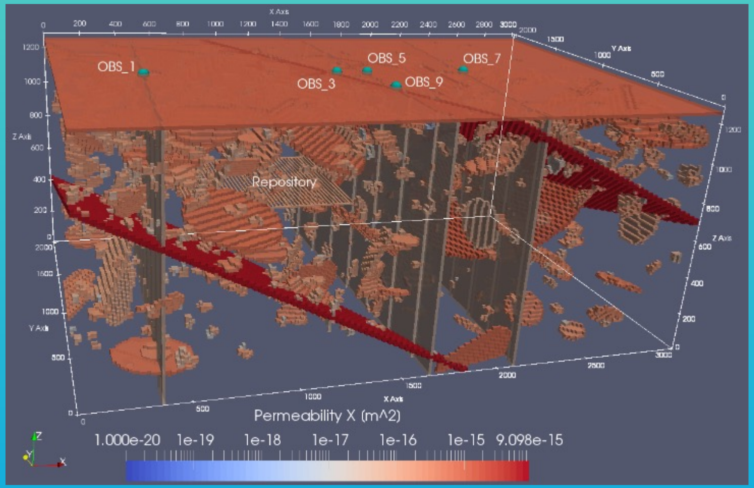
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.



Geologic Disposal Safety Assessment (GDSA) Overview

U.S. Nuclear Waste Technical Review Board

Fall Workshop

November 3-4, 2021

Emily Stein

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA

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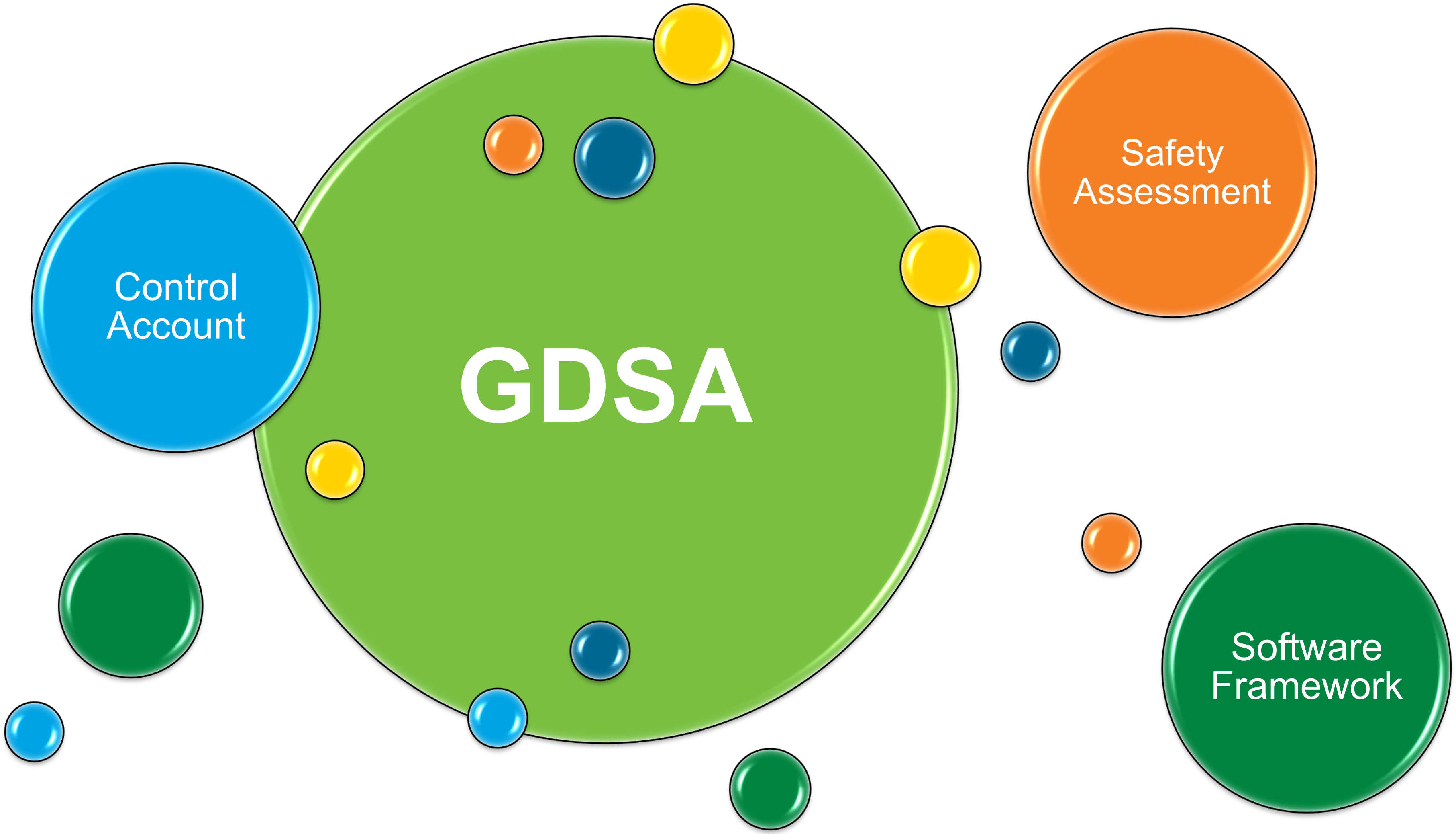
Outline

- What is GDSA?
- Objectives
- Prioritization
- Challenges
- 5-year Plan

What is Geologic Disposal Safety Assessment or GDSA?



Spent Fuel and Waste Science and Technology Disposal Research Control Accounts

Disposal Research

- Argillite R&D
- Crystalline R&D
- Salt R&D
- Engineered Barrier System R&D
- Inventory and Wasteform Characteristics and Performance
- International Collaborations
- **Geologic Disposal Safety Assessment**
- Direct Disposal of Dual Purpose Canisters
- Technical Support for Underground Research Laboratory Activities

Scope of the GDSA Control Account

Geologic Disposal Safety Assessment (GDSA)

- **GDSA Framework Development (SNL)**
- **Repository Systems Analysis (SNL)**
- **Uncertainty and Sensitivity Analysis Methods (SNL)**
- **PFLOTRAN Development (SNL)**
- **Modeling and Integration (LANL, LBNL, ORNL, PNNL)**
- **Geologic Modeling (LANL, INL)**

Sandia National Laboratories

BERKELEY LAB

INL Idaho National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

OAK RIDGE National Laboratory

Pacific Northwest NATIONAL LABORATORY

Post-closure Safety Assessment

1. Introduction, Purpose, and Context

2. Safety Strategy

2.1 Management Strategy
a. Organizational/mgmt. structure
b. Safety culture & QA
c. Planning and Work Control
d. Knowledge management
e. Oversight groups

2.2 Siting & Design Strategy
a. National laws
b. Site selection basis & robustness
c. Design requirements
d. Disposal concepts
e. Intergenerational equity

2.3 Assessment Strategy
a. Regulations and rules
b. Performance goals/safety criteria
c. Safety functions/multiple barriers
d. Uncertainty characterization
e. RD&D prioritization guidance

3. Technical Bases

3.1 Site Selection
a. Siting methodology
b. Repository concept selection
c. FEPs Identification
d. Technology development
e. Transportation considerations
f. Integration with storage facilities

3.2 Pre-closure Basis
a. Repository design & layout
b. Waste package design
c. Construction requirements & schedule
d. Operations & surface facility
e. Waste acceptance criteria
f. Impact of pre-closure activities on post-closure

3.3 Post-closure Bases (FEPs)

3.3.1 Waste & Engineered Barriers Technical Basis
a. Inventory characterization
b. WF/WP technical basis
c. Buffer/backfill technical basis
d. Shafts/seals technical basis
e. UQ (aleatory, epistemic)

3.3.2 Geosphere/ Natural Barriers Technical Basis
a. Site characterization
b. Host rock/DRZ technical basis
c. Aquifer/other geologic units technical basis
d. UQ (aleatory, epistemic)

3.3.3 Biosphere Technical Basis
a. Biosphere & surface environment:
- Surface environment
- Flora & fauna
- Human behavior

4. Disposal System Safety Evaluation

4.1 Pre-closure Safety Analysis
a. Surface facilities and packaging
b. Mining and drilling
c. Underground transfer and handling
d. Emplacement operations
e. Design basis events & probabilities
f. Pre-closure model/software validation
g. Criticality analyses
h. Dose/consequence analyses

4.2 Post-closure Safety Assessment
a. FEPs analysis/screening
b. Scenario construction/screening
c. PA model/software validation
d. Barrier/safety function analyses and subsystem analyses
e. PA and Process Model Analyses/Results
f. Uncertainty characterization and analysis
g. Sensitivity analyses

4.3 Confidence Enhancement
a. R&D prioritization
b. Natural/anthropogenic analogues
c. URL & large-scale demonstrations
d. Monitoring and performance confirmation
e. International consensus & peer review
f. Verification, validation, transparency
g. Qualitative and robustness arguments

5. Synthesis & Conclusions
a. Key findings and statement(s) of confidence
b. Discussion/disposition of remaining uncertainties
c. Path forward

Sevougian et al. 2019b

Assumptions for GDSA Development

- Individual performance standard
- Probabilistic risk assessment
- Separation of aleatory and epistemic uncertainty
- Biosphere may be prescribed
- Prioritize features, events, and processes that are likely to occur regardless of site and design specifics
- Provide a quantitative estimate of the performance of the disposal system for comparison to regulatory standards

Assessment Strategy

a. Regulations and rules
b. Performance goals/safety criteria
c. Safety functions/multiple barriers
d. Uncertainty characterization
e. RD&D prioritization guidance

Post-closure Technical Bases

Waste & Engineered Barrier

a. Inventory characterization
b. Wasteform and waste package
c. Buffer and backfill
d. Shafts and Seals
e. Aleatory and epistemic uncertainty

Geosphere/Natural Barrier

a. Site characterization
b. Host rock and disturbed rock zone
c. Aquifer and other geologic units
d. Aleatory and epistemic uncertainty

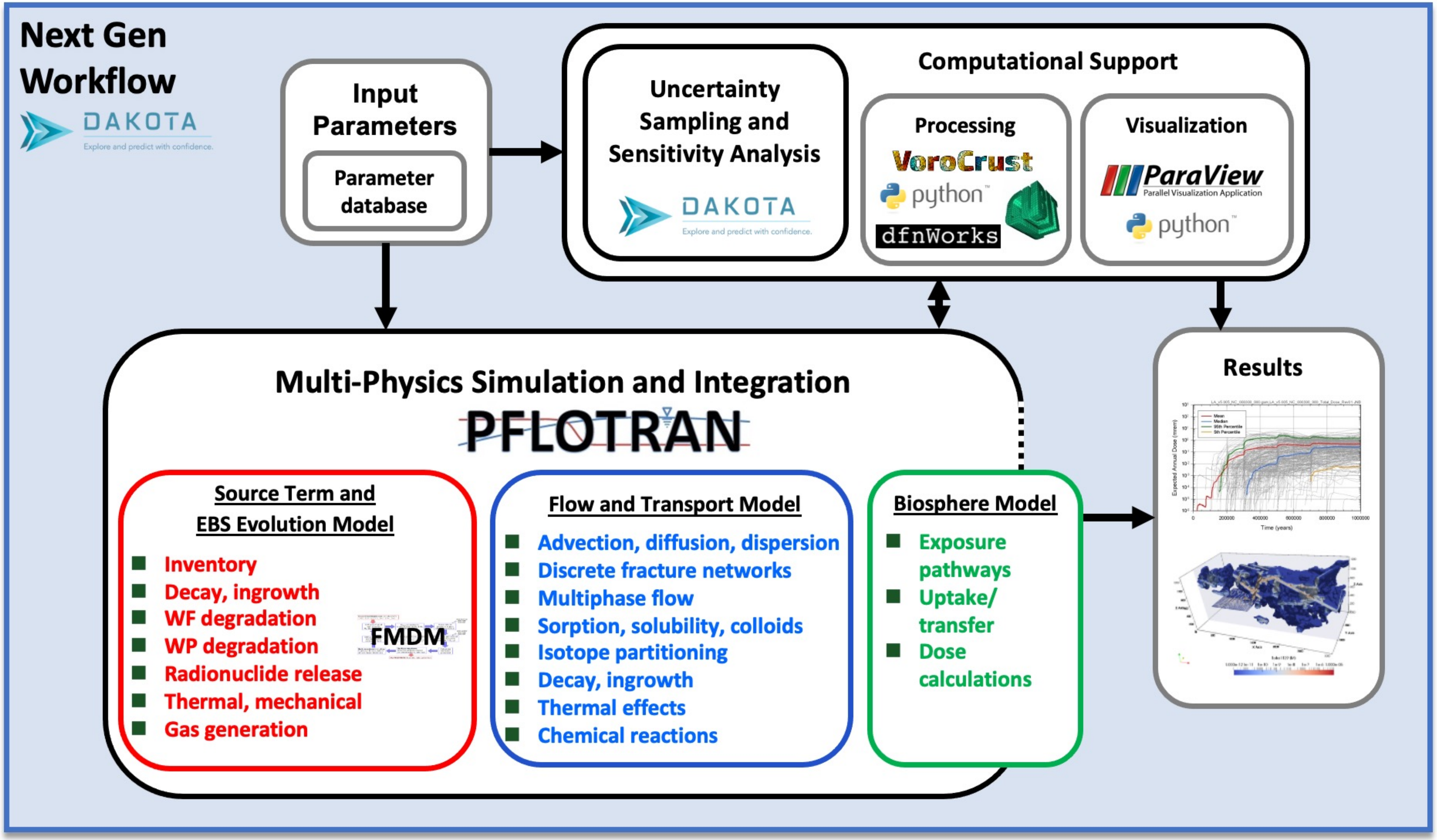
Biosphere

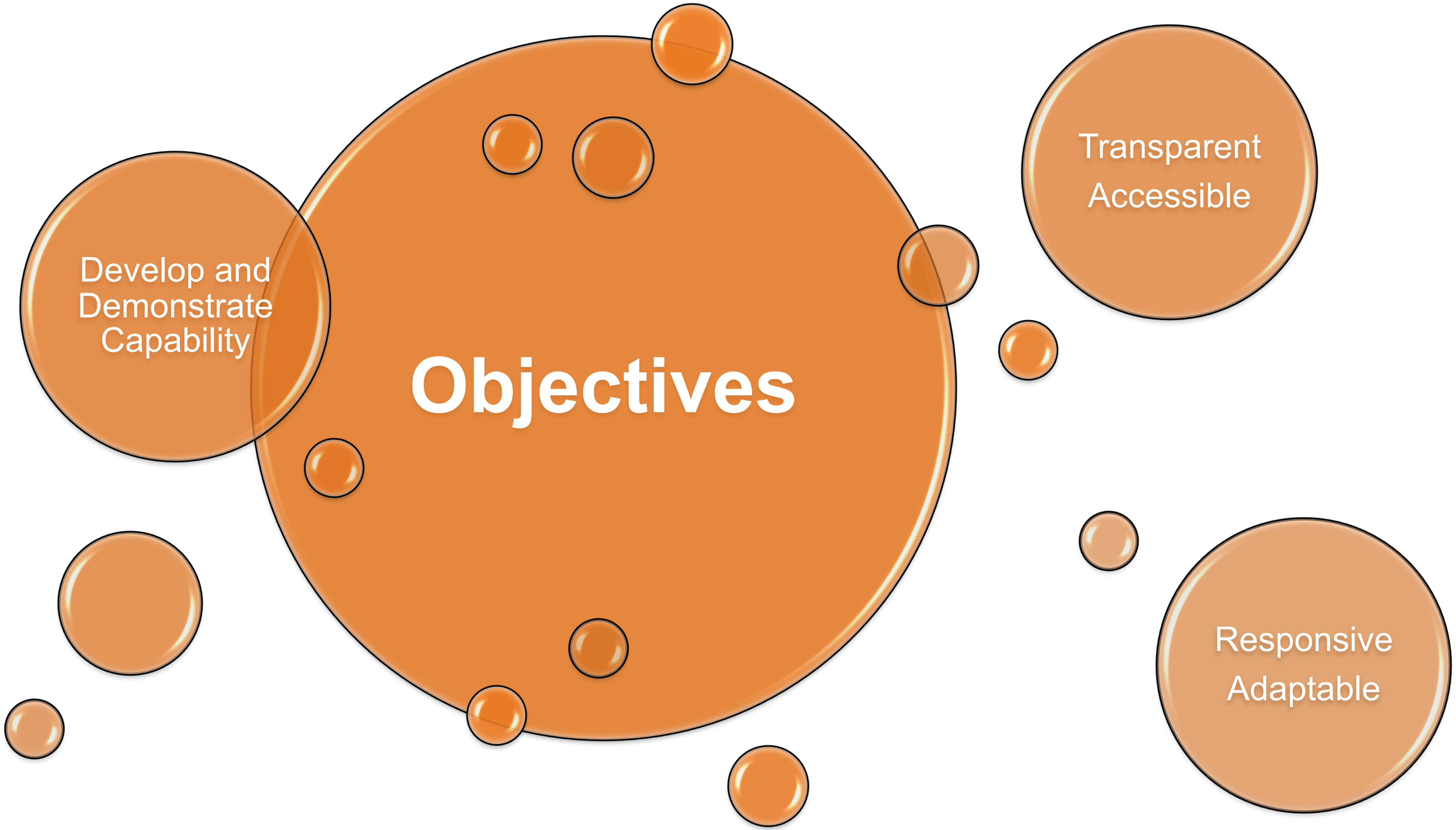
a. Surface environment
b. Flora and fauna
c. Human behavior

Post-closure Safety Assessment

a. FEPs analysis/screening
b. Scenario construction/screening
c. PA model/software validation
d. Barrier and subsystem analyses
e. PA and process model analyses
f. Uncertainty characterization and analysis
g. Sensitivity analysis

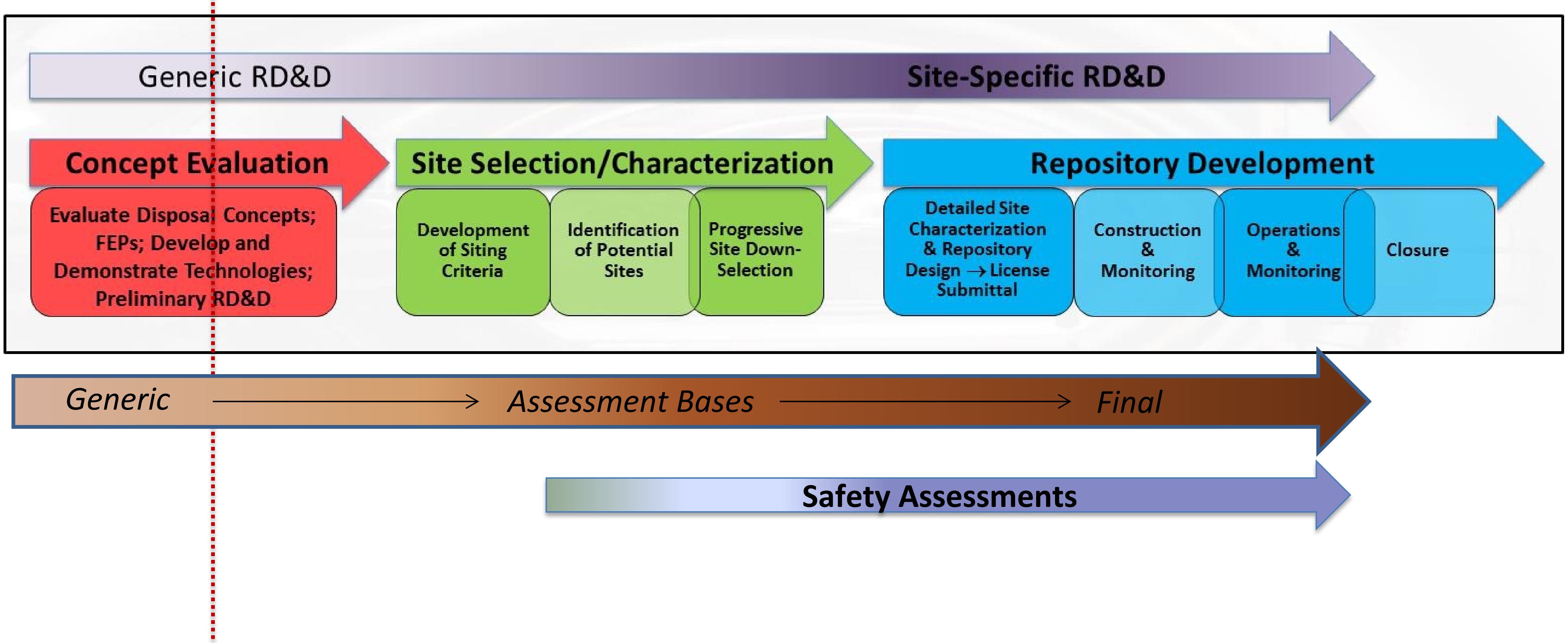
GDSA Framework




Develop and Demonstrate Capability
Objectives
Transparent Accessible
Responsive Adaptable

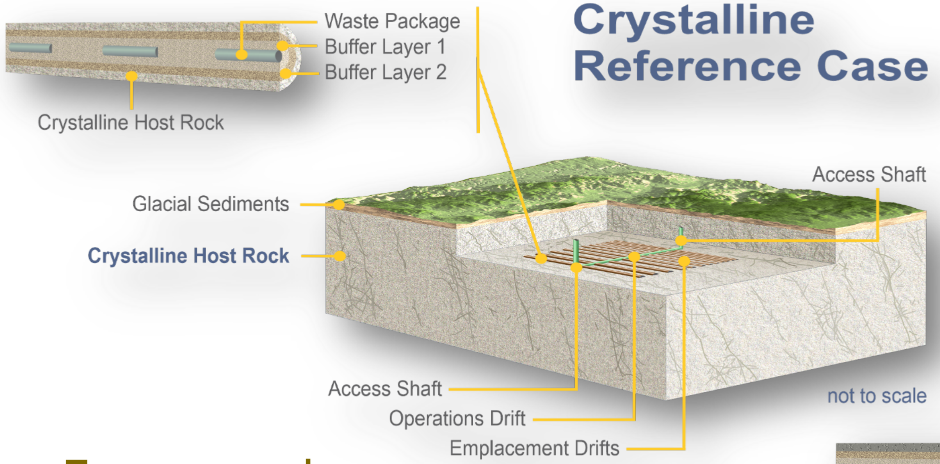
Stages of a Deep Geologic Disposal Program

U.S. Program Currently:
- *Concept Evaluation stage*
- *"Generic" stage*



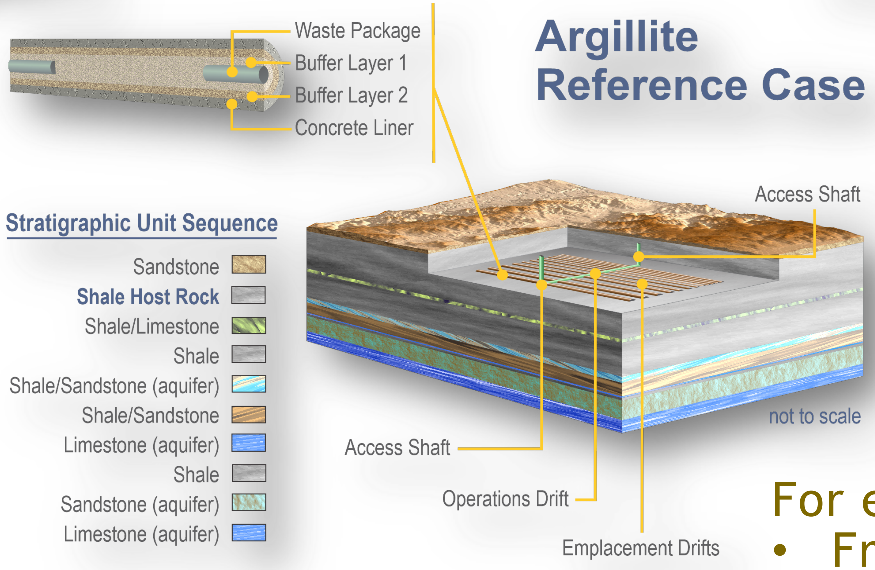
Generic Host Rock Systems

Crystalline Reference Case



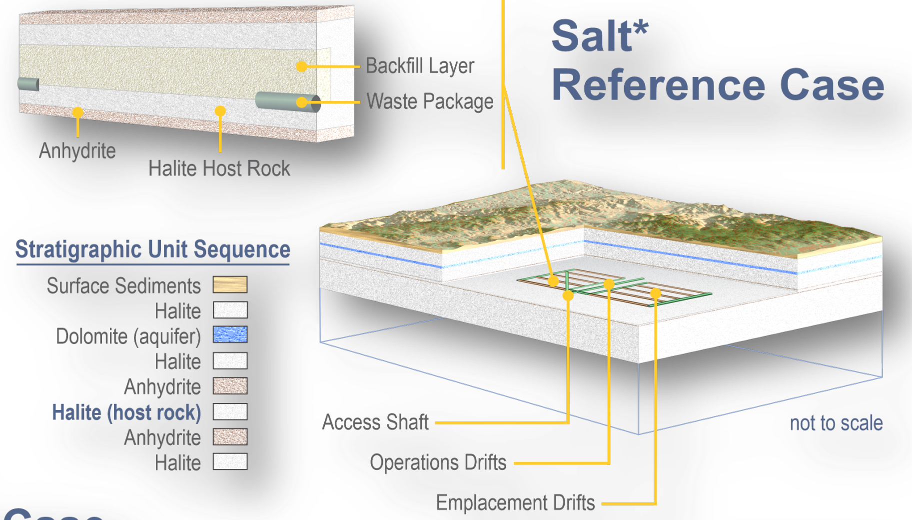
For example:
- Sweden
- Finland

Argillite Reference Case



For example:
- France
- Switzerland

Salt* Reference Case



*2019 commercial waste case

Also considered by:
- Germany
- The Netherlands

These host rocks were identified in the early US siting program as well (DOE 2012).

Multiple Barriers

Overall performance relies on multiple components; different disposal concepts emphasize different barriers

- Natural barriers prevent or delay water from reaching waste form
- Engineered barriers prevent or delay water from reaching waste form
- Slow degradation of waste form limits exposure to water
- Near Field: water chemistry limits aqueous concentrations
- Natural and engineered barriers prevent or delay transport of radionuclides to the human environment

Time (radioactive decay)

Why GDSA Framework?

- Be flexible to changes in design, geometry, or geology
- Represent three-dimensional geometry
- Facilitate two-way coupling
- Integrate process models transparently
- Leverage high-performance computing to
  - Allow more detailed representation
  - Reduce computational costs (of all of the above)
  - Enable probabilistic calculations (given the computational cost)
- State-of-the-art

Vaughn et al. 2012

Why GDSA Framework?

PFLOTRAN

- High-performance computing
- Open source
- Sequentially coupled flow and transport
- Global implicit reactive transport

DAKOTA

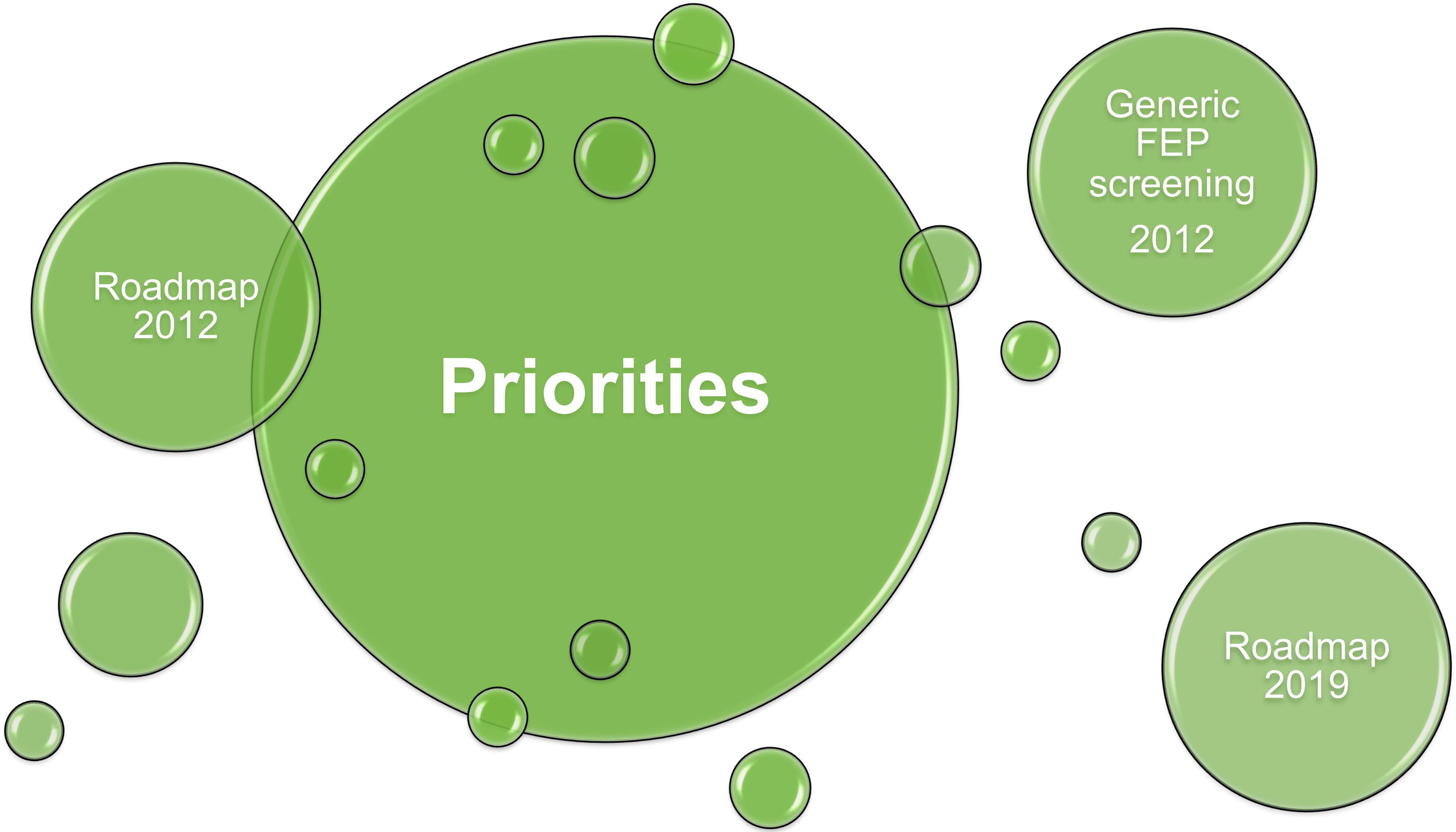
- High-performance computing
- Open source
- Latin hypercube sampling
- Aleatory and epistemic uncertainty

GDSA Objectives

- Develop and demonstrate capability
  - Geologic modeling, multiphysics simulation, uncertainty and sensitivity analysis, workflow

that is

- Responsive to advances in
  - Process understanding, computer hardware and software, simulation and analysis methods
- Adaptable to
  - Generic site and design constraints
  - Site- and design-specific technical bases
  - Evolution of the safety assessment strategy
- Transparent
  - Developed and distributed in an open-source environment with public documentation
- Accessible
  - Laptop, workstation, and high-performance computing



Generic FEP screening 2012
Roadmap 2012
Priorities
Roadmap 2019

Evolution of GDSA Framework and Reference Cases

2012
- Roadmap (DOE 2012)
- Requirements (Freeze & Vaughn 2012)
- Generic FEPs (Vaughn et al. 2012)

2013
- Salt reference case with PFLOTRAN & DAKOTA (Freeze et al. 2013)

2014
- Multiphase flow added to PFLOTRAN (Sevougian et al. 2014)

2015
- Shale reference case
- Fuel Matrix Degradation (FMD)
- Glass dissolution (Mariner et al. 2015)

2016
- Crystalline reference case
- dfnWorks
- Isotope partitioning
- Wasteform process model (Mariner et al. 2016)

2017
- Well water ingestion
- QA test suite
- Analytical derivatives (Mariner et al. 2017)

2018
- Variance-based sensitivity analysis
- Stepwise linear regression
- Alluvial reference case (Mariner et al. 2018)

2019
- Roadmap Update (Sevougian et al. 2019a)
- High-temperature shale simulations
- Swelling stress (Sevougian et al. 2019b)

2020
- FMD surrogates (Mariner et al. 2020a)
- Advanced solvers
- Next Gen Workflow (Mariner et al. 2020b)
- DECOVALEX Task F (LaForce et al. 2020)
- Biosphere model (Condon et al. 2020)

2021
- Dual porosity
- Criticality (Nole et al. 2021)
- International sensitivity analysis report (Swiler et al. 2021)

Planning/Prioritization Disposal Research (DR) Activities Overview

- Used Fuel Disposition (UFD) Campaign 2012 Roadmap
  - Features, Events, and Processes (FEP) gap assessment synthesis
  - Synthesize into High Priority Topics for UFD Campaign work planning
  - 2012 Roadmap Report (Rev. 01; 2012)
- 2019 Roadmap Update
  - Review/prioritize DR Activities for progress, gaps, and recent Program Direction
    - Begin assessment of DR R&D Program in FY2017
  - 2019 Roadmap Update Report (Rev. 01; 2019)
- Development of SFWST Disposal Research Five-year Plan (2020, 2021)
  - Incorporate/address updated priorities
  - Identify short-term primary objectives (1-2 years; relatively certain)
  - Provide longer-term vision (3-5 years; general guide)

2012 Roadmap – Cross Cutting Issues

- **Disposal System Modeling (High)**
  - Enable risk-informed, probability-based performance assessment
  - Provide a capability for evaluating disposal system performance to inform R&D prioritization
  - Support simple and complex integrated generic disposal system models
- Site Screening and Selection Tools (Medium)
  - Unified geospatial database and visualization tool

DOE 2012

2012 Generic FEP screening

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 Disturbed Rock Zone (DRZ))
- Waste package degradation (corrosion processes, mechanical damage, early failures)
- Evolution/degradation of engineered barrier system (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

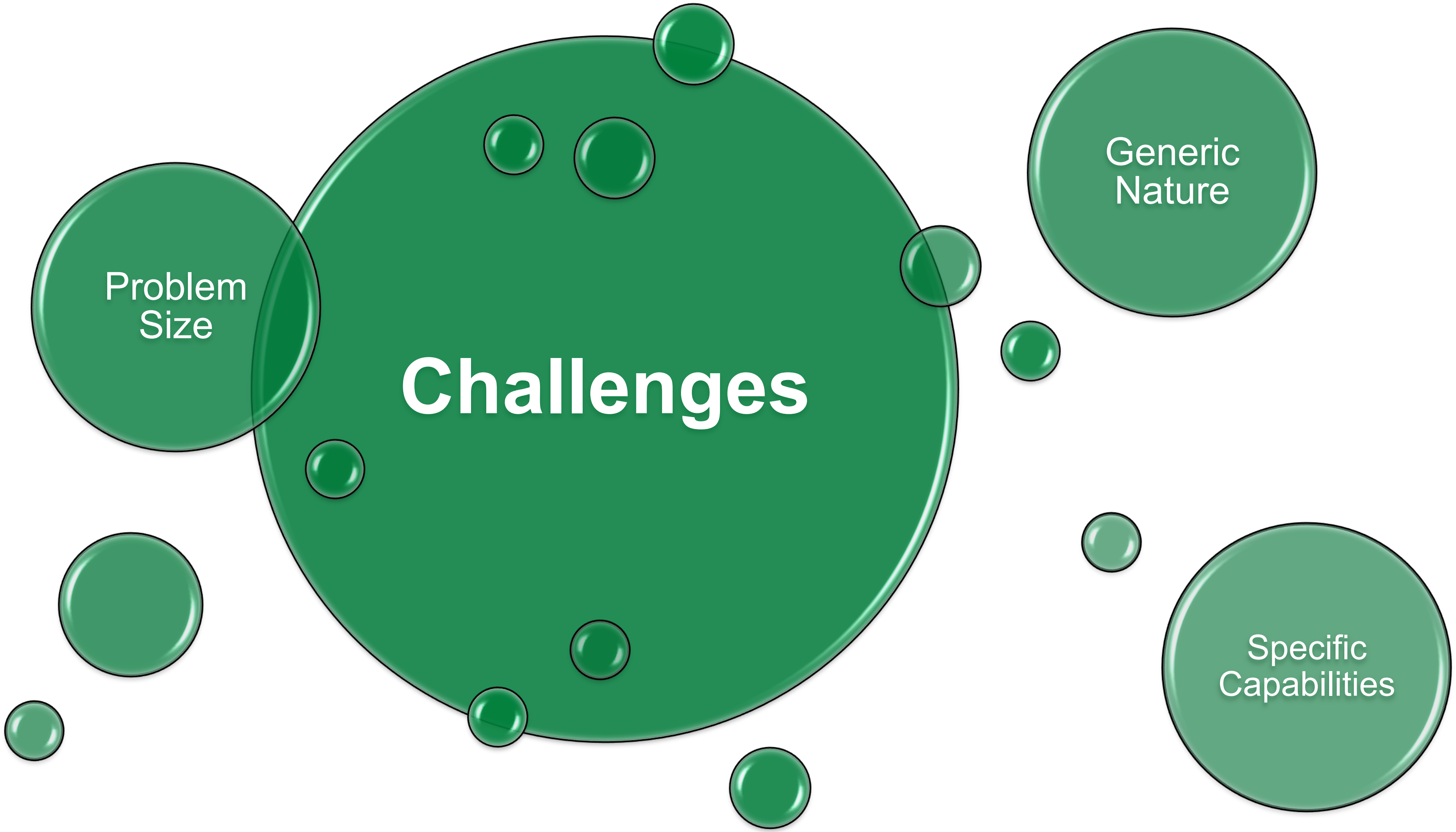
Receptor (Biosphere)
- Dilution due to mixing of contaminated and uncontaminated waters
- Receptor characteristics (basis for converting radionuclide concentrations in groundwater to dose)

Vaughn et al. 2012

2019 Roadmap Update – High Impact R&D Topics

- **High-temperature impacts**
- Buffer and seal studies
- Coupled processes in salt
- Gas flow in the engineered barrier system
- **Criticality**
- **Waste package degradation**
- In-package chemistry
- **Generic performance assessment models**
- **Radionuclide transport**

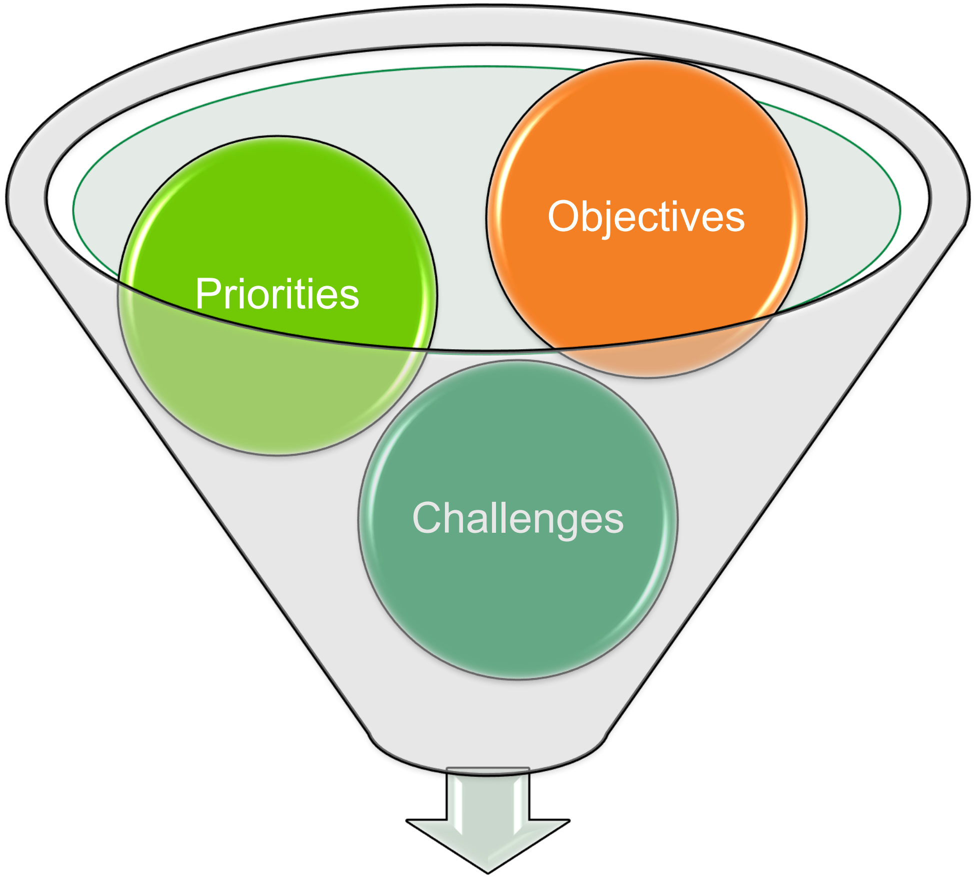
Sevougian et al. 2019


Problem Size
Challenges
Generic Nature
Specific Capabilities

Challenges

- Generic nature of the problem
- Size of problem
  - 3D comprehensive model domain
  - Long time scale (1 million years)
  - Number of radionuclides
  - Uncertainty propagation
- Resolution of near-field processes
- Specific modeling capabilities
  - High-temperature multiphase flow
  - Computationally efficient implementation of the Fuel Matrix Degradation Model
- Workflow

Objectives, Priorities, and Challenges Shape the 5-year Plan



5-year plan

Research Thrusts in 5-Year Plan

- **Advanced simulation capability**
- **State-of-the-art uncertainty and sensitivity analysis methods**
- **Traceable, user-friendly workflow**
- **Repository systems analysis**
- Geologic framework modeling

Sassani et al. 2021

Advanced Simulation Capability

- **Recent Accomplishments**
  - Advanced linear and nonlinear solvers
  - Waste package criticality
  - High-temperature effects
  - Fracture-matrix diffusion
  - Surrogates for the Fuel Matrix Degradation Model
  - Biosphere prototype

- **Next 1-2 Years**
  - High-temperature simulation capability
  - Material-specific waste package degradation models
  - Buffer and backfill evolution
  - Biosphere pathways
  - dfnWorks capability
  - Geologic meshing

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Mariner, Nole, Hyman, & Condon

Uncertainty and Sensitivity Analysis (U/SA)

- **Recent Accomplishments**
  - Advance U/SA of crystalline reference case
  - Led international comparison of SA methods
  - Demonstrate potential of multifidelity methods

- **Next 1-2 Years**
  - Increase computational efficiency
  - Increase understanding of system behavior
  - Metrics for assessing goodness of surrogates
  - International best-practices

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★ **Swiler**

Workflow

- **Recent Accomplishments**
  - Next Generation Workflow (NGW)
  - Expansion of software verification testing (”QA test suite”)

- **Next 1-2 Years**
  - Increase automation through NGW
  - Release the “QA test suite”
  - Develop geologic meshing workflow

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  - Develop geologic meshing workflow

★ **Mariner, Nole**

Repository Systems Analysis

- **Recent Accomplishments**
  - Conceptual models and simulations that account for high-temperature impacts
  - Initiate 4-year international performance assessment comparison (DECOVALEX-2023 Task F)
  - Growing collaboration with Germany, Netherlands, and United Kingdom regarding salt FEPs and scenario development

- **Next 1-2 Years**
  - Simulation and analysis of salt and crystalline reference cases developed in Task F
  - Drive development of process models
    - Bentonite evolution
    - Waste package degradation
    - Salt consolidation and creep

Repository Systems Analysis

- **Recent Accomplishments**
  - Conceptual models and simulations that account for high-temperature impacts
  - Initiate 4-year international performance assessment comparison (DECOVALEX-2023 Task F)
  - Growing collaboration with Germany, Netherlands, and United Kingdom regarding salt FEPs and scenario development

- **Next 1-2 Years**
  - Simulation and analysis of salt and crystalline reference cases developed in Task F
  - Drive development of process models
    - Bentonite evolution
    - Waste package degradation
    - Salt consolidation and creep

LaForce, Stein

Topics for this meeting

- GDSA Framework - Mariner
- PFLOTRAN - Nole
- dfnWorks - Hyman
- Fuel Matrix Degradation Model - Mariner
- Biosphere Model - Condon
- Uncertainty and Sensitivity Analysis - Swiler
- Reference Case Simulation - LaForce
- DECOVALEX-2023 Task F - Stein

References

Condon, C. A., B. A. Napier, S. Ghosh, W. C. Weaver and C. B. Varnum-Lowry, 2020. *GDSA Biosphere Model Software Requirements Document*. PNNL-30280, Pacific Northwest National Laboratory, Hanford, WA

DOE, 2012. *Used Fuel Disposition Campaign Disposal Research and Development Roadmap*. FCRD-USED-2011-000065 Rev 1, U.S. Department of Energy, Washington, D.C.

Freeze, G. A. and P. Vaughn, 2012. *Development of an Advanced Performance Assessment Modeling Capability for Geologic Disposal of Nuclear Waste: Methodology and Requirements*. SAND2012-10208, Sandia National Laboratories, Albuquerque, NM

Freeze, G. A., W. P. Gardner, P. Vaughn, S. D. Sevougian, P. E. Mariner, V. Mousseau and G. E. Hammond, 2013. *Enhancements to Generic Disposal System Modeling Capabilities*. FCRD-UFD-2014-000062; SAND2013-10532P, Sandia National Laboratories, Albuquerque, NM

LaForce, T., K. W. Chang, F. V. Perry, T. S. Lowry, E. Basurto, R. S. Jayne, D. M. Brooks, S. Jordan, E. R. Stein, R. C. Leone and M. Nole, 2020. *GDSA Repository Systems Analysis Investigations in FY2020*. SAND2020-12028R, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., W. P. Gardner, G. Hammond, S. D. Sevougian and E. R. Stein, 2015. *Application of Generic Disposal System Models*. FCRD-UFD-2015-000126; SAND2015-10037R, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., E. R. Stein, J. M. Frederick, S. D. Sevougian, G. E. Hammond and D. G. Fascitelli, 2016. *Advances in Geologic Disposal System Modeling and Application to Crystalline Rock*. FCRD-UFD-2016-000440 / SAND2016-9610R, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., E. R. Stein, J. M. Frederick, S. D. Sevougian and G. E. Hammond, 2017. *Advances in Geologic Disposal System Modeling and Shale Reference Cases*. SFWD-SFWST-2017-000044 / SAND2017-10304R, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., E. R. Stein, S. D. Sevougian, L. J. Cunningham, J. M. Frederick, G. E. Hammond, T. S. Lowry, S. Jordan and E. Basurto, 2018. *Advances in Geologic Disposal Safety Assessment and an Unsaturated Alluvium Reference Case*. SFWD-SFWST-2018-000509; SAND2018-11858R, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., T. M. Berg, C. Chang, B. J. Debusschere, R. C. Leone and D. T. Seidl, 2020. *Surrogate Model Development of Spent Fuel Degradation for Repository Performance Assessment*. SAND2020-10797, Sandia National Laboratories, Albuquerque, NM

Mariner, P. E., M. Nole, E. Basurto, T. M. Berg, K. W. Chang, B. J. Debusschere, A. C. Eckert, M. S. Ebeida, M. Gross, G. Hammond, J. Harvey, S. Jordan, K. L. Kuhlman, T. LaForce, R. C. Leone, W. C. McLendon, M. M. Mills, H. Park, F. V. Perry, A. Salazar, D. T. Seidl, S. D. Sevougian, E. R. Stein and L. P. Swiler, 2020. *Advances in GDSA Framework Development and Process Model Integration*. SAND2020-10787R, Sandia National Laboratories, Albuquerque, NM

Nole, M., R. C. Leone, H. Park, M. Paul, A. Salazar, G. Hammond and P. Lichtner, 2021. *PFLOTRAN Development FY2021*. SAND2021-8709R, Sandia National Laboratories, Albuquerque, NM

Sassani, D., 2020. *Technical Approach and Prioritization of Activities*. U. S. Nuclear Waste Technical Review Board Fall 2020 Meeting, December 2-3, 2020, Virtual Meeting

Sassani, D., J. Birkholzer, C. Camphouse, G. A. Freeze and E. R. Stein, 2021. *SFWST Disposal Research R&D 5-Year Plan – FY2021 Update*. M2SF-21SN010304054; SAND2021-12491R, Sandia National Laboratories, Albuquerque, NM

Sevougian, S. D., G. A. Freeze, W. P. Gardner, G. E. Hammond and P. E. Mariner, 2014. *Performance Assessment Modeling and Sensitivity Analyses of Generic Disposal System Concepts*. FCRD-UFD-2014-000320; SAND2014-1765, Sandia National Laboratories, Albuquerque, NM

Sevougian, S. D., P. E. Mariner, L. A. Connolly, R. J. MacKinnon, R. D. Roger, D. C. Dobson and J. L. Prouty, 2019. *DOE SFWST Campaign R&D Roadmap Update*. M2SF-19SN010304042 SAND2019-5179R, Sandia National Laboratories, Albuquerque, NM

Sevougian, S. D., E. R. Stein, T. LaForce, F. V. Perry, T. S. Lowry, L. J. Cunningham, M. Nole, C. B. Haukwa, K. W. Chang and P. E. Mariner, 2019. *GDSA Repository Systems Analysis Progress Report*. M2SF-19SN010304051 SAND2019-5189R, Sandia National Laboratories, Albuquerque, NM

Swiler, L. P., E. Basurto, D. M. Brooks, A. C. Eckert, R. C. Leone, P. E. Mariner, T. Portone, M. L. Smith and E. R. Stein, 2021. *Uncertainty and Sensitivity Analysis Methods and Applications in GDSA Framework (FY2021)*. Sandia National Laboratories, Albuquerque, NM

Vaughn, P., G. A. Freeze, J. Lee, S. Chu, K. D. Huff, W. M. Nutt, T. Hadgu, R. Rogers, J. L. Prouty, E. L. Hardin, B. Arnold, E. Kalinina, W. P. Gardner, M. Bianchi, H. H. Liu and J. Birkholzer, 2012. *Generic Disposal System Model: Architecture, Implementation, and Demonstration*. FCRD-UFD-2012-000430; SAND2013-1539P, Sandia National Laboratories, Albuquerque, NM