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
November 4 and 5, 2020
Online Virtual Meeting

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SAND2020-xxxx PE

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Acknowledgements

Mohamed Ebeida, Kris Kuhlman, Tara LaForce, Paul Mariner, Michael Nole, Heeho Park, Frank Perry, Alex Salazar

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)
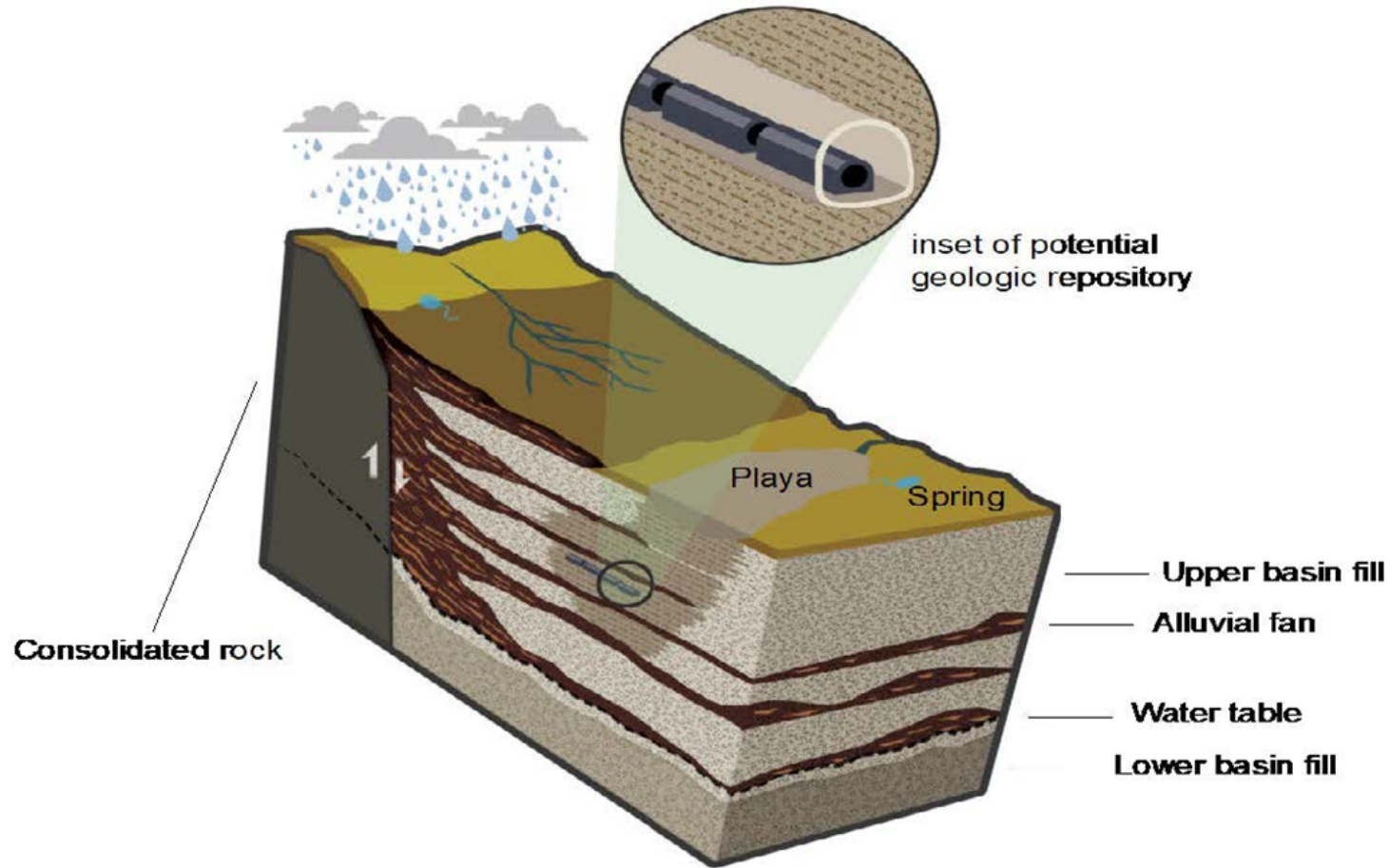- Resulting capabilities are broadly applicable
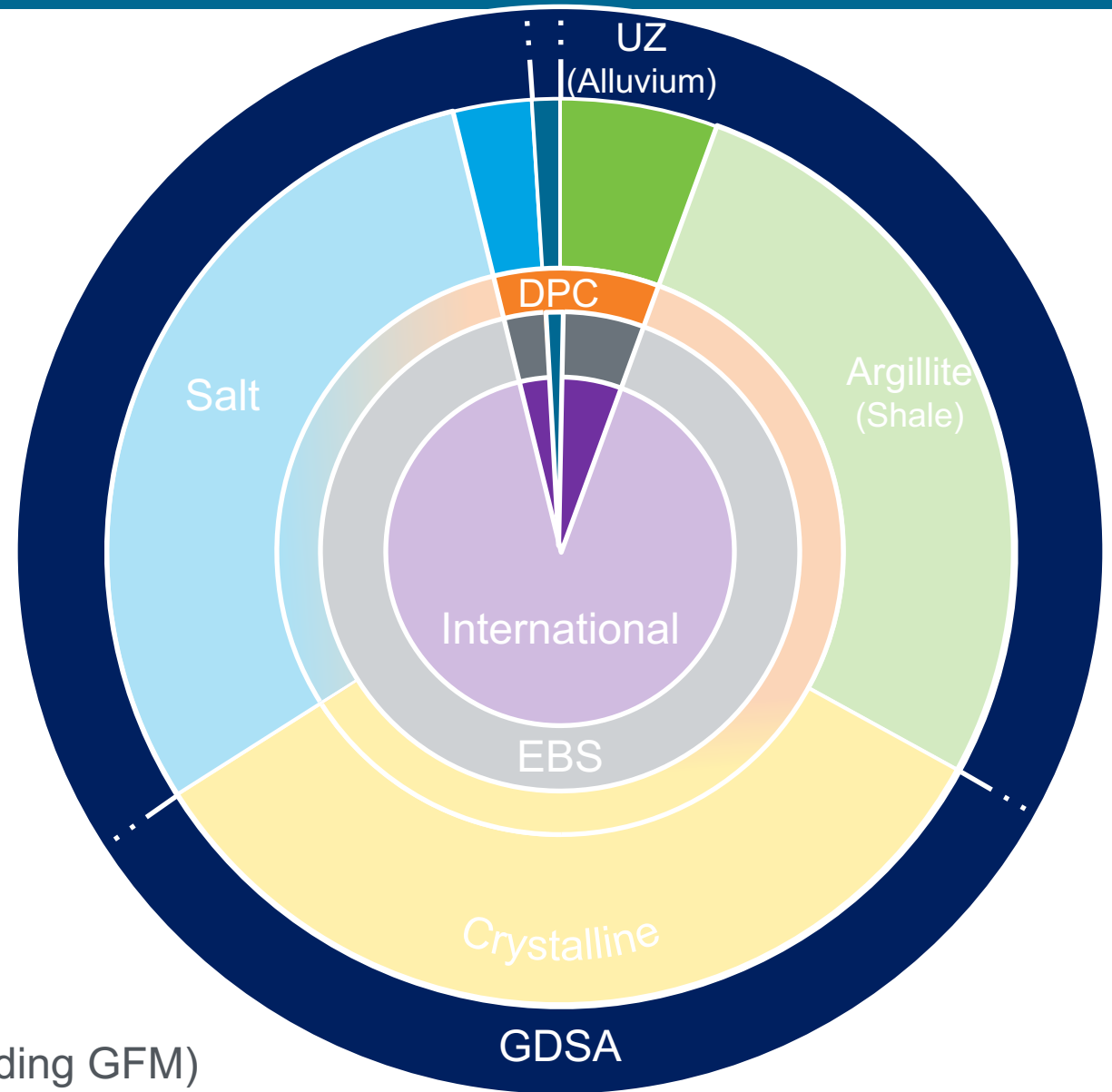
UZ = Unsaturated Zone
DPC = Dual Purpose Canisters
EBS = Engineered Barrier System
GDSA = Geologic Disposal Safety Assessment (including GFM)

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

inset of potential geologic repository

Consolidated rock

Playa

Spring

Upper basin fill

Alluvial fan

Water table

Lower basin fill
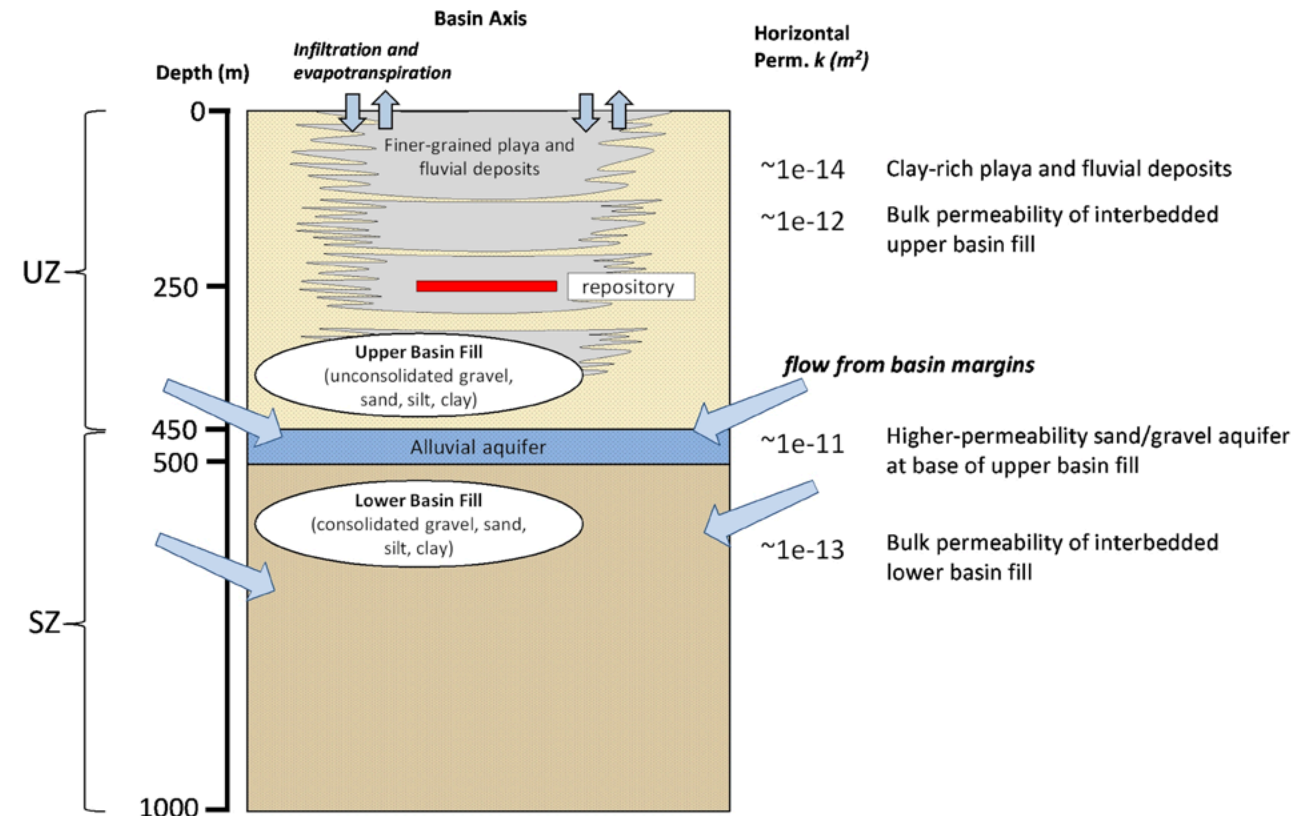
Mariner et al. 2018

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
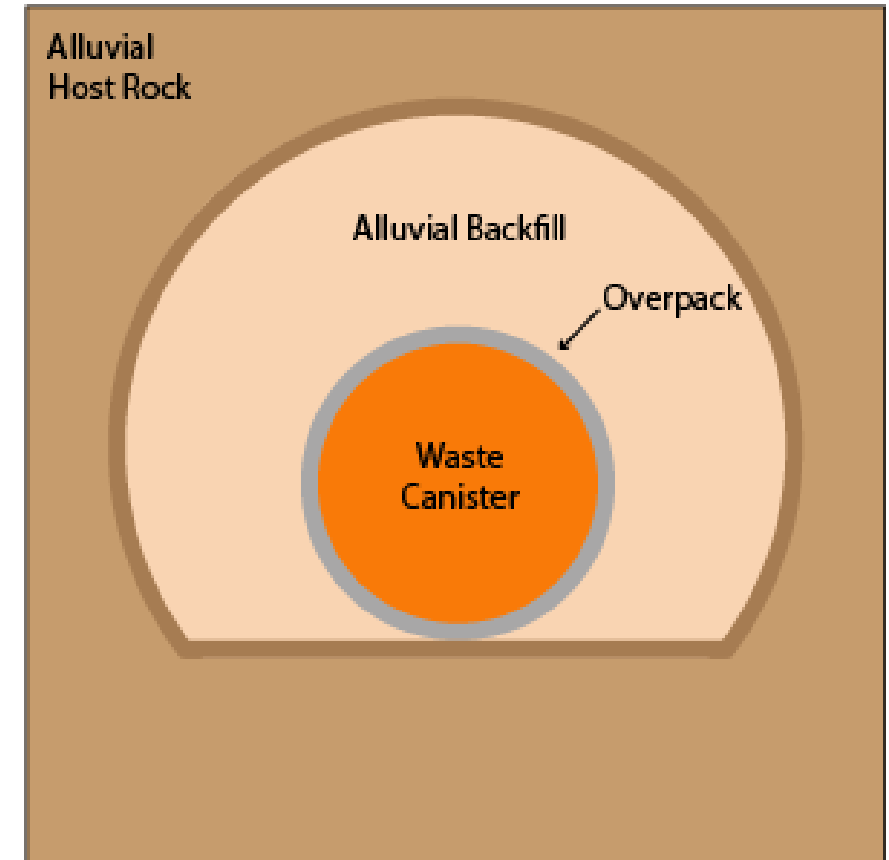
Sevougian et al. 2019

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

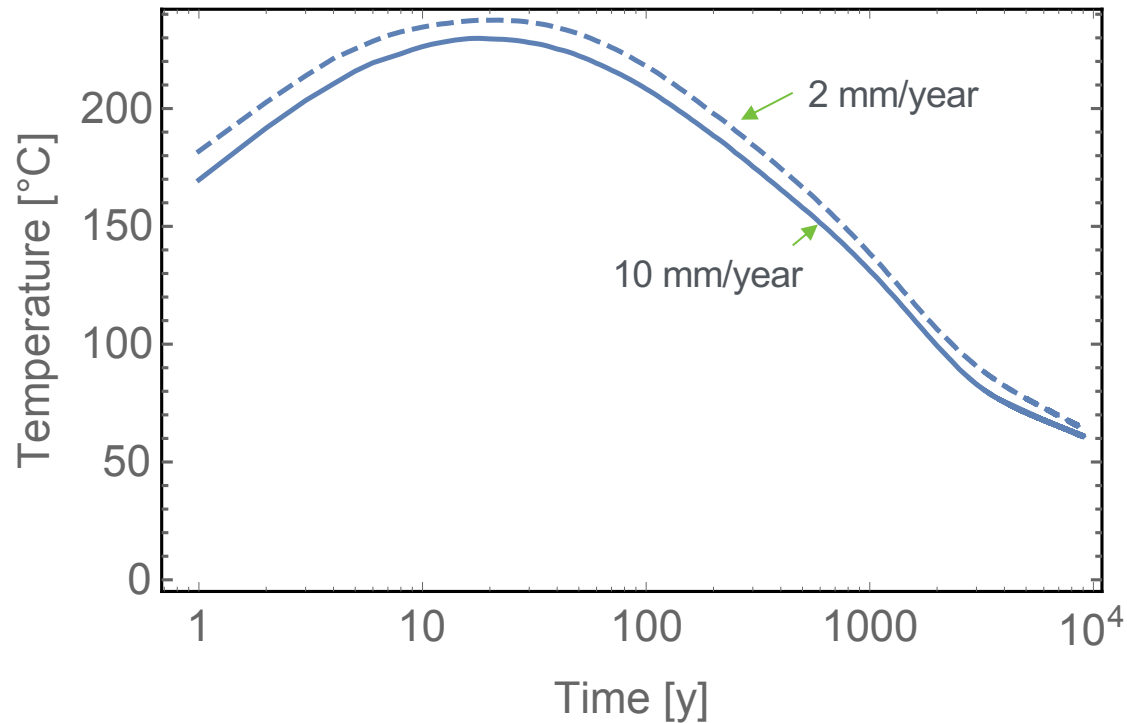# Priority R&D – DPC Criticality Consequence Analysis

- 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
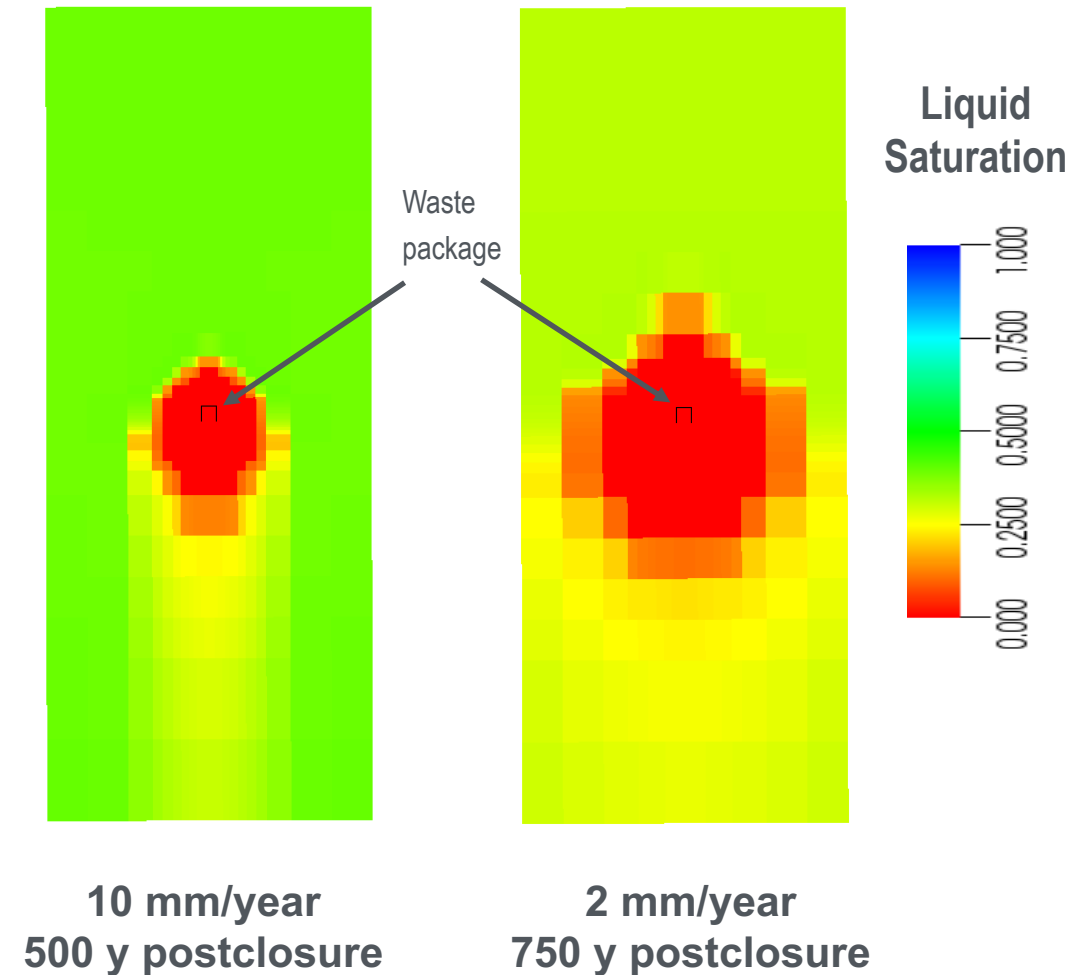 - Range of power outputs for criticality event
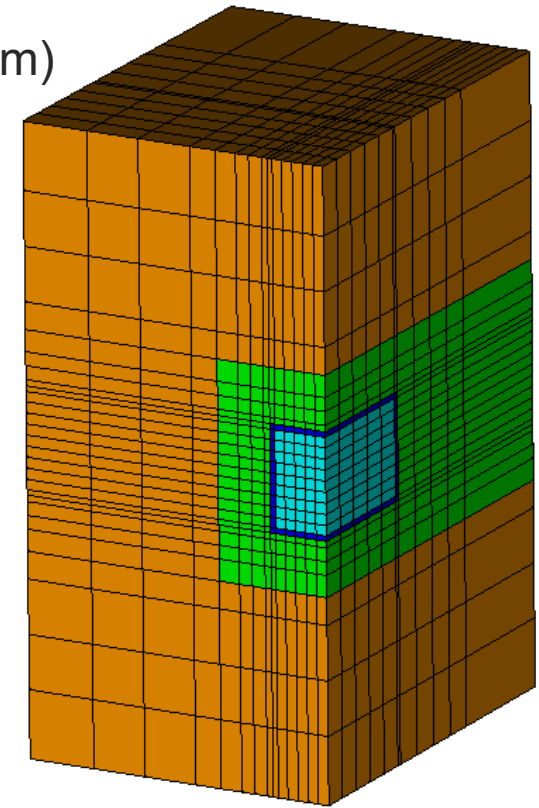
Price et al. 2019; Price 2020

Temperature up to 9000 y

2 mm/year

10 mm/year

Maximum dryout
40 m x 80 m vertical cross sections

Liquid Saturation

Waste package

10 mm/year
500 y postclosure

2 mm/year
750 y postclosure

Price et al. 2019; Price 2020

2 mm/year 100 W event
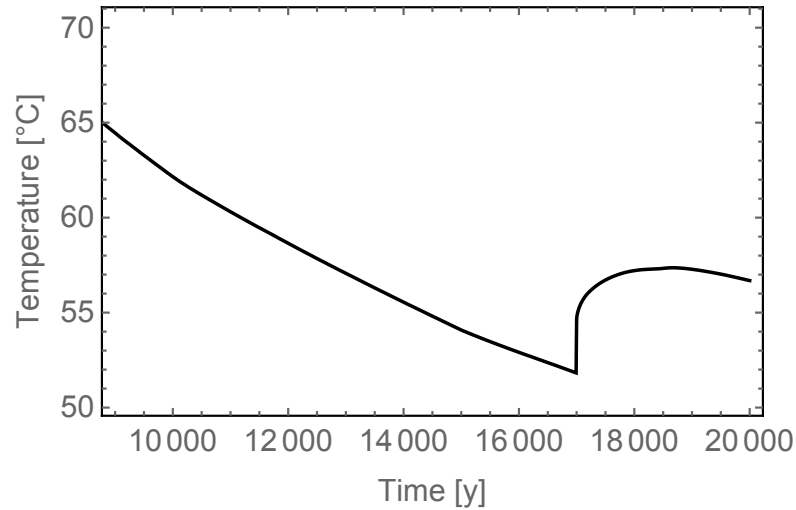
10 mm/year 400 W event
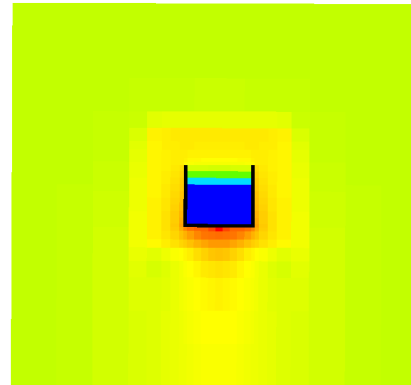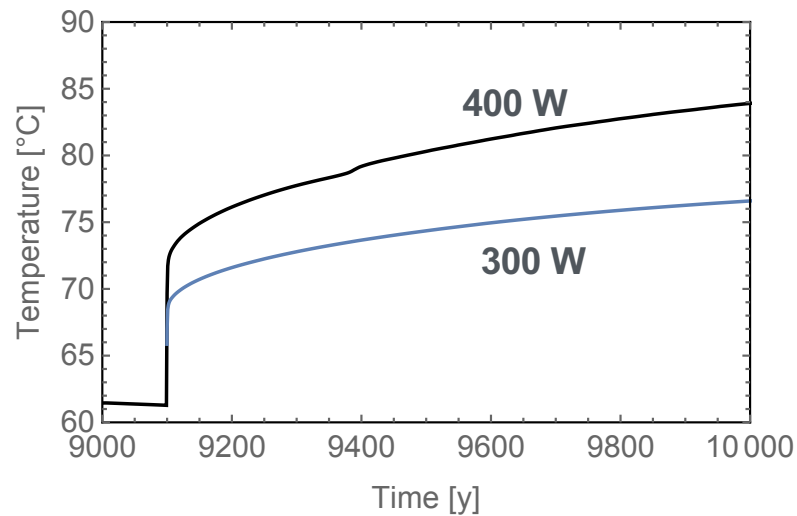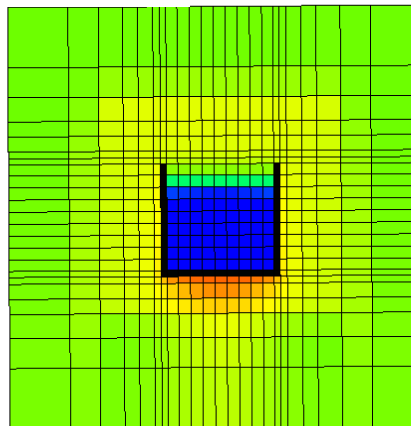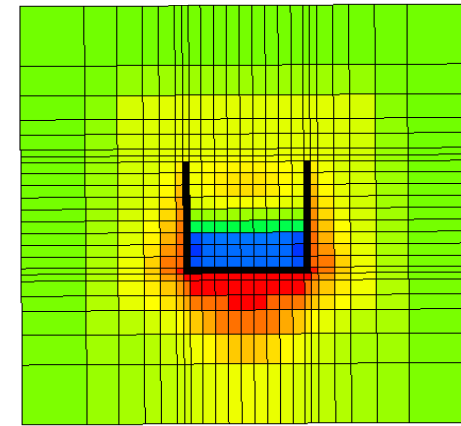
17,000 y

18,000 y

9100 y

9310 y

Liquid Saturation

Price et al. 2019; Price 2020

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

Computational Support

Input Parameters
- Parameter database

Uncertainty Sampling and Sensitivity Analysis
DAKOTA
Explore and predict with confidence.

Pre-/Post-Processing
python
dfnWorks

Visualization
ParaView
Parallel Visualization Application
VisIt

Multi-Physics Simulation and Integration
PFLOTRAN

Source Term and EBS Evolution Model
- Inventory
- Decay, ingrowth
- WF degradation
- WP degradation
- Radionuclide release
- Thermal, mechanical
- Gas generation

FMDM

Flow and Transport Model
- Advection, diffusion, dispersion
- Discrete fracture networks
- Sorption, solubility, colloids
- Isotope partitioning
- Decay, ingrowth
- Thermal effects
- Chemical reactions

Biosphere Model
- Exposure pathways
- Uptake/ transfer
- Dose calculations

Results

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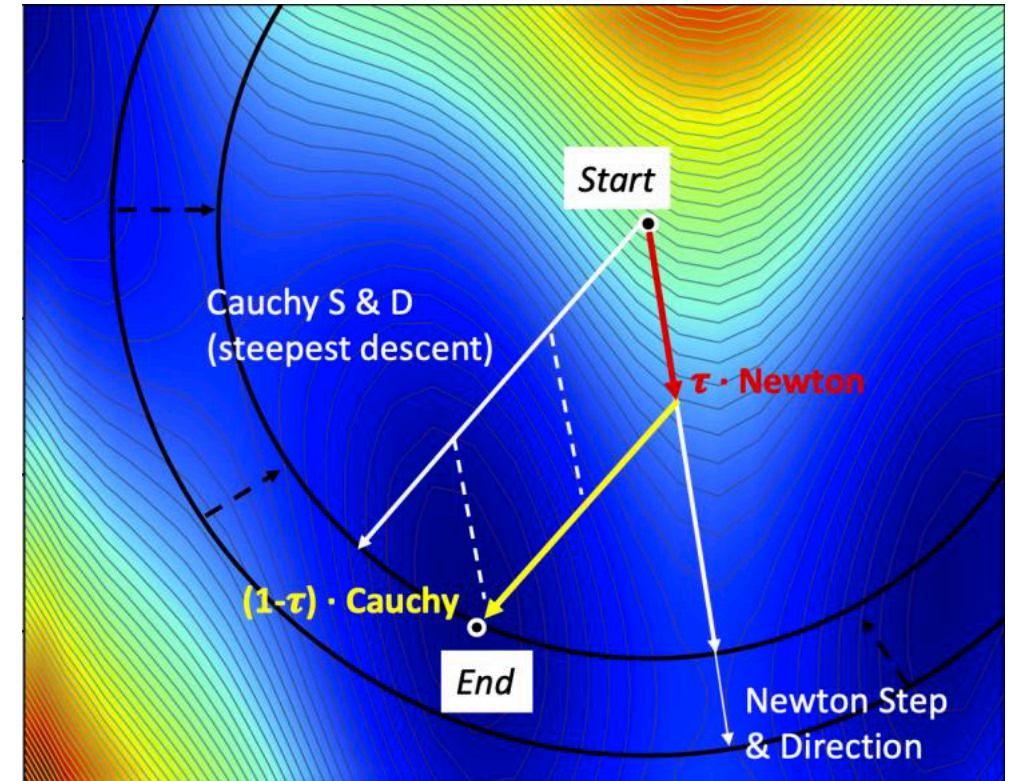
A demonstration of the NTRDC method. The algorithm corrects the appropriate Newton step-and-direction by reducing the trust region and adds Cauchy step-and-direction if the solution update can be improved further in the same iteration.

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

Brine Availability Test in Salt (BATS)
Core sample thermal conductivity
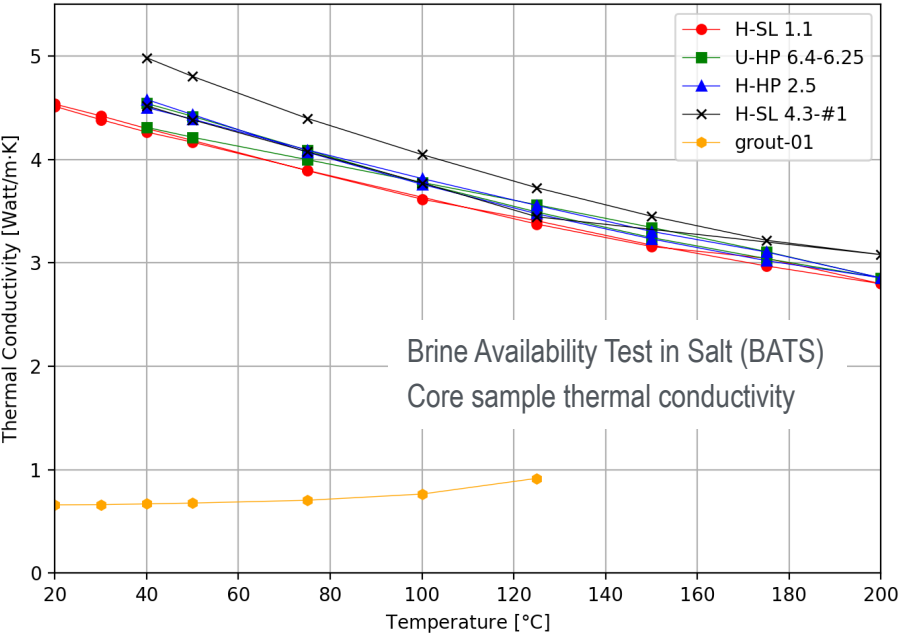
Kuhlman et al. 2020;
LaForce et al. 2020

| 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)
	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)
	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)
	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
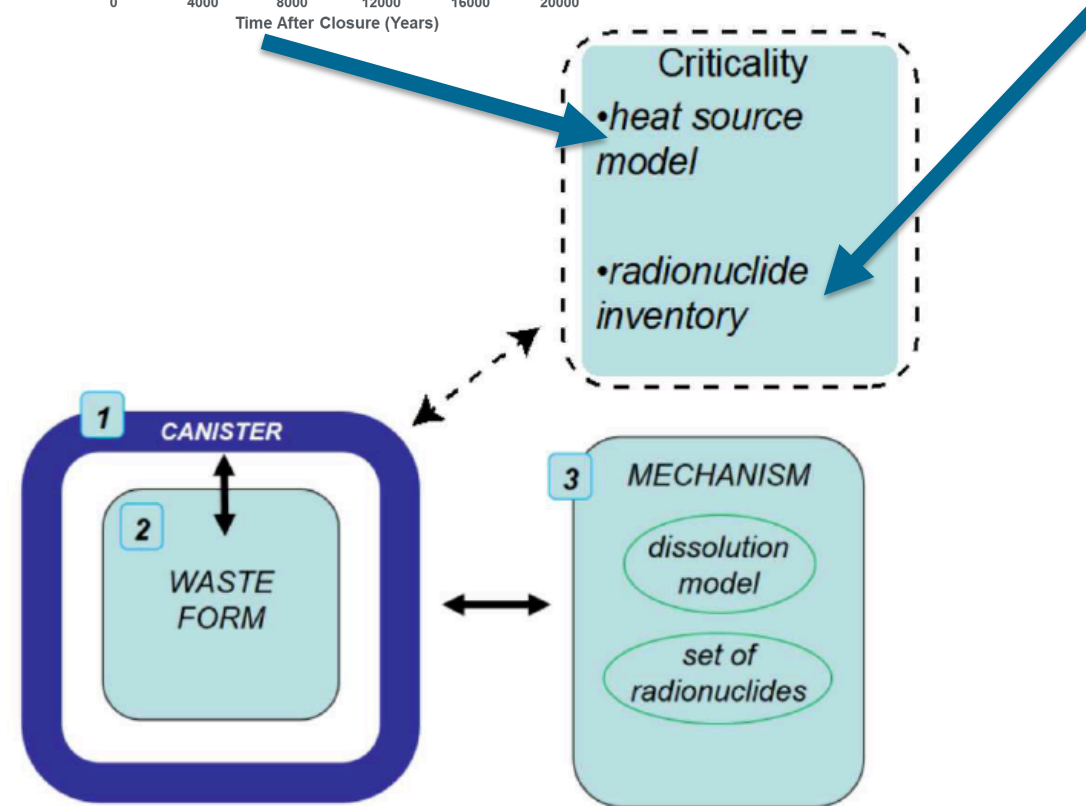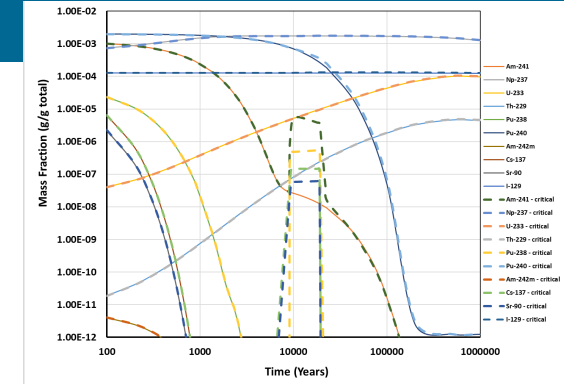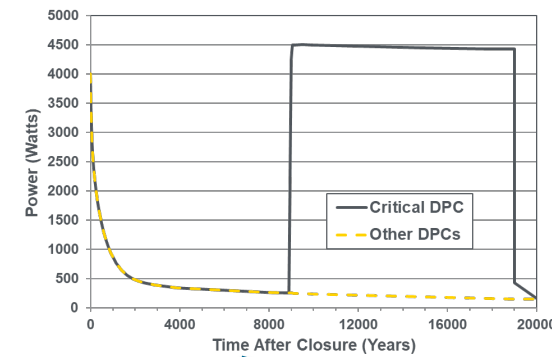
Price et al. 2019
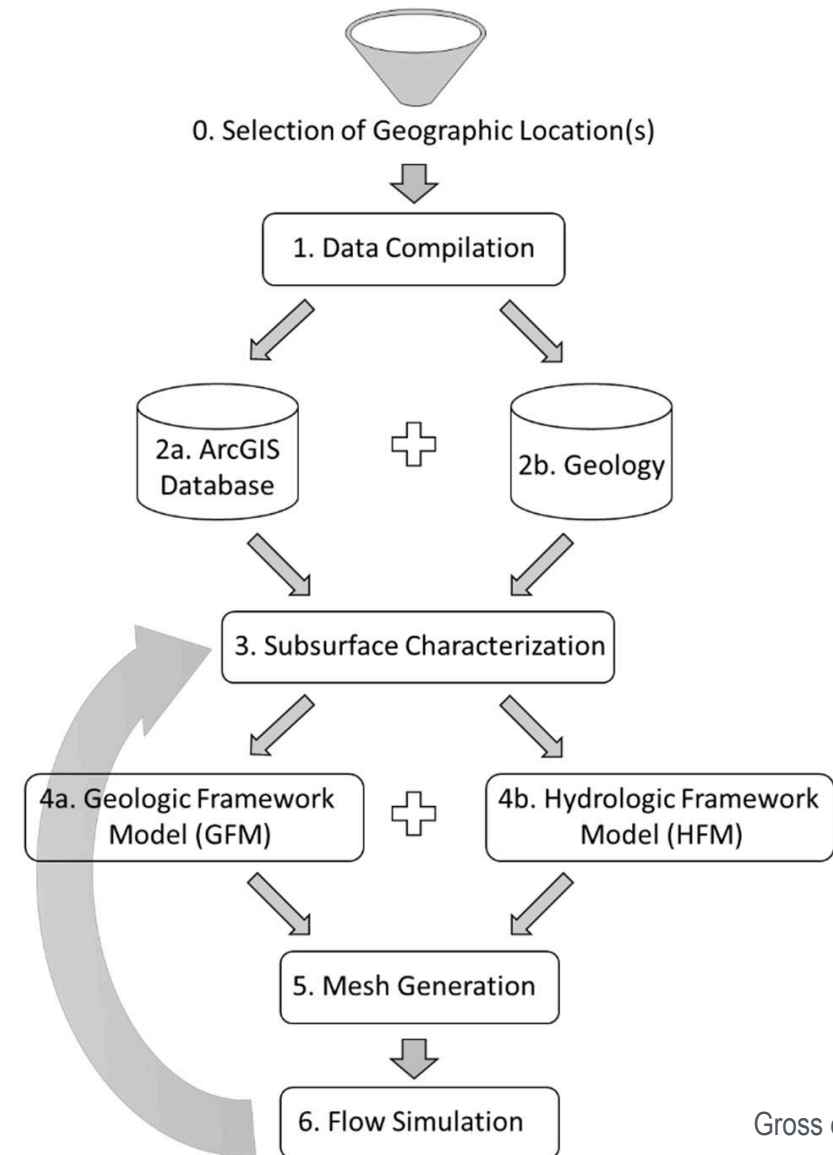
Fuel Matrix Degradation Model (FMDM)

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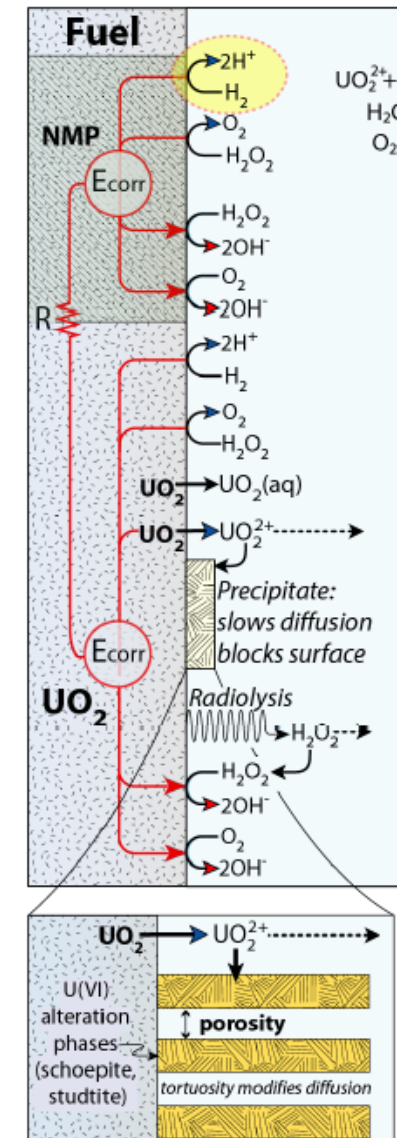
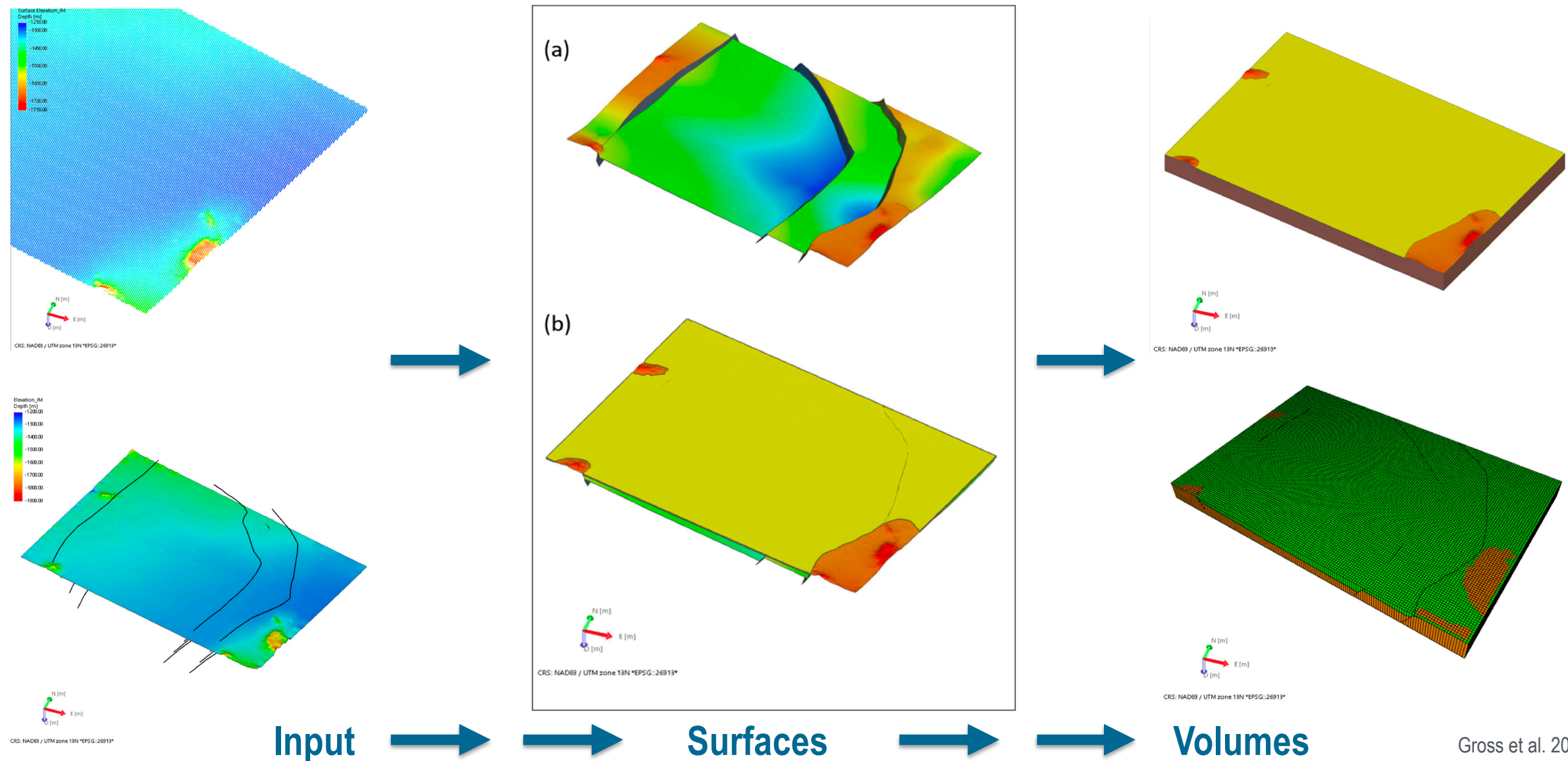(Jerden et al. 2018; Mariner et al. 2020)

- 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

0. Selection of Geographic Location(s)

1. Data Compilation

2a. ArcGIS Database

2b. Geology

3. Subsurface Characterization

4a. Geologic Framework Model (GFM)

4b. Hydrologic Framework Model (HFM)

5. Mesh Generation

6. Flow Simulation

Gross et al. 2019

Input → → **Surfaces** → → **Volumes**

Gross et al. 2020

- ## Lithofacies
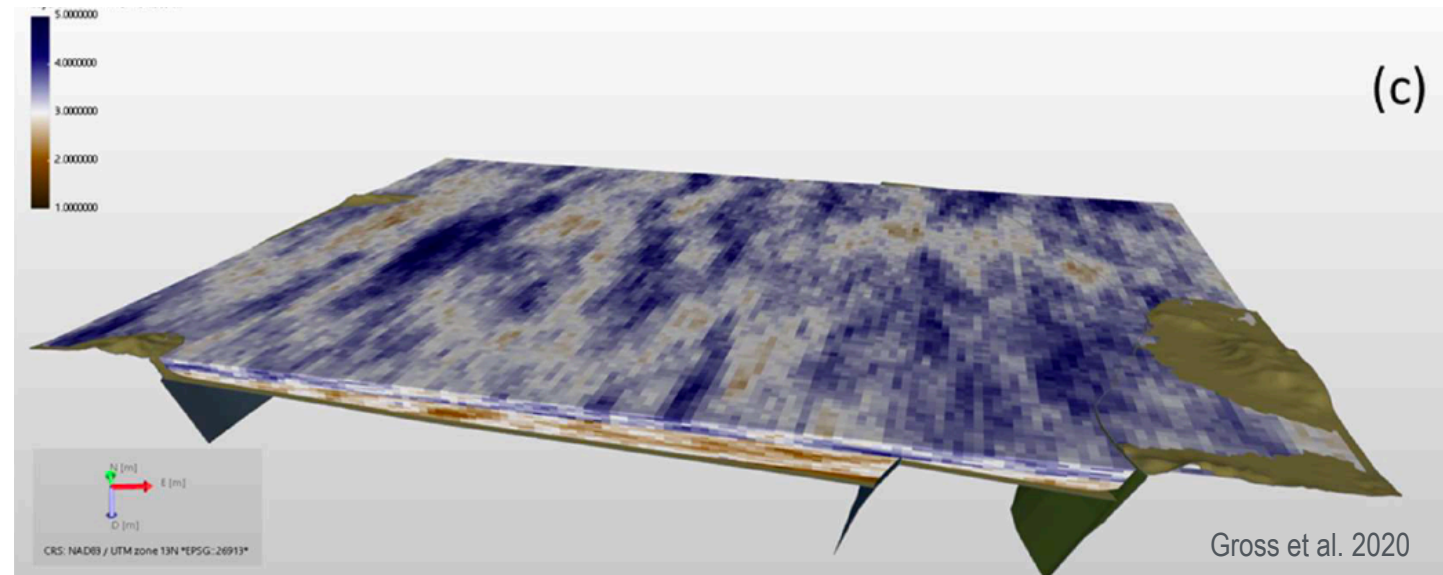 - 3 alluvial facies
  - Bedrock

(a)
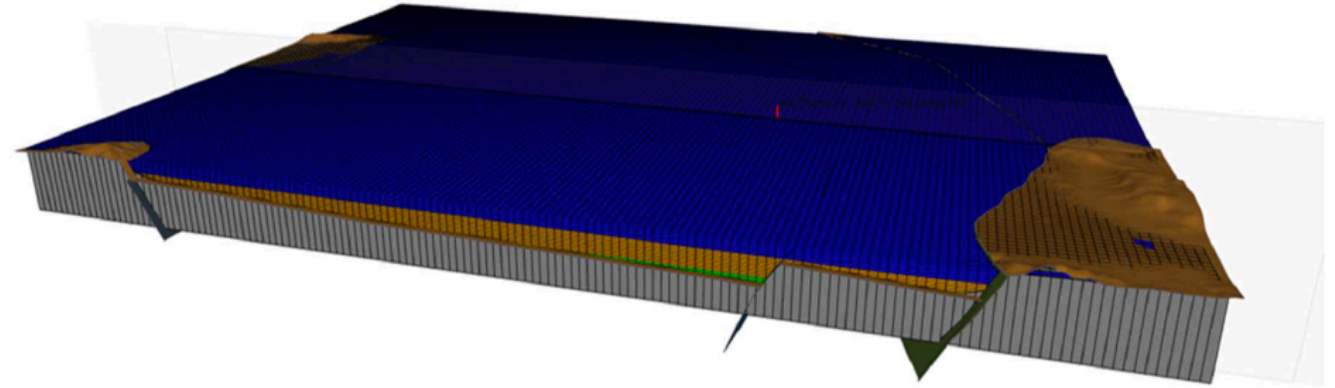
- ## Geostatistical distributions describe hydrologic properties
  - Porosity
  - Permeability

(c)

Gross et al. 2020

GFM to Computational Mesh

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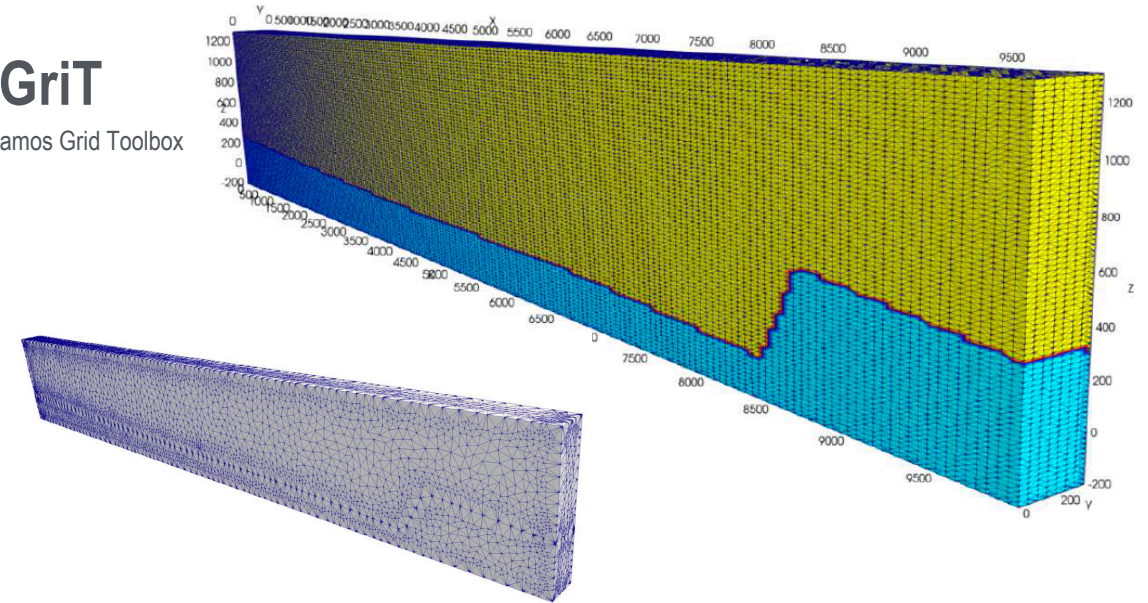 - Automate information processing and workflow to create computational mesh from GFM
  - Versatile tools for user-controlled generation of Voronoi mesh using Delauney triangulation
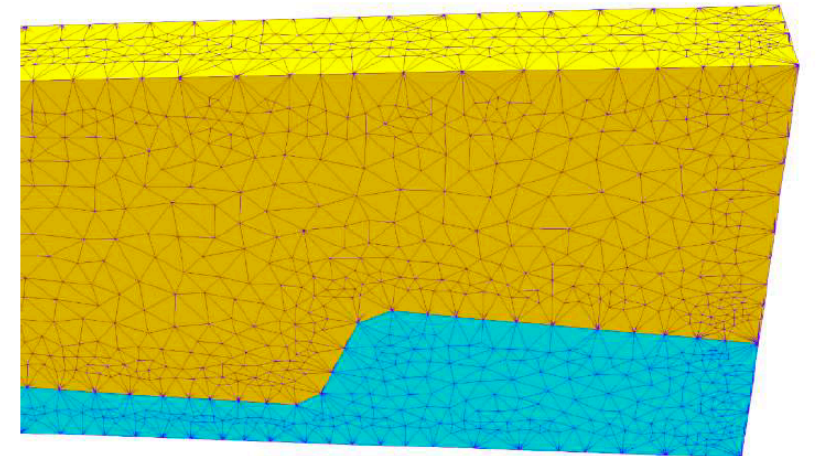
- ## VoroCrust
  - The first provably correct algorithm for conforming Voronoi tessellation
  - Automated algorithm simplifies meshing

LaGriT

Los Alamos Grid Toolbox
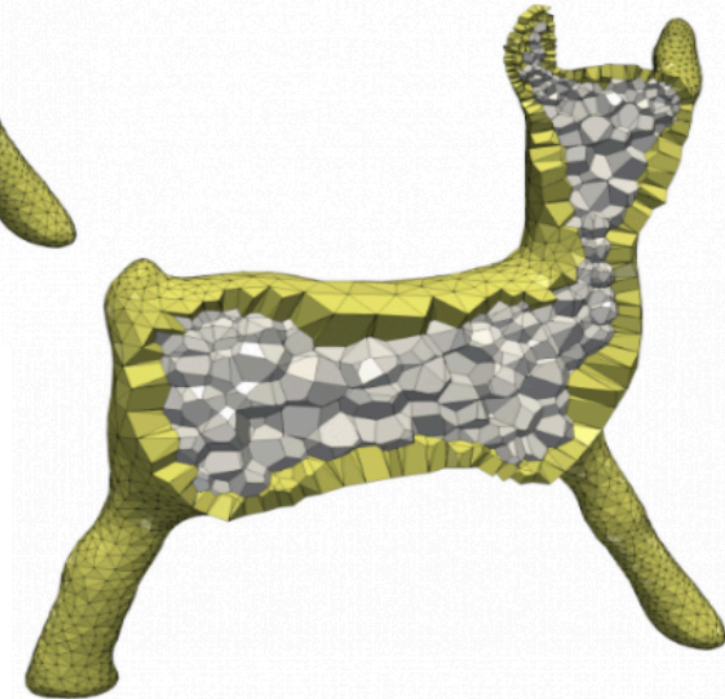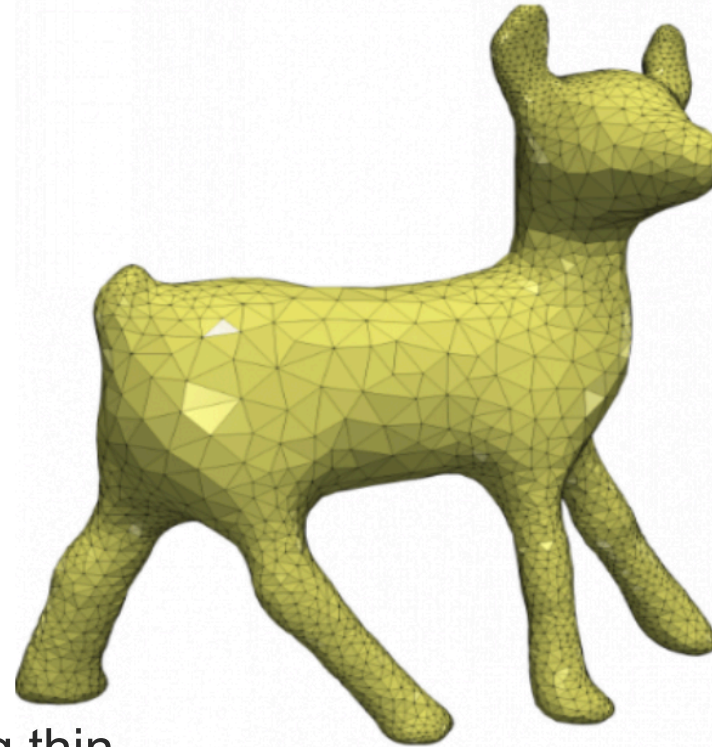
Vorocrust

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

**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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