Cleaning Up the Cold War: Simulating Uranium Migration at the Hanford 300 Area

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SciDAC 2010

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Chattanooga, TN

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MOTIVATION

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Motivation Behind Subsurface Simulation

- DOE currently facing:
  - Expensive cleanup of contaminated sites
  - Accelerated development schedule for alternative energy
- Benefits of subsurface simulation to DOE:
  - Evaluation of environmental impact and viability of alternative energy sources
  - Evaluation of remediation alternatives
  - Reduced cleanup costs
  - Reduced liability to stakeholders

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Characteristics of the Subsurface Geosciences Problems

- Multi's
  - Multiprocess: physical, biological and geochemical (2-4)
  - Multiphase (e.g. 2-3)
  - Multiscale/Multicontinuum (e.g. 10-100)
  - Multicomponent (e.g. 10-20)
  - Multirealization (e.g. 1000-10,000)
    - Stochastic simulation
    - Uncertainty quantification
- Discretization of governing PDEs results in the solution of large tightly-coupled nonlinear systems of equations

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HANFORD 300 AREA

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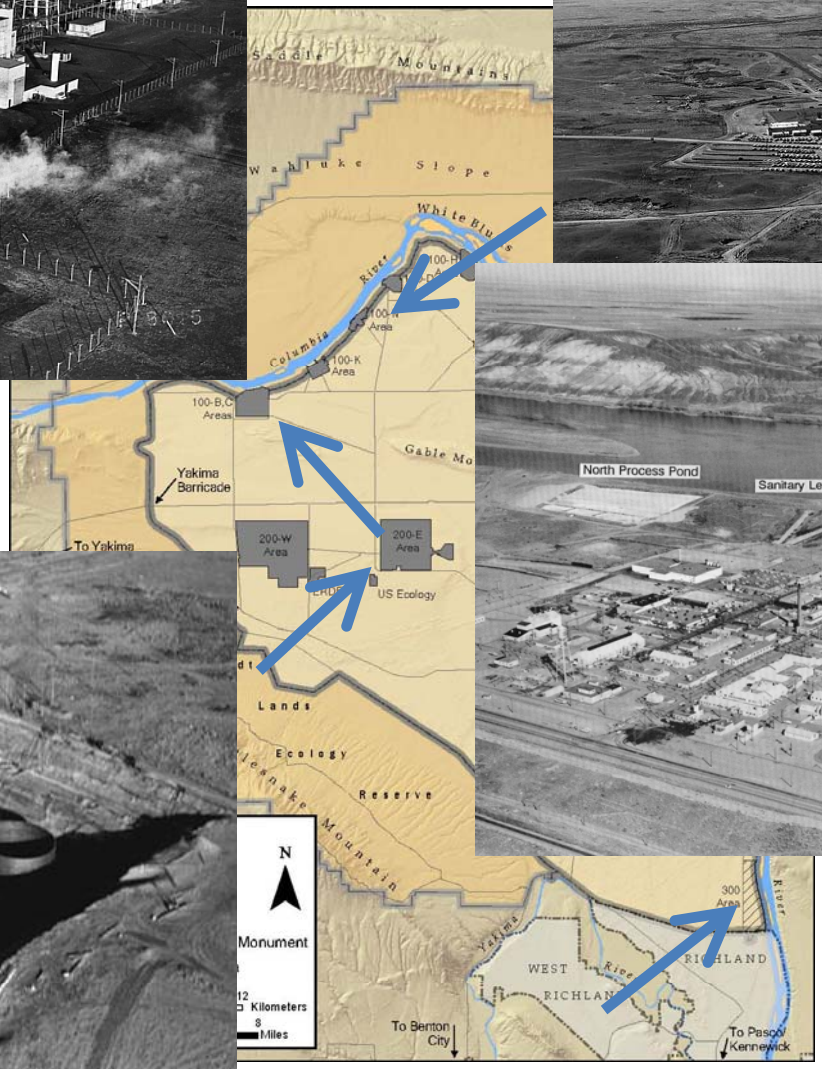
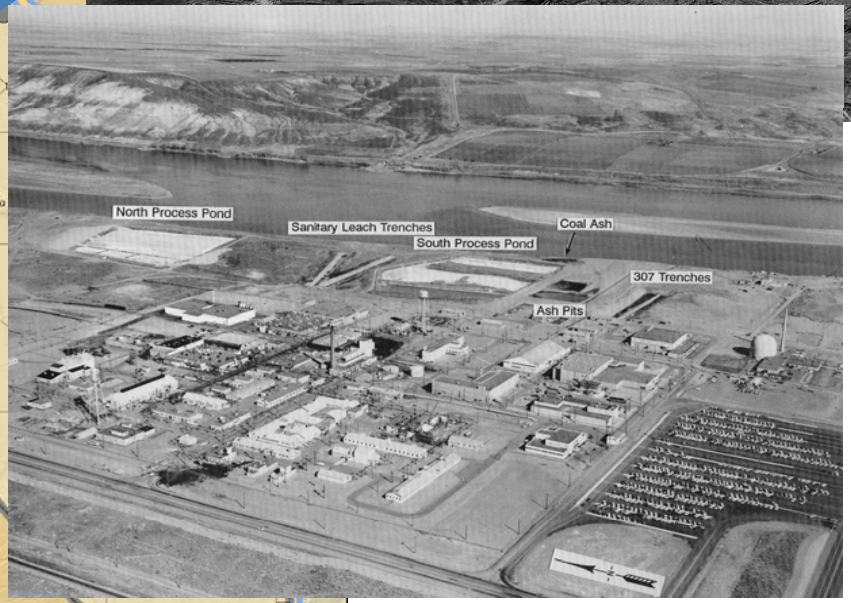
ashingto





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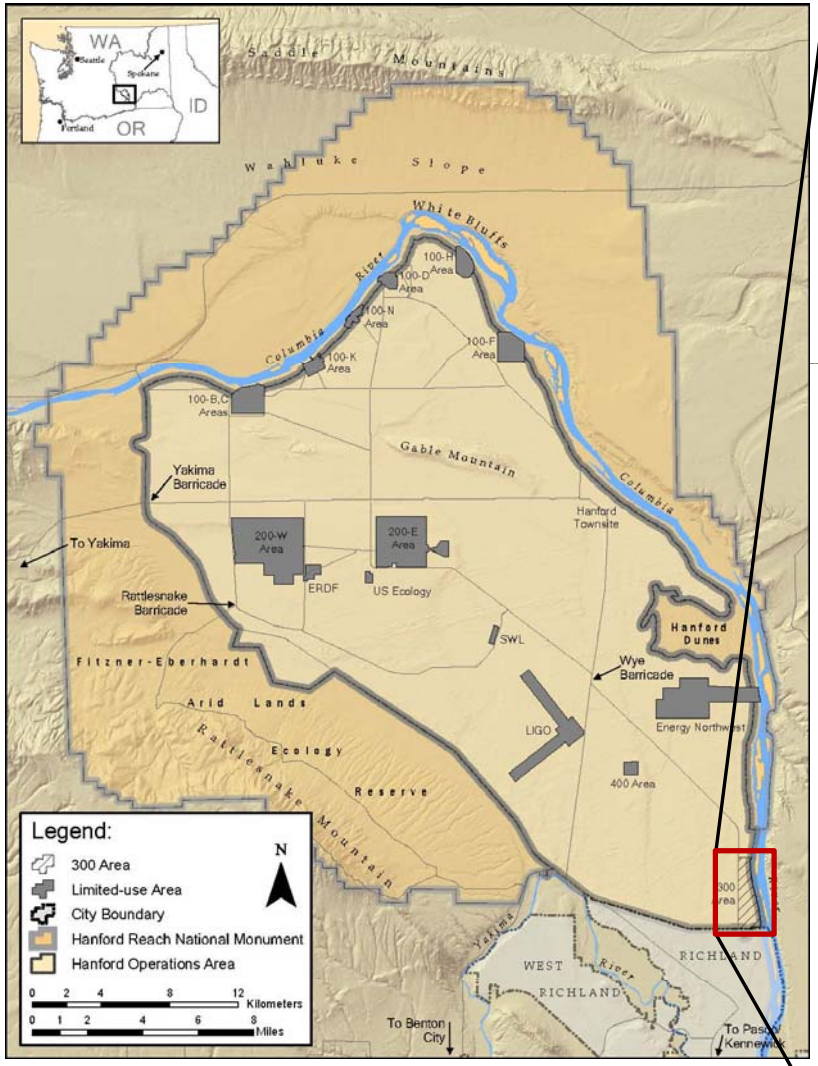
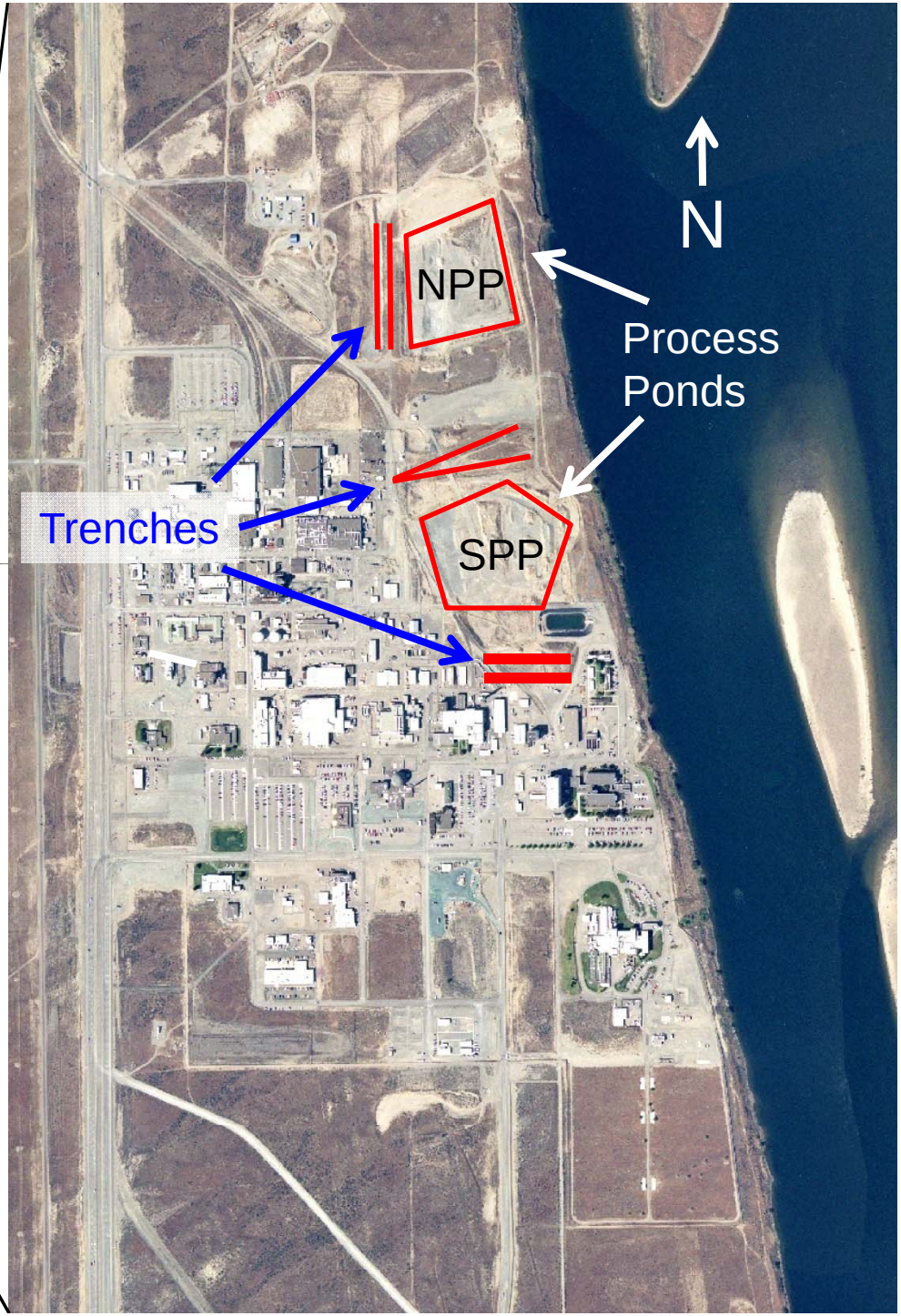
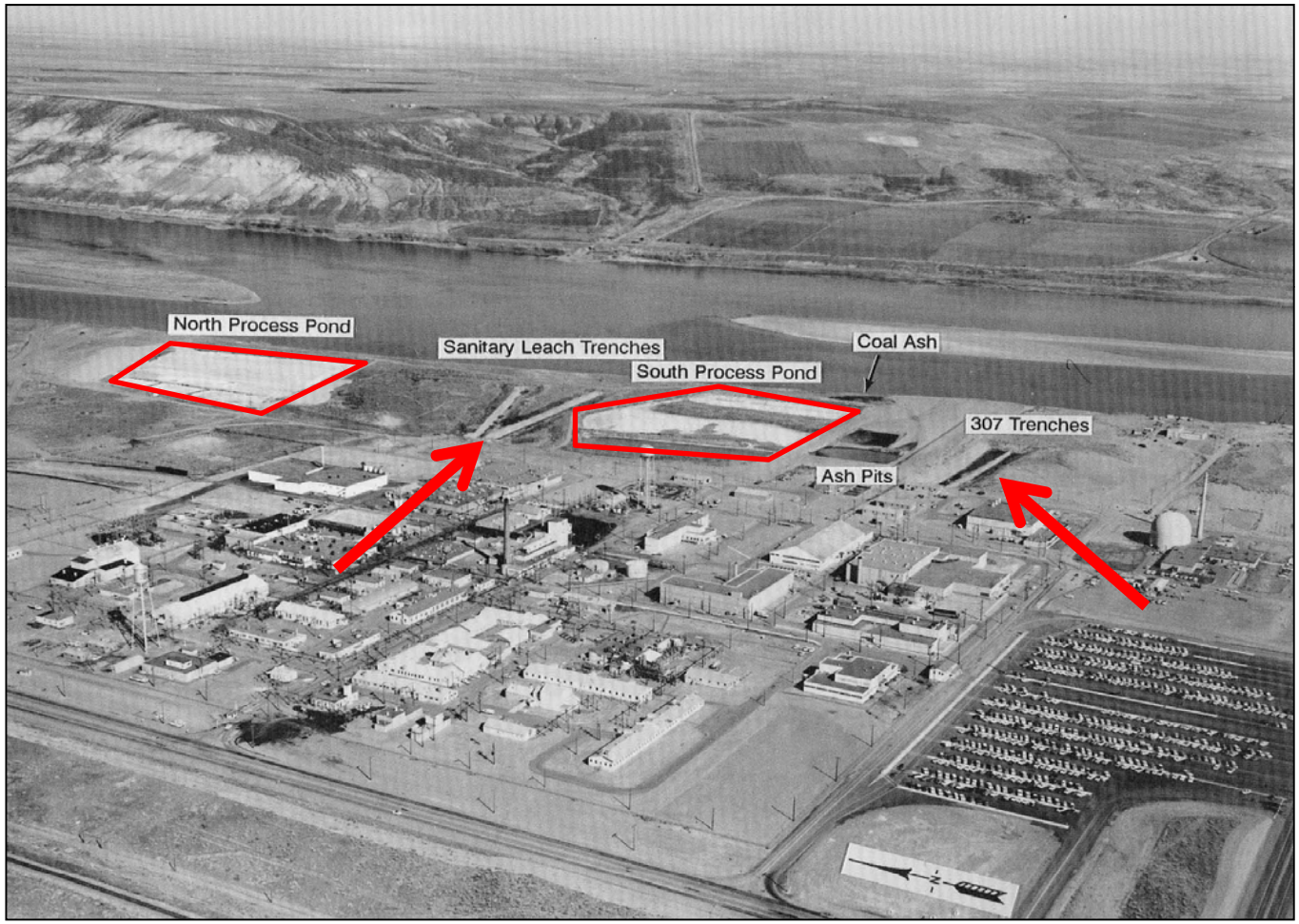
Hanford 300 Area



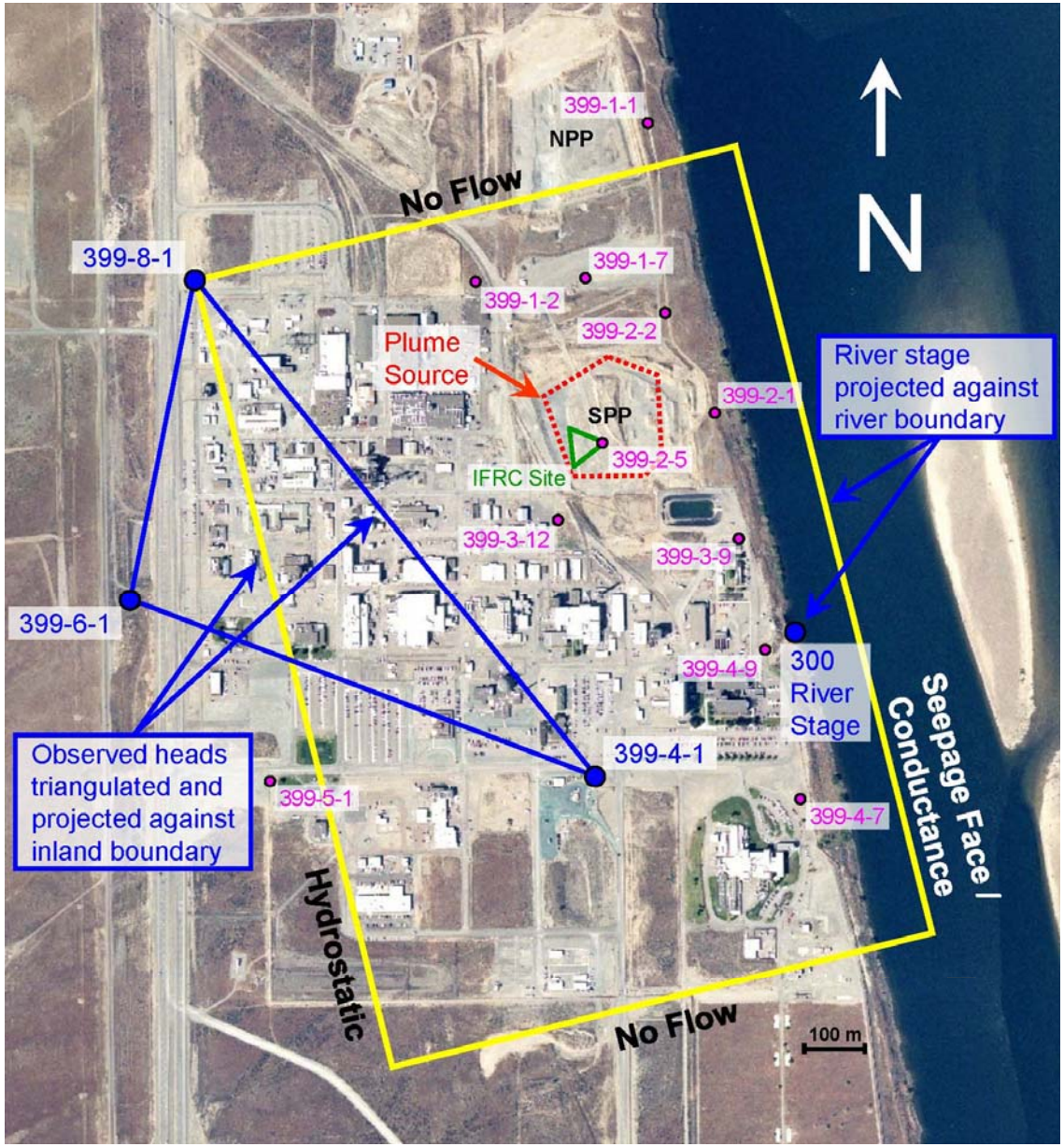


Hanford 300 Area: ~1962

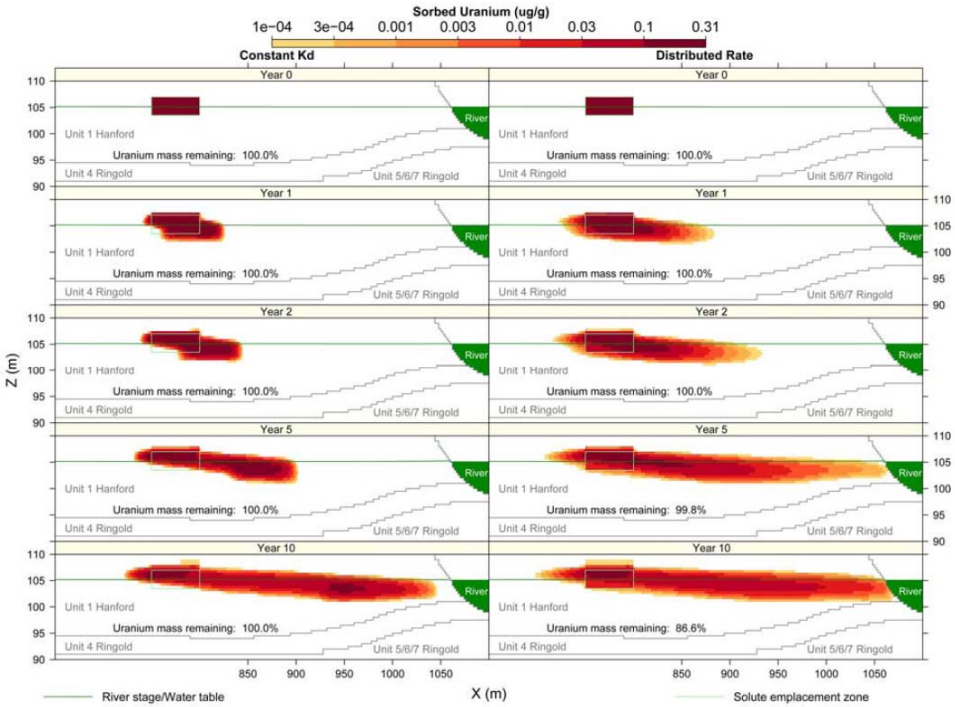


Hanford 300 Area Conceptual Model

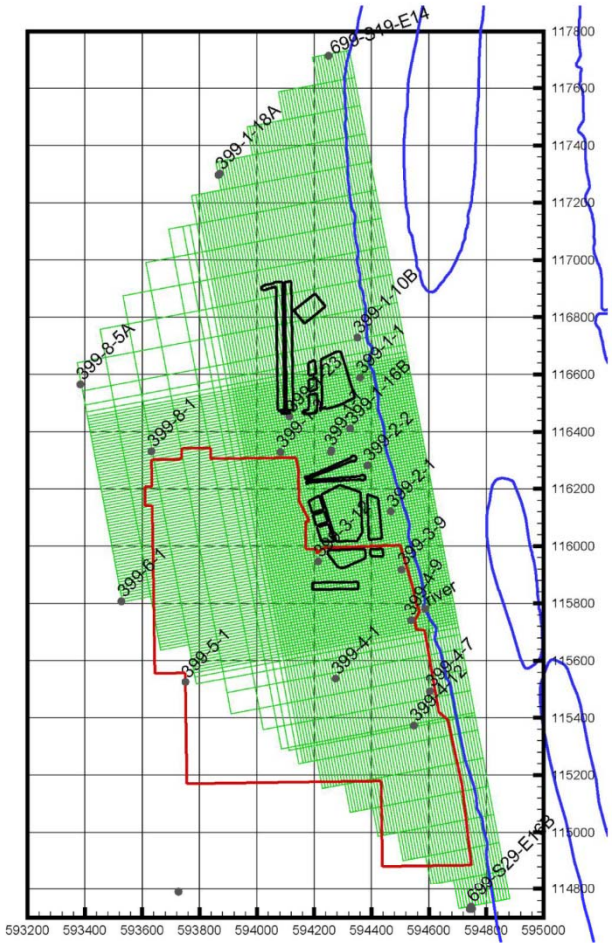
- Problem domain:
  - 900×1300×20m
  - $\Delta x/\Delta y = 5$ m
  - $\Delta z = 0.5$ m
  - 1.87M grid cells
  - 15 chemical species
  - 28M dofs total
- 1-year simulation:
  - $\Delta t = 1$ hour
- Computing
  - 4096 cores (single realization)
  - 40960 cores (10 realizations)
  - 5-10 hour runtime



Previous 2D/3D Simulations of the 300 Area

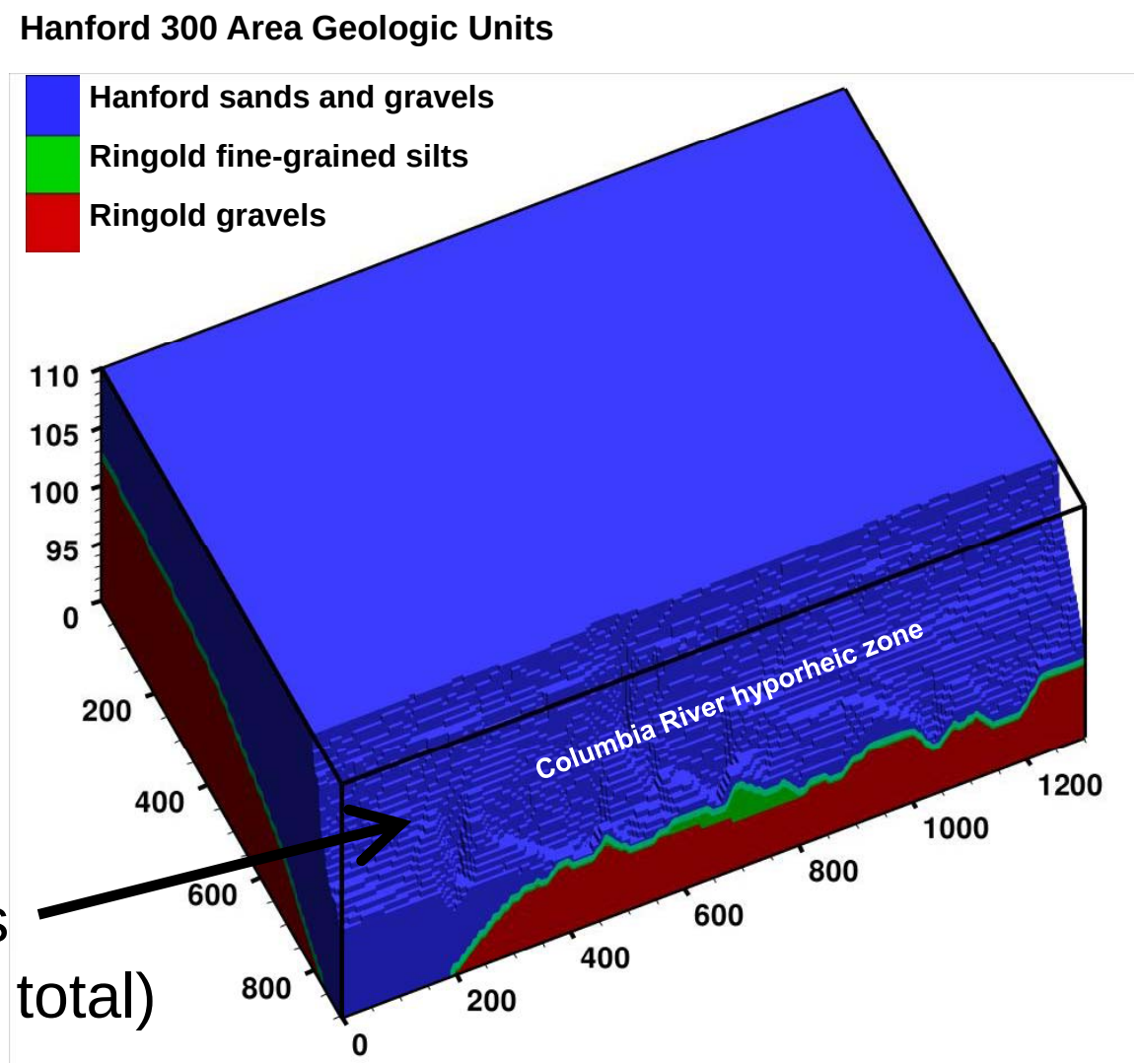


Yabusaki et al., 2008



Williams et al., 2008

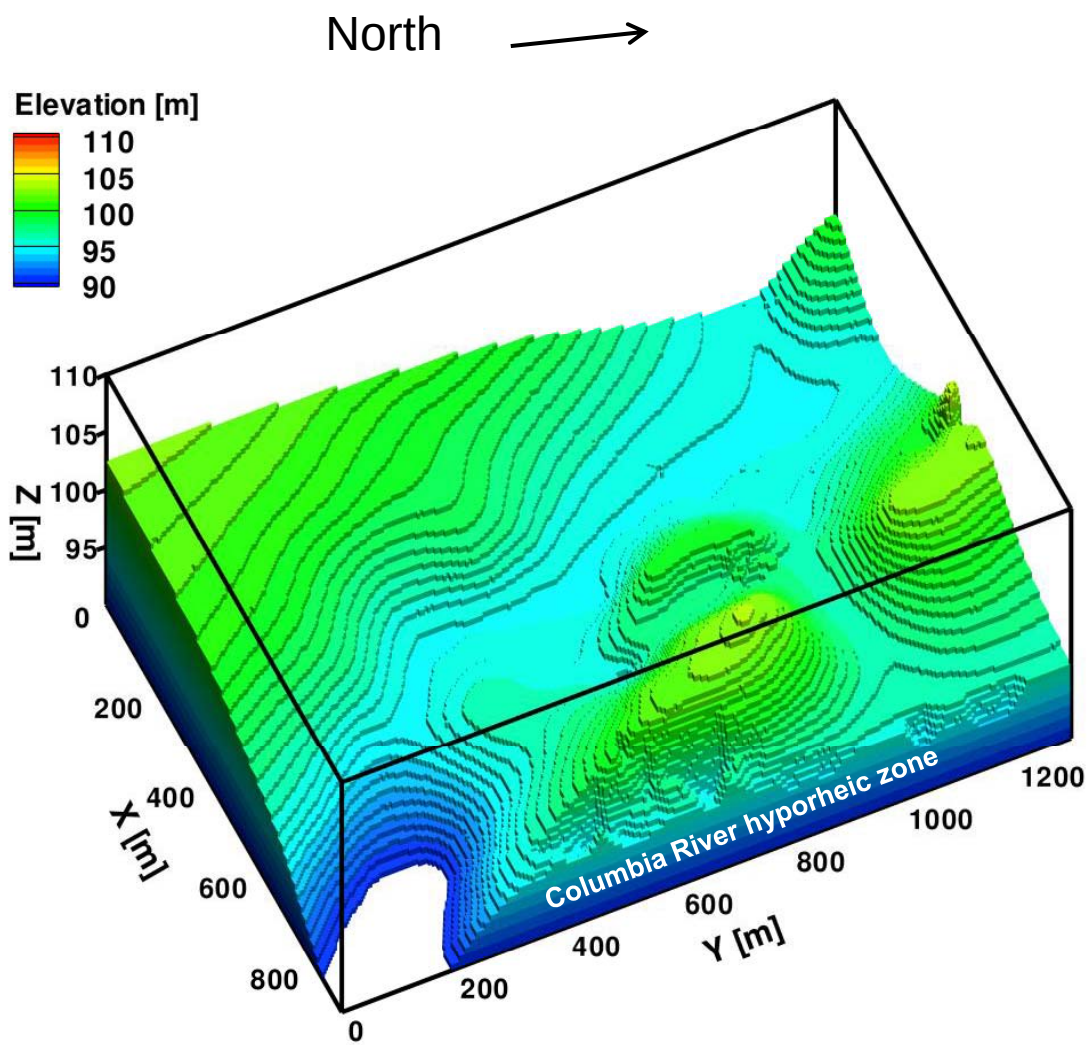
Hanford 300 Area: Geology



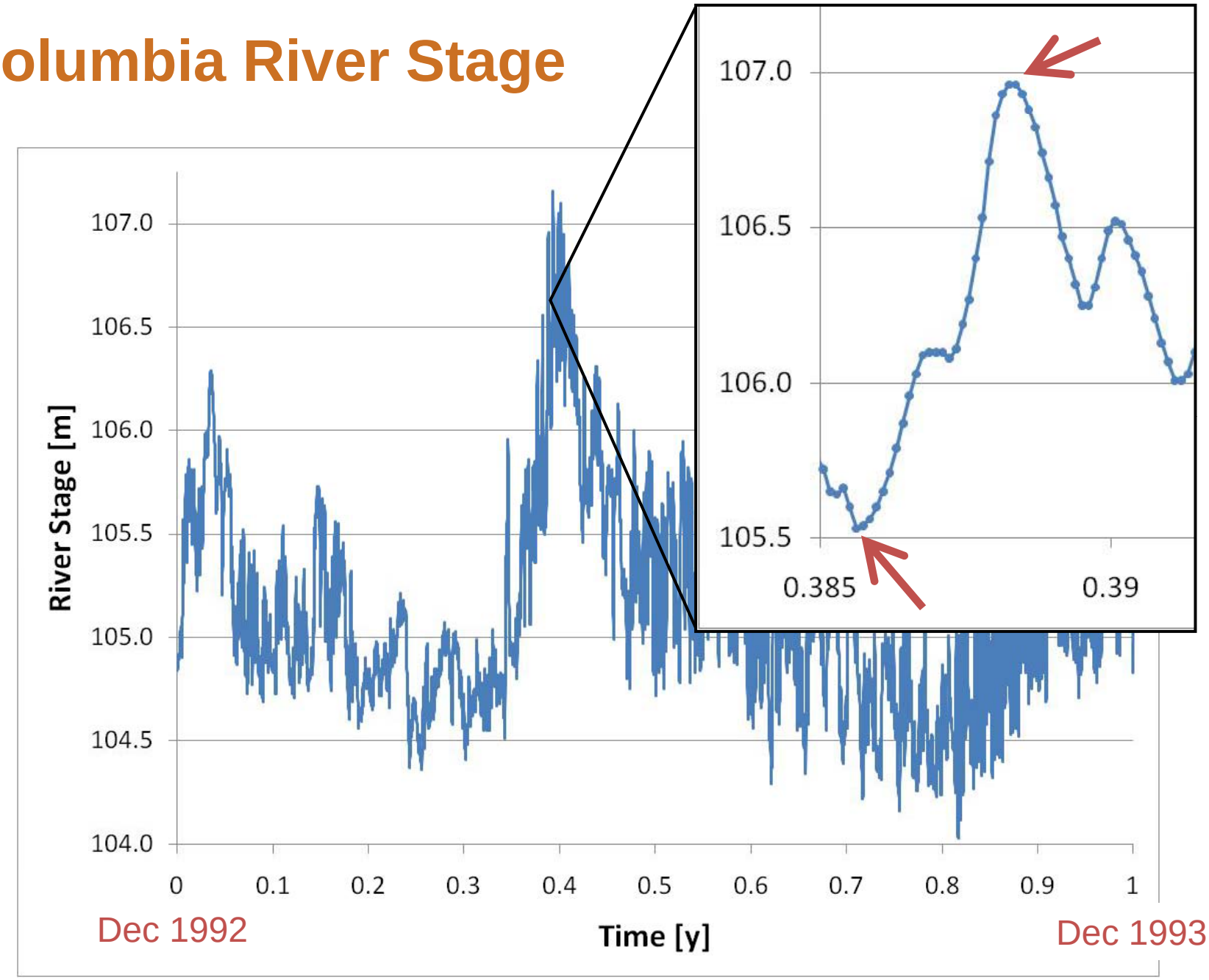
Inactive grid cells (6-7% of total)

Hanford 300 Area: Representative Excavation

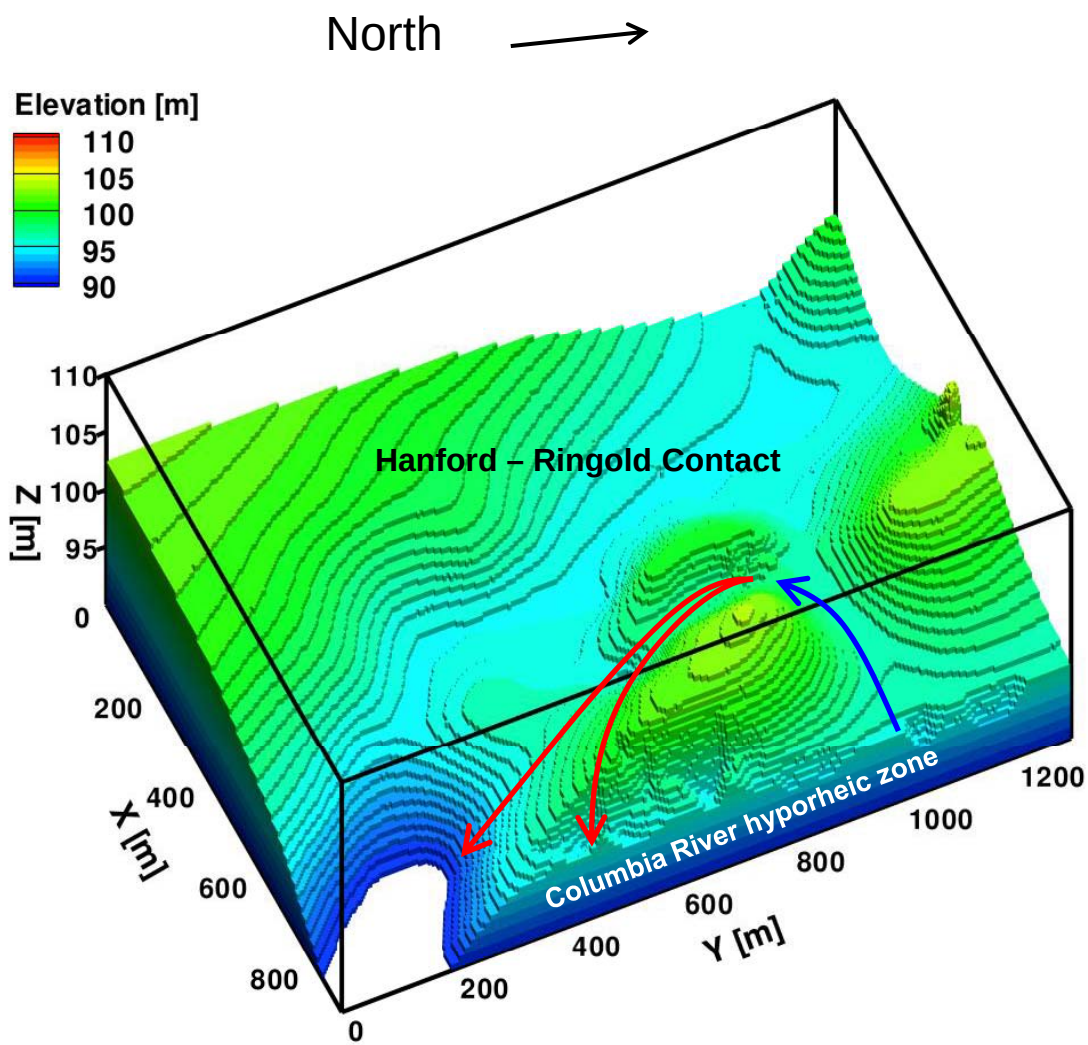
Hanford – Ringold Contact



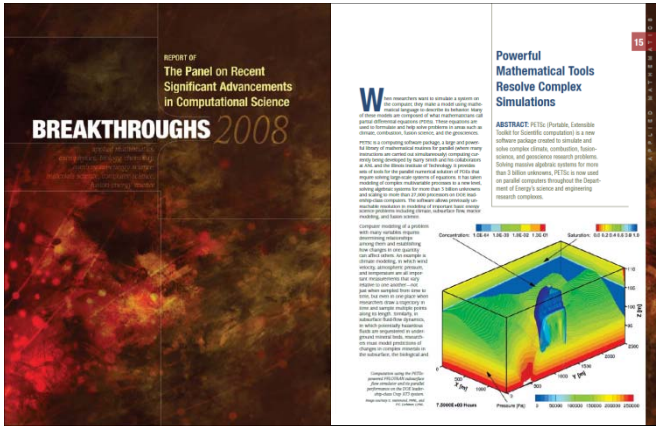
Columbia River Stage



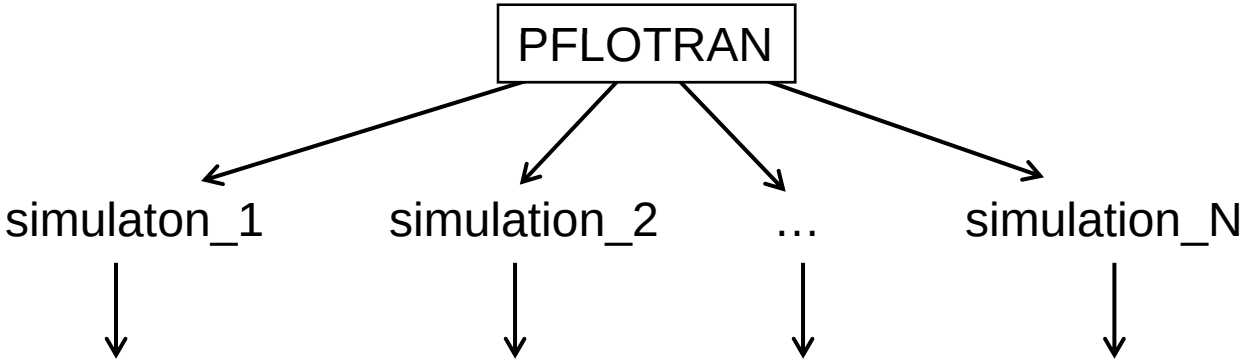
River – Groundwater Interaction



PFLOTRAN



- Petascale reactive multiphase flow and transport code
- Object-oriented Fortran9X, parallel HDF5 IO, PETSc
- Adaptive mesh refinement through SAMRAI
- Demonstrated performance:
  - Maximum # processor cores: 131,072 (ORNL's Jaguar)
  - Maximum problem size: 2 billion degrees of freedom
- Multi-realization simulation capability



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PFLOTRAN
Governing Equations

- Variably-saturated flow (laminar Darcy flow)

$$\frac{\partial}{\partial t}(\varphi s \rho) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{q}) = Q_w$$

$$\boldsymbol{q} = -\frac{k k_r}{\mu} \boldsymbol{\nabla} (P - \rho g z)$$

- Geochemical transport

$$\frac{\partial}{\partial t}(\varphi s \Psi_j + \Psi_{S,j}) + \boldsymbol{\nabla} \cdot \boldsymbol{\Omega}_j = -\sum_m \nu_{jm}^{\min} I_m$$

$$\boldsymbol{\Omega}_j = (\boldsymbol{q} - \varphi s D \boldsymbol{\nabla}) \Psi_j$$

$$\Psi_j = C_j + \sum_{i=1}^{N_X} \nu_{ji} (\gamma_i)^{-1} K_i \prod_{j'=1}^{N_c} (\gamma_{j'} C_{j'})^{\nu_{j'i}}$$

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Hanford 300 Area Conceptual Model: Geochemistry

- 15 primary aqueous species (28 M degrees of freedom):

  H^+, Ca^{2+}, Cu^{2+}, Mg^{2+}, UO_2^{2+}, K^+, Na^+, HCO_3^-, Cl^-, F^-, HPO_4^{2-}, NO_3^-, SO_4^{2-} and 2 tracers

- 88 secondary aqueous complexes

  $CaUO_2(CO_3)_3^{2-}$, $Ca_2UO_2(CO_3)_{3(aq)}$ (dominant U(VI) species)

- 2 surface complexes with surface site $>SOH$

  $>SOUO_2OH$, $>SOHOU_2CO_3$ (Bond et al. 2007)

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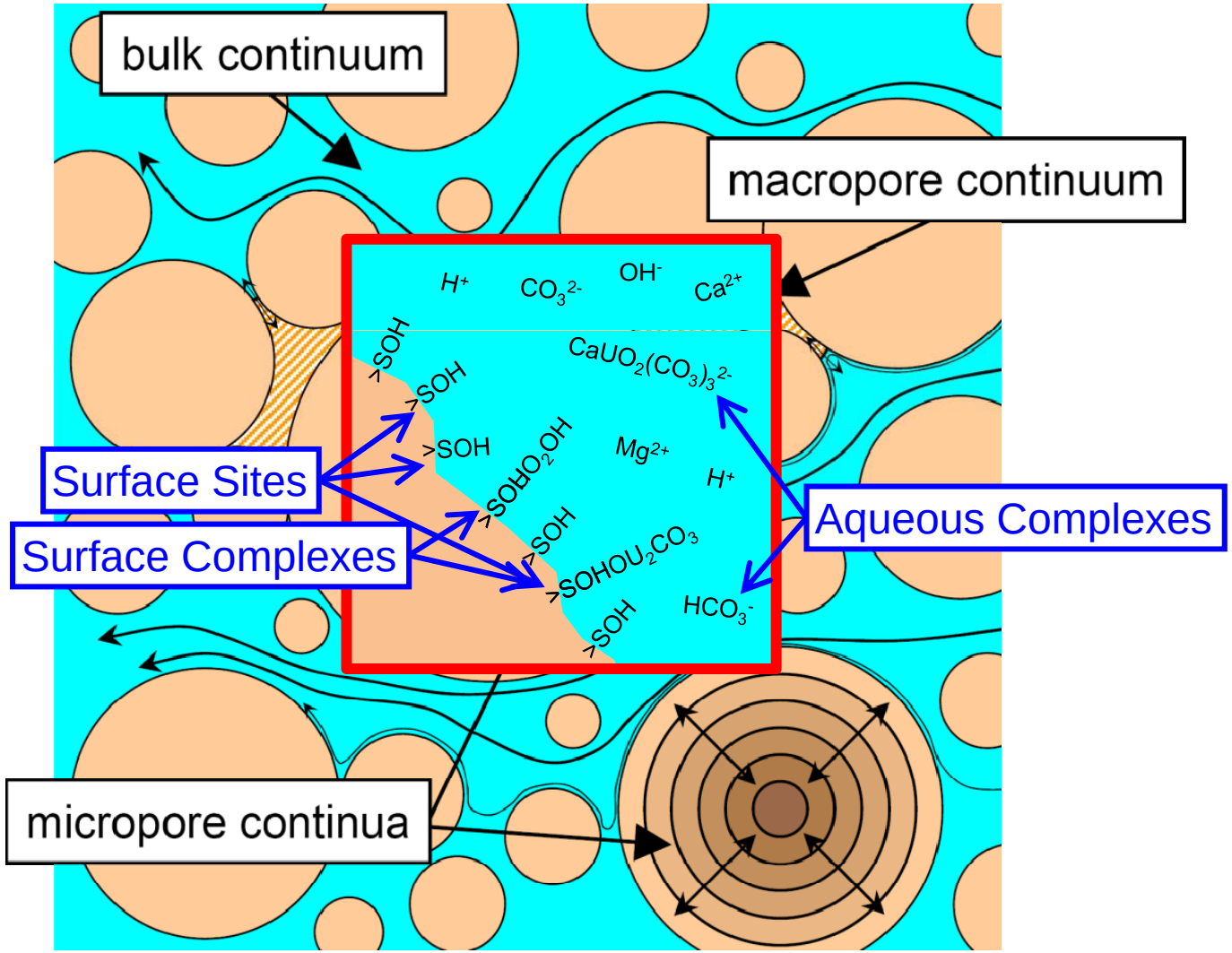
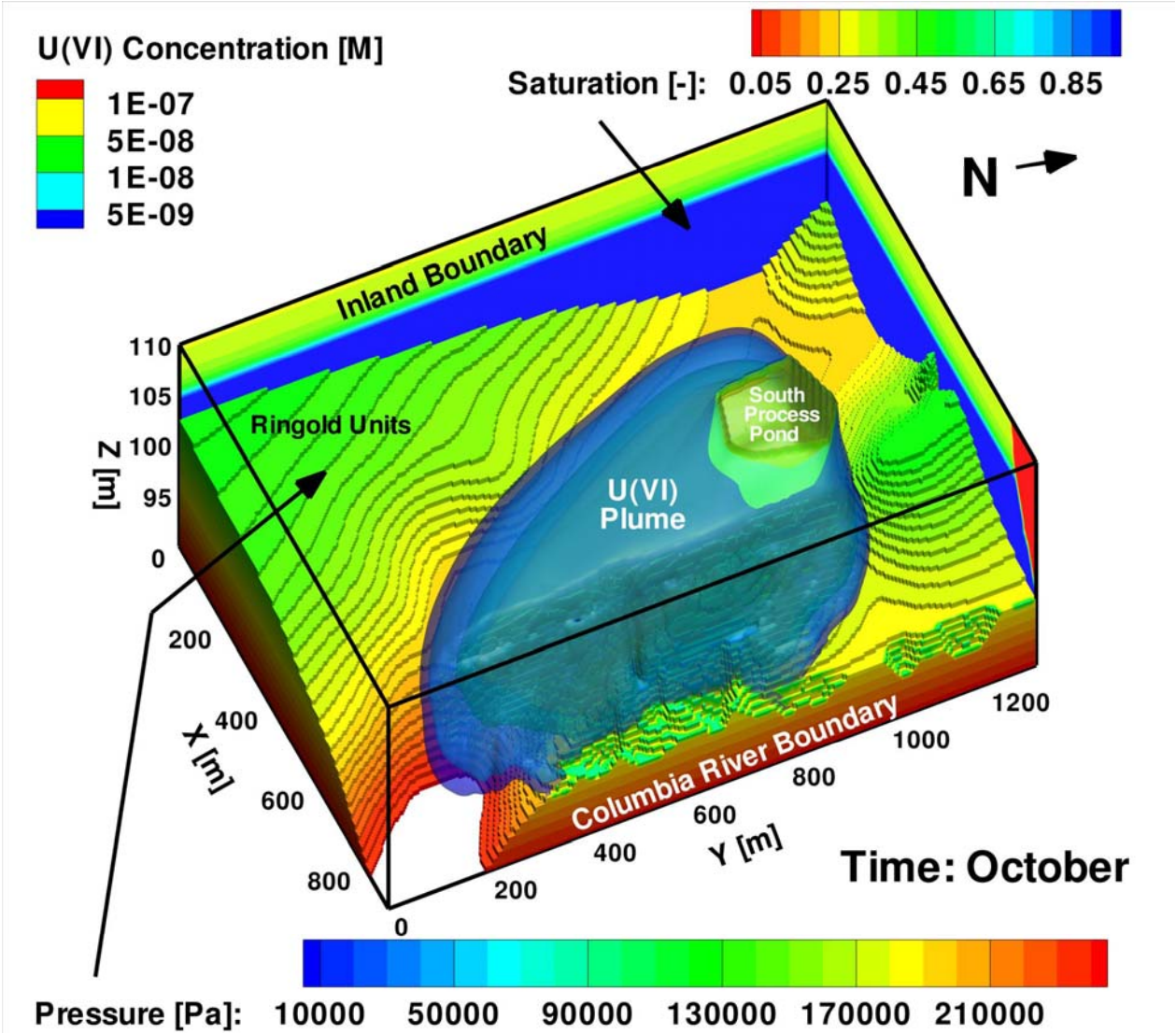
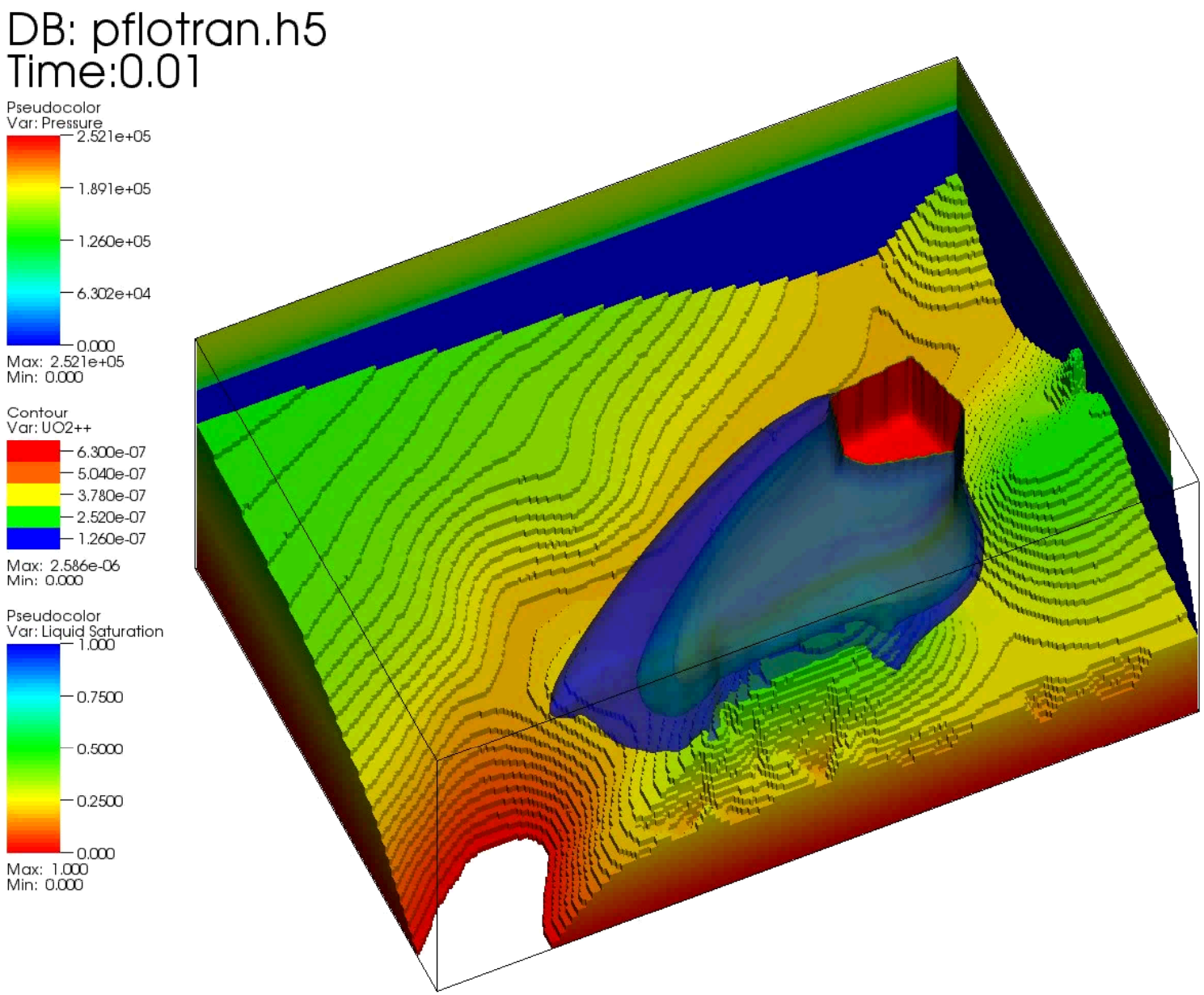
Surface Complexation



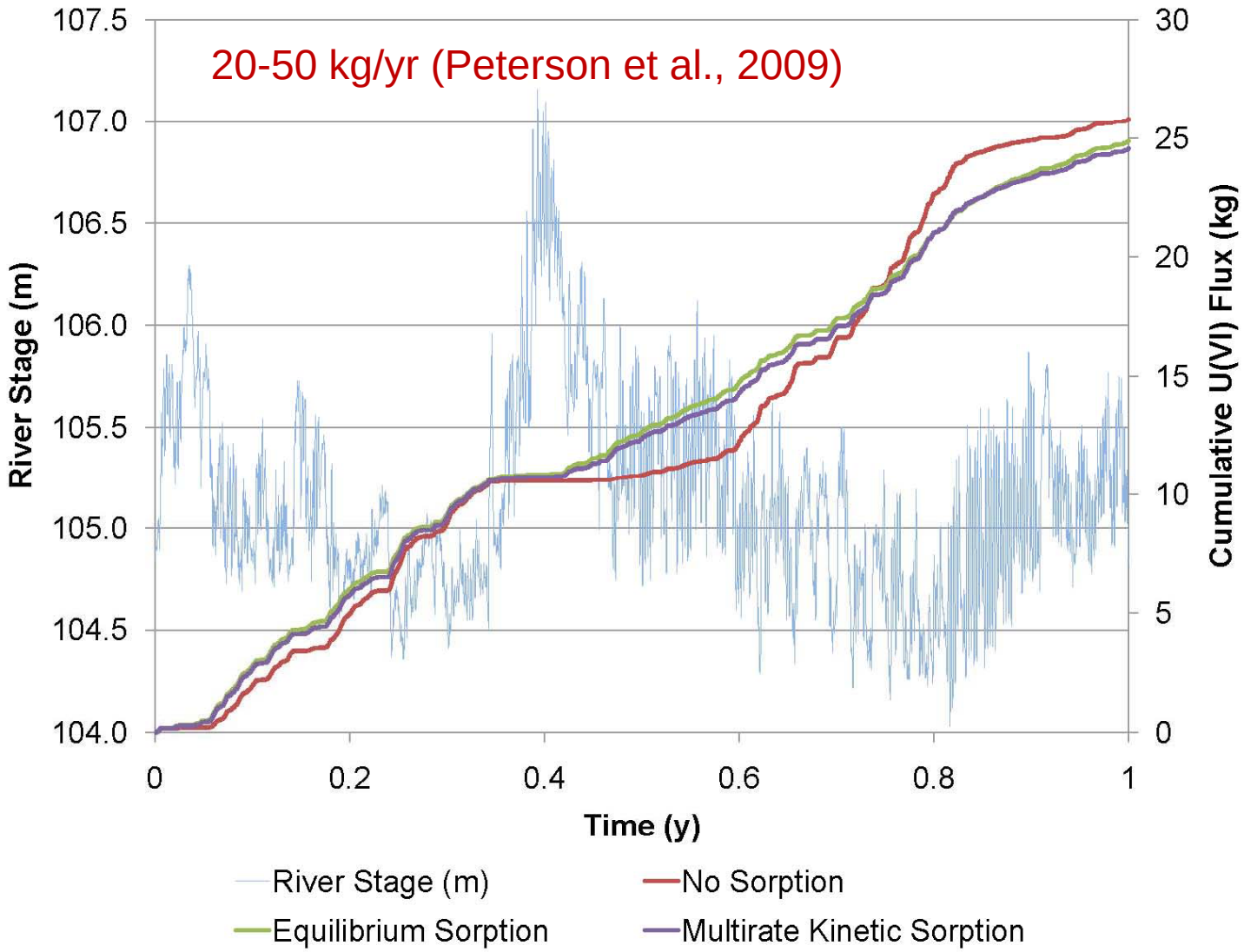
Hanford 300 Area Plume (October Timeframe)



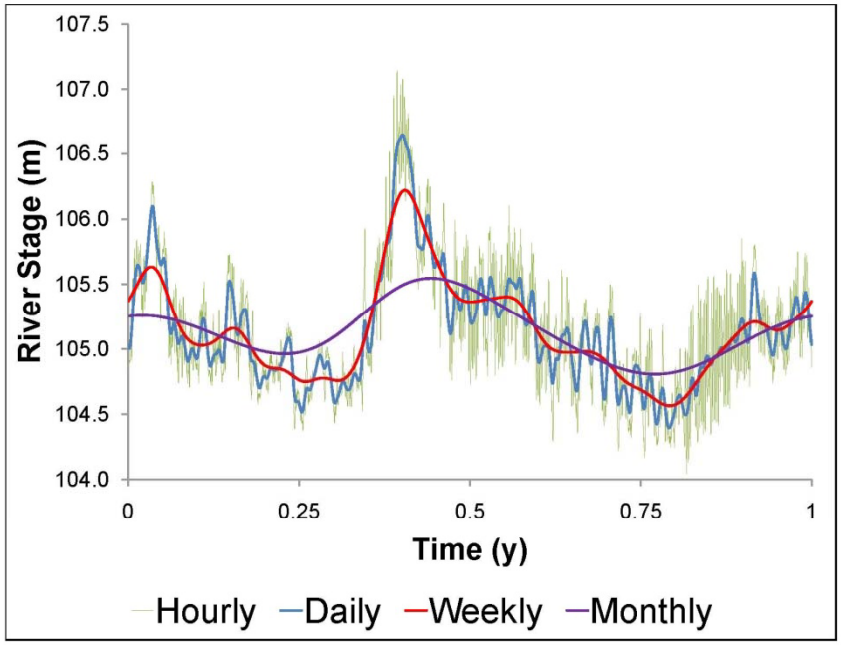

DB: pflotran.h5
Time:0.01
Pseudocolor
Var: Pressure
2.521e+05
1.891e+05
1.260e+05
6.302e+04
0.000
Max: 2.521e+05
Min: 0.000
Contour
Var: UO2++
6.300e-07
5.040e-07
3.780e-07
2.520e-07
1.260e-07
Max: 2.586e-06
Min: 0.000
Pseudocolor
Var: Liquid Saturation
1.000
0.7500
0.5000
0.2500
0.000
Max: 1.000
Min: 0.000

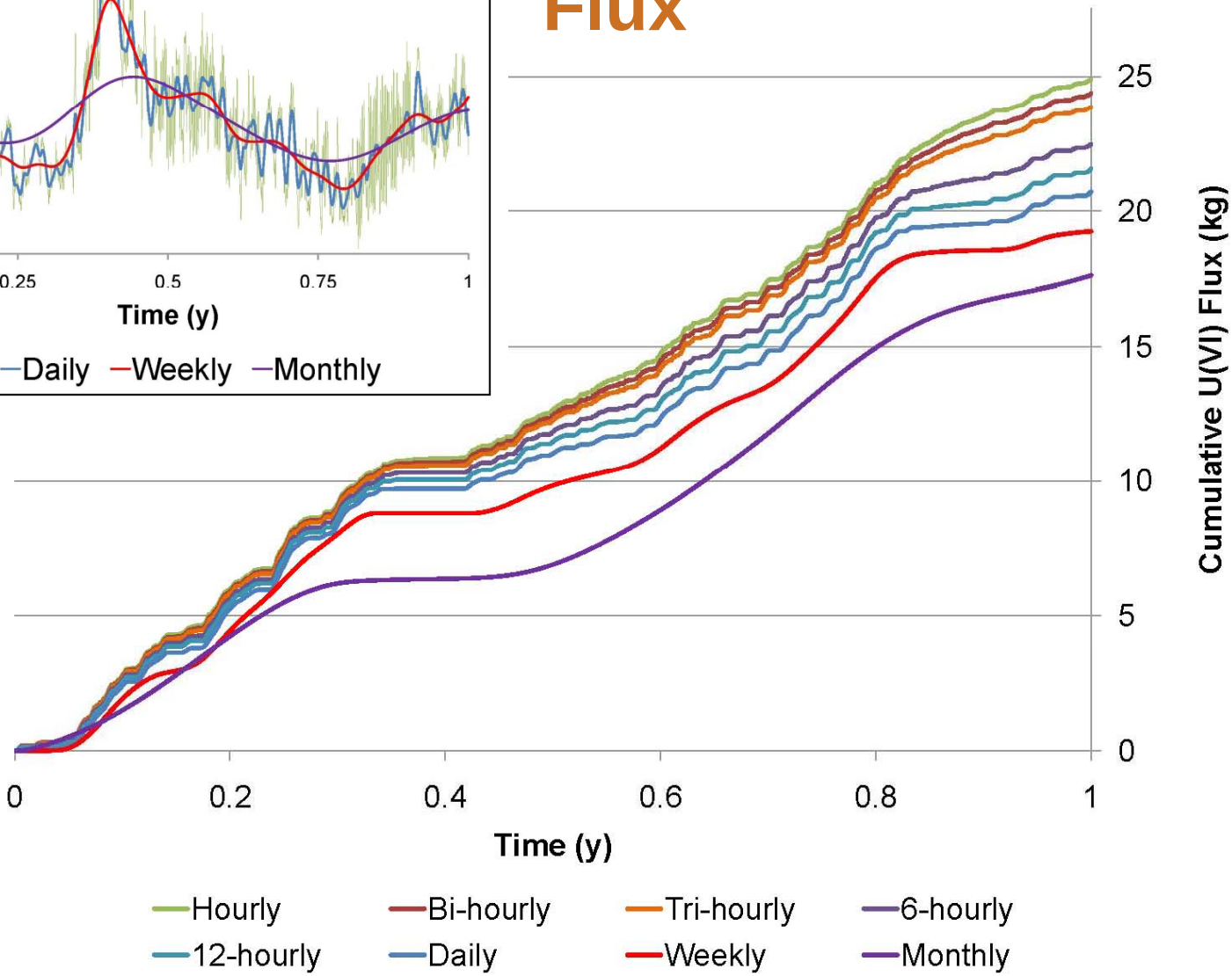
Cumulative U(VI) Flux to Columbia River

(Hammond and Lichtner, Water Resources Research, 2010)



Effect of Smoothing River Stage on U(VI) Flux





Motivation for Stochastic Simulation of the Hanford 300 Area

- U(VI) migration at site is highly sensitive to:
  - transient groundwater flow velocities
  - transient, directional K_Ds
- Groundwater flow plays key role in U(VI) migration
  - Hydrology well-constrained at boundaries
  - Uncertainty in magnitude and distribution of internal velocities
- Stochastic simulations enable:
  - Incorporation of site-specific permeability data
  - Better quantification of flow velocity uncertainty

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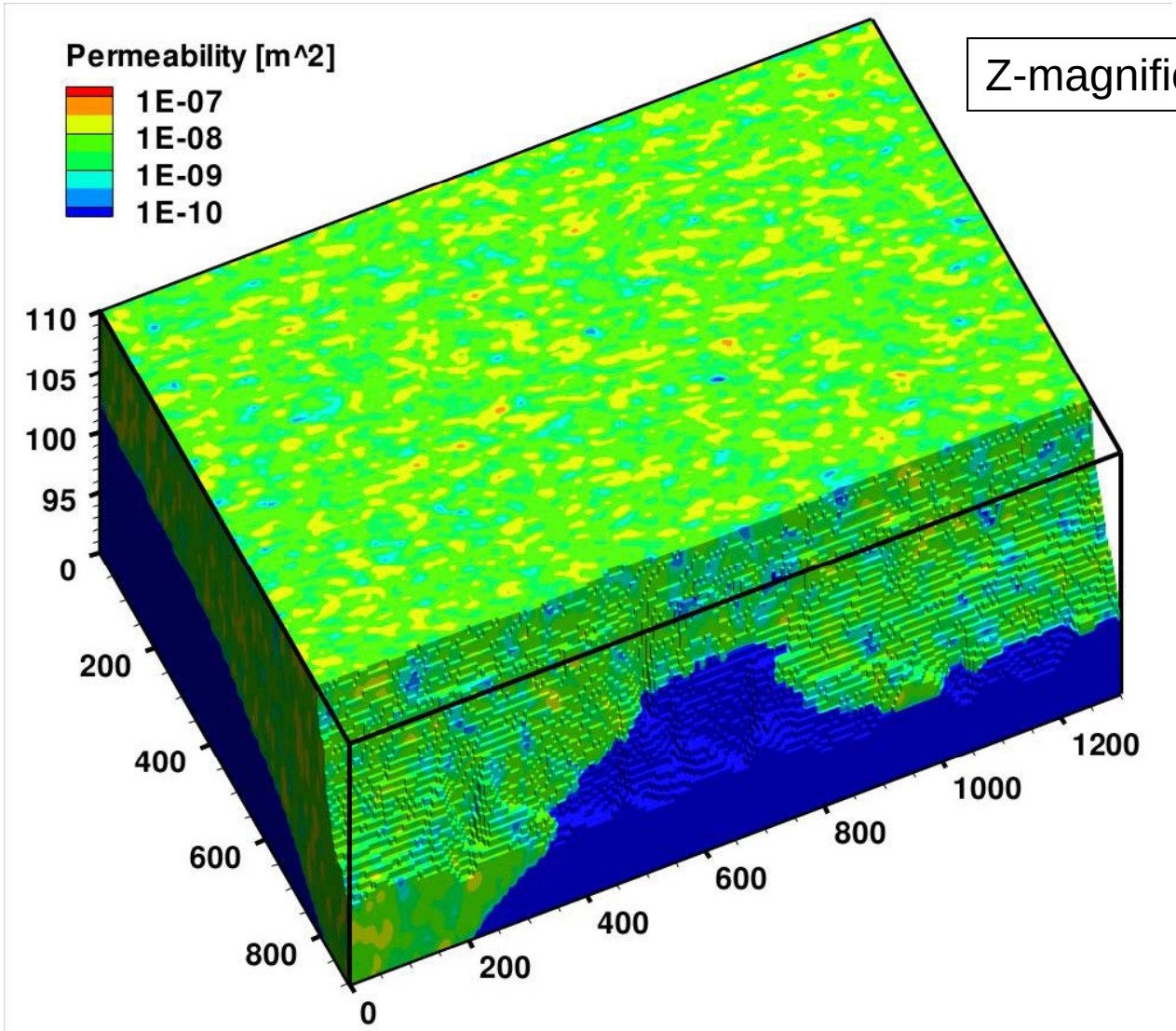
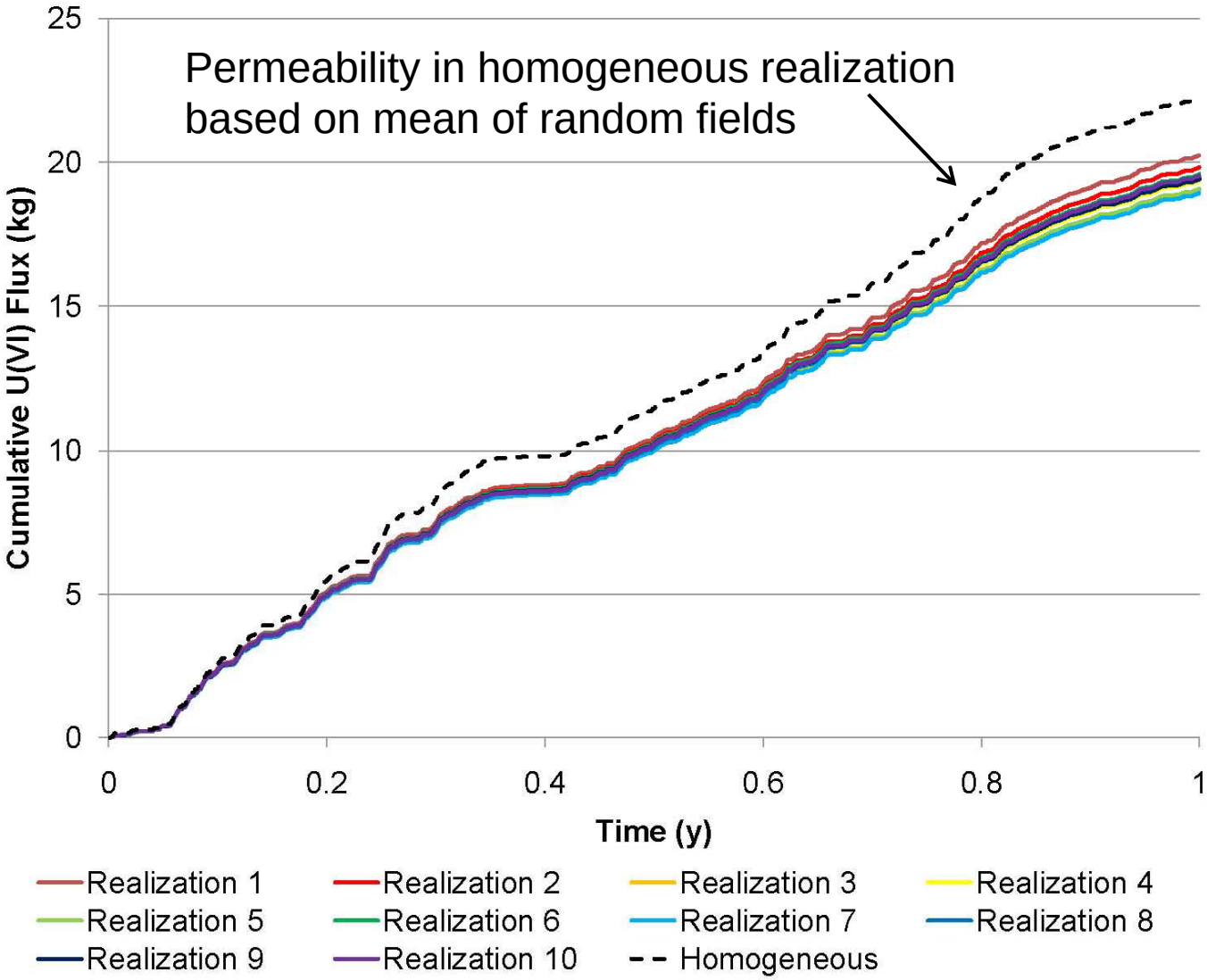
Heterogeneous Permeability Field



Z-magnification = 32.5x

Cumulative U(VI) Flux for Stochastic Sims.

(Hammond et al., Journal of Contaminant Hydrology, 2010)



PFLOTRAN PERFORMANCE

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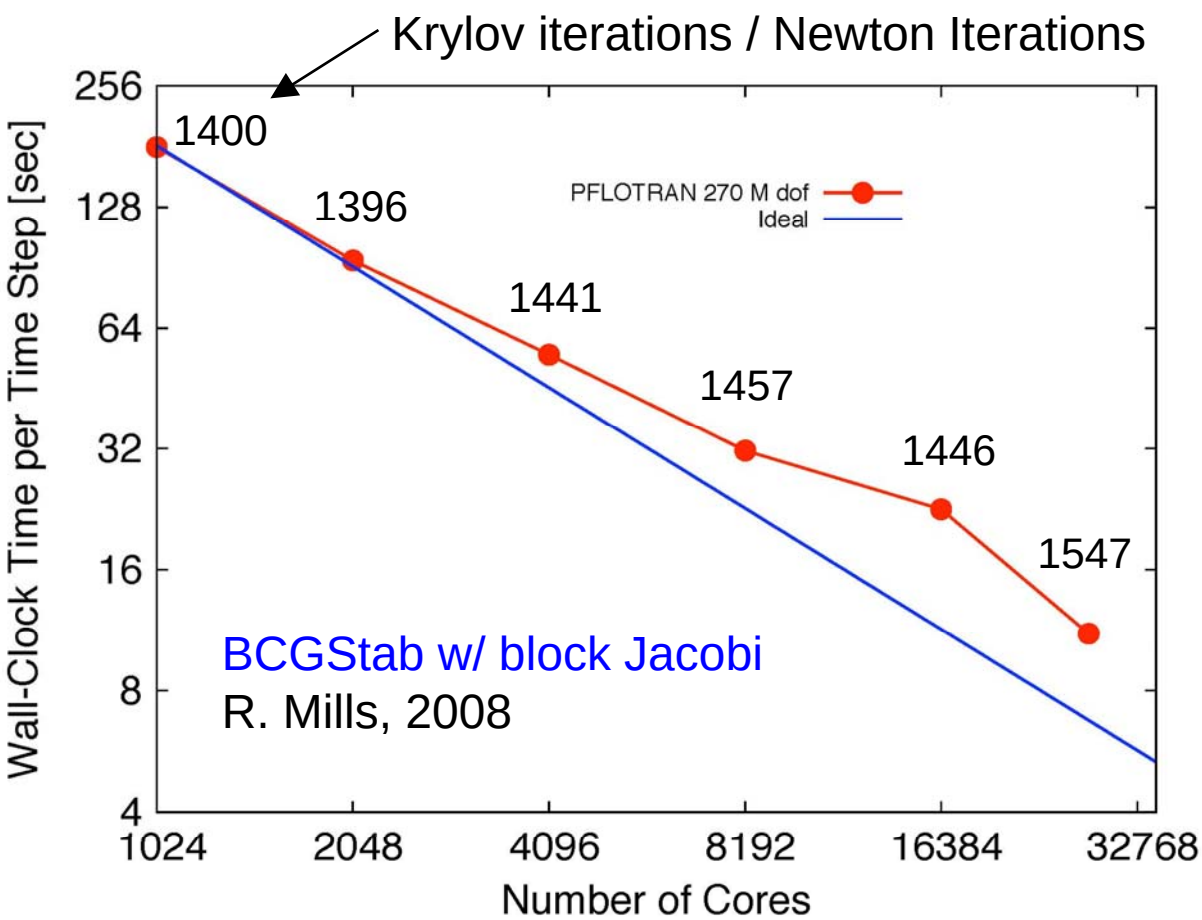
Hanford 300 Area Groundwater Flow: Strong Scaling – Jaguar XT4
270M Degrees of Freedom



Overall 60% efficient

Physics

(1-2% of overall time)

- 75% efficient (wall clock)

Solvers

(96% of overall time)

- 90% efficient (iteration count)
- 64% efficient (wall clock)

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Hanford 300 Area Groundwater Flow: Weak Scaling or Scaled Speedup – Jaguar XT4
~16200 Degrees of Freedom per Processor Core

BCGStab w/ block Jacobi

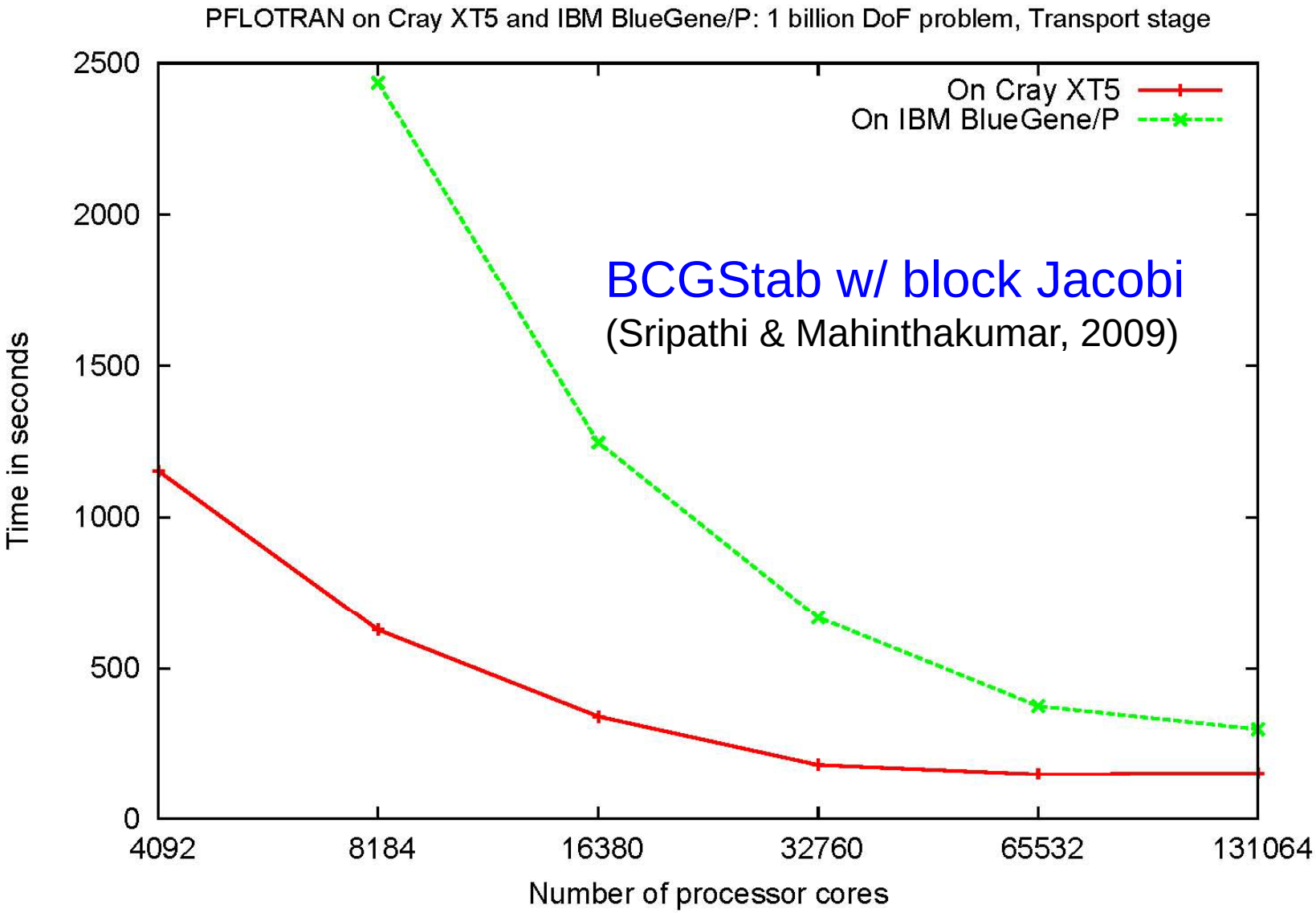
R. Mills, 2008

Processor Cores	4000	8000
Problem Size (dofs)	64.8 million	129.6 million
Problem Size / Processor Core	16200	16204
Krylov Iterations / Newton Iterations	418.4	462.6 (10.6% difference)
Nonlinear Solver Wall Clock Time (sec)	2531	2844 (12.4% difference)

Poor "weak" scalability

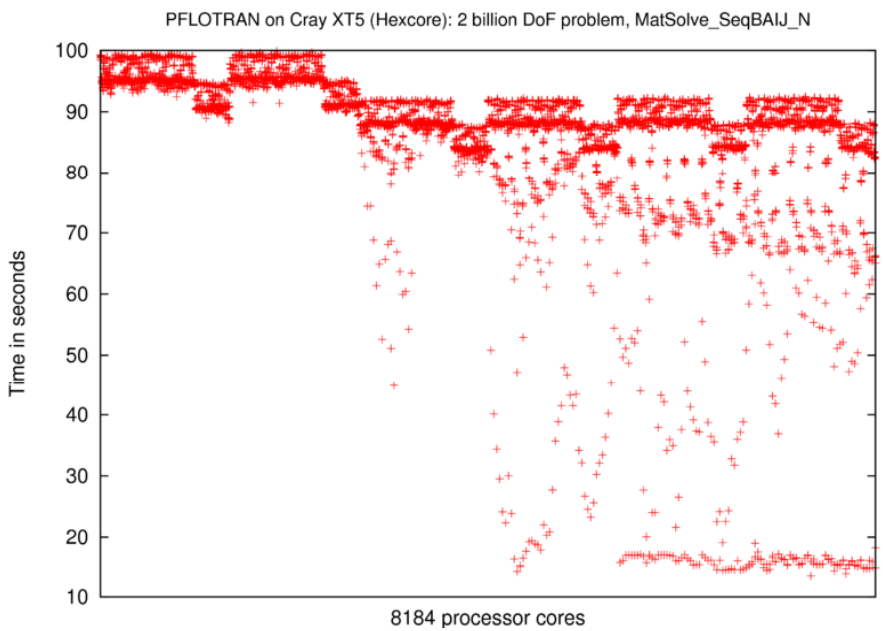
Load imbalance, global reductions?

Cray XT5 vs. BlueGene/P (Strong Scalability)
PFLOTRAN Geochemical Transport (1B dofs)

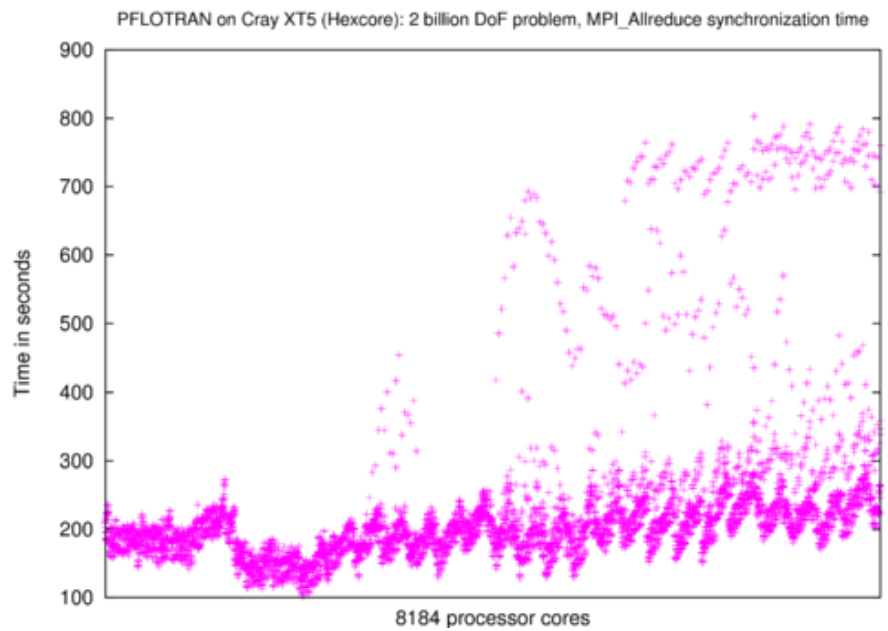


Impact of Inactive Grid Cells:
2 billion dof problem on 8192 cores

MatSolve_SeqBAIJ_N



MPI_Allreduce sync time



(Sripathi & Mahinthakumar, NC State
http://www.secure-water.org/wiki)

Acknowledgements

- Department of Energy Office of Science
  - SciDAC-2 program groundwater project
    - Office of Advanced Scientific Computing Research (ASCR)
    - Subsurface Biogeochemical Research Program (BER)
  - INCITE program (supercomputing)
    - Jaguar supercomputer – National Center for Computational Sciences (NCCS) at Oak Ridge National Laboratory (ORNL)

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