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

Spent Fuel and Waste Science and Technology (SFWST)

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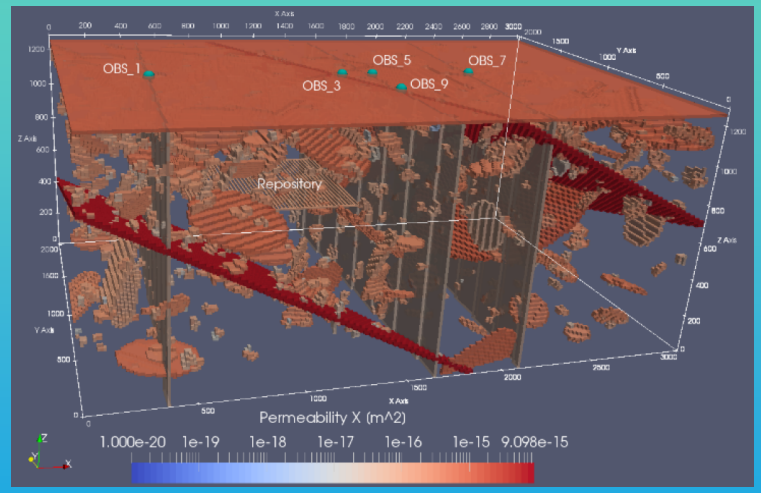

Advanced Simulation Capability 1: Foundational Capability – GDSA Framework

U.S. Nuclear Waste Technical Review Board

Fall Workshop

November 3-4, 2021

Paul Mariner

Sandia National Laboratories

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SAND2021-XXXX PE

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Outline

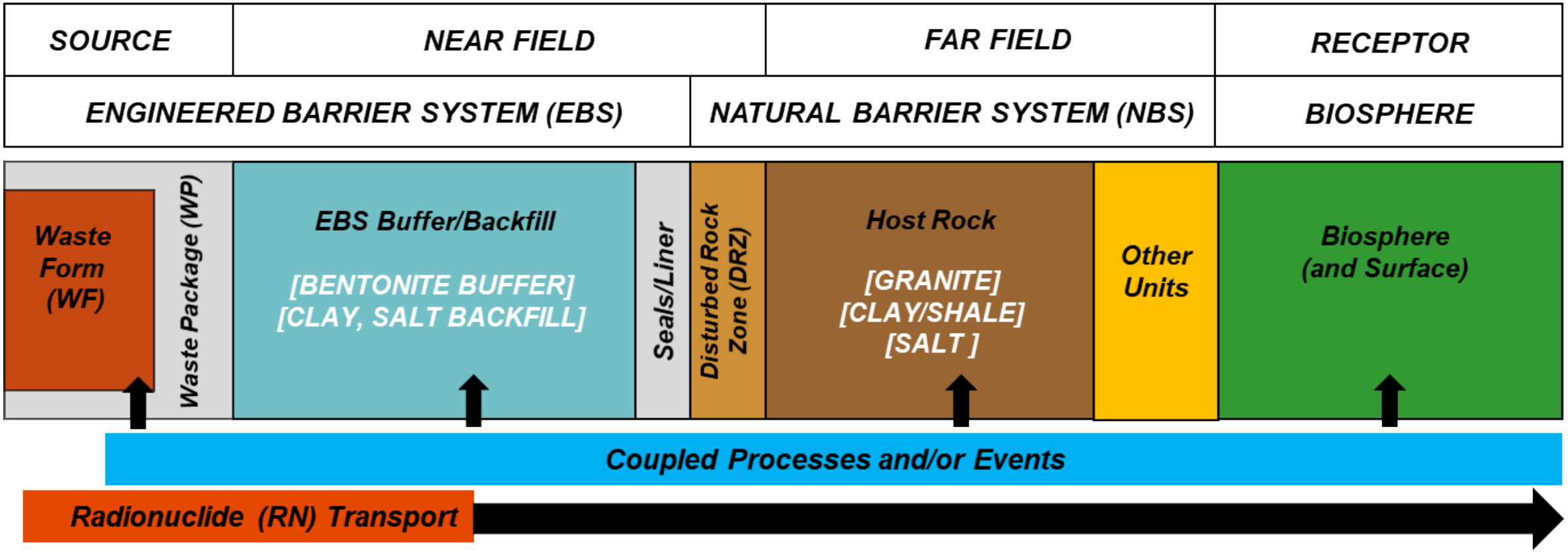
- GDSA Framework
- GDSA Framework applications
- Performance metrics
- Capability development

GDSA Framework

Objective

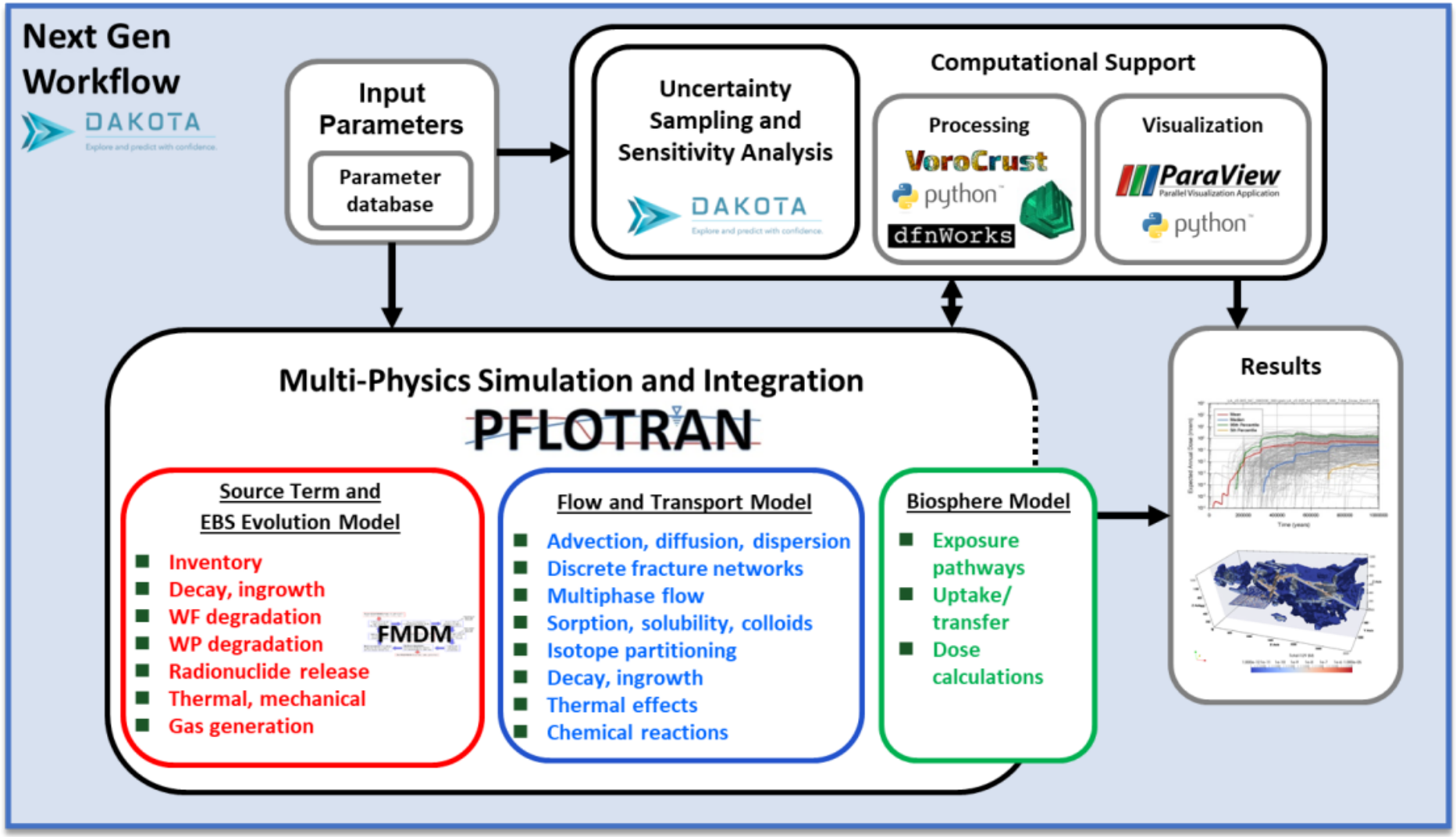
- Develop a disposal system modeling and analysis capability (Geologic Disposal Safety Assessment (GDSA)) that supports the integrated modeling of detailed coupled processes controlling disposal system performance of deep geologic repositories, including uncertainty.
- The system-level modeling capability will:
  - Integrate updated conceptual models of subsystem processes and couplings
  - Interface with site characterization data organized in a geologic framework model
  - Develop and apply uncertainty quantification (UQ) and sensitivity analysis (SA) methods
  - Leverage existing computational capabilities (e.g., meshing, visualization, high-performance computing (HPC)) where appropriate
  - Be developed and distributed in an open source environment

GDSA Framework – Conceptual



Freeze et al. 2013

GDSA Framework – Computational

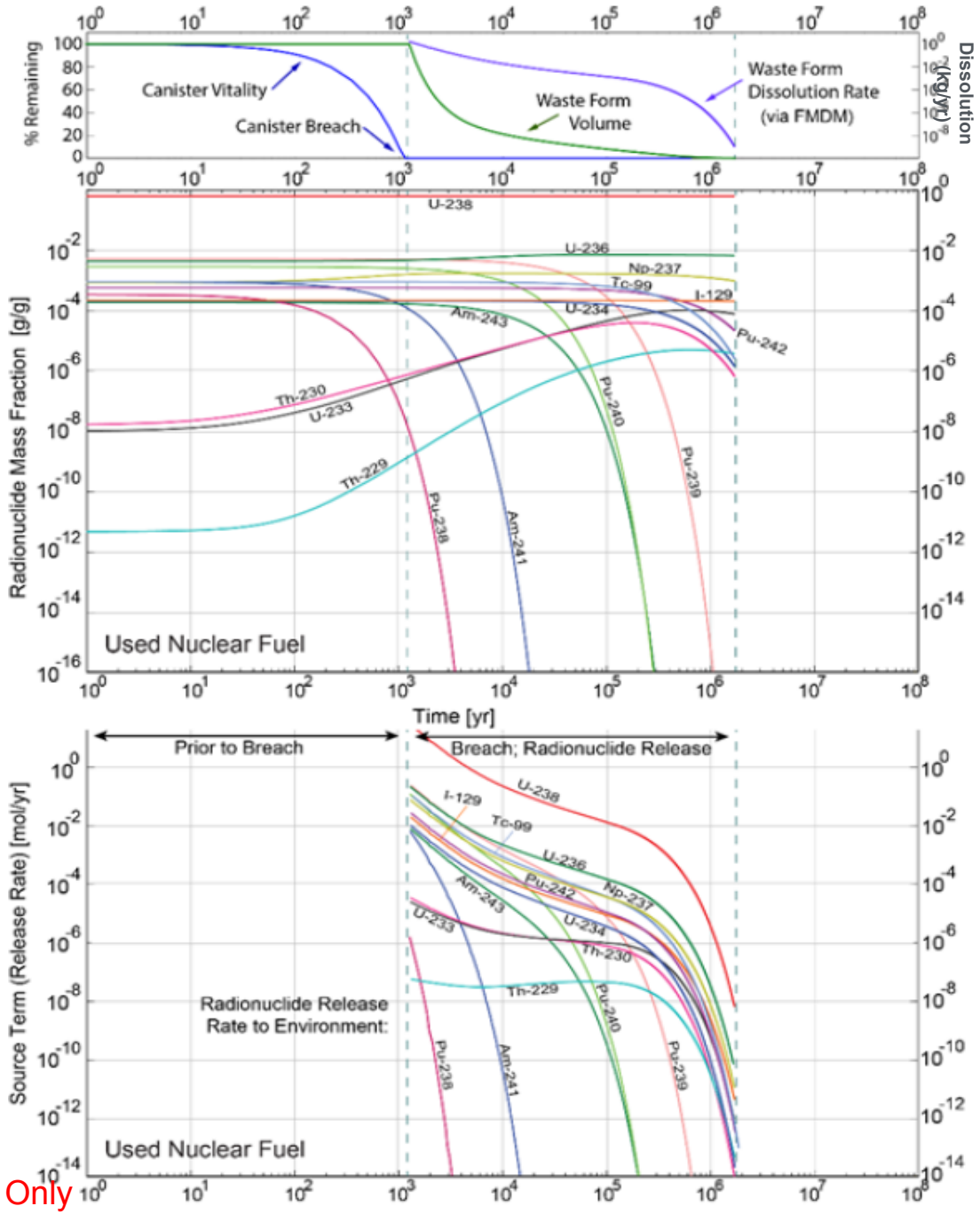


International Influences

- International working groups
  - DECOVALEX (international group working on DEvelopment of COupled models and their VALidation against Experiments)
  - Nuclear Energy Agency (NEA) salt and crystalline clubs
  - An informal international joint sensitivity analysis group (JOSA)
  - Membership in underground research laboratory (URL) programs
- Available literature
  - Published models, reports, and analyses
- International forums / interactions
  - Conferences, journal publications, manuscript review

Source Term Capabilities

- Waste form inventory
- Decay and ingrowth
- Instant release fractions
- Spent nuclear fuel (SNF) degradation
  - Fuel matrix degradation model (FMDM) surrogate (radiolysis, electro-kinetic reactions, alteration layer growth, diffusion of reactants through the alteration layer)
  - Fractional dissolution rate
  - Defense SNF (instantaneous)
- High-level radioactive waste (HLW) glass degradation
  - Transition state theory (TST)
  - Kienzler dissolution
- Custom (e.g., surface area specific)



Mariner et al.

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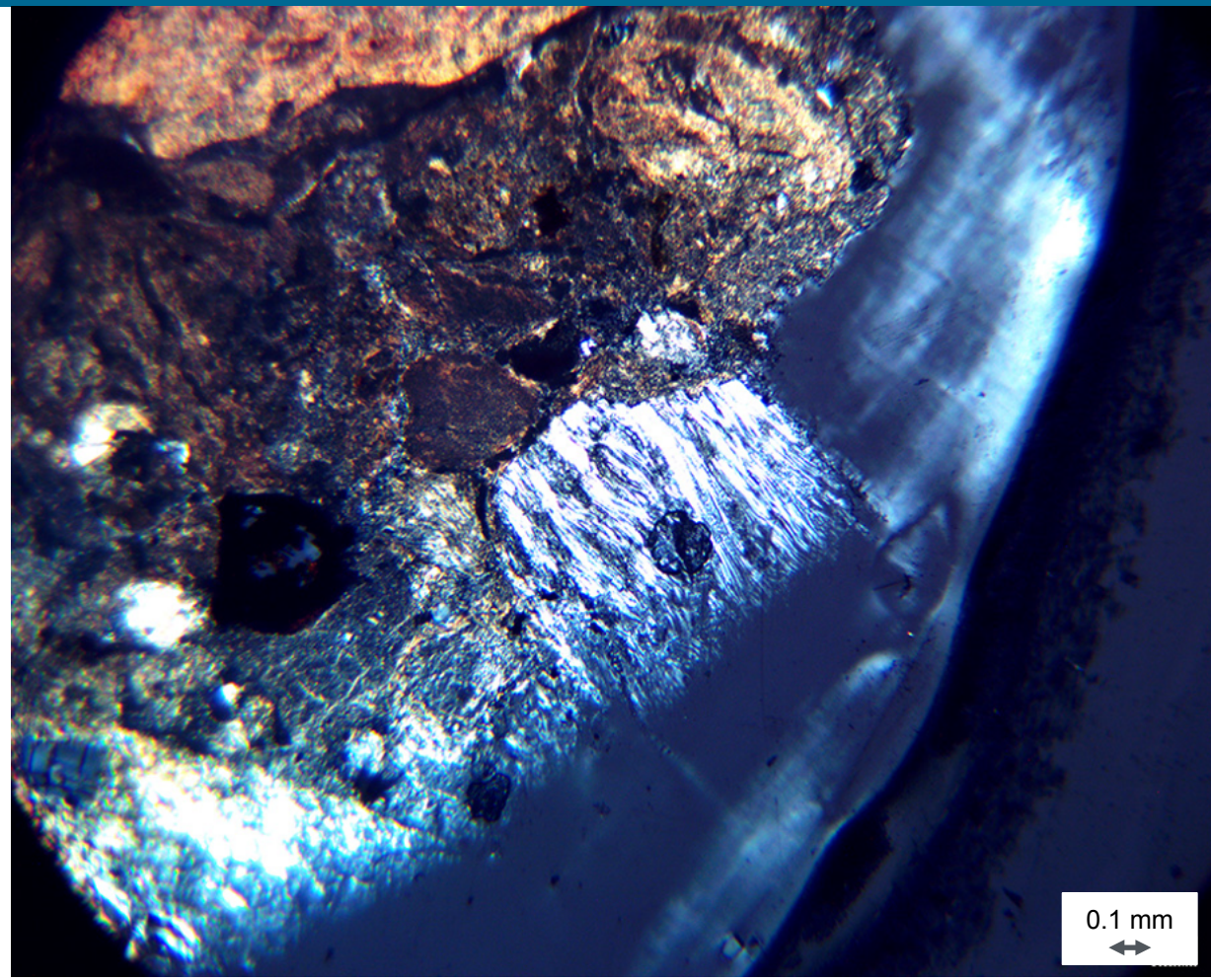
WP, EBS, and DRZ Model Capabilities

- Waste package (WP) objects
  - Allows simulation and monitoring of each WP individually
- WP degradation
  - General corrosion (temperature-dependent) or specified WP breach times
- Buffer behavior and evolution
  - Temperature-dependent characteristic curves
  - Radionuclide adsorption and diffusion
  - Water imbibition and swelling
  - Smectite-to-illite transition
- Disturbed rock zone (DRZ)
  - Buffer swelling effects on DRZ permeability



Caporuscio et al. 2019

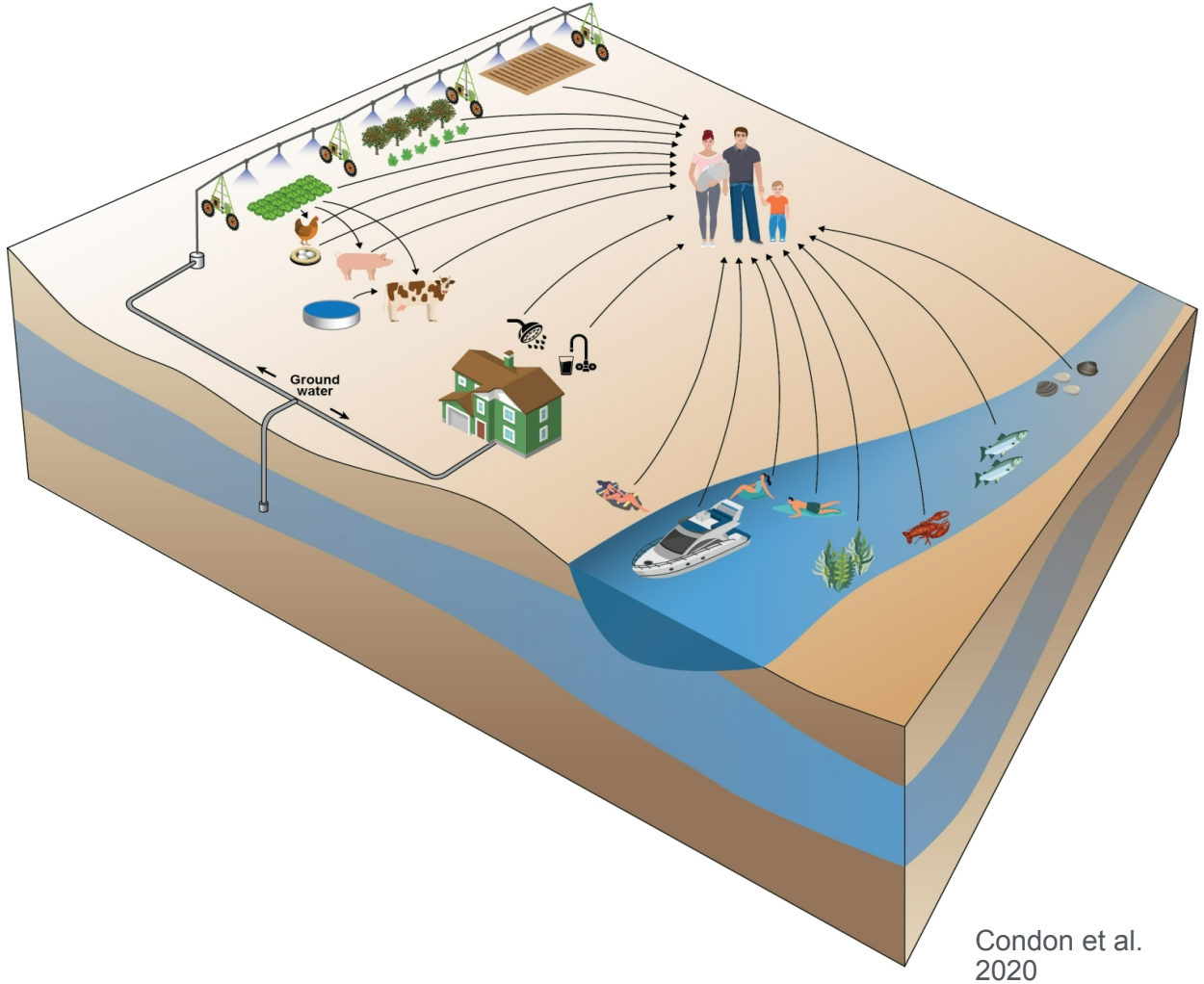
Smectite altering to sericite (muscovite/illite) in a sample from an inner bentonite block of a Grimsel heater test

Flow and Transport Capabilities

- Thermal-hydrological-chemical (THC)
- Multiphase flow (water and gas)
  - Saturated, unsaturated
- Fractured rock
  - Discrete fracture networks (DFNs)
  - Equivalent continuous porous medium (ECPM)
  - Fracture-matrix interaction
- Solute transport
  - Advection, dispersion
  - Decay, ingrowth, partitioning (sorption, solubility limits)

Biosphere Capabilities

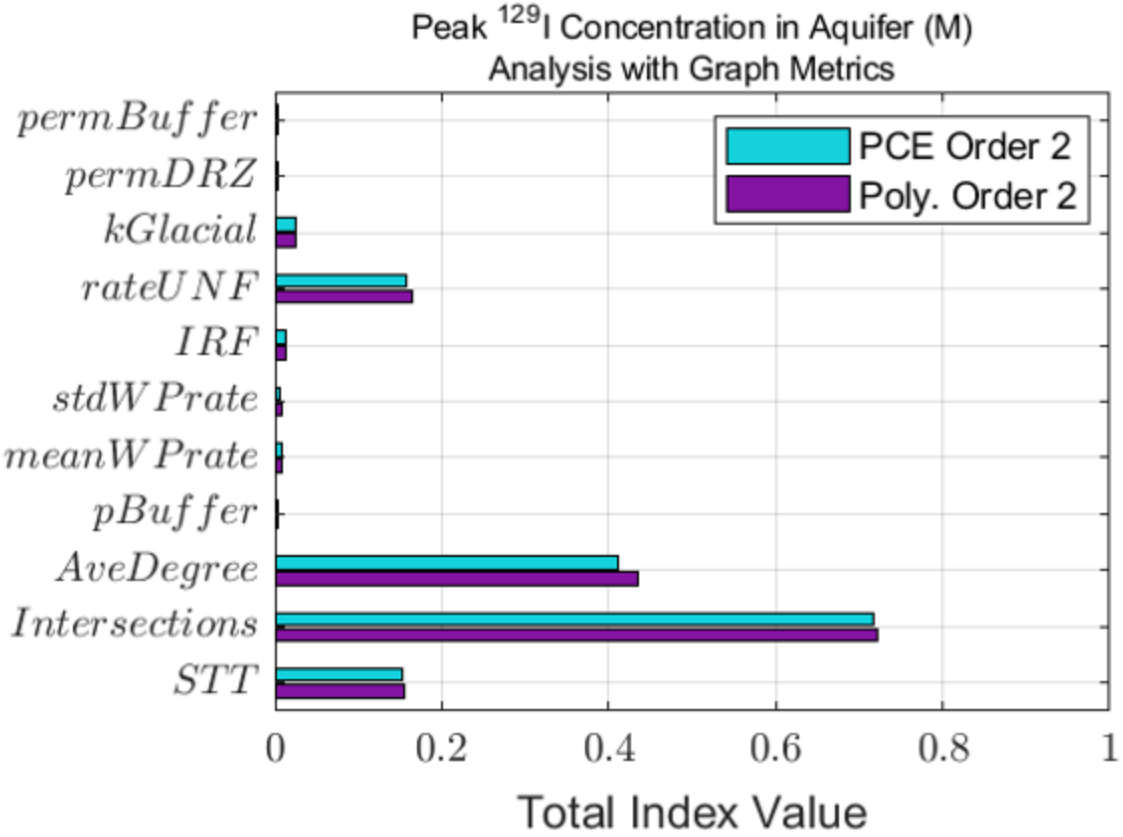
- Well water capture
  - Includes enhancement factors for short-lived radionuclides (e.g., radon-222)
- Water ingestion dose model
  - International
- Biosphere model (in progress)
  - Multiple pathways
  - Various dose mechanisms
  - Bioaccumulation
  - Decay and ingrowth



Condon et al. 2020

Uncertainty Capabilities

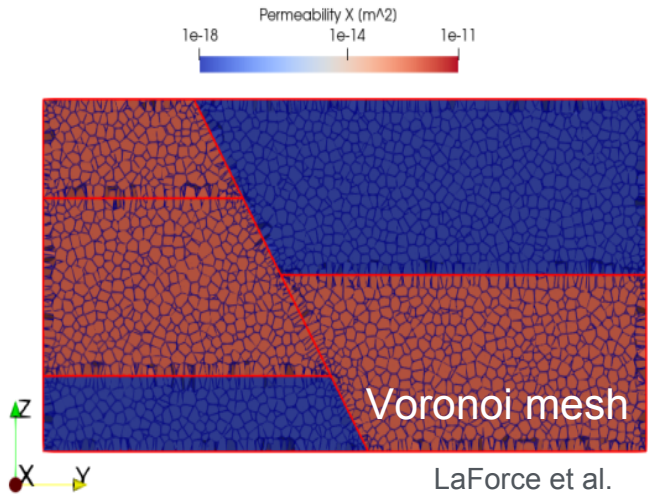
- Uncertainty propagation
  - Random, Latin Hypercube Sampling
  - Aleatory and epistemic loops
- Statistical characterization of output, quantities of interest (QoI)
  - Mean, median, percentiles, etc.
- Sensitivity analysis
  - Correlation, interaction, and variance analysis
  - Identification of input importance
  - Ranking of sources of uncertainty



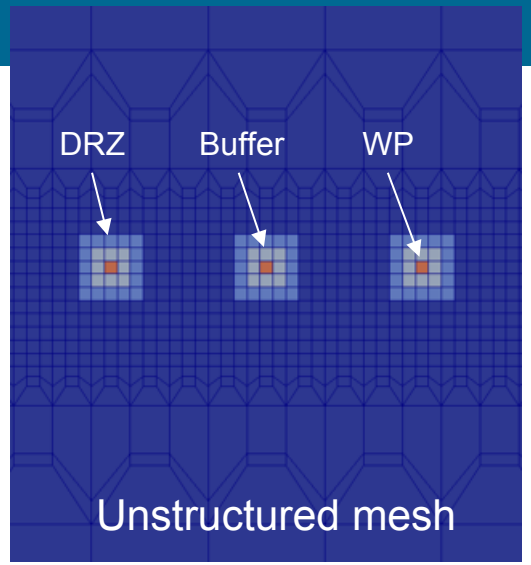
Swiler et al. 2021

Meshing and Fracture Network Capabilities

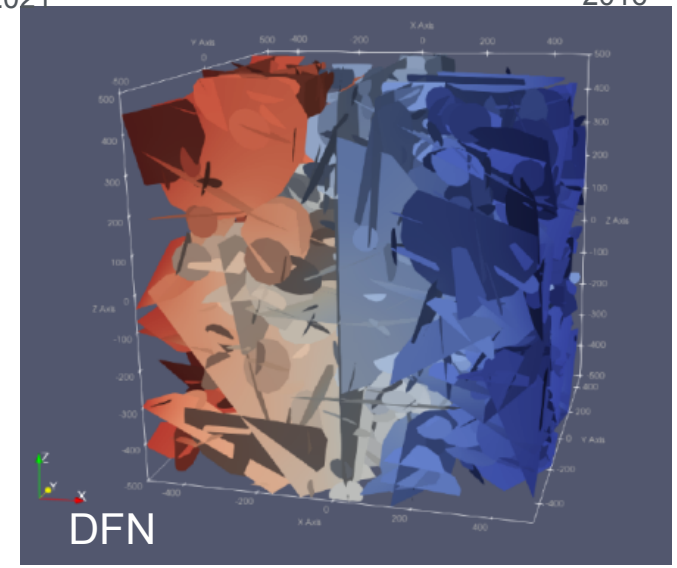
- Meshing
  - Traditional (structured, simple unstructured)
  - Voronoi (enhanced visualization, local grid refinement)
- Discrete Fracture Networks (DFNs)
  - Introduces significant spatial heterogeneity
  - Matrix diffusion and adsorption



LaForce et al. 2021



Mariner et al. 2016



LaForce et al. 2021

Generic FEP screening (from Vaughn et al. 2012)

Source (Inventory and Waste Form)
- Radionuclide inventory (heat generation, decay and ingrowth)
- Waste form degradation (dissolution processes)
- Gas generation
- Radionuclide release and transport (mobilization, early release [e.g., from gap and grain boundaries], precipitation/dissolution)

Near Field (Waste Package, Buffer, Backfill, Seals/Liner, and DRZ)
- Waste package degradation (corrosion processes, mechanical damage, early failures)
- Evolution/degradation of EBS components and DRZ
- Effects from rockfall, drift collapse (e.g., salt creep)
- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Chemical interactions (aqueous speciation, mineral precipitation/dissolution, reaction with degraded materials, surface complexation, radiolysis)
- Thermal effects on flow and chemistry
- Effects from disruptive events (seismicity, human intrusion)

Far Field (Host Rock and Other Units)
- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Effects of fracture flow (e.g., dual porosity/permeability, discrete fracture)
- Groundwater chemistry

Receptor (Biosphere)
- Dilution due to mixing of contaminated and uncontaminated waters
- Receptor characteristics (basis for converting radionuclide concentrations in groundwater to dose)

Key

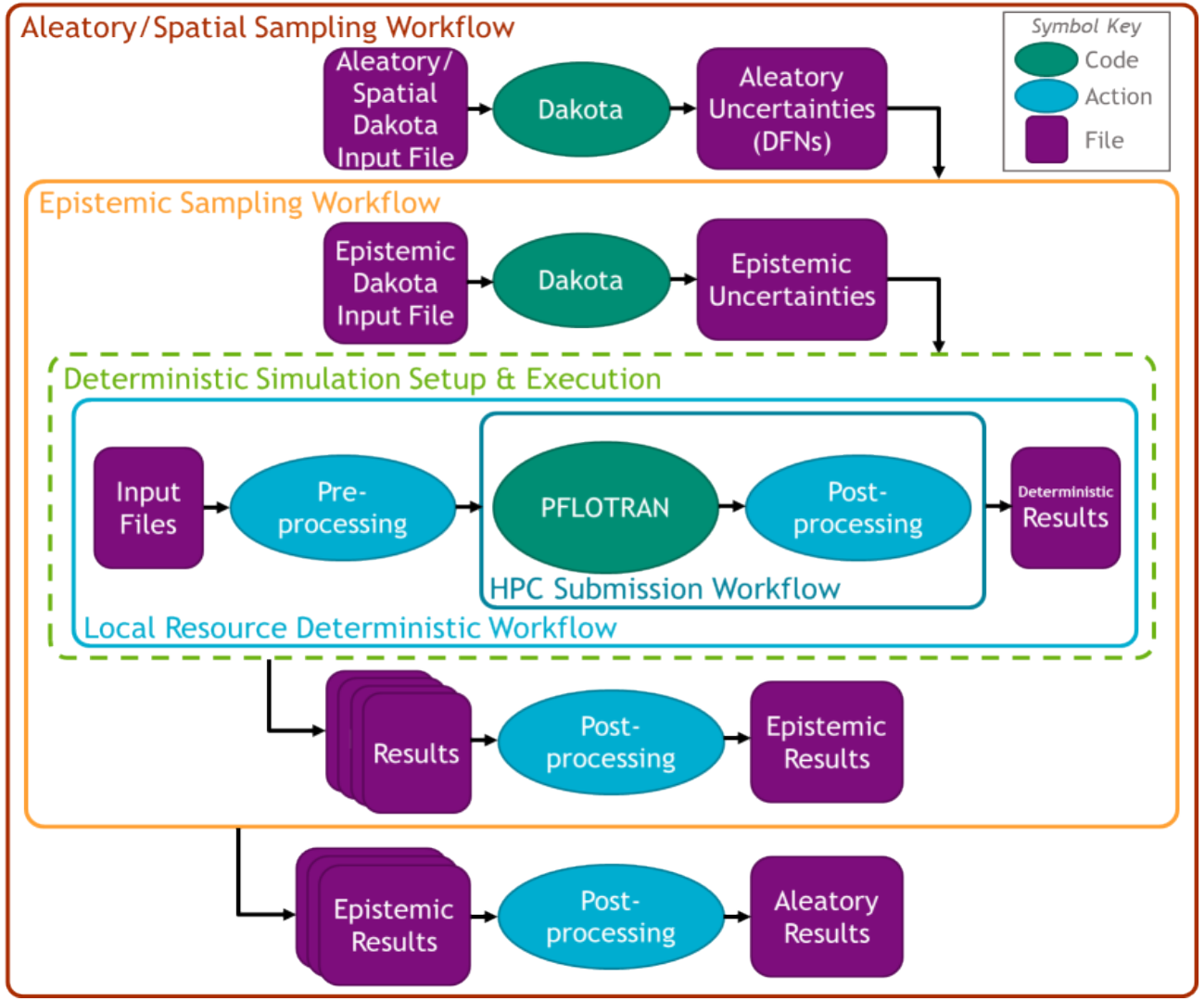
Red = FEP included, at least to some degree

Black = FEP capability lacking or excluded so far

- Features, Events, and Processes (FEPs)
  - Many excluded FEPs (or yet-to-be-implemented FEPs) are chemical, mechanical, and disruptive FEPs

Next Gen Workflow Capabilities

- Workflow
  - Autonomously executes all GDSA Framework's major components
  - Graphic object-oriented interface shows
    - How all components are linked
    - Status of each component during a simulation
  - Executes post-processing calculations
  - Facilitates transparency and reproducibility

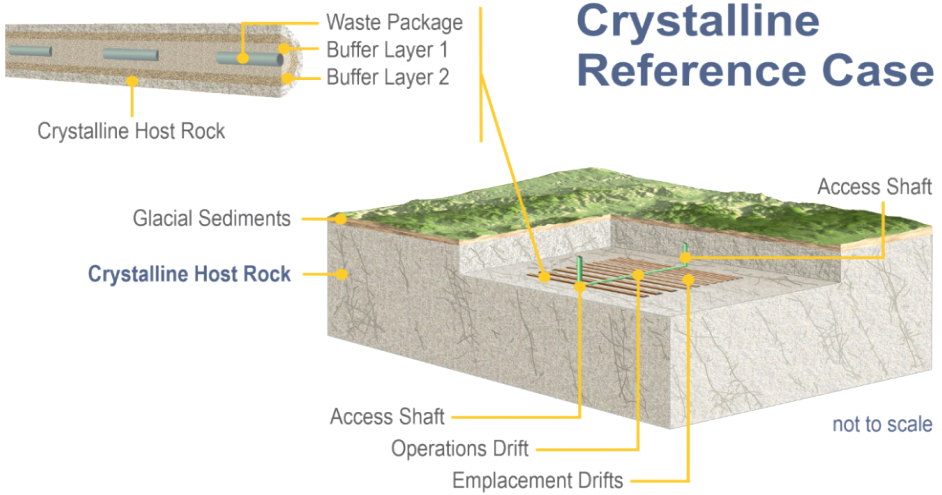


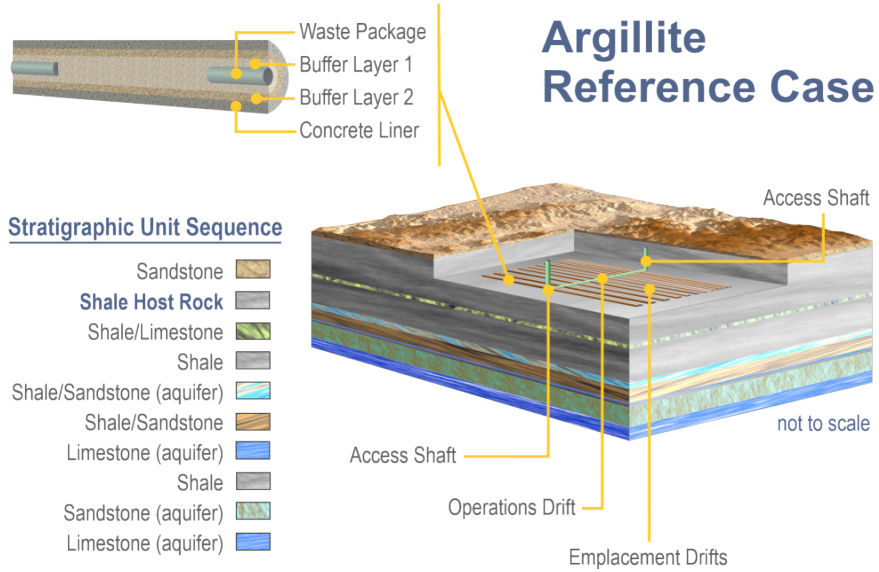
Swiler et al. 2021

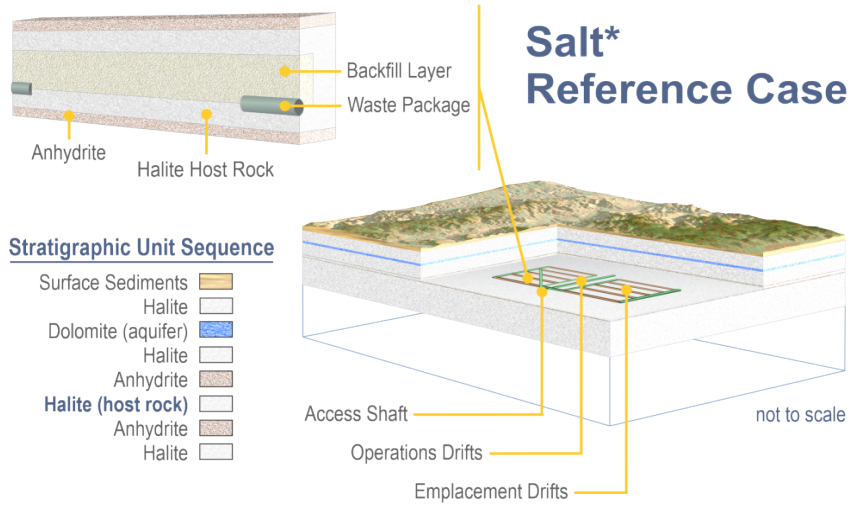
GDSA Framework Applications

GDSA Framework Applications – Total System

- Study and assess
  - Total system performance
  - Importance of included FEPs







*2019 commercial waste case

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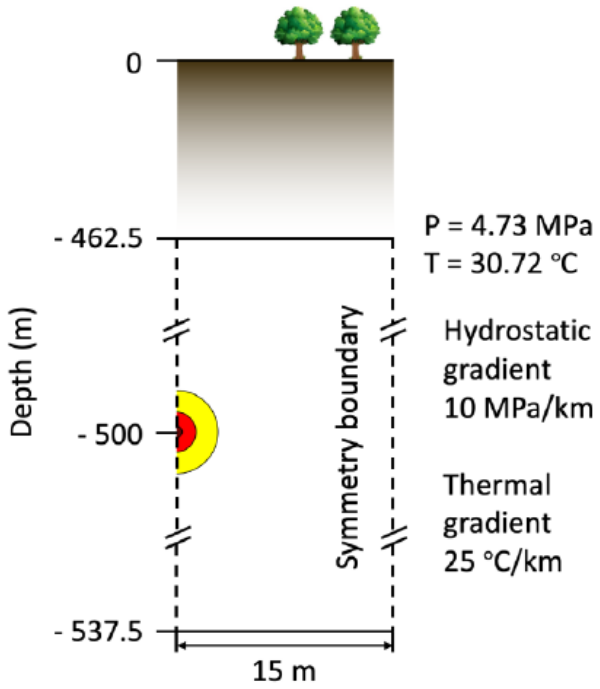
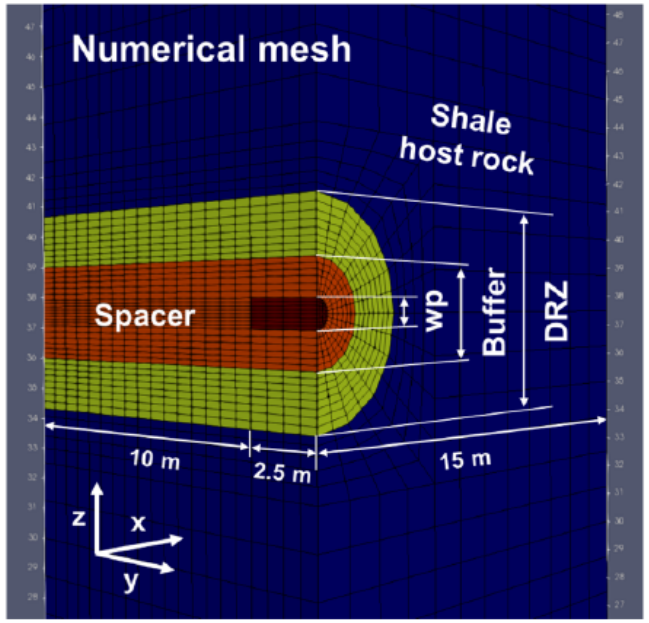
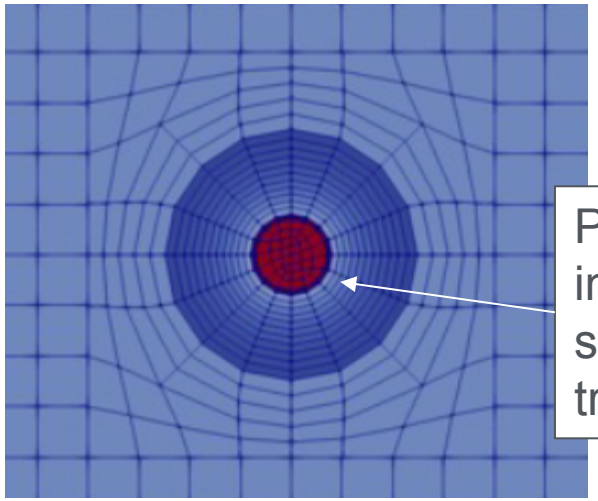
GDSA Framework Applications – Subsystems

- Higher fidelity simulations of subdomains of reference cases
- Assess effects of FEPs too expensive to simulate in total system simulations





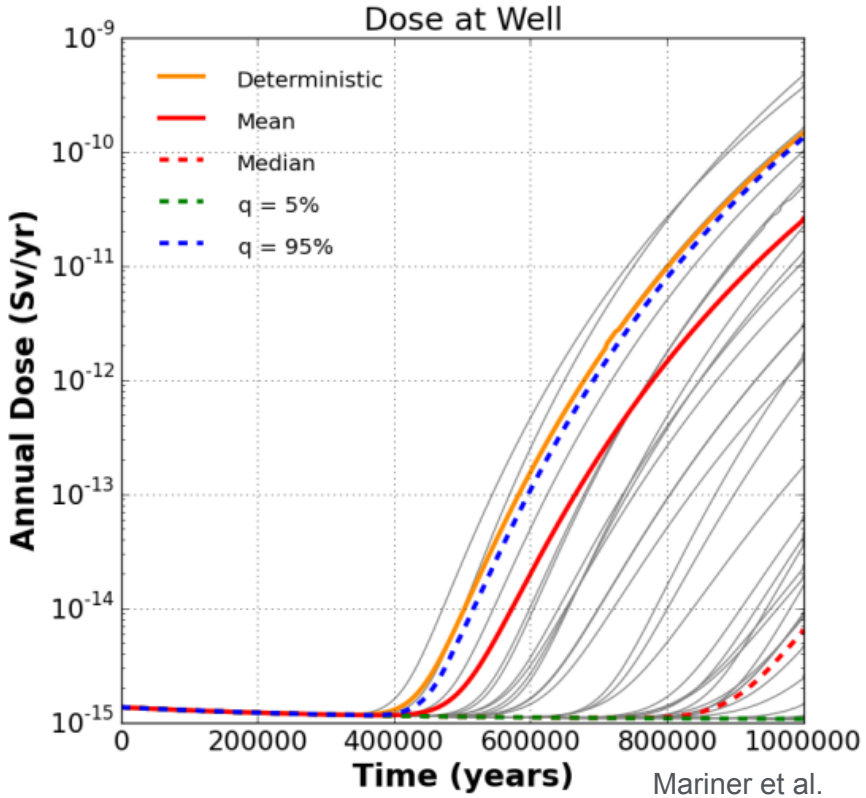


Nole et al. 2021

Performance Metrics

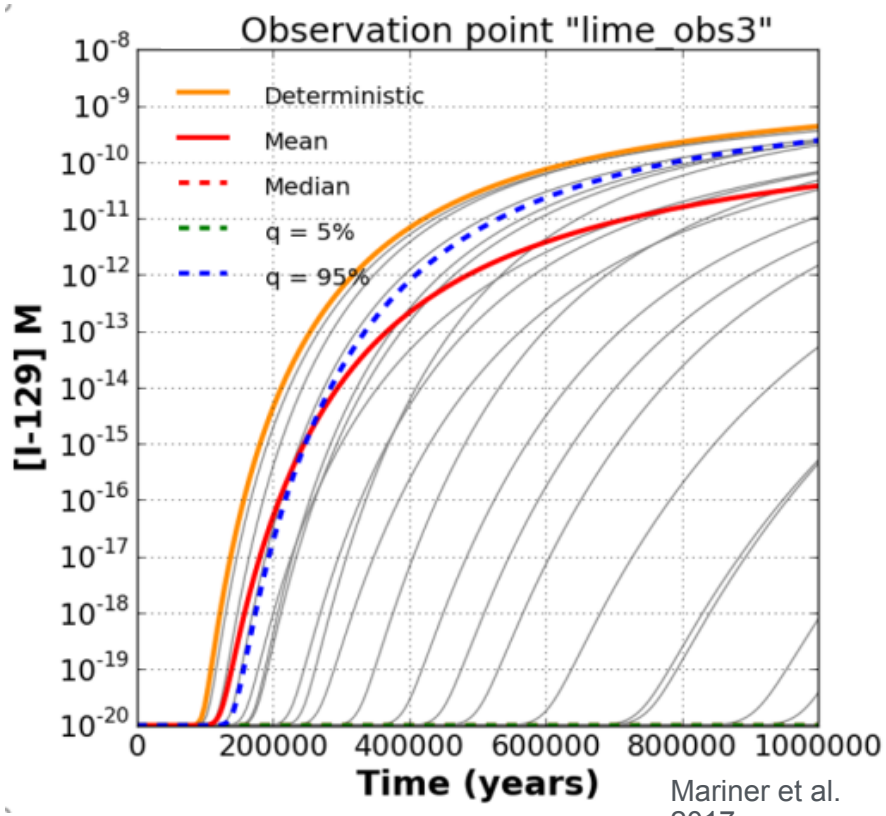
Performance Metrics – Total System

- Annual dose to receptor over time



Mariner et al. 2017

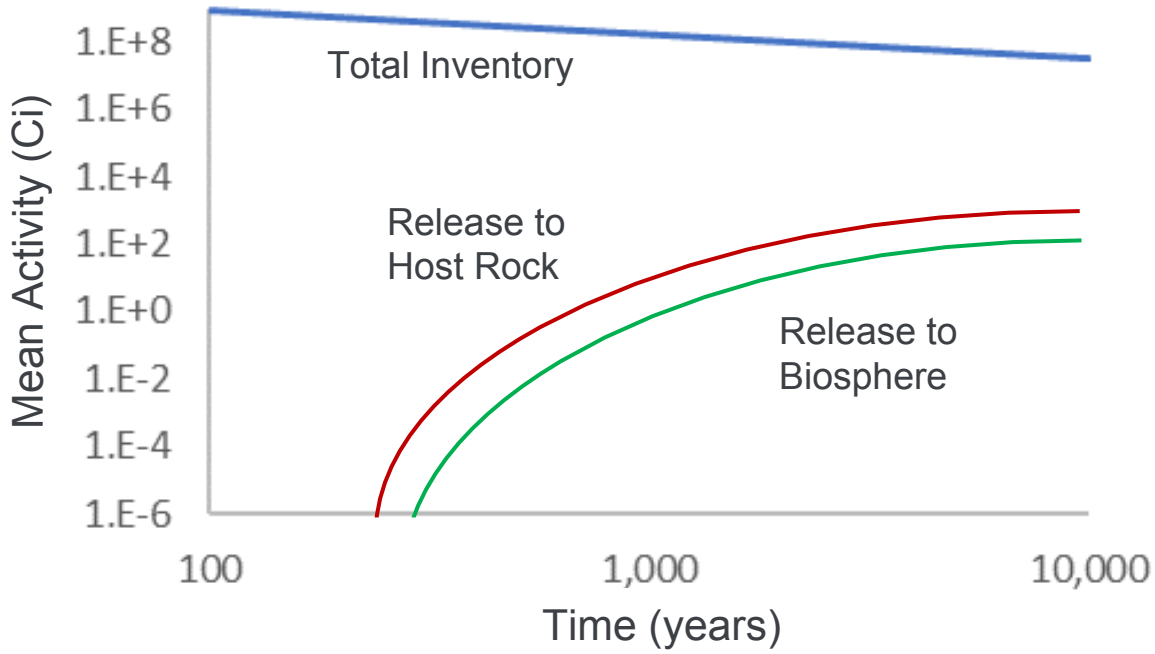
- Radionuclide concentration (or total activity) in aquifer



Mariner et al. 2017

Performance Metrics – Multiple Barriers

- Engineered Barrier System (EBS)
  - Mean release to host rock versus total inventory activity
- Combined EBS and Natural Barrier System (NBS)
  - Mean release to biosphere versus total inventory activity



Process Model Integration

Integration	Guided by
Scope	Roadmap, FEP analysis, 5-yr disposal research plans
Importance	Scope, simulations, experience, literature
Feasibility	Analysis of inputs, outputs, code constraints
Readiness	Screening questions
Decision	Readiness screening and prioritization considerations

Capability Development

Capability Development – Types

- Feature / process model development
  - Coupled / internalized
  - Reduced-order / surrogate
- Solvers
  - Convergence, speed
- Preprocessors / postprocessors
  - Meshing, discrete fracture networks, performance metric calculations, uncertainty and sensitivity analysis
- Verification
  - Testing, documentation
- Reproducibility, transparency, user-friendliness

Model Capability Development – Importance and Readiness

- Will the model have significant effects on important repository performance metrics and/or provide important answers to key questions?
- Are all model assumptions affecting the validity of the model acceptable for the intended use?
- Does the model cover the necessary ranges of input values?
- Is there a better model or approach with more defensible assumptions that covers the same or larger range of applicability?
- Does the standalone model converge and produce sensible and defensible results over the entire multi-dimensional sample space of application?

Model Capability Development – Prioritization

- Importance to 5-yr plan and roadmap
- Importance to reference case(s)
- A balance of
  - Required level of effort
  - Available resources

Summary

Summary

- GDSA Framework development guided by
  - Roadmap, FEPs analysis, 5-yr plans
  - International influences
- Model capability development decisions rely on
  - Readiness considerations
  - Prioritization considerations

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Questions