IFRC Project Meeting: Adaptive mesh refinement and plume scale modeling

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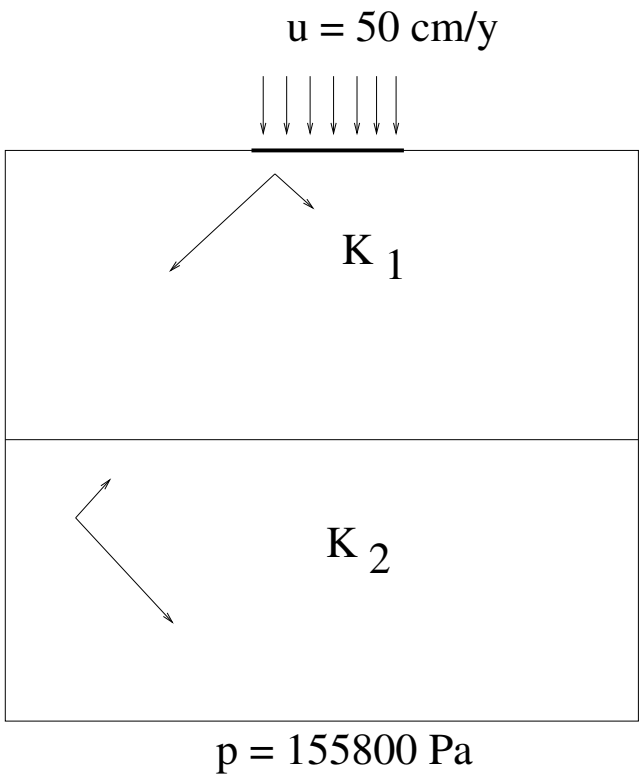
Advances in PFLOTRAN

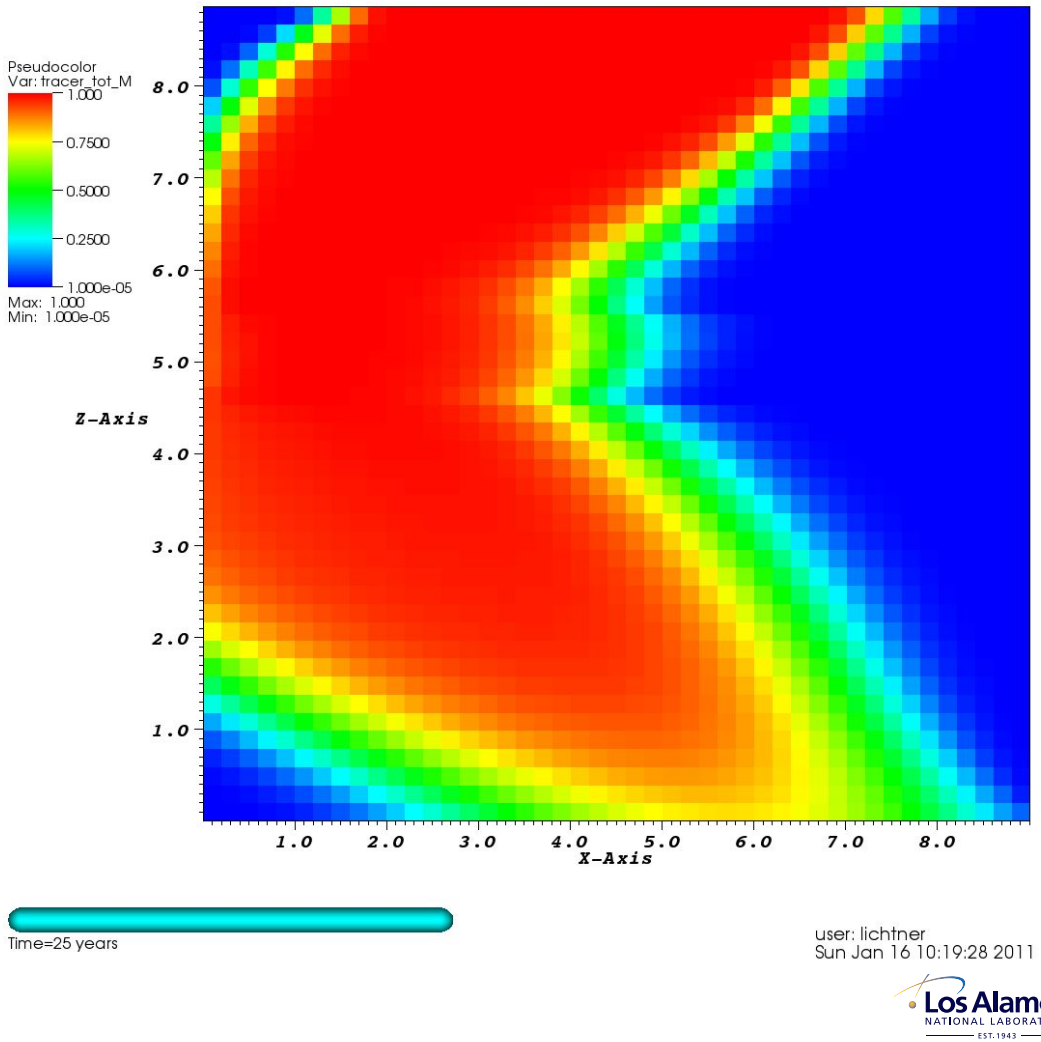
- Non-diagonal permeability tensor using MFV
- Solute Age
- AMR
- Multiple Continuum (in progress)

MFV (Mimetic Finite Volume) Permeability Tensor



$$\boldsymbol{K}_{1,2} = \begin{pmatrix} 7.75 \times 10^{-12} & \pm 3.90 \times 10^{-12} \\ \pm 3.90 \times 10^{-12} & 3.25 \times 10^{-12} \end{pmatrix}$$

Anisotropy 10:1



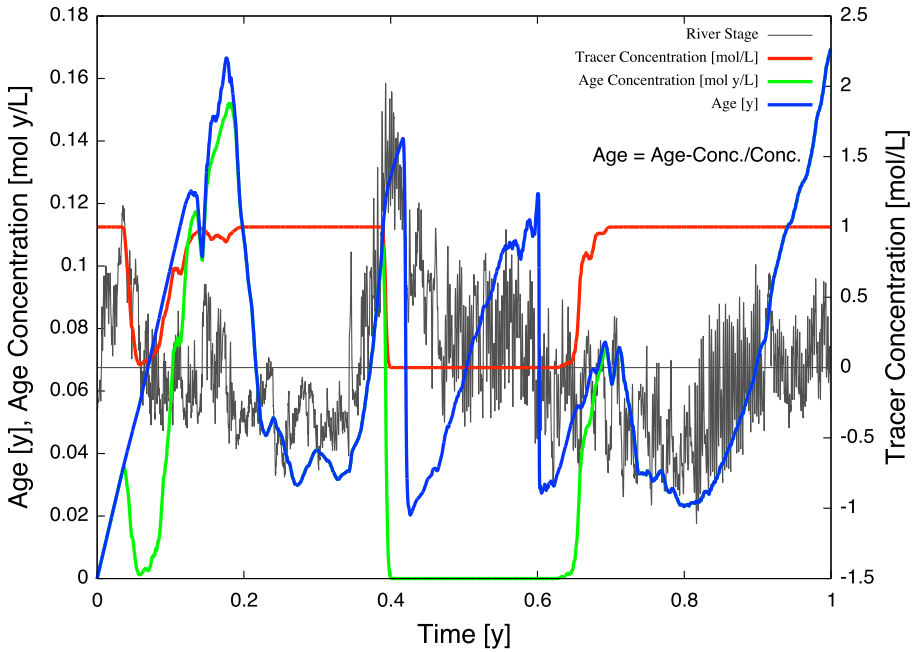
Tracer Age

- Tracer Concentration C:

$$\frac{\partial}{\partial t}\varphi s_l C + \nabla \cdot \left(\boldsymbol{q} C - \varphi s_l D \nabla C \right) = Q$$

- Tracer Age A:

$$\frac{\partial}{\partial t}\varphi s_l A C + \nabla \cdot \left(\boldsymbol{q} A C - \varphi s_l D \nabla A C \right) = \varphi s_l C$$



AMR (Adaptive Mesh Refinement)

- Put nodes only where needed to maintain accuracy while reducing the number of degrees of freedom (orders of magnitude reduction in DOFs compared to finest grid)
- Significant saving in computation cost and memory
- Track moving fronts
- SAMR (Structured Adaptive Mesh Refinement) represents a locally refined mesh as a union of logically rectangular meshes
- Disadvantages: not easy to implement; need special solvers (multilevel)

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SAMRAI: Structured Adaptive Mesh Refinement Application Interface

- **Parallel C++ SAMR Framework**
  - Patch-based
  - Multiple refinement levels
  - Parallel data transfer between refinement levels
  - Uniform Local Grid
  - Different data representations: cell, face, node, edge, ...
  - Jacobian-Free FV methods
  - Multilevel solvers
  - Parallel I/O using HDF5
  - Visit parallel visualization tool
- **Interface between PFLOTRAN F90 and C++**
- **Interface between PETSc and SAMRAI**

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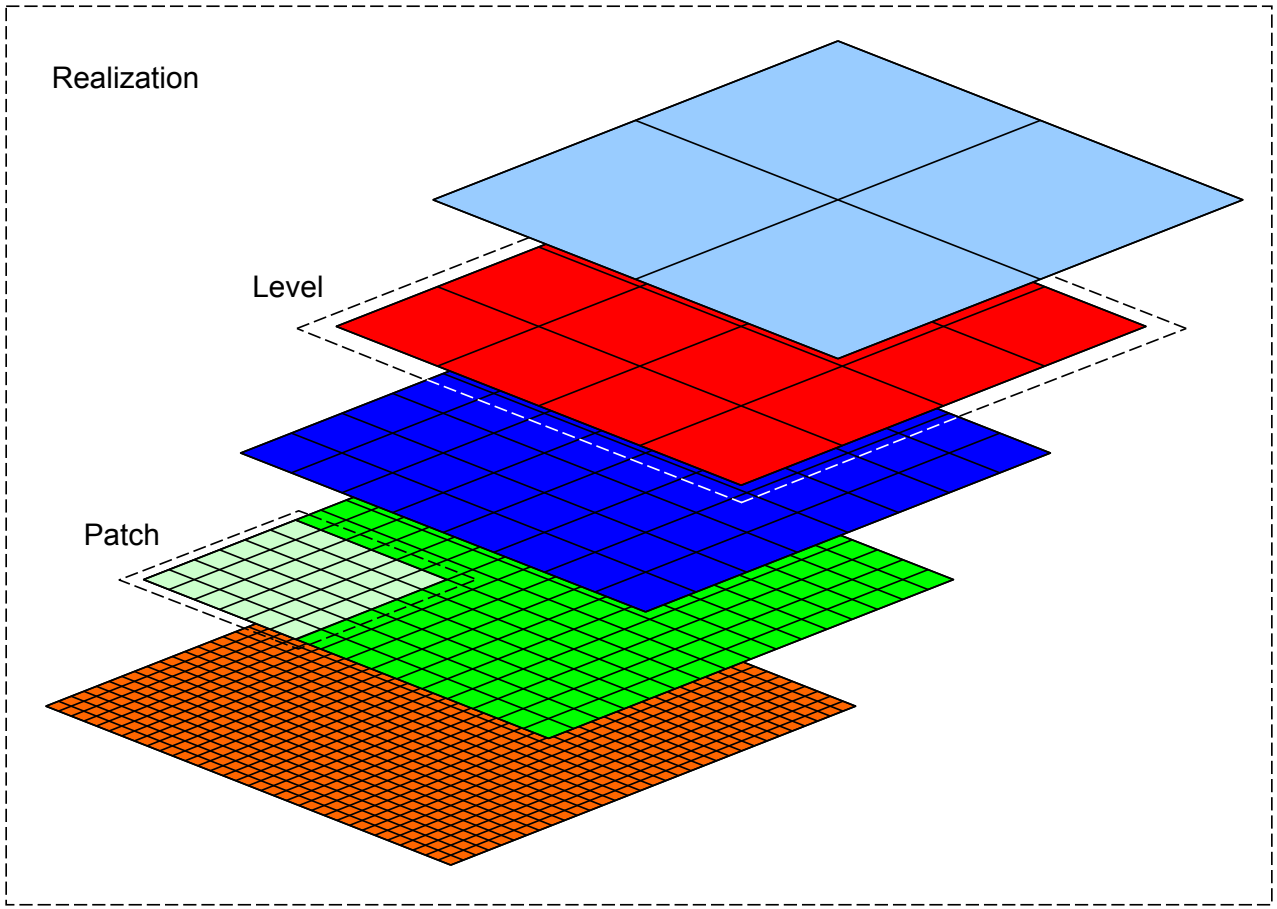
PFLOTRAN AMR Implementation

- **Patch-based SAMRAI grid**



SAMRAI Framework Mesh Hierarchy (Rich Hornung, LLNL)

Structured mesh hierarchy defined using "index spaces"

- Each finer level relates to a coarser level by a "refinement ratio"

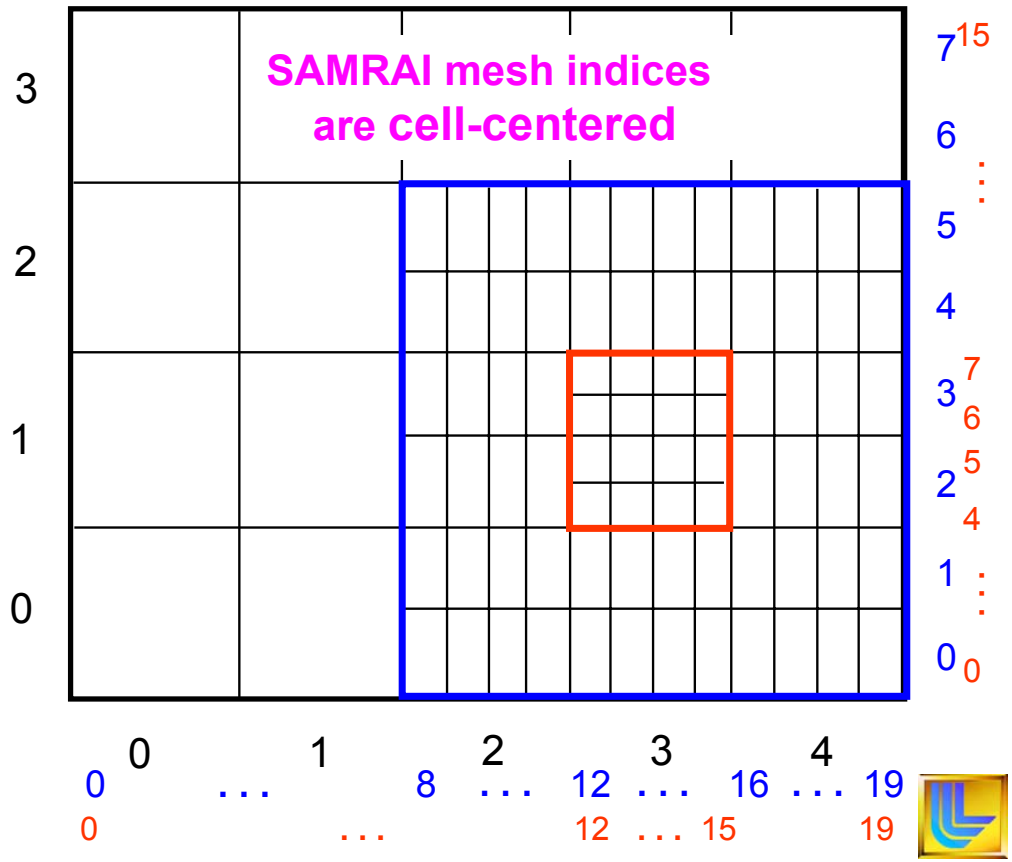
Coarsest Level
global index space …(0,0) - (4,3)
patch ……..(0,0) - (4,3)

Refinement ratio = (4,2)

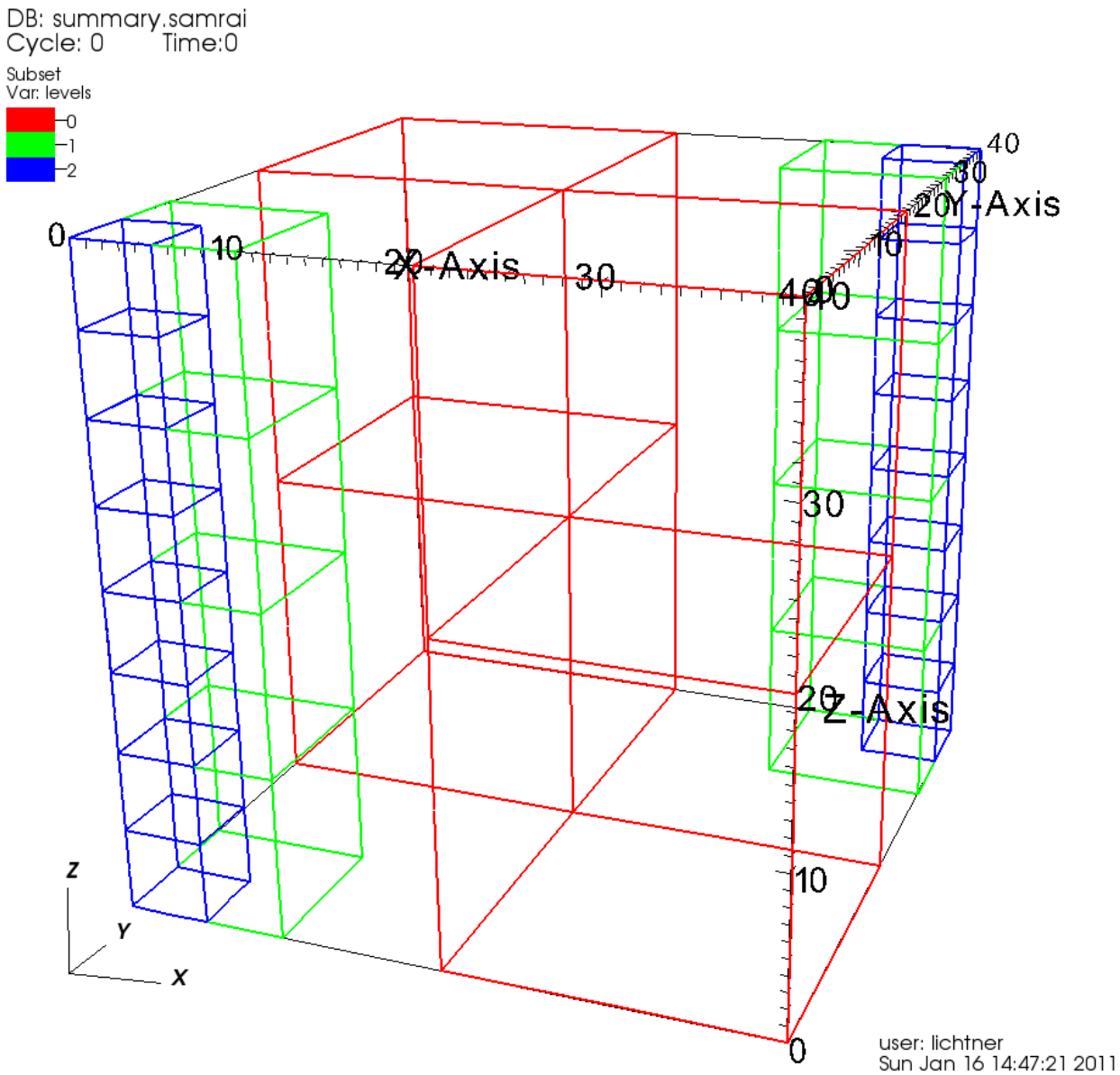
Intermediate Level
global index space … (0,0) - (19,7)
patch ……(8,0) - (19,5)

Refinement ratio = (1,2)

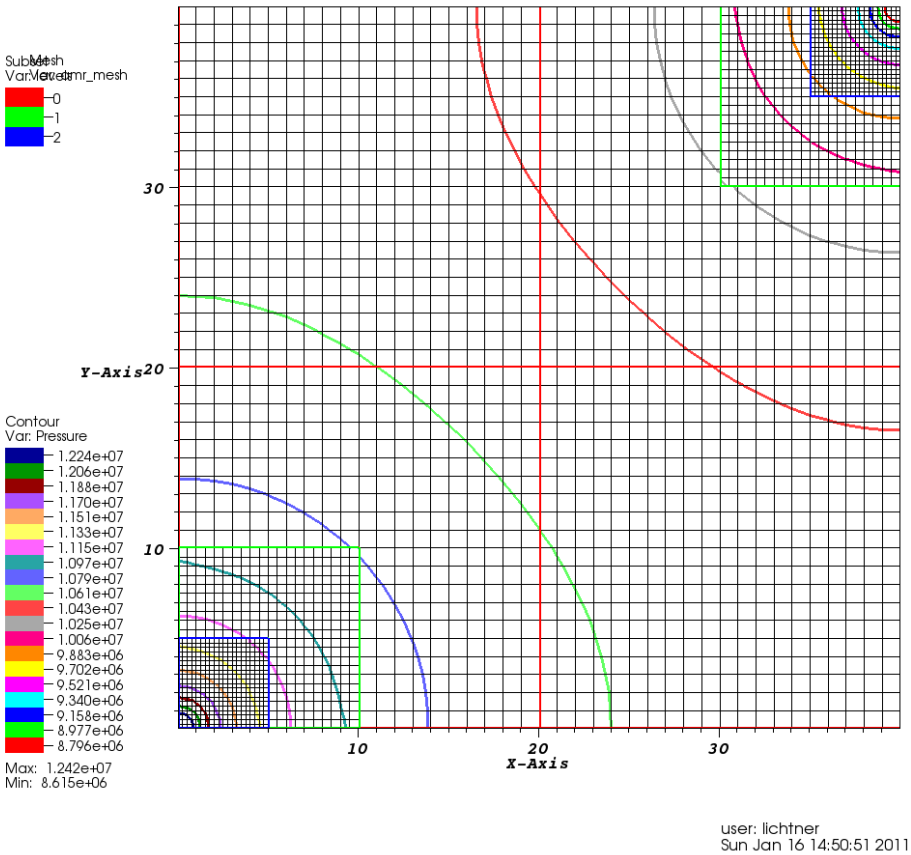
Finest Level
global index space… (0,0) - (19,15)
patch …….. (12,4) - (15,7)

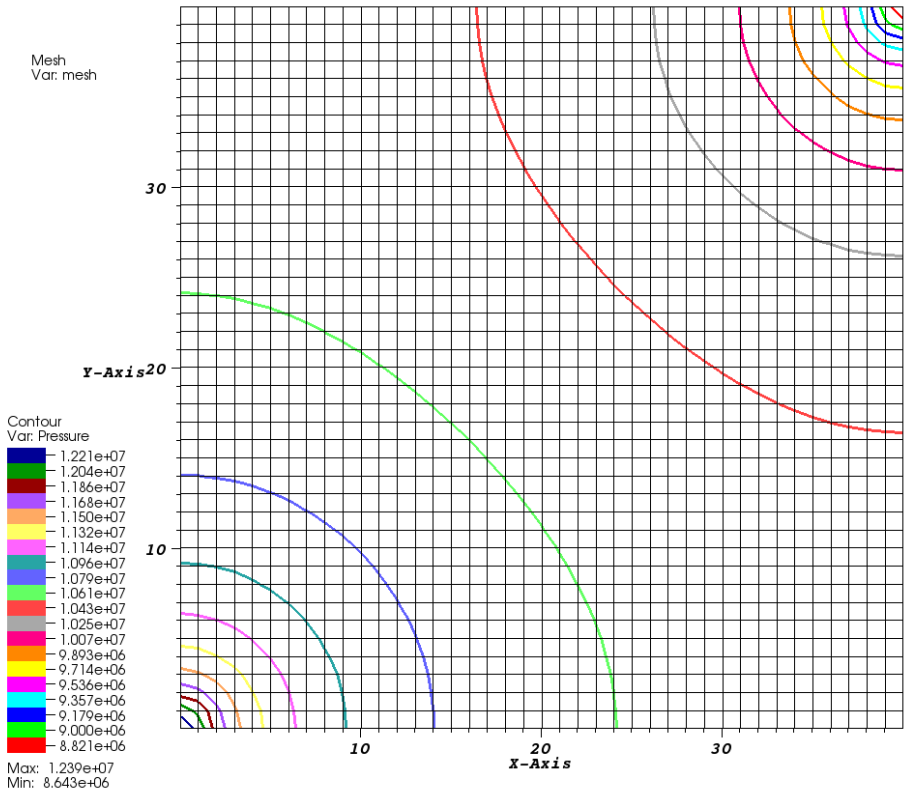


5-Spot Well Pattern: Refinement Levels



5-Spot Well Pattern: Comparison of Pressure Field

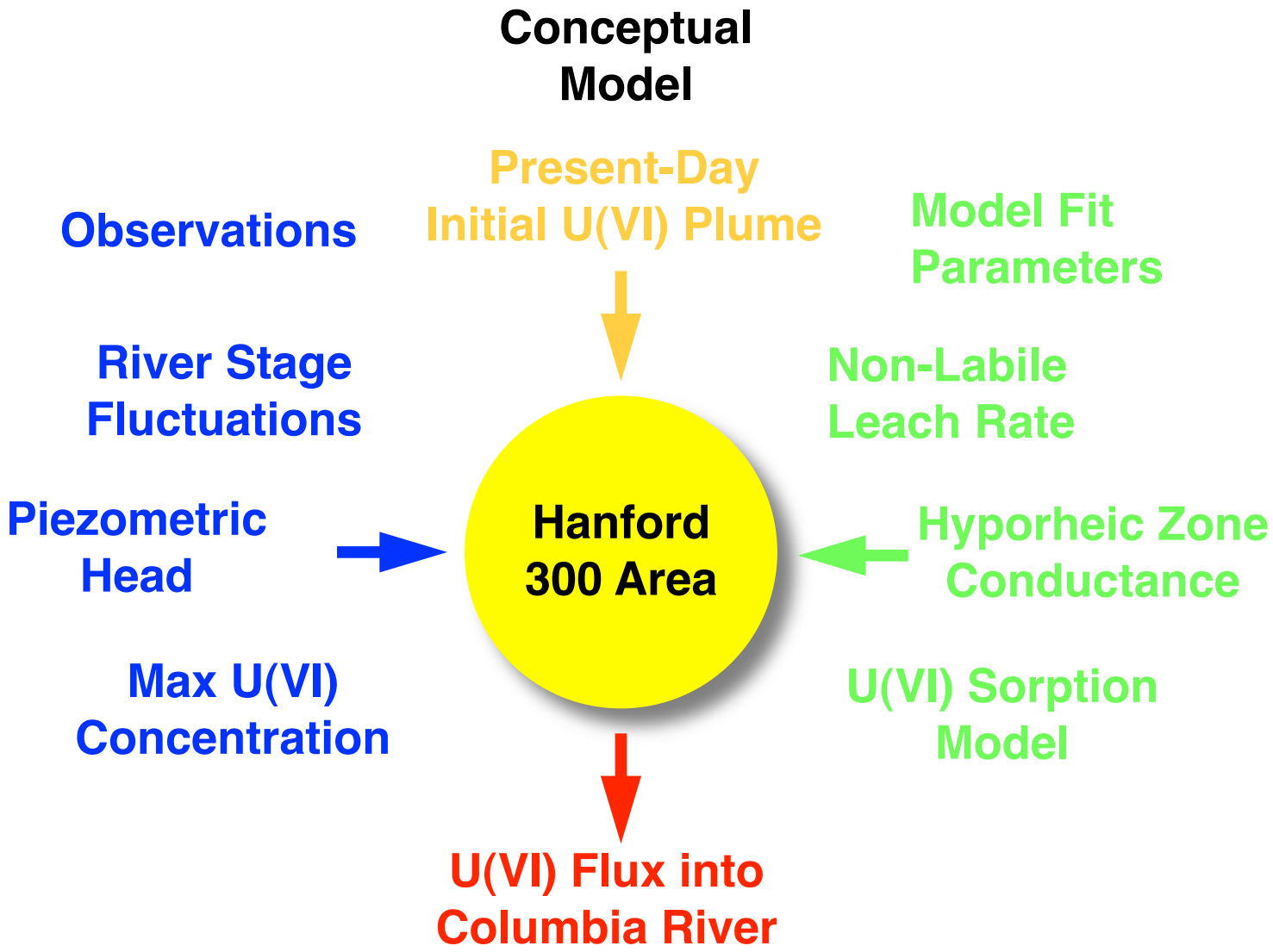




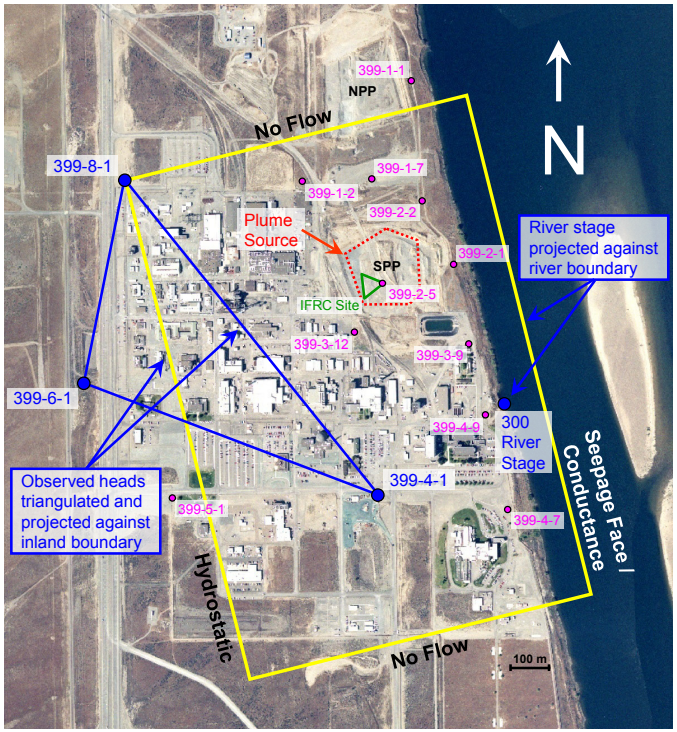
Plume & Site-Scale Models

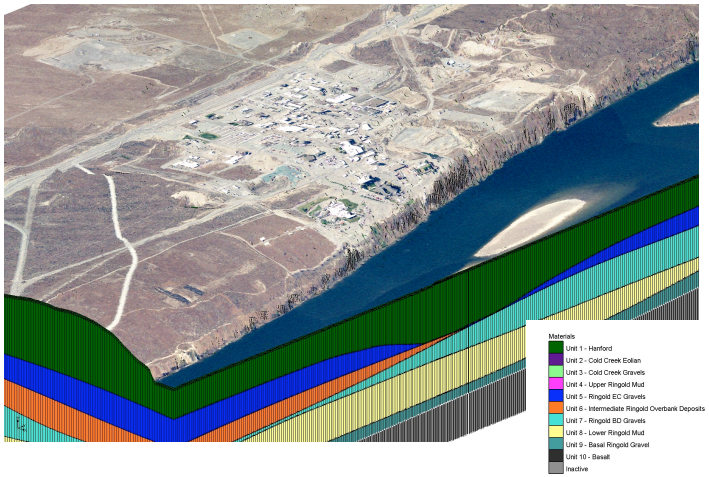
- **Hanford 300 Area Plume-Scale Model**
  - Time scale: years
  - Domain size: 900 m $\times$ 1300 m $\times$ 20 m
  - High resolution grid: 5 m $\times$ 5 m $\times$ 0.5 m
  - Nodes: 1.872M
- **IFRC Site-Scale Domain**
  - Time scale: hours
  - Domain size: 80 m $\times$ 80 m $\times$ 20 m
  - Grid Size: $\sim$ 1 m

Plume-Scale Conceptual Model



Hanford 300 Area Modeling Domain





- Domain size: $900\text{m} \times 1300\text{m} \times 20\text{m}$
- Grid size: $\Delta x = \Delta y = 5\text{m}$
  $\Delta z = 0.5\text{m}$
- Flow: $N_{\text{dof}} = 1.872\text{M}$
  $= 180 \times 260 \times 40$
- Reactive Transport: $N_{\text{dof}} = 28.08\text{M}$
  $= 180 \times 260 \times 40 \times 15$

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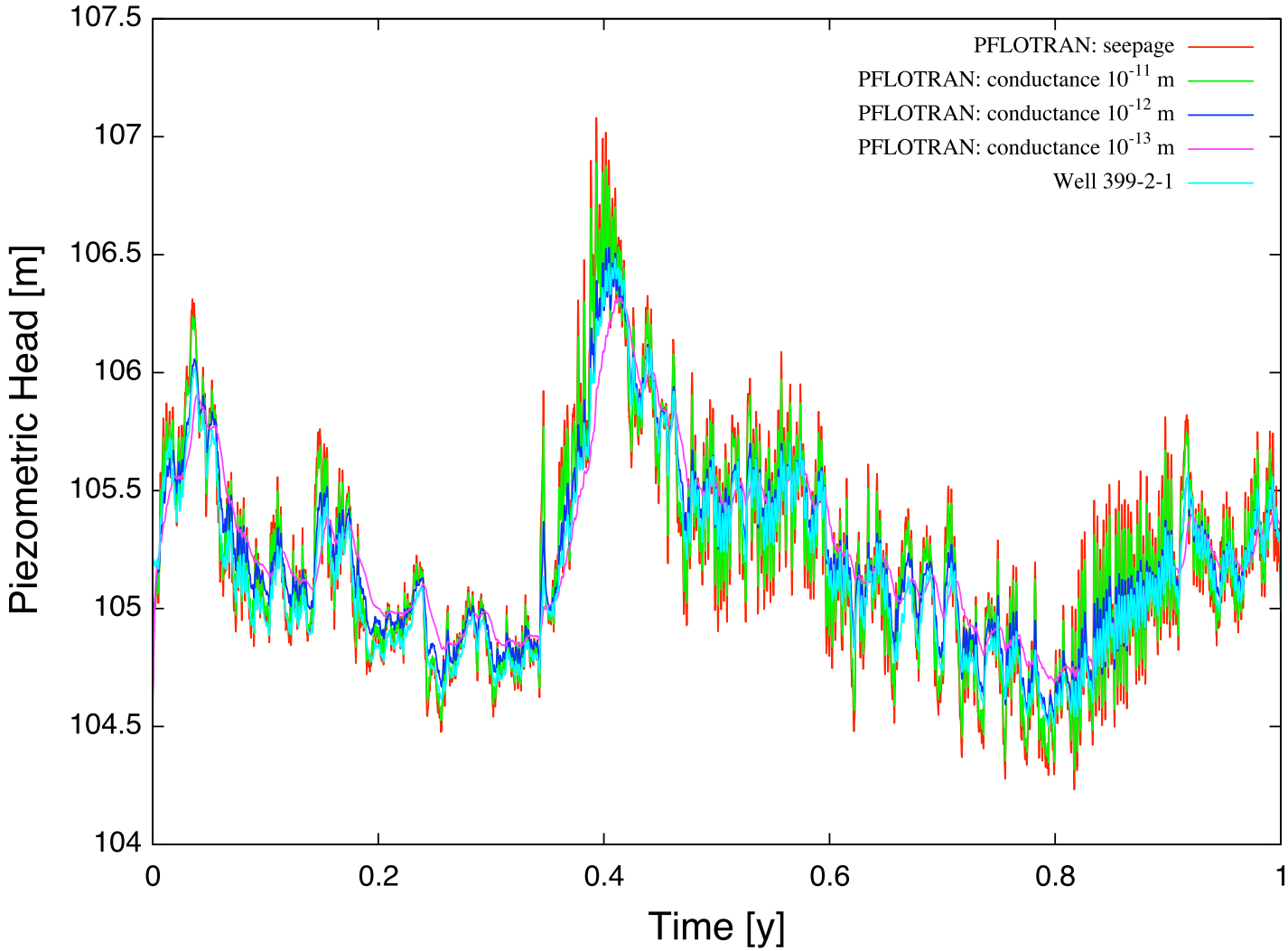
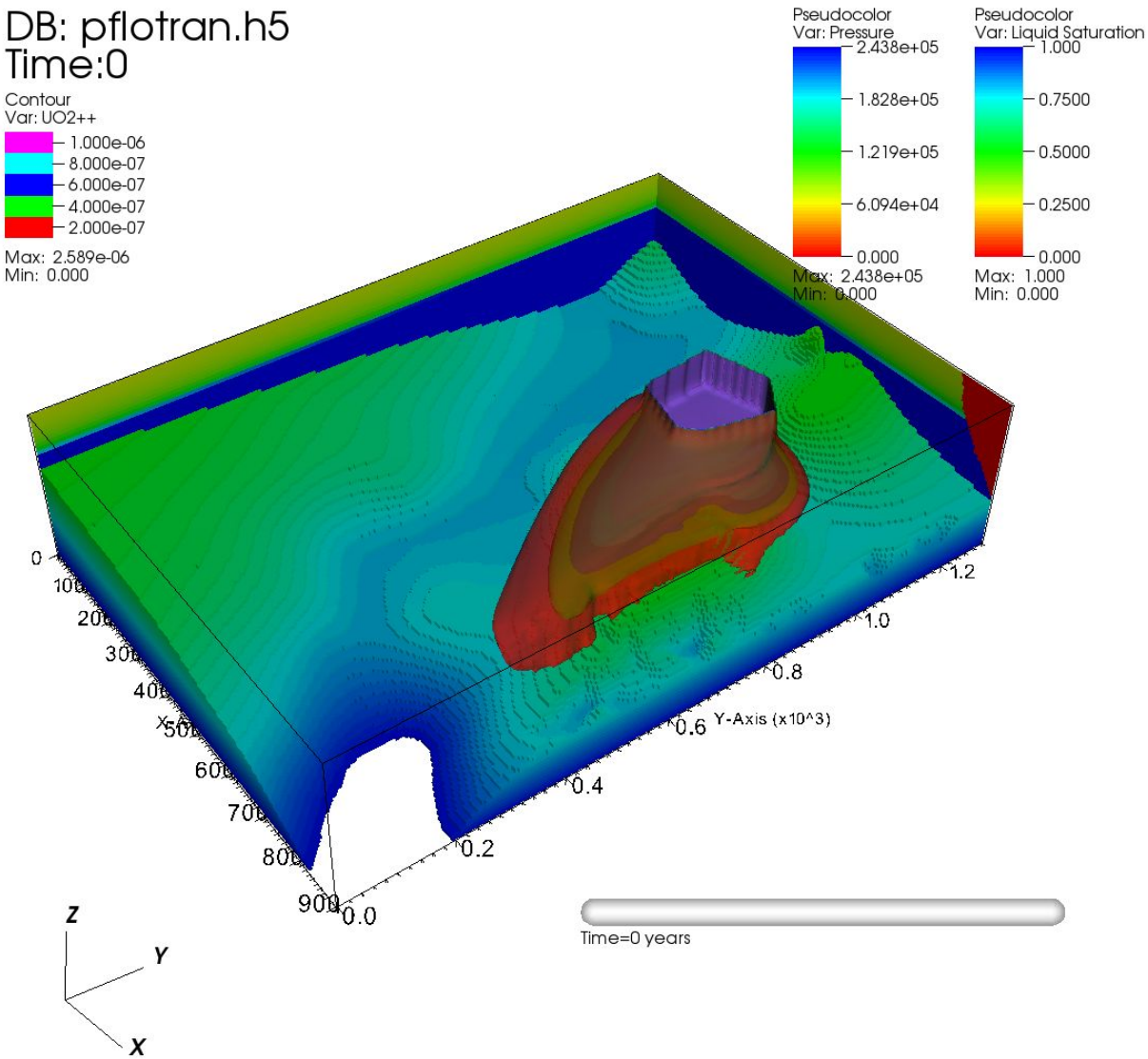
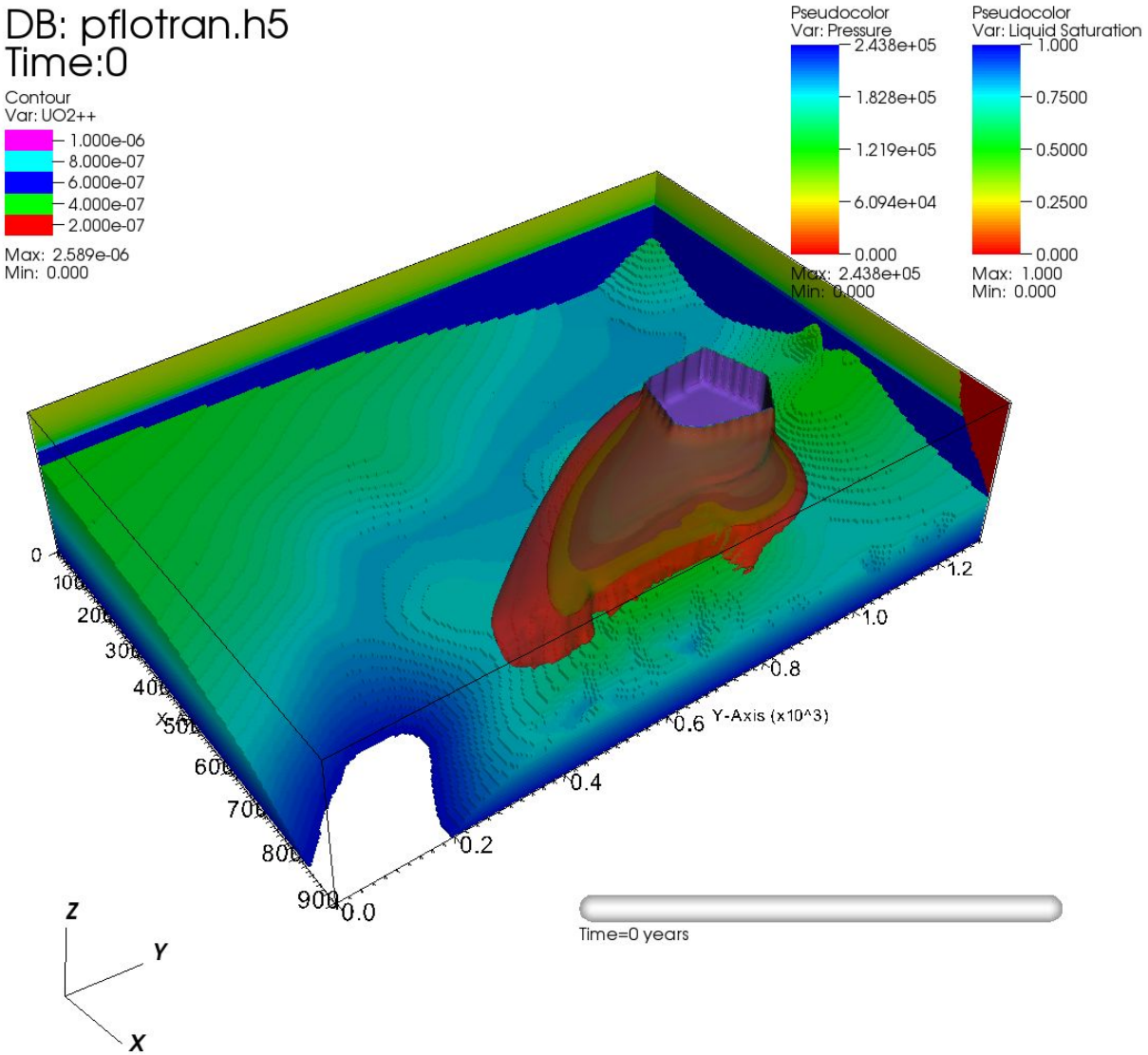
Hyporheic Zone Conductance: Predicted and Measured Head at Well 399-3-12



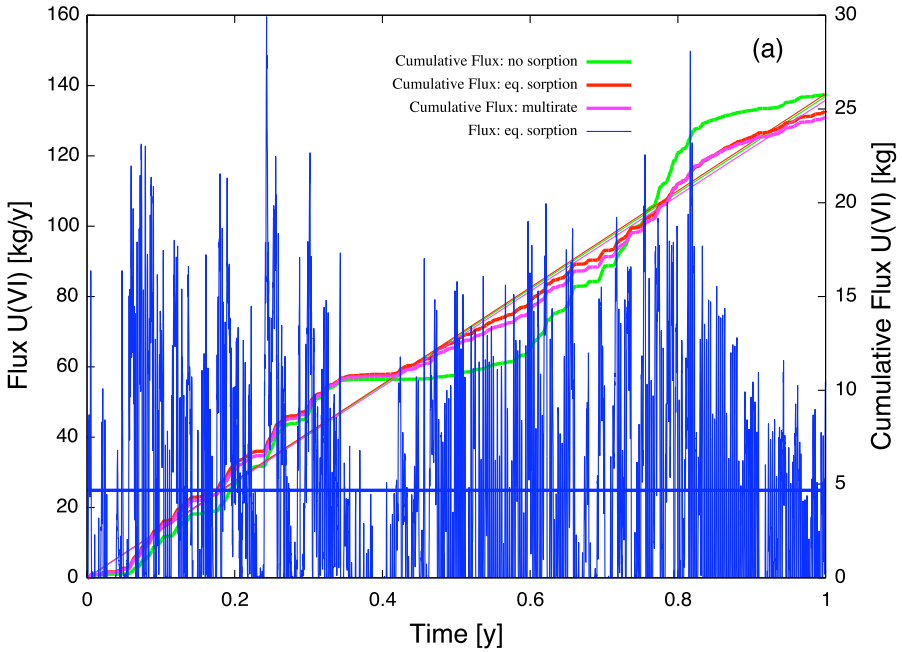
U(VI) Plume: Multirate Model

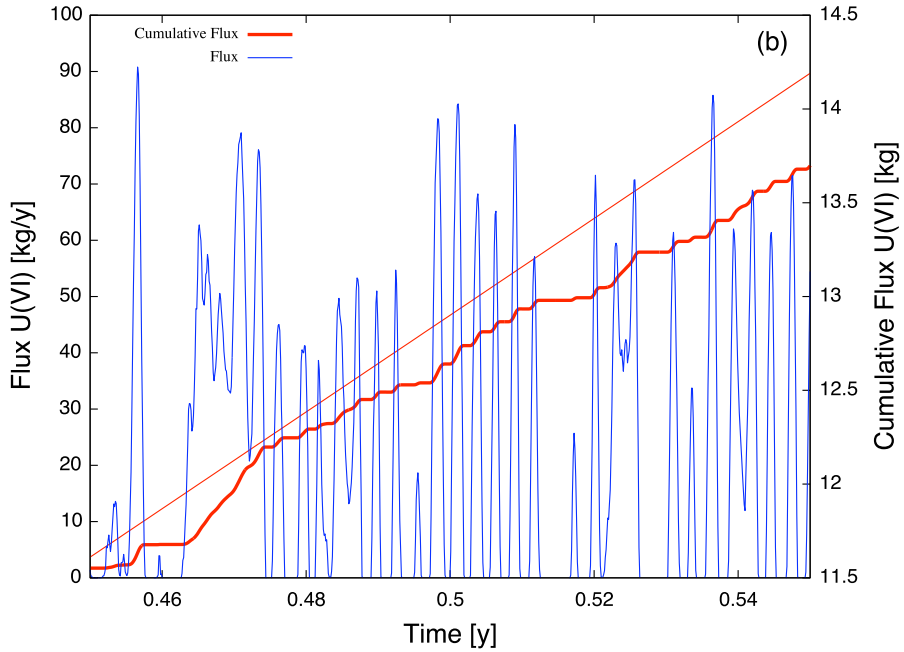


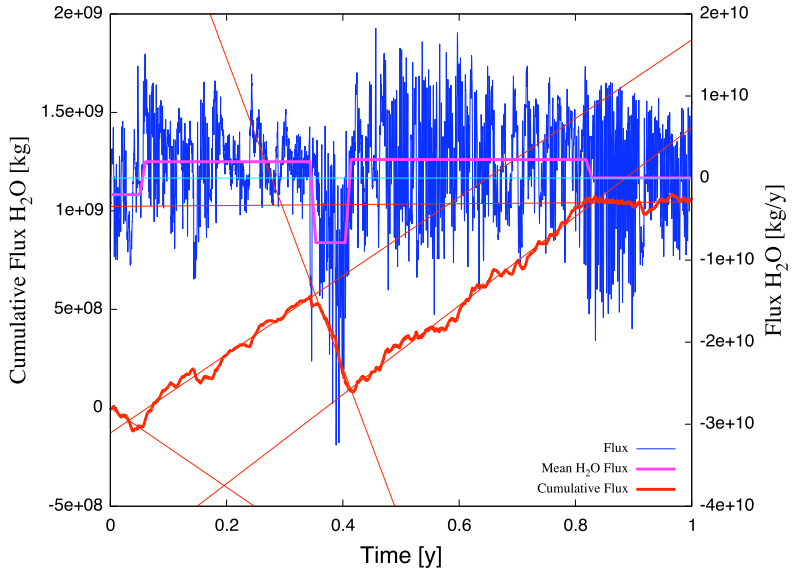
U(VI) Plume: No Sorption



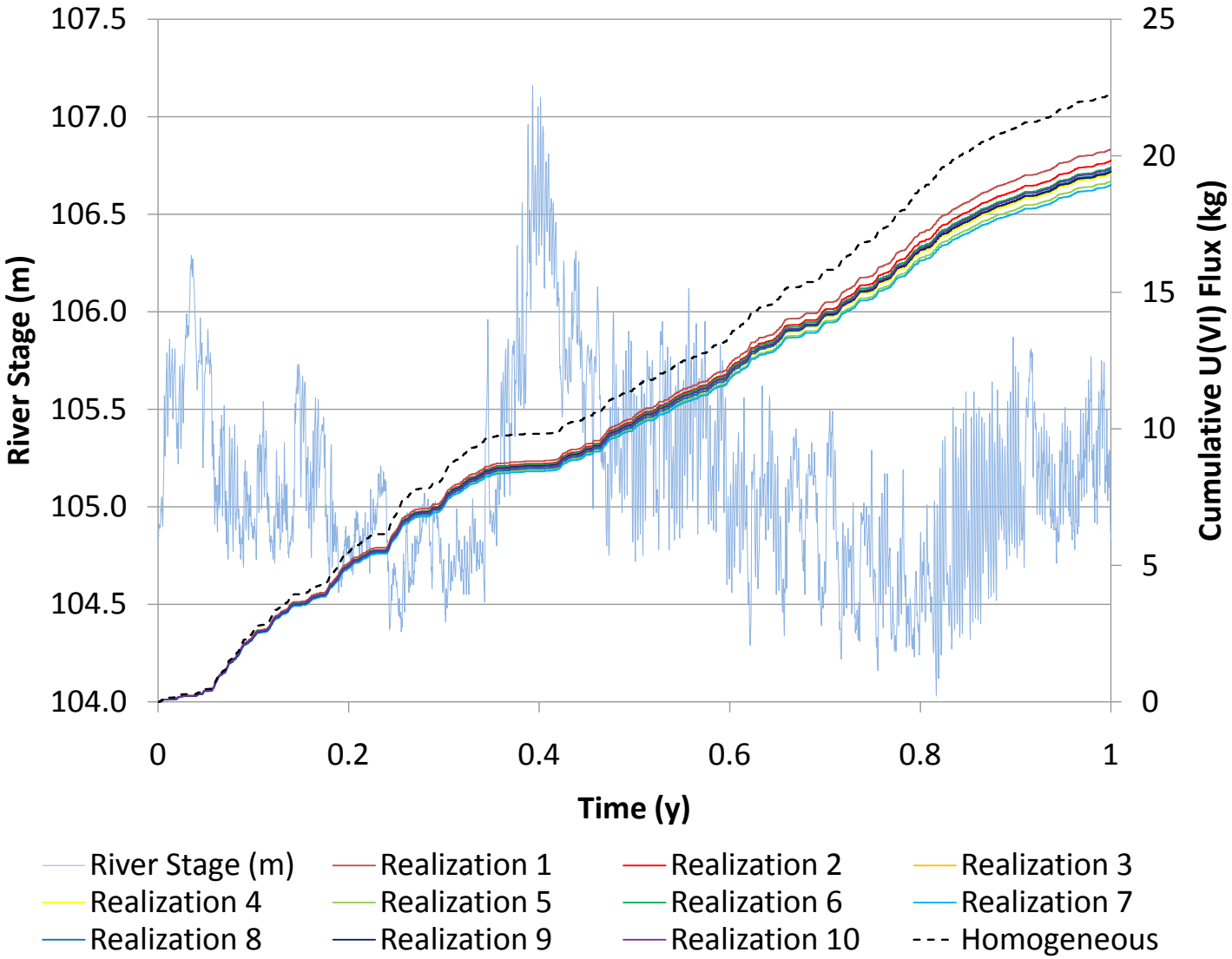
Predicted U(VI) & H_2O Flux to Columbia River



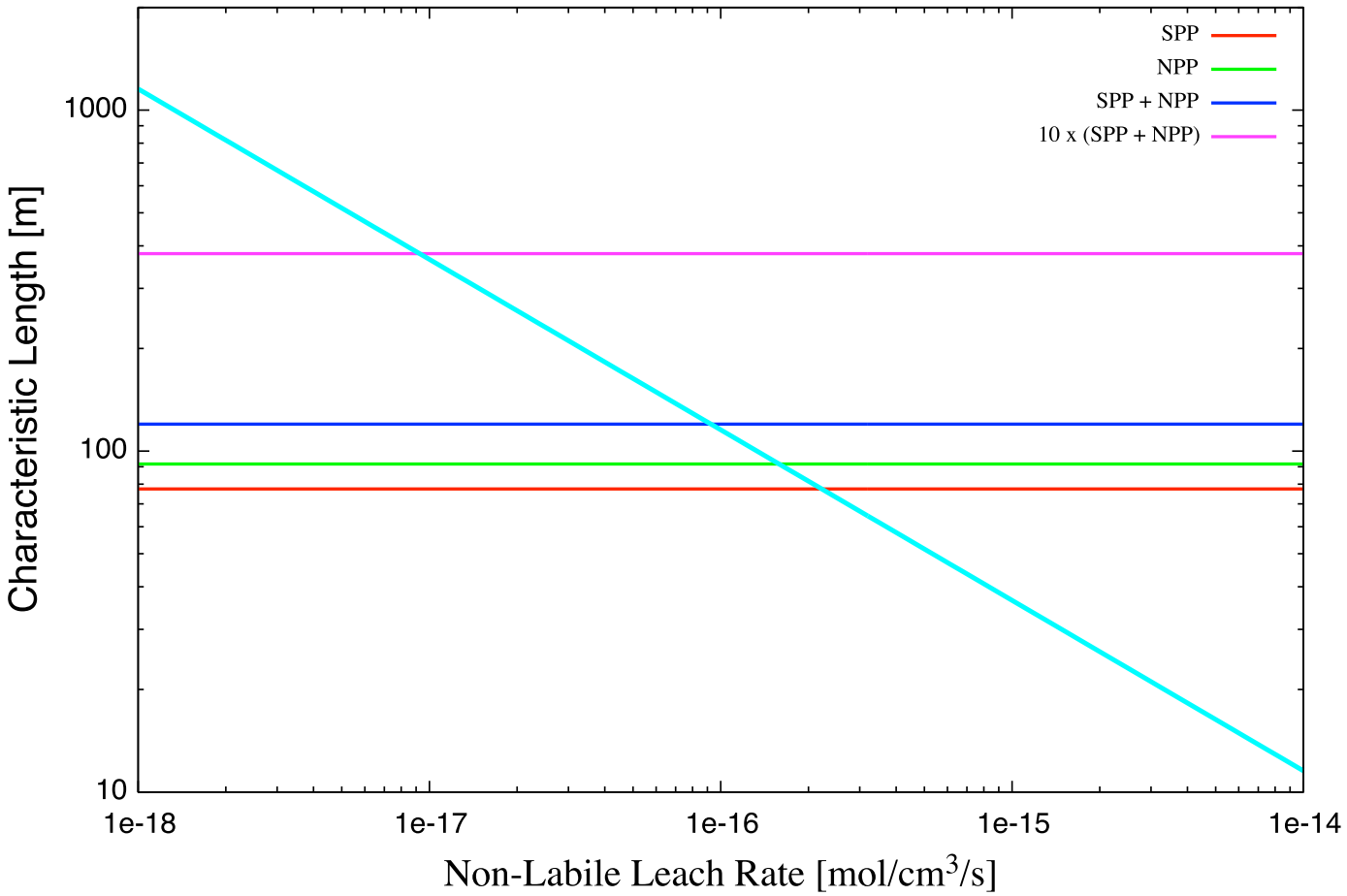




Heterogeneity

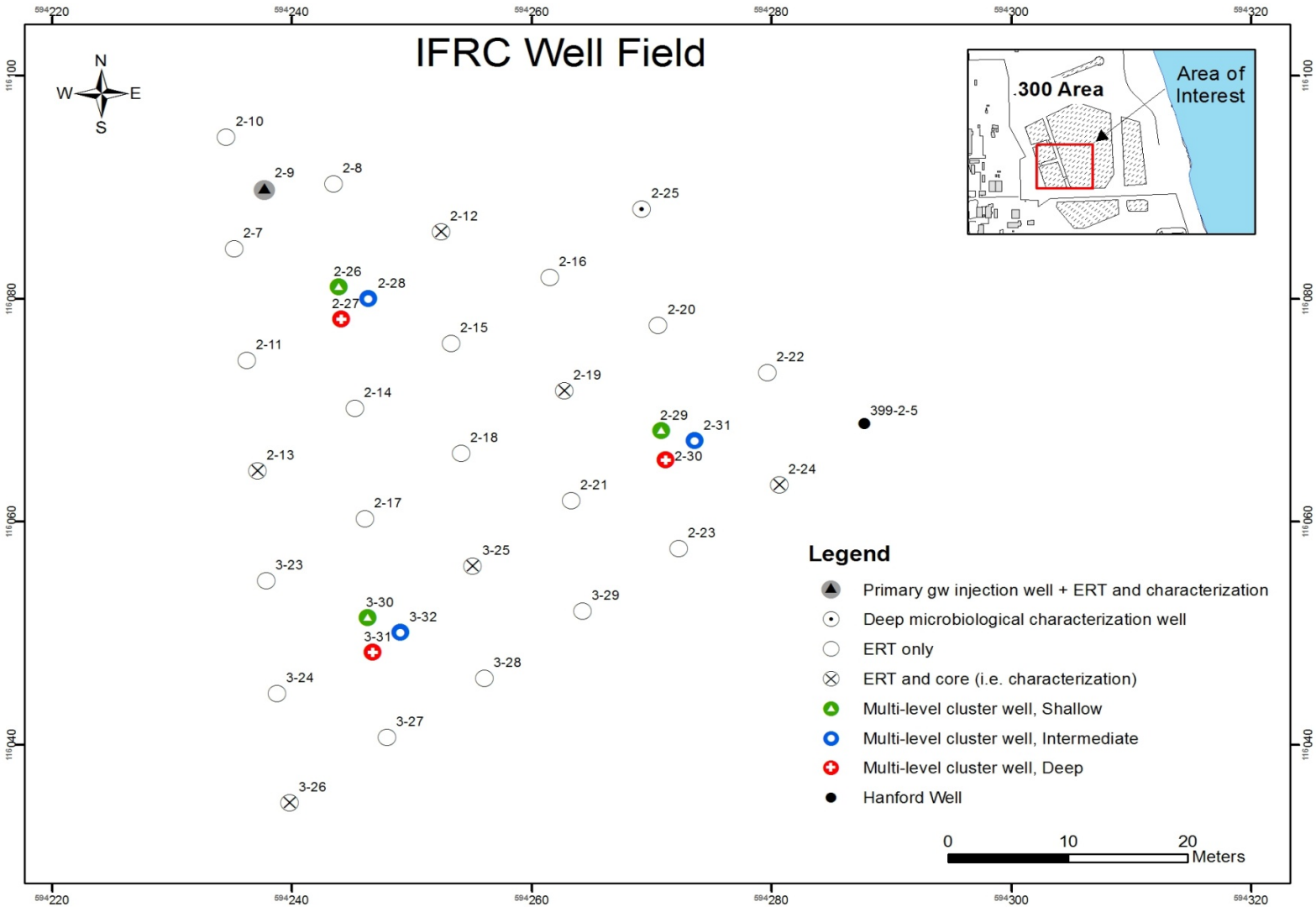


Global Mass Conservation: Non-Labile Leach Rate



50 kg/year U(VI) flux into Columbia River: $\mathcal{R} = V \cdot \mathcal{L}$

IFRC Site


IFRC Well Field
N
W
E
S
.300 Area
Area of Interest
2-10
2-9
2-8
2-25
2-12
2-7
2-16
2-26
2-28
2-27
2-20
2-15
2-11
2-22
2-19
2-14
399-2-5
2-29
2-31
2-18
2-13
2-30
2-24
2-21
2-17
2-23
3-25
3-23
3-29
3-30
3-32
3-31
3-28
3-24
3-27
3-26
Legend
Primary gw injection well + ERT and characterization
Deep microbiological characterization well
ERT only
ERT and core (i.e. characterization)
Multi-level cluster well, Shallow
Multi-level cluster well, Intermediate
Multi-level cluster well, Deep
Hanford Well
0
10
20
Meters

Modeling Site-Scale IRFC Experiments using Plume-Scale Domain

- **Embed IFRC site in plume-scale domain using AMR**
- **Boundary conditions:**
  - Account for hourly river fluctuations
  - Triangulate data from wells 399-8-1, 6-1, & 4-1
- **Multicomponent chemistry:**
  Na-K-Ca-Fe-Mg-Br-N-CO_2-P-S-Cl-Si-U-Cu-H_2O
  ($\sim$15 primary species)
- **Incorporate highly heterogeneous sediments** (fine sand, silt, coarse gravels, cobbles)
- **Include multiscale processes** (μm–m)

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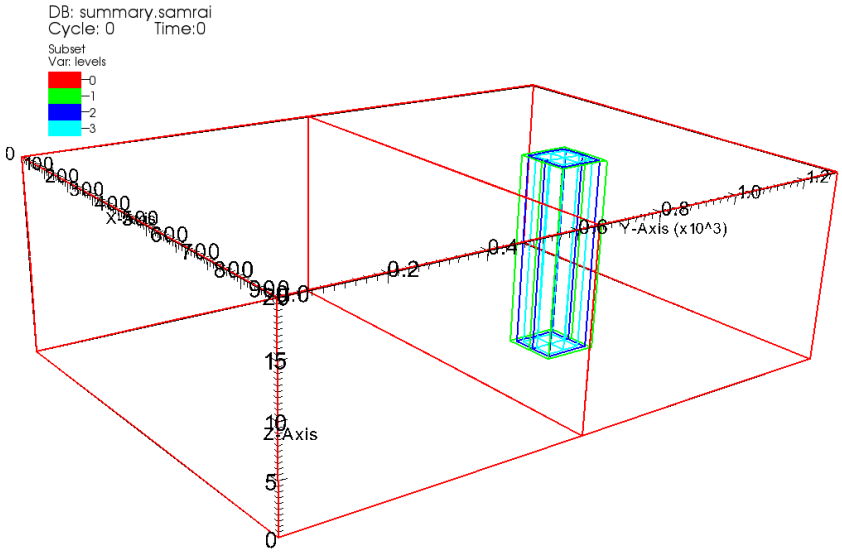
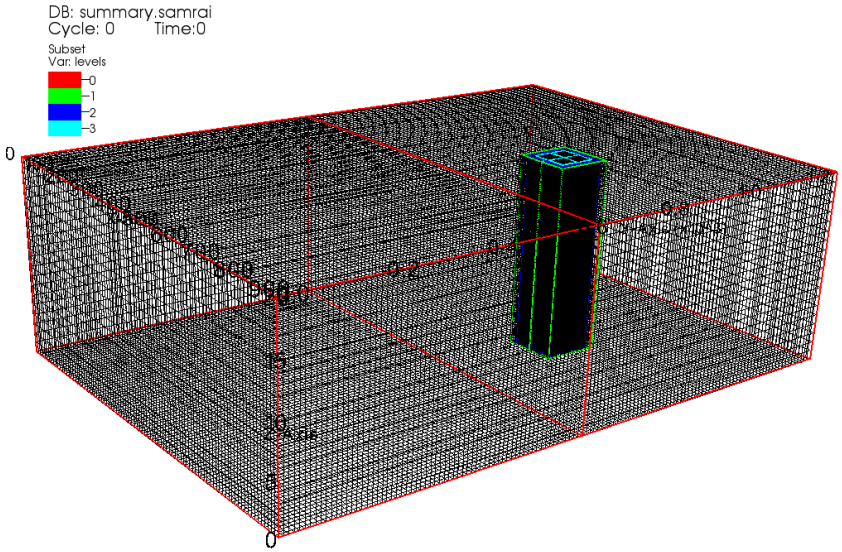
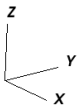
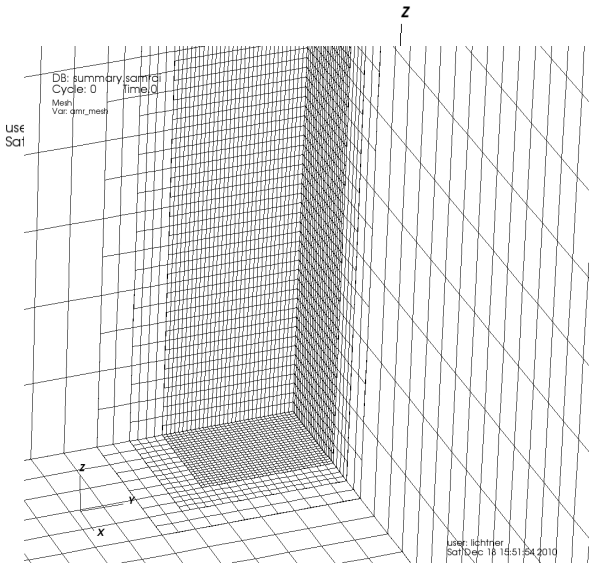
IFRC Site Model: SAMRAI Grid









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Sat Dec 18 14:16:10 2010

SAMRAI Grid Statistics

GRID STATISTICS	N_{dof}
Total DOF:	939,600
Total Relative Number of DOF:	0.0078
DOF, level 3:	655,360
DOF, level 2:	46,080
DOF, level 1:	7,040
DOF, level 0:	231,120
Grid points, level 3:	655,360
Grid points, level 2:	128,000
Grid points, level 1:	23,040
Grid points, level 0:	234,000

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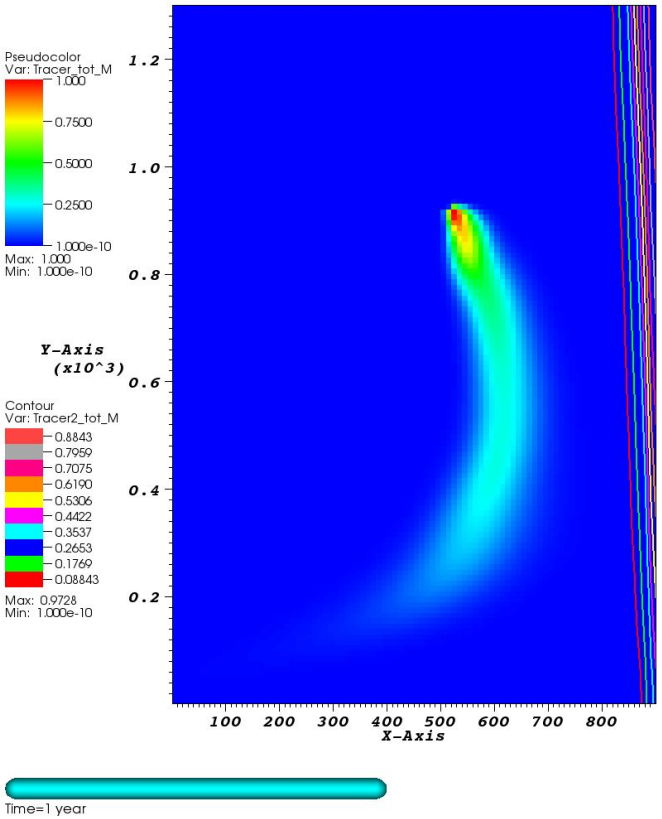
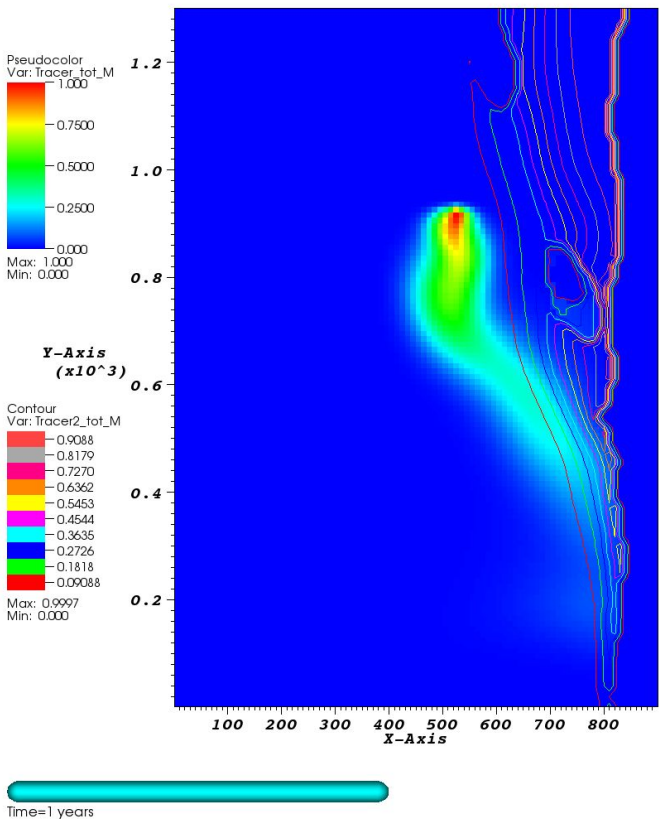
Tracer Injection Plume at Well 399-2-9



Time=1 year



Time=1 years

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Sun Jan 16 10:05:48 2011

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Future Directions

- Apply AMR to IFRC experiments with concurrent river stage and inland well data
- Use site-scale IFRC experiments to calibrate plume-scale model
- Implement heterogeneous U(VI) distribution, permeability and porosity fields
- Estimate non-labile U(VI) leach rate
- Use multiple continuum model explicit diffusion pathway with sorption/mineral dissolution/precipitation

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