# Cementitious Barriers Partnership: Demonstration of Coupling and Code Integration

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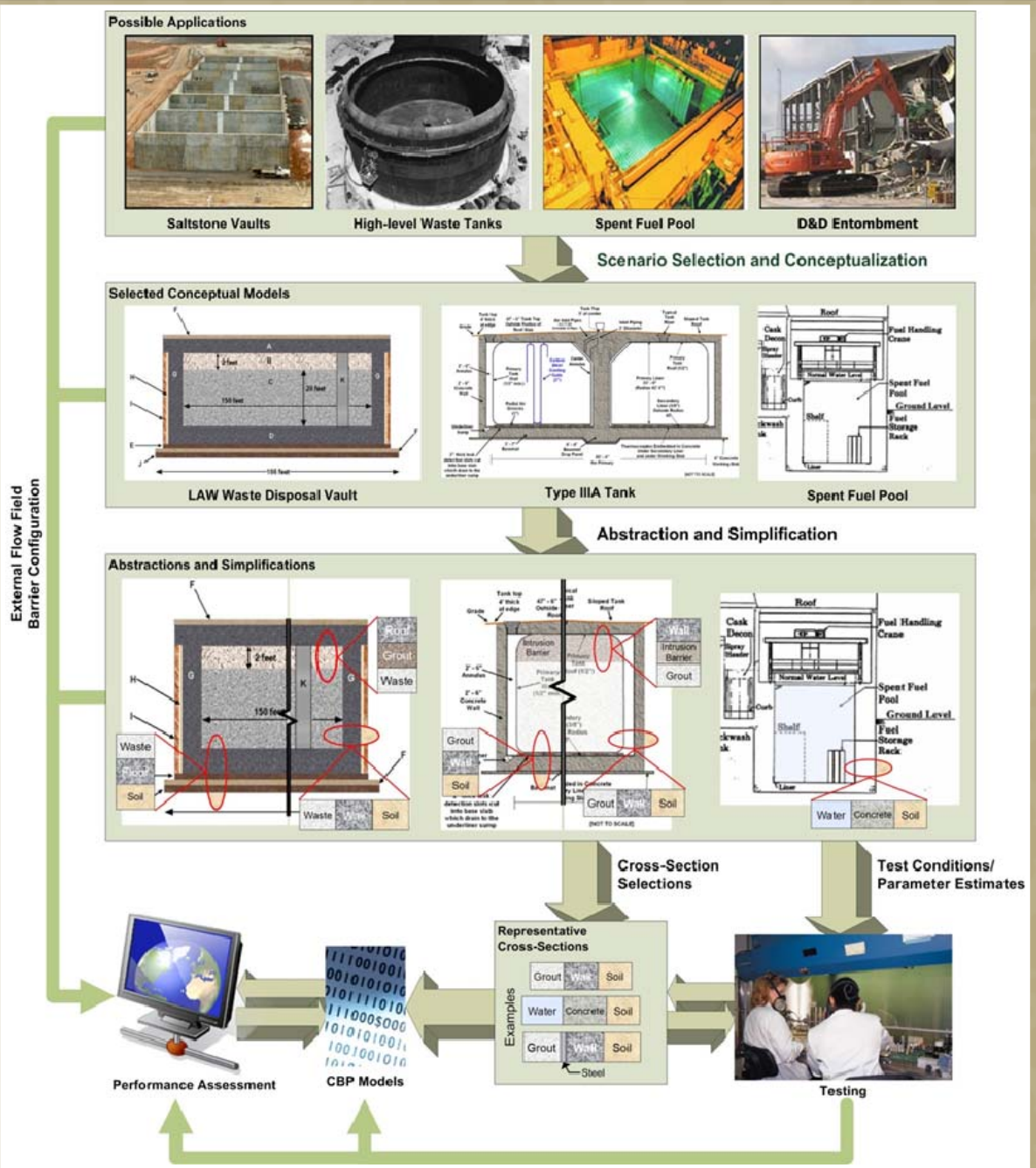
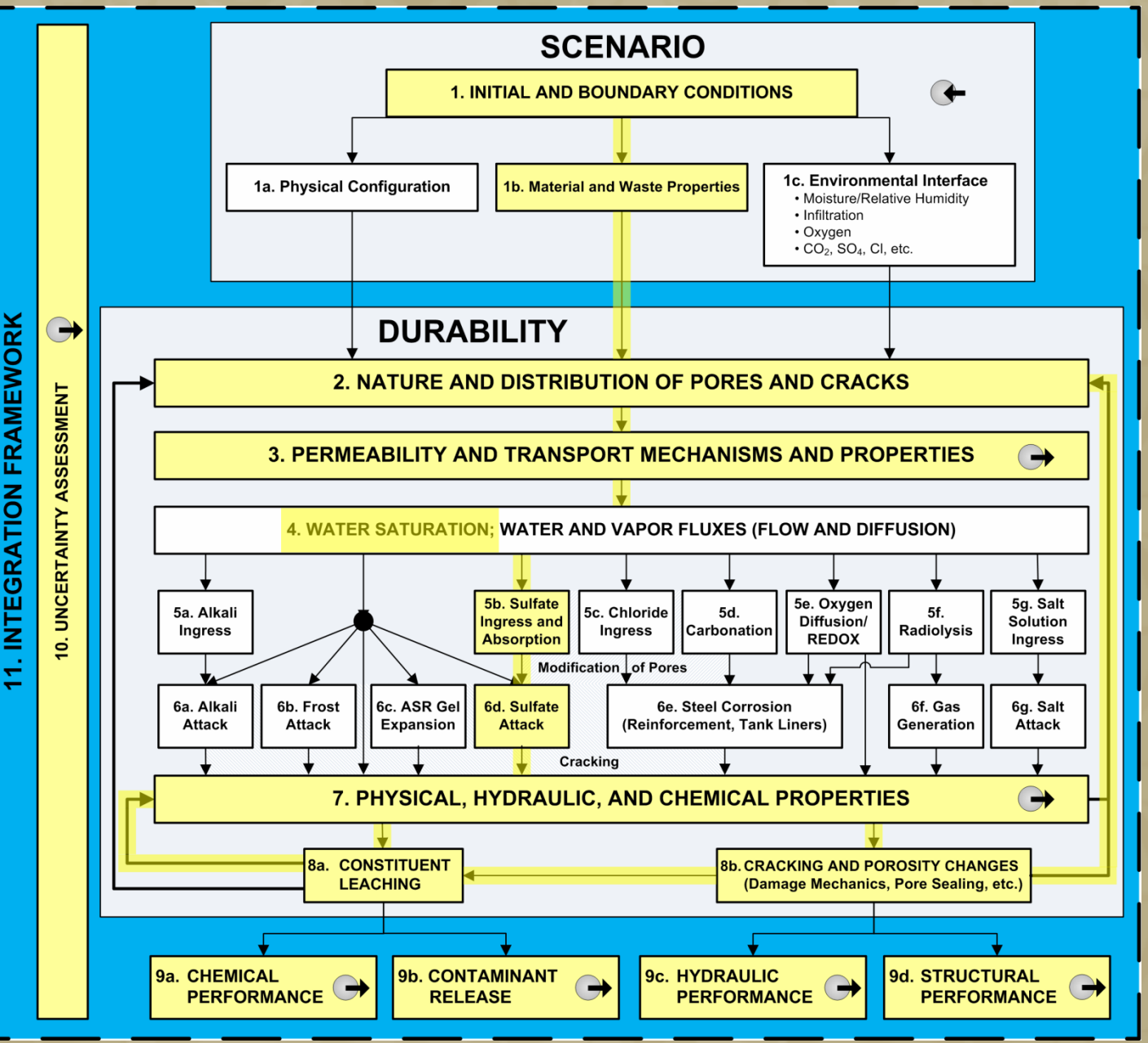



# Linking Prototype Cases to Performance Models through System Abstraction and Validated by Laboratory and Field Testing

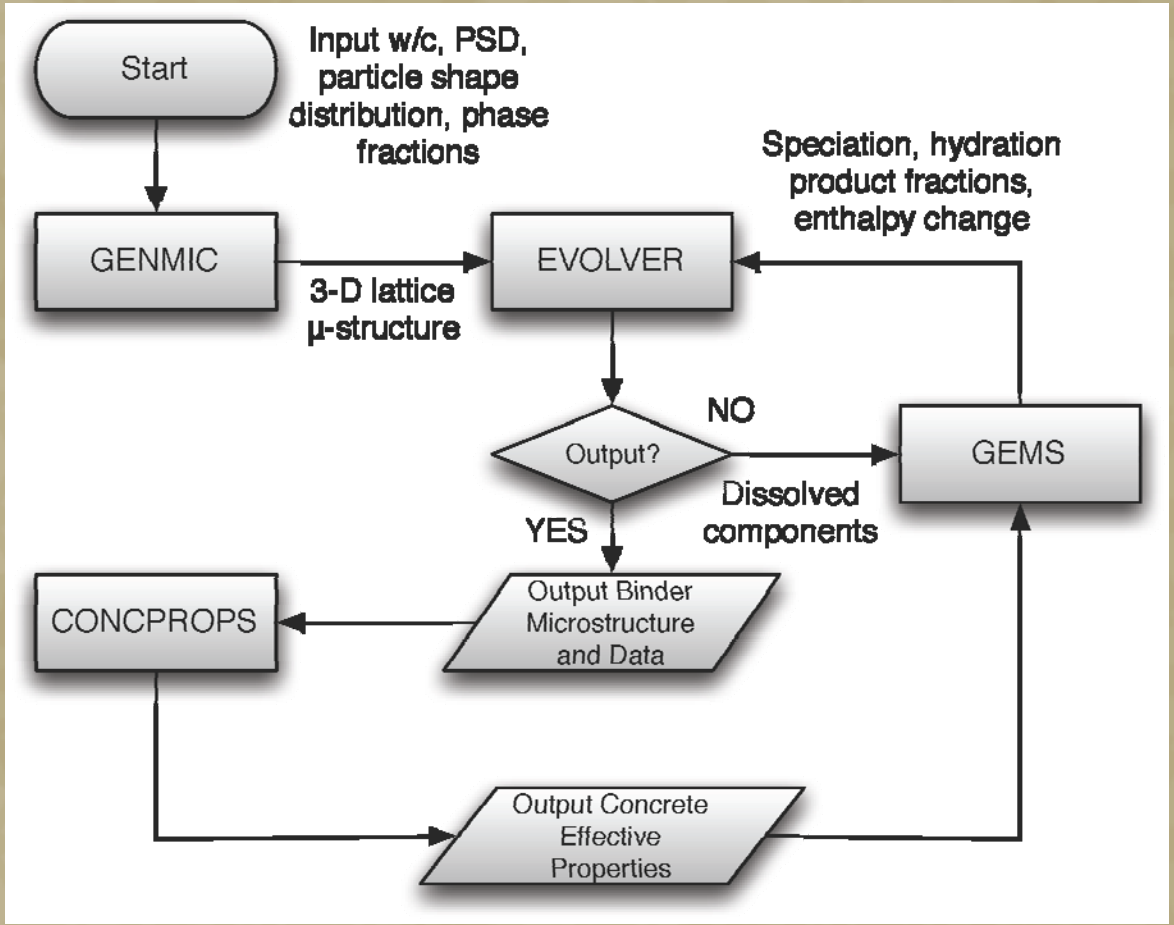
# Sulfate Attack as a "Proof of Principle" for Coupling of Phenomena



# THAMES (NIST)

- **Virtual "micro-probe" of microstructure**
  - Constructs time-dependent 3-D virtual microstructures of a cementitious binder during hydration or degradation
  - Computes important engineering properties of a concrete made from a binder at prescribed times
- **Planned model improvements**
  - Embed geochemical modeling code (GEMS) into microstructure module
  - Improve hydration microstructure growth rules
  - Parallelize THAMES code
  - Incorporate microstructure impact on GEMS boundary conditions
  - Incorporate degradation reactions and effects on microstructure
  - Improve predictions for more complex systems

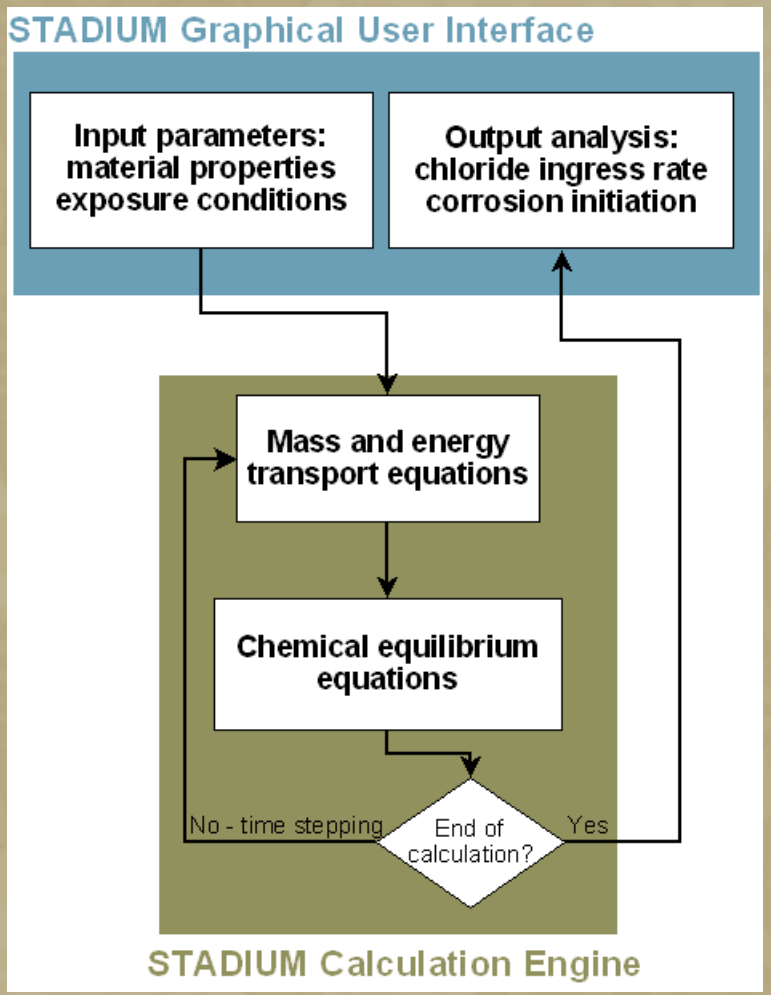
# THAMES Overview



# STADIUM® (SIMCO Technologies)

- **Simulates ionic transport in saturated/unsaturated, isothermal/non-isothermal cementitious materials**
  - Simulates contaminant ingress, ionic leaching in pore solution, and modifications to microstructure of cementitious material
  - Accounts for electrical coupling between ions and activity gradients and dissolution/precipitation due to the high paste reactivity
  - Main components: ionic transport, electrodiffusion potential conservation, moisture transport, and energy conservation
  - Test results and methods available that relate directly to model predictions and validation
- **Planned model improvements**
  - Model damage due to sulfate exposure
  - Model effect of pore solution viscosity
  - Model effect of pore solution density of highly concentrated solutions
  - Model carbonation and acid exposure and resulting secondary species

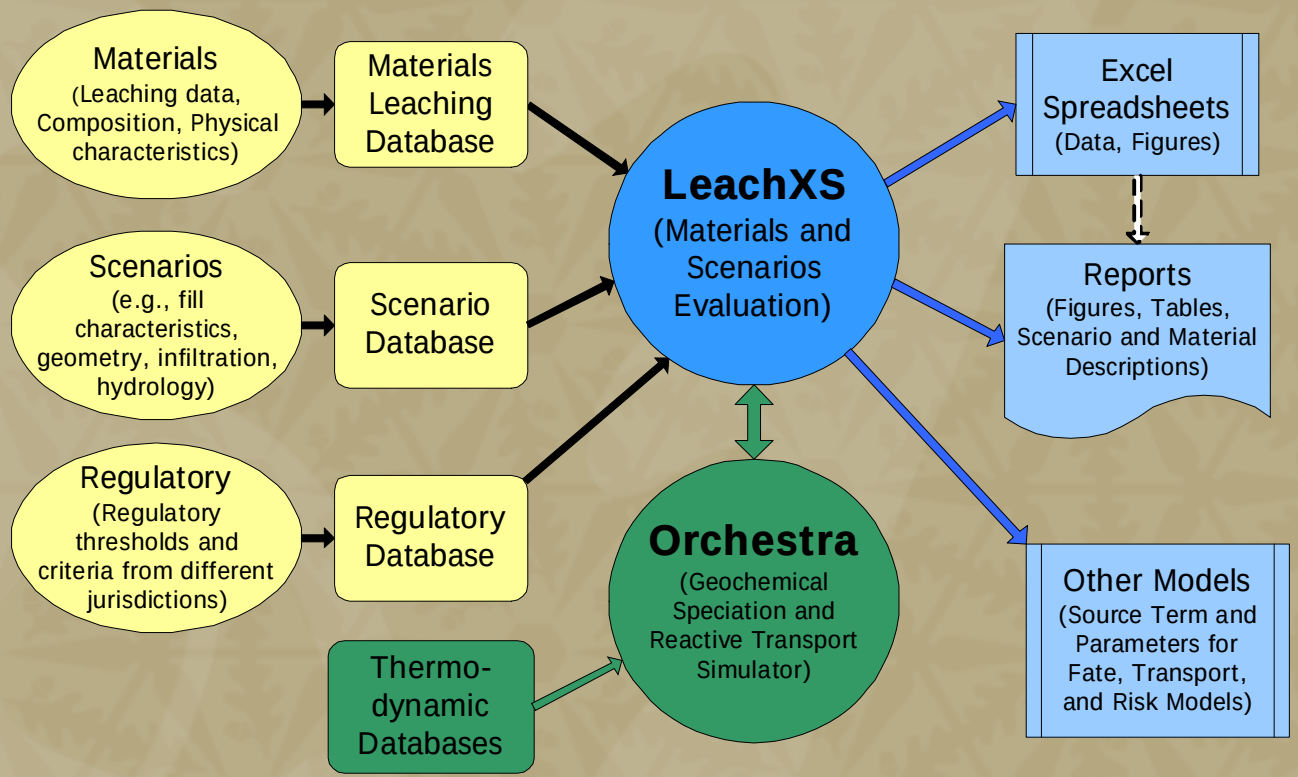
# STADIUM Overview



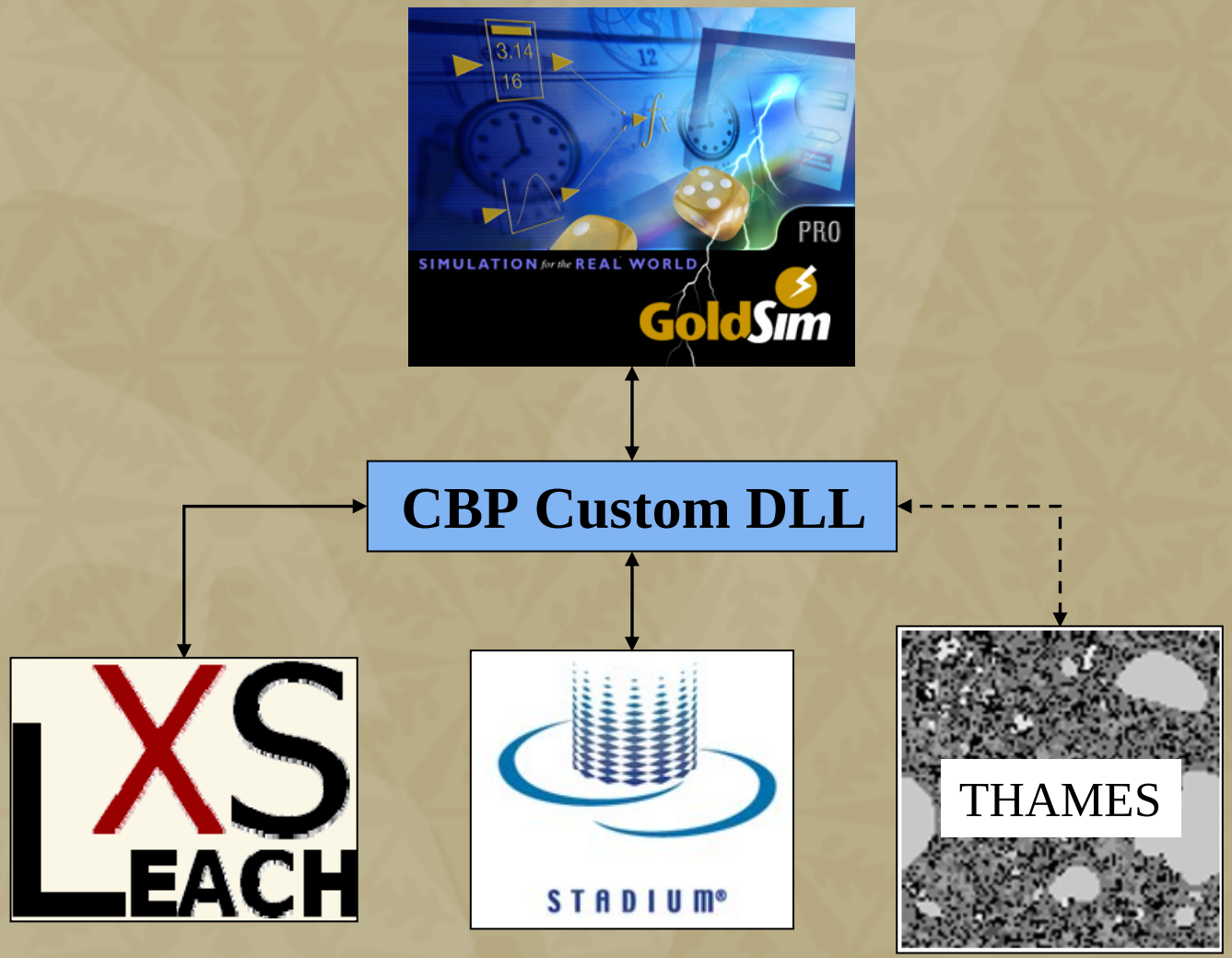
# LeachXS™/ORCHESTRA (ECN)

- **LeachXS is a database/expert decision support system for characterization and environmental impact assessment**
  - Includes leaching results for 600+ materials (cements, concretes, stabilized wastes, soils), scenarios, and regulations
  - Assists evaluation and lab guidance, data management /evaluation, source term description, impact evaluation, and decision analysis
  - Geochemical speciation and chemical reaction/transport modeling integrated into LeachXS using ORCHESTRA model
- **Planned model improvements**
  - Parallelize LeachXS/ORCHESTRA equilibrium module calculations
  - Incorporate radionuclides and decay in LeachXS/ORCHESTRA
  - Evaluate chemical model performance by comparing with pH dependent solubility and diffusion data
  - Account for chemical model uncertainty on transport predictions
  - Account for impact of variable saturation and intermittent wetting
  - Account for effects of physical and chemical heterogeneity

# LeachXS/ORCHESTRA Overview



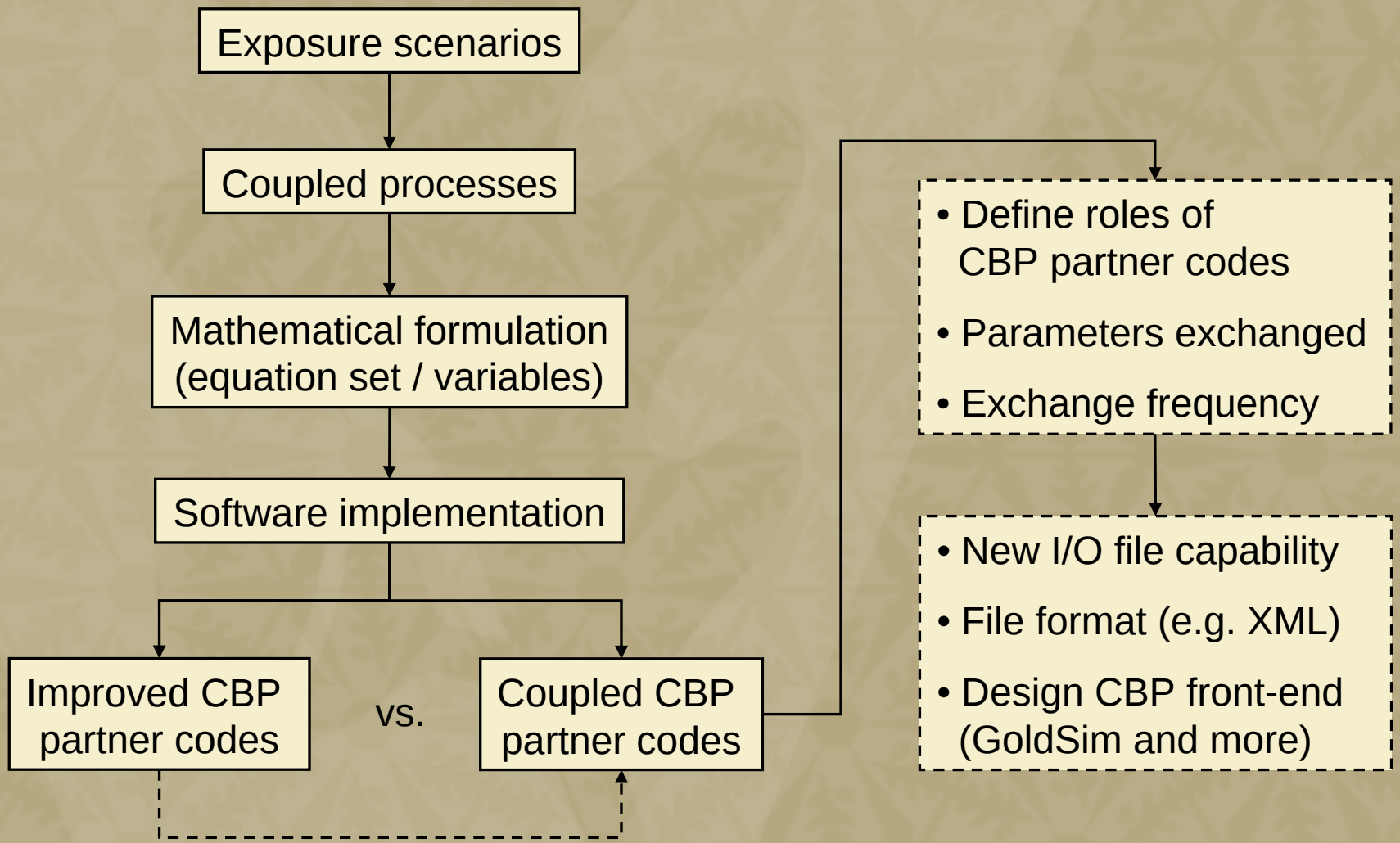
# Integrated Model Description



# Integrated Model General Design Principles

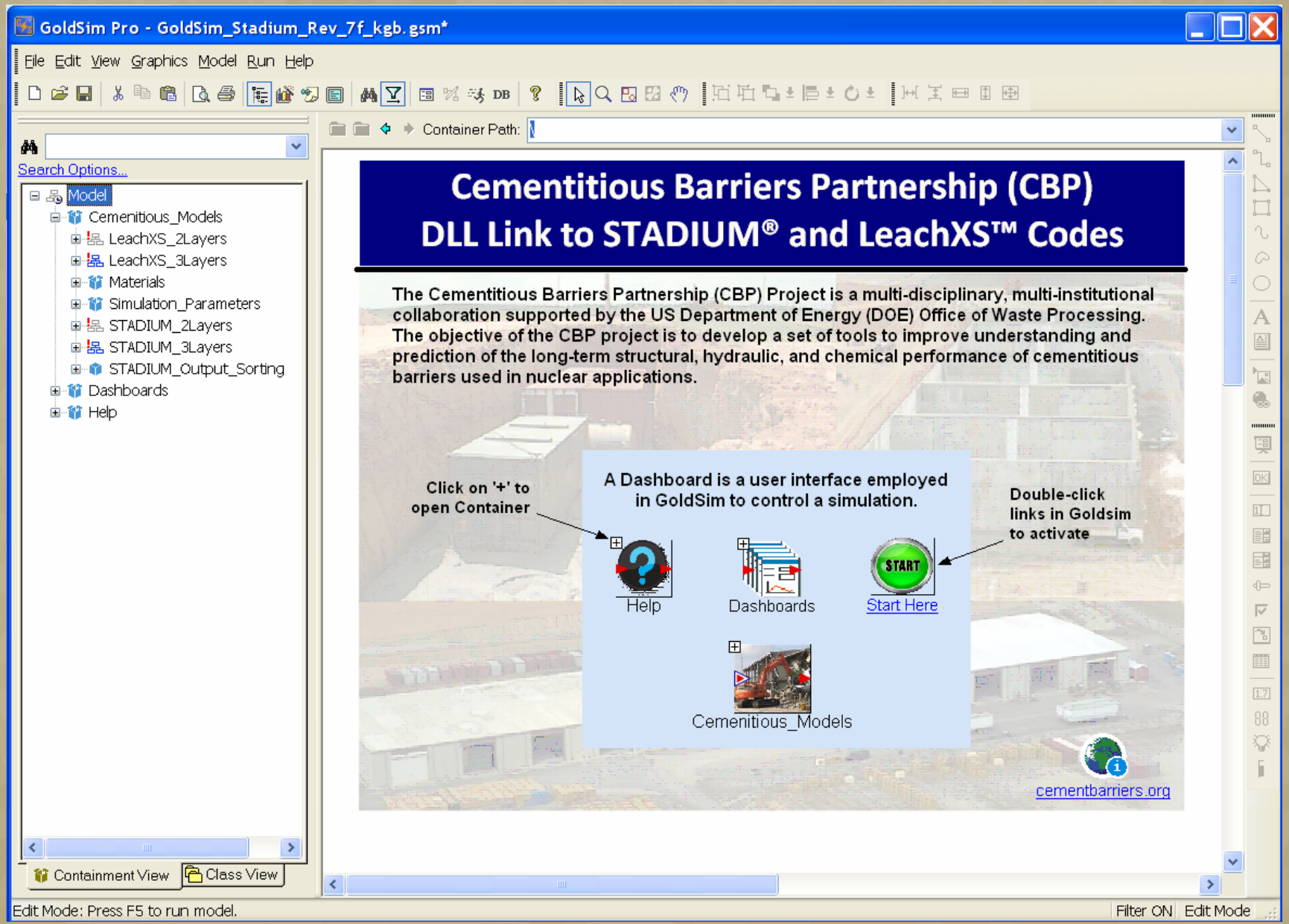
- **Model development proceeding in phases**
  - Weakest appropriate coupling amongst models
- **Parallel improvement of partner codes and coupling**
  - Influence, but stay within, CBP partners' main code development paths
  - Accept reasonable extant duplication of functionality (e.g., bulk chemistry), but require consistency
- **Data and I/O considerations**
  - Common repository (database) for common data
  - Common data formats, so an output can be an input
  - Common graphics format
  - Consistent mesh/node generation

# Coupling Decisions and Software Integration



# Integrated Model Development

- **Phase I: Use existing CBP partner codes "as is"**
  - Minimal coupling
- **Phase II: Coupling through functions**
  - Modest coupling where appropriate
  - Enhanced I/O needed in partner codes
  - Use "system call" DLLs using instructions file (at run time)
- **Phase III: Selected coupling at each timestep**
  - Strongest coupling / synchronization
  - Call partner codes as DLL subroutines (object code level)


GoldSim Pro - GoldSim_Stadium_Rev_7f_kgb.gsm*
File Edit View Graphics Model Run Help
Container Path:
Search Options...
Model
Cementitious_Models
LeachXS_2Layers
LeachXS_3Layers
Materials
Simulation_Parameters
STADIUM_2Layers
STADIUM_3Layers
STADIUM_Output_Sorting
Dashboards
Help
Containment View
Class View
Cementitious Barriers Partnership (CBP)
DLL Link to STADIUM® and LeachXS™ Codes
The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the US Department of Energy (DOE) Office of Waste Processing. The objective of the CBP project is to develop a set of tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers used in nuclear applications.
Click on '+' to open Container
A Dashboard is a user interface employed in GoldSim to control a simulation.
Double-click links in Goldsim to activate
Help
Dashboards
START
Start Here
Cementitious_Models
cementbarriers.org
Edit Mode: Press F5 to run model.
Filter ON
Edit Mode

GoldSim Pro - GoldSim_Stadium_Rev_7f_kgb.gsm*

File Edit View Graphics Model Run Help

Container Path: \Dashboards\STADIUM_Control

Search Options...

- Model
  - Cemenitious_Models
    - LeachXS_2Layers
    - LeachXS_3Layers
    - Materials
    - Simulation_Parameters
    - STADIUM_2Layers
    - STADIUM_3Layers
    - STADIUM_Output_Sorting
  - Dashboards
    - Build_Mesh
    - LeachXS_Control
    - Simulation_Control
    - STADIUM_Control
    - STADIUM_More_Options
    - ViewSTADIUMResults
  - Help

Containment View | Class View

# STADIUM® Run Controls Dashboard

## Scenario Options

**Option 1: Two-layer system** ☑

| | | | | |
|---|---|---|---|---|
| Layer 1: | Salt Waste Type 2 | 10 m | 0.05 | Concentration RSD |
| Layer 2: | Concrete Type 2 | 15 m | 0.05 | Concentration RSD |

**Option 2: Three-layer system** ☐

| | | | | |
|---|---|---|---|---|
| Layer 1: | Salt Waste Type 1 | 5 m | 0.05 | Concentration RSD |
| Layer 2: | Concrete Type 2 | 10 m | 0.05 | Concentration RSD |
| Layer 3: | Soil Type 1 | 20 m | 0.05 | Concentration RSD |

Generate Mesh | View Geometry | More Options

Exit GoldSim

## General Run Settings

| | |
|---|---|
| Initial Time Step, sec | 5000 |
| Max Time Step, sec | 432000 |
| Step Adapt Factor | 1.5 |
| Step Adapt Criterion | 0.005 |
| Total number of nodes | 101 |

Check to Save STADIUM® Output ☑

## View STADIUM® Results

View Results

## Simulation Controls

Browse Model | Run Simulation

Simulation Settings | Simulation Controls

Edit Mode: Press F5 to run model.

Scale: 100% | Filter ON | Edit Mode

# CBP DLL Subroutine

- **Avoid need for low-level programming by user**
  - Put generic executable content in pre-compiled subroutine (DLL)
  - Put application content in "instructions file" read at run-time
  - Primary instructions: PUT (create input), EXE (execute file), GET (retrieve input), and LOG (record)
- **Provide flexible, user-friendly access to partner code input and output files via instructions file**
  - Row selection by number, label, value
  - Field selection by number
- **Used to couple STADIUM and LeachXS/ORCHESTRA to GoldSim model**

# Uncertainty Analysis

- **Sources of uncertainty**
  - Inherent variability
  - Data uncertainty
  - Model uncertainty
- **Approaches to uncertainty management**
  - GoldSim has sensitivity and uncertainty analysis capabilities
  - More advanced capabilities will be used to evaluate model uncertainty impacts

# Summary of Uncertainty Analysis

- Uncertainties due to physical variability, data uncertainty, and model uncertainty must be considered
- Several methods available for uncertainty propagation through computational models
- Methods for model uncertainty and error quantification currently under study
- Bayesian framework appears attractive for managing various uncertainties
- Methods for epistemic uncertainty under investigation
- Application to large problems (time-dependent, complicated multi-physics) needs investigation (accuracy, computational effort, uncertainty quantification, confidence assessment)