Used Fuel Disposition Campaign

Introduction and Objectives for

GDSA ⇔ Process Model Integration

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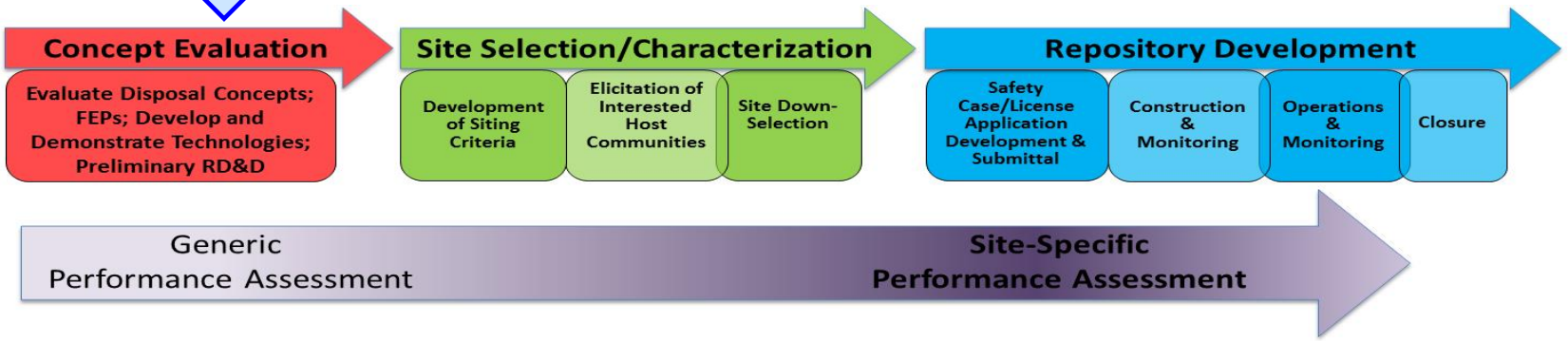
Outline

- Timeline and context
- PA model philosophy
- Linkages: PA model ⇔ process models
- Model integration template
- Goals of this session
- Agenda

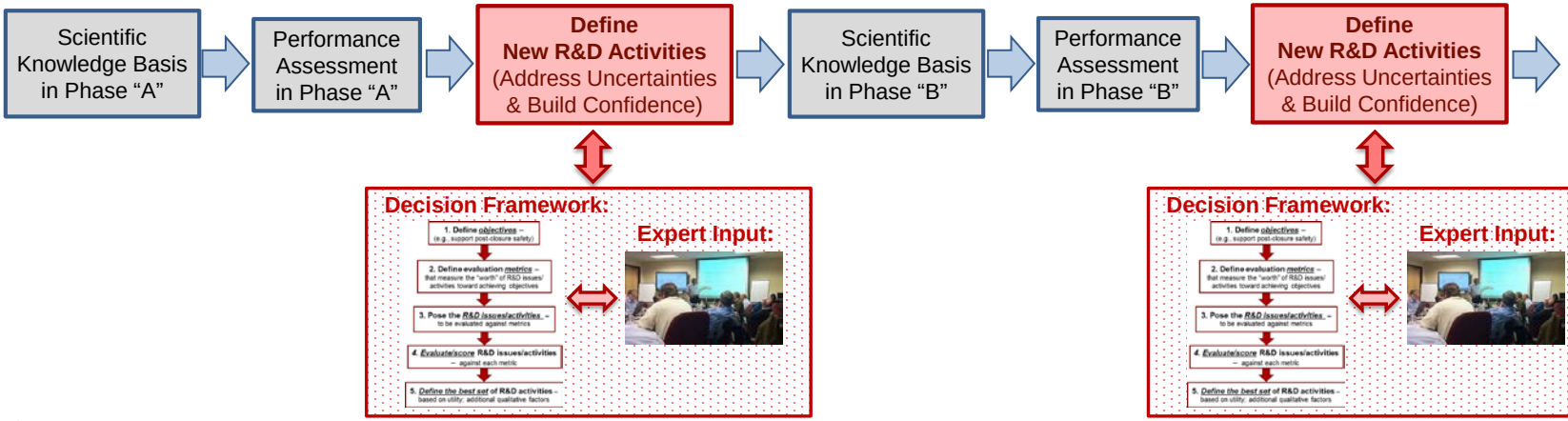
Timeline and Context

You are here



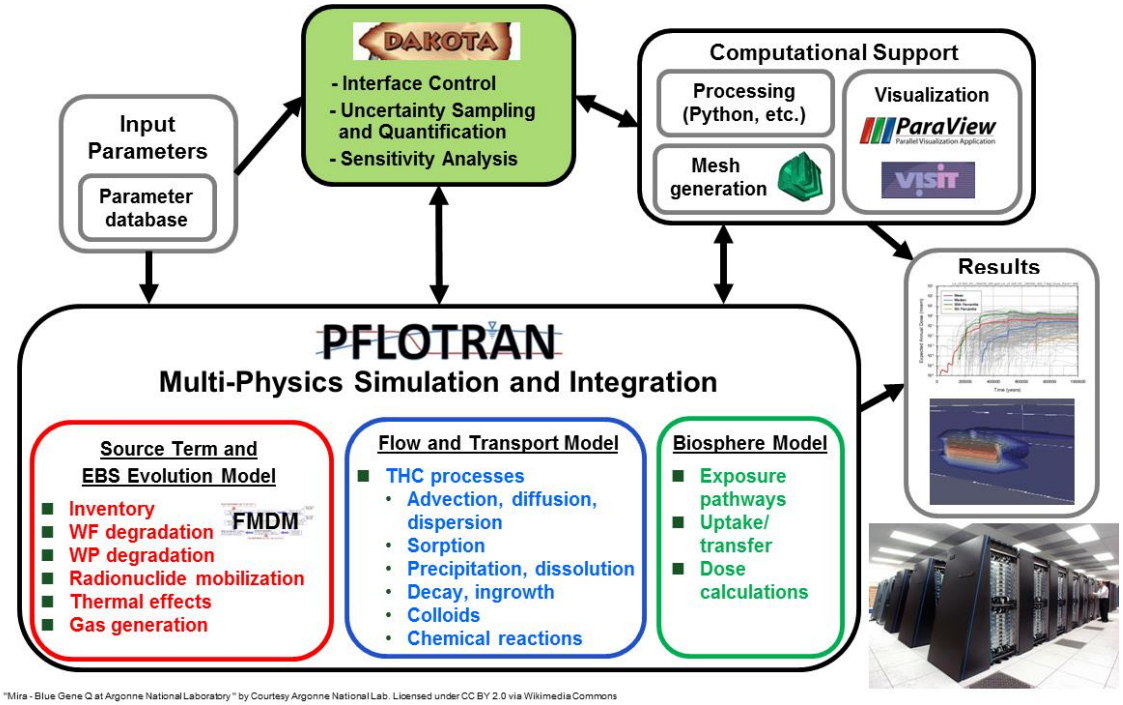
Performance Assessment Functions

1. **<u>Evaluate</u> potential disposal concepts/sites in various host rock media throughout the timeline**
2. **Help <u>prioritize</u> modeling and testing RD&D activities:**



GDSA-PA Philosophy

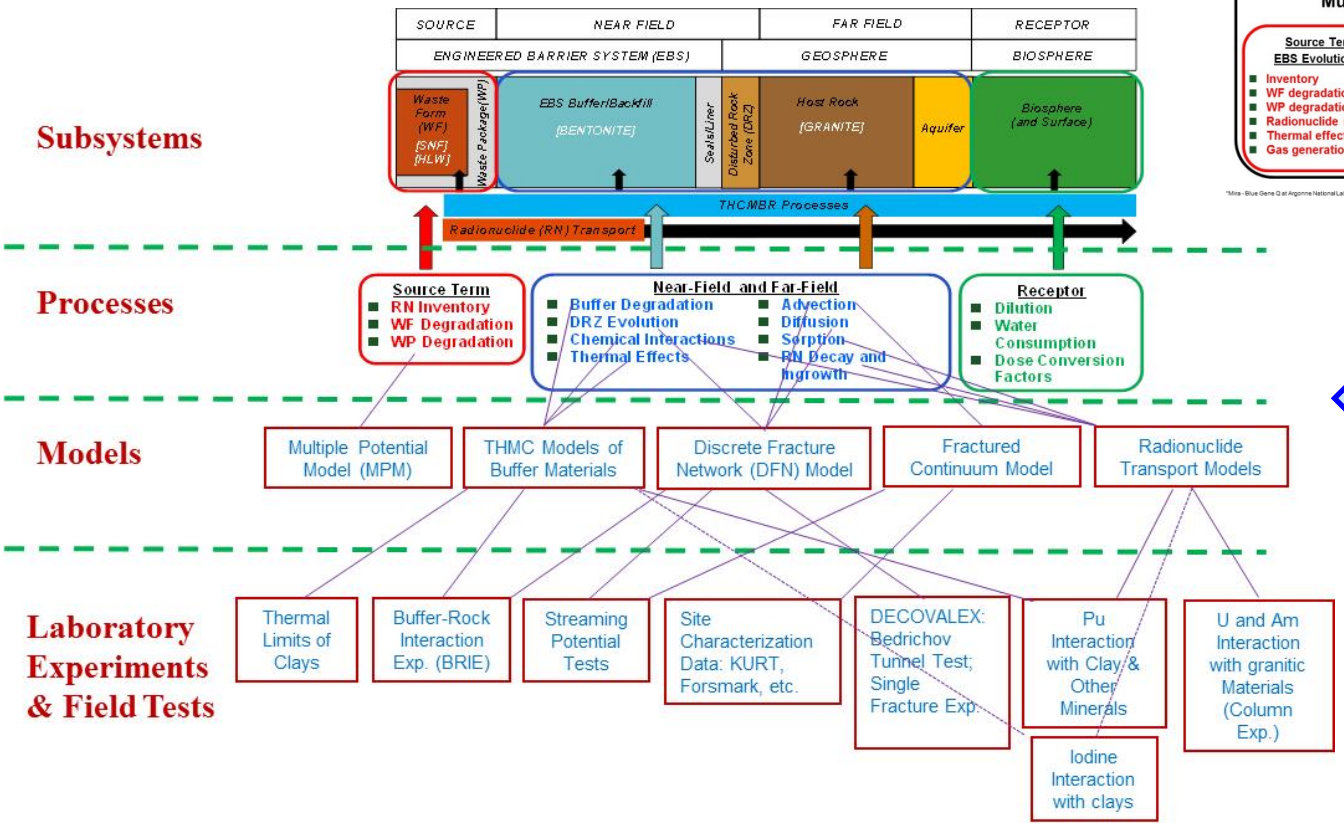
- **Direct representation in PA model of significant coupled multi-physics processes in three dimensions (3-D), over a large heterogeneous domain**
  - *Lessening reliance on assumptions, simplifications, and process abstractions*
- **Realistic spatial resolution of features and processes**
  - *Explicit representation of all waste packages*
- **Appropriate quantification and propagation of uncertainties, based on model form and data availability at various spatial scales**



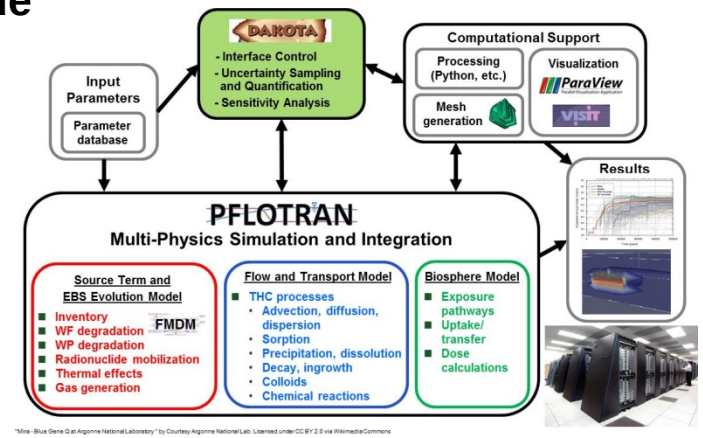
"Mira - Blue Gene Q at Argonne National Laboratory" by Courtesy Argonne National Lab. Licensed under CC BY 2.0 via Wikimedia Commons

Linkages: GDSA ⇔ Process Models

- **Crystalline workscope structure (based on FEPs):**
  - Generally applicable to other concepts/media: clay, salt, DBH



- **GDSA workscope/ model/code structure:**



Process Model Integration Template

Model Integration Template – Integration with PA

1.	**Name of Model:**
2.	**Principal Investigator(s) and Affiliation:**
3.	**Brief Model Description:** • Describe the processes and/or events considered in the model, as well as the applicable feature (e.g., waste form, DRZ, etc.), i.e., include a description of the FEP or FEPs addressed by this model.
4.	**R&D Issue(s) and Safety Case Objectives Addressed by This Model:** • How will the modeled FEP(s) affect repository performance (especially biosphere dose) in a meaningful way? • Why is it important from a regulatory perspective? • Describe the current "state of the art" knowledge regarding the issue(s) addressed and why this particular model advances the state of the art in an important way.
5.	**Proposed method for coupling this model to the PA model**[1] • Direct coupling or abstraction? • Time scale of transient modeled processes (10 years, 100 years…. 1,000,000 years?). • Degree of abstraction: reduced dimensionality; simplified representation; response surface. • Key environmental inputs required from the PA model (and its coupled submodels) and key outputs delivered by this model. • Are there other models you are aware of that are not being developed, which are needed for your model or for PA?
6.	**Real time integration horizon: estimate how long before the proposed model is ready for integration with PA and how long the integration activities might take?** • Are there intermediate steps or degrees of coupling with PA, e.g., can you couple a certain version of your model in an expedited fashion and then go to the next more detailed version—please describe how

[1] The PA simulation framework is based on PFLOTRAN, which is a parallel Fortran 2003/2008 code running in an HPC environment. A desired goal is to reduce the level of "abstraction" required, relative to previous PAs, like Yucca Mtn. However, your model must have reasonable run times in relation to all other parts of the PA model.

In 2015 (last FY):

- **17 templates received from process modelers**
- **4 additional templates internal to GDSA**
- **10 chosen for additional information**

Thank you!
But please update, as the model evolves!

Objective and Goal: This Session

- **<u>OBJECTIVE</u>: Facilitate the integration of UFD process modeling with GDSA by addressing:**
  - (1) *Integration progress* made during FY 2016, and
  - (2) *How* the process model can be coupled to the GDSA-PA Framework in FY17 and beyond.
- **<u>GOAL</u>: The outcome of this session is envisioned to be a rough scope/timeline for integration of process models with GDSA-PA, with an emphasis on FY17 workscope.**
- **<u>METHODS</u>: Response surfaces are NOT the preferred coupling method. Direct coupling or reduced-order mechanistic models (ROMs) are preferred.**

Agenda

3:50 – 3:55 Introduction and Objectives (Sevougian)

3:55 – 4:15 LIGHTNING Talks on Ongoing FY2015-16 Integration (5 min per talk)

1. Density dependence on salinity – **crystalline (deep borehole)** (**Hammond**)
2. DFN Model – **crystalline** (**Stein/Makedonska**)
3. Colloid-facilitated transport model (progress and future work) – **all media** (**Reimus**)
4. CSNF degradation model (FMDM) – **all media** (**Jerden**)

4:15 – 5:20 LIGHTNING Talks on Possible New FY17 Integration Workscope (5 min/talk)

5. Salt coupled THM processes (TOUGH-FLAC) – **salt** (**Rutqvist**)
6. THC Processes in salt – **salt** (**Stauffer**)
7. TOUGH-FLAC/BBM/RBSN models – **argillite and/or crystalline (deep borehole)** (**Rutqvist**)
8. THMC model (illitization) and THM model (TPHM Hooke's) – **argillite** (**Zheng**)
9. DFN enhancements – **granite** (**Viswanathan**)
10. Waste package degradation – **argillite and/or crystalline** (**Jove-Colon**)
11. Waste package and waste form degradation – **all media** (**Frederick**)
12. Glass degradation – **all media** (**Rieke**)
13. Grid refinement – **all media** (**Alzraiee/Hammond**)
14. THM processes in salt (PFLOTRAN-Adagio) – **salt** (**Park/Hammond**)
15. A control variate method for performance assessment – **all media** (**MacKinnon**)
16. Remaining process model gaps – **all media** (**Mariner**)

5:20 – 5:40 Integration discussion (All)

Herr
Hammond