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Spent Fuel and Waste Science and Technology (SFWST)

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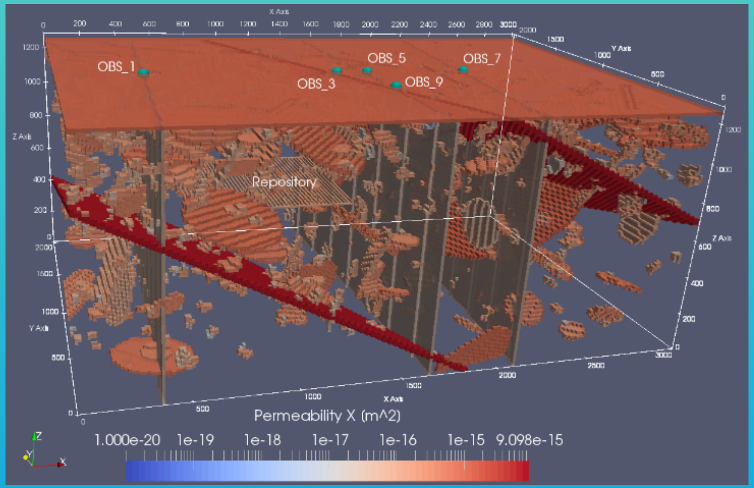


# Prioritization of Cross-Cutting Research & Development Activities: Unsaturated Alluvium Reference Case, Disposal of Dual Purpose Canisters, and Geologic Disposal Safety Assessment

U.S. Nuclear Waste Technical Review Board
Fact-Finding Meeting
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Online Virtual Meeting

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ENERGY NNSA

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## Legal Notice

# Acknowledgements

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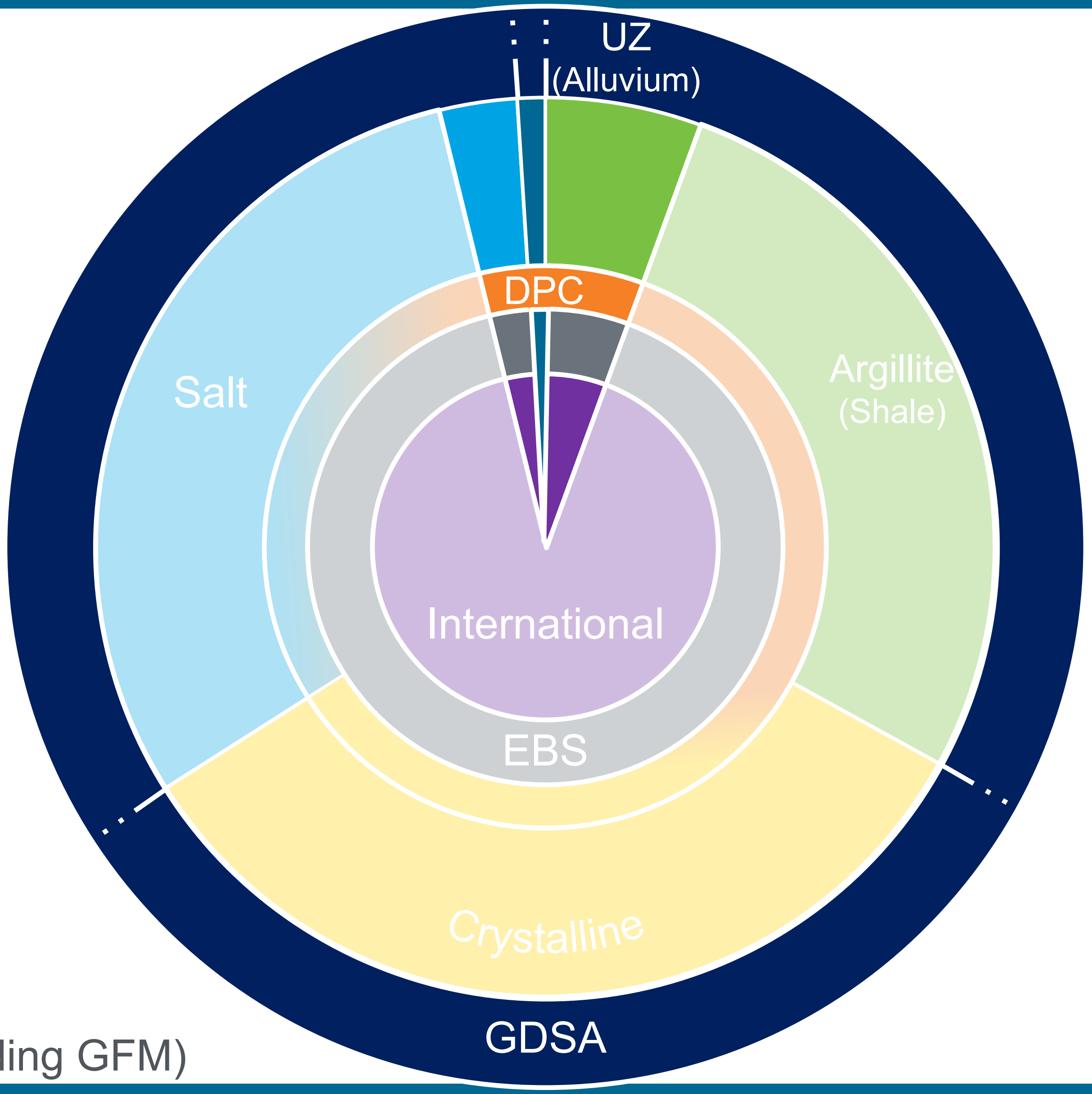
Michael Gross, Elizabeth Miller, Terry Miller

Zhufeng Fang, Scott Painter

# R&D Priorities

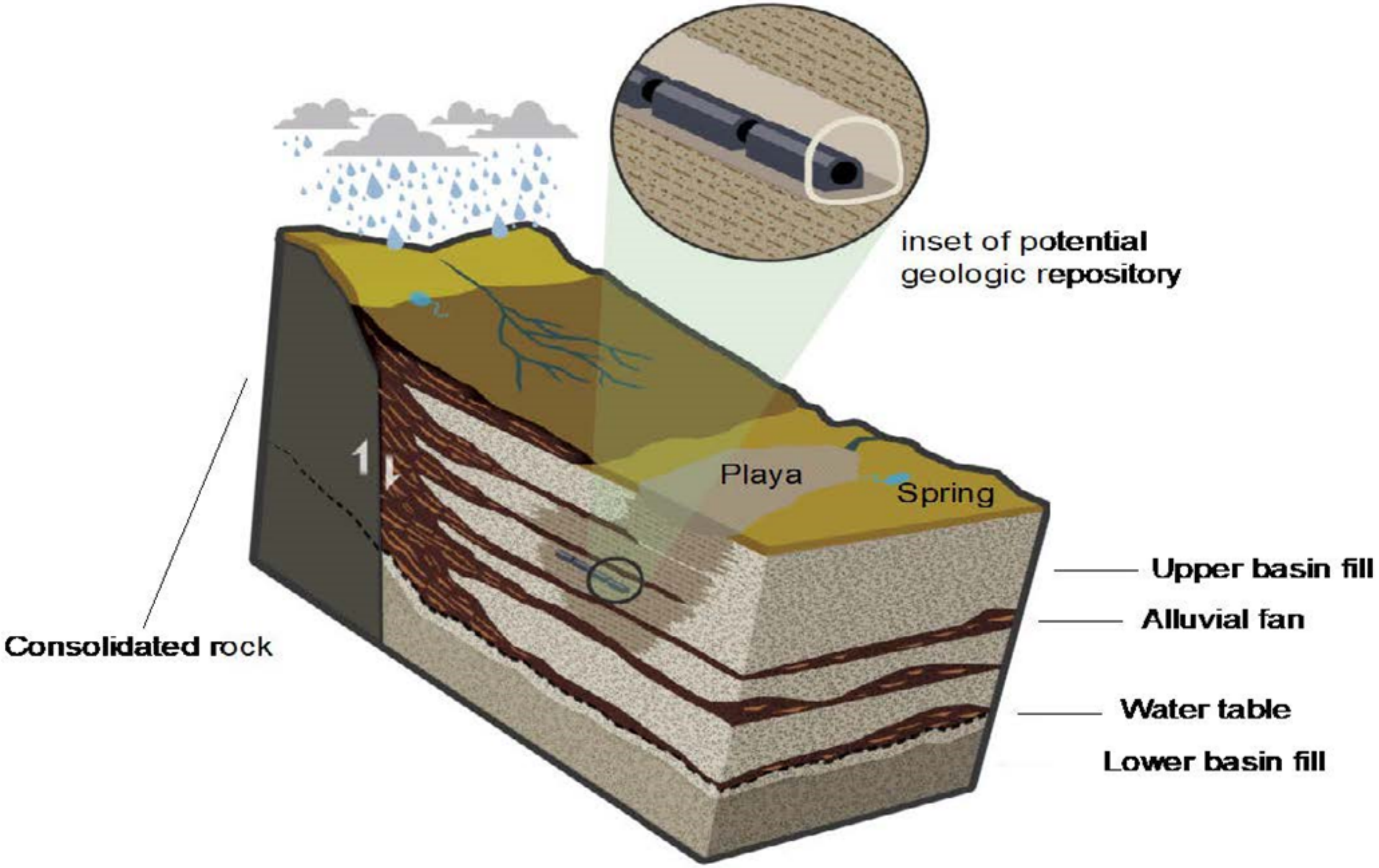
- Unsaturated alluvium reference case is not associated with a host rock R&D program
- Concept of a deep geologic repository in the unsaturated zone (UZ) is used to improve understanding and drive capability development
- Within Geologic Disposal Safety Assessment (GDSA) and Direct Disposal of Dual Purpose Canisters (DPC)
- Resulting capabilities are broadly applicable




UZ = Unsaturated Zone
DPC = Dual Purpose Canisters
EBS = Engineered Barrier System
GDSA = Geologic Disposal Safety Assessment (including GFM)

# Host Rock Characteristics

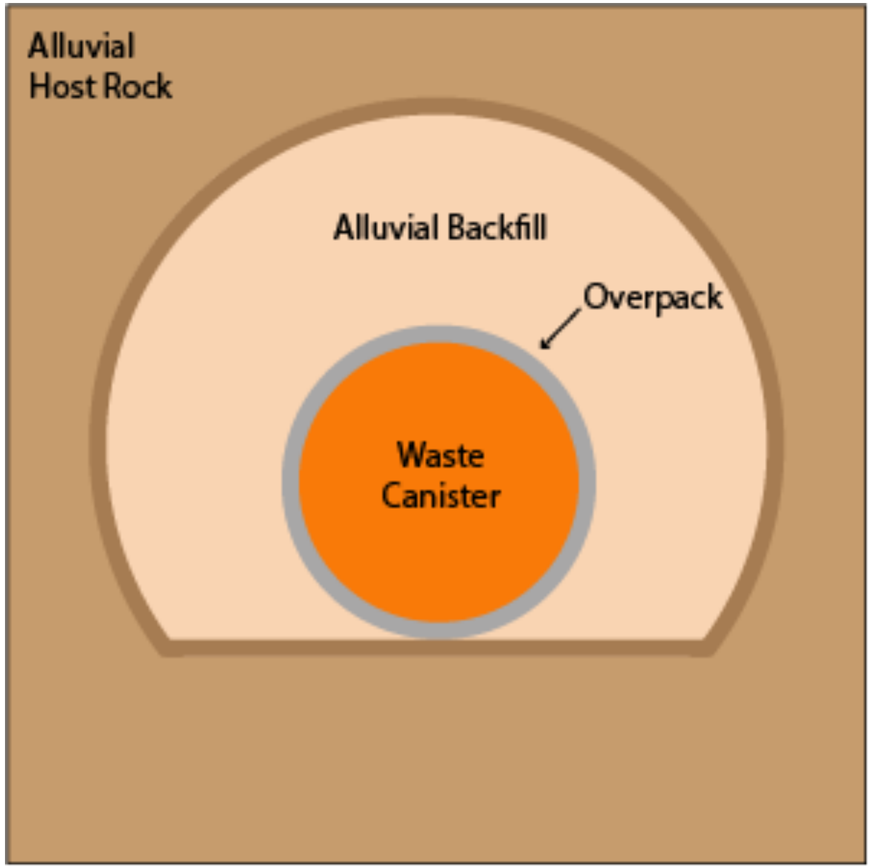
- Repository above the water table
- Complex stratigraphy and structure
- Lithologic heterogeneity
- Perched water tables and local aquifers
- Oxidizing in repository; reducing at some depth below water table




Mariner et al. 2018

# Disposal Concept

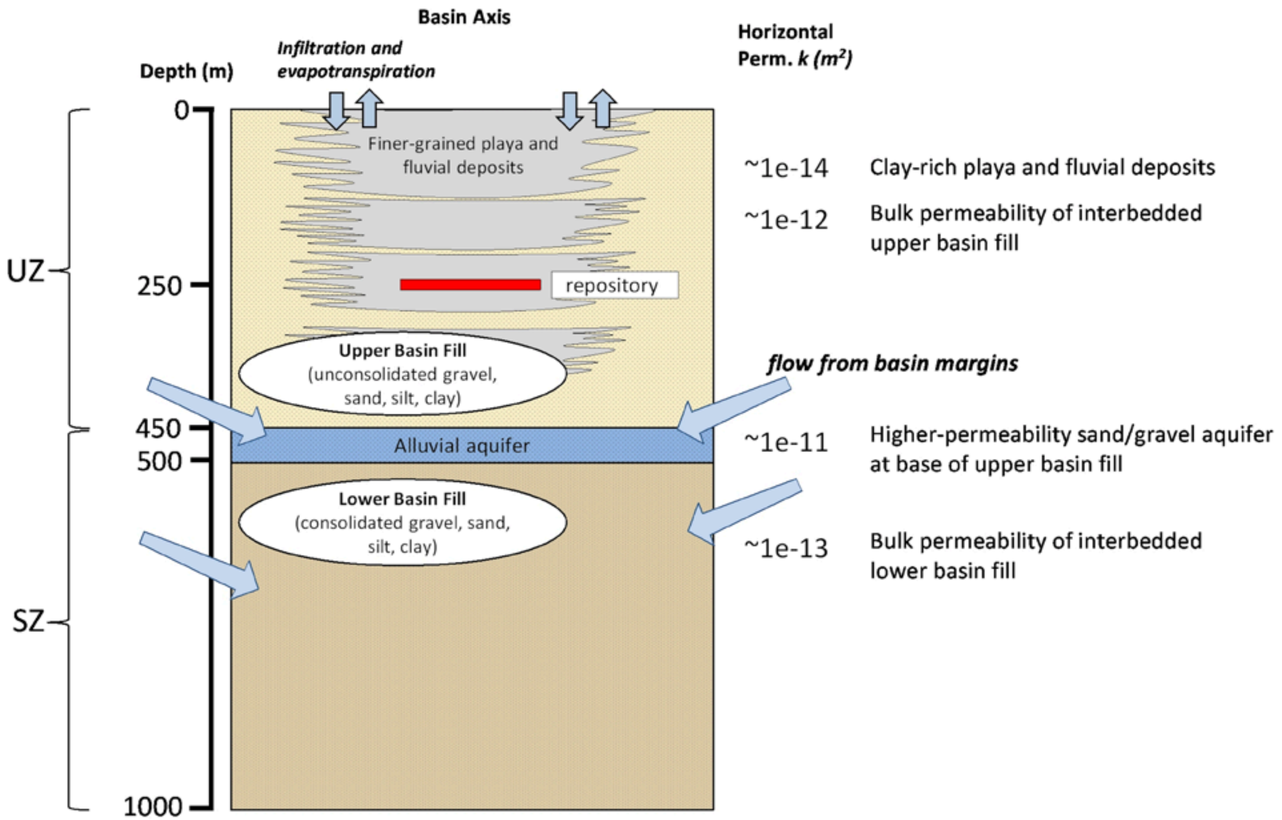
- Direct disposal of Dual Purpose Canisters (DPCs)
  - e.g., containing 24 or 37 pressurized water reactor (PWR) assemblies
- Overpack provides mechanical strength and appropriate protection against corrosion
- Crushed alluvium backfill provides shielding and protects against rockfall
- Thermal management achieved through waste package loading, aging, and spacing
- Maintain temperature <100 ºC and water saturation > 0 along axes of pillars




Sevougian et al. 2019

# Post Closure Safety Strategy

- Containment
  - Corrosion resistant overpack
  - Low water saturation
- Limited Transport
  - Deep water table
  - Low effective permeability ($k_{eff}$)
- Dilution
  - In saturated zone
- Climate variability (arid to pluvial)
  - In some locations recharge has not occurred over the last 100,000 y
  - Under pluvial conditions, downward liquid flux may be 5 to 10 mm/yr
  - Saturation would increase only until $k_{eff}$ balances the infiltration rate



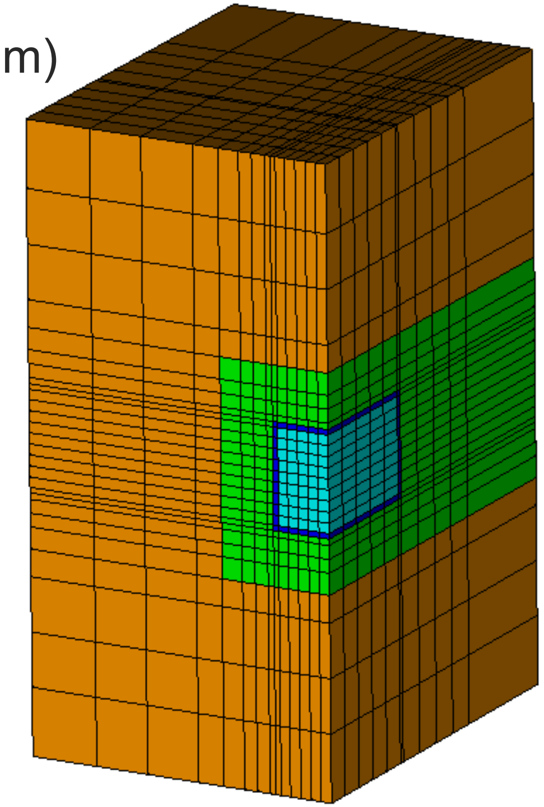

Mariner et al. 2018; Perry et al. 2018

# Knowledge and Capability Gaps

- Criticality Consequence Analysis for Direct Disposal of DPCs
  - What is the power output that can be sustained before driving water out of the package?
  - What are impacts to radionuclide inventory?
  - What are impacts to disposal system?
- Integrated DPC/GDSA Process Model Capability Development
  - Heat and radionuclide source terms associated with criticality event
  - Numerical methods for solution of highly nonlinear partial differential equations
  - Temperature-dependent properties and processes
- Geologic Framework Modeling (GFM) Capability Development
  - Complex structure and stratigraphy
  - Spatial heterogeneity
  - Workflow from GFM to flow and transport simulation
- Geologic meshing

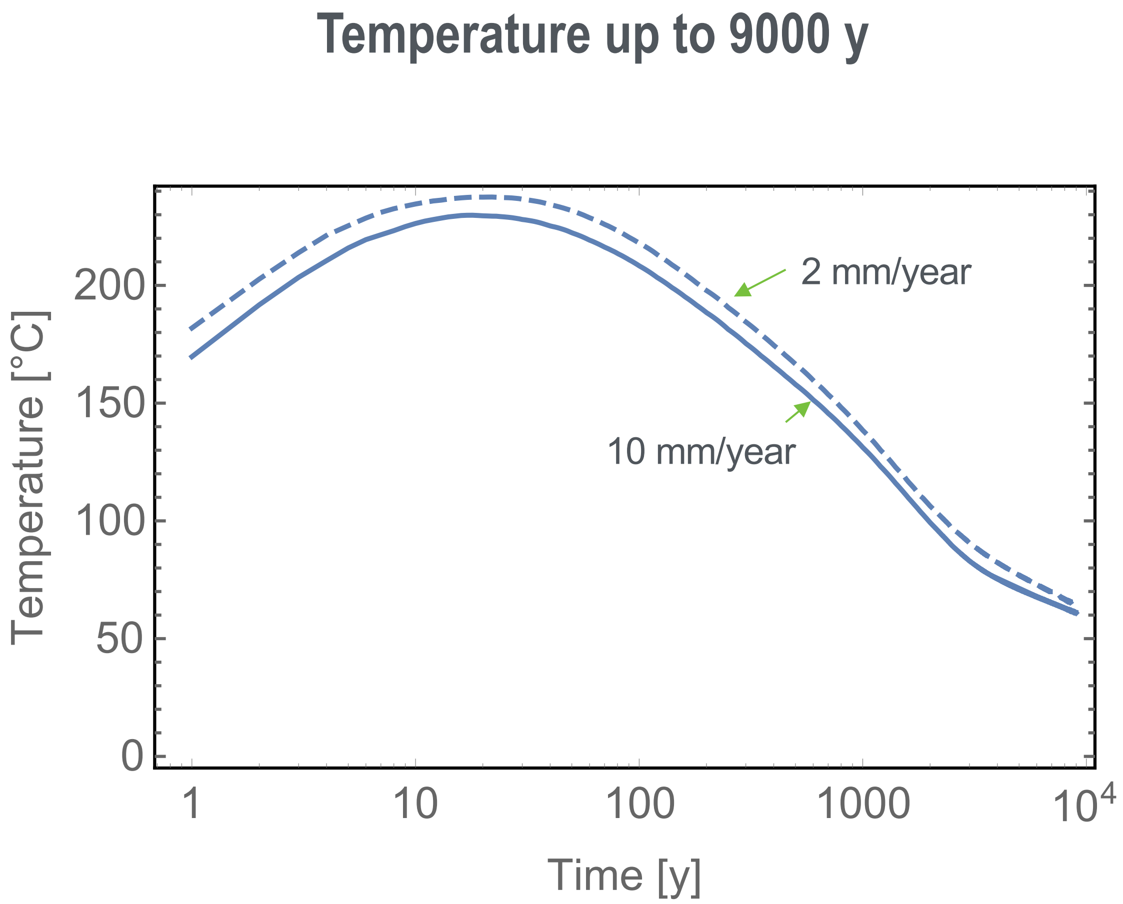
# Priority R&D – DPC Criticality Consequence Analysis

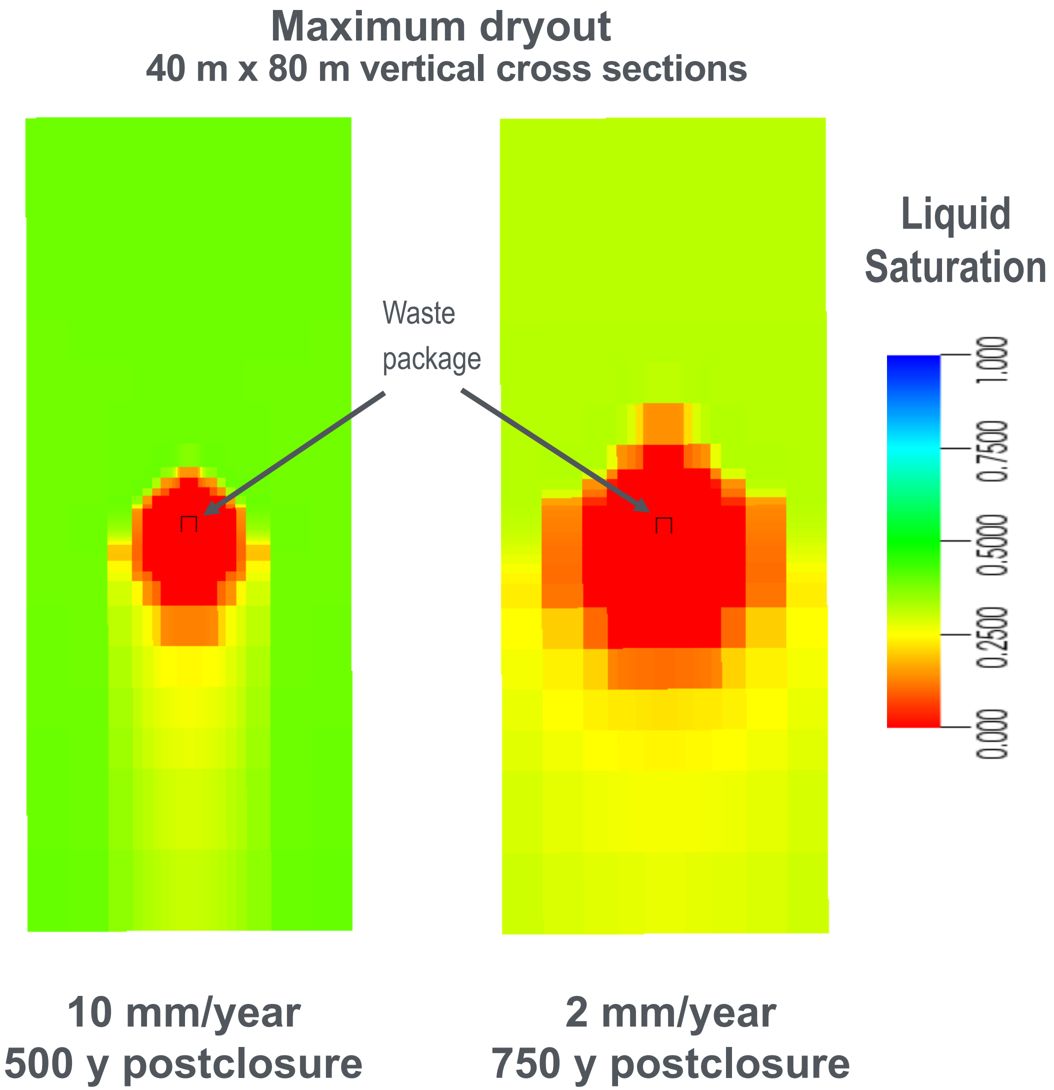
- Geometry
  - Consistent with GDSA Unsaturated Alluvium reference case (Sevougian 2019; Hardin and Kalinina 2016)
  - 40 m drift spacing, 40 m center-to-center spacing within drift
  - Square cross-section for drift (4m x 4m) and DPC (1.67 m x 5 m x 1.67 m)
  - 0.1 m overpack/shell
- Properties
  - Permeability $10^{-14}$ $m^2$ (alluvium) $10^{-13}$ $m^2$ (backfill)
  - Thermal conductivity  = 1 W/(m·K) (dry) and 2 W/(m·K) (wet)
  - Canister internals = hydraulic properties of backfill
- Scenario
  - Postclosure with 37-PWR assembly and backfilled drifts in place
  - Top of DPC shell breached at 9000 years allowing water to enter
  - Initiate criticality event when canister is filled with water
- Cases
  - 10 mm/year and 2 mm/year percolation into waste package
  - Range of power outputs for criticality event



Price et al. 2019; Price 2020

# 37-PWR DPC in Unsaturated Alluvium: Before Breach

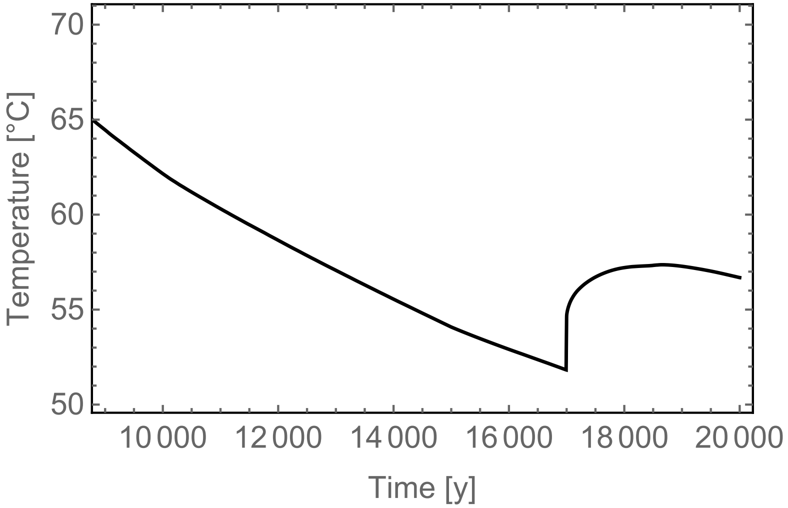


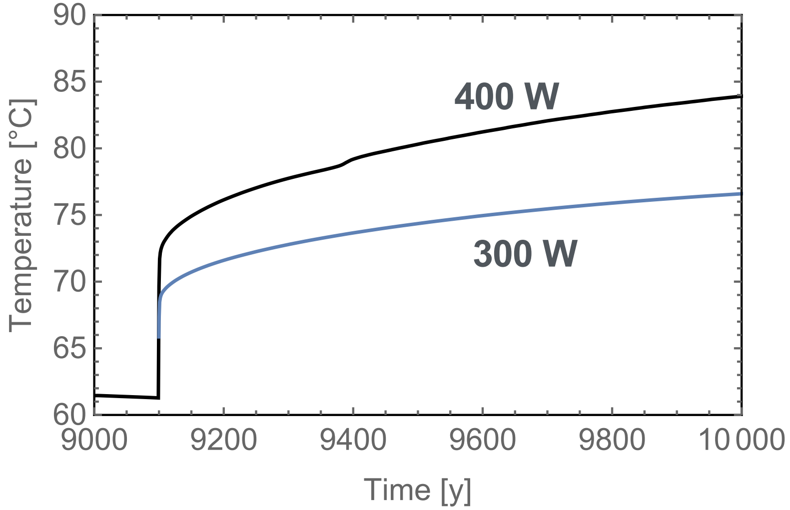

Price et al. 2019; Price 2020

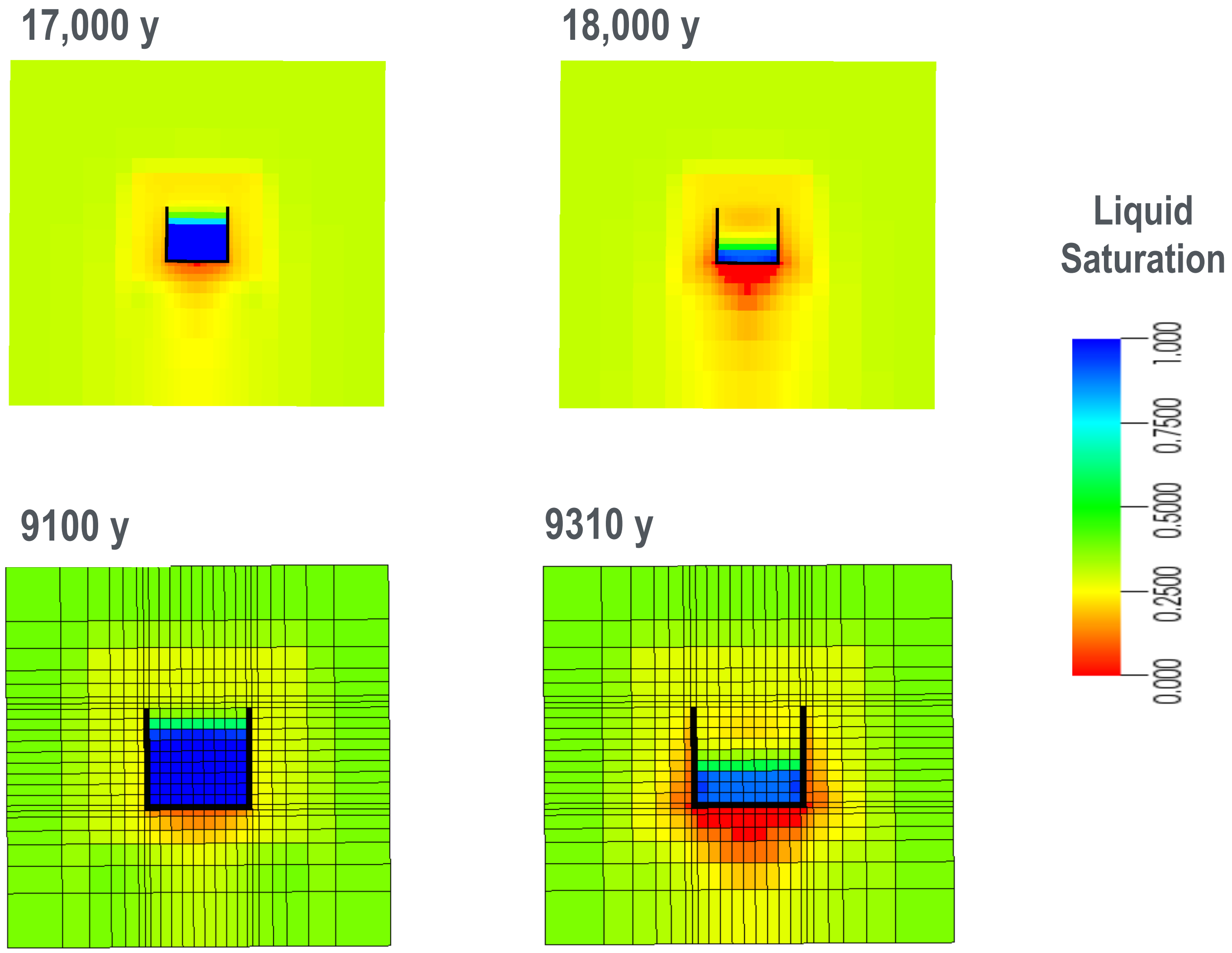
# 37-PWR DPC Hypothetical Criticality Events

**2 mm/year**
**100 W event**




**10 mm/year**
**400 W event**

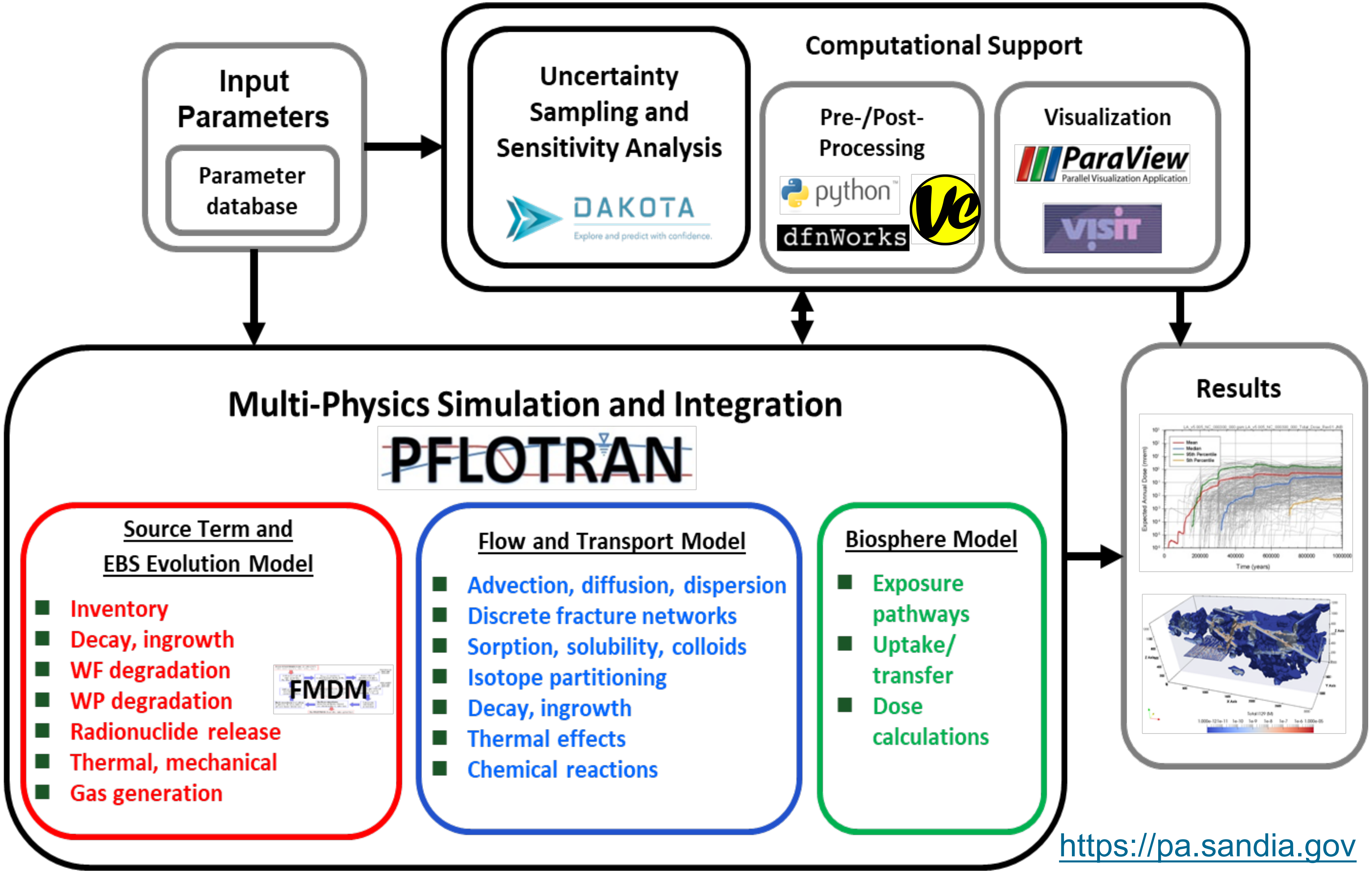



Price et al. 2019; Price 2020

# Priority R&D – Simulation Capability for High Temperature Systems

- GDSA Framework
  - Open-source software
  - Leverages high-performance computing
  - Transparent model development and implementation



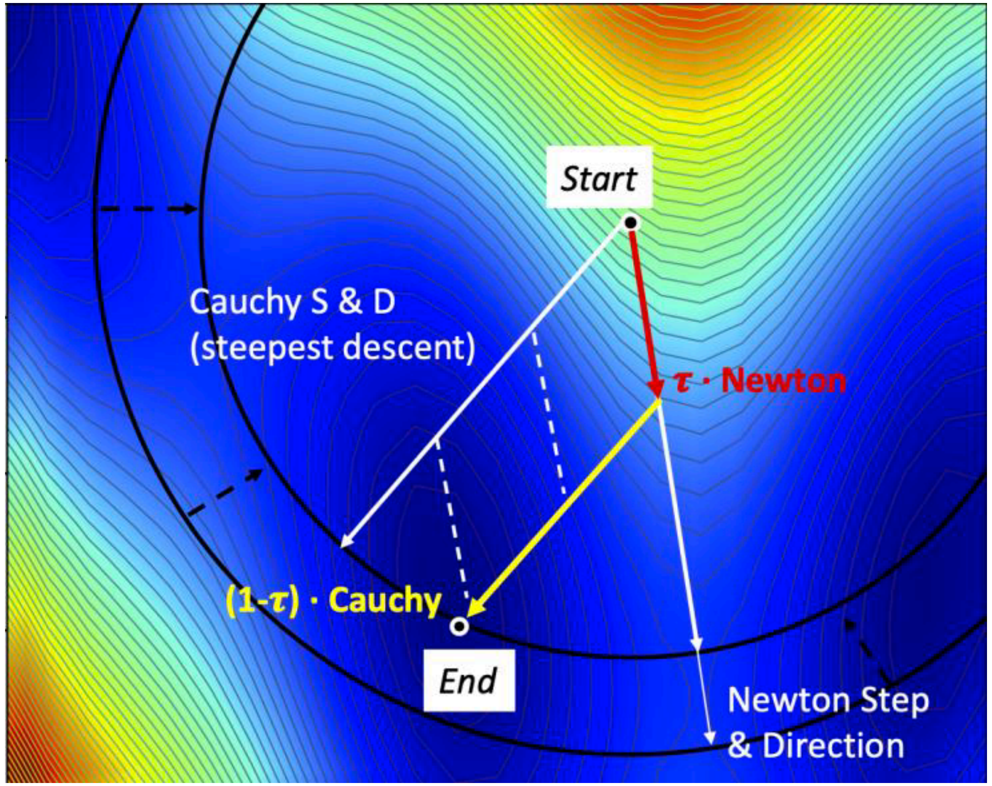

https://pa.sandia.gov

# Advanced Nonlinear Solvers

## Minimize the residual of a multi-dimensional function

1. Newton Step and Direction overshoots.
2. Newton Trust Region (NTR) truncates the step to keep it within the region in which minimum is predicted to exist.
3. Cauchy Step and Direction follows the steepest descent.
4. Newton Trust Region Dogleg Cauchy (NTRDC) combines NTR with Cauchy to find the minimum in a single iteration.

NTRDC reduces computation time by a factor of approximately 35.

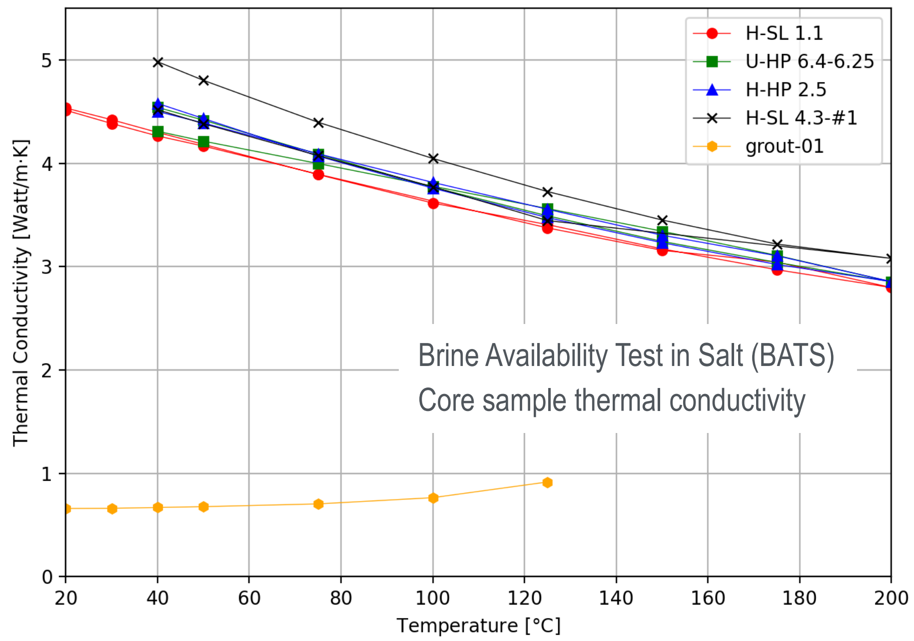



A demonstration of the NTRDC method. The algorithm corrects the appropriate Newton step-and-direction by reducing the trust region and adds Cauchy step-and-direction if the solution update can be improved further in the same iteration.

Mariner et al. 2020

# Temperature-Dependent Thermal Conductivity

- Temperature-dependent processes
  - Corrosion
  - Mineralogical changes
  - Aqueous speciation (radionuclide solubilities)
  - Thermal expansion of solids
  - Buoyancy-driven fluid flow

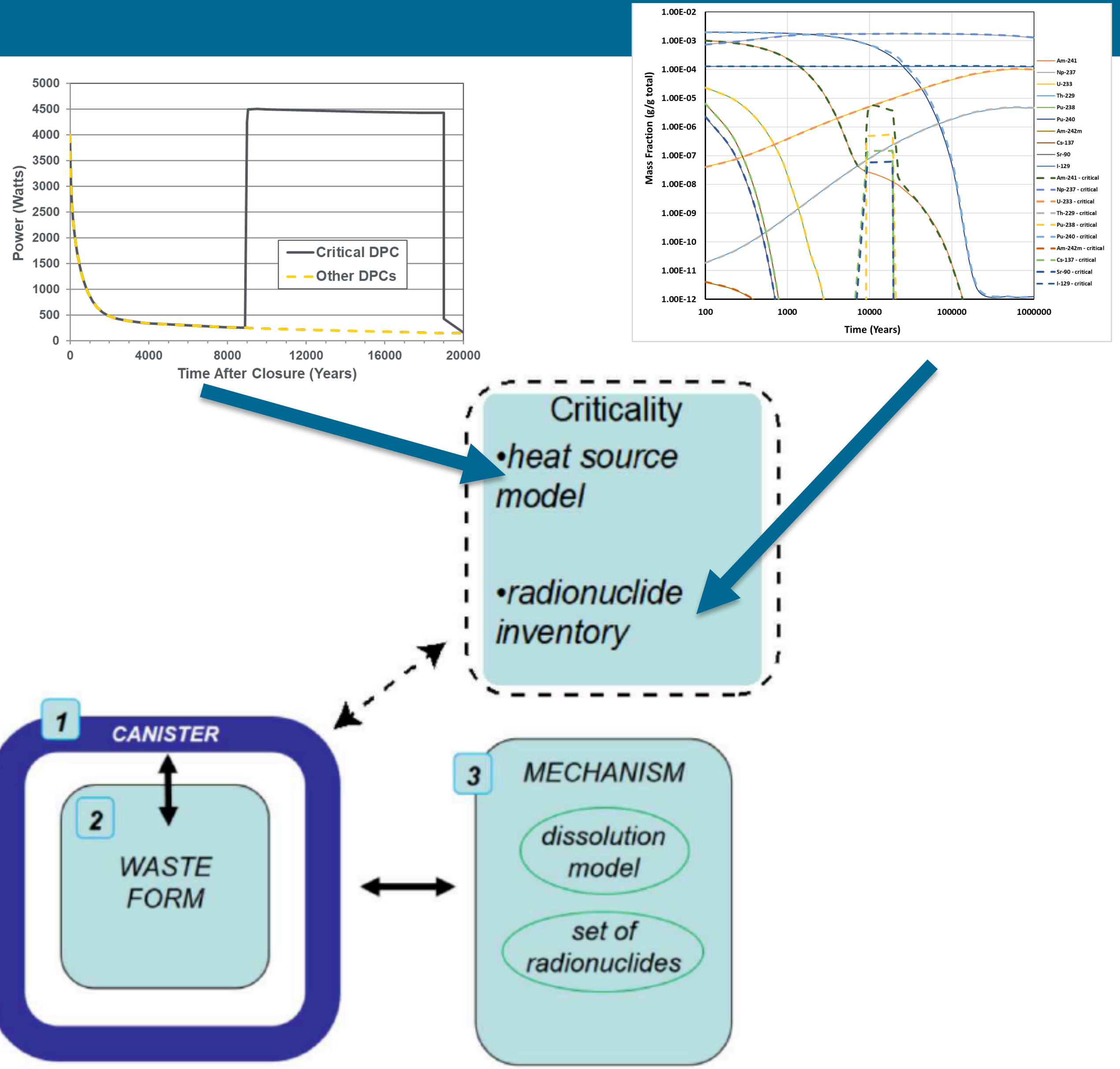



Kuhlman et al. 2020;
LaForce et al. 2020

| Name | Function |
|---|---|
| Default | $\kappa_T^D(S_l)=\kappa_T^{dry}+\sqrt{S_l}\left(\kappa_T^{wet}-\kappa_T^{dry}\right)$ (24) |
| Constant | $\kappa_T=\kappa_T^C$ (25) |
| Linear Resistivity | $\kappa_T(S_l,T)=\dfrac{\kappa_T^D(S_l)}{a_1+a_2(T-T_{ref})}$ (26)<br>Granite, basalt, shale, and salt |
| Cubic Polynomial | $\kappa_T(S_l,T)=\kappa_T^D(S_l)\left[1+\beta_1(T-T_{ref})+\beta_2(T-T_{ref})^2+\beta_3(T-T_{ref})^3\right]$ (27)<br>Various soils at temperatures up to 1700 °C |
| Power Law | $\kappa_T(S_l,T)=\kappa_T^D(S_l)\left(\dfrac{T-T_{ref}}{300}\right)^{\gamma}$ (28)<br>Crystals, ceramics, and engineering materials |

# Criticality Submodule

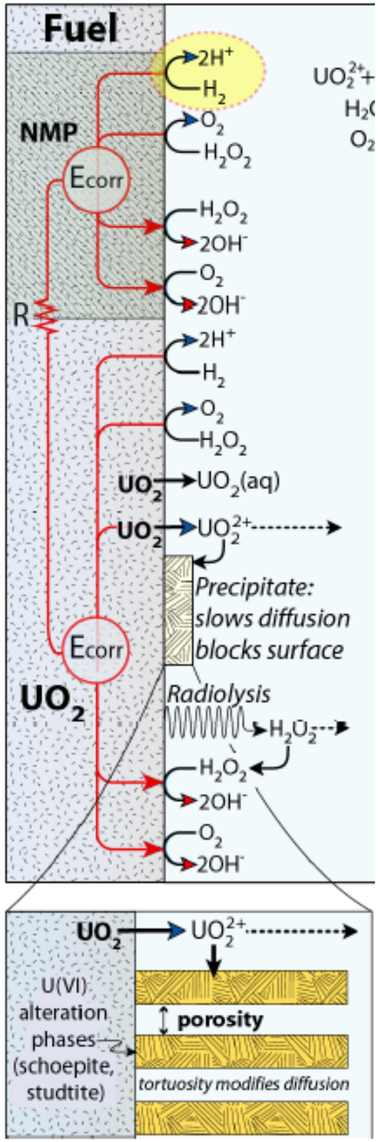
- Capability added to PFLOTRAN's Waste Form Process Model
- Reads files containing
  - Power as function of time
  - Radionuclide inventory as function of time
- Future: integrate with neutronics calculations to model criticality power output as a function of water saturation




Price et al. 2019

# Fuel Matrix Degradation Model (FMDM)

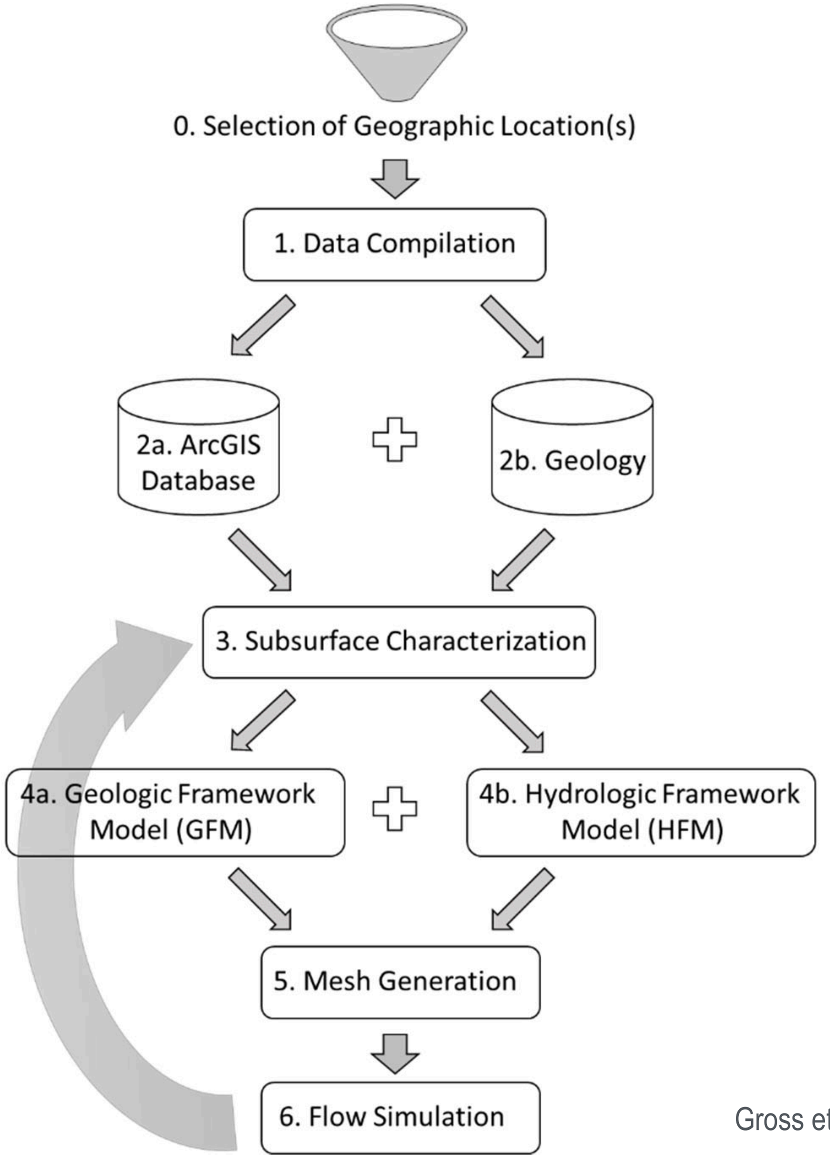
- 1-D reactive transport model to simulate dissolution of spent nuclear fuel (SNF) as a function of
  - Radiolysis
  - Diffusion of reactants through growing alteration layer
  - Interfacial corrosion potential
- GDSA Framework integration:
  - Implement efficient numerical methods for mechanistic coupling
  - Speed computation using machine-learned surrogate models
  - Future: Couple to evolution of in-package chemistry given specific conditions
  - Future: Model validation against SNF dissolution experiments




(Jerden et al. 2018; Mariner et al. 2020)

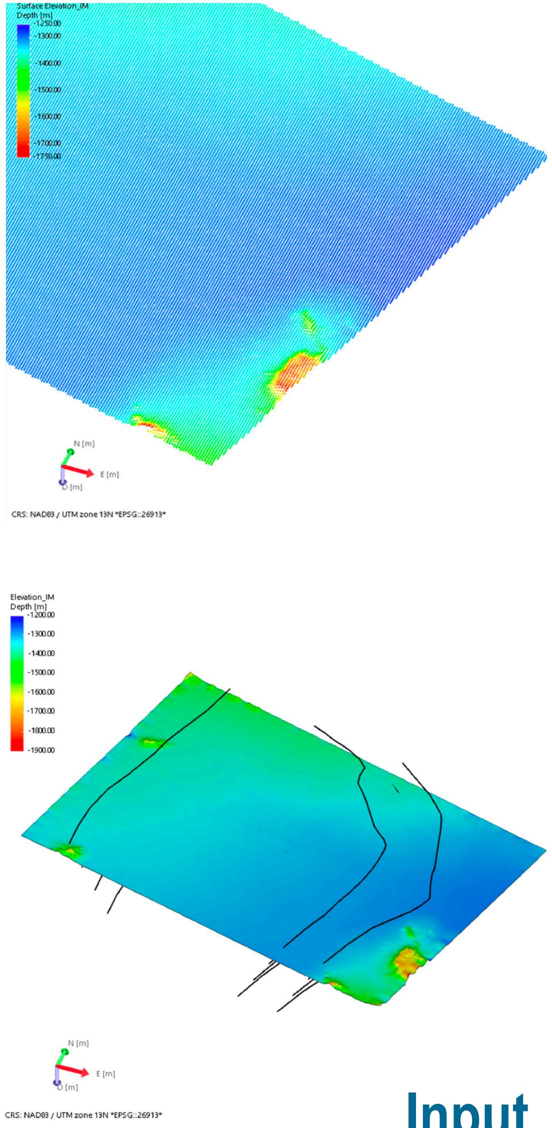
# Priority R&D – 3-Dimensional Geologic Framework Model (GFM)

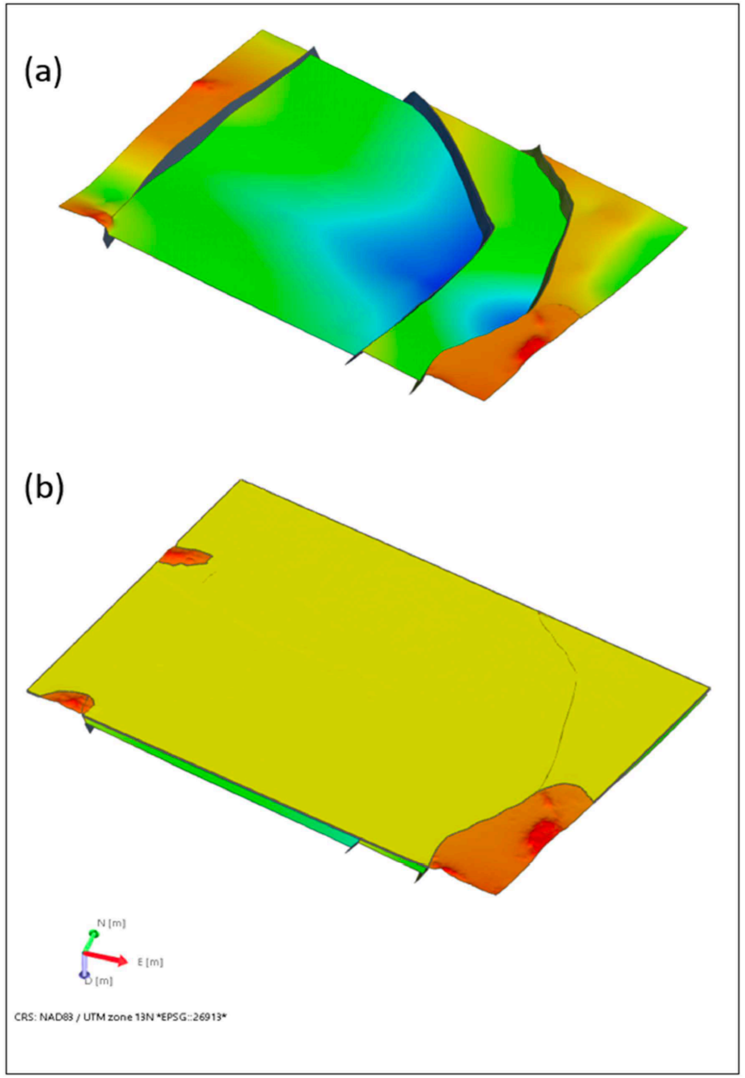
- Constructed from surfaces (stratigraphic horizons, faults) derived from 3D seismic surveys and borehole data
- Informed by digital elevation maps, geologic maps, cross sections, and conceptual models
- May also hold lithologic data, hydrologic data
- Iteration improves subsurface characterization

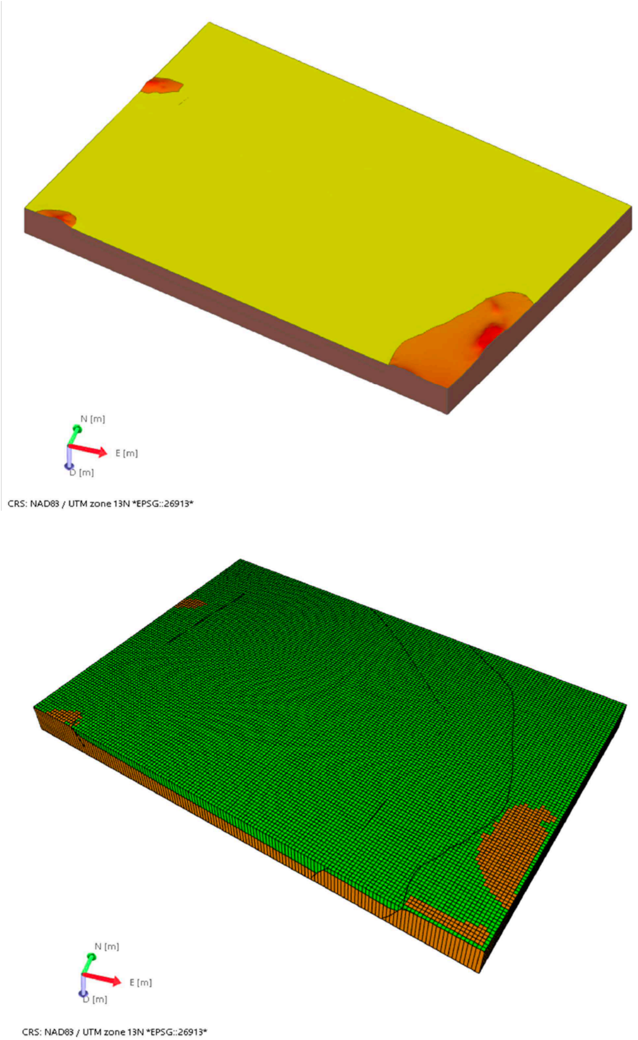



Gross et al. 2019

# Complexity Makes Alluvial Basin GFM a Useful Test Case





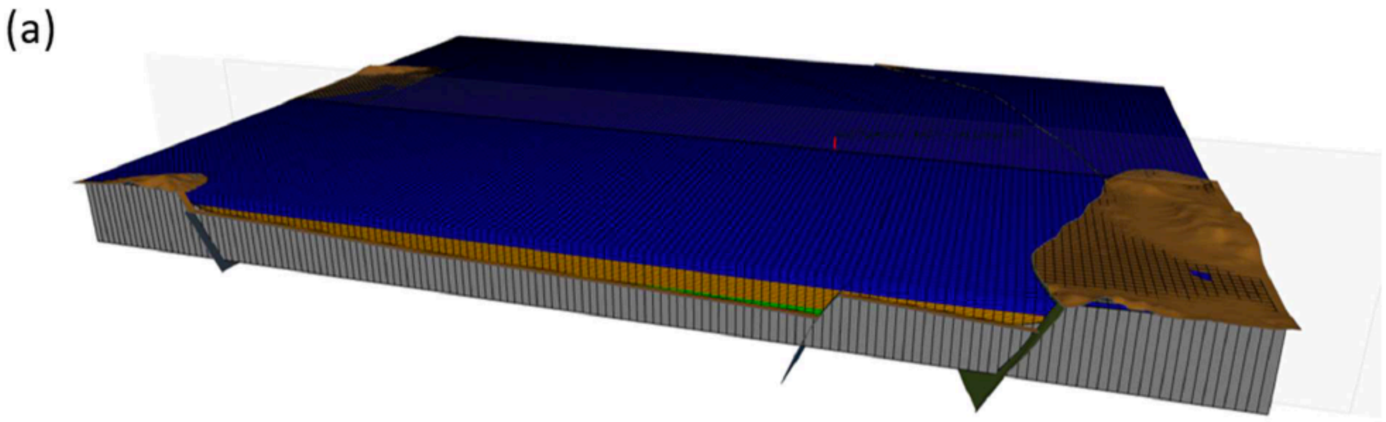



Input → → Surfaces → → Volumes

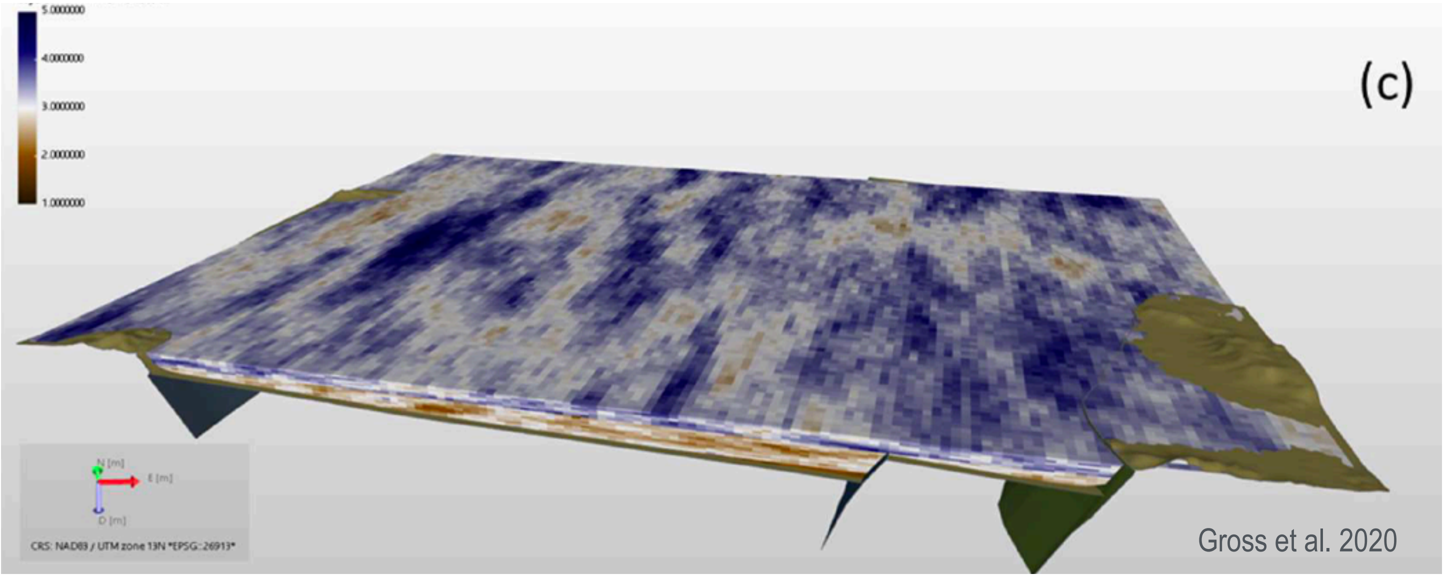
Gross et al. 2020

# Adding Lithofacies and Hydrologic Properties

- Lithofacies
  - 3 alluvial facies
  - Bedrock




- Geostatistical distributions describe hydrologic properties
  - Porosity
  - Permeability

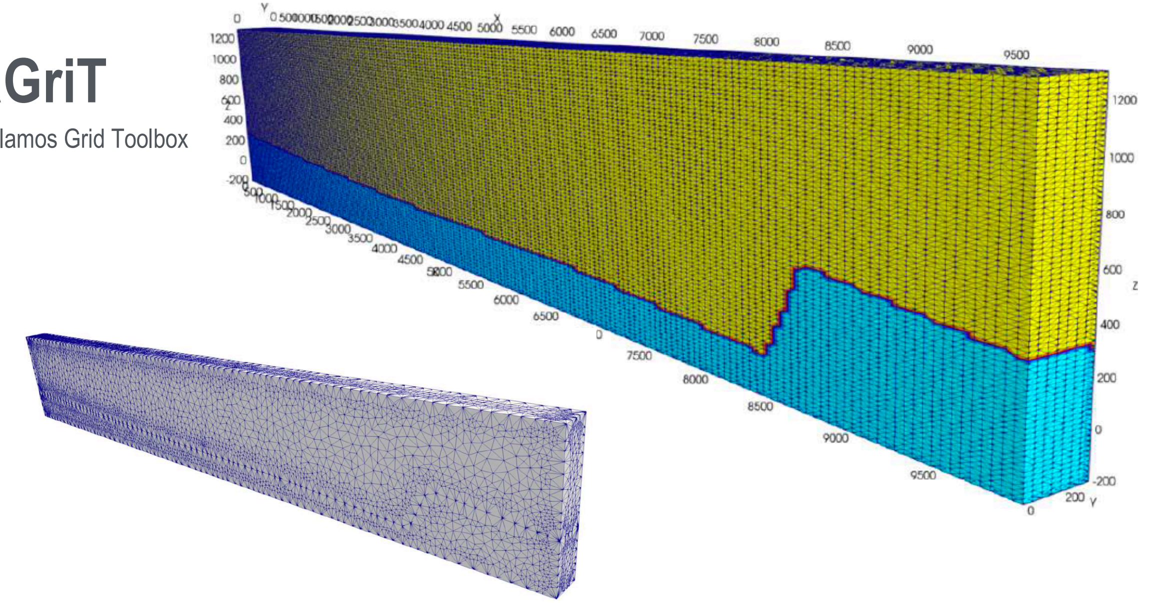


# GFM to Computational Mesh

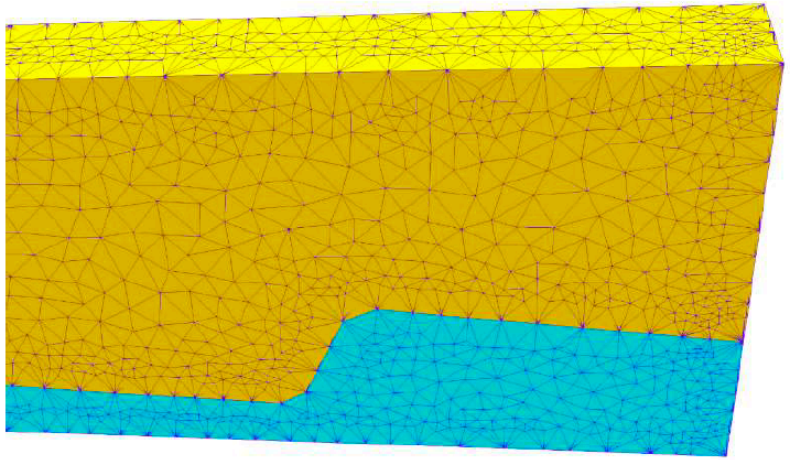
- LaGriT
  - Automate information processing and workflow to create computational mesh from GFM
  - Versatile tools for user-controlled generation of Voronoi mesh using Delauney triangulation
- VoroCrust
  - The first provably correct algorithm for conforming Voronoi tessellation
  - Automated algorithm simplifies meshing

**LaGriT**

Los Alamos Grid Toolbox



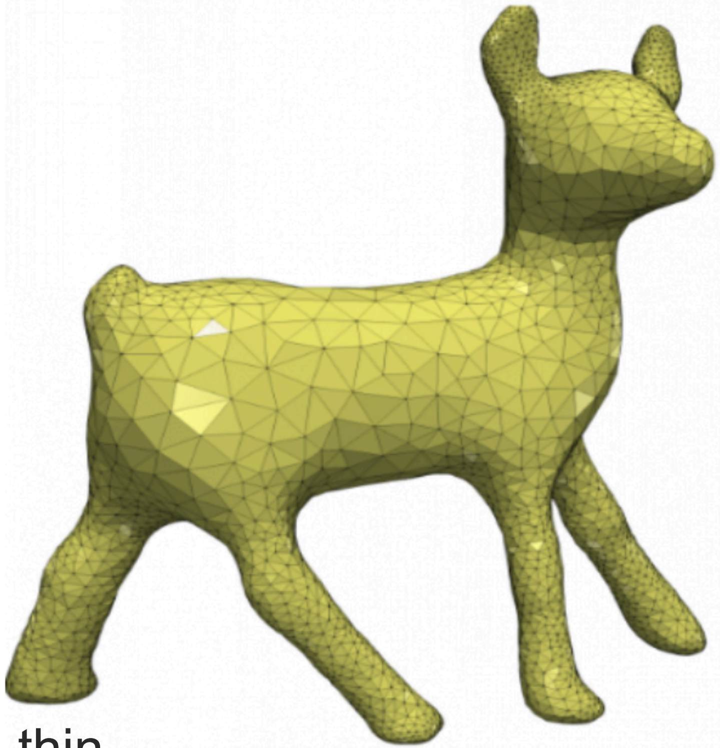
**Vorocrust**

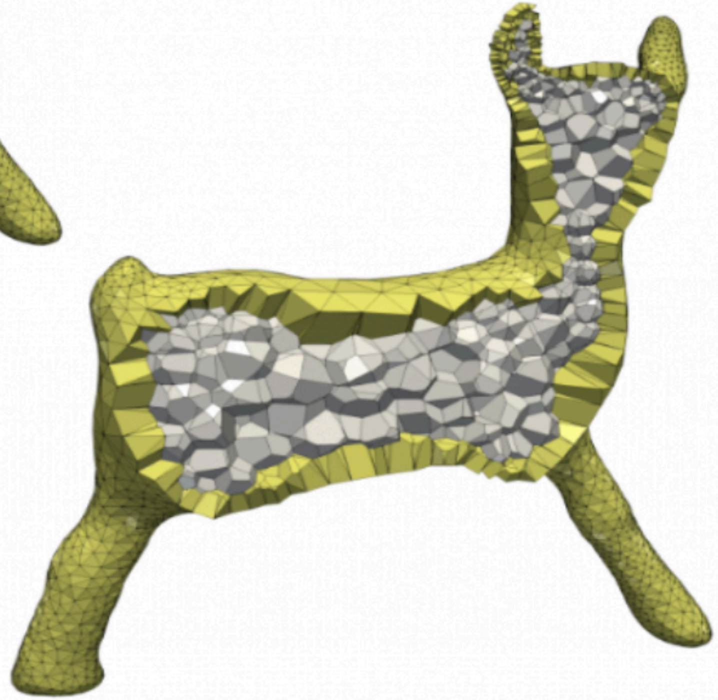


Gross et al. 2020

# VoroCrust Development

- User-friendliness
  - User-controlled mesh specifications
  - Input and output formats
  - User manual and website
- Computational efficiency
  - Parallelization
- Advanced capability
  - Anisotropic Voronoi cells for meshing thin features and stratigraphic layers





Mariner et al. 2020

https://vorocrust.sandia.gov

# Priority R&D – Forward Look at GDSA-DPC Integration

**Prioritization of Cross-Cutting Research & Development Activities:**
**High-Temperature Shale Reference Case, Disposal of Dual Purpose Canisters, and Geologic Disposal Safety Assessment**

- Representative waste package loading using UNF ST&NDARDS database
- Temperature dependent reactions
  - Mineralogy
  - Aqueous speciation
  - Radionuclide solubility and sorption
- Corrosion models
  - Temperature-dependent, material-specific
  - Waste package
  - Cladding
  - Neutron absorbers
- Thermal-Hydrological-Mechanical evolution of the near field

Price 2020; Freeze and Howard 2020; Stein et al. 2020

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