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Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems

Examples of how high performance computing can facilitate these discoveries.

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Outline

- The BRN for Geosciences:
  - Purpose and Organizing Principals
  - Scientific Challenges
    - Scientific Grand Challenges
    - Priority Research Directions
- What we can do now with HPC (petascale focus)?
  - Introduce selected examples

Basic Research Needs for Geosciences

- Purpose and Organizing Principles
  - Sponsored by the Geosciences Research Program within the Office of Basic Energy Sciences.
    - Organizers DePaolo (LBL) and Orr (Stanford)
  - Driving principal was that long-term geologic sequestration represented an critical limitation to advancing the Nation's new energy future.
    - Geologic sequestration of greenhouse gases (CO_2)
    - Nuclear waste disposal.

Basic Research Needs for Geosciences

- Purpose and Organizing Principles
  - Focus was on long-term deep geologic sequestration of greenhouse gases and nuclear wastes.
  - Panelists selected primarily based upon their expertise in these areas:
    - Multiphase flow and transport
    - Imaging geologic systems
    - Colloidal and nanoparticle transport
    - Interfacial and actinide chemistry
    - Limited biogeochemistry (extreme conditions)
  - Near surface environmental remediation not emphasized.
    - Many identified science challenges also applicable

Basic Research Needs for Geosciences

- Scientific Grand Challenges
  - **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.
  - **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.
  - **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.

Basic Research Needs for Geosciences

- Priority Research Directions
  - Mineral-Water Interface Complexity and Dynamics.
    - Theme of moving from statics to dynamics to examine long term interfacial changes and reactivity.
  - 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.
  - Biogeochemistry in Extreme Subsurface Environments
    - Geologic waste disposal creates unique environments (acidic conditions – CO_2; high temperature, high radiation, with reduced metals – nuclear waste) for microbial communities.

Basic Research Needs for Geosciences

- Priority Research Directions
  - 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.
      - Development of smart tracers, electromagnetic imaging of the subsurface
  - 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.
  - 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.

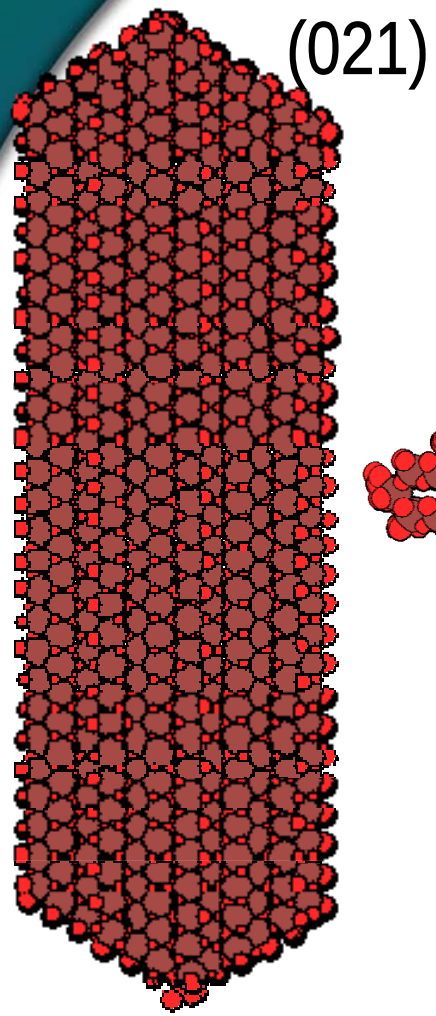
What we can do now with HPC (toward petascale) computing

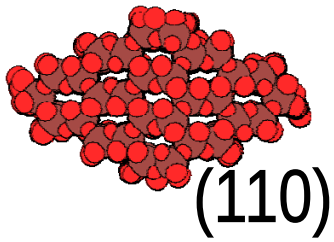
Examples:

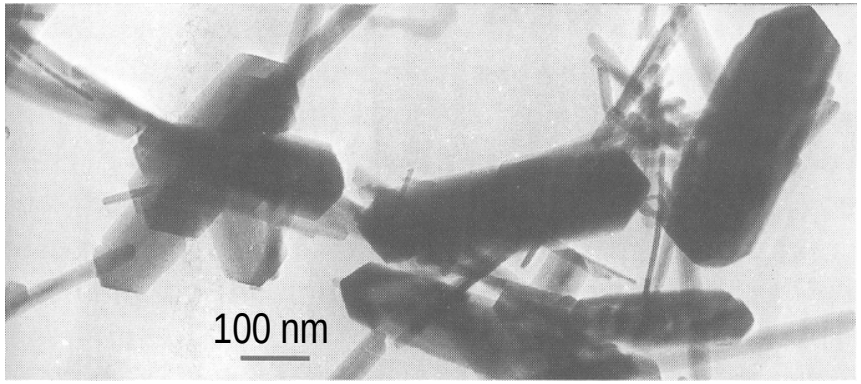
Mineral-Water Interface Complexity and Dynamics

- **Science Challenge**: The Edge Effect: Can overall mineral behavior be resolved into contributions from individual surfaces?
- **HPC Application**: Molecular Dynamics Simulations of Solvated Goethite Nanoparticles Protonated to Neutral Charge (Rustad and Felmy GCA 6, 1405, 2005)
  - Simulations of goethite particles with the same total overall surface area but different ratios of 021/110 surfaces.
  - Using a dissociating model for liquid water.

Mineral reactivity being the sum of surfaces (Goethite morphology in laboratory samples)



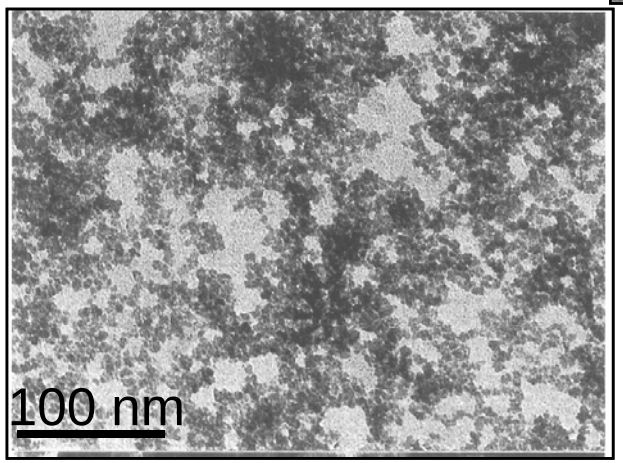




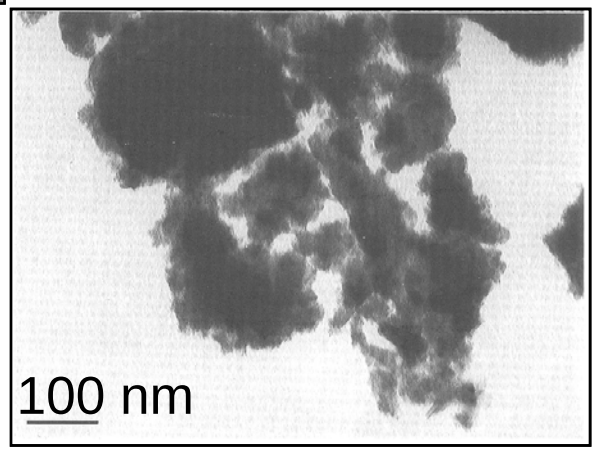
Cornell and Schwertmann
Iron Oxides in the Laboratory
VCH, Weinheim 1991

Natural Sample Complexity

Goethite a-FeOOH



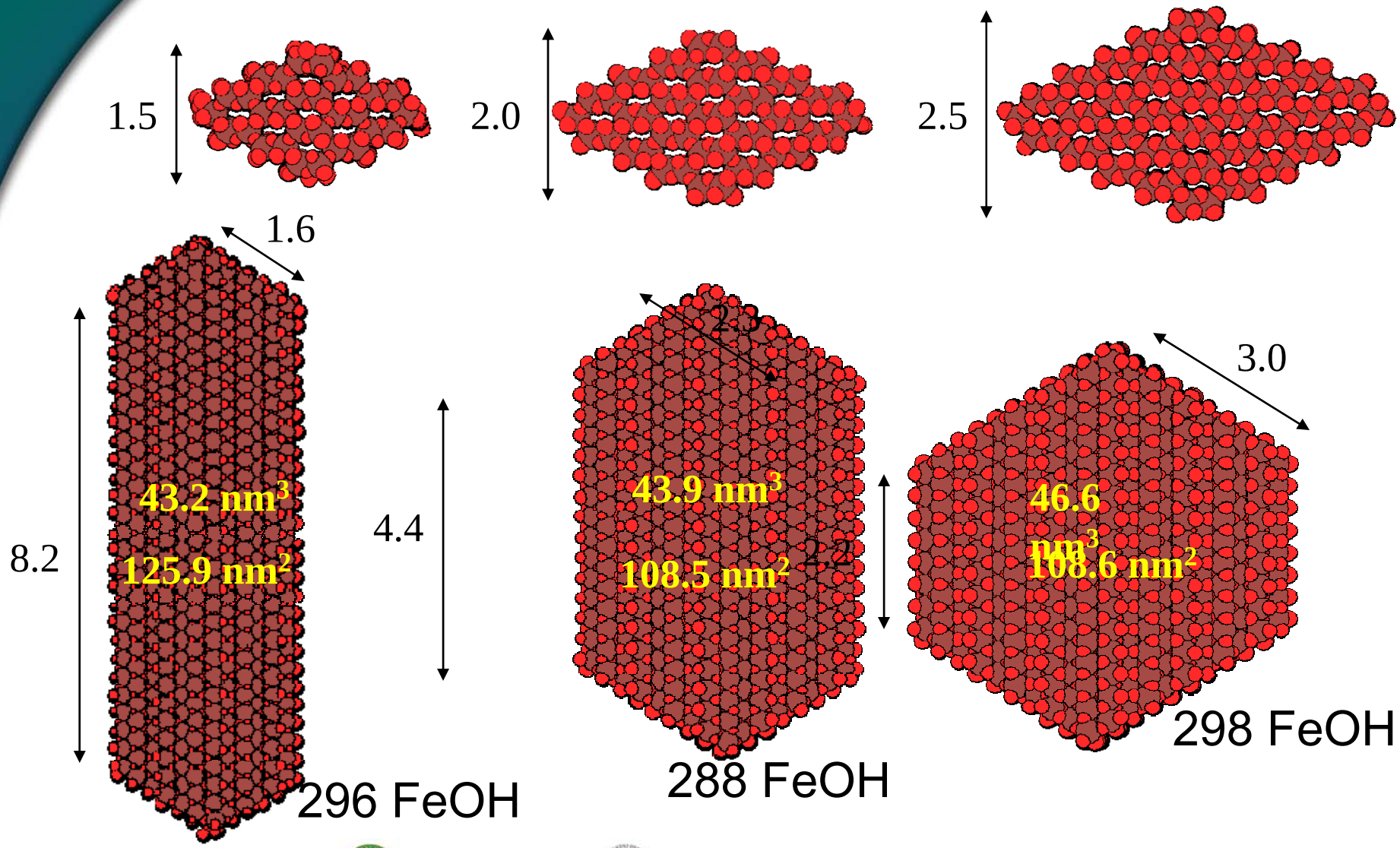
6-line Ferrihydrite



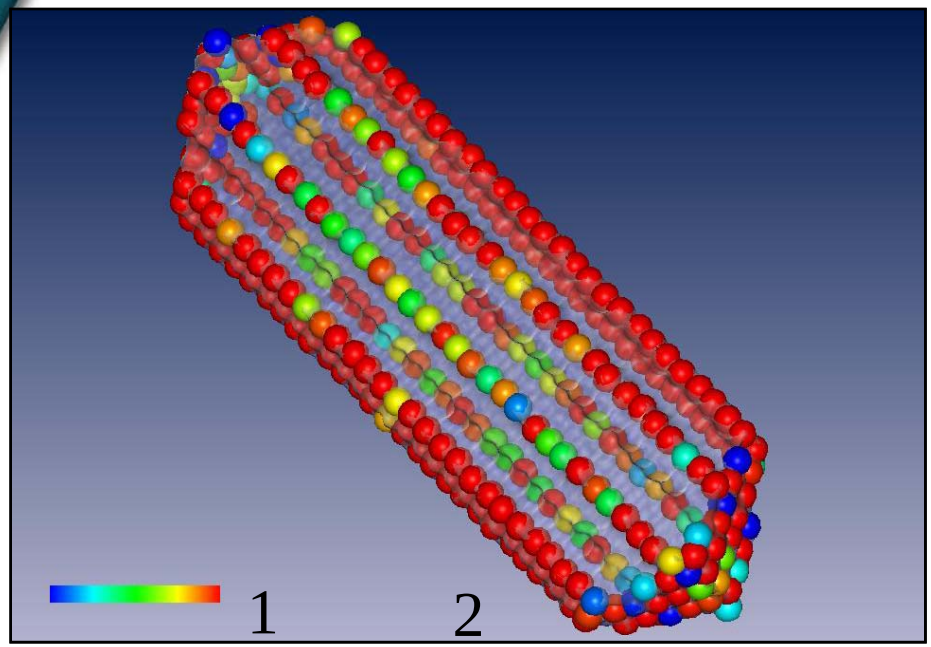
2-line Ferrihydrite

Molecular Dynamics Simulations of Solvated Goethite Nanoparticles Protonated to Neutral Charge

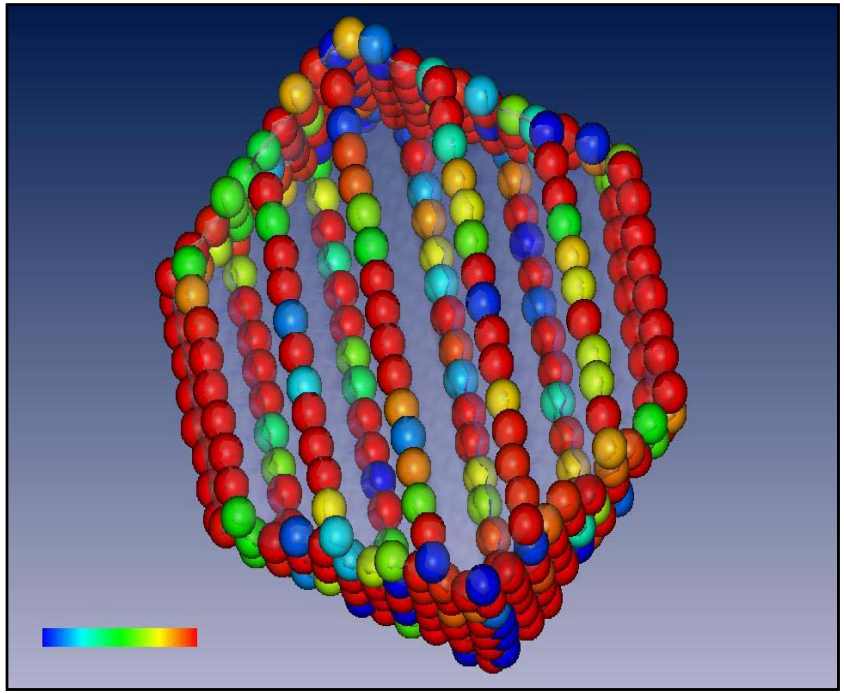
(Rustad and Felmy GCA 6, 1405, 2005)



MD Simulations of Model Goethite Nanoparticles Calculated Proton Distributions for Different Particle Shapes



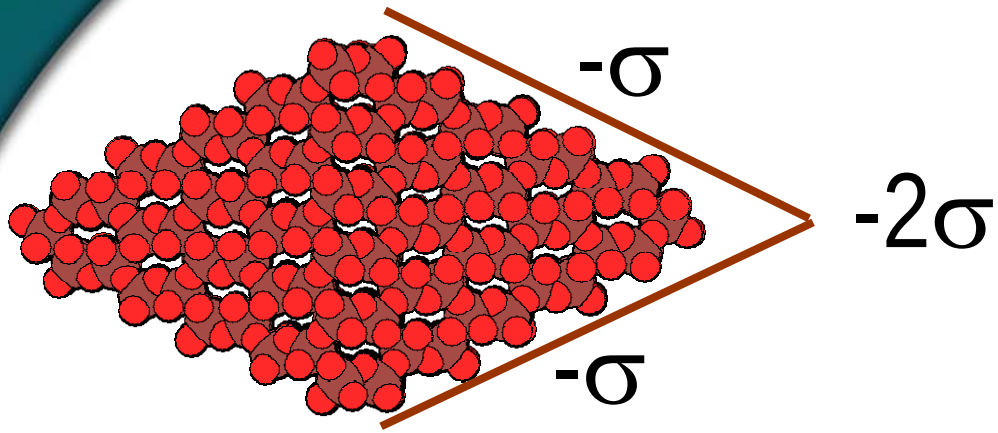
Acicular



Equant

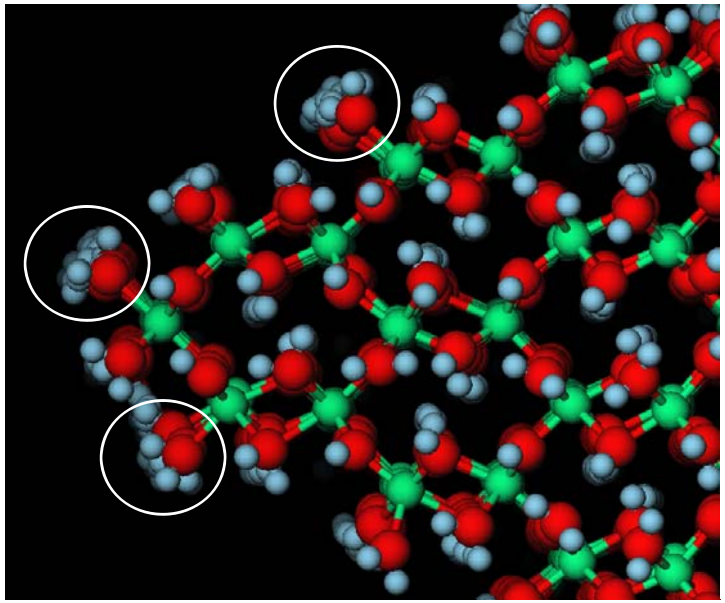
No relationship to original 110/021 ratio

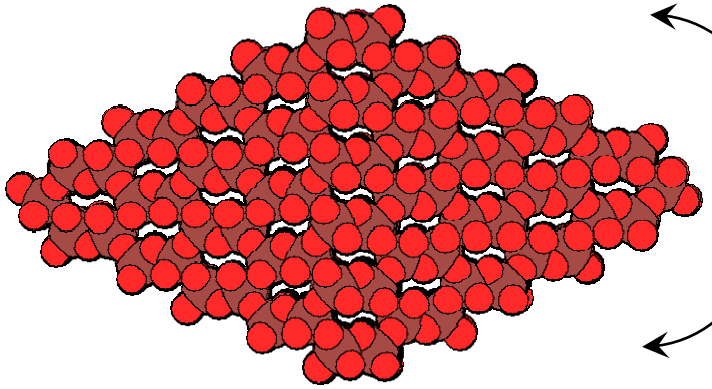
Why do Protons Accumulate Non-homogeneously on the Particles?



Charge Deficit

Crystal Chemical



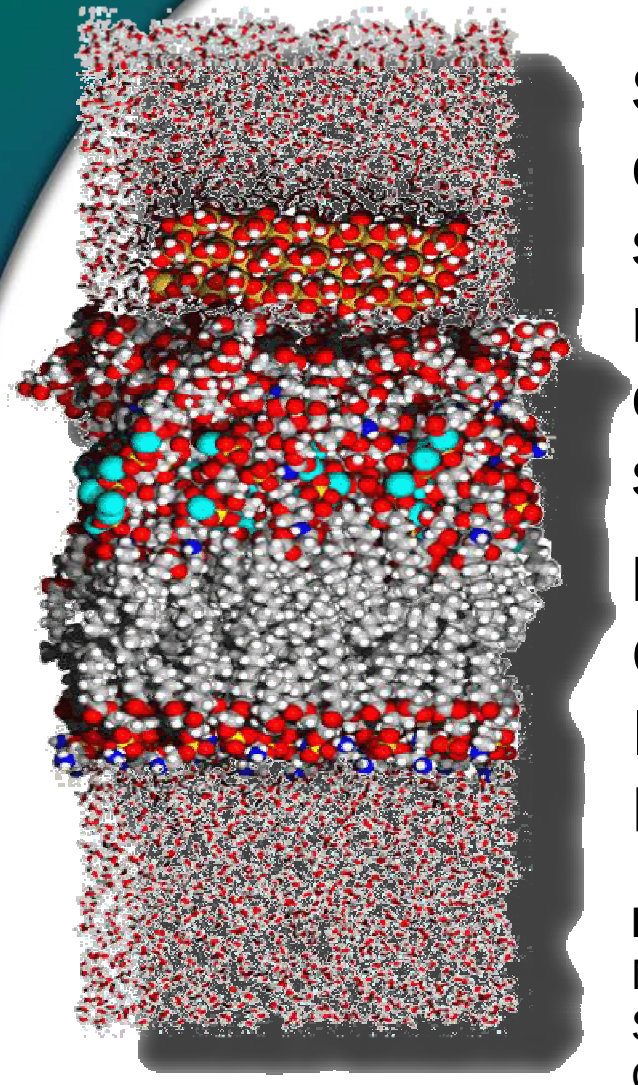


High Dielectric

Benefits of HPC

Challenges people to think.

Biogeochemistry in Extreme Subsurface Environments



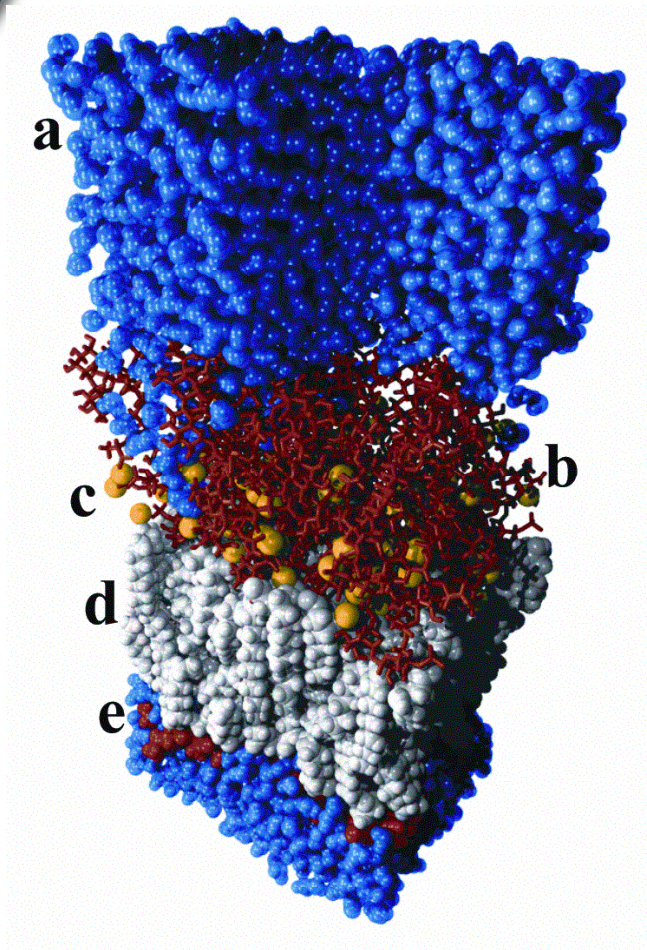
Science Challenge: What microbial communities evolve under extreme subsurface conditions and what unique reactions will occur between these organisms, subsurface minerals, and solutions?

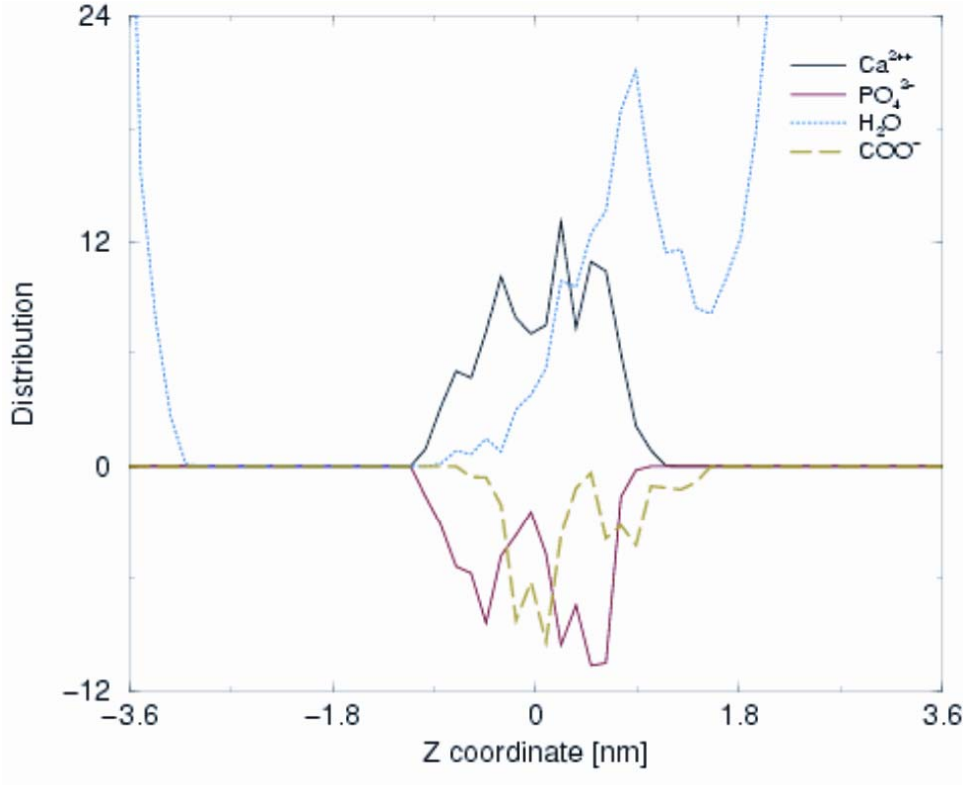
HPC Application: Characterization of Geochemical Reactions at the Interface between Microbial Membranes and Mineral Surface

R. M. Shroll, and T. P. Straatsma, "Molecular Basis for Microbial Adhesion to Geochemical Surfaces: Computer Simulation of *Pseudomonas aeruginosa* Adhesion to Goethite",Biophysical Journal, **84**, 1765-1772 (2003).

Towards a new geochemical model for metal binding on microbial surfaces

(Solvated *P. aeruginosa* Membrane)



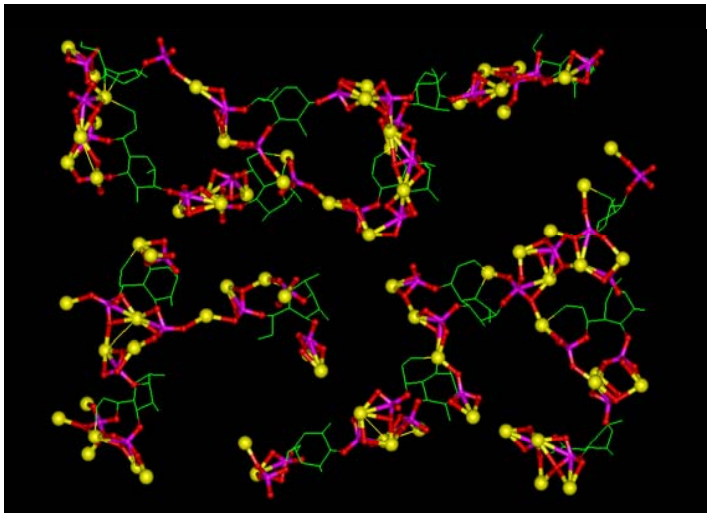


Axial distribution of functional groups and water in the outer membrane of *P. aeruginosa*.

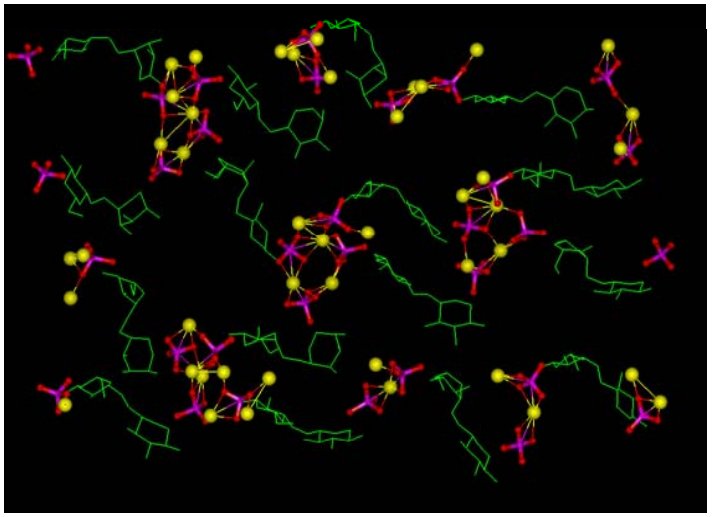
Metal-Ligand Clustering in *P. aeruginosa membrane*

Do such clusters form precursors for biomineralization reactions in natural systems?

Outer Core



Inner Core

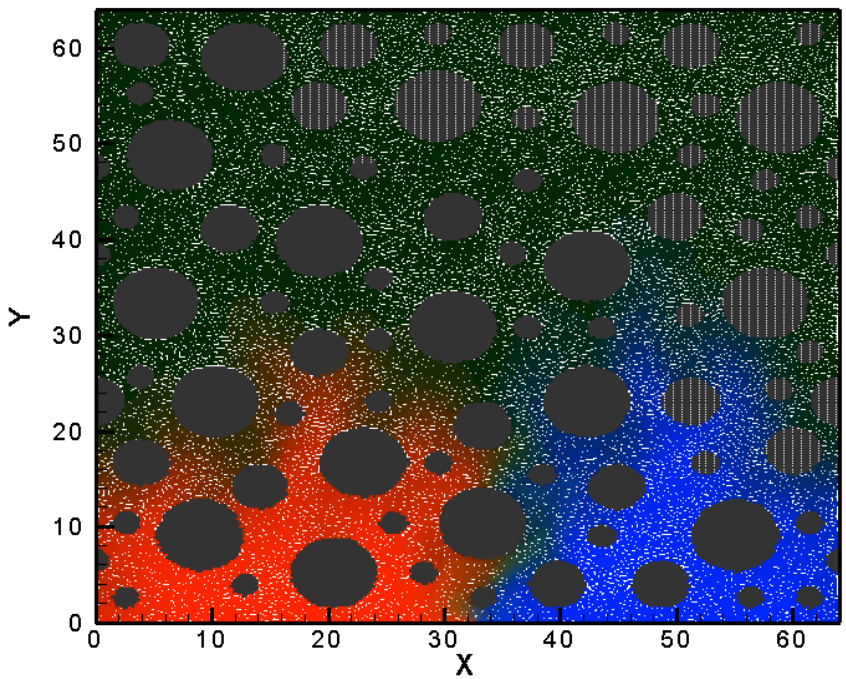


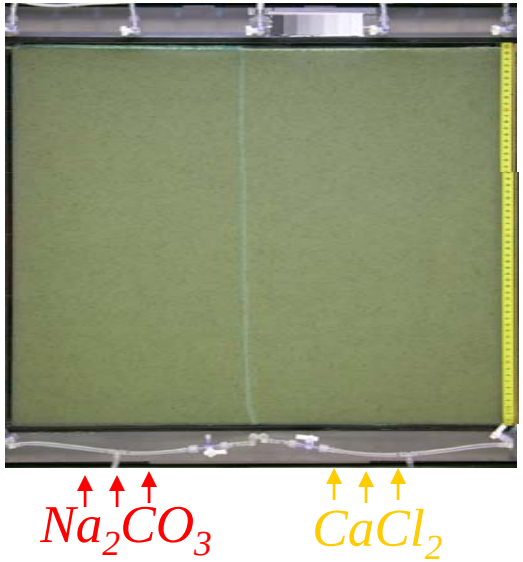
Transport Properties and In Situ Characterization of Fluid Trapping, Isolation, and Immobilization

- **Science Challenge**: Prediction of coupling between mineral precipitation and flow in complex geologic systems.
- **HPC Application**: Pore-scale modeling of coupled transport and reaction using Smoothed Particle Hydrodynamics (SPH)

Transport Properties and In Situ Characterization of Fluid Trapping, Isolation, and Immobilization

Side-by-side injection of reacting solutions into two halves of a two-dimensional granular porous medium.



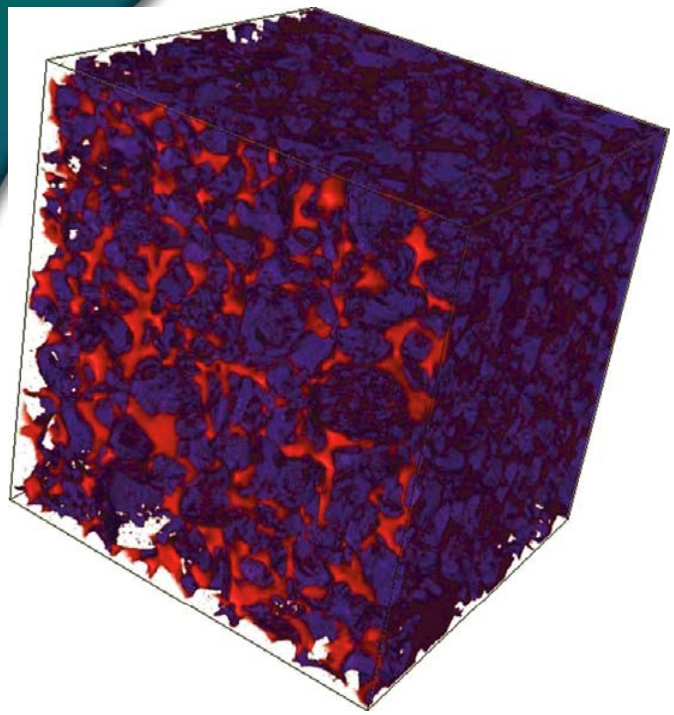


Smoothed Particle Hydrodynamics (SPH) simulation of solute transport, mixing and precipitation reaction

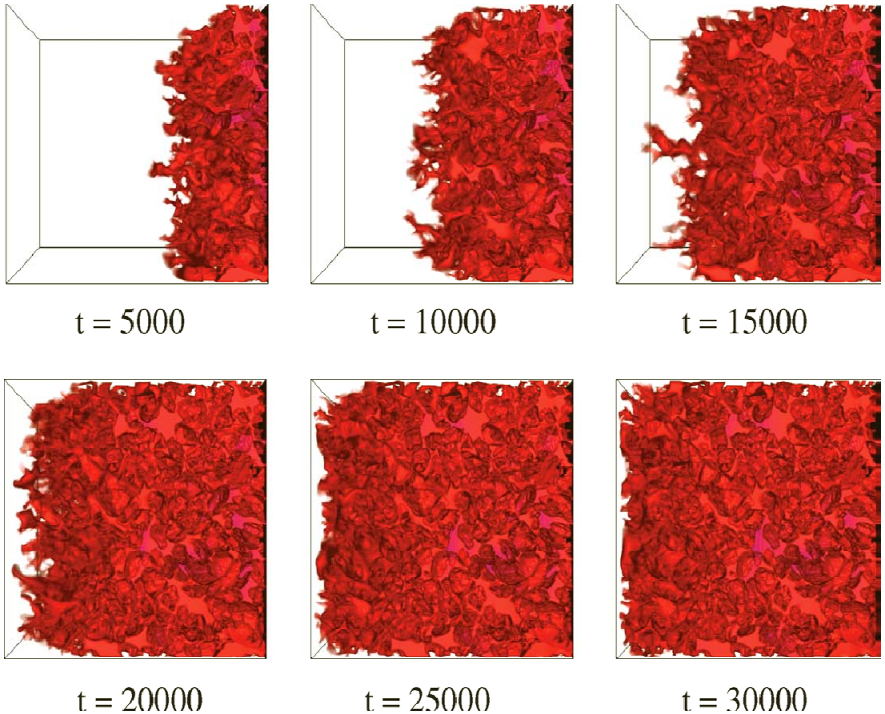
Transport Properties and In Situ Characterization of Fluid Trapping, Isolation, and Immobilization

- **Example:** Multiphase flow in subsurface systems
- **Science challenge**: Unraveling the influence of introduced non-aqueous solvents (supercritical CO_2) on the displacement of subsurface brines, the trapping of solution in pores or fractures, and projections of small scale fracturing or flow paths.
- HPC Application: Large scale lattice Boltzmann simulations of multiphase flow.
  - Explicit finite difference method that does not require a parallel solver and very little message passing in streaming the particle distribution function.
  - Large scale smoothed particle hydrodynamics simulations
  - Use geometries from high resolution x-ray tomography and/or model geometries

Large-scale Lattice Boltzmann Simulations of Complex Fluids

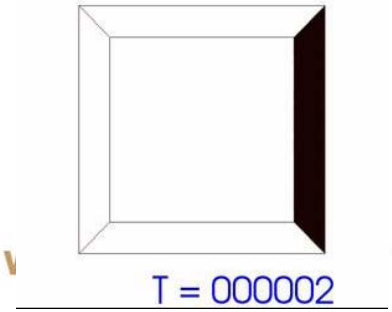


Bentheimer sandstone,
512×512 ×512
4.9 μm resolution



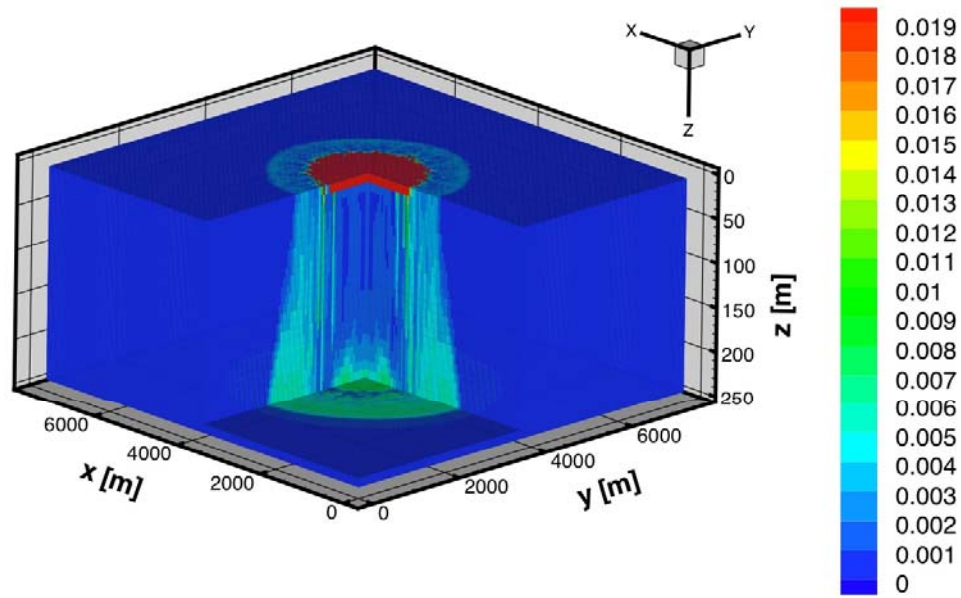
Harting *et al*., Philosophical Trans. Roy. Soc. 363, 1895-1950 (2005).

Linking of X-Ray tomography imaging with Lattice-Boltzmann simulations of multiphase flow. Enhanced imaging experiments needs to be married with advances in HPC.



Modeling CO_2 Sequestration at the basin scale

- Extensive fingering occurs due to the density instabilities caused by the heavier CO_2+brine fluid.
- The red colored region corresponds to a separate supercritical CO_2 phase where the brine is saturated with CO_2.
- Essential for challenging and refining conceptual models of CO_2 reservoir emplacement.



Plot of dissolved CO_2 after an elapsed time of 300 years following injection of supercritical CO_2 into a sandstone reservoir. No flow boundary conditions are imposed at the top and bottom of the domain.

Dynamic Imaging of Flow, Transport and Fluid Identification

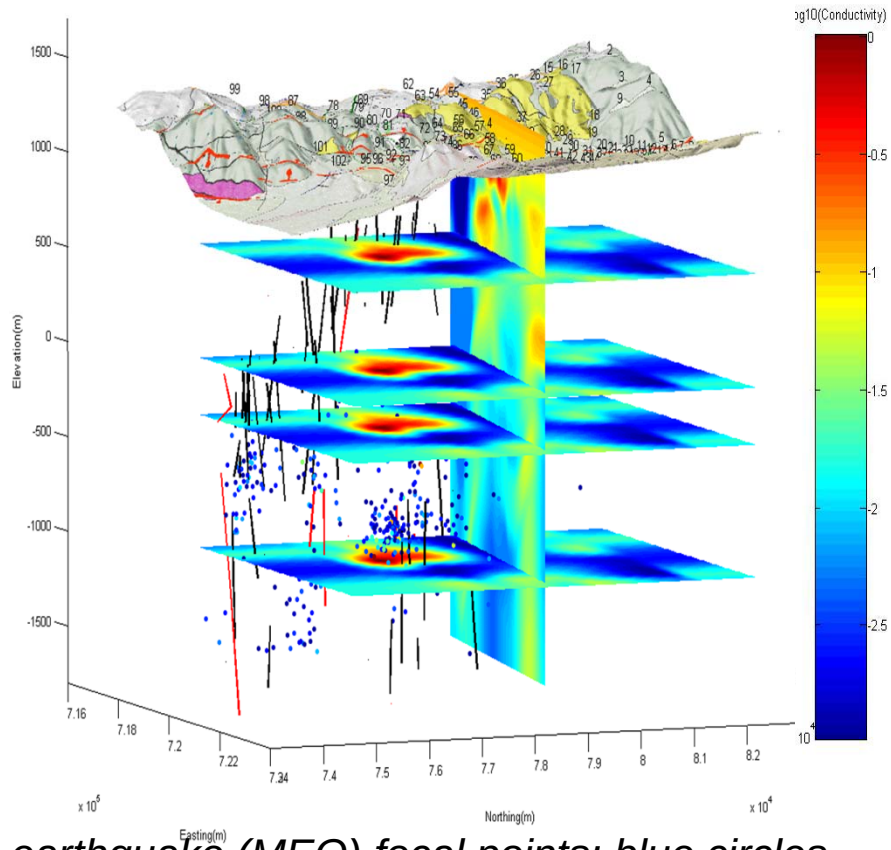
- **Example**: 3D geophysical Imaging.
- **Science Challenge**: Utilizing large geophysical data sets to render a meaningful image of the deep subsurface geology through a non-linear imaging process.
  - 3D data sets extremely expensive to obtain
- **HPC Application**: Large scale 3D subsurface imaging experiments
  - Current technology
    - Near petascale (32,000 cores IBM BG/L)
  - 12-18 months applications of petascale computing
    - 100,000s of cores do able.
  - 3-5 years
    - Large scale multi-scale, multi-physics imaging, appraisal, and uncertainty quantification.
    - Petascale and beyond

3D Geophysical Imaging
(geothermal reservoir characterization)

- 3D electrical conductivity subsurface map of the Coso geothermal reservoir (Southeastern California).

  Depth range 3Km from the surface.

  Lateral scale 6kmX8km.
- The central conductive (red) feature in model is a magmatic intrusive with well production on the boundaries associated with high temperature fractures.



Micro earthquake (MEQ) focal points: blue circles
Well production intervals: black linear segments
Well injection intervals: red linear segments.

Summary

- HPC (including petascale) can facilitate scientific and technical discoveries in several areas of importance to Geosciences.
  - Dynamic Imaging of Flow and Transport
  - Transport Properties and In Situ Characterization of Fluid Trapping, Isolation, and Immobilization
  - Mineral-Water Interface Complexity and Dynamics
  - Biogeochemistry in Extreme Subsurface Environments
- Can challenge the way we think about representing and studying geochemical and geologic systems.
- Can provide a vision for what is possible.
  - Not a tool for the masses