Computational Sciences at NREL

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Computational Sciences Center Director

Outline

- Background
- C.S. at NREL
- Capabilities and Expertise
- Next Steps

Background

- NREL's newest Center: The Computational Sciences Center was formed in March 2002.

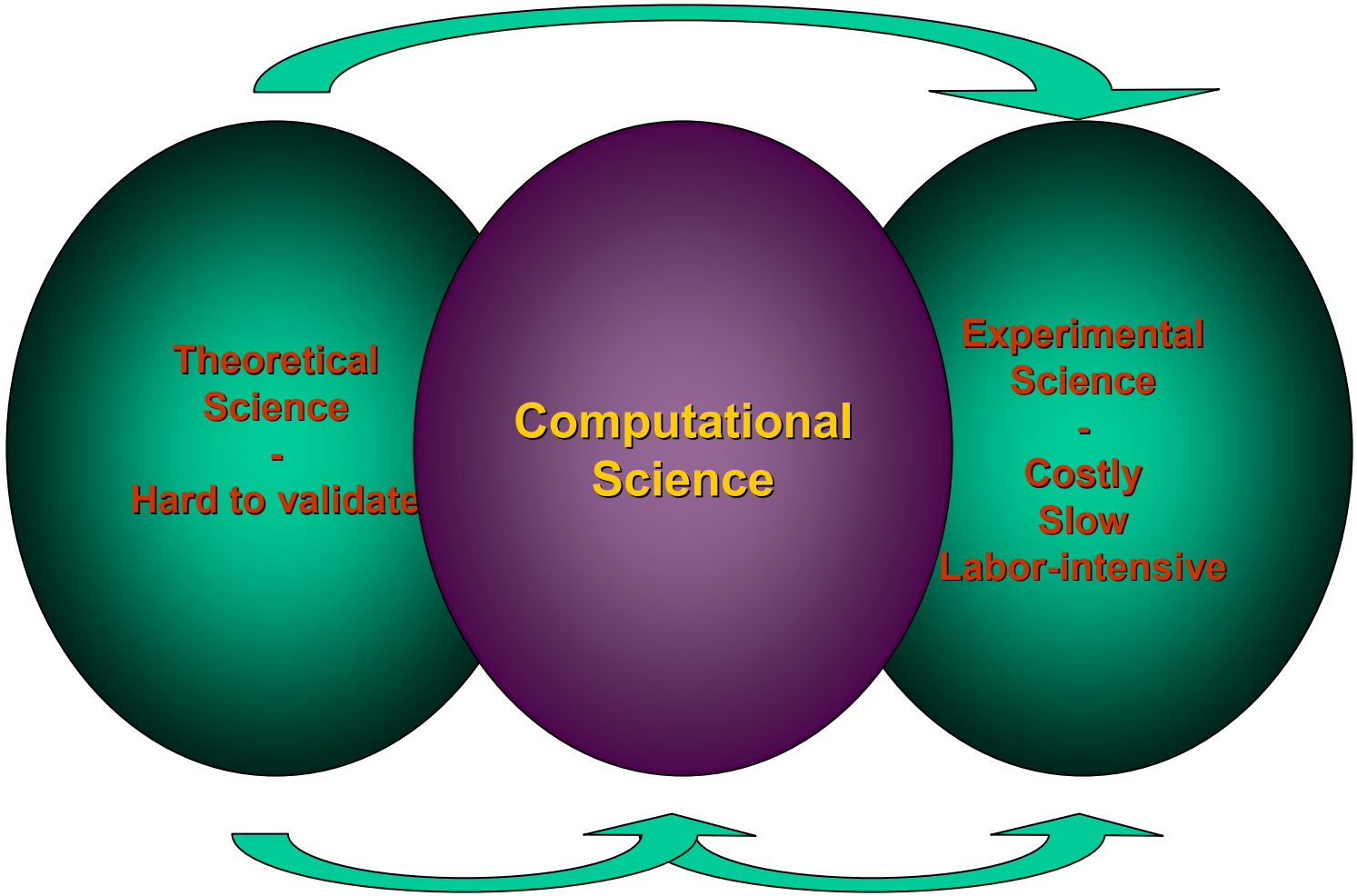
- Mission: perform world-class computational science research and provide high performance computing capabilities, leadership, and expertise enabling advances in the leading edge of renewable energy and energy efficiency technologies.
  - Support for large-scale modeling, simulation, & visualization
  - Collaboration with other Labs and Universities

Computational Sciences at NREL

- Computation is an equal and indispensable partner, along with theory and experiment, in the advance of science and engineering.
- Numerical simulation enables the study of complex systems and natural phenomena that would be too expensive or dangerous, or even impossible, to study by direct experimentation.
- Explore more of the design space than is feasible through prototyping.

C.S. Improves the Scientific Process

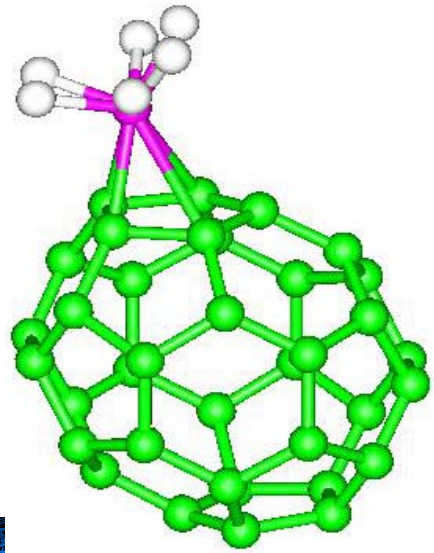
Traditional scientific process moved from the theoretical to the experimental.

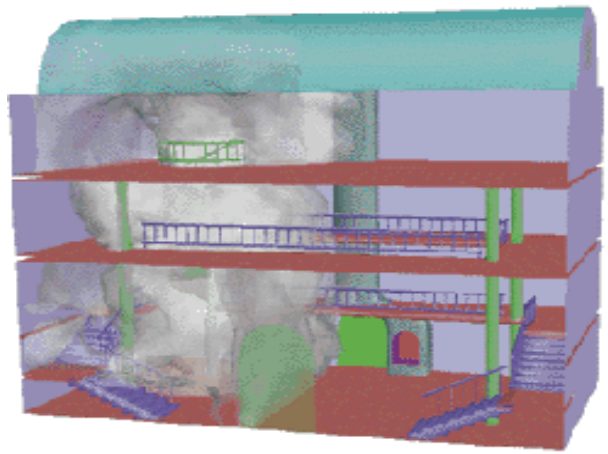


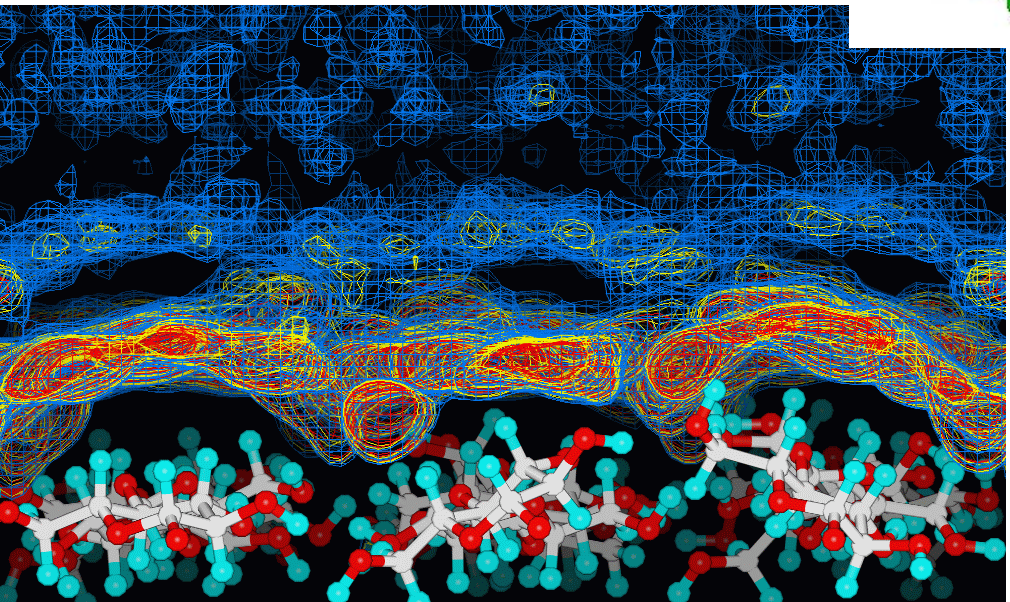
Computational science creates a model of the experimental environment resulting in reduced cost, accelerated cycle time, and increased research effectiveness.

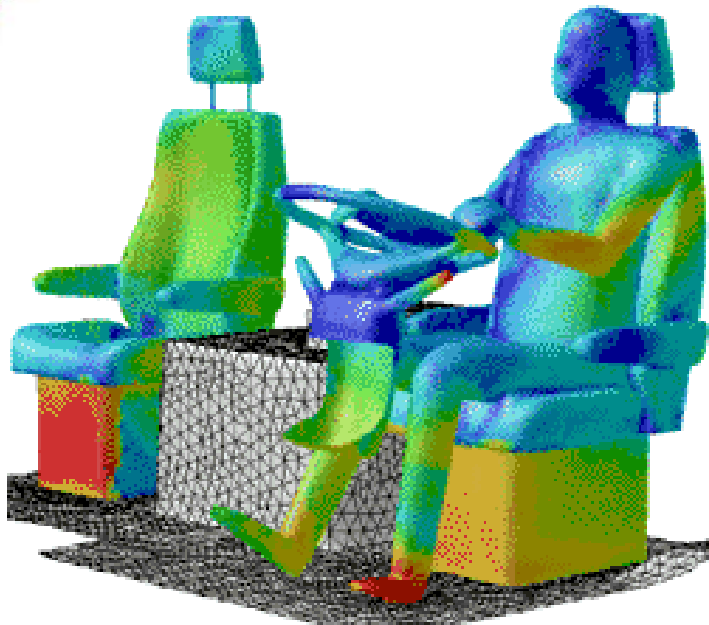
Laboratory-wide Opportunities

H_2 Binds to Iron-Doped C_{36}









C.S. Focus Areas

- **Simulation**: Numerical methods & algorithms
  - Computational fluid dynamics (wind, buildings, trans.)
  - Computational biology & chemistry (biomass, H2)
  - Structural mechanics (buildings, wind, trans.)
  - Solid State Physics (basic science, PV)
- **Data**:
  - Analysis and Visualization (all centers)
- **Integration and Work Flow**:
  - Tools, Systems, and Enterprises (all centers)

Staff

- Sr. computational scientist (physics)
- Computational Scientist (solid state theory)
- HPC system manager
- Post doc (mathematics)

Capabilities

- 64 Processor IBM computer.
- 20 PE Linux cluster test bed.
- Delivery of new HPC system in July – ~10x performance of IBM.
- New SuperNode system.
- Wide variety of modeling software
  - Fluids, Heat transfer, Chemistry, Molecular Dynamics, etc)
- Prototype stereo visualization system.

Outreach

Building relationships with Universities.

- Nanoscience grant from SC, UTenn.
- Assisting School of Mines subcontractors in biomass conversion.
- Expertise in simulation and modeling for photobiology – H_2 production from algae (Univ of Illinois).
- HFI – collaboration with ASU, UIUC

- Establishing a culture of high performance computing at NREL, sharing with Universities.

Computational Photobiology

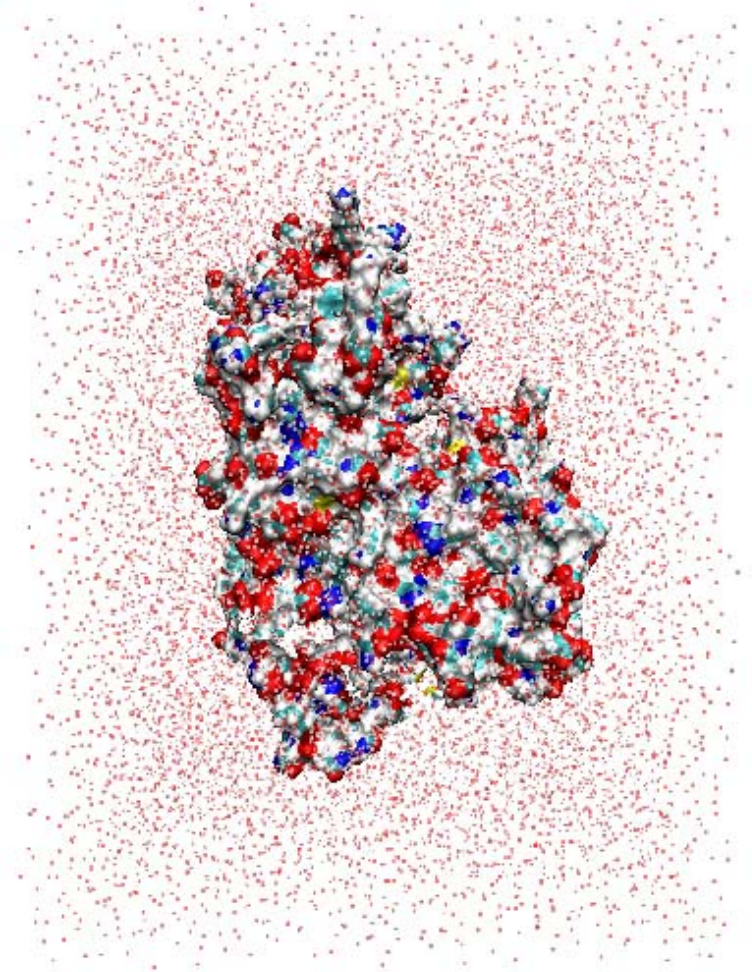
- Goal: Use Molecular Dynamics simulation to identify and understand the O_2 and H_2 diffusion mechanism. Simulation results guide genetic modification to Algal Hydrogenase to optimize H_2 production.

- Who: Paul King (Basic Sciences Post Doc), Jordi Cohen (UIUC), Kwiseon Kim, Wes Jones

- Progress: Modeling protein in water
  - 57,000 atoms including 9,000 atom protein and explicit water molecules.
  - Molecular Dynamics via enhanced sampling
    - H2 diffusion: ~0.2 ns (20 hrs on 20 CPUs)
    - O2 diffusion: longer ~5ns (8 days on 20 CPUs)

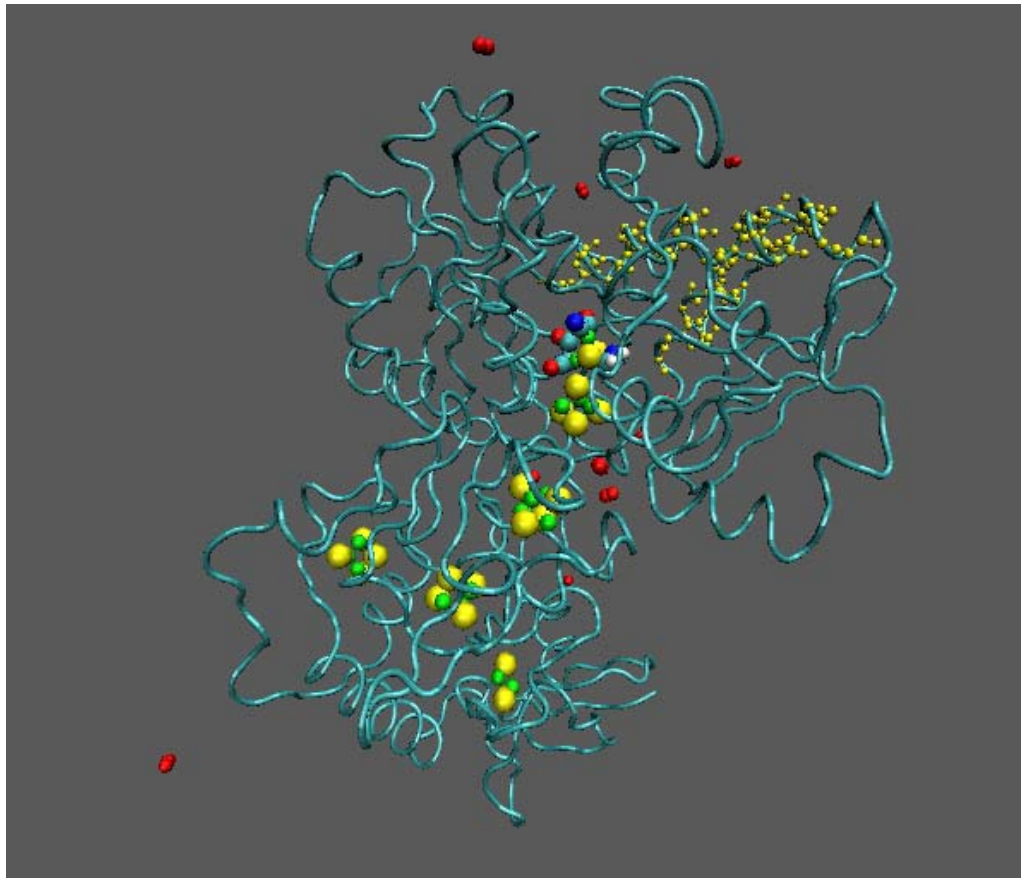
Need to run many times with different configurations, very large computational requirements.

Cp1 molecule in water



Molecular modeling set up
~57,000 atoms including
~9,000 atom protein and
explicit water molecules.

Snapshot of H_2 diffusion simulation



Cp1 (blue tubes) with H2 (red), active site metal clusters (HC1) are shown (large yellow)

Next Steps

- Look for joint funding opportunities and grants with NREL researchers.
- Expand relationships with Universities.
- Currently supported by Lab overhead.
- Need annual programmatic support from EERE and SC for sustained success.

Summary

- Investing in Computational Sciences to increase expertise and capability in high performance computing is integral to fulfilling NREL's mission.
- Computational Sciences is making great progress in a very short amount of time.