Used Fuel Disposition Campaign

Generic Disposal Systems Analysis (GDSA)

Paul Mariner, Glenn Hammond, Emily Stein, David Sevougian, and Jennifer Frederick

Sandia National Laboratories

2016 UFD Group Meeting

UNLV, Las Vegas, Nevada

June 8, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2016-5393 PE

Session Agenda

- 1:30 – GDSA overview : objectives, work, and FY16 accomplishments (Mariner)
- 1:45 – GDSA simulation framework: PFLOTRAN (Hammond)
- 2:00 – Isotope chemistry and source term (Mariner)
- 2:15 – Source term implementation and demonstration (Frederick)
- 2:30 – GDSA process model integration (Sevougian)
- 2:35 – GDSA mined repository in crystalline rock (Stein)
- 3:00 – GDSA planning for FY17 (Mariner)

Used Fuel Disposition Campaign

GDSA Overview – Objectives, Work, and FY16 Accomplishments

Paul Mariner, Glenn Hammond, Emily Stein, David Sevougian, and Jennifer Frederick

Sandia National Laboratories

2016 UFD Group Meeting

UNLV, Las Vegas, Nevada

June 8, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2016-5393 PE

Presentation Outline

- FY16 GDSA objectives, scope, and methodology
- GDSA model structure and capabilities
- Capabilities added or improved in FY16
- Process model integration in FY16
- New GDSA model application for crystalline rock
- FY16 GDSA deliverable

GDSA Work Package Participants

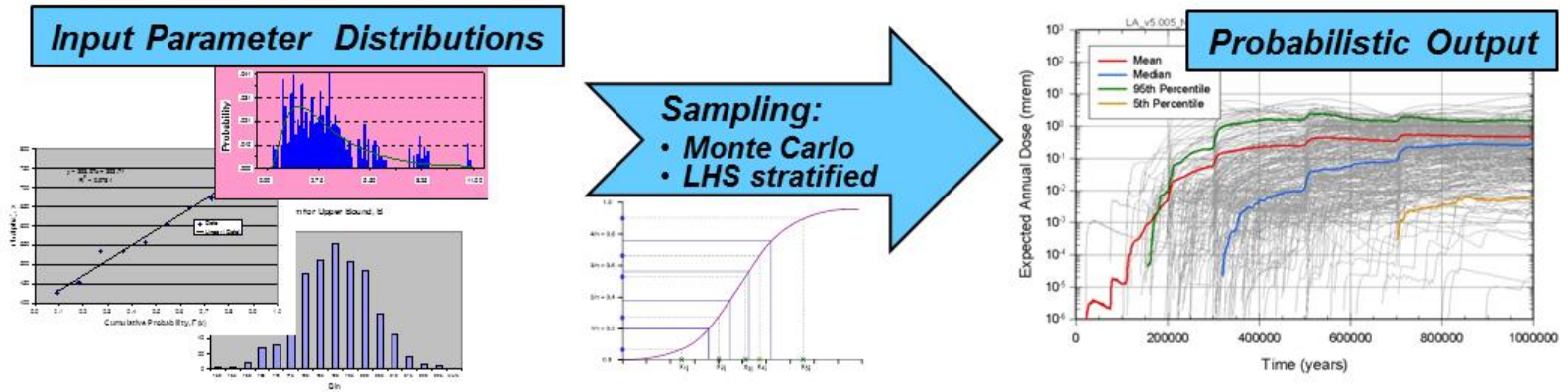
- **DOE**
  - Mark Tynan
- **SNL (code development, PA model implementation)**
  - Glenn Hammond, Emily Stein, Jenn Frederick, Dave Sevougian, Paul Mariner, Peter Lichtner (contractor)
- **Other contributors of special mention**
  - SNL: Bob MacKinnon, Geoff Freeze, Carlos Jove-Colon, Yifeng Wang, Teklu Hadgu, Elena Kalinina, Kris Kuhlman
  - LANL: Hari Viswanathan, Satish Karra, Nataliia Makedonska, Jeffrey Hyman, Frank Perry, Paul Reimus
  - LLNL: Zavarin

GDSA Scope (WBS 1.02.08.03.04)

- **Objective**
  - Develop a disposal system modeling and analysis capability that supports the prioritization of Disposal Research (DR) and the evaluation of disposal system performance, including uncertainty, for a range of disposal options (e.g., salt, argillite, crystalline, deep borehole).
- **FY16 tasks**
  - Upgrade models for baseline isotope behavior (e.g., phase-partitioning, decay, release).
  - Integrate subsystem conceptual models, developed under other DR work packages, into the GDSA-PA system model architecture (e.g., colloid transport, non-Darcy flow, discrete fracture model, waste package degradation).
  - Perform simulations of selected reference case demonstration problems and conduct sensitivity analyses to inform R&D planning.

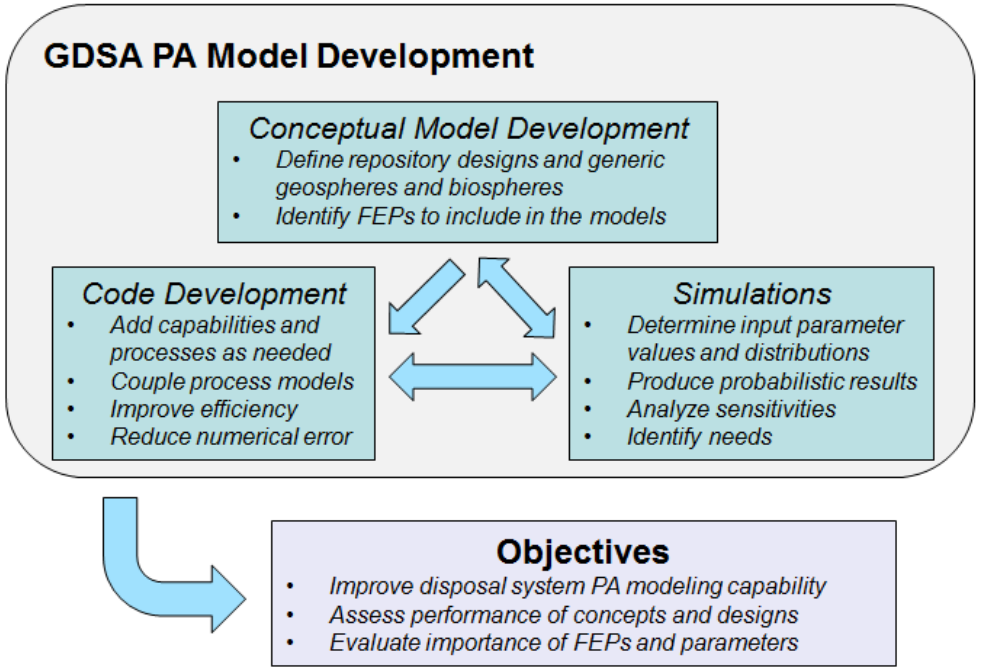
GDSA Objectives

- **Improve disposal system PA modeling capability**
  - *Provide a tool for realistic spatial-temporal probabilistic representation of radionuclide release and transport in 3D*
  - *Reduce the use of conservative assumptions and process abstractions*
  - *Improve the coupling of multi-physics processes*
  - *Minimize numerical error and error due to model form*
  - *Enhance transparency in process modeling*
  - *Provide useful tools for sensitivity analysis and uncertainty quantification*
- **Assess performance of generic concepts/designs (salt, DBH, granite, …)**
- **Evaluate importance of FEPs and model parameters**

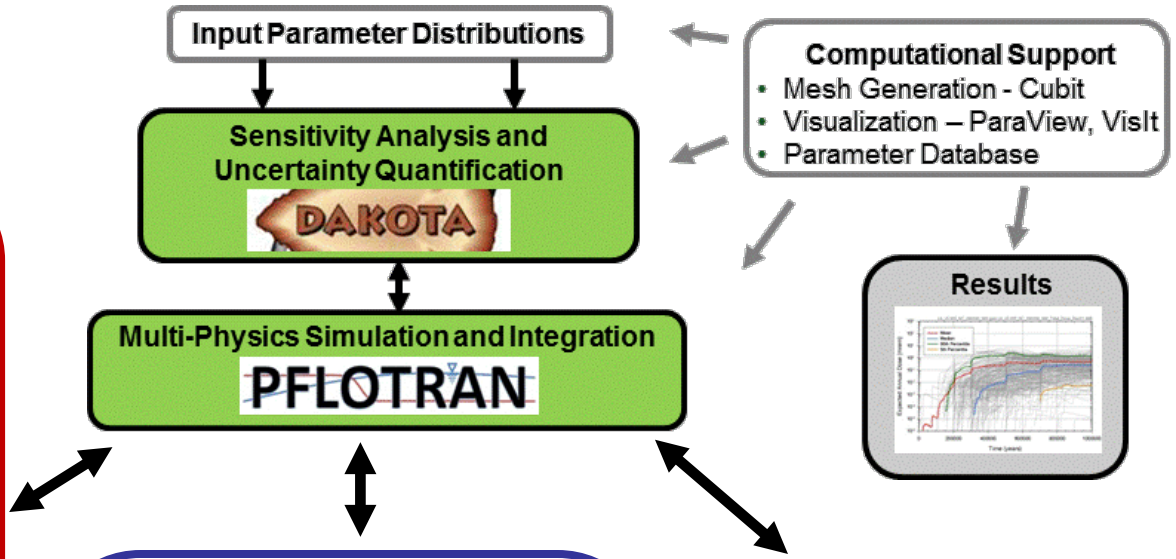


GDSA PA Model Development Methodology

- **Conceptual model development (e.g., repository in salt, clay, granite, etc.)**
  - *Define dimensions of the generic geosphere and biosphere*
  - *Define full-scale layout of the generic repository, guided by generic reference cases developed in UFD Campaign*
  - *Identify Features, Events, and Processes (FEPs) to include in the PA model*
- **Code development**
  - *Add capabilities as needed to simulate the conceptual model*
  - *Integrate with other UFD work packages where possible*
- **Simulations**
  - *Assess importance of FEPs and parameters on radionuclide migration and safety*
  - *Evaluate code performance*
- **Iterate**
  - *Learn from simulations*
  - *Improve code and model to achieve overall objectives*



Current GDSA Model Capabilities and Framework



Source Term and EBS Evolution Model

- Inventory
  - Decay & ingrowth
- High resolution of spatial and temporal representation of processes and couplings:
  - UNF degradation

Fuel Matrix Degradation Model

FMDM

- HLW glass degradation
- WP degradation
- Radionuclide release
- Thermal effects
- Gas generation

Flow and Transport Model

- Spatial and temporal representation of THC processes
  - Advection, diffusion, dispersion
  - Solubility limits
  - Isotope partitioning
  - Decay & ingrowth
  - Fractured rock

Discrete Fracture Network

dfnWorks

- Chemical reactions
- Colloids

Biosphere Model

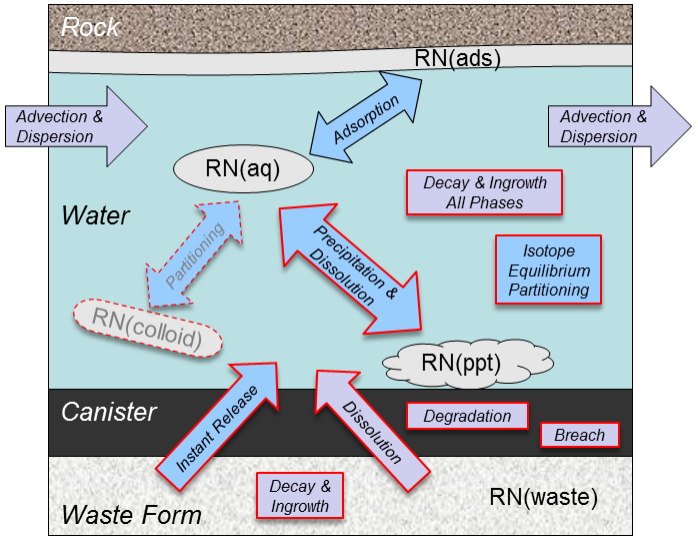
- Exposure pathways
- Uptake/transfer factors
- Radionuclide concentrations in aquifer

Green fill indicates separate code

Red text indicates area of major advances this year

FY16 Progress in GDSA Process Modeling

- **Process models completed in FY16**
  - *Equilibrium isotope solubility and partitioning (aqueous, sorbed, and precipitate phases)*
  - *Decay & ingrowth (waste form, aqueous, sorbed, and precipitate phases)*
  - *Waste package degradation and breach framework with default degradation model*
  - *Multiple waste form dissolution models*
  - *Discrete fracture network mapping tool*
  - *Solution density model*

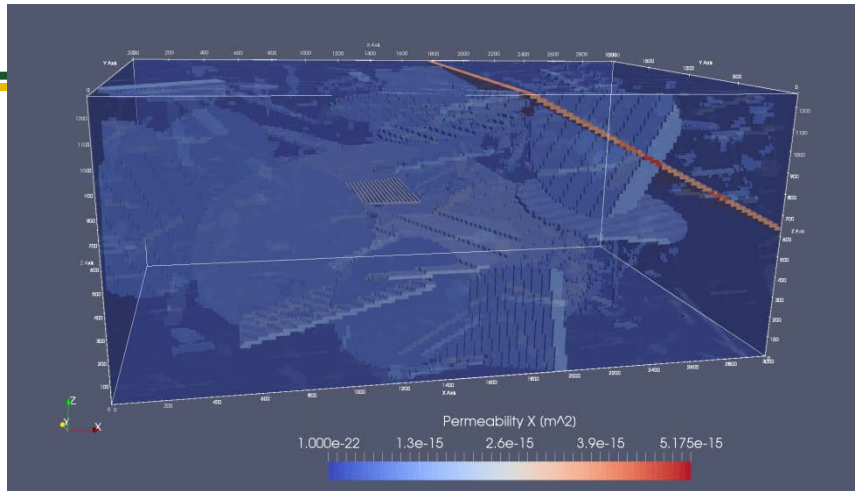


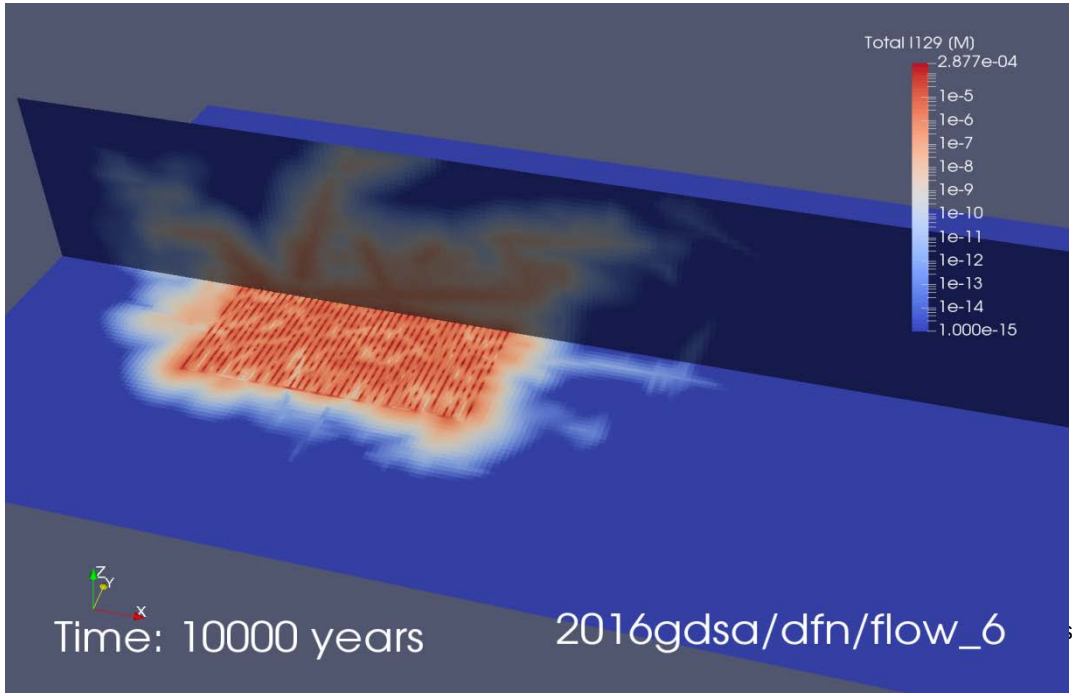
- **Process model integration in FY16**
  - *Fracture network modeling (LANL and SNL)*
  - *Colloids (LANL, LLNL)*
  - *FMDM (fuel dissolution) enhancements (ANL)*
  - *Defense repository, deep borehole, salt repository work packages*
  - *Selection of additional process models for integration*
    - *GDSA integration templates*
    - *GDSA integration session*

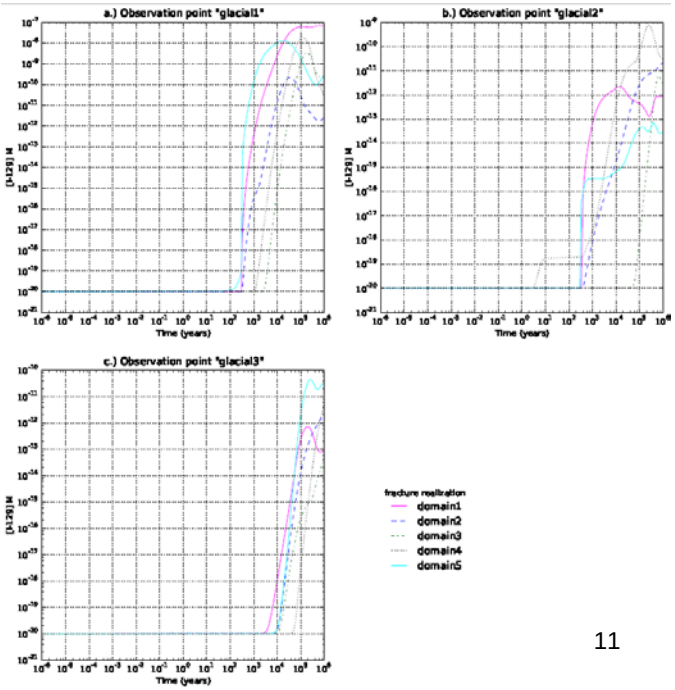
Used Fuel Disposition

FY2016 GDSA PA Modeling and Analysis

- **Crystalline host rock repositories**
  - Commercial, defense, deep borehole
  - Full 3-D, unstructured grids
- **Discrete fracture network (DFN)**
  - Generated by dfnWorks, LANL
  - DFNs mapped to unstructured grid
- **Uncertainty and sensitivity analyses**



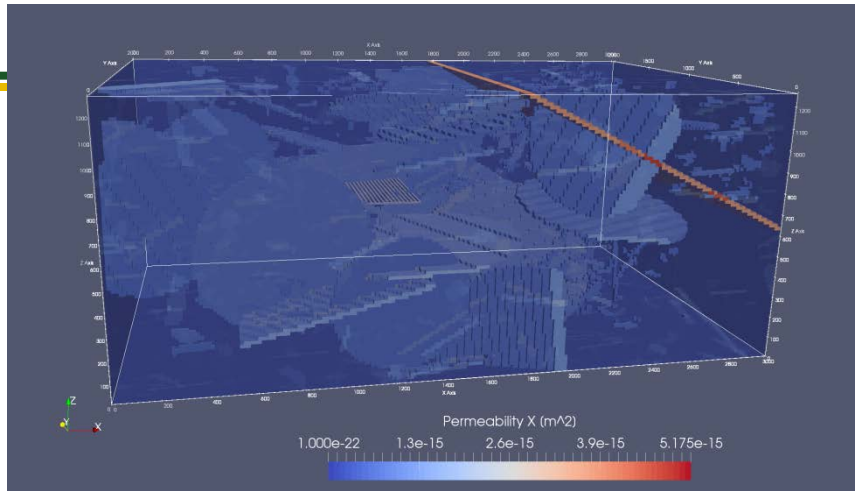


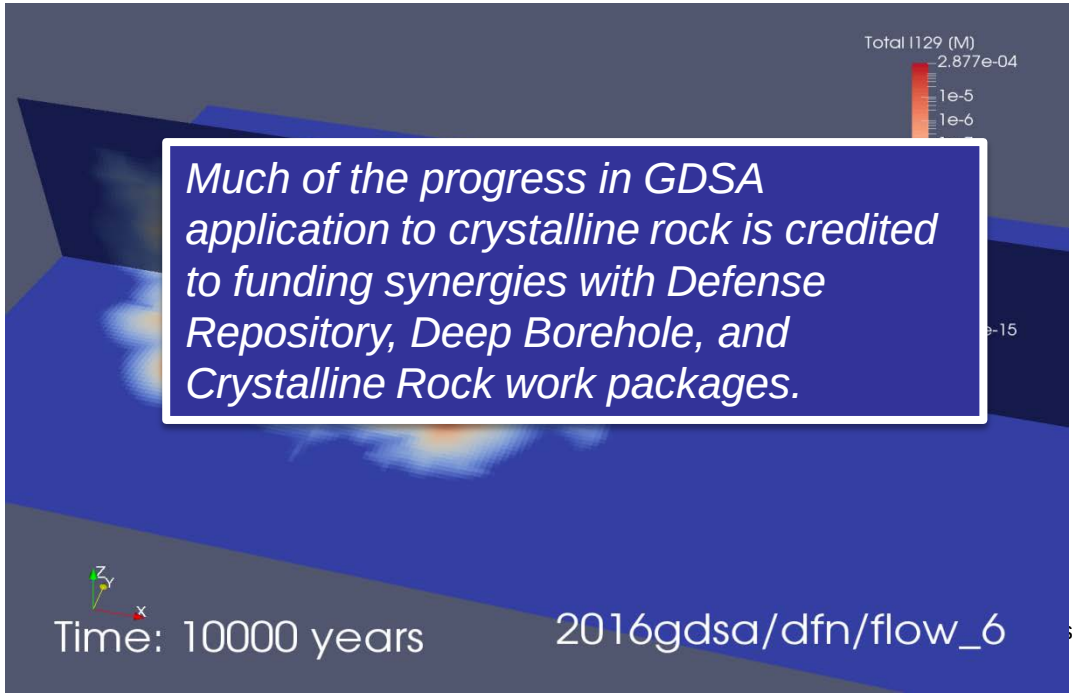


Used Fuel Disposition

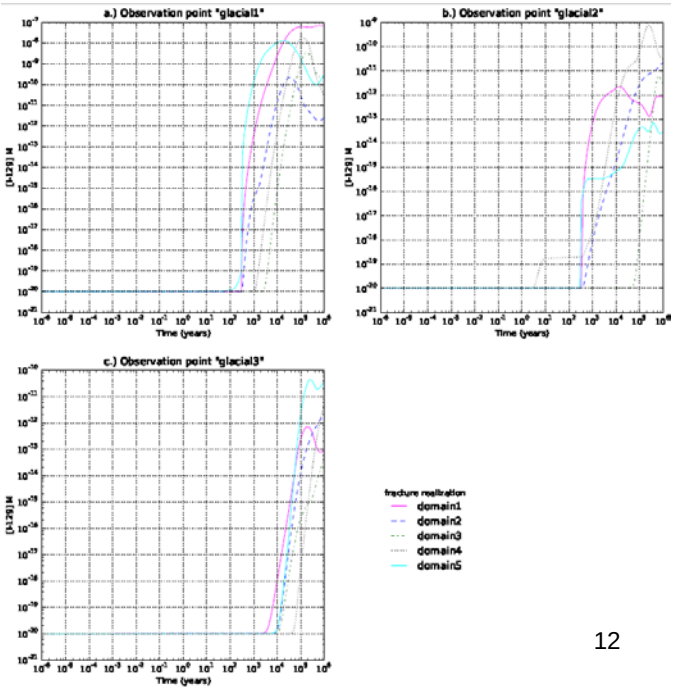
FY2016 GDSA PA Modeling and Analysis

- **Crystalline host rock repositories**
  - Commercial, defense, deep borehole
  - Full 3-D, unstructured grids
- **Discrete fracture network (DFN)**
  - Generated by dfnWorks, LANL
  - DFNs mapped to unstructured grid
- **Uncertainty and sensitivity analyses**





Much of the progress in GDSA application to crystalline rock is credited to funding synergies with Defense Repository, Deep Borehole, and Crystalline Rock work packages.



FY2016 GDSA Deliverable

- **Level M3 milestone report**
  - M3FT-16SN080304011
  - GDSA modeling capability and reference case development
  - September 2016