Scientific Challenges in Geosciences

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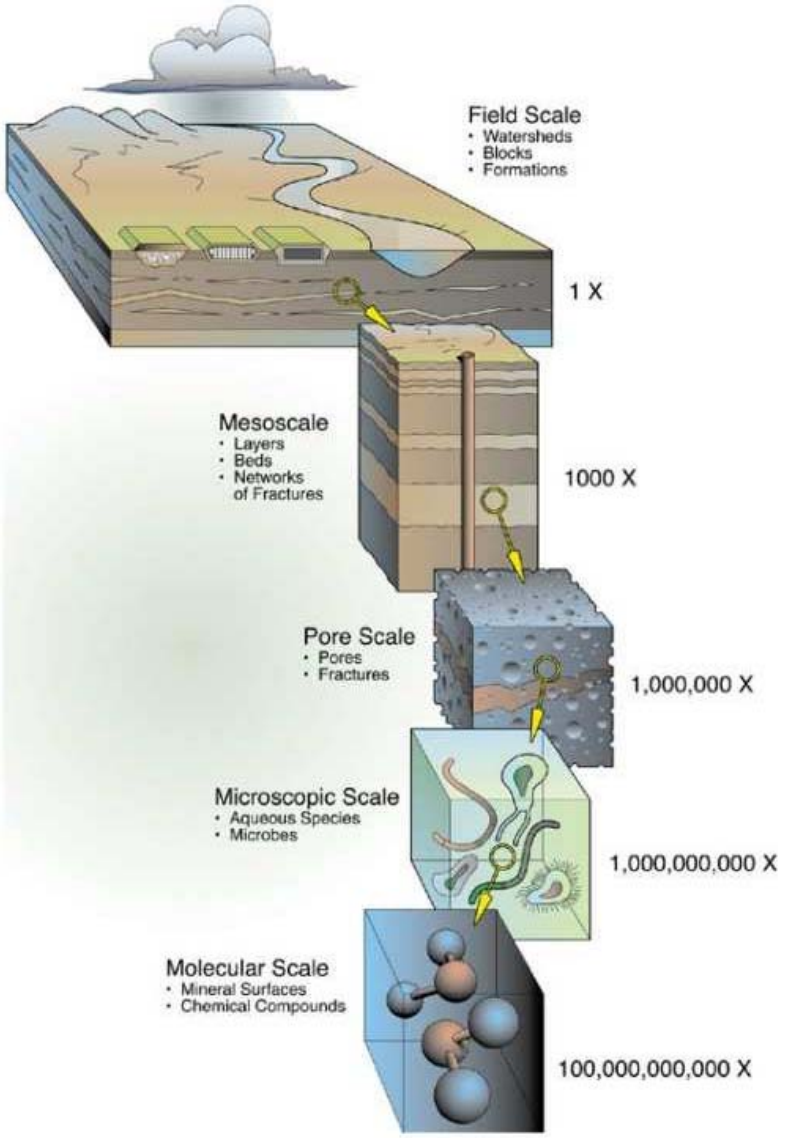
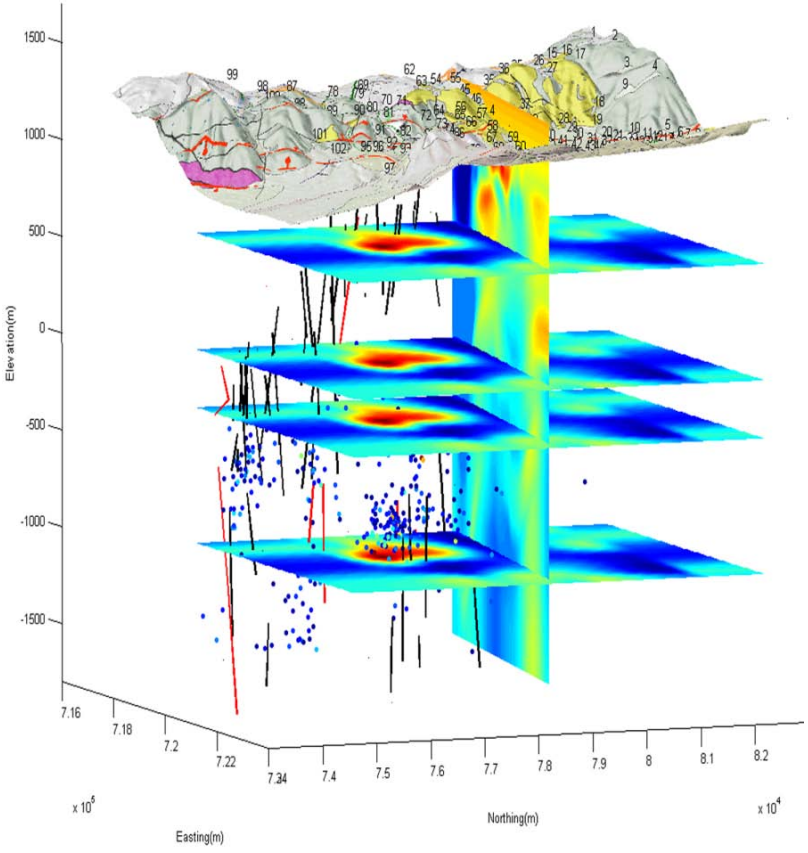
Scientific Challenges in Geosciences

- Cover a broad range of time and length scales
  - Large field scale simulation of CO_2 sequestration, oil and gas recovery, and enhanced geothermal development
  - Microscale processes involving fracture flow in rocks or pore flow in sediments
  - Molecular level processes that provide mechanistic insight into geochemical reactions.
- Requires a diverse technical expertise
  - Imaging of geologic systems
  - Multiphase fluid flow and transport
  - Colloid and interfacial chemistry
- Highlighted in 2007 workshop report
  - "Basic Research Needs in Geosciences: Facilitating 21st Century Energy Systems



Basic Research Needs in Geosciences

- Grand Challenge: **Integrated Characterization, Modeling, and Monitoring of Geologic Systems**
  - Site characteristics must be know across a range of scales (pore to kilometer), modeling is an essential tool, and long term security requires linking modeling to monitoring of the site.
- Priority Research Direction: **Transport Properties and In Situ Characterization of Fluid Trapping, Isolation, and Immobilization**
  - Fluid immobilization single most important factor in assessing geologic CO_2 storage locations. Yet our knowledge of low permeability flow, porosity changes due to mineralization, or detecting small cracks or fractures is limited.



Geothermal reservoir characterization by 3D Geophysical Imaging

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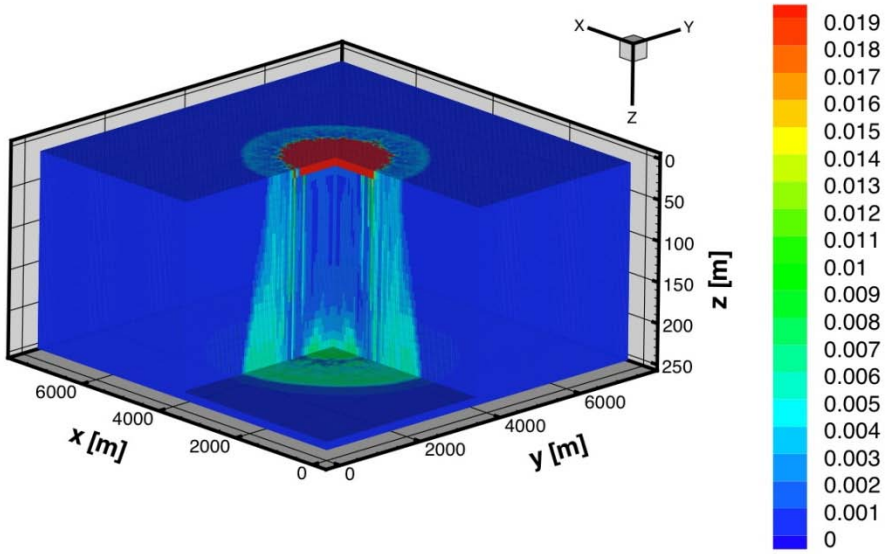
Basic Research Needs in Geosciences

- Grand Challenge**: Simulation of Multiscale Systems for Ultra-Long Times**
  - Geologic sequestration requires establishing the safety and security of the site for hundreds of years to as long as a million years.
- Priority Research Direction**: Fluid-Induced Rock Deformation.**
  - CO_2 injection induces large pressure transients that affect thermal, mechanical, hydrological and chemical states of subsurface volumes that can span hundreds of kilometers. Accurate forecasting of these effects requires improved understanding of rock stress-strain and flow response to fluid induced pressure changes.



Modeling CO_2 sequestration at the Basin Scale
Plot of dissolved CO_2 after an elapsed time of 300 years following injection of supercritical CO_2 into a sandstone reservoir.

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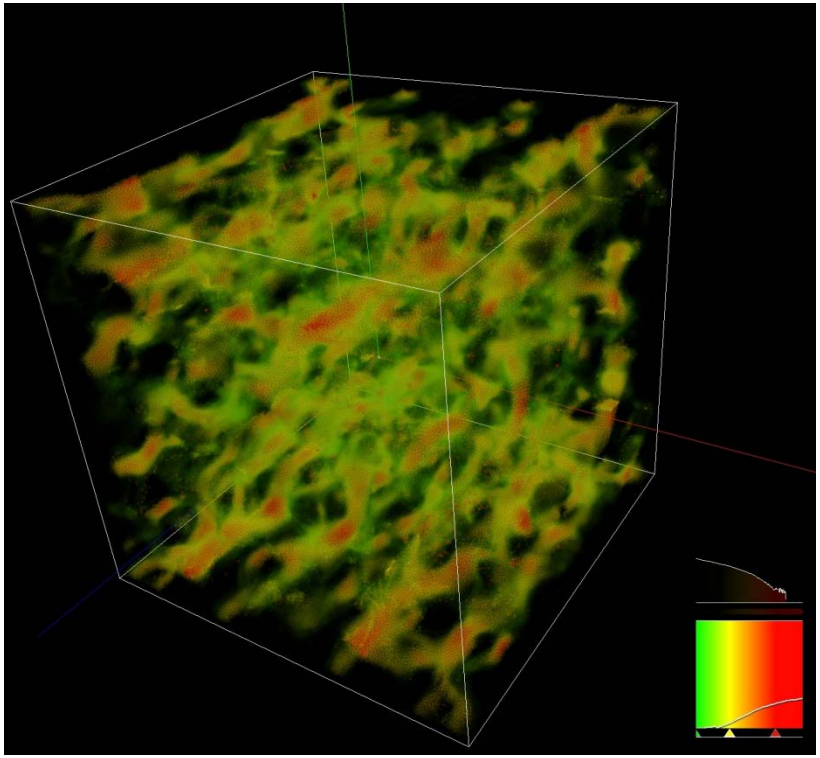
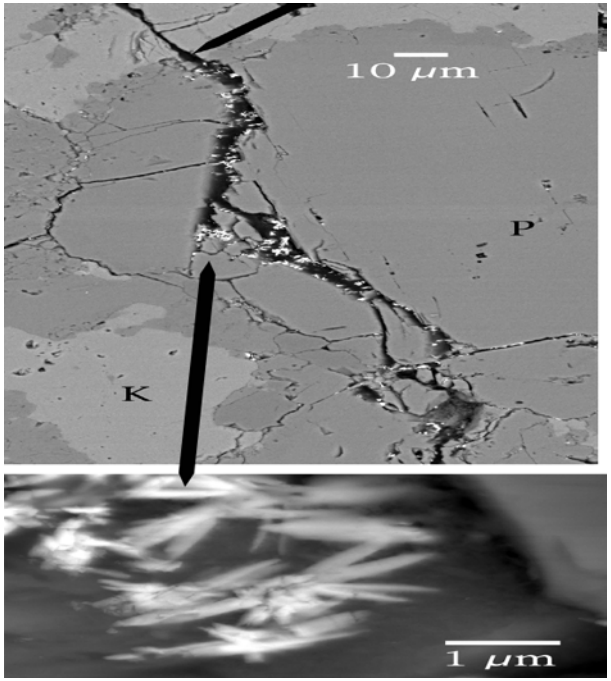
Basic Research Needs in Geosciences

- **Priority Research Direction: Dynamic Imaging of Flow and Transport**
  - Real-time dynamic imaging of flow, transport, and chemical reactions *in situ* essential for managing wastes in the subsurface.



SPH Simulation of 3D Pore scale flow



Uranyl silicates within microfractures of a single granitic clast at the micron observation scale.

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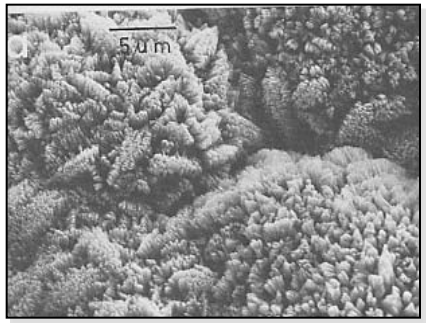
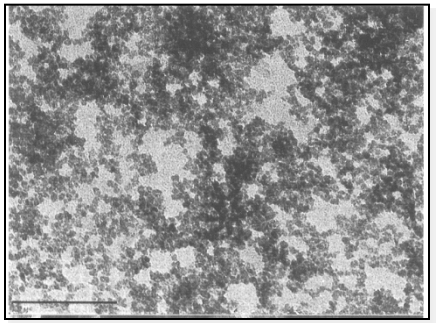
Basic Research Needs in Geosciences

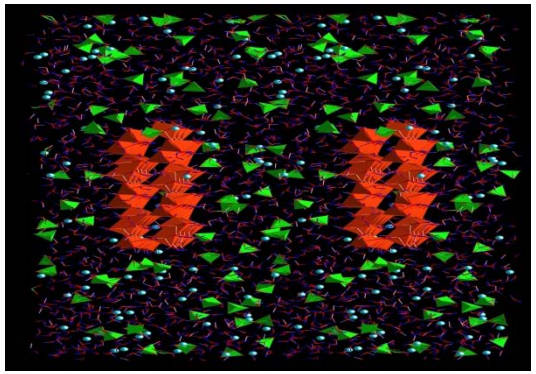
- Grand Challenge**: Computational Thermodynamics of Complex Fluids and Solids.**
  - Prediction of long-term reaction rates from short term experiments, the influence of mixed-multicomponent solvents, and better theories of interfacial reactivity and dynamics.
- Priority Reseach Direction**: Mineral-Water Interface Complexity and Dynamics.**
  - Theme of moving from statics to dynamics to examine long term interfacial changes and reactivity.
- Priority Research Direction**: Nanoparticle and Colloid Chemistry and Physics**
  - Ultra low levels of actinide nanoparticles (10^{-14}M) can drive the repository performance assessment, yet we have no unified theory for colloid/nanoparticle transport in the subsurface.

Goethite



6-line Ferrihydrite





MD simulation of goethite particles in $NaClO_4$ solutions
(Cover picture for Director's Perspective
2001 NERSC annual report)

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Future Trends

- Experiment and Theory need to go hand in hand.
  - Laboratory and field characterization will increase
    - Field scale – enhanced electrical, magnetic and well data; as well as efforts to develop new and unique subsurface probes (nanophase – chemical characterization).
    - Microscale – advanced instrumentation for characterizing pore structure, fluid composition, mineral assemblages, and microfluidics
    - Molecular scale – next generation synchrotron facilities, advanced NMR, XPS, TEM, non-linear optics … for determining molecular structure and composition.
  - Computational methods will be challenged to interpret these data sets and project future impacts.
    - Especially important in Geosciences since the systems can be quite complex

Future Trends

- Move from statics to dynamics
  - Current focus at molecular scale examining interfacial reactivity and electron transfer (redox).
  - Molecular simulation limited to bond breaking/formation and there is a need to couple to hydrodynamics to better predict reaction rates and mechanisms.
- Ability to treat increasingly complex materials
  - The ability to synthesize increasingly complex materials with known structure will greatly facilitate model development and reliability
  - Crucial impact on geosciences

Multiscale Simulations

Yucca Mt.

field

Finite Element Analysis and Continuum Methods

Detail

molecular fragments

Mesoscale Modeling

atoms

Molecular Mechanics

e

Quantum Mechanics

Application

Waste Repository PA Requirement

log Distance (m)

6 3 0 -3 -6 -9

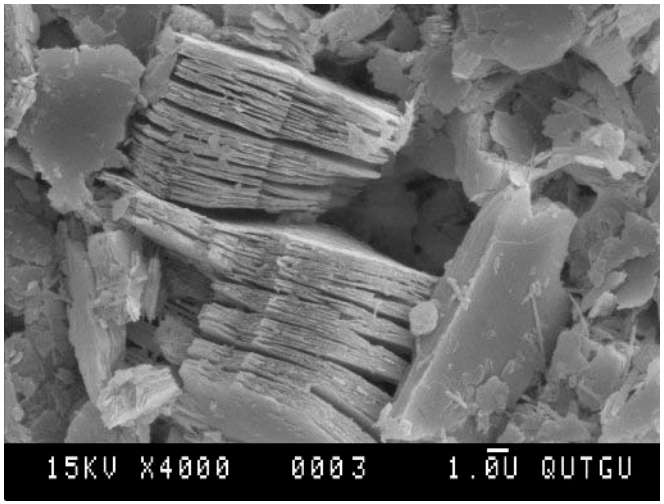
km m mm μm nm Å

-15 fs -12 ps -9 ns -6 μs -3 ms 0 s 3 min 6 day 9 year 12 ka 15 Ma

log Time (s)

Computational Challenges in Molecular Geochemistry

- Complex chemistry with multicomponent systems, disorder, and vacancies
  - Need capabilities to do calculations on large representative systems.
- Nanocrystalline materials (less than 1 μm grain size)
  - Surface structures at 10-100nm often govern surface reactivity
  - Significant electrostatic fields (double layer) associated with surface structures
- Accumulation of protons at the surface controls sorption processes
  - Dissociative model for water allows H_3O+, OH- formation
  - Protonation/deprotonation of surface functional groups.



Clay minerals in deep-sea sediments exhibiting layer structure and reactive edge sites

- Non-equilibrium Processes
  - Redox processes, mineral dissolution and nucleation/growth kinetics
  - Intermediates in reaction control rates (difficult to experimentally evaluate)

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Current Research Programs (AR Felmy PI)

- Molecular Mechanisms of Interfacial Reactivity in Near Surface and Extreme Geochemical Environments (5 projects total).
  - Coupled Surface and Solid-State Charge and Ion Transport Dynamics at Mineral/Water Interfaces (K.M. Rosso, S. Kerisit, P Meakin)
    - Kinetic Monte Carlo and *ab initio* molecular dynamics simulations of surface structures
    - A*b initio* calculations of parameters in electron transport rate theory (reorganization energy, electronic coupling matrix elements…)
  - The Influence of Reaction Pathways on Reduction of U(VI) to U(IV): The Role of the Intermediate U(V) Species (E.S. Ilton, P.S. Bagus)
    - Simulation of U Core level spectroscopies for interpretation of XPS spectra.
  - Development and Application of Next Generation Parameter Free Petascale Simulation Technology for Solution Species, Nanoparticles and Geochemical Interfaces (E.J. Bylaska, J.H. Weare).
    - Development of *ab initio* Molecular Dynamics
- SISGR: The Role of Interfacial Processes on Mineral Transformations in Wet Supercritical CO_2 (J.R Rustad, D.A. Dixon)
  - Development of a molecular dynamics model for orthosilicate surfaces
  - DFT calculations of CO_2/water surface interactions.