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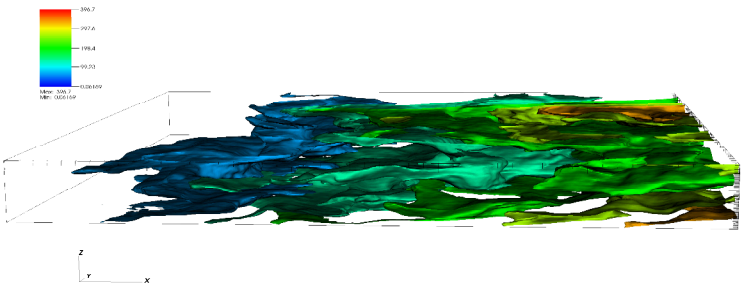

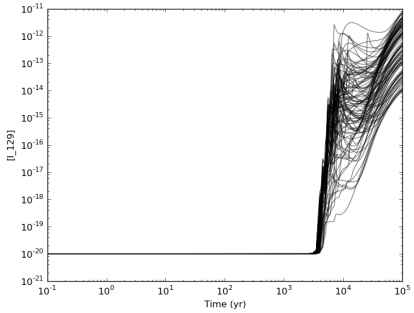

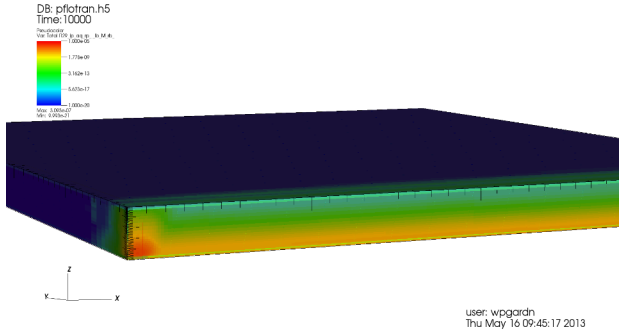

High Performance Simulation of Environmental Tracers in Heterogeneous Domains

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U.S. DEPARTMENT OF ENERGY

NNSA Nuclear Security Administration

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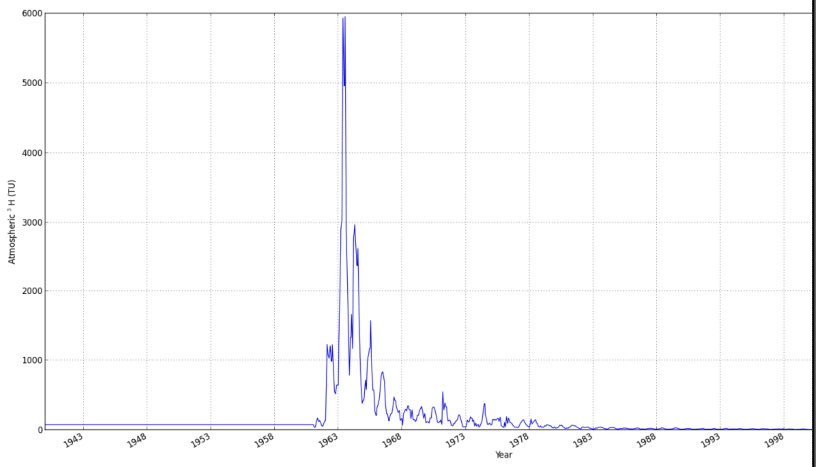
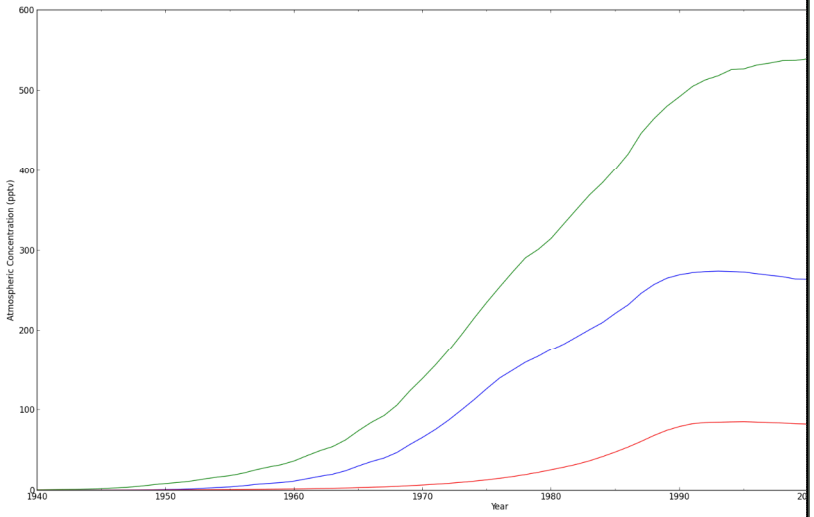
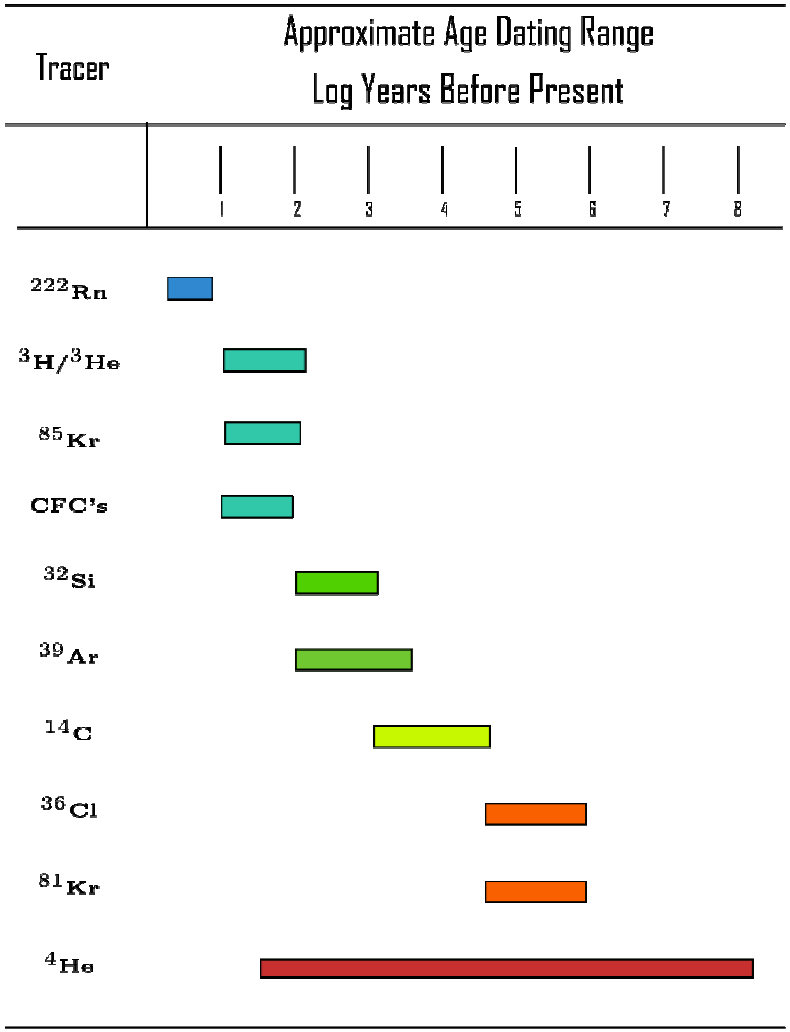
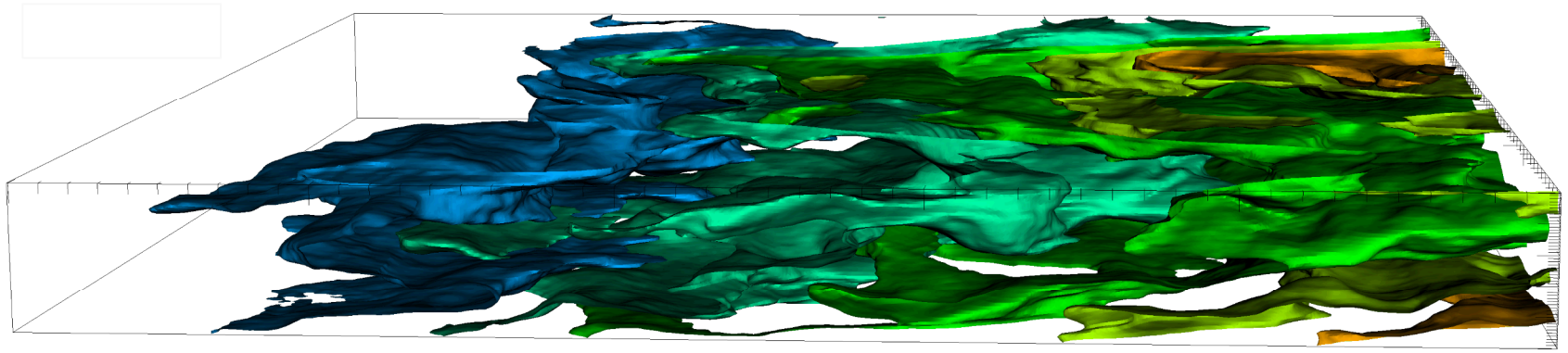
Environmental tracers – the basics







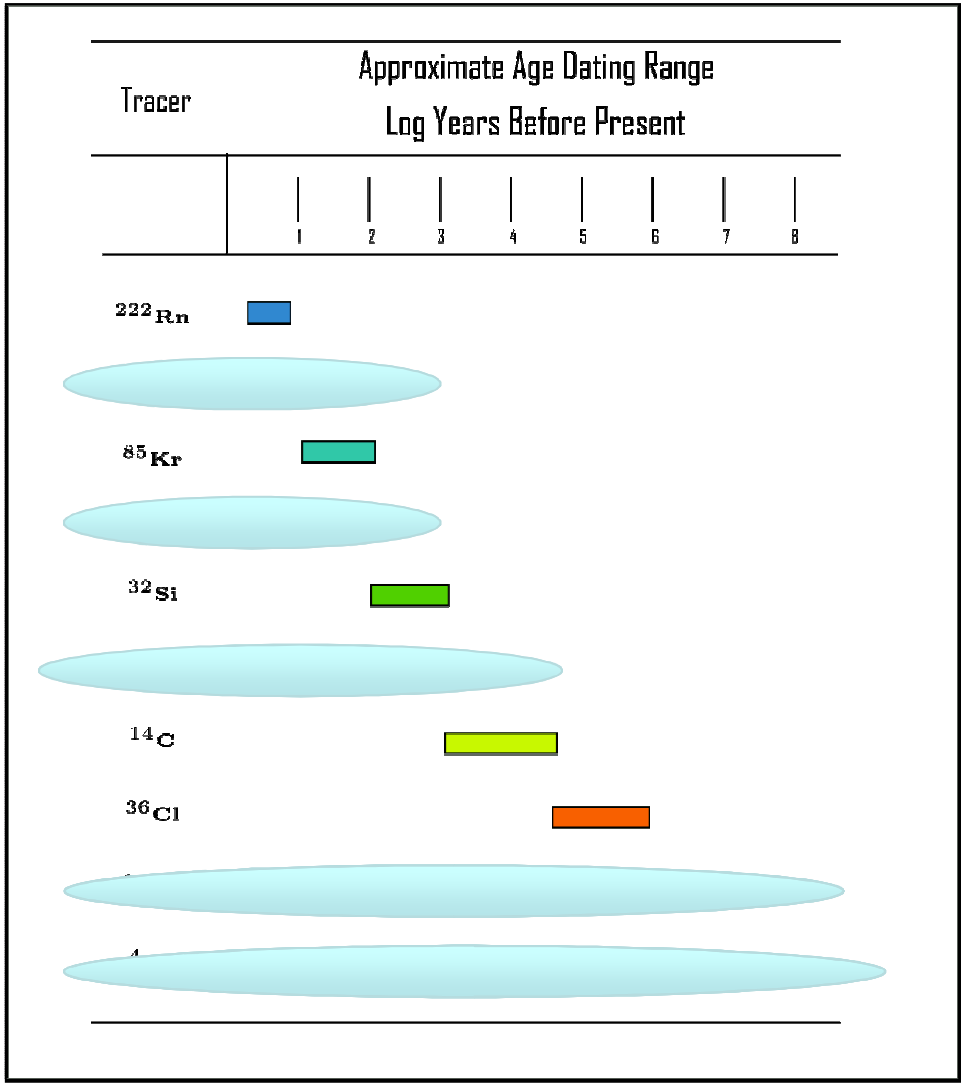
Modeling age



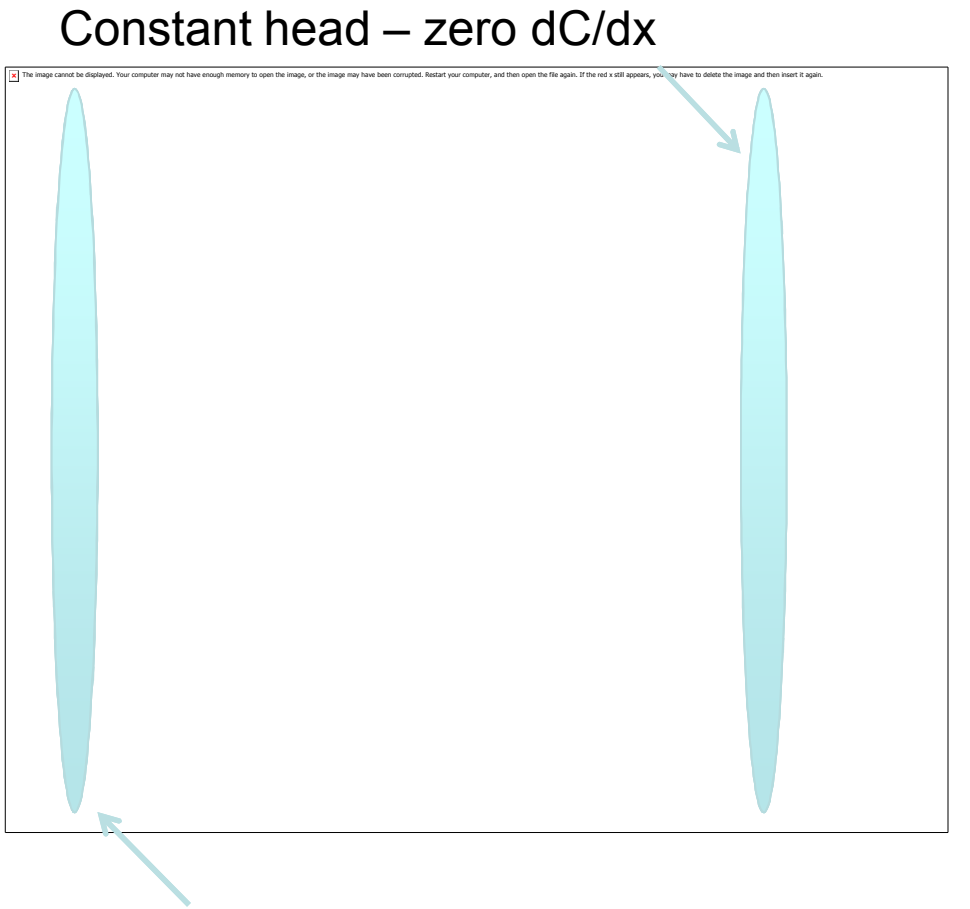
- How do we incorporate age and tracer information in a model?
  - Theory exists to model groundwater mean age and age distribution throughout a reservoir.
- Modeled mean age and apparent age for single tracers have been utilized
  - Problem – in order to calculate age from the tracer concentration we have to assume the age distribution!
- Concentrations of a single tracers have been used to constrain models
  - Problem – A single tracer cannot resolve different age mixtures
  - Need to model multiple species to resolve age mixtures, but 3-D modeling of tracer transport is expensive

High Performance Modeling of Environmental Tracers

- Using PFLOTRAN
  - Massively-parallel flow and reactive transport code
  - Simulate of a suite of tracers
    - $^{3}H/^{3}He$, CFC11, CFC12, CFC113, SF_6,^{39}Ar,^{81}Kr,^{4}He
    - Mean groundwater age
  - Large travel time span
  - More cam be added
- High Resolution 3-D Simulations
- Calibration and uncertainty quantification
  - DAKOTA and PEST coupled to PFLTORAN



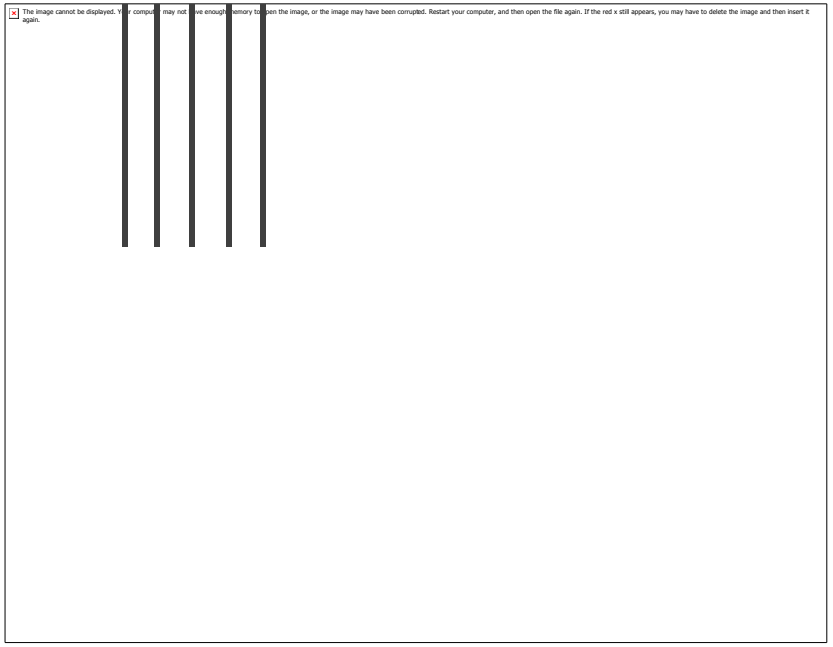
Synthetic Heterogeneous Permeability Field



- Heterogeneous field created with sequential Gaussian simulation
- Uniform correlation lengths of 20 m in x, y and z (3-D only)
- Considered lognormal permeability distributions with 1 and 2 orders of magnitude standard deviation
- Constant porosity

2-D Transport

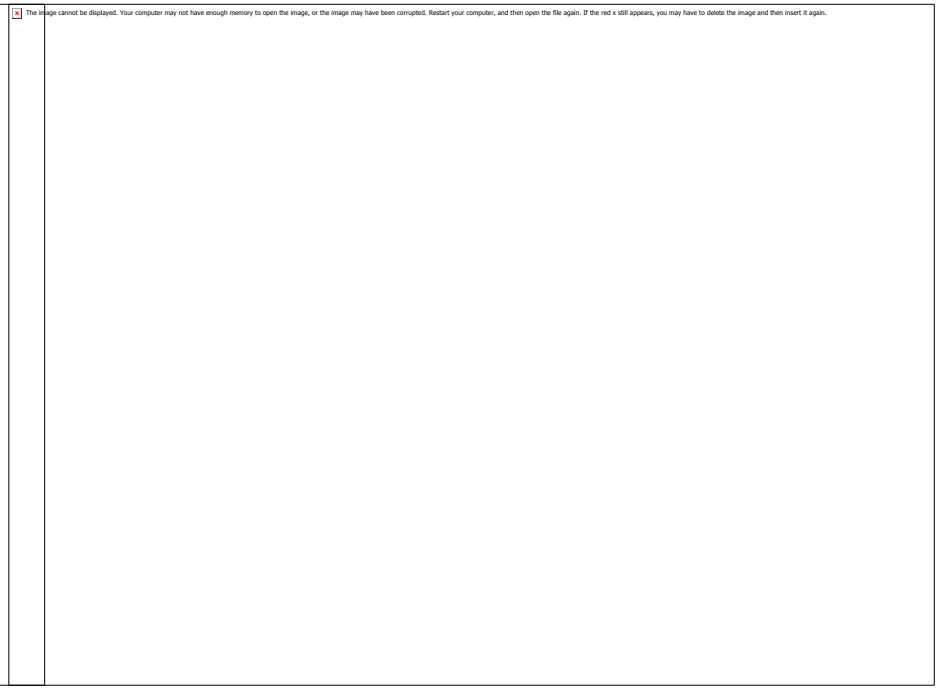
Lets look at spatial distribution of age along slices at increasing flow lengths in the x-direction



Simulate Concentration of Tracer

Tracer derived apparent age derived from measured concentration

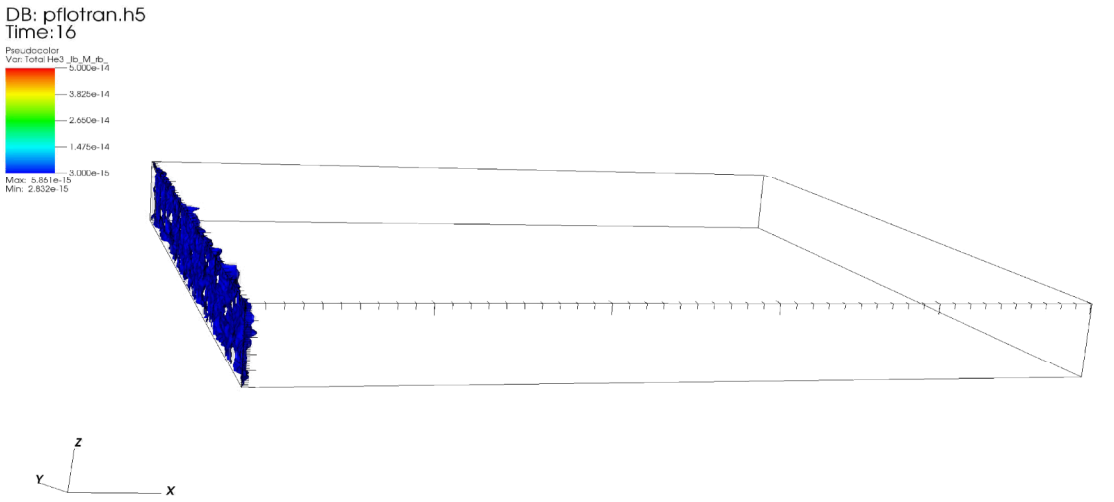
Spatial Bias of Mean Age and Age Variance

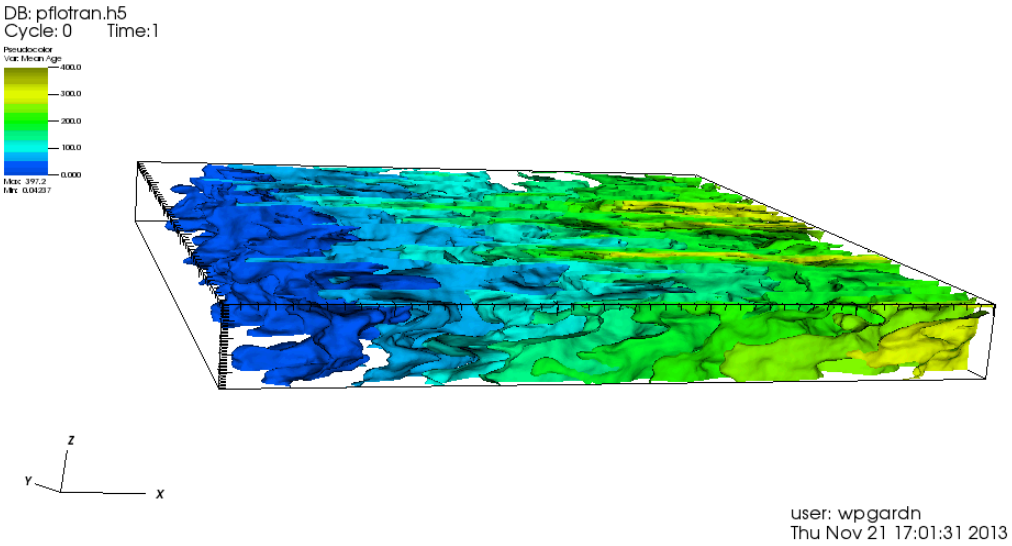


1s heterogeneity field – distinct bias in mean and variance in spatial age distribution

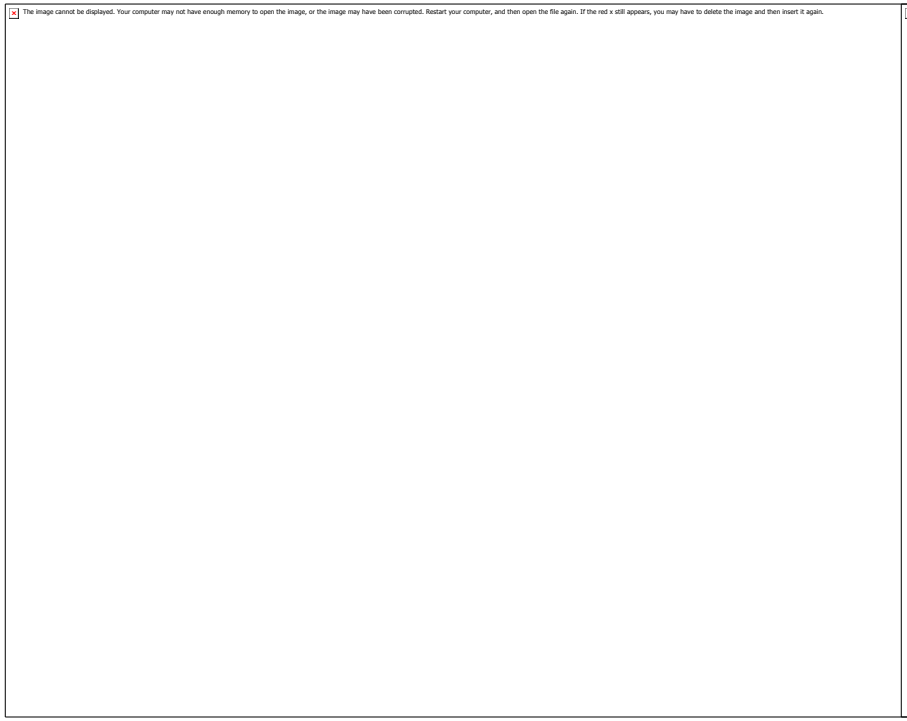
Increasing heterogeneity increases the Observed bias

High resolution 3-D domain





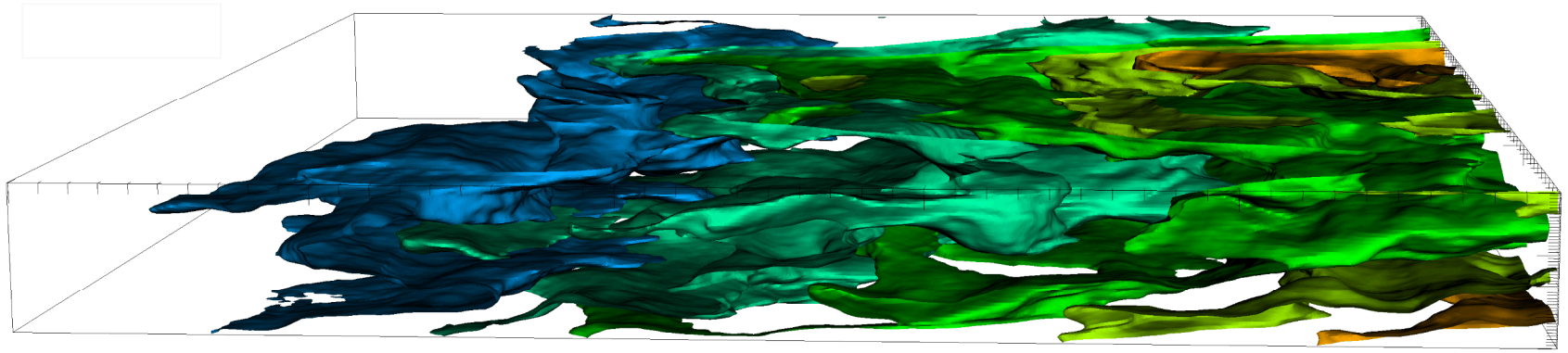
Effect of Adding the 3rd Dimesion



Difference in mean age and age variance for 2-D and 3-D simulations with 1σ Lognormal standard deviation

Difference in mean age and age variance for 2-D and 3-D simulations with 2σ Lognormal standard deviation

Conclusions



- We show that simulation of many tracer species in high-resolution, three-dimensional heterogeneous domains is possible
- We report on simulations with meshes over 10 million nodes, and simulation time periods over 100,000 years, which can be run with wall clock times less than two hours when spread over 800 processors
- Simulated random permeability fields were used to explore tracer transport through heterogeneous 2-D and 3-D fields for many different tracers
- Significant heterogeneity exists in the spatial distribution of mean age even in relatively homogenous domains after flow path lengths 25 times the spatial correlation length
- Tracer-derived ages show systematic biases toward younger ages when the groundwater age distribution contains water older than the maximum tracer age
- The addition of the third dimension increases connectivity by adding another degree of freedom for groundwater flow
  - Mean age and spatial variance in age is decreased in 3-D systems relative to 2-D systems
- Environmental tracer concentrations for multiple tracers can be used to constrain models
  - Use the direct data – not a very complex abstraction