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Modelling Approaches and Issues

Peter C. Lichtner

Los Alamos National Laboratory

Office of Science
U.S. DEPARTMENT OF ENERGY
Environmental Remediation Sciences

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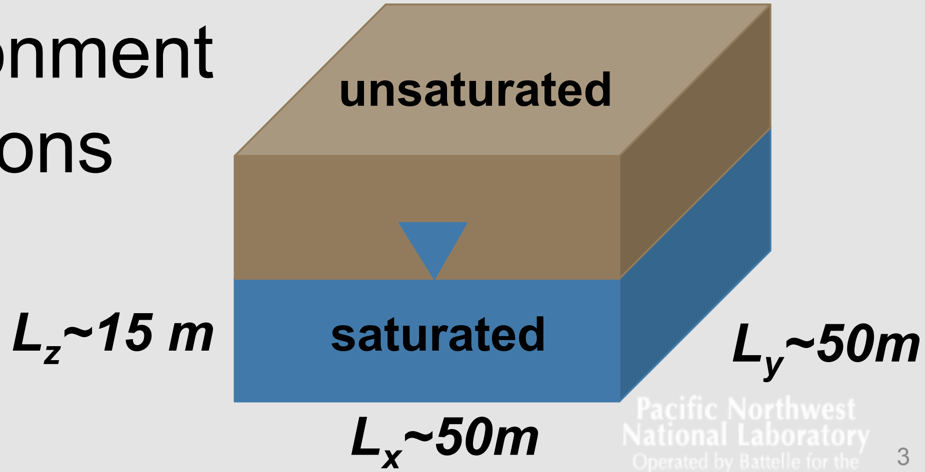
Outline

- Modeling Challenges
- Site Characterization
  - Physical and chemical properties
  - U(VI) Source Term
- Scale Up
- Multiscale Models
- Need for High Performance Computing

Modeling Challenges

- 3D Domain: length and time scales
  - field scale domain (5-50m)
  - hourly river fluctuations, ~year predictions
- Complex chemistry: Na-K-Ca-Fe-Mg-Br-N-CO_2-P-S-Cl-Si-U-Cu-H_2O (~15 primary species)
- Multiscale processes (μm-m)
- Highly heterogeneous sediments
  - fine sand, silt; coarse gravels; cobbles
- Variably saturated environment
- Initial & boundary conditions



Site Characterization

- Porosity, permeability, relative permeability and capillary pressure relations
- U(VI) concentration in aqueous and solid phases
- Surface complexation site density
- Mineral surface areas, rate constants and abundances
- Multiscale model parameters
- Geostatistical model to generate multiple realizations

U(VI) Source Term

- Vadose zone source
- Release mechanisms
  - Fluctuating water table
  - Mineral dissolution
  - Desorption
  - Diffusion
- Infiltration
  - Chinook (~200 mm/d 1985)
  - Mean 200 mm/y

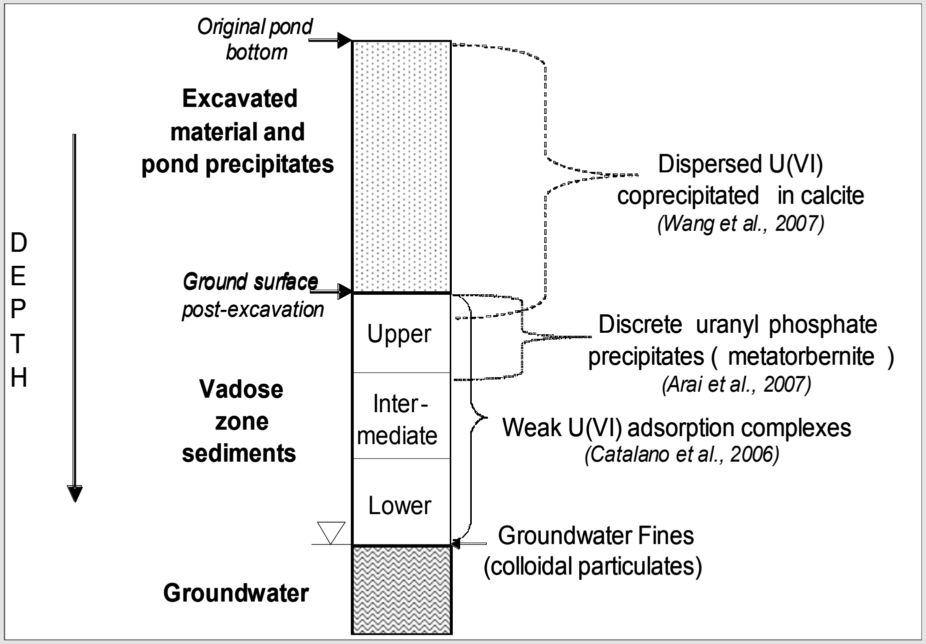
Sub-Grid Scale Model

- Mineral form (kinetic dissolution)
  - Co-precipitation of U(VI) with calcite
  - Metatorbernite [$Cu(UO_2)_2(PO_4)_2 \cdot 8H_2O$]

- Sorbed form (surface complexation-local equilibrium)

- Intra-granular diffusion

- Sub-domain distribution

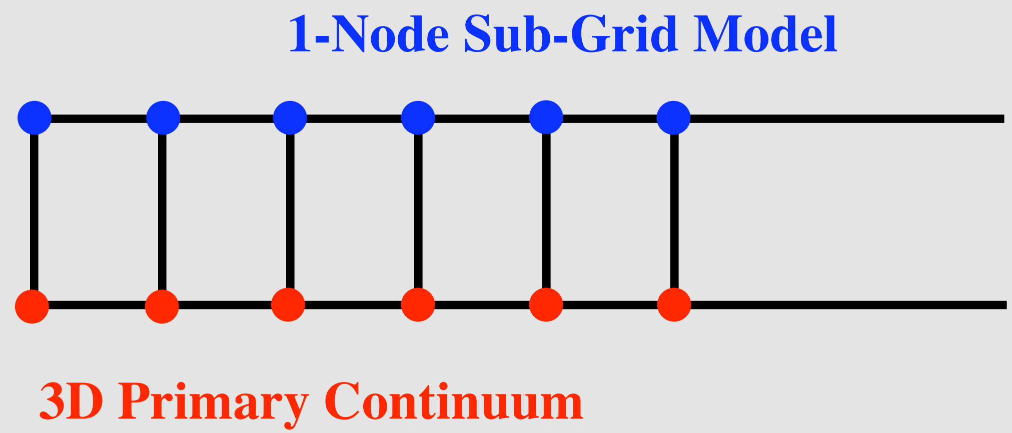


Scale Up

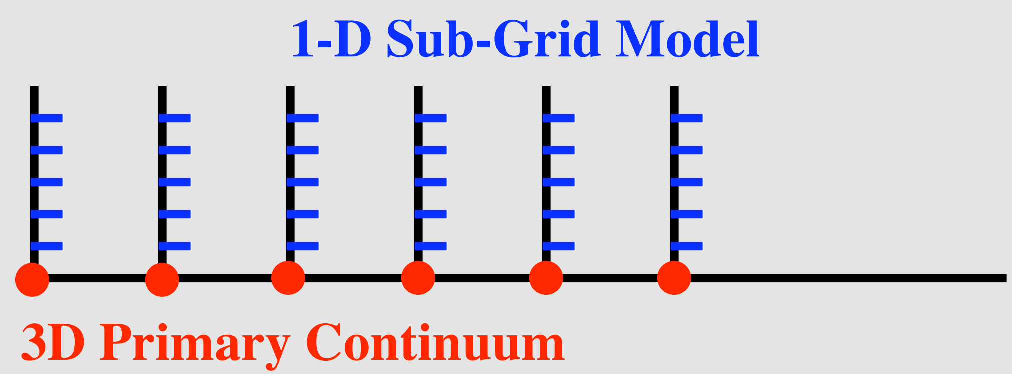
- Spatial
  - Small column ⇒ large column ⇒ field
  - Core scale (column support data): 1-10 cm
  - Field domain size: $L \sim 5\text{-}50$ m
- Temporal
  - Highly fluctuating river stage (~hourly)
  - Time step Δt: 1 hour = 1.14×10^{-4} years
  - 8.76×10^{6} time steps to reach 1000 years
- Methods
  - Geostatistical methods to extrapolate between wells
  - Fitting to column experiments
  - Time averaging

Multiscale Models

- Multirate model



- Multiple interacting continuum model



Two-Domain Model

- Primary continuum:

$$\frac{\partial}{\partial t}\epsilon_\alpha\varphi_\alpha R_j^\alpha\Psi_j^\alpha + \boldsymbol{\nabla}\cdot\epsilon_\alpha\boldsymbol{\Omega}_j^\alpha = -\epsilon_\alpha\sum_m \nu_{jm} I_m^\alpha - \Gamma_j^{\alpha\beta}\left(\Psi_j^\alpha - \Psi_j^\beta\right)$$

- Secondary continua:

$$\frac{\partial}{\partial t}\epsilon_\beta\varphi_\beta R_j^\beta\Psi_j^\beta + \boldsymbol{\nabla}\cdot\epsilon_\beta\boldsymbol{\Omega}_j^\beta = -\epsilon_\beta\sum_m \nu_{jm} I_m^\beta + \Gamma_j^{\alpha\beta}\left(\Psi_j^\alpha - \Psi_j^\beta\right)$$

- Mineral mass transfer: $\dfrac{\partial\varphi_s^\alpha}{\partial t} = \overline{V}_s I_s^\alpha, \quad \dfrac{\partial\varphi_s^\beta}{\partial t} = \overline{V}_s I_s^\beta$

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Multiple Interacting Continuum Model

- Primary continuum (α = *primary fluid*):

$$\frac{\partial}{\partial t}\epsilon_\alpha \varphi_\alpha R_j^\alpha \Psi_j^\alpha + \nabla \cdot \epsilon_\alpha \boldsymbol{\Omega}_j^\alpha = -\epsilon_\alpha \sum_m \nu_{jm} I_m^\alpha - \sum_\beta a_{\alpha\beta}\Omega_j^{\alpha\beta}$$

- Secondary continua (β^{th} continuum):

$$\frac{\partial}{\partial t}\epsilon_\beta \varphi_\beta R_j^\beta \Psi_j^\beta + \nabla \cdot \epsilon_\beta \boldsymbol{\Omega}_j^\beta = -\epsilon_\beta \sum_m \nu_{jm} I_m^\beta$$

- Boundary conditions:

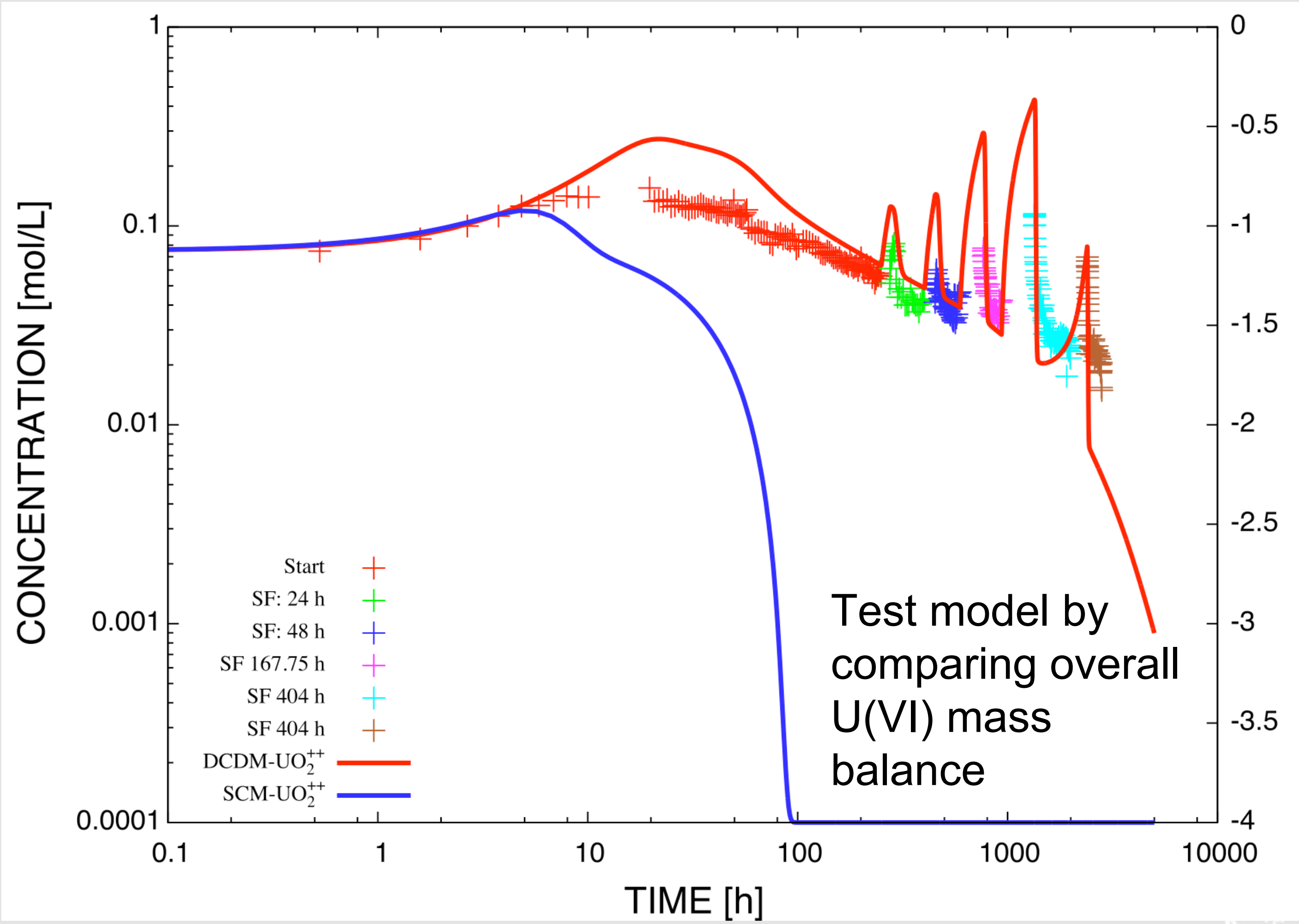
$$\Psi_j^\beta(0,\, t\,|\boldsymbol{r}) = \Psi_j^\alpha(\boldsymbol{r},\, t), \qquad \Omega_j^{\alpha\beta} = -\varphi_\beta D_\beta \left(\frac{\Psi_j^\alpha - \Psi_j^\beta}{d_{\alpha\beta}}\right)$$

- Mineral mass transfer:

$$\frac{\partial \varphi_s^\alpha}{\partial t} = \overline{V}_s I_s^\alpha, \qquad \frac{\partial \varphi_s^\beta}{\partial t} = \overline{V}_s I_s^\beta$$

Hanford Large Column Exp. NPP1-14

Multiscale Model of Hanford Large Column Exp.



Number of Degrees of Freedom

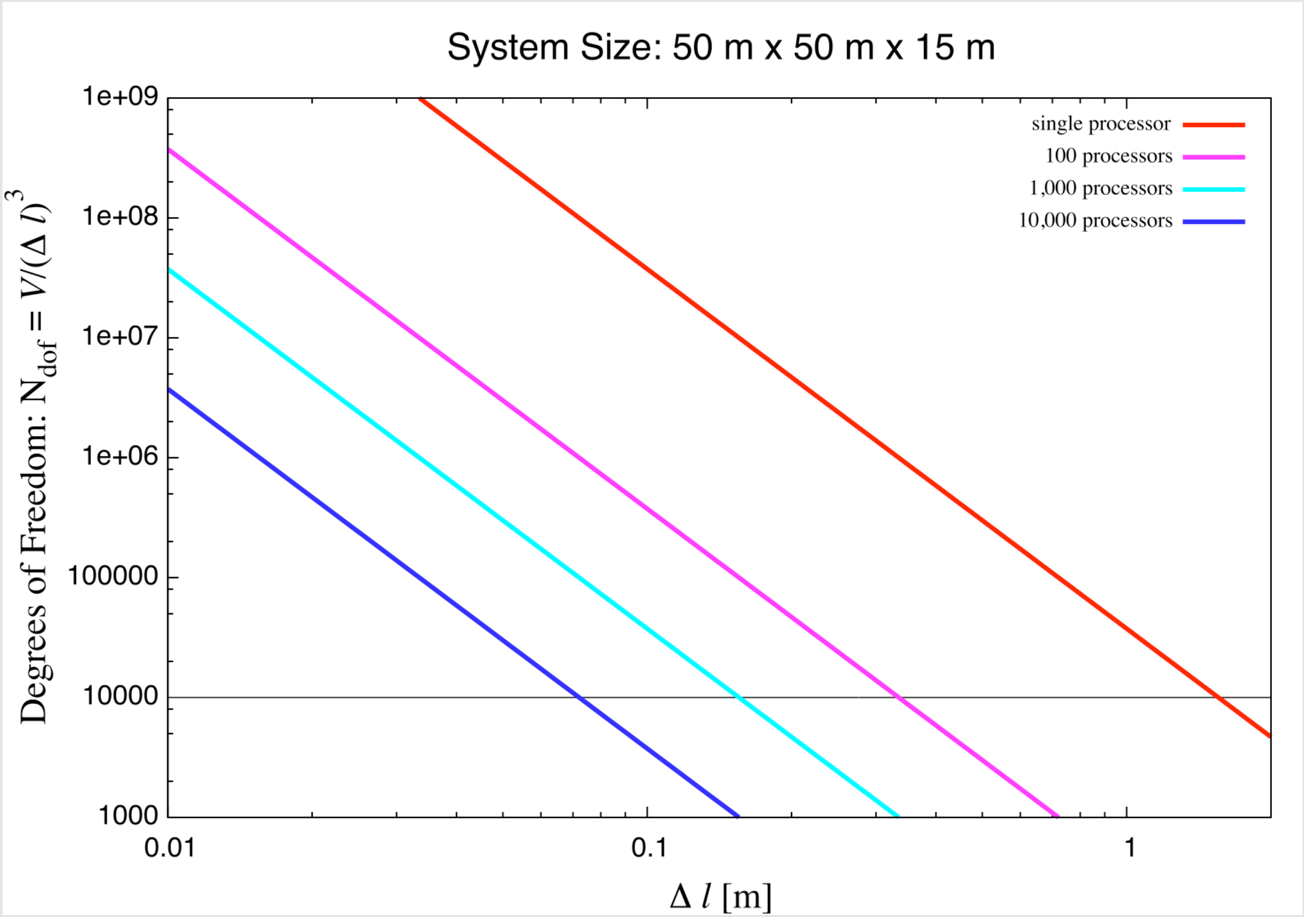
$$N_{\mathrm{dof}} = \underbrace{N \times N_c}_{\mathrm{primary}} + \underbrace{N \times N_c \times N_M \times N_K}_{\text{sub-grid continuua}}$$

		Storage
N	= Number of primary domain nodes	(3D: 10^7)
N_K	= Number of sub-grid classes	(10)
N_M	= Number of nodes in each class	(10)
N_C	= Number of chemical components	(15)
	total:	1.5×10^{10}

- Employ sub-grid model only where needed
- Combine with adaptive mesh refinement
- Use efficient numerical schemes to rigorously "decouple" primary and secondary continua
  - Operator splitting
  - Fully implicit

Computational Resources

- Degrees of Freedom



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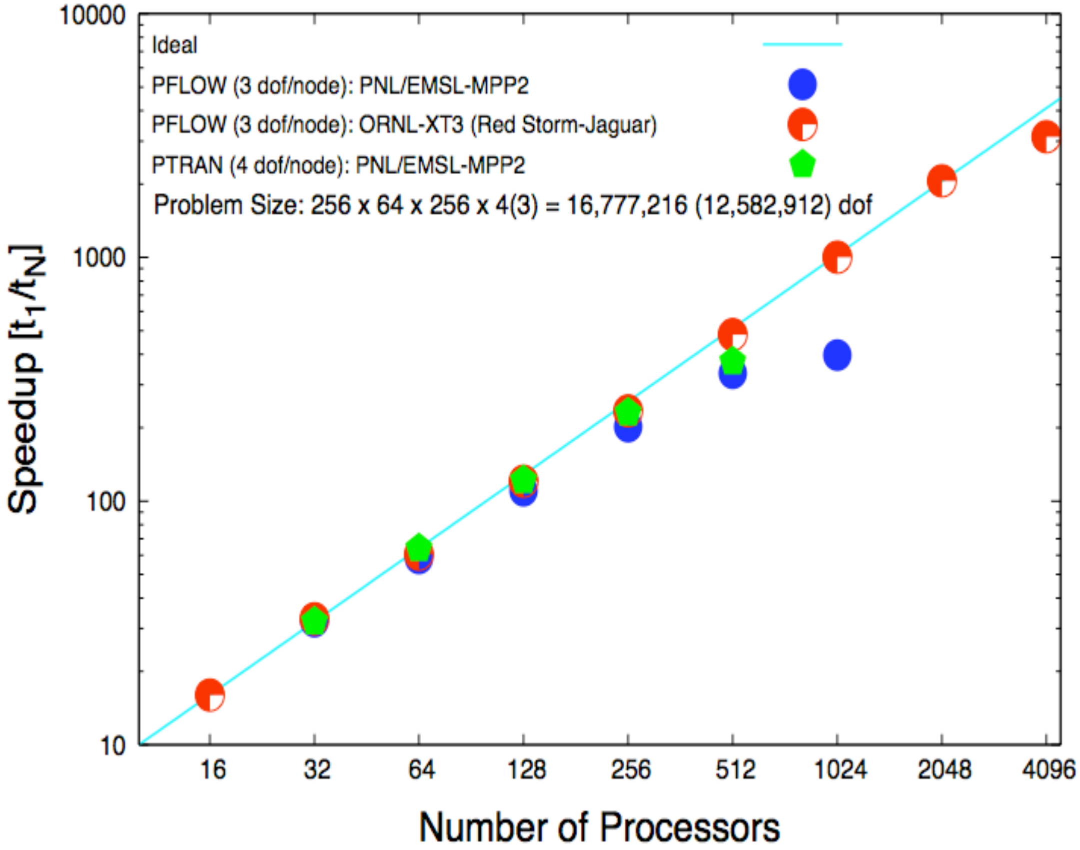
PFLOTRAN Parallel Efficiency on PNNL MPP2 and ORNL Jaguar XT3

Jaguar: 11,508 dual-core 2.6GHz AMD Opteron processors, 4 GB of memory (2 GB per core) for a total of 46 TB, 600 TB of scratch space, Cray Seastar router through Hypertransport interconnected in a 3D-torus topology providing very high bandwidth, low latency, and extreme scalability.



Multirate Model

- Sorption model:

$$\frac{\partial}{\partial t}\varphi C_j + \nabla\cdot\boldsymbol{F}_j = -\sum_\beta \Gamma_j^\beta\left(f_\beta K_j^d C_j - S_j^\beta\right)$$

$$\frac{\partial S_j^\beta}{\partial t} = \Gamma_j^\beta\left(f_\beta K_j^d C_j - S_j^\beta\right)$$

- Not clear how to include mineral precipitation and dissolution

Time Step Control

- Groundwater velocity: q ~ 500 m/y (Darcy Vel.)
- Porosity = 0.25, v_{pore} ~ 2 km/y
- CFL = $v\ \Delta t/\Delta l$ ~ 1, Δt = 1 hour, Δl ~ 20 cm