Pore-Scale Reactive Transport Simulation

A Computational Opportunity for Scientific Discovery

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Scientific Impacts and Opportunities in Computing
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Reactive Transport

- Movement and transformation of fluids in the subsurface is relevant to several DOE missions (e.g., CO_2 sequestration, hydrocarbon recovery, legacy waste stewardship, high-level waste isolation).
- Fluid flow, solute transport (advection, diffusion) and reactions are intimately coupled in many cases.
- Natural systems are highly heterogeneous at multiple scales
- There is inherent disparity between “process” and “phenomenon” scales

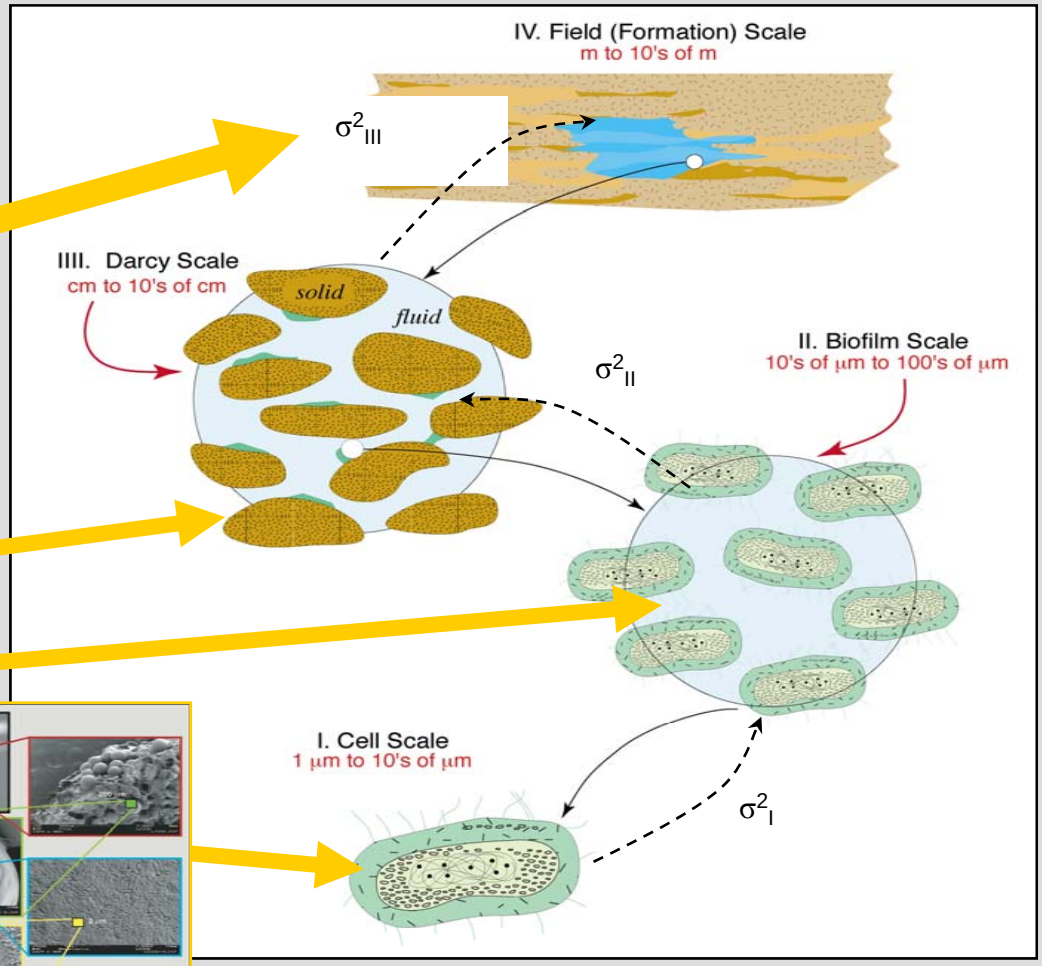
Disparity between "process" and "phenomenon" scales

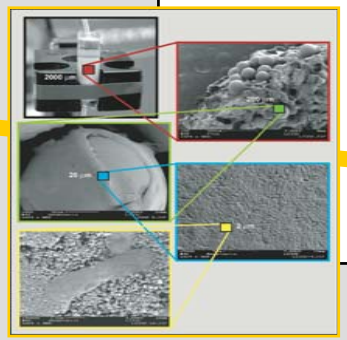
Phenomena:

- Concentration of contaminant metals measured in well water
- Changes in bulk flow rate

Processes:

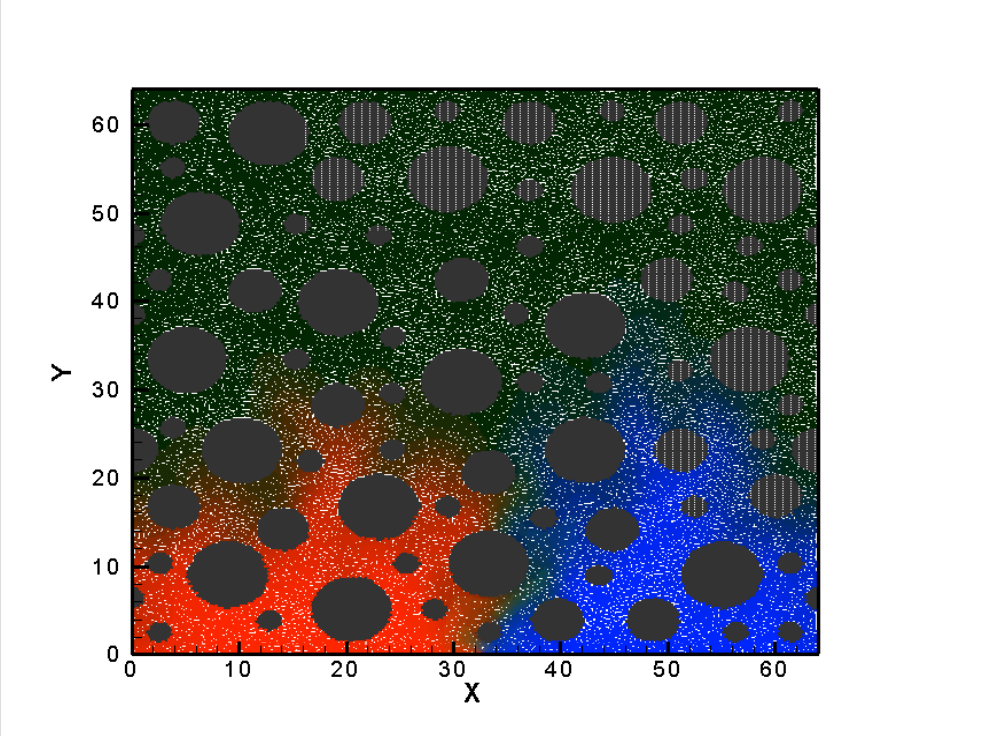
- Precipitation or sorption of reactants/products on solid surfaces; pore clogging
- Substrate and metabolite diffusion in biofilms
- Cellular metabolism and electron transfer





Critical Issues:

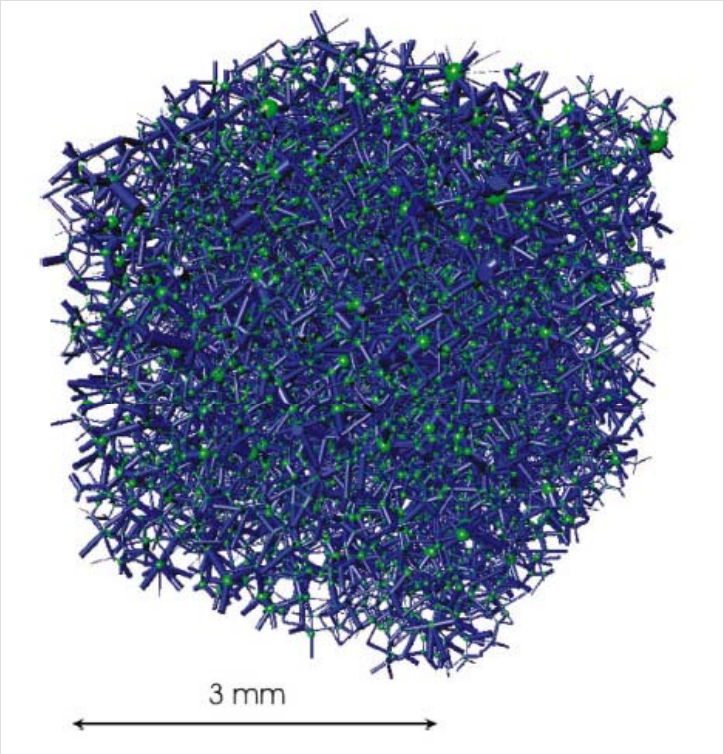
- Mass transfer / mixing limitations mean that local concentrations do not equal average concentrations
- Effective reaction rates are not equal to experimentally measured (complete mixing) and cannot yet be rigorously quantified
- Local coupling strongly affects macroscopic behavior and properties in complex ways
- Characterization data are far from complete (at local and macroscopic scales)



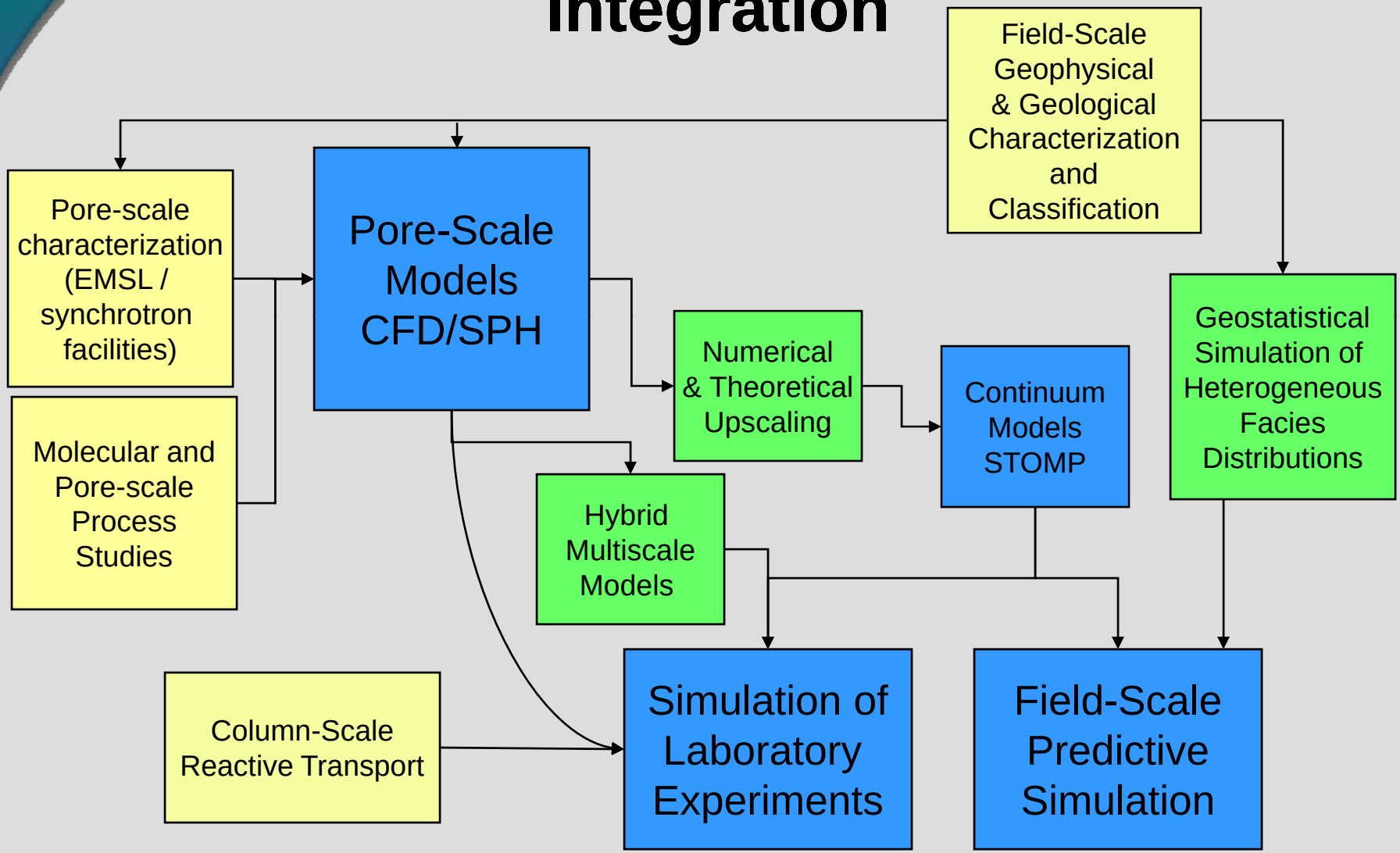
Why Pore-Scale Modeling?

- "…It is important to have a reliable physically based tool that can provide plausible estimates of macroscopic properties. Any theoretical or numerical approach to this problem not only needs a *detailed understanding* of mechanisms at the pore level but also an accurate and realistic characterization of the *structure* of the porous medium."

  Piri and Blunt, Phys. Rev. E, 026310, 2005



Conceptual Framework for Scale Integration



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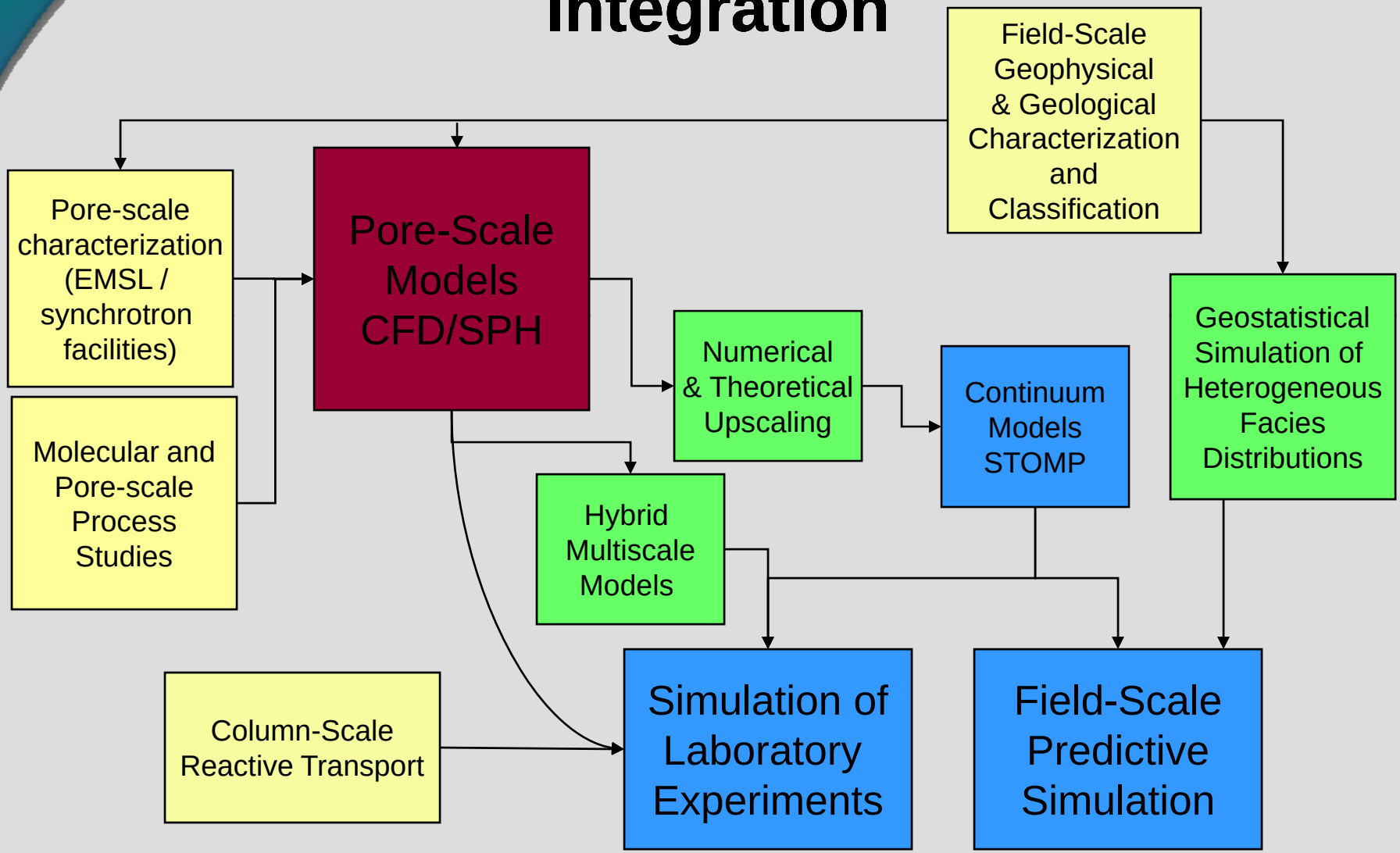
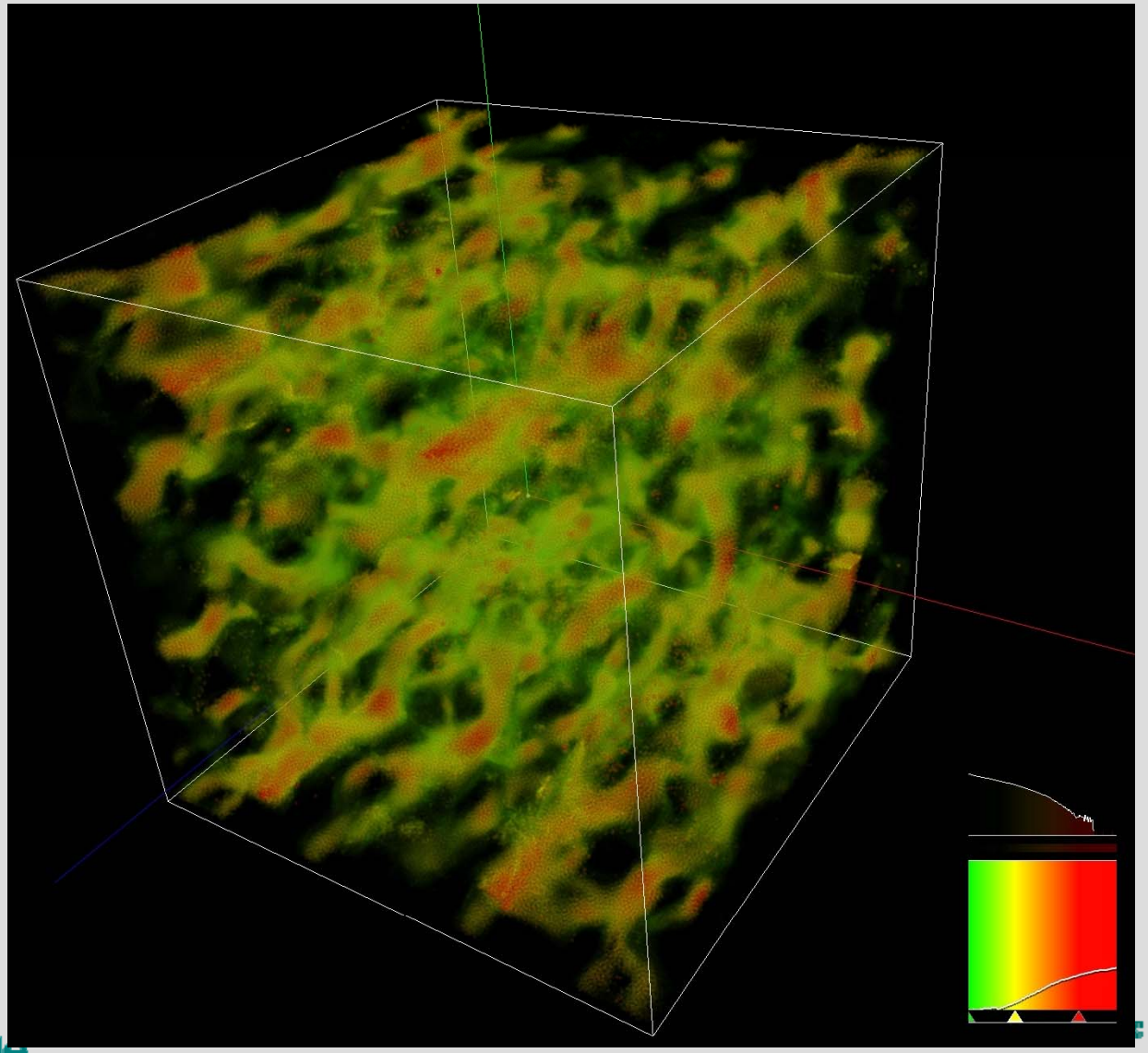


3D SPH Flow Simulations

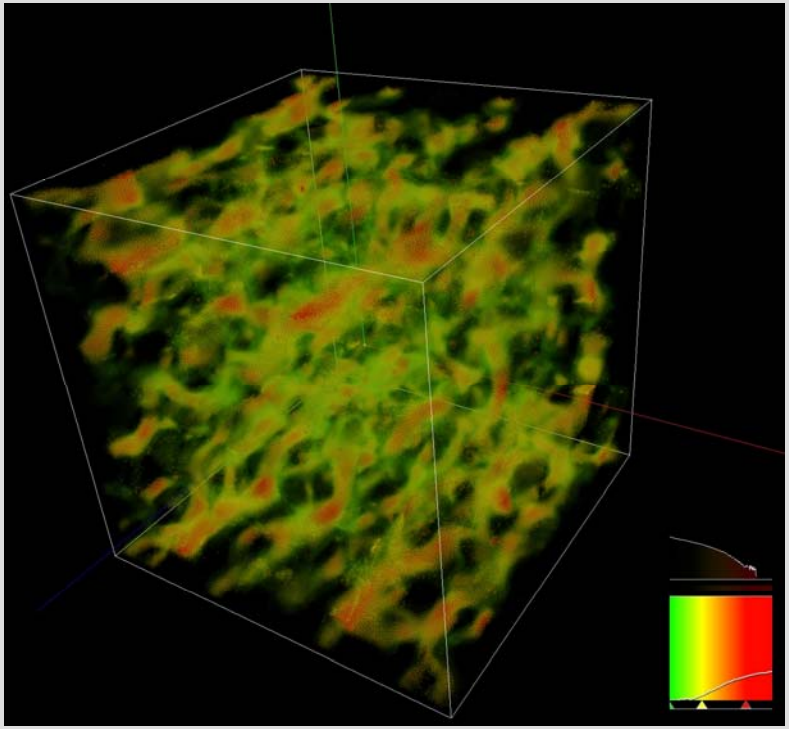


Simulation by Bruce Palmer (PNNL)

Visualization courtesy of Kwan-Liu Ma and students (UC Davis)

Particle-Based Simulations

- Only local communication required (within smoothing kernel distance)
- No solver required – explicit method
- Expect good scaling properties
- Current run on MPP2 (PNNL/EMSL) with 7 million particles on ~500 processors
- Received new ERCAP allocation at NERSC – will be doing scaling studies to 1000's – 10000's cores.



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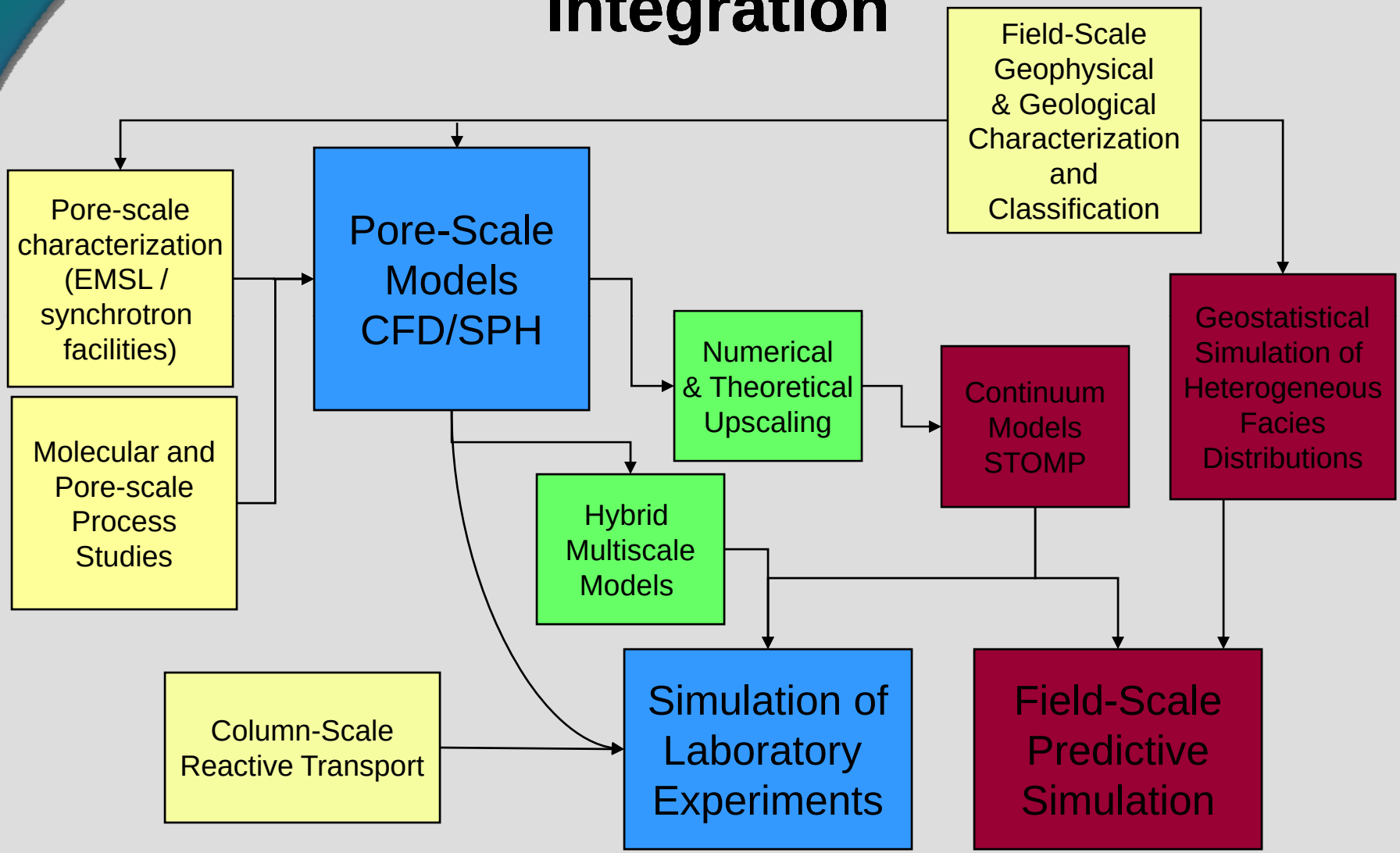
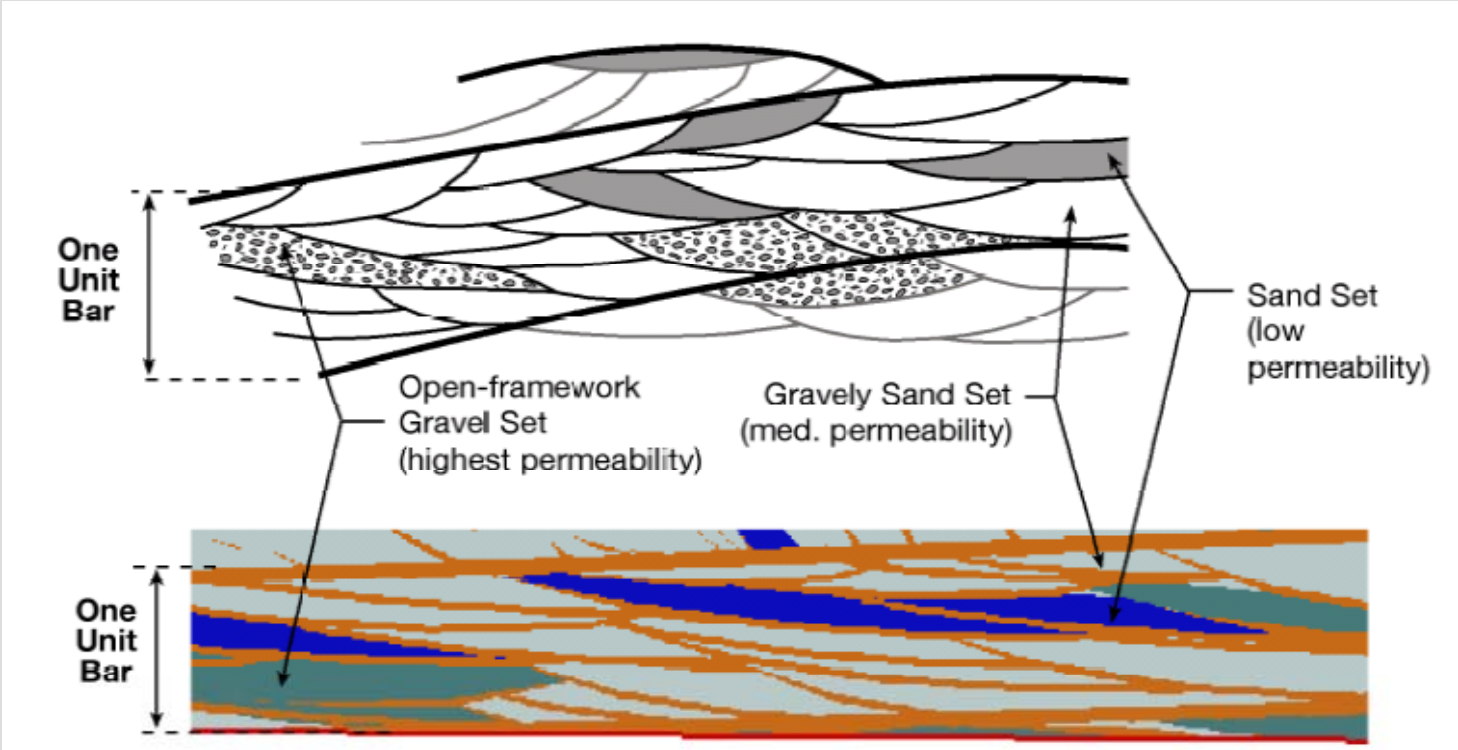


Field-Scale Simulation

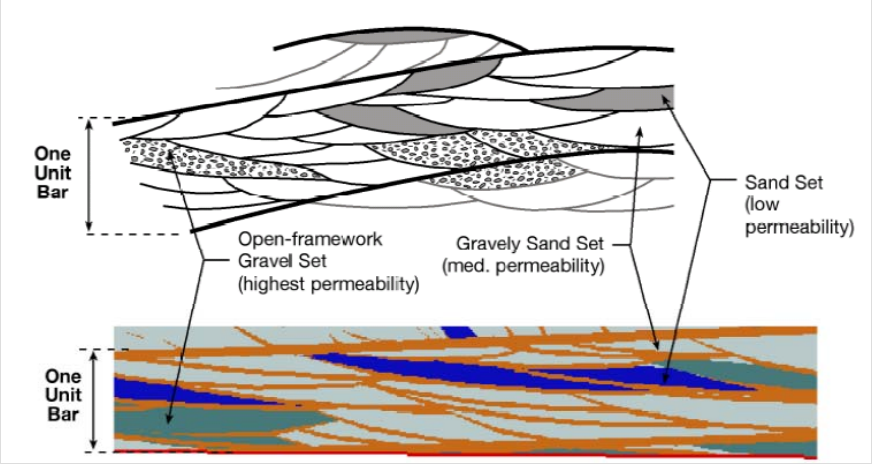
- Simulation of geologically realistic heterogeneous aquifer structure at high spatial resolution

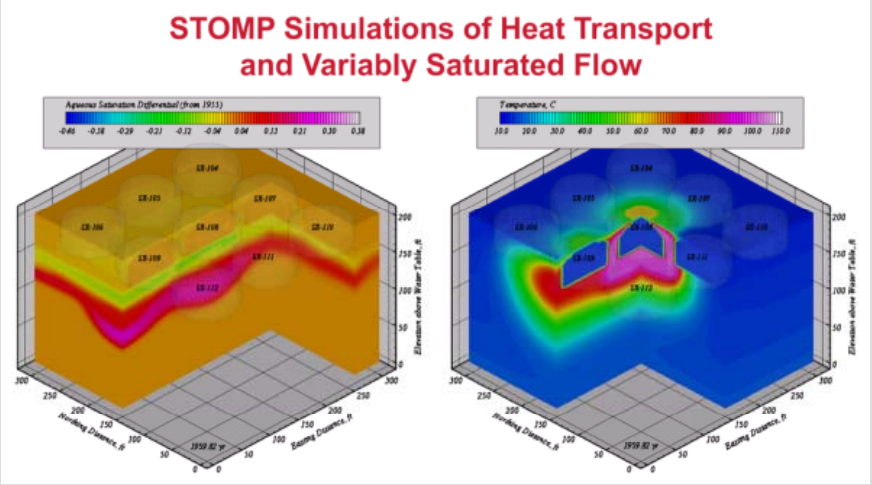
Figure courtesy of Robert Ritzi, Wright State Univ.



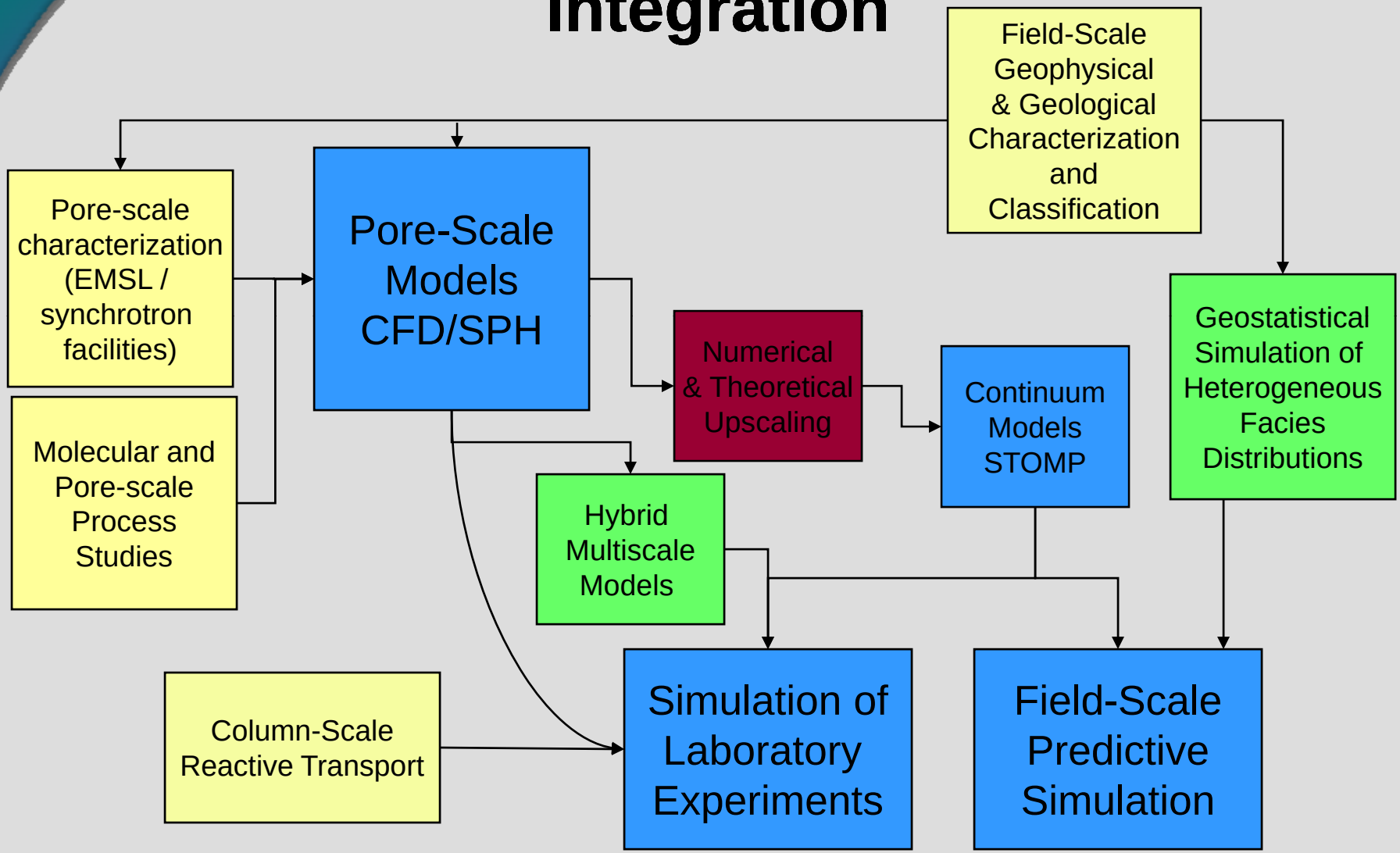
Field-Scale Simulation

- Geometric / geologic simulation method will create km-scale 3D domain with cm-scale resolution; up to 10^{13} grid elements.
- Currently solving flow and reactive transport on the order of 10^{8} grid elements (STOMP/CRUNCH simulation) on 2000 processors.
- Putting STOMP within CCA framework for portability and transparent model linkage with other SciDAC technologies (grid / solver / visualization).

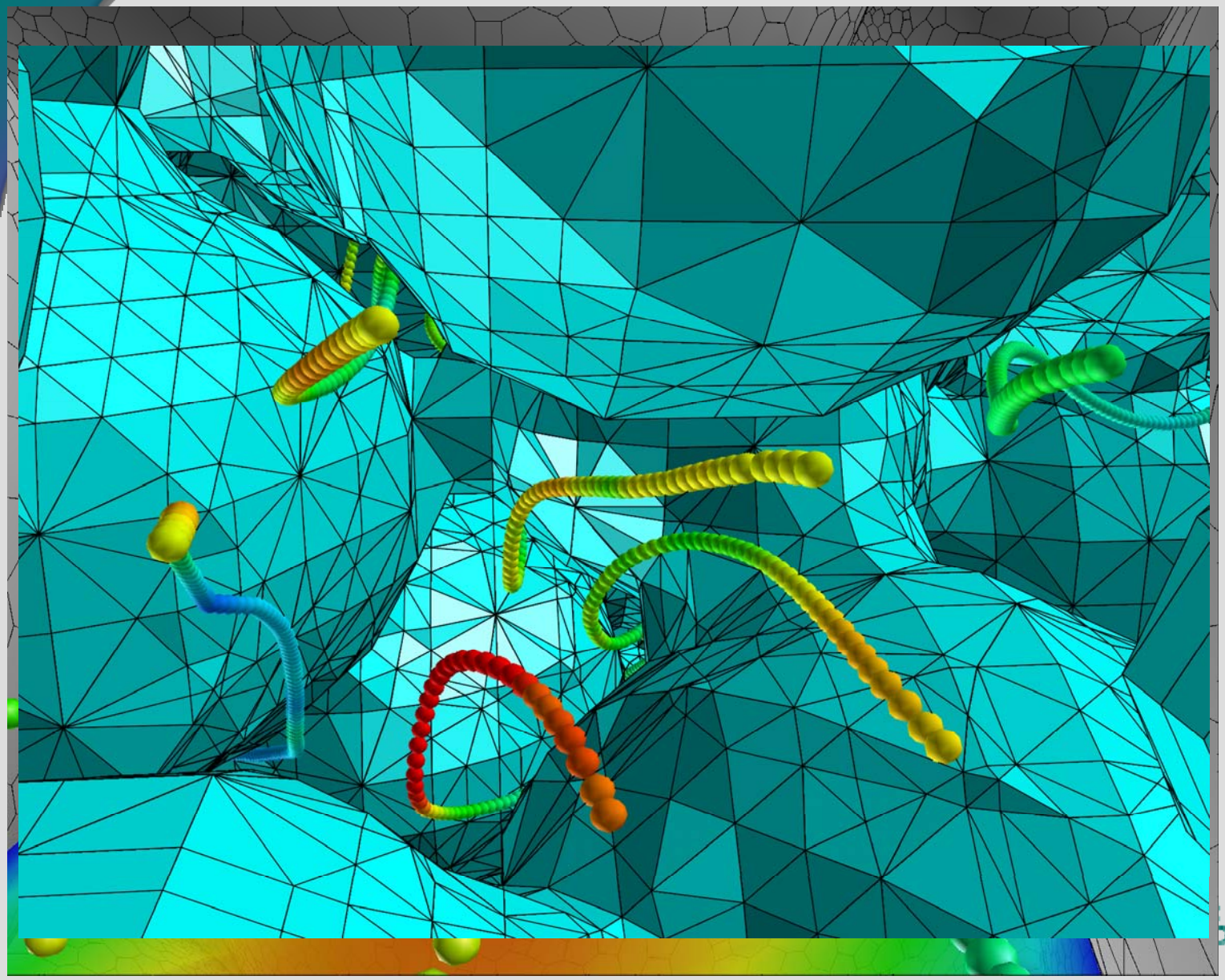




Conceptual Framework for Scale Integration



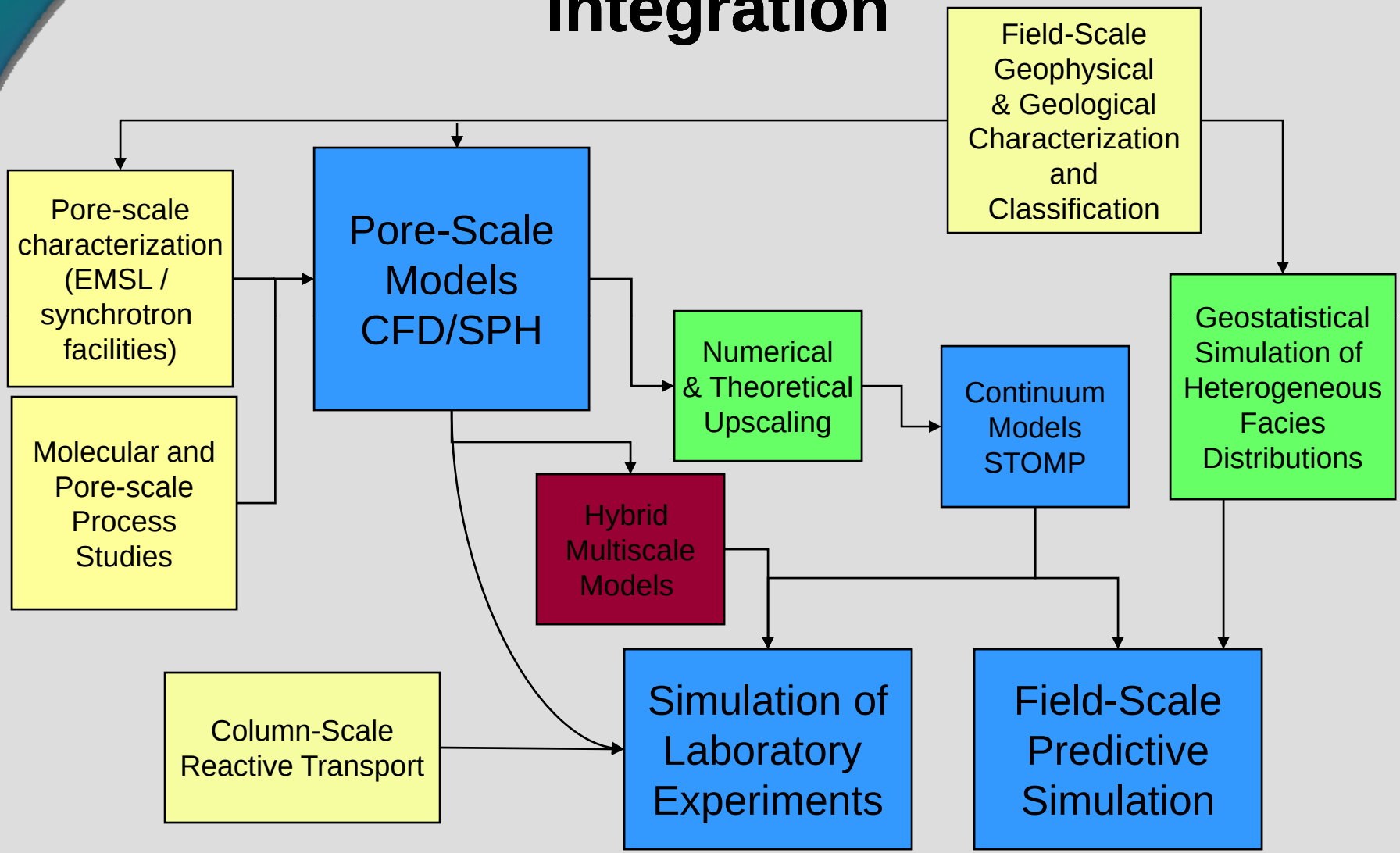
3D CFD Flow Simulations



Simulations by Tao Fu and Cindy Rakowski (PNNL)

Visualizations by John Serkowski (PNNL)

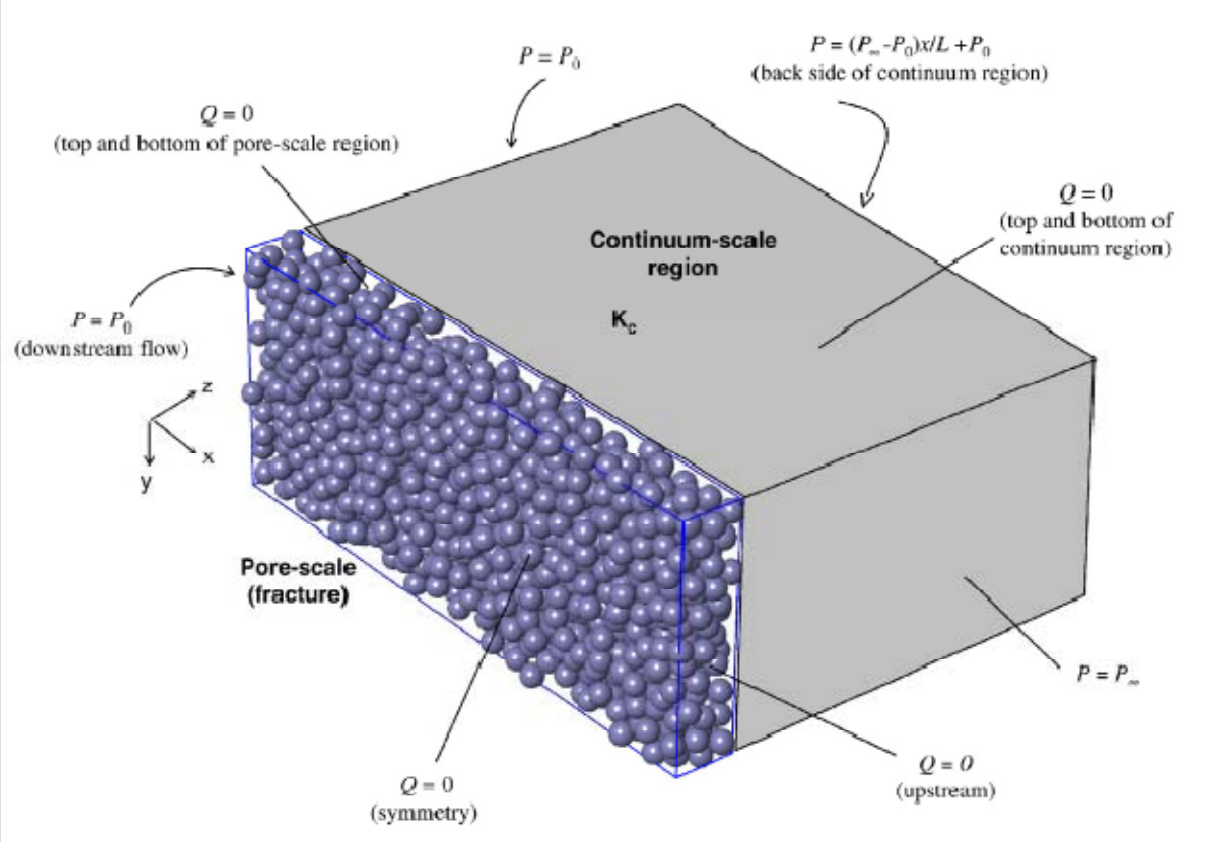
Conceptual Framework for Scale Integration



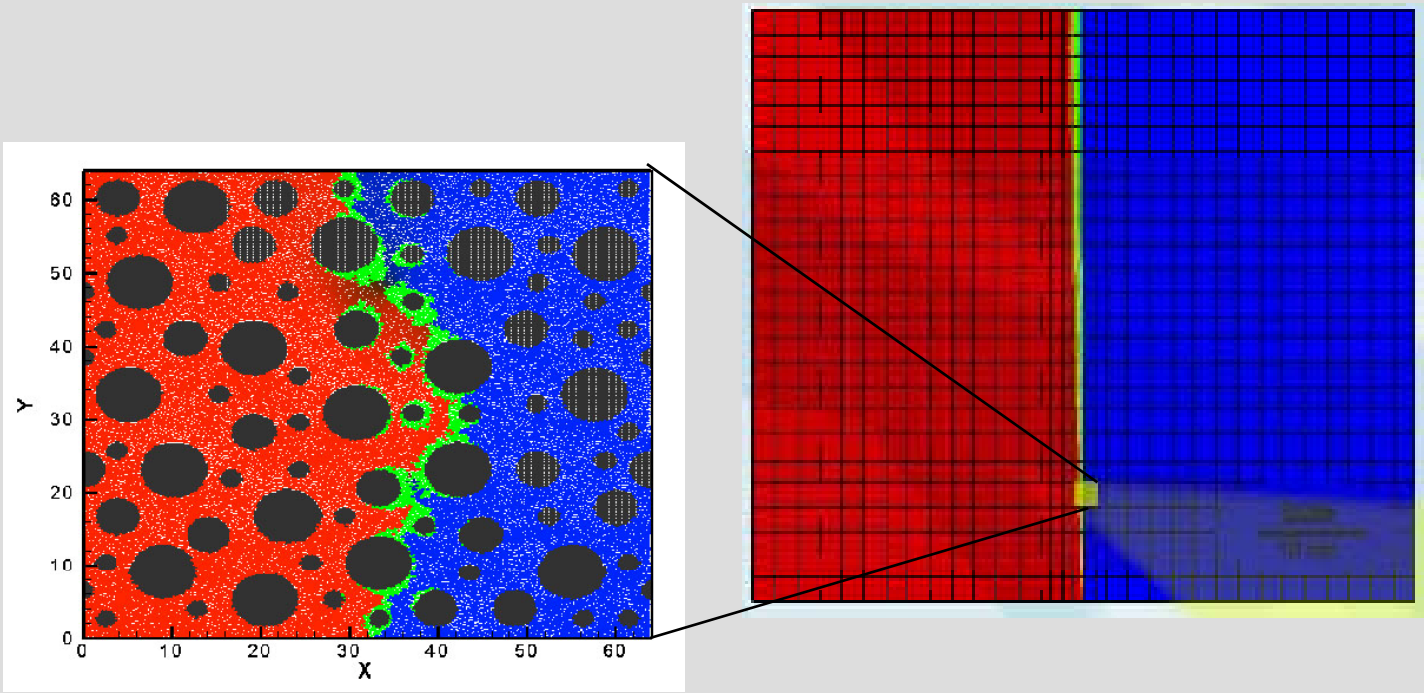
Hybrid Modeling

From Balhoff et al. 2007

Two porous media of contrasting permeability (e.g., sand-filled fracture and relatively impermeable matrix). Network pore model in pore-scale region; continuum model in matrix region.



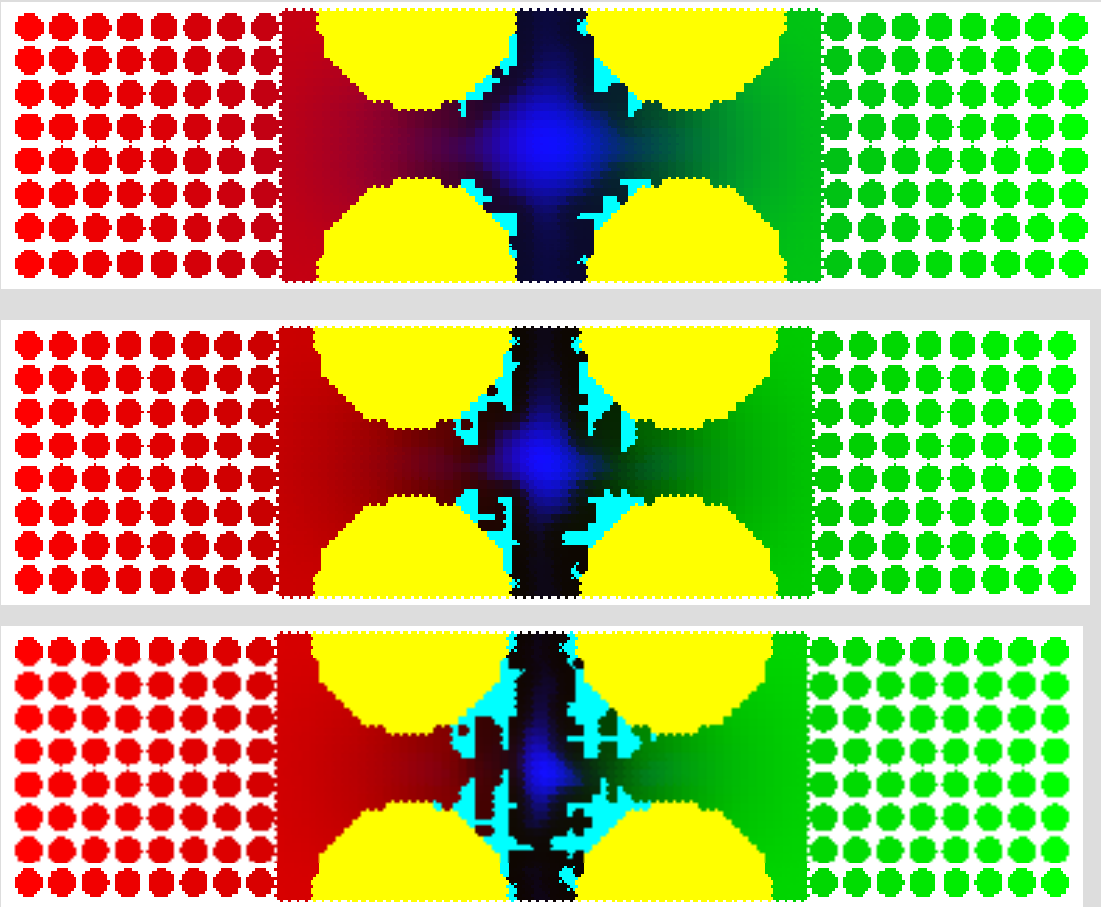
Application to Mixing/Reaction Problem



First Hybrid (Continuum-Pore) Model

Tartakovsky, A. M., D. M. Tartakovsky, T. D. Scheibe and P. Meakin, "Hybrid simulations of reaction-diffusion systems in porous media," submitted to *SIAM Journal on Scientific Computing*, in revision.

- SPH at both scales
- No advection; mixing by diffusion only and heterogeneous reaction
- Also working on a coupled SPH / FE model



Acknowledgments

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  - Daniel Tartakovsky (UC San Diego)
  - Brian Wood (Oregon State University)
  - Robert Ritzi (Wright State University)