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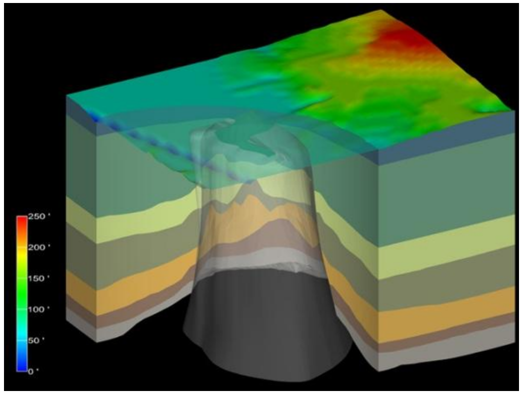

Site Investigations: Characterization of System Heterogeneity and Classical Statistical Methods

IAEA Training Course – July 1-5, 2013

Bill Arnold

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

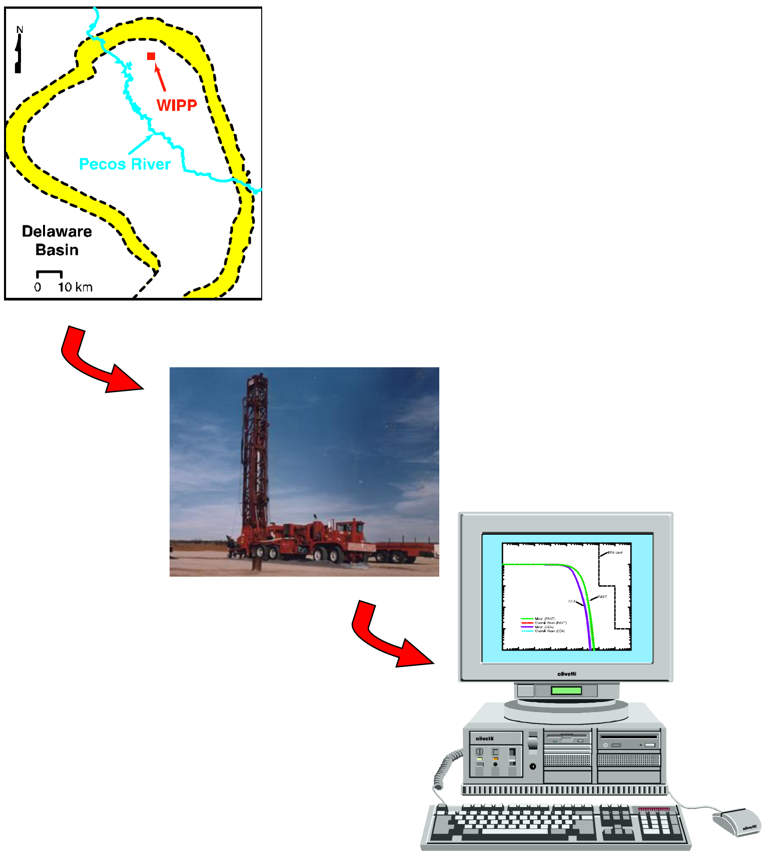
- **Introduction**
- **Geology**
- **Hydrology**
- **Geochemistry**
- **Geophysics**
- **Classical Statistics**

Introduction

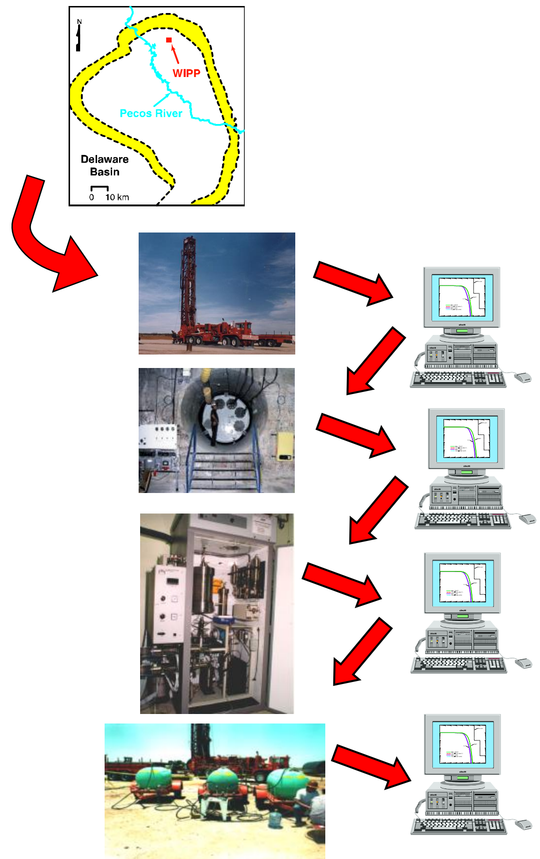
- **Site investigations serve various roles during waste repository development**
  - **Early confidence that the site is viable**
  - **Identify important features, events, and processes that form the basis of the site conceptual model**
  - **Characterization of geosphere components and quantification of parameters used in the safety assessment**
  - **Assess the variability and uncertainty in the natural system**
- **Ideally, site characterization activities are guided and prioritized by relevance to safety of the disposal system**
- **Following the initial phase of site characterization, further investigations are done in an iterative fashion**

Introduction

Classical Approach

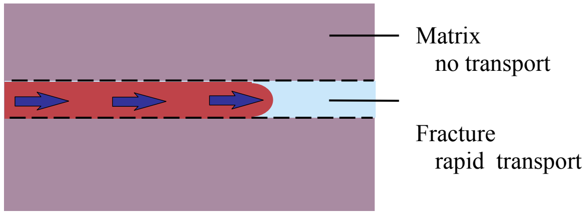


Iterative Approach

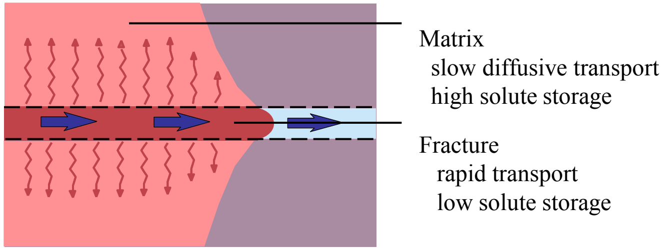


Introduction – Conceptual Model

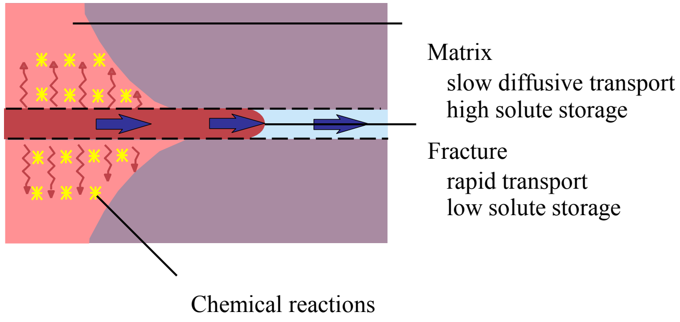
Fracture-
Only
Transport



Double-Porosity
Nonreactive Transport
(Physical Retardation)



Double-Porosity
Reactive Transport
(Physical and Chemical Retardation)



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Introduction – Conceptual Model

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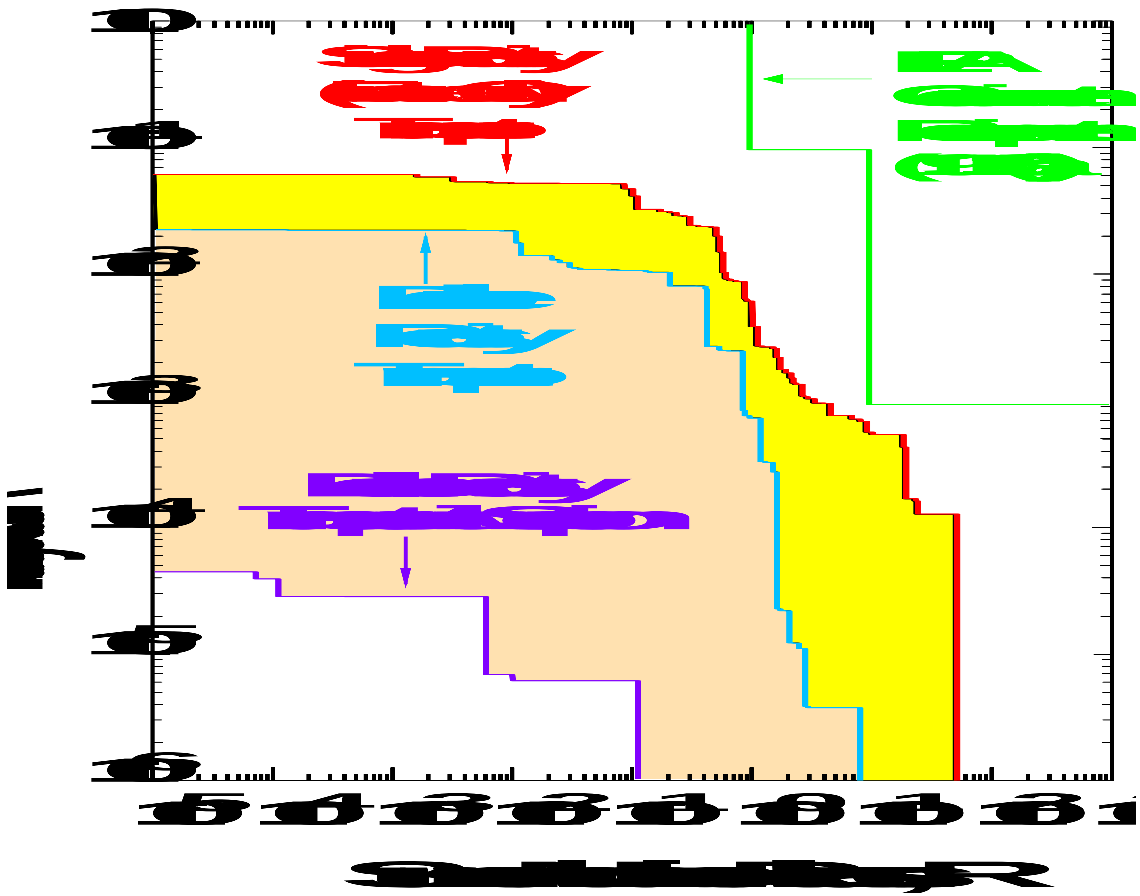
Conceptual model of fracture transport within the Culebra Dolomite has a strong influence on WIPP PA results.



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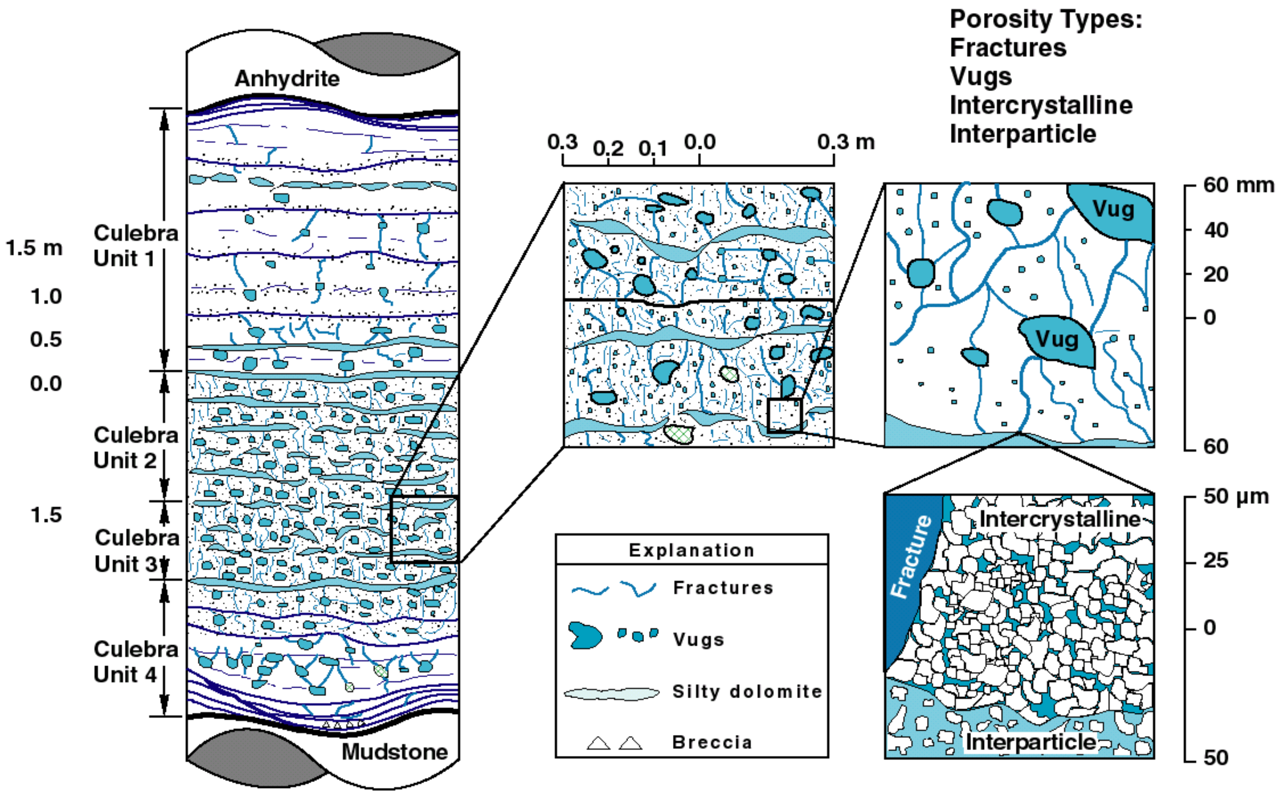
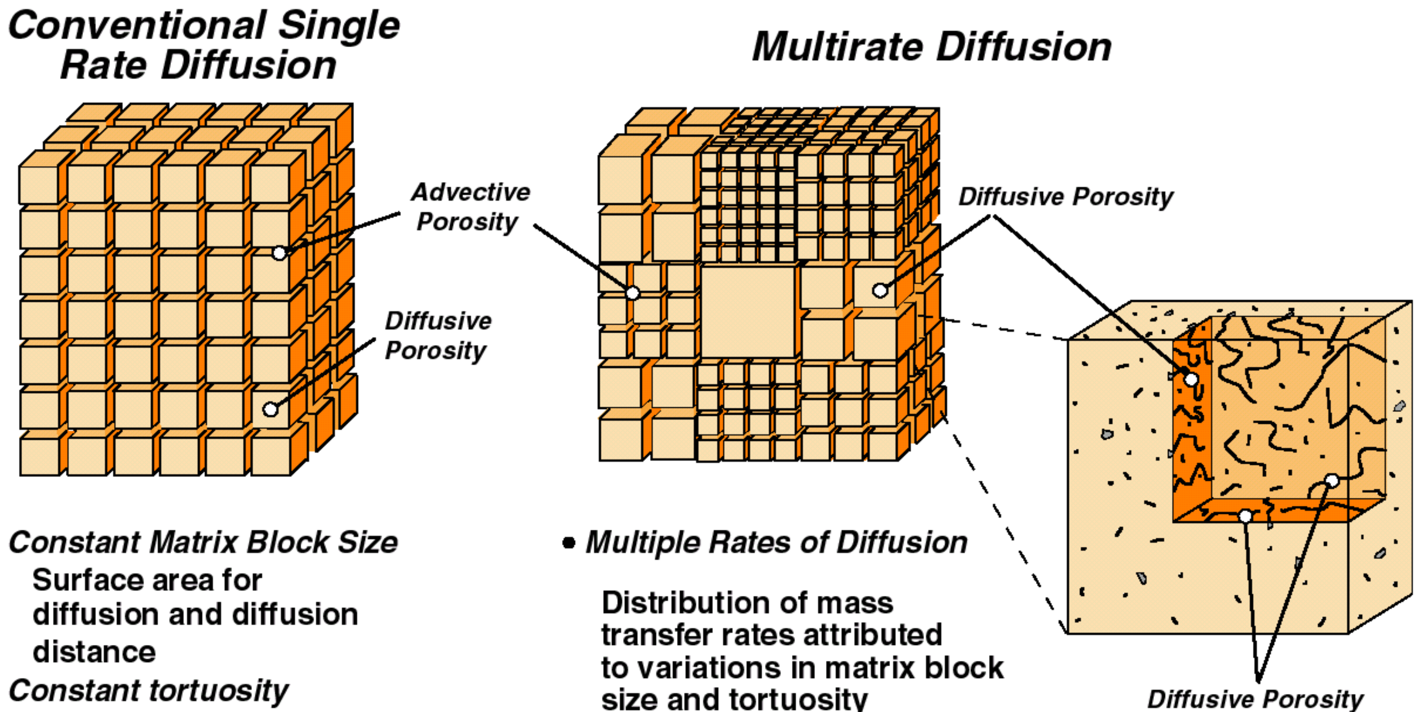
Introduction – Conceptual Model

Refined Conceptual Model of Geology



Introduction – Conceptual Model

Multirate Diffusion Model Conceptualization

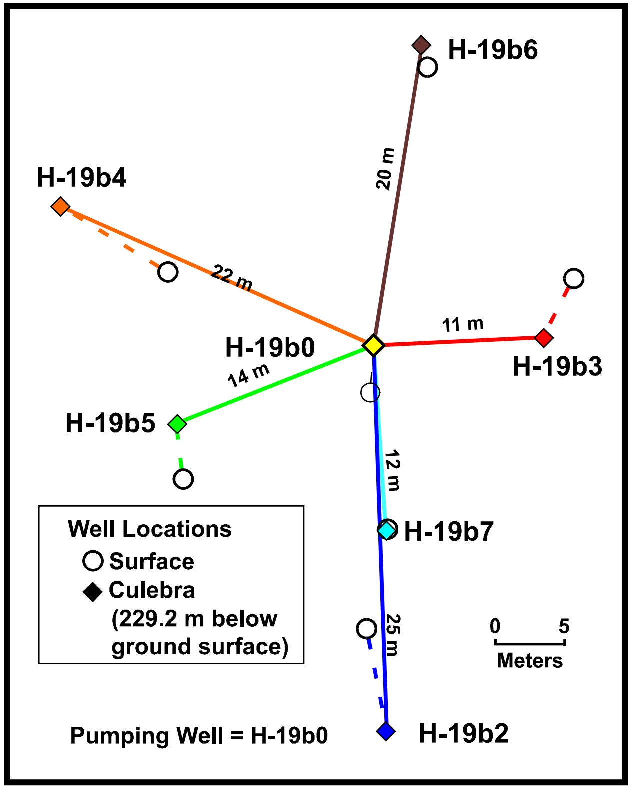


- ***Constant Matrix Block Size***
  Surface area for diffusion and diffusion distance
- ***Constant tortuosity***
  Tortuous nature of "matrix" pores

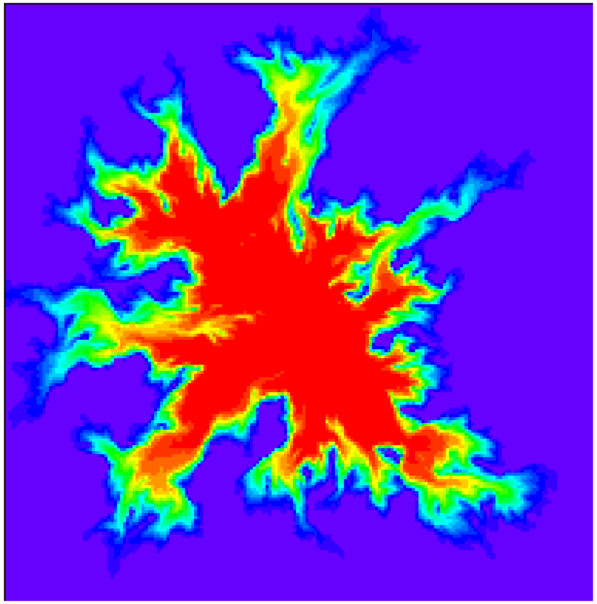
- ***Multiple Rates of Diffusion***

  Distribution of mass transfer rates attributed to variations in matrix block size and tortuosity

Introduction – Conceptual Model



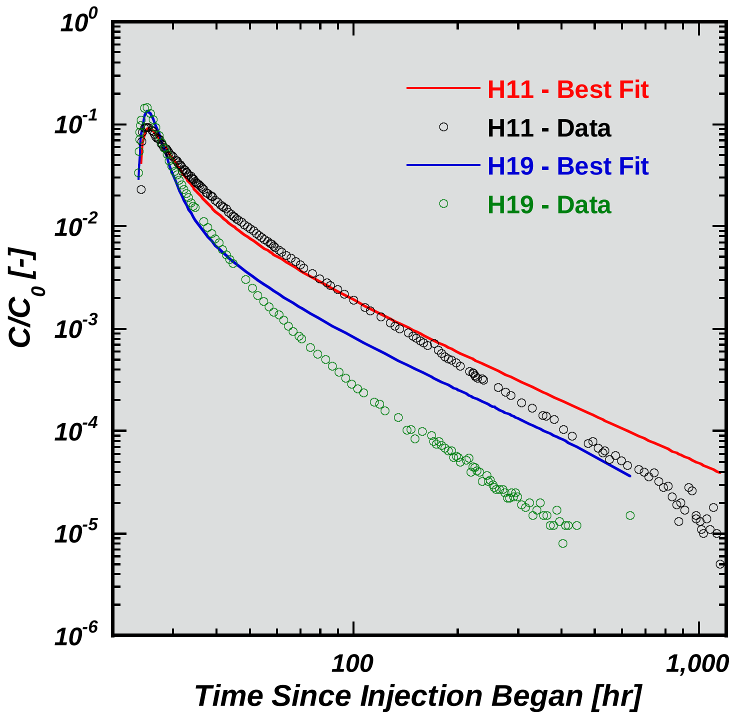
Well layout for 7- well convergent flow tracer test



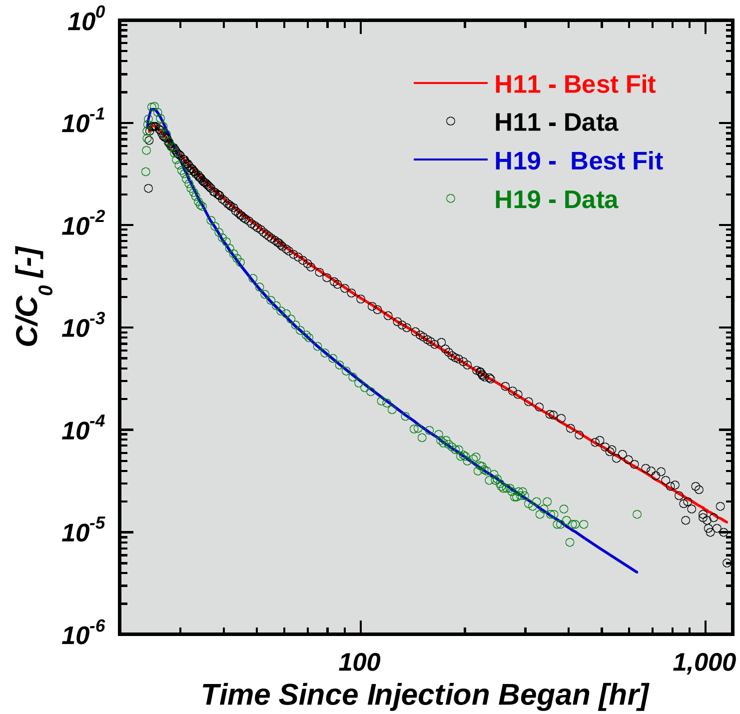
Numerical simulations for design of single-well injection/withdrawal tracer test

Introduction – Conceptual Model

Single-Well Injection Withdrawal Test Results



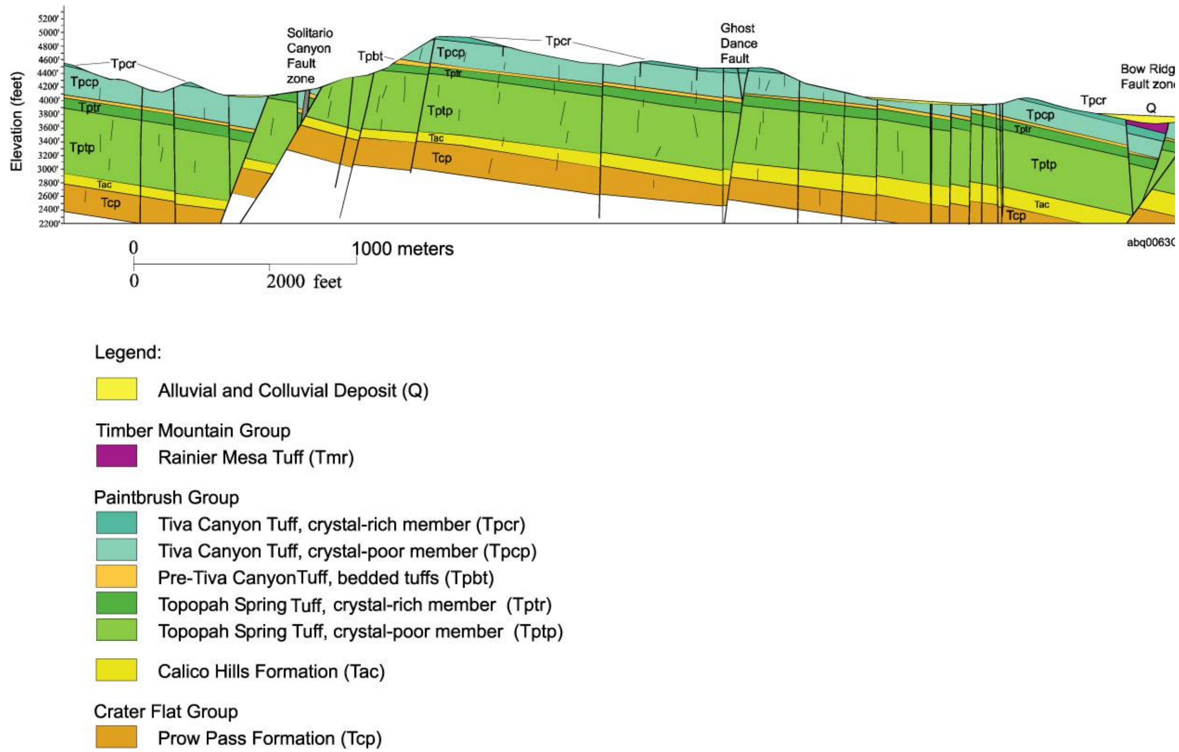
Single-diffusion rate model cannot capture tailing behavior



Multirate-diffusion model provides excellent fits throughout time range

Geology - Lithology

- **Standard geological interpretation typically involves designating lithologic or lithostratigraphic units based on rock type.**
- **Variability of lithology and physical parameters is much greater among units than within units.**
- **However, systematic and random variability within units can be significant.**



Geology - Structure

- **Geological structures, including faulting and folding, are important aspects of disposal system heterogeneity.**
- **Faults constitute discontinuities that may be preferential pathways for fluid flow or barriers to flow because of fault gouge and offsets in stratigraphy.**
- **Although faults are often simply conceptualized as planar features, they typically have variable strike, dip, fracturing, and gouge structure.**
- **Example figure is from the Yucca Mountain site.**

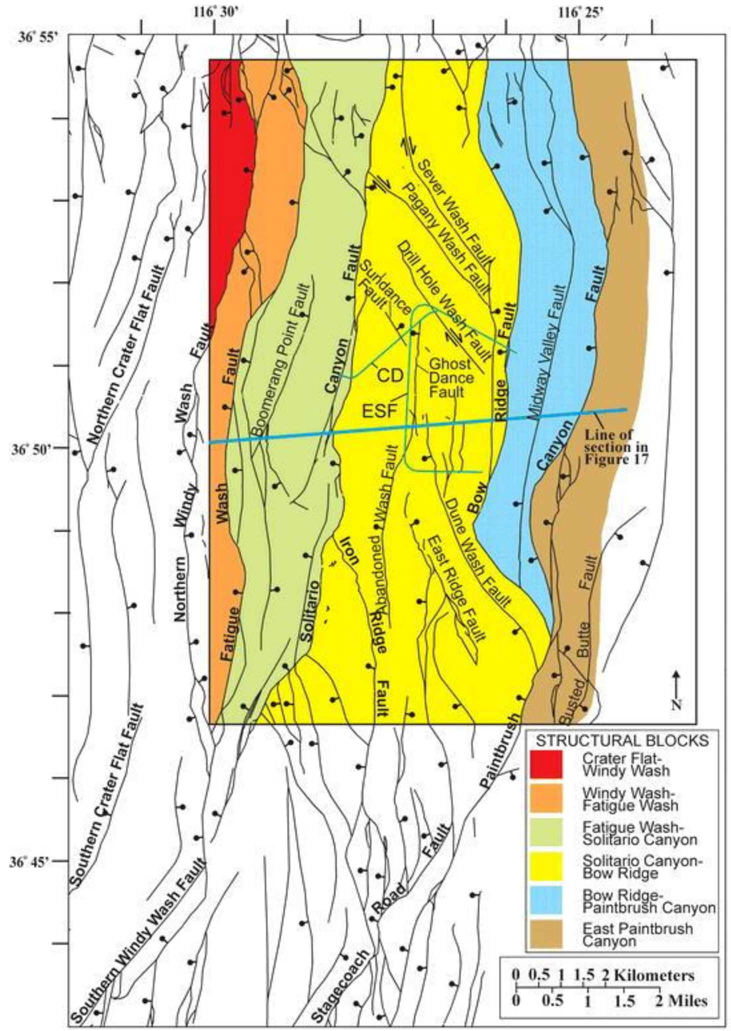
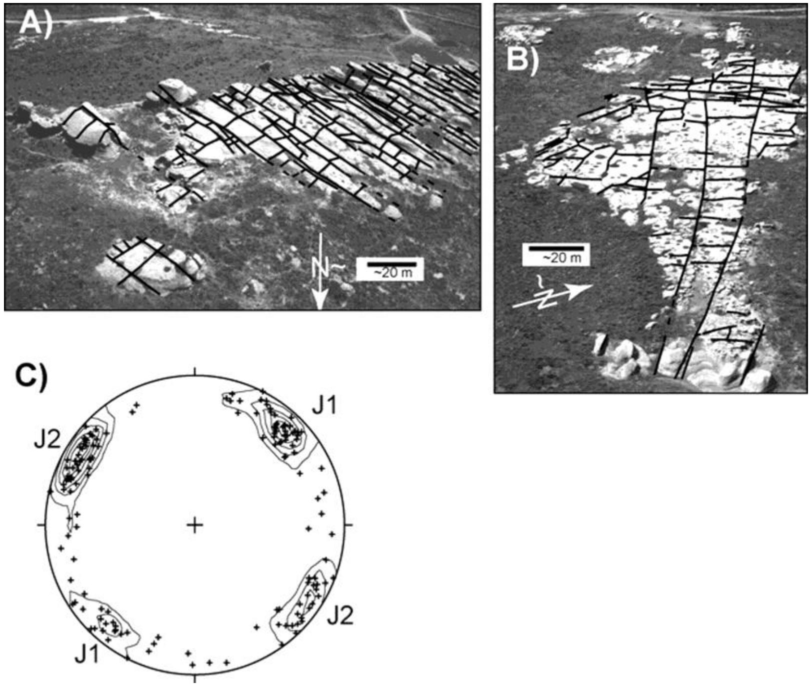


Figure 16

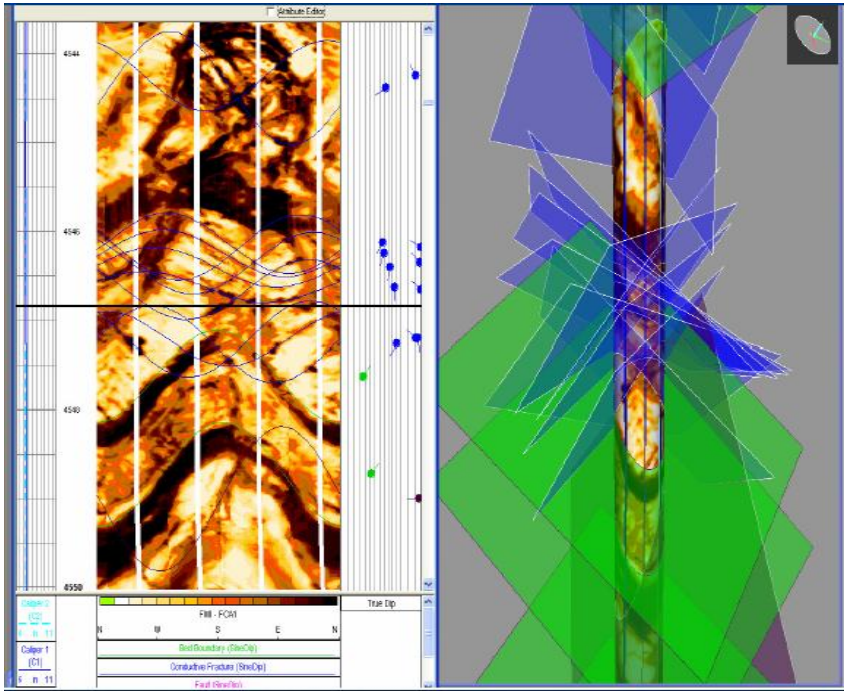
Geology – Fracture Network

- Tectonic fractures are often nearly planar features that occur in preferred orientations determined by the stress state at the time of fracture formation.
- Statistical characterization of fracture orientation data typically indicates multiple populations, sometime forming mechanically defined conjugate sets.
- Statistical characterization of fractures is often limited by observational limitations (1D, sometimes 2D, rarely 3D), particularly with regard to fracture length statistics.



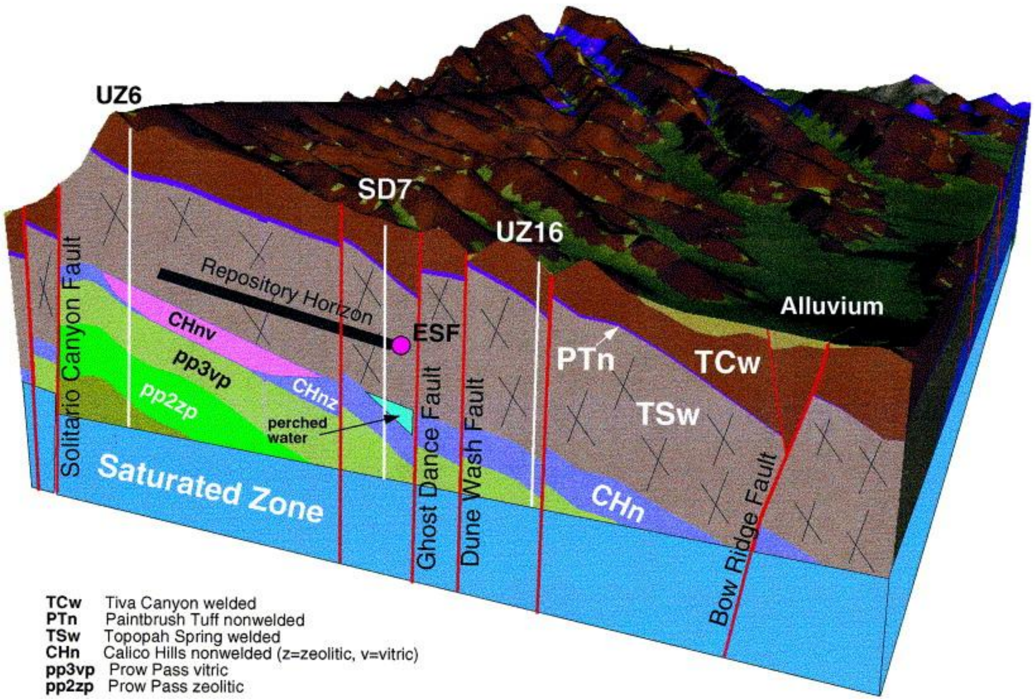
Geology – Fracture Network

- **Fracture networks are typically highly variable due to the complexity of superimposing multiple fracture sets and random variations in fracture spacing and aperture.**
- **Borehole logging methods such as FMI (shown in the example figure) provide automated identification of fracture orientations and estimates of fracture aperture.**
- **Fracture orientations tend to be normally distributed; fracture spacing, length, and aperture tend to be lognormally distributed.**



Geology – Mineralogy

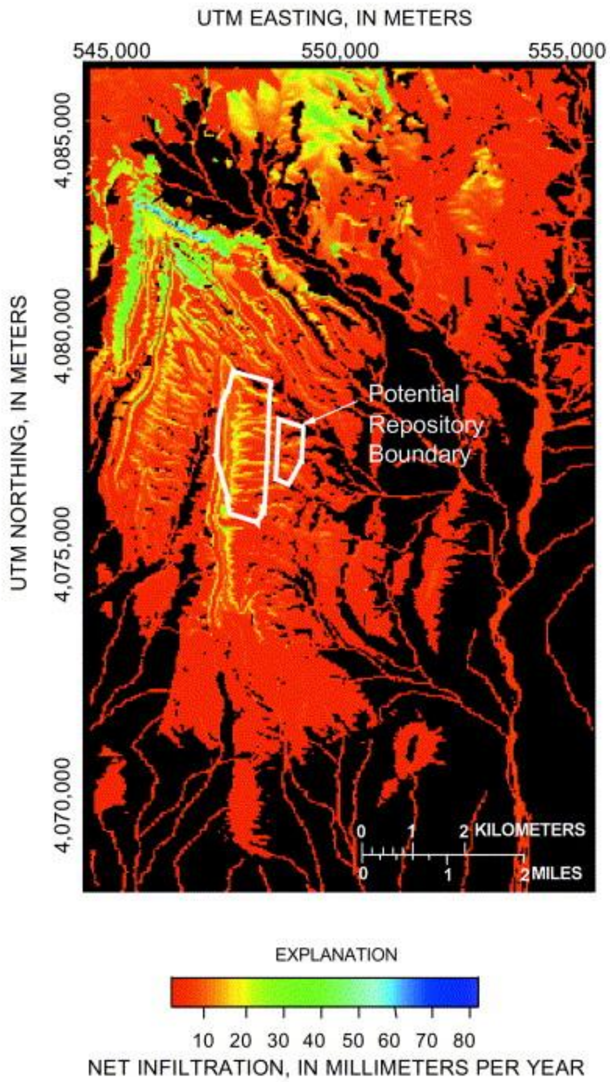
- **Variations in mineralogy may have important impacts on repository performance, especially with regard to radionuclide sorption.**
- **The example figure shows the distribution of zeolitic and vitric tuffs in the vadose zone at Yucca Mountain.**
- **Sorption coefficients for zeolitic tuff are much higher for some radionuclides.**
- **Spatial variability in zeolite content is complex, related to volcanic stratigraphy and paleohydrology.**



TCw Tiva Canyon welded
PTn Paintbrush Tuff nonwelded
TSw Topopah Spring welded
CHn Calico Hills nonwelded (z=zeolitic, v=vitric)
pp3vp Prow Pass vitric
pp2zp Prow Pass zeolitic

Hydrology – Surface Water

- **Variability in surface water hydrology is both spatial and temporal.**
- **Temporal variability can occur on the scale of individual rain/flood events and on much longer time scales for stream channel migration.**
- **Spatial variability may be significant to repository science due to enhanced infiltration under stream channels, particularly in arid climates, such as Yucca Mountain.**



Hydrology – Groundwater Recharge

- Recharge into groundwater flow systems tends to occur over a large percentage of the land surface under most conditions
- The rate of recharge can be highly variable and depends on:
  - Local precipitation
  - Local evapotranspiration and cover vegetation
  - Runoff of precipitation
  - Depth of soil and hydraulic conductivity of bedrock
  - Hill slope steepness and orientation
- Recharge can also occur from surface water features
  - Lakes
  - Streams and rivers

Hydrology – Groundwater Recharge

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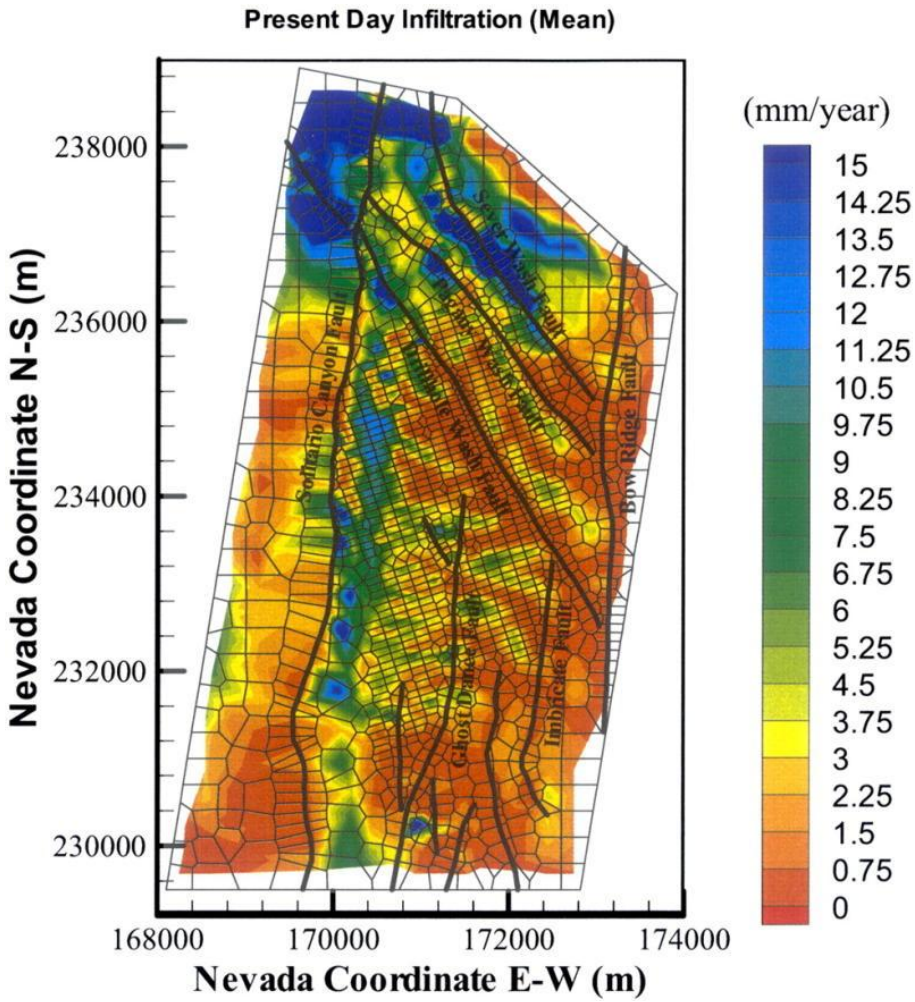
- **Groundwater infiltration and recharge can be highly variable, particularly in arid regions like Yucca Mountain**
- **Chloride mass balance is a simple method that can be used to estimate recharge in simple systems (porous media flow in the vadose zone).**



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Hydrology – Groundwater Discharge

- Discharge tends to occur over a small percentage of the area of a groundwater flow system
- Discharge can occur at:
  - Springs
  - Surface seeps
  - Desert playas
  - Phreatophyte zones
  - Lakes
  - Rivers
  - Ocean
  - Pumping wells

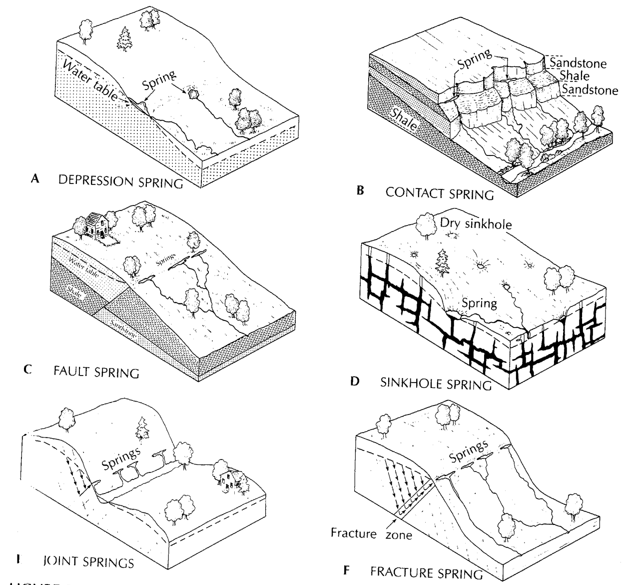
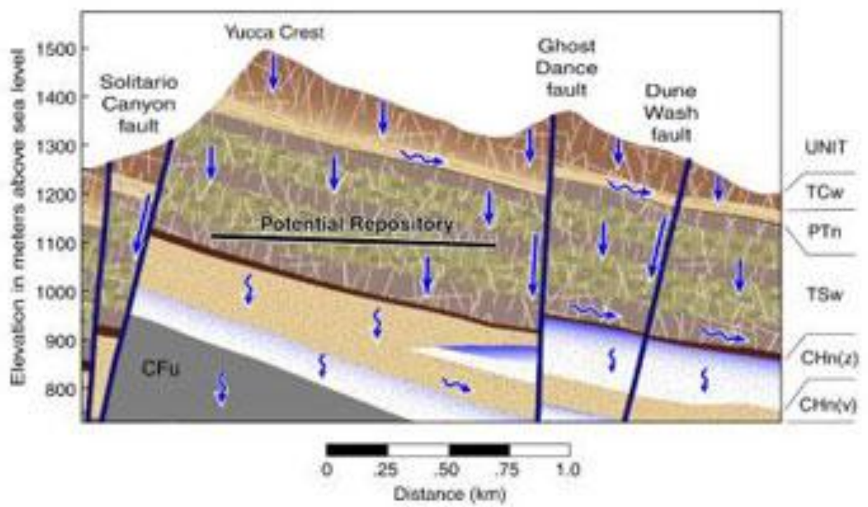


FIGURE 7.11
Types of springs.

Hydrology – Vadose Zone

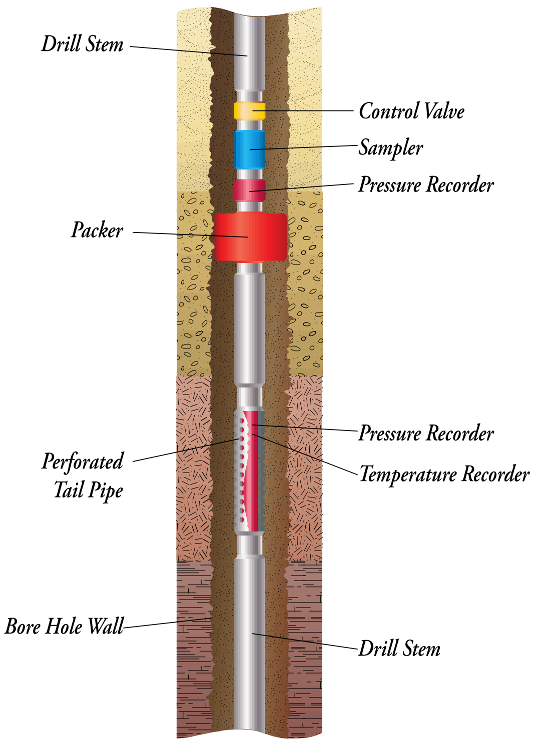
- Unsaturated groundwater flow in the vadose zone may be highly variable, as caused by heterogeneity in material properties.
- Gravity-driven flow dominates in fractures, but capillary forces in the rock matrix may influence the downward migration of groundwater.
- Capillary flow dominates flow in dipping porous units, such as the PTn unit shown in the figure from Yucca Mountain.
- Perched water forms where infiltration rates exceed the hydraulic conductivity of the medium

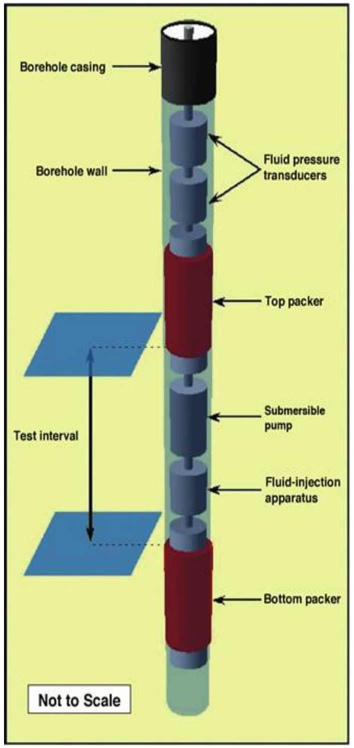


Geologic cross-section with flow patterns

Hydrology – Well Testing

- Numerous hydraulic testing methods are used in wells to estimate the permeability.
- Testing results typically show significant heterogeneity even within single hydrogeologic units.
- Spatial scale of testing is important; smaller-scale slug tests generally show more variability than larger-scale pump tests.
- Because permeability may vary by many orders of magnitude, heterogeneity in this parameter may be one of the most significant factors in site characterization.





Geochemistry – Hydrochemistry

- **Natural groundwater chemistry can be highly variable, depending on geology and flow history of the groundwater**
- **Total Dissolved Solids (TDS) is a gross measure of groundwater quality**
- **TDS generally increases along flow paths, with depth and age**
- **Anion concentrations evolve along flow paths as shown at right**

Class	TDS (mg/L)
Fresh	0–1,000
Brackish	1,000–10,000
Saline	10,000–100,000
Brine	>100,000

Travel along flow path ⟶

$$HCO_3^- \longrightarrow HCO_3^- + SO_4^{2-} \longrightarrow SO_4^{2-} + HCO_3^- \longrightarrow SO_4^{2-} + Cl^- \longrightarrow Cl^- + SO_4^{2-} \longrightarrow Cl^-$$

Increasing age ⟶

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Geochemistry – Environmental Tracers

- Naturally occurring stable isotopes of oxygen and hydrogen vary systematically in precipitation and groundwater
- Variations can be used to identify timing of recharge, effects of evaporation, water rock interactions, and hydrothermal effects

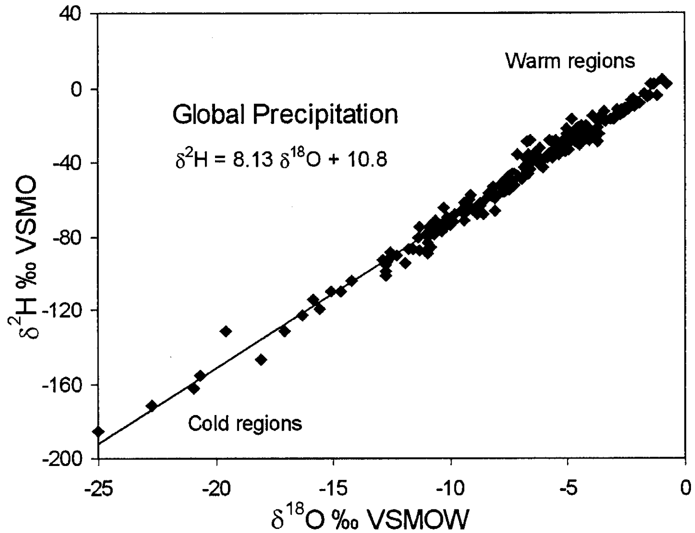

Fig. 2-1 The meteoric relationship for ^{18}O and ^{2}H in precipitation. Data are weighted average annual values for precipitation monitored at stations in the IAEA global network, compiled in Rozanski et al. (1993).

Geochemistry – Environmental Tracers

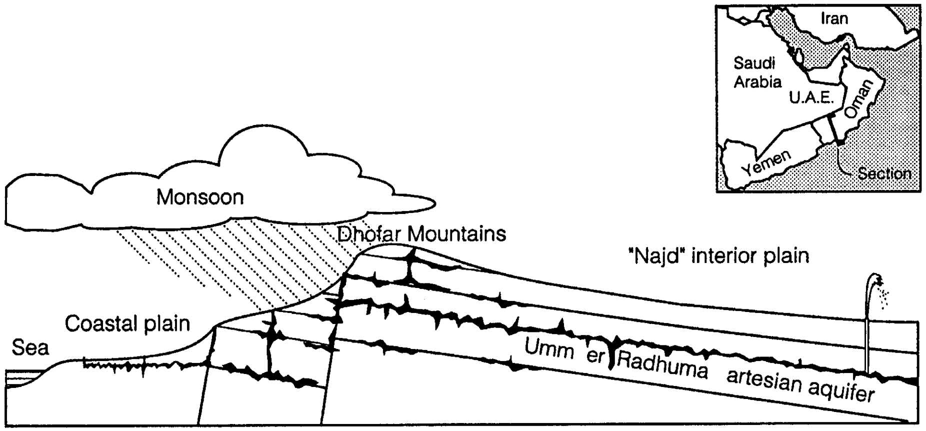

Fig. 8-11 Schematic geological cross section through the coastal plain, Dhofar Mountains and "Najd" interior plain. (10 × vertical exaggeration). The Umm er Radhuma formation hosts an extensive fissured limestone aquifer with artesian groundwater (from Clark et al., 1987).

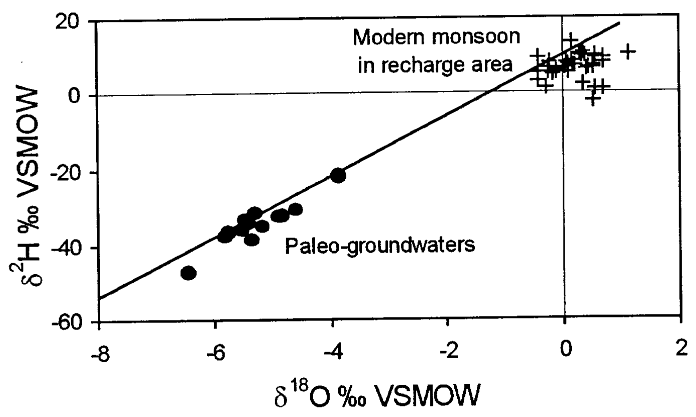

Fig. 8-12 Stable isotope signature of modern and paleogroundwaters in southern Oman.

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Geochemistry – Environmental Tracers

Table 1-3 The environmental radioisotopes

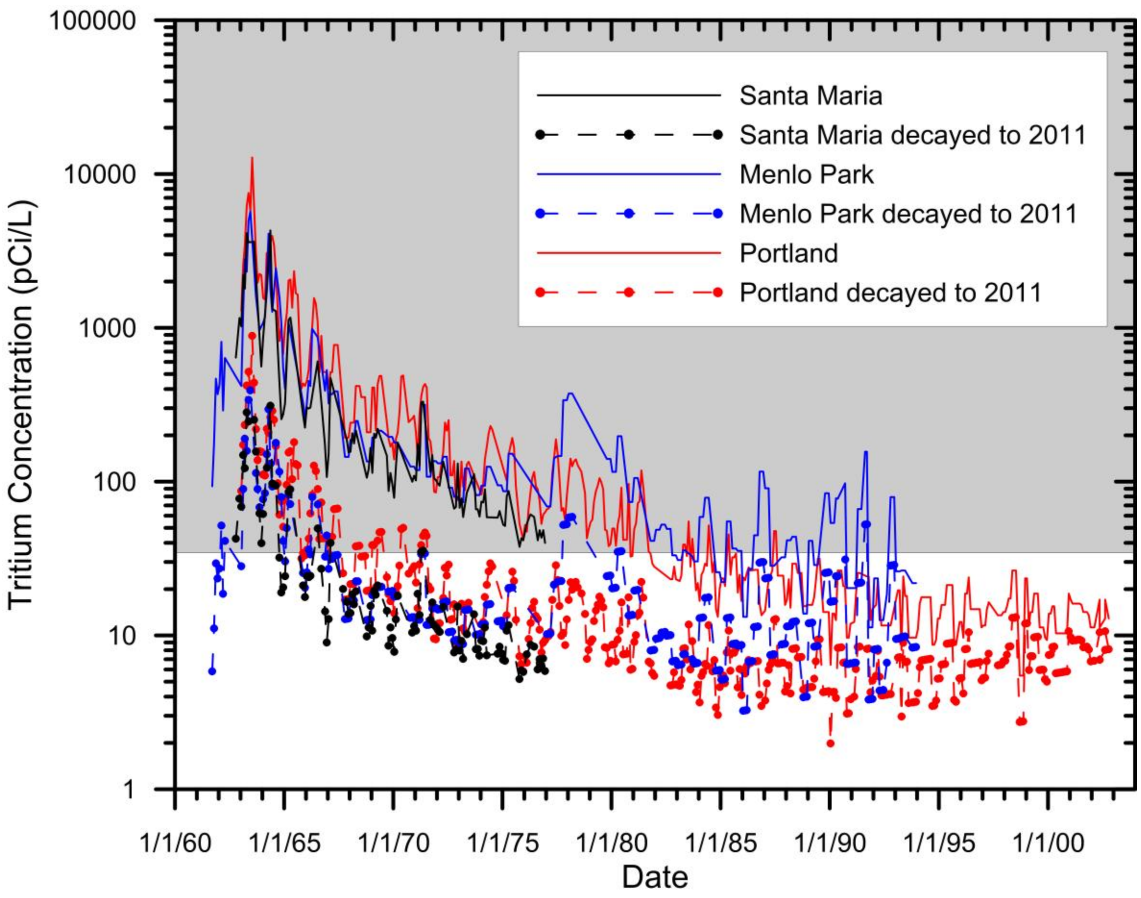
Isotope	*Half-life (years)*	*Decay mode*	*Principal Sources*	*Commonly measured phases*
^{3}H	12.43	β^-	Cosmogenic, weapons testing	H_2O, CH_2O
^{14}C	5730	β^-	Cosmogenic, weapons testing, nuclear reactors	DIC, DOC, CO_2 $CaCO_3$, CH_2O
^{36}Cl	301,000	β^-	Cosmogenic and subsurface	Cl^-, surface Cl-salts
^{39}Ar	269	β^-	Cosmogenic and subsurface	Ar
^{85}Kr	10.72	β^-	Nuclear fuel processing	Kr
^{81}Kr	210,000	ec	Cosmogenic and subsurface	Kr
^{129}I	$1.6 \cdot 10^7$ yr	β^-	Cosmogenic, subsurface, nuclear reactors	I^- and I in organics
^{222}Rn	3.8 days	α	Daughter of ^{226}Ra in ^{238}U decay series	Rn gas
^{226}Ra	1600	α	Daughter of ^{230}Th in ^{238}U decay series	Ra^{2+}, carbonate, clays
^{230}Th	75,400	α	Daughter of ^{234}U in ^{238}U decay series	Carbonate, organics
^{234}U	246,000	α	Daughter of ^{234}Pa in ^{238}U decay series	UO_2^{2+}, carbonate, organics
^{238}U	$4.47 \cdot 10^9$	α	Primordial	UO_2^{2+}, carbonate, organics

β^- - beta emission.

α - alpha emission.

ec - electron capture.

Geochemistry – Environmental Tracers



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Geochemistry – Redox Chemistry

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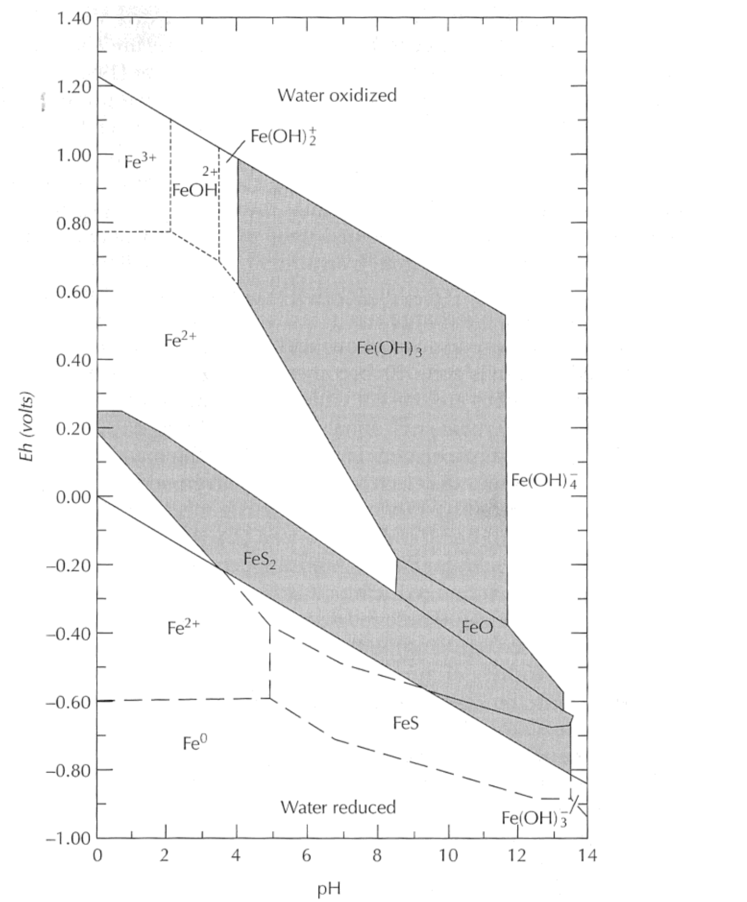
- **Reduction-oxidation (redox) conditions can have large impacts on groundwater chemistry and contaminant movement**
- **Shallow groundwater is generally oxidizing and deeper groundwater is generally reducing**
- **Local variations in redox state can occur due to several factors**



▲ FIGURE 9.4
Stability fields based on Eh and pH for solid and dissolved forms of iron in an aqueous solution of 56 μg/L iron, 96 mg/L of sulfur as SO_4^{-2}, 61 mg/L carbon dioxide as HCO_3^- at 25°C, and 1 atm pressure. *Source: J. D. Hem, U.S. Geological Survey Water-Supply Paper 2254, 1985.*

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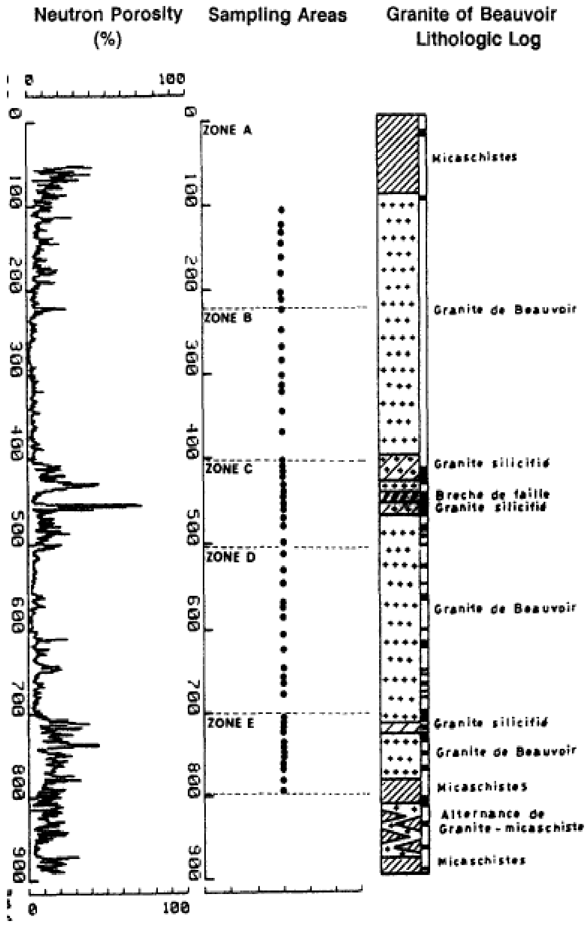
Geochemistry – Groundwater Colloids

- **Colloid-facilitated radionuclide transport in groundwater may be a significant mechanism for rapid migration of some radionuclides.**
- **Strongly sorbing radionuclides, particularly Pu and Am, may sorb to natural groundwater colloids.**
- **In addition, intrinsic colloids consisting of or with embedded actinides may form by the degradation of spent nuclear fuel or high-level waste glass.**
- **The concentrations and mineralogical composition of colloids may vary significantly in groundwater flow systems and are related to rock type, hydrochemical composition, and ionic strength in the system.**

Geophysical – Physical Properties

- Several physical properties require characterization during site investigations, including fracture porosity, matrix porosity, bulk density, and sorption coefficients.
- Variability in porosity and bulk density in most geological systems is small relative to variability in permeability, and has a smaller impact on modeling of repository performance.
- Variability in values of sorption coefficient may be relatively larger, particularly in heterogeneous geological systems.



from Gallé (1994)

Geophysical – Thermal Properties

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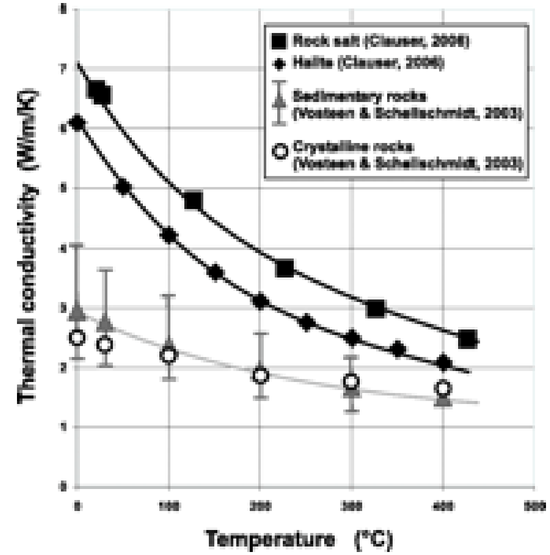
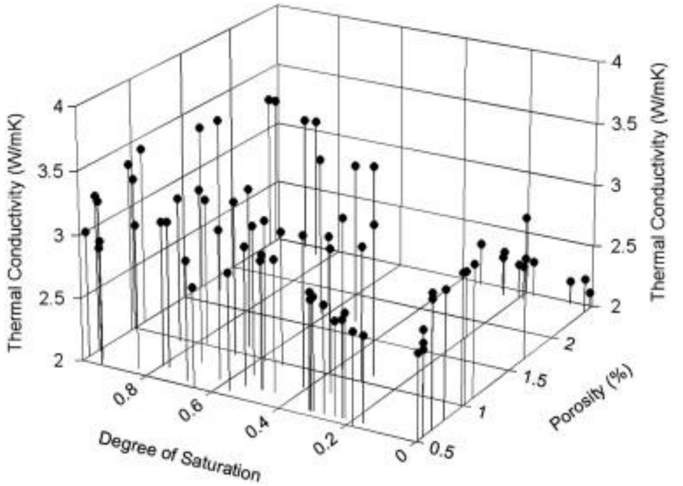
- Thermal conductivity and heat capacity are important parameters in modeling for thermal management of repository heat.
- Variability in thermal properties of host rock tends to be small relative to other parameters, but may have significant impact on peak temperatures in the repository.
- Thermal conductivity vary with porosity, liquid saturation, and temperature, with saturation and temperature being dynamic state variables.





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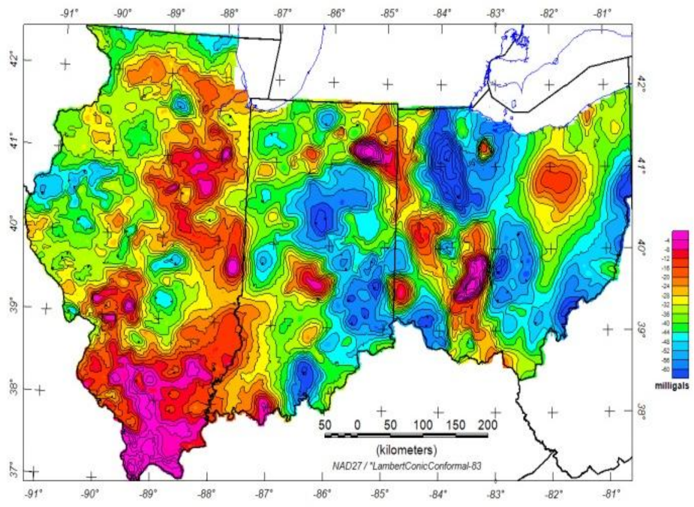
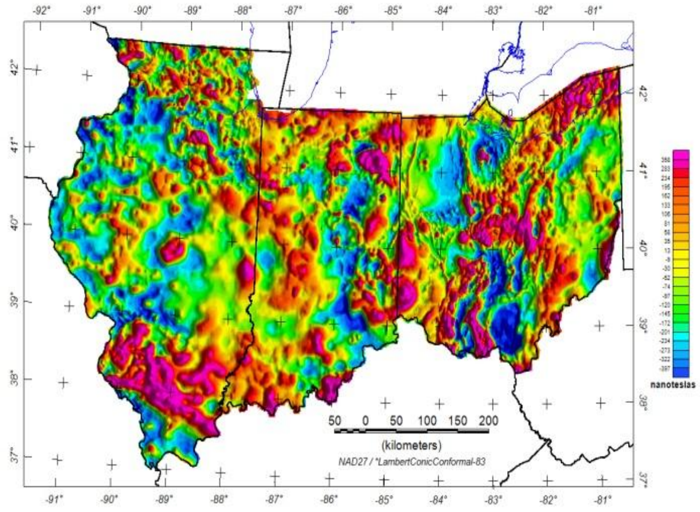
Geophysical – Surface-Based

- **Airborne and surface based geophysical surveys, such as gravity and magnetic anomaly can provide information on geological variability at depth, at regional- to site-specific scales.**
- **Interpretation of geophysical results is usually non-unique.**

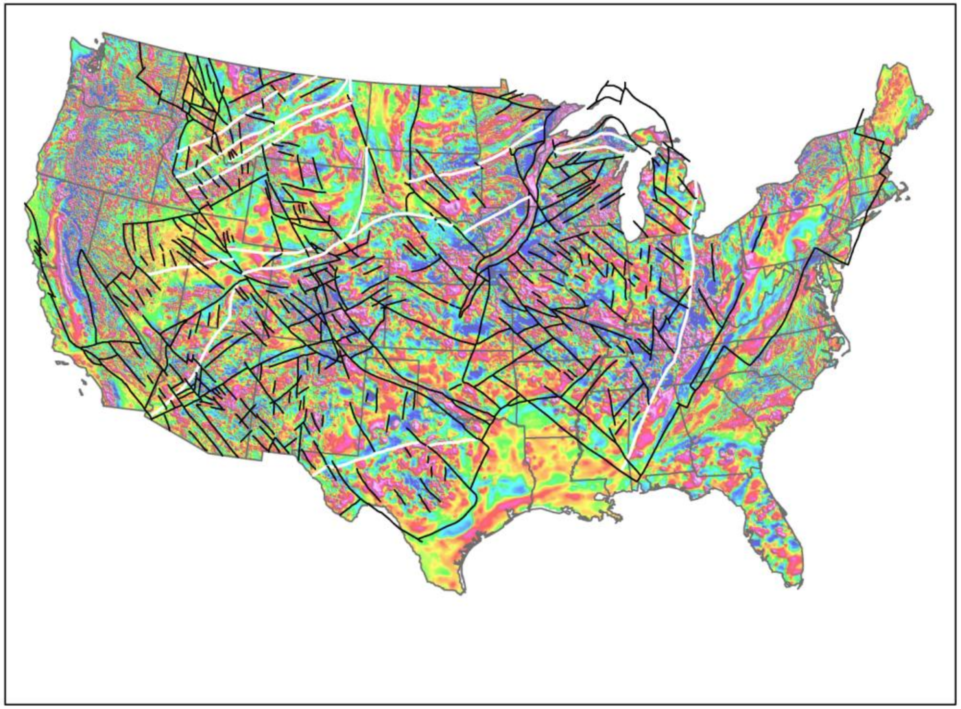




Example gravity (left) and magnetic (right) anomaly maps of Illinois, Indiana and Ohio (Daniels et al., 2008).

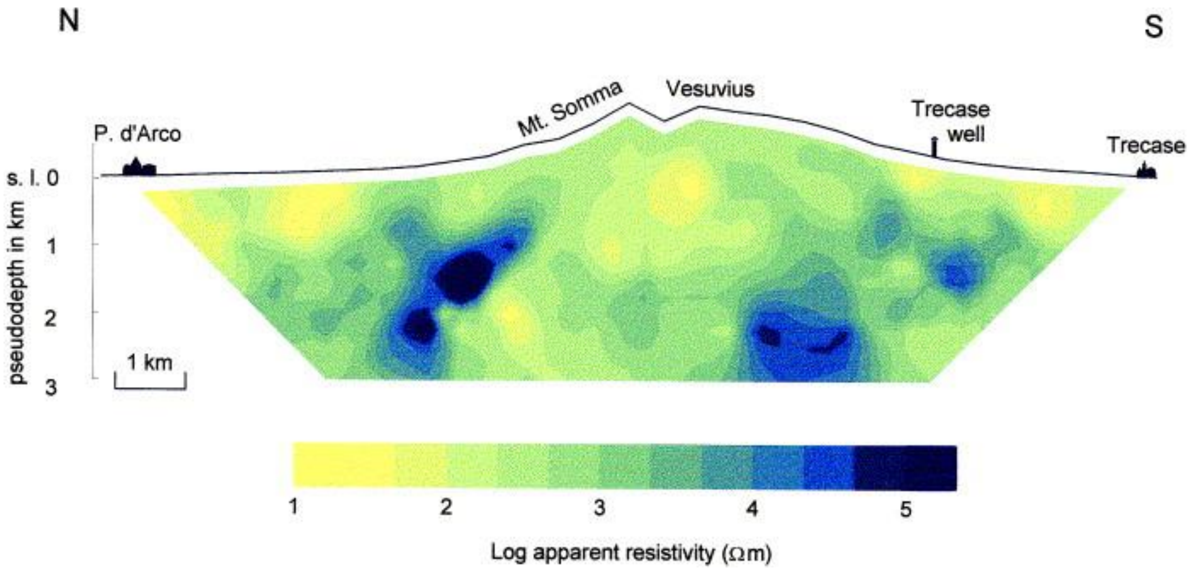
Geophysical – Surface-Based

- **Discontinuities in geophysical measurements (e.g., aeromagnetic survey shown in figure) are often the basis for interpretation of deeply buried structural features, such as faults.**



Geophysical – Surface-Based

- **Higher resolution geophysical methods along survey lines (e.g., electric resistivity sounding shown in figure) may produce much more refined measures of variability at the site scale.**



Dipolar geoelectrics apparent resistivity pseudosection showing a coarse horizontal set of alternating conductive and resistive bodies. (Di Maio et al., 1998).

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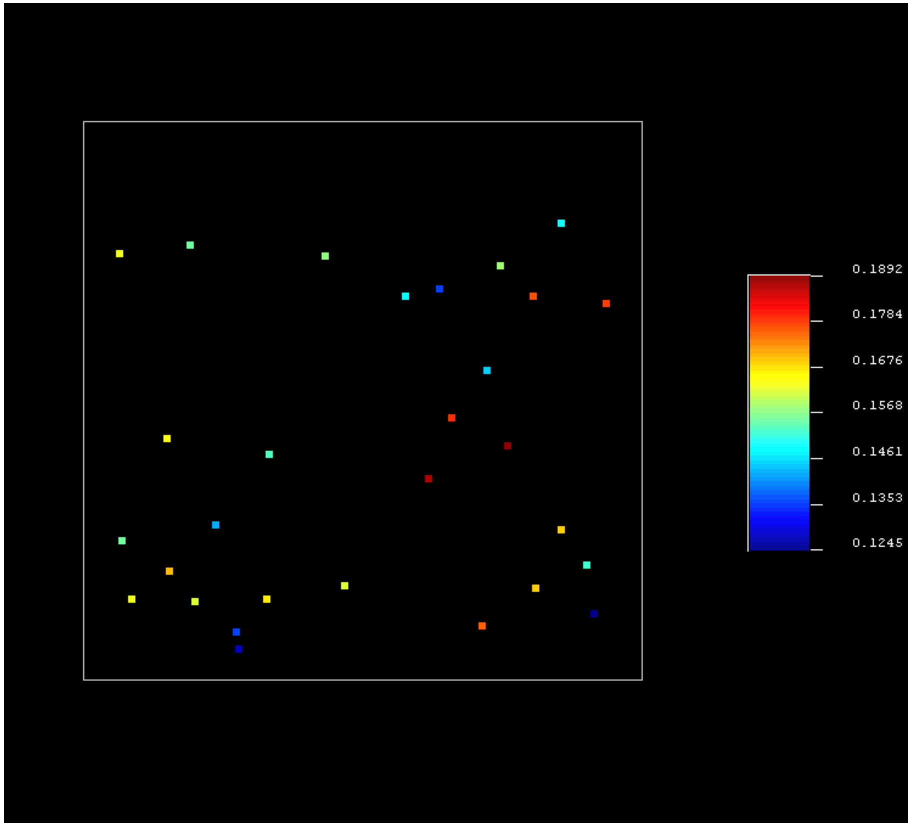
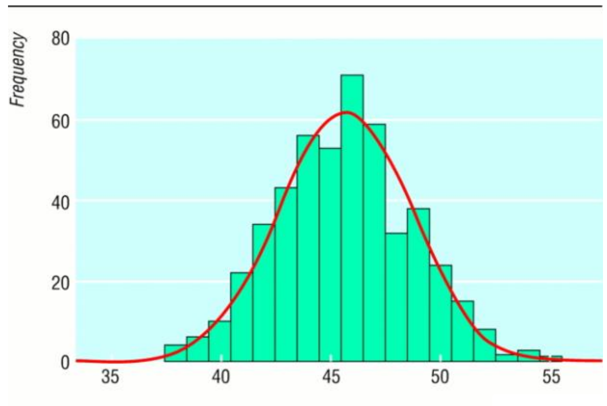
Classical Statistics – Data Visualization

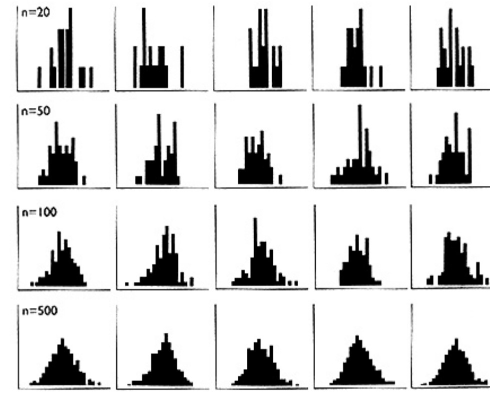
- **Classical statistics approaches the data as a population of values and discards any information about the spatial or temporal location of the value.**
- **Classical statistical analysis provides information on the variability, distribution, and potential correlation of the variables, allows extrapolation to extreme values, and serves as the basis for hypothesis testing.**
- **Classical statistics does not provide insights into spatial correlation and associated impacts on physical processes**

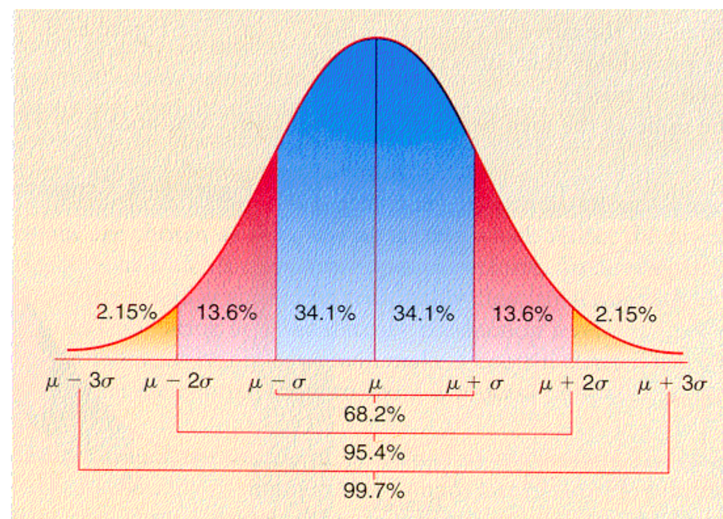


Classical Statistics – Parametric

- **Parametric classical statistics characterizes variability using one of several idealized mathematical functions (e.g., normal distribution).**
- **These idealized distributions provide a powerful set of tools for analyzing and testing the data, but may be inadequate for some variables and processes.**
- **Variables from additive processes tend to a normal distribution and those from multiplicative processes tend to a log-normal distribution (both common in earth sciences).**

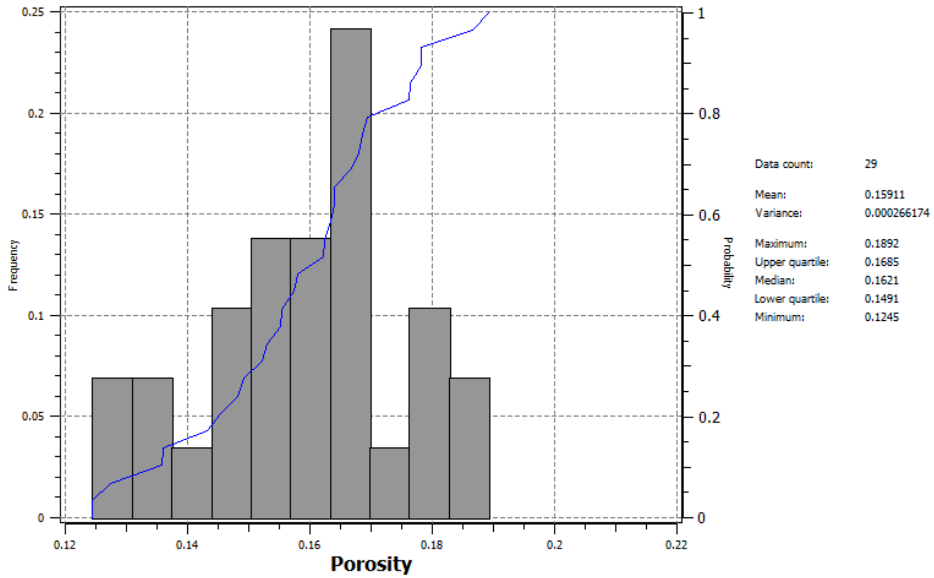






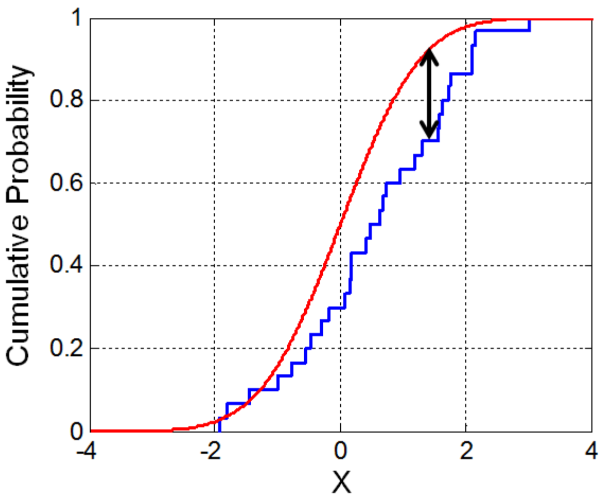
Classical Statistics – Nonparameteric

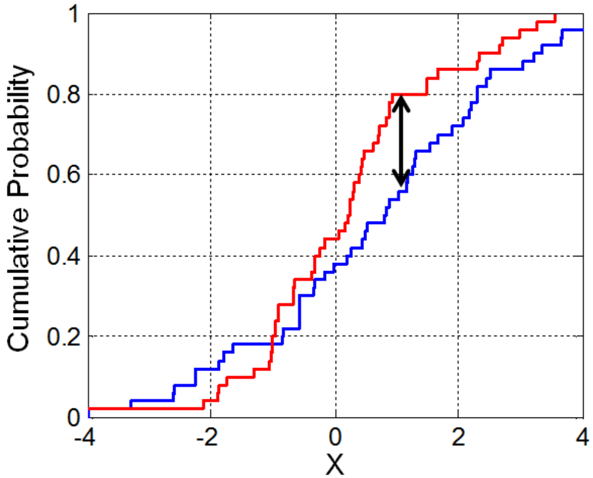
- **Nonparametric statistical methods make no assumptions about the mathematical form of the underlying distribution of the variable.**
- **May be more appropriate for limited sample size because distribution form is not readily discernible.**
- **May be more appropriate for empirical distributions that have long or irregular tails.**



Classical Statistics – Hypothesis Testing

- **A large number of parametric and nonparametric methods are available for hypothesis testing in classical statistics.**
- **Although in classical statistics hypothesis testing is often an important component of statistical analyses, in repository geosciences and geostatistics hypothesis testing is often of lesser importance.**
- **Example figures illustrate the simple and useful Kolmogorov-Smirnov test for determining if an experimental distribution is equivalent to a reference parametric distribution or to another nonparametric distribution.**





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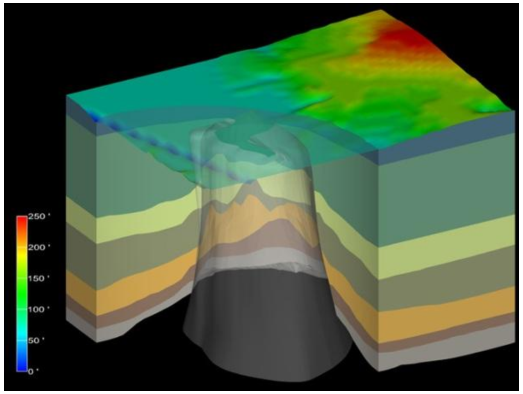

Exercise 3: Spatial Estimation and Simulation

IAEA Training Course – July 1-5, 2013

Bill Arnold

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

IAEA International Atomic Energy Agency

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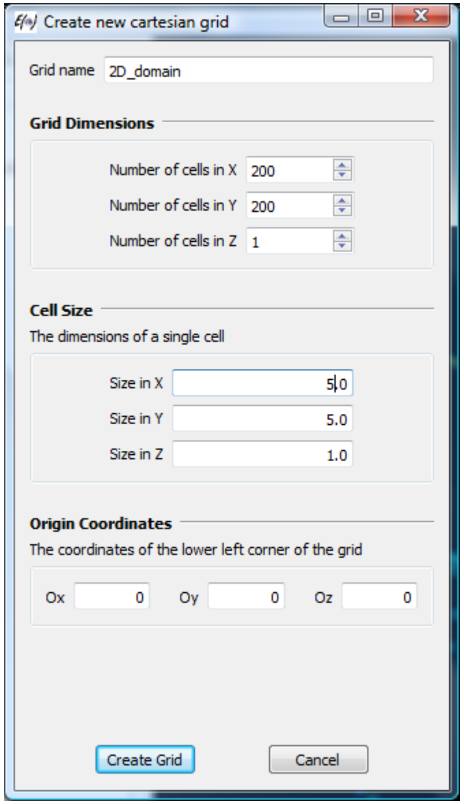
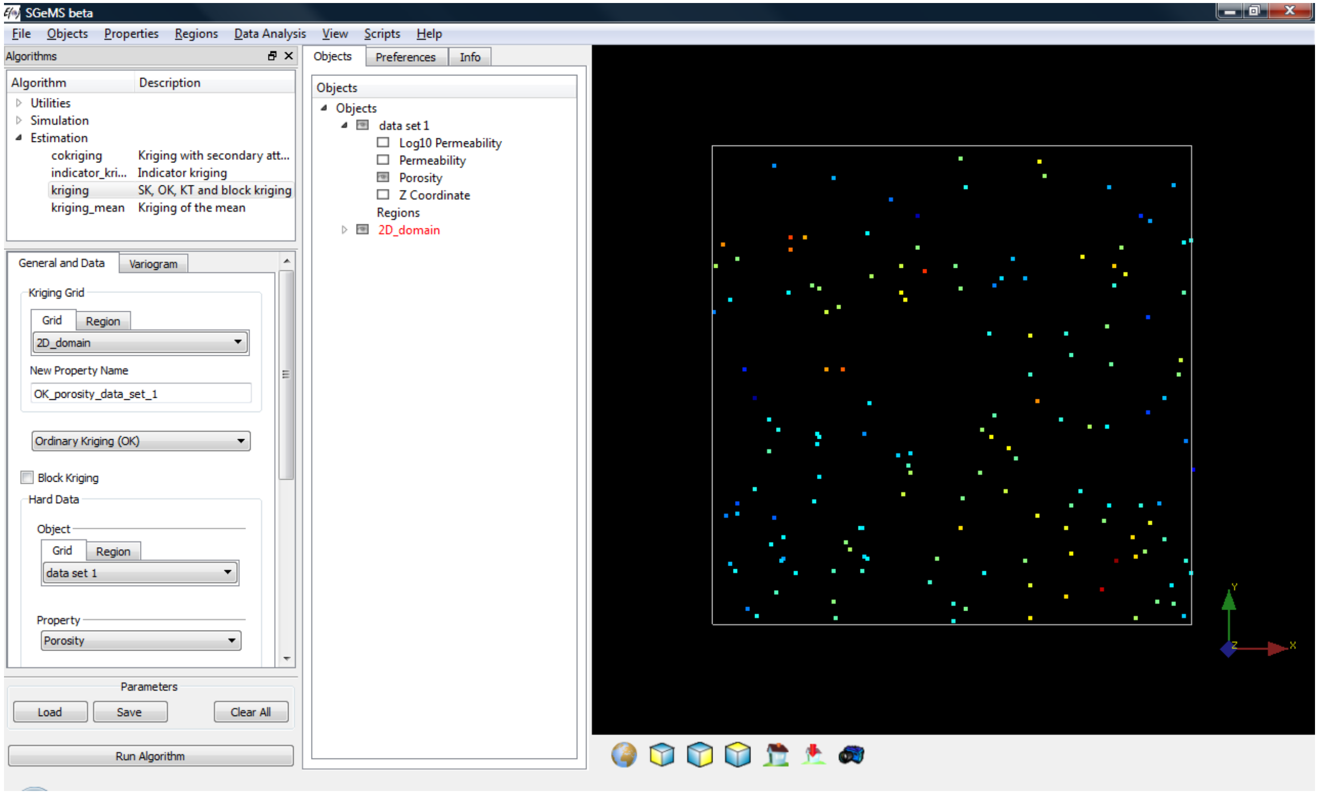
SGeMS – Spatial Estimation

- Load the data sets that were used in the exploratory data analysis exercise.
- Create a 2D grid to use as the basis for the kriging of the 2D data sets by choosing the "New Cartesian Grid" option under the "Objects" pulldown menu.
- Name the grid and specify the number and dimensions of cells in the x, y, and z directions. The model domain is 1,000 m by 1,000 m and the origin should be (0.0, 0.0).



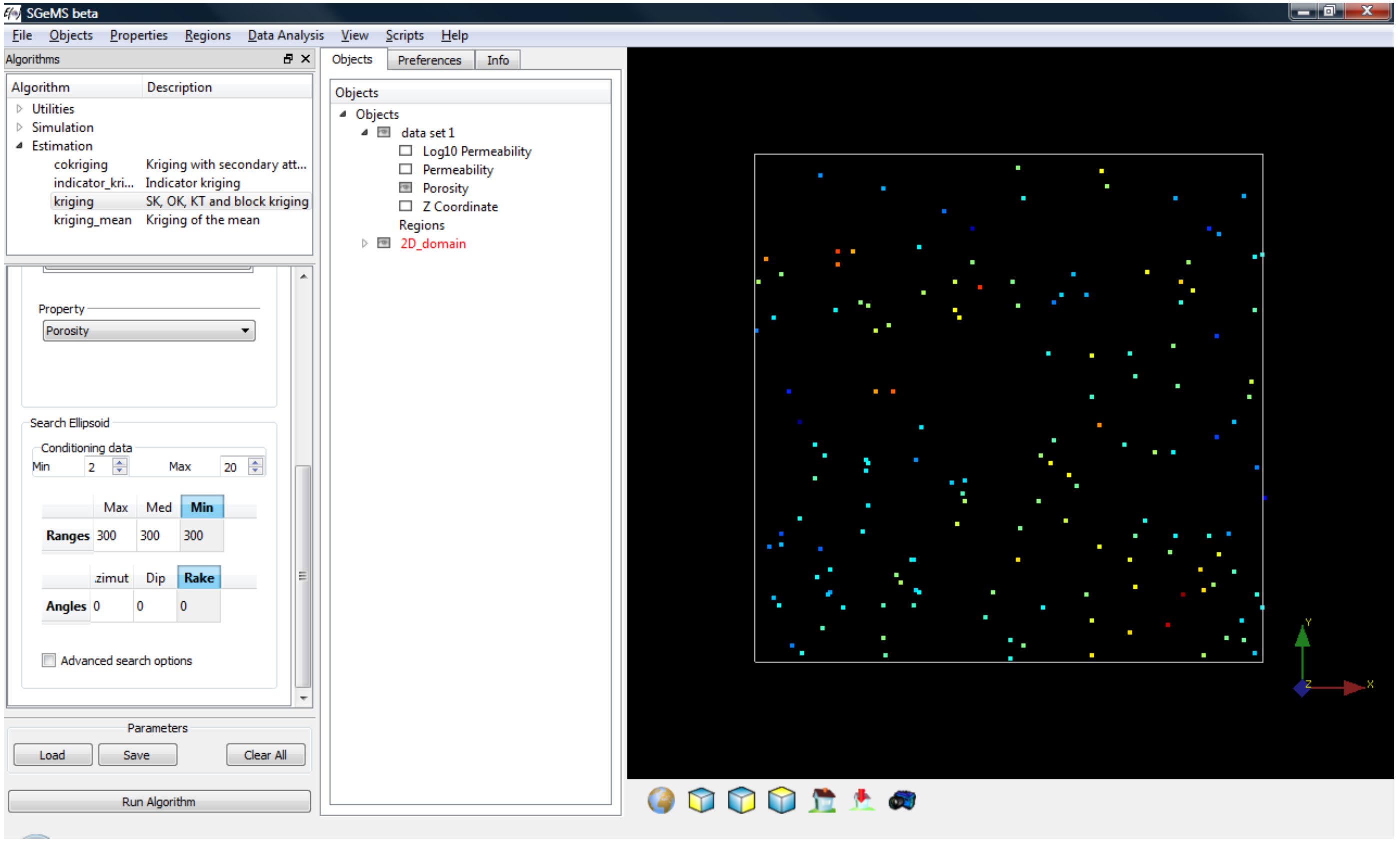
SGeMS – Spatial Estimation

- Choose “kriging” under the “Estimation” option in the “Algorithms” window.
- Select the grid that you created under the Kriging Grid area and type in a new property name for the kriging output that you will be generating.
- Choose “Ordinary Kriging” from the dropdown menu, and select the data set name and property (porosity) from the “Object” and “Property” dropdown menus.



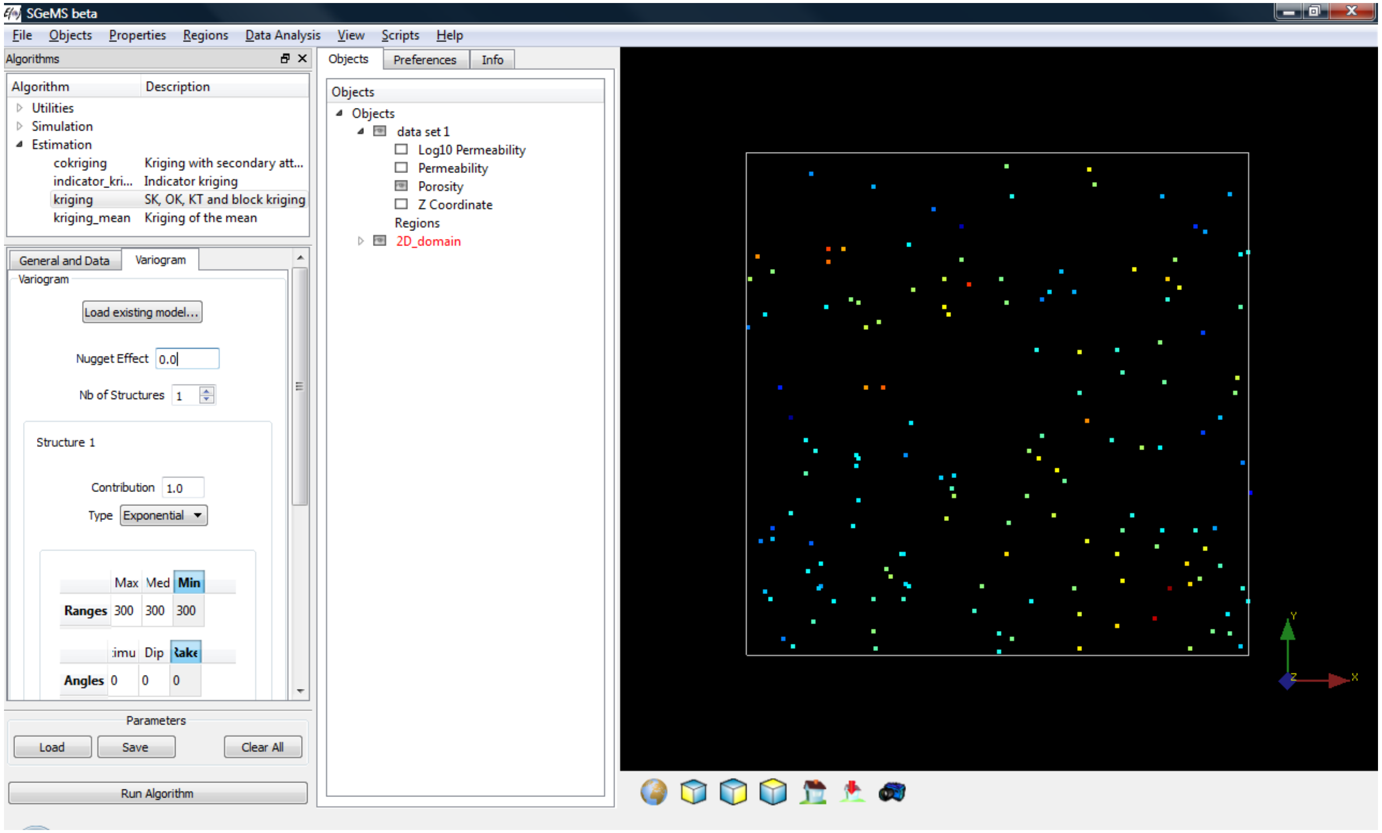
SGeMS – Spatial Estimation

- **Scroll down in the kriging entry window and enter the "Search Ellipsoid" information, including number of conditioning data, search ranges, and search ellipsoid orientation.**



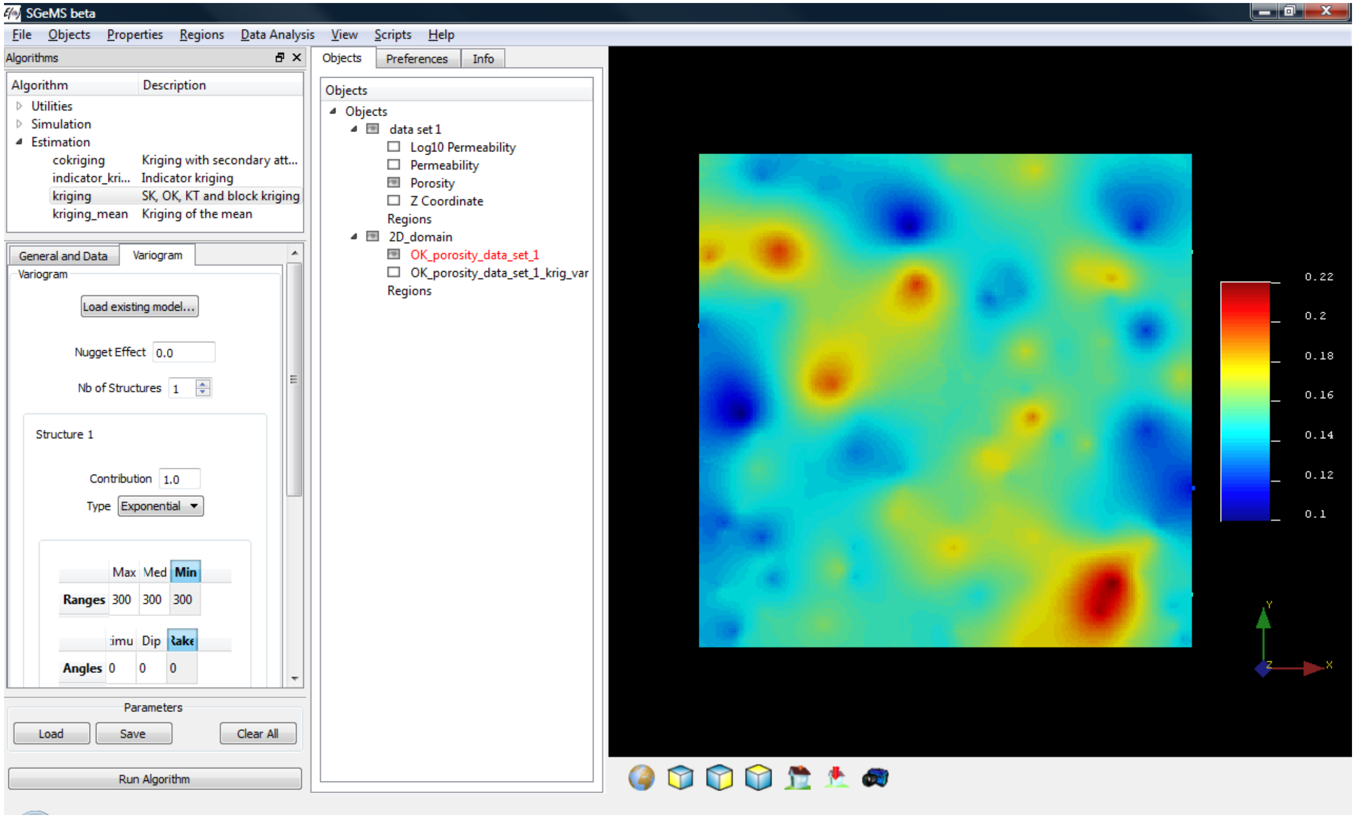
SGeMS – Spatial Estimation

- Now choose the "Variogram" tab in the kriging window and enter the data to be used in the kriging.
- You can enter the kriging parameters from your notes on the variogram analysis or load them as an existing model if you saved them to a file
- Press the "Run Algorithm" button to run the ordinary kriging algorithm



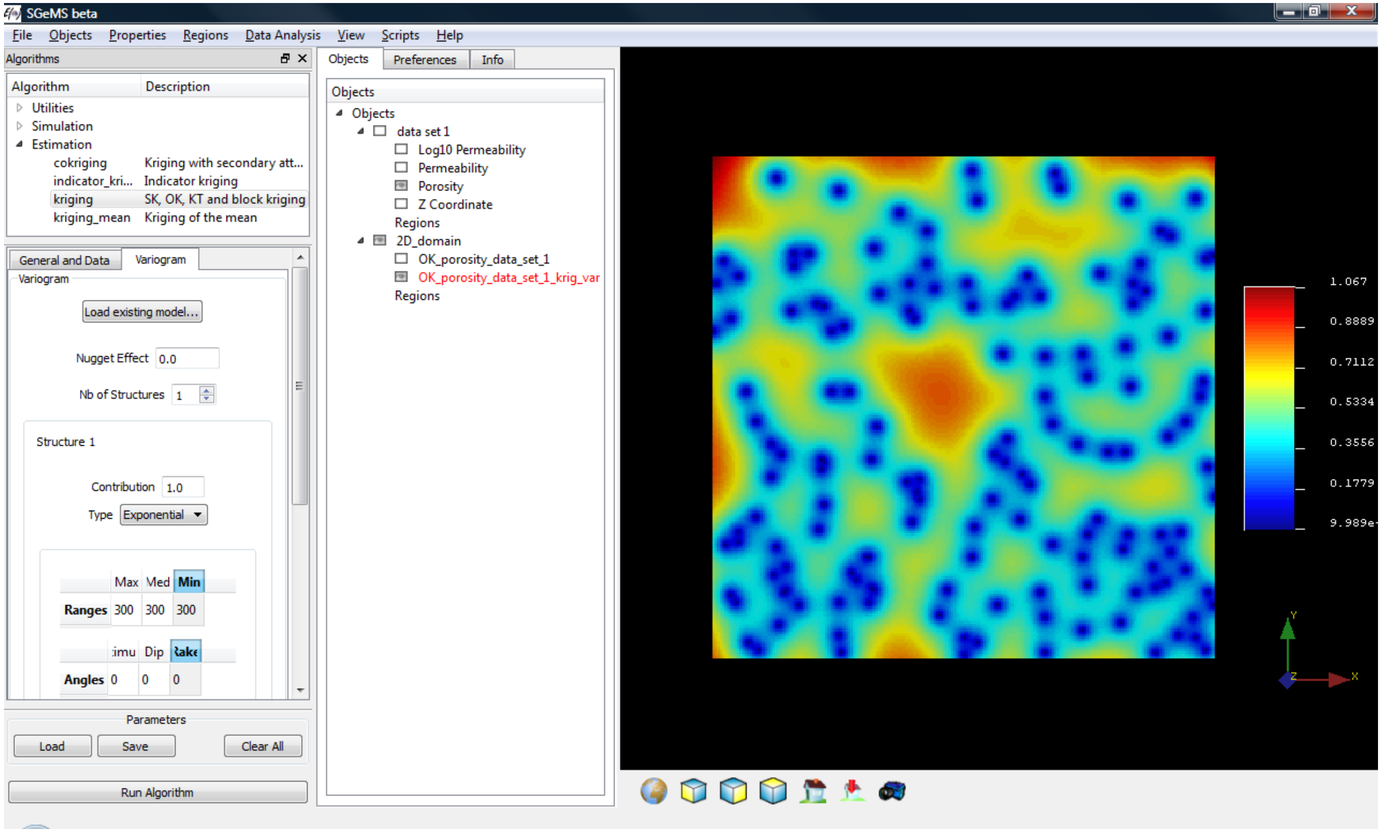
SGeMS – Spatial Estimation

- Expand the grid name item in the "Objects" window and note that two new properties have been generated for the kriged porosity values and the kriging variance.
- Select the kriged porosity values to visualize the estimated porosity field and add a color scale.
- Toggle the porosity field on and off to verify that the hard data have been honored.



SGeMS – Spatial Estimation

- Now visualize the kriging variance by selecting that property in the “Objects” window.
- Redo the spatial estimation exercise for different parameters, using different kriging methods, and varying the search radius and variogram parameters.
- Practice exporting visualization images with the snapshot tool and saving the kriging results to an output file.



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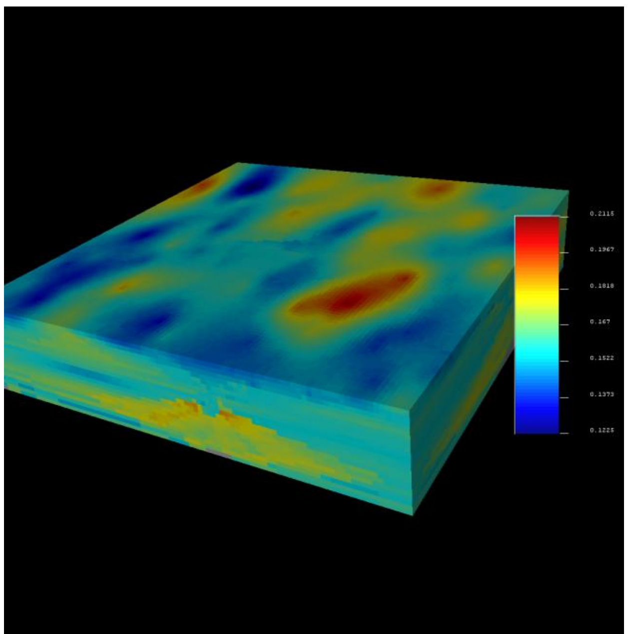
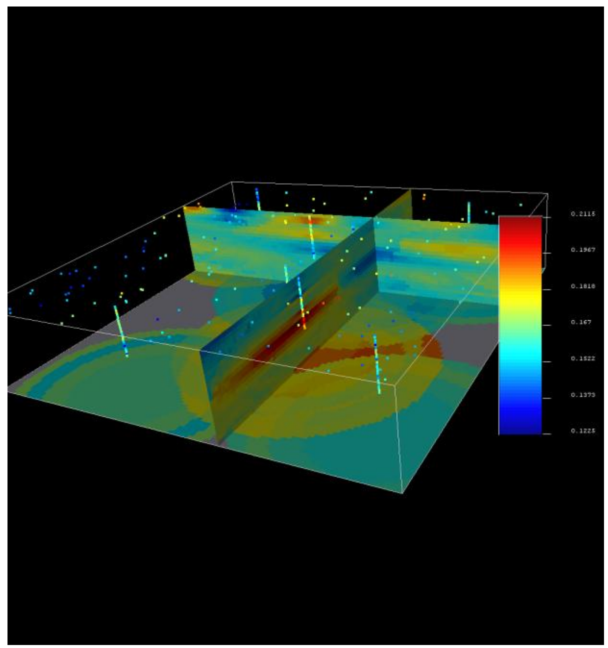
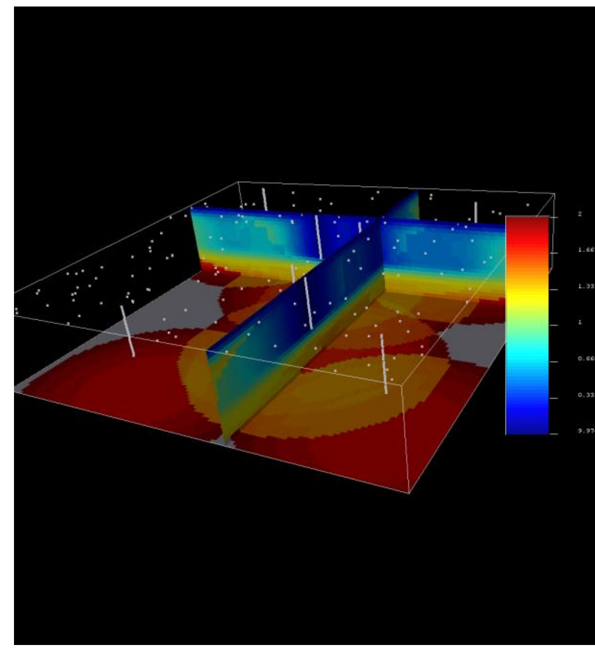
SGeMS – Spatial Estimation

- **Conduct the kriging exercise using the "data_set_2_2D.dat" and "data_set_3_3D.dat" data sets.**
- **Practice using the visualization window and the slicing tool to understand the kriging output in three dimensions.**
- **Practice saving and exporting the results of the spatial estimation exercises.**

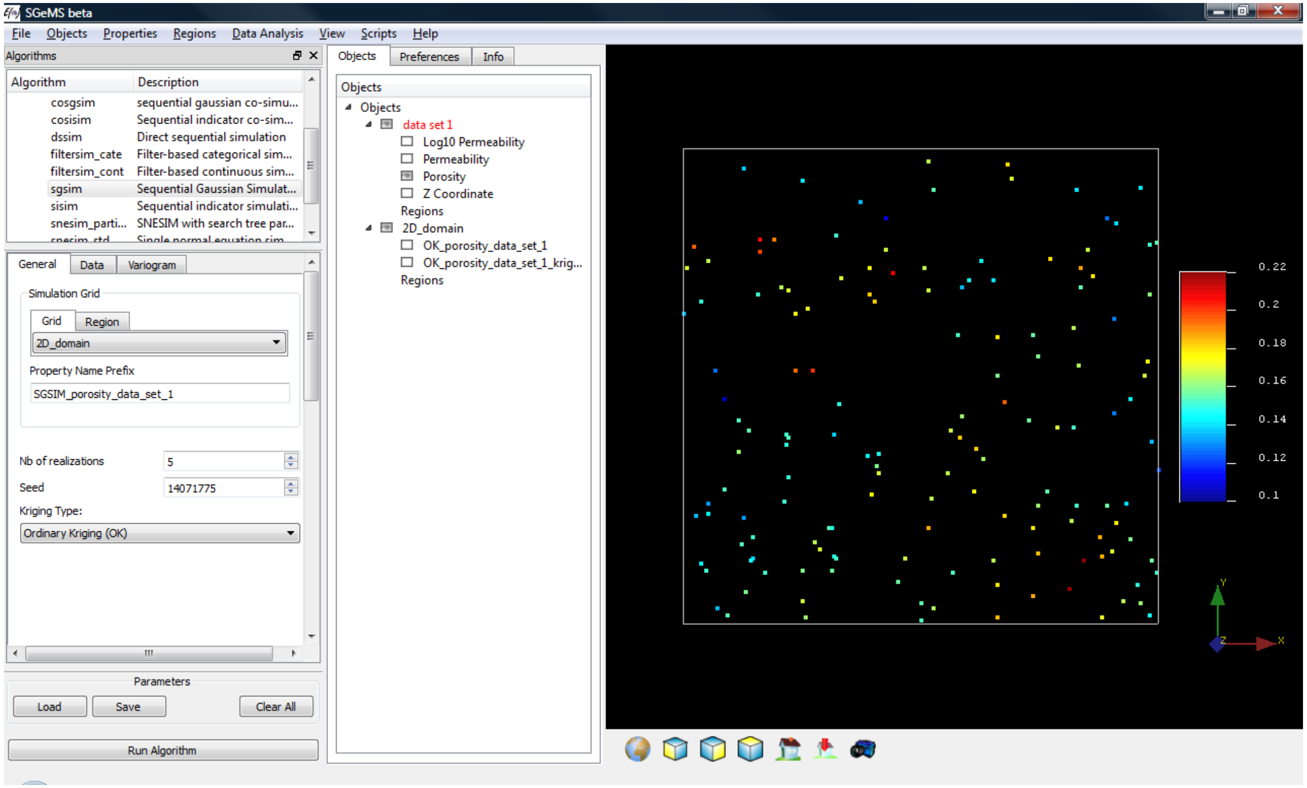






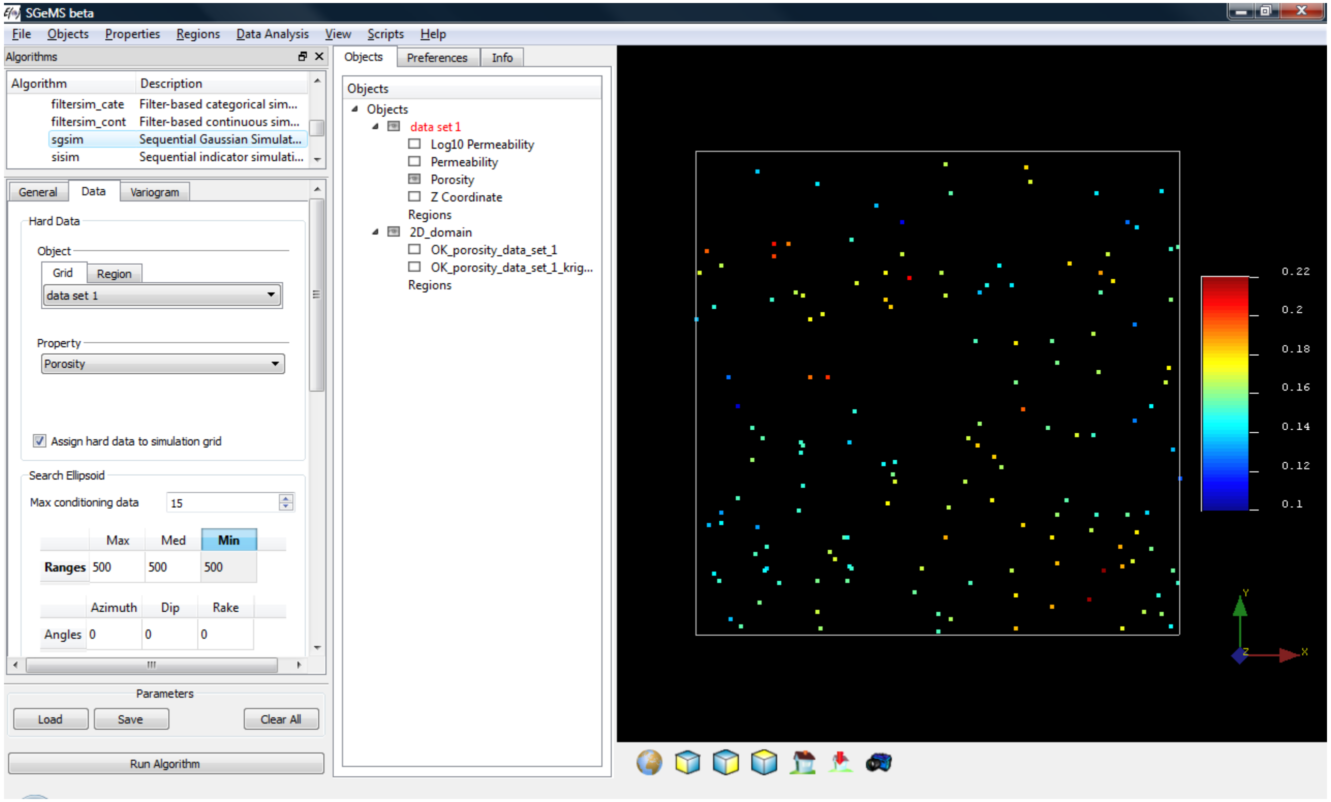
SGeMS – Spatial Simulation

- **Choose the "sgsim" option under the "Simulation" heading in the "Algorithm" window to conduct sequential Gaussian simulation for data set 1.**
- **Use the same 2D grid that you created for the kriging exercise (or create a new grid with a different resolution).**
- **Assign a property name, choose the number of realizations, enter a random seed, and choose "Ordinary Kriging" for the kriging type.**



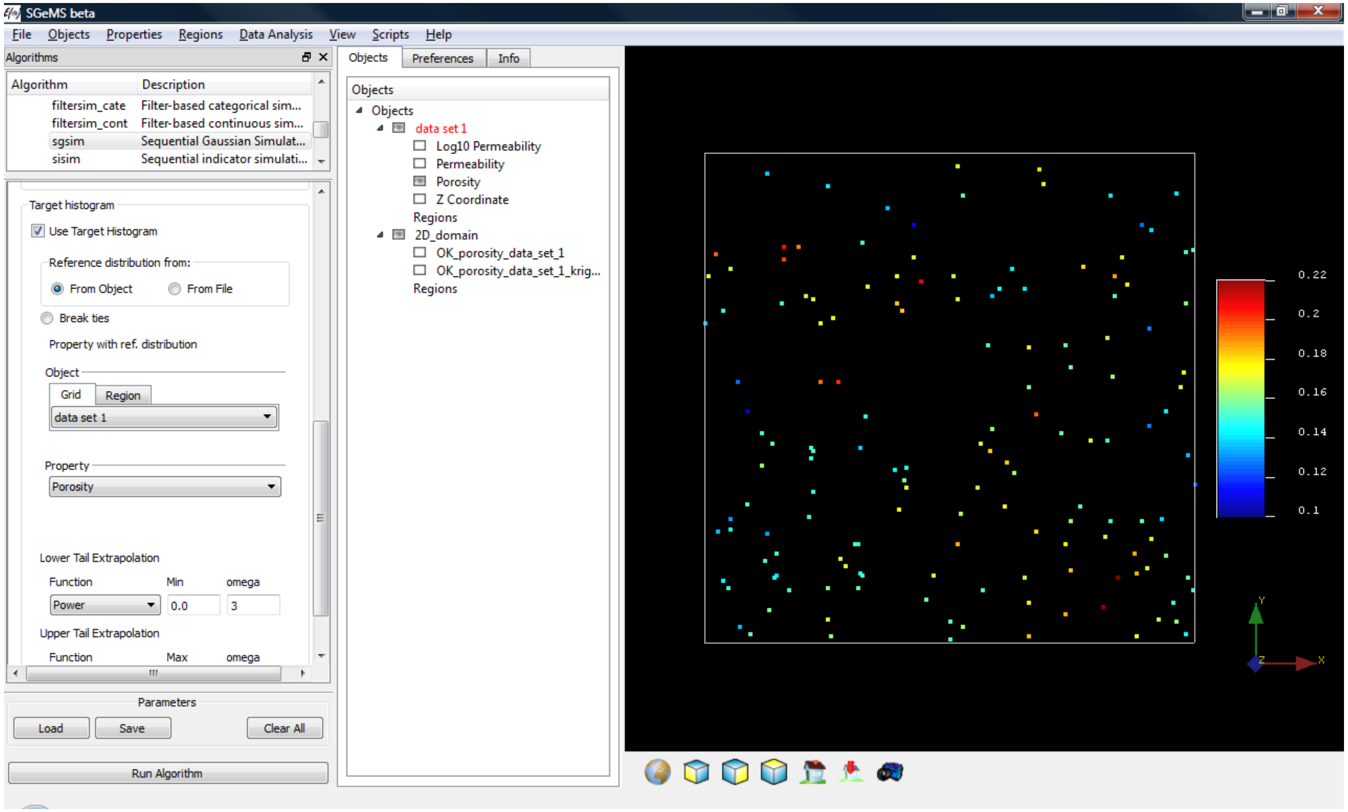
SGeMS – Spatial Simulation

- Under the "Data" tab specify the object containing the hard data, the property to be simulated (start with porosity), and check "Assign hard data to simulation grid".
- Next enter the search ellipsoid parameters, including the maximum number of conditioning data, the ranges, and the search ellipsoid orientation angles.



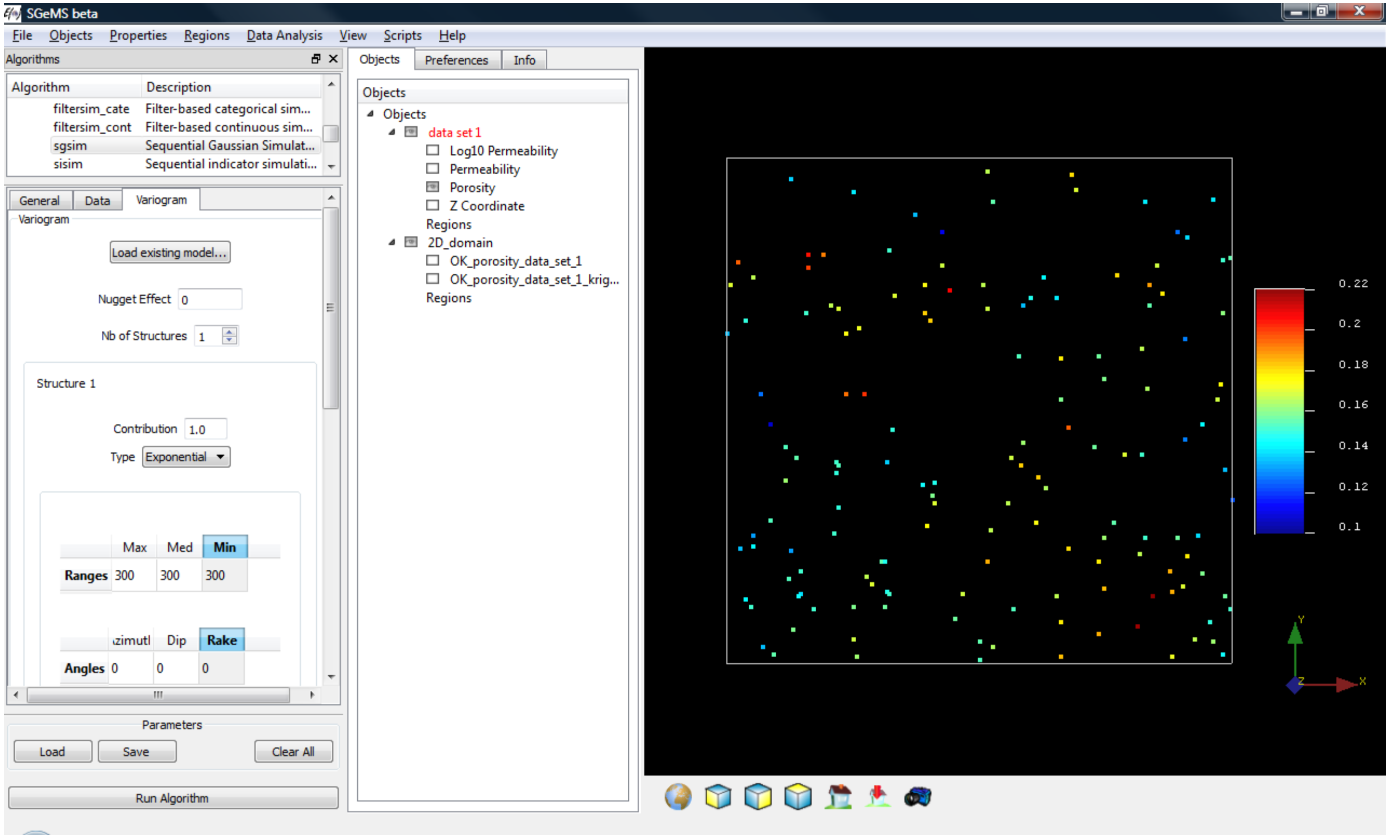
SGeMS – Spatial Simulation

- Scroll down the data tab to enter the target histogram parameters.
- The target histogram will be defined by the values in the data set file by choosing that object under the "Grid" tab and by choosing porosity as the "Property".
- Enter the minimum (0.0) and maximum (0.5) values for the tail extrapolation based on the physical limits of the property of interest (porosity in this case).



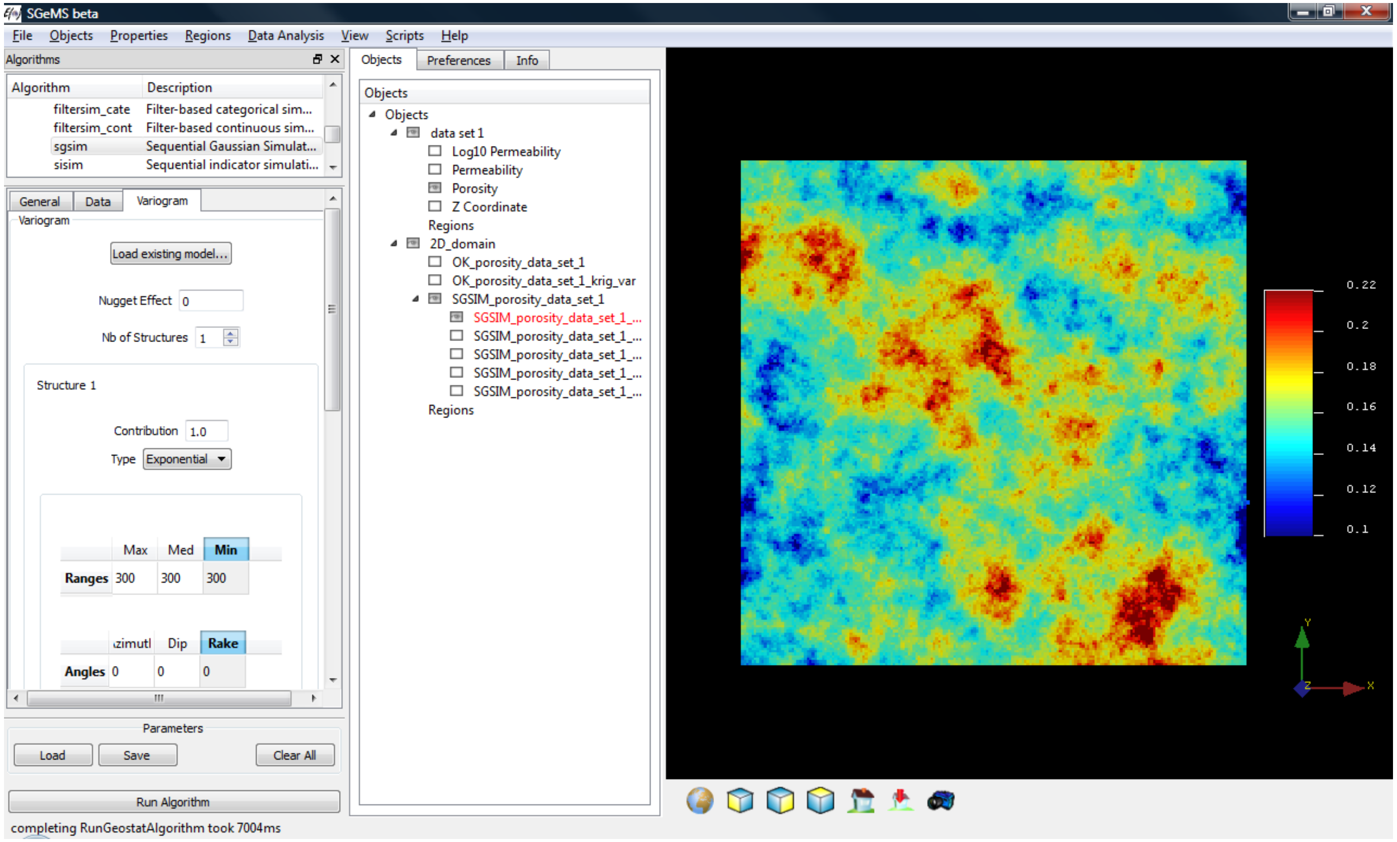
SGeMS – Spatial Simulation

- **Enter the variogram model to be used in the simulation under the "Variogram" tab, including model type, ranges, and ellipsoid angles.**
- **Push the "Run Algorithm" button to run the SGSIM simulator.**



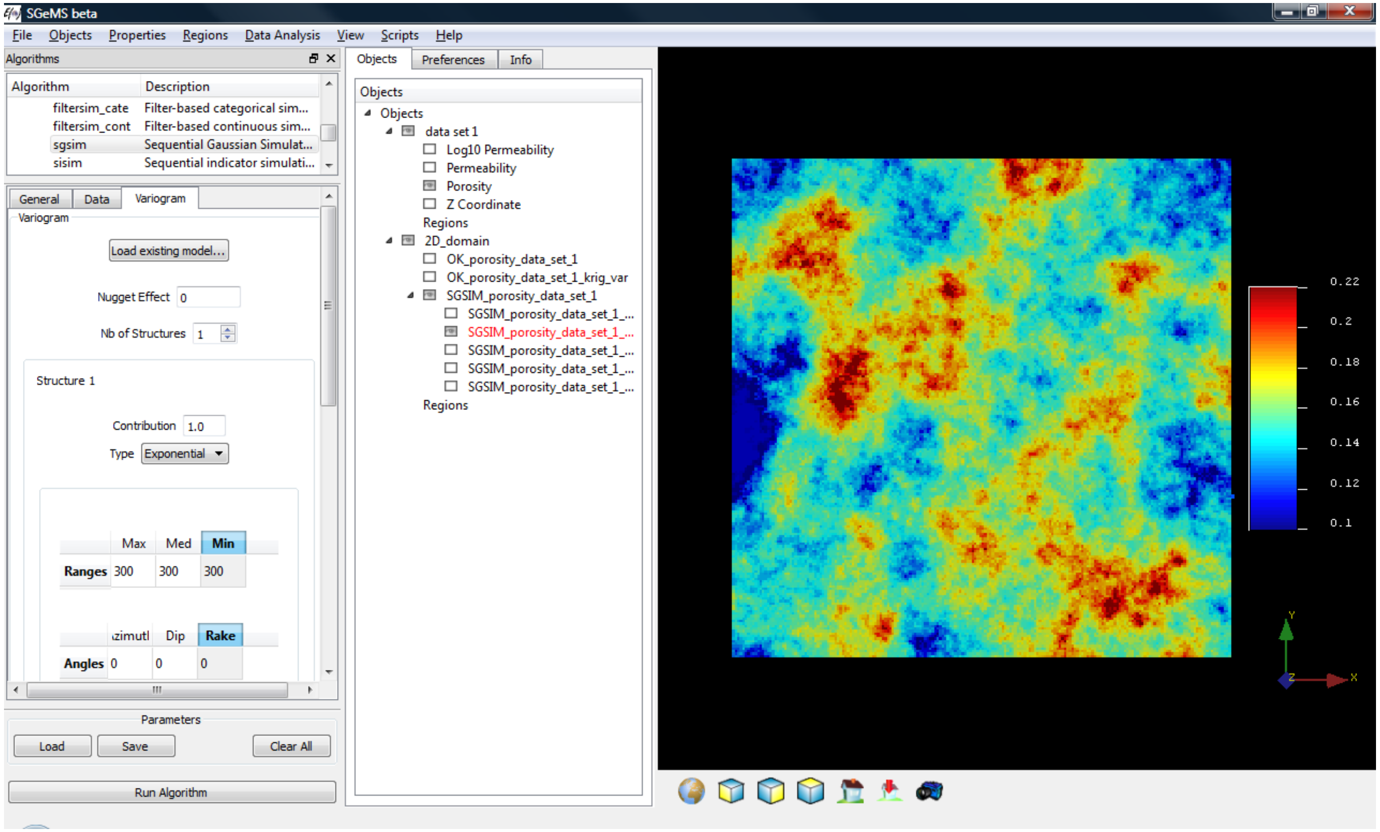
SGeMS – Spatial Simulation

- Note that a new object has been created under the 2D grid name that contains separate sub-objects for each of the realizations generated by SGSIM
- Click on the first realization to visualize the results. Note that you will have to reset the color scale under the "Preferences" tab to be consistent with the color bar.



SGeMS – Spatial Simulation

- **Click on the other SGSIM realizations to visualize the variations among them and visually compare the simulation results to the kriging results.**
- **Note that you will need to reset the color scale for each of the realizations to the same range to make meaningful comparisons among the realizations.**



SGeMS – Spatial Simulation

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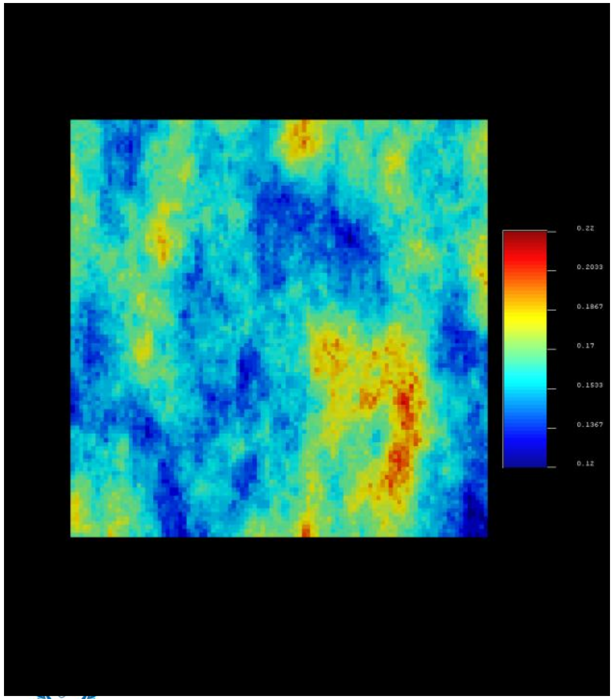
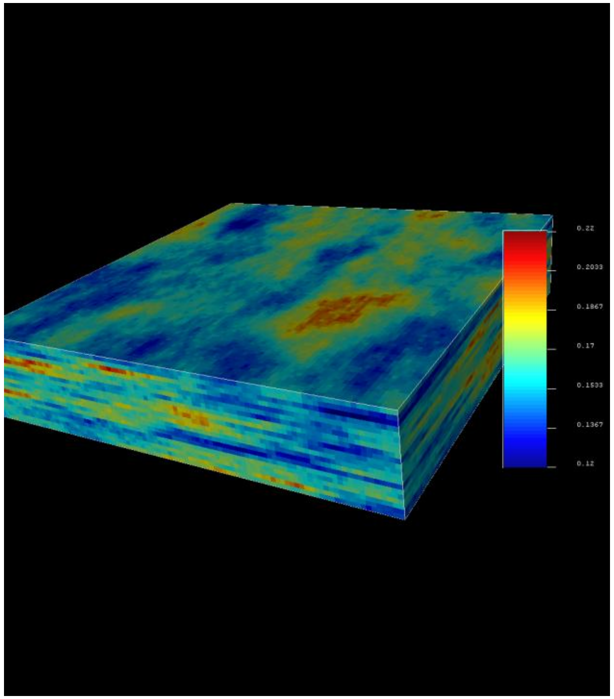
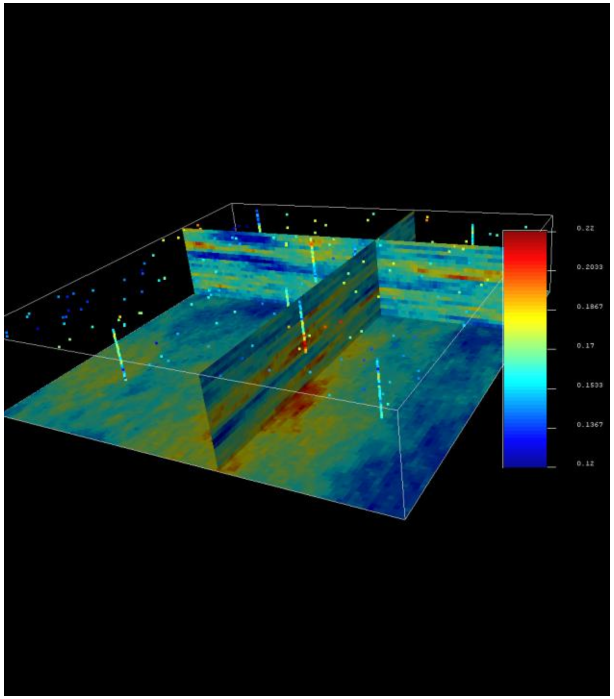
- **Conduct the simulation exercise using the “data_set_2_2D.dat” and “data_set_3_3D.dat” data sets.**
- **Practice using the visualization window and the slicing tool to understand the sequential Gaussian simulation output in three dimensions.**
- **Perform spatial simulations for other parameters and try changing various inputs to SGSIM to observe the impacts on the results.**







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