Advanced Simulation Capability for Environmental Management (ASCEM) Overview and Example Application

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What is ASCEM?

- **Advanced Simulation Capability for Environmental Management**
  - Modeling toolset currently under development for understanding and predicting subsurface contaminant fate and transport

- **Organized into three thrust areas**
  - **High Performance Computing** – open-source, high performance simulator (Amanzi)
  - **Platform** – tools that facilitate model setup and simulation execution (Akuna)
  - **Applications** – demonstrate the tools through applications to real sites

- **Completed initial user release of toolset**

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ascemdoe.org
User Environment

Akuna

[Diagram showing the User Environment with components like Velo, Connection, Toolset, Agni, and HPC Computing Environment]
Application to Hanford BC Cribs

- Former plutonium production site
  - Waste disposed from 1956 to 1958 to 6 cribs
  - Funnel-shaped with sloping sides (~3 x 3 m wide)
- Located a few meters bgs
- Thick vadose zone (~107 m)
- Primary contaminant of concern $^{\text{99}}$Tc
- Traditional remediation technologies are ineffective
- Evaluate uncertainty impact on remediation

(Rucker and Fink 2007)
**Problem Description**

- **Boundary Conditions**
  - > 10 million gallons liquid waste released at 6 cribs
    - 1956 – 1958
    - $^{99}$Tc primary contaminant
    - Source concentrations $\sim 10^6$ pCi/L
  - Recharge at surface
  - Water table boundary at the bottom of the domain

- 320 m x 280 m x 107 m (~455K grid blocks)

- Executed simulation from 0 – 2008
  - 0 – 1956 period to attain steady state flow field
  - 1956 – 2008 transient
Major Stratigraphy
Generated 100 realizations of three-dimensional lithofacies distributions using geostatistical model

- Identified by k-means cluster analysis of $^{232}$Th and $^{40}$K data (spectral gamma log data)
- Three lithofacies identified, log data from 5 wells
Geologic Realizations

- Selected 10 realizations for demonstration
- Layering is the same, but small-scale variability in heterogeneities captured
Property Assignments and Boundary Conditions

Hydraulic Property Input

Boundary Condition Input
Parameter Estimation

- Permeability and porosity estimation
- Moisture content and $^{99}$Tc measured in 2008 at Boreholes A & C
- Data obtained from database, accessed through web interface, and exported to Akuna
Parameter Estimation

Borehole A Tc-99 Concentration

Borehole A Moisture Content

Borehole C Moisture Content

Elevation (m)

Concentration (Ci/L)

Moisture Content

Observed
GR 01
GR 02
GR 03
GR 04
GR 05
GR 06
GR 07
GR 08
GR 09
GR 10
Simulation 1956 – 2008

Tc-99 (pCi/L)

Facies 1  Facies 2  Facies 3

Year = 1956

through Crib 15, 17, 19 at y=122.5

through Crib 14, 16, 18 at y=117.5

through Borehole A and near Crib 17, 18
Uncertainty Quantification

- Varied recharge rate for 100 simulations for 2012 – 3000
  - Rates represent management actions (1 – 75 mm/yr)
    - Soil desiccation
    - Surface barriers
    - No-action
    - Soil flushing
- Metrics
  - Peak concentration and arrival time at water table
  - Time at which a threshold concentration is exceeded
- Launched on 9600 processor cores, 96 per simulation

Screenshot from UQ Toolset: Histogram of Recharge Rates
Uncertainty Quantification

- Time to peak occurs within 200 years, small variation with recharge rate
  
  a) Mean and 95% confidence intervals for $^{99}$Tc breakthrough at boreholes A and C
  
  b) Histogram of time to reach peak concentration
Uncertainty Quantification

- Compare breakthrough curves for one conceptual model realization to all 10
  - Confidence intervals are wider when 10 realizations of the conceptual model are considered
  - Upper bound is ~85% higher at Borehole A for all ten models than for GR01

Mean and 95% confidence intervals for the $^{99}$Tc breakthrough curve at Boreholes A and C for single and multiple geologic realizations
Conclusions

- ASCEM facilitates model setup, execution, analysis, and visualization
- High performance computing enables multiple realizations of complex model through reduction in computational time
- Simulations of BC Cribs provides insight on controlling processes and properties for $^{99}$Tc transport in the subsurface
  - Baseline conditions for “no action” alternative
  - Variation in recharge rate from soil desiccation and surface barriers
  - Variability in conceptual models impacted the magnitude of peak concentrations, but had minor impact on arrival times
Thank You!

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