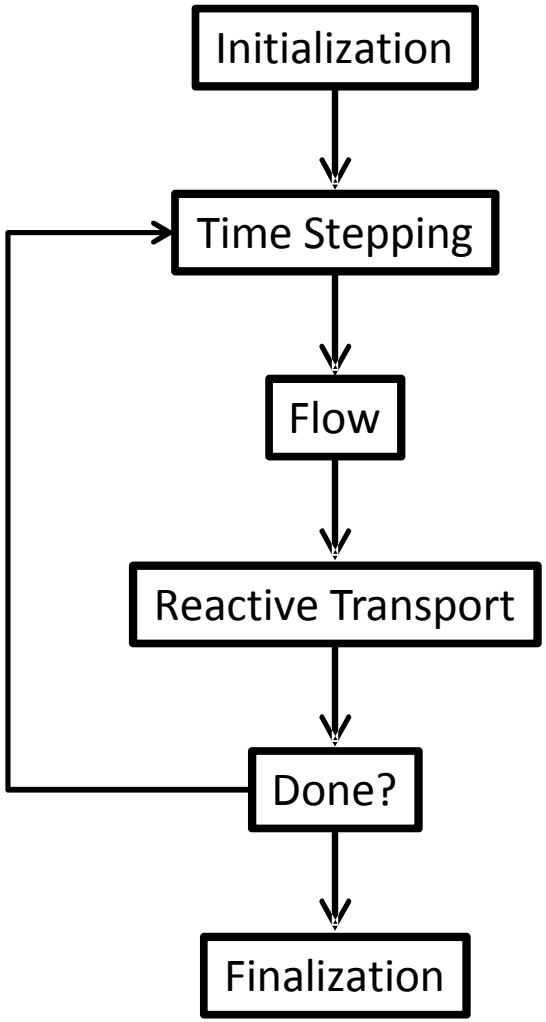
Data Assimilation



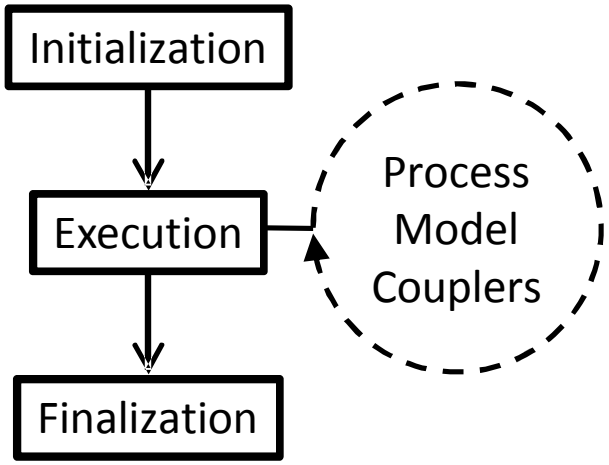
Xingyuan Chen, PNNL, 2011

Traditional Process Model Coupling

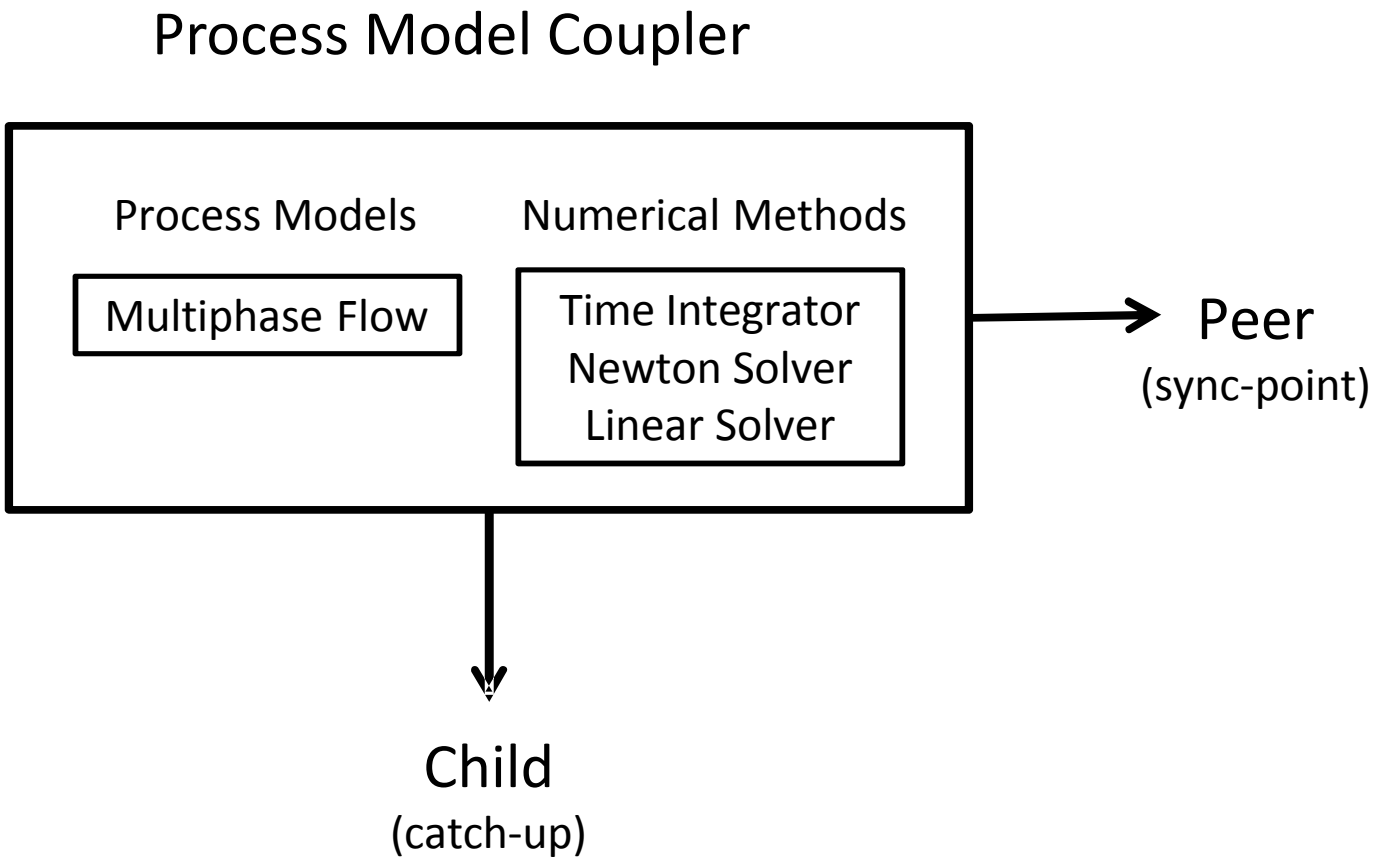
Traditional Time Stepping Loop



PFLOTRAN Workflow

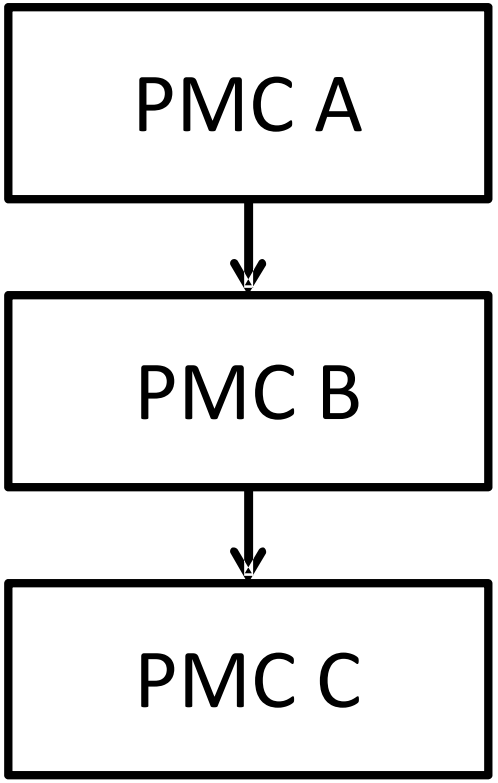


Process Model Coupling



Hypothetical PMC Coupling

PMC = Process Model Coupler



Hypothetical PMC Coupling

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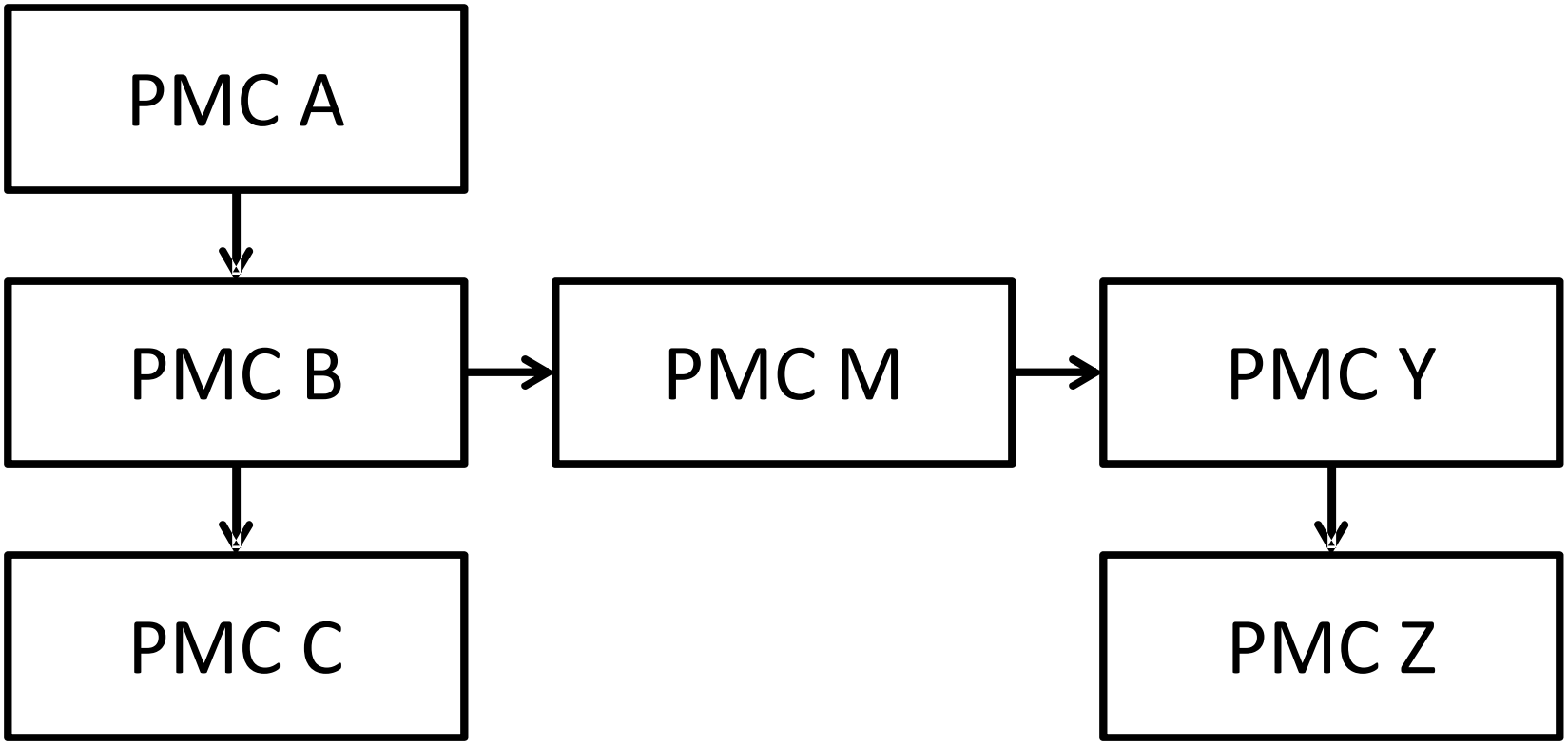
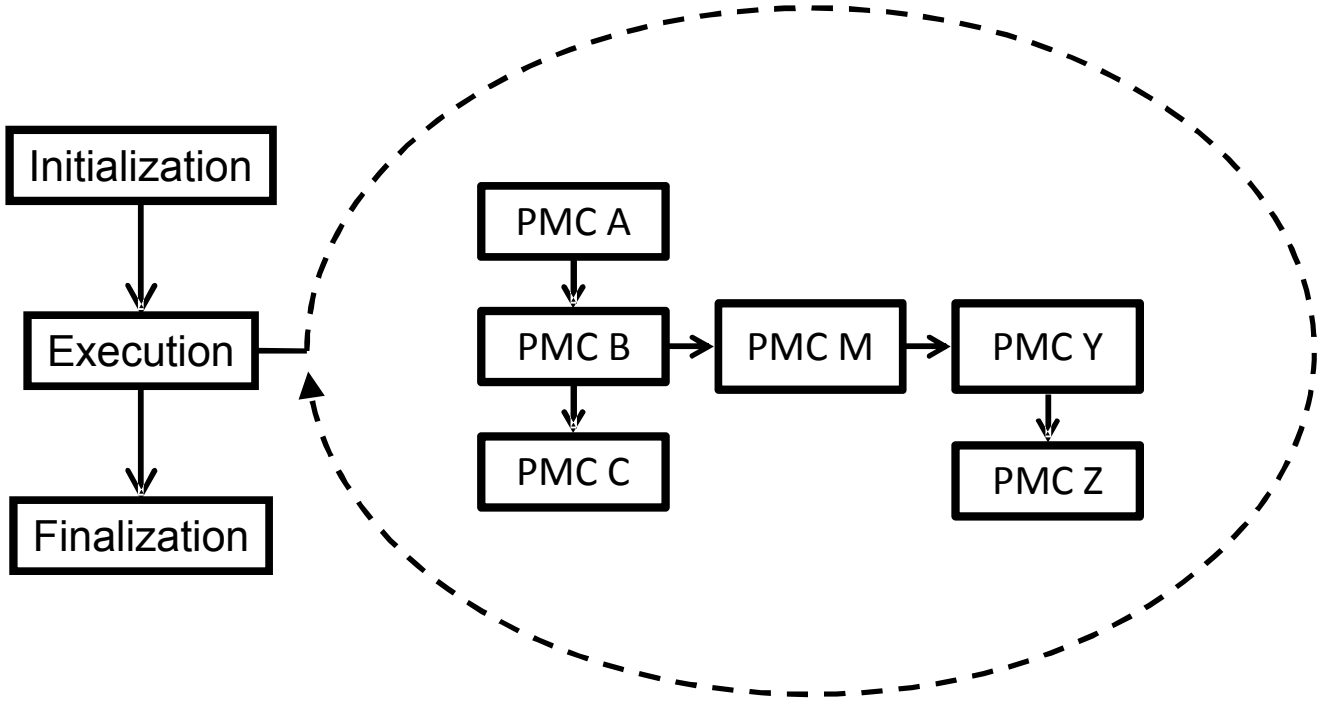


PFLOTRAN Workflow



Flexible Process Model Coupling

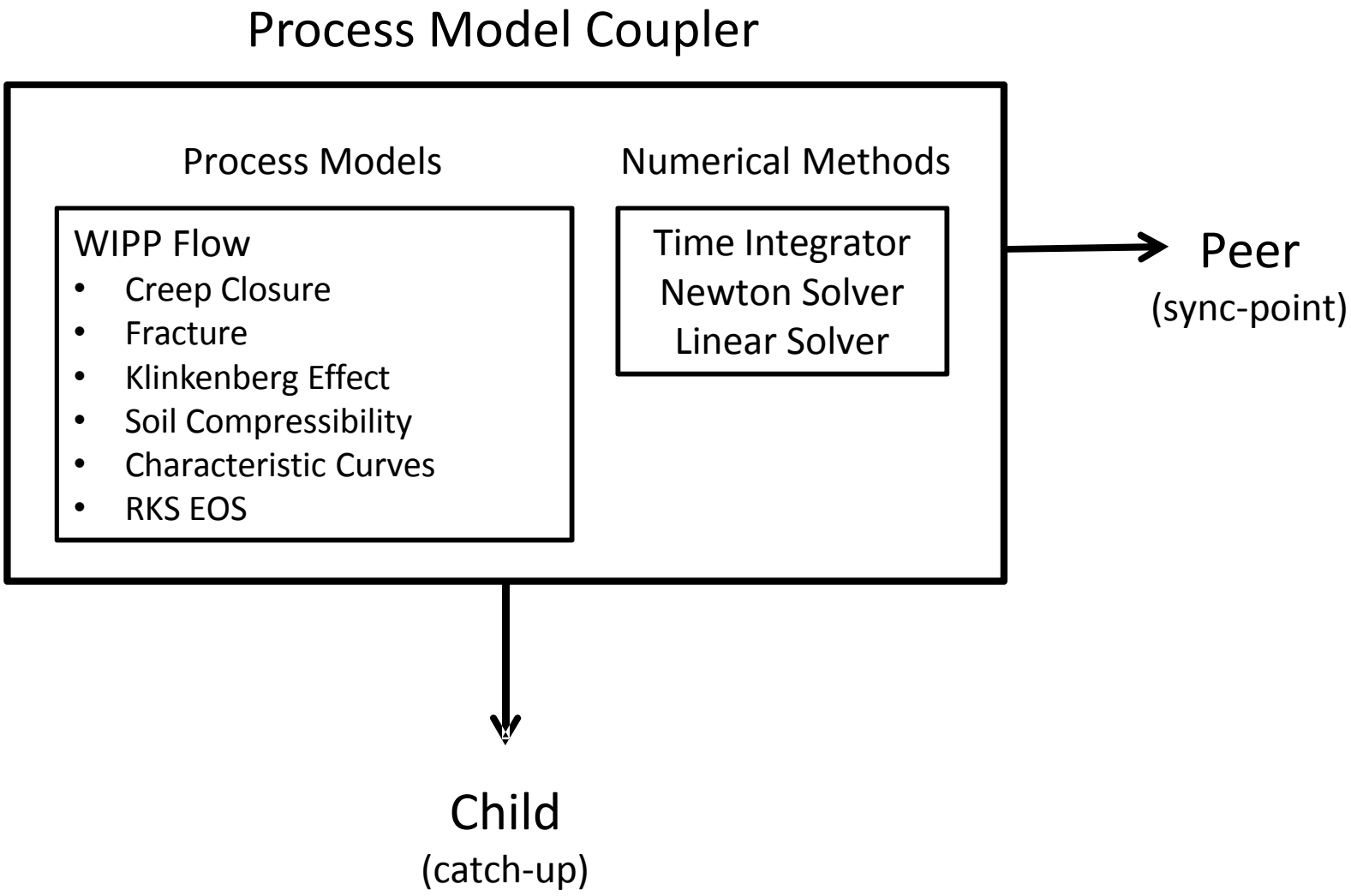
Sandia National Laboratories

- 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.

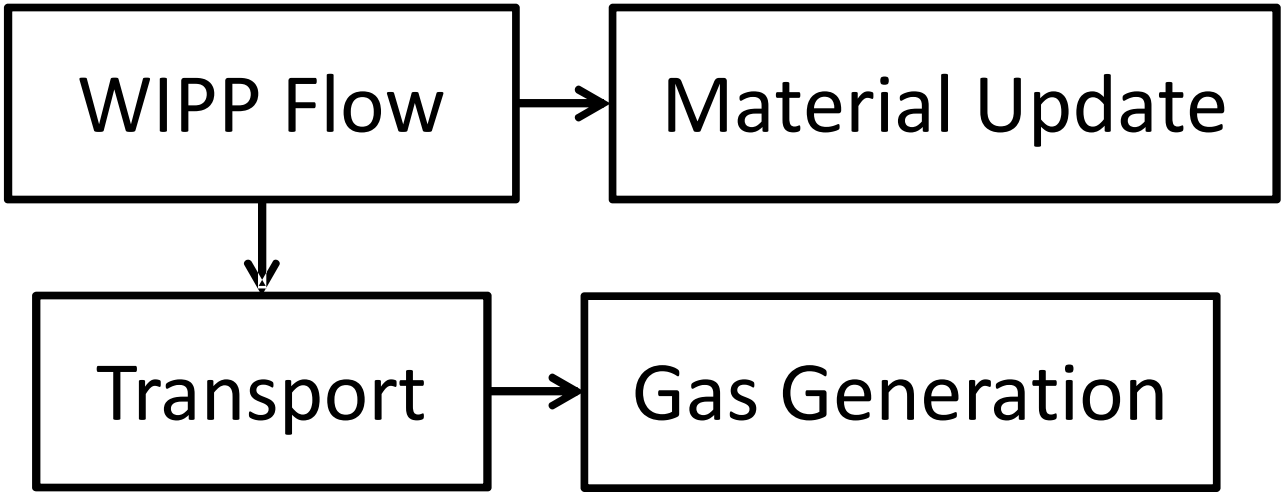
WIPP Process Models

- Two-phase flow
  - Immiscible
  - Isothermal
- WIPP-specific capability
  - Characteristic curves: capillary pressure, relative permeability = f(liquid saturation)
  - Creep closure: porosity = f(liquid pressure, time)
  - Fracture processes: permeability, porosity = f(liquid pressure)
  - $H_{2(g)}$ generation: gas source = f(liquid saturation, time)
  - Klinkenberg effect: gas permeability = f(gas pressure)
  - Soil compressibility: porosity = f(liquid pressure)
  - Redlich-Kwong-Soave equation of state: gas density = f(gas pressure)
  - Modification of material properties at select points in time

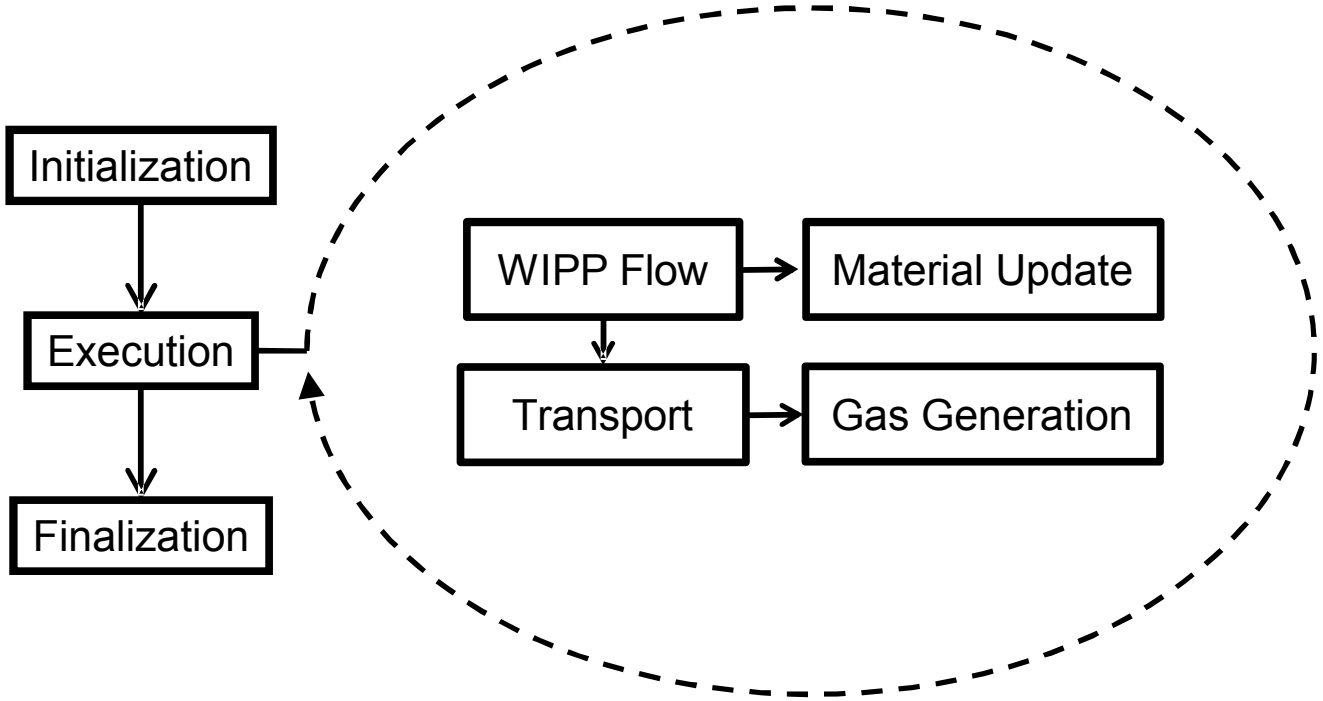
WIPP Process Model Coupling



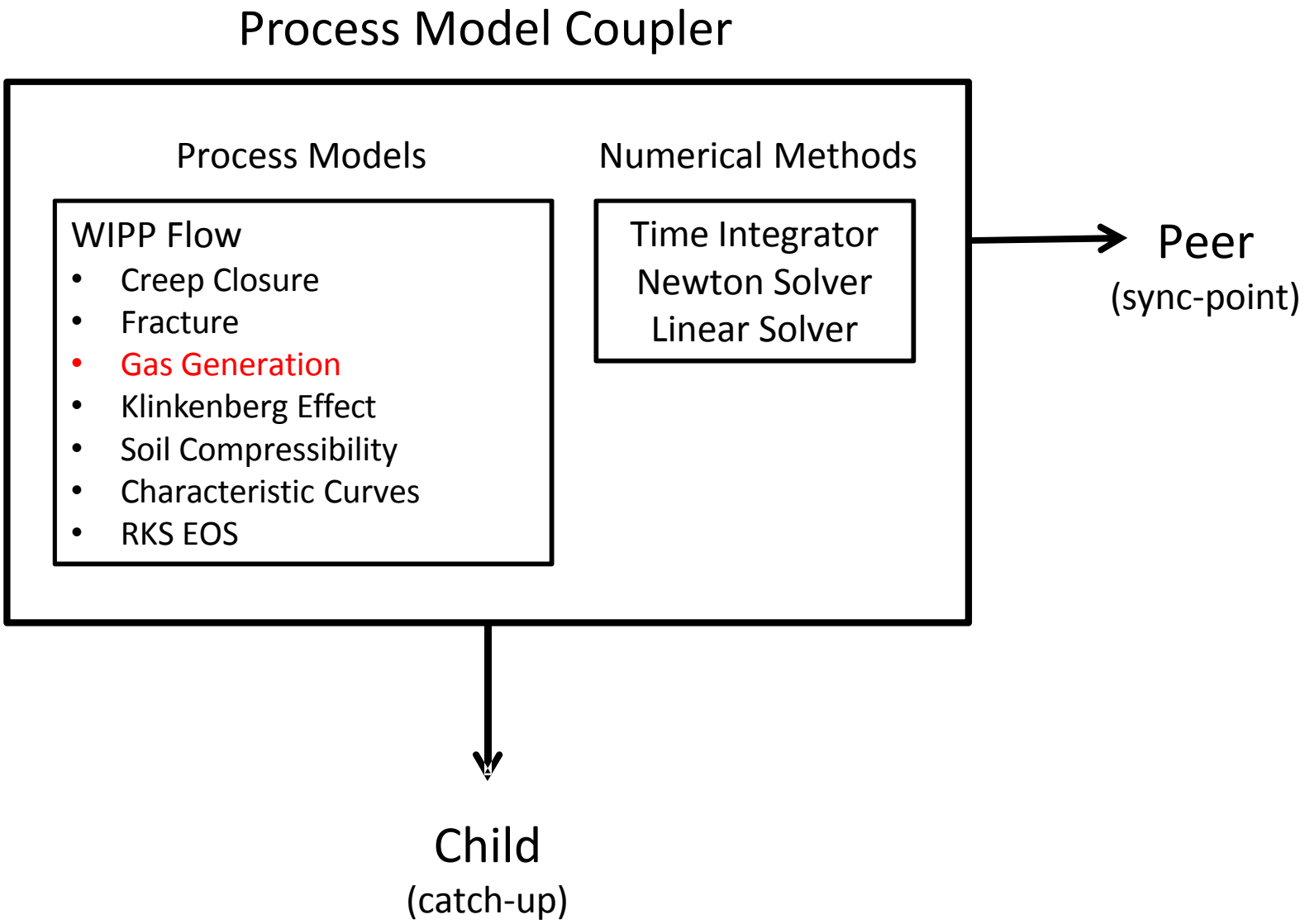
WIPP Process Model Coupling



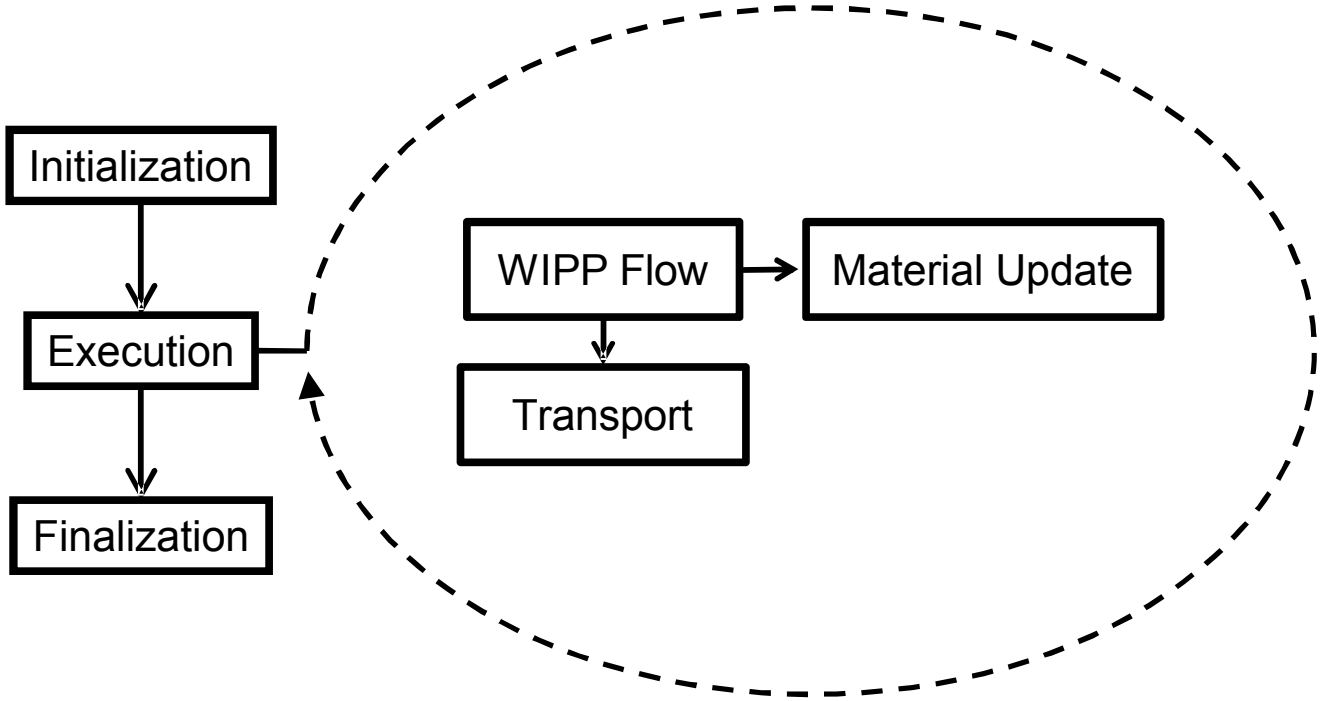
Current WIPP Workflow



WIPP Process Model Coupling



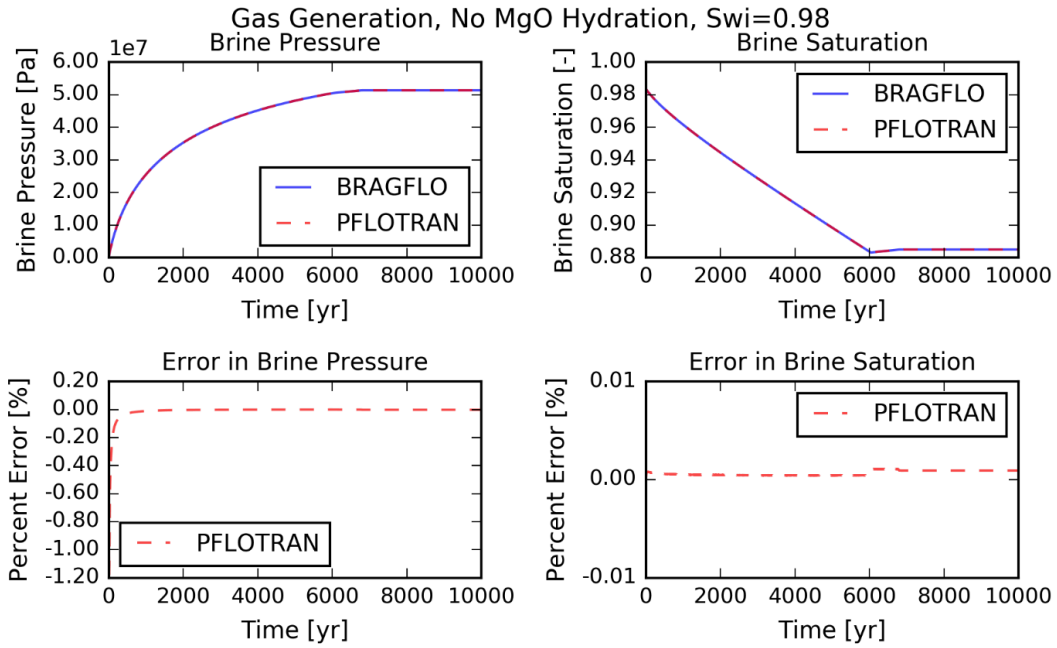
Future WIPP Workflow



Process Model Implementation

- Code development
  - Transport is straight-forward
  - Flow has required more work
- Validation/Verification Testing
  - Against BRAGFLO, NUTS, analytical solutions
  - Single-cell
  - Multi-cell

Sample test for gas generation (pressure and saturation compared)



Summary

- SNL is further developing the existing PFLOTRAN code for application to WIPP PA
  - Potential repository layout changes require 3-D representation

- Process model workflow has been an important part of the development

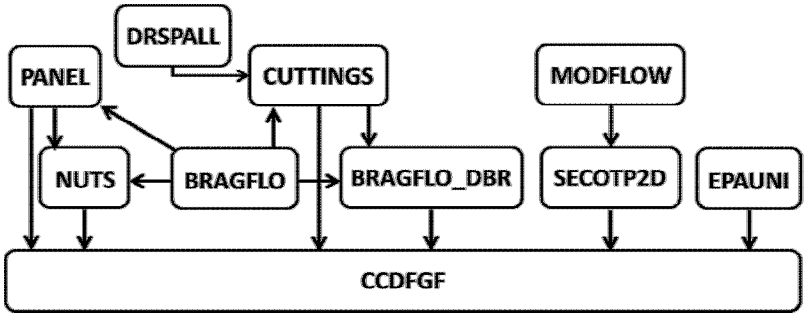
- Thanks to WIPP PA PFLOTRAN development team

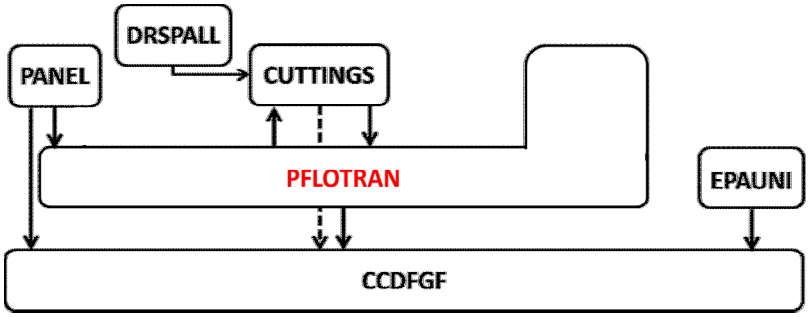
James Bethune
Brad Day
Michael Feng
Jennifer Frederick
Sungtae Kim
Heeho Park
Ramesh Sarathi
Emily Stein

Sandia National Laboratories

Questions?

PA Code Map/Description





Codes	Description
BRAGFLO	Simulates porous media flow in and surrounding the repository over 10,000 years
NUTS	Calculates radionuclide transport in the Salado Formation including the repository
BRAGFLO-DBR	Predicts release from the repository to the environment via borehole intrusion
MODFLOW	Used to calculate flow field away from the repository in the Culebra member of the Rustler Formation
SECOTP2D	Computes radionuclide transport in fractured porous media (Culebra)
PFLOTRAN	Massively parallel reactive flow and transport model for describing surface and subsurface processes

Current PA vs PFLOTRAN

Codes	Current PA	PFLOTRAN
BRAGFLO (porous media flow)	- Immiscible (gas/liquid) - Isothermal - Two-phase flow	- **Miscible** - **Anisothermal** - Multiphase Flow - **Diffusion**
NUTS (radionuclide transport)	- Multicomponent transport - Single porosity - Constant sorption - Single continuum model	- **Biogeochemical Transport** - Dissolution/precipitation - **Multi-rate sorption** - **Multi-continuum model**
General Comparison	- **2D** - Structured grid - **Parallel with single core simulations** - Limitations on simulation size - Many I/O interfaces required - Network of coupled 2D simulations - **Simplified process models and coarse mesh** for quicker overall calculation time	- **3D** - Unstructured/structured grid - **Massively parallel** - Simulation size only depends on hardware capability - Need to develop WIPP-specific functionalities - **Detailed process models and high mesh resolution**, but overall PA calculation may be longer

Other Advantages of PFLOTRAN

- **Open source development**
  - A broad research community that leverages innovation in subsurface and computational sciences.
- In-house code development expertise
  - **Multiple Sandians are PFLOTRAN developers with authorization to commit changes to the code.**
- Managed under a modern support infrastructure
  - **Distributed source control management through Mercurial**
  - **Central, open source repository resides on Bitbucket**
  - Comprehensive regression and unit testing using Python
  - Automated building and testing through Buildbot
- PFLOTRAN HDF5 file formats
  - **Compatible with open source visualization tools** (i.e. VisIt and Paraview)