Visualization in Molecular Science

Ray Bair Visualization Frameworks Workshop 6/2/03

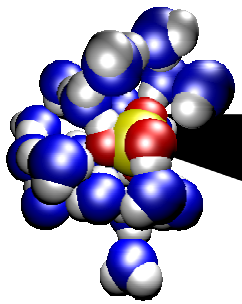
- Structural features and relationships are central to understanding the chemical and physical properties of molecules and their interactions
  - Absolutely necessary, but not sufficient
- Over 100 years, visualizing of the invisible
  - from schematic drawings (Kekule's benzene)
  - to ball-and-stick model sets
  - to sophisticated molecular modeling environments
- Established community conventions
  - 2D and 3D representations of molecular properties (e.g., atomic positions, volume, electron density, charge)

State of the Practice

- Visualization is an integral part of molecular science problem solving at all stages
  - Computation design, monitoring, and analysis
- Ubiquitous desktop visualization capabilities
  - Many similar tools offer base functionality
  - Quickly render 10^5-10^6 atom systems
  - Experience building interactive frameworks [arch. *matters*]
- Lack of powerful mol. sci. viz components
  - Significant limitations to commercial frameworks, e.g., AVS, Molecular Inventor, web viewers
  - Scarce tools for high performance mol. sci. rendering on high rez (tiled/immersive) devices

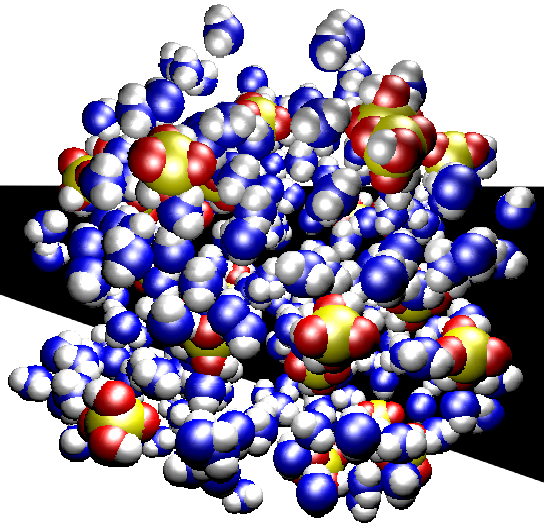
Physically accurate calculations challenge visualization capabilities and paradigms

1997



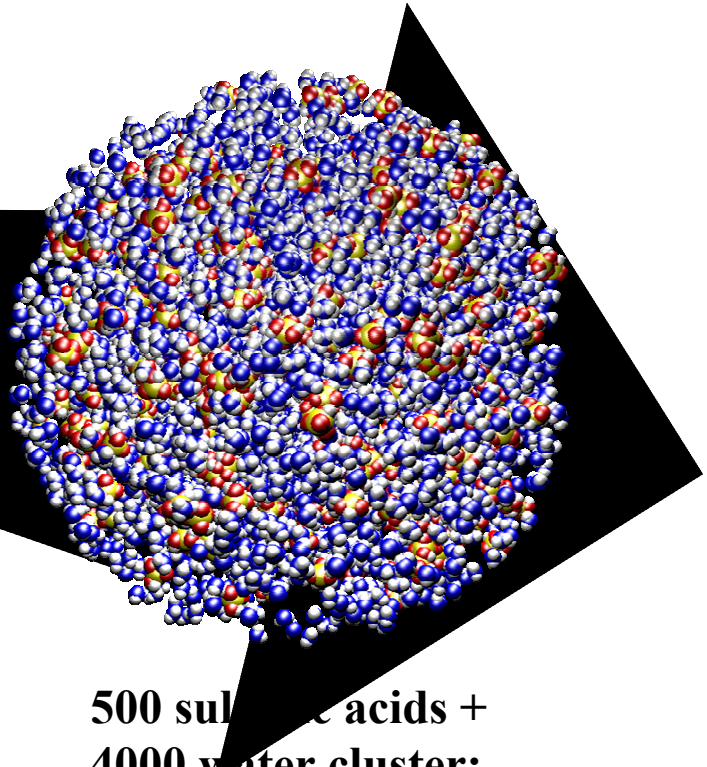
Sulfuric acid + 20 water cluster; this is the critical size cluster for nucleation

2003



250 Sulfuric acid + 250 water cluster; nucleated particle with growth

2006

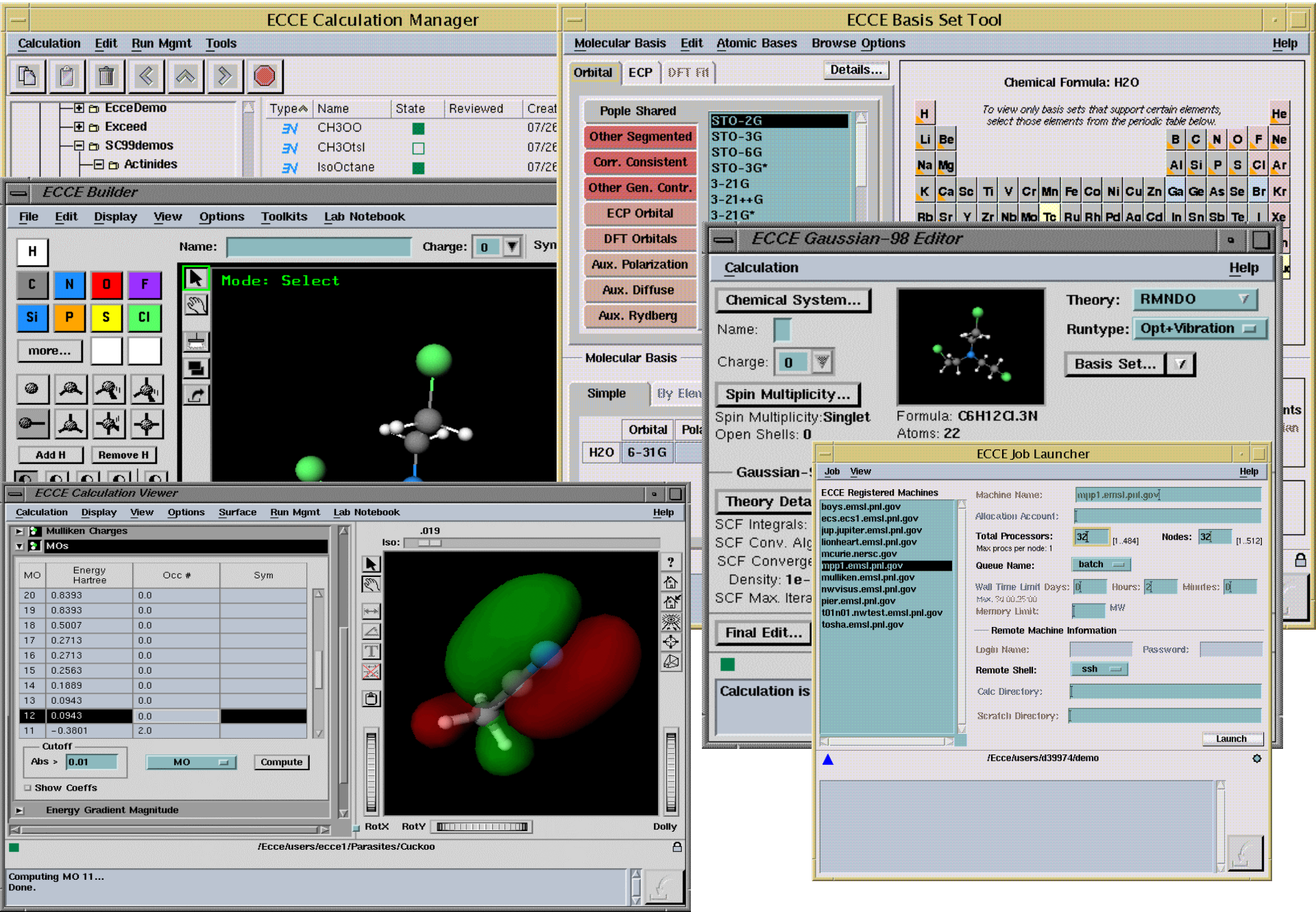


500 sul[illegible]c acids + 4000 water cluster; a nanodroplet of sulfuric acid

***Chemical Dynamics*:**

Nucleation of Aerosols

Challenges

- Tera-scale computers enable simulation of processes that cannot be visualized on desktop, or elsewhere
  - Conveying (often dynamic) relationships between molecules and parts of molecules is paramount
  - Display resolution is part of the problem
- Need high quality, parallel, portable, real time visualization tools for large molecular dynamics (e.g., protein/DNA)
  - Display structures together with properties (e.g., temp., velocity)
- Interactive remote visualization increasingly important
  - Remote real time data stream filtering as Grid service
- Tools/frameworks must integrate smoothly with the whole PSE/collaboratory environment
  - Data & computation management, collaboration, …

Extensible Computational Chemistry Environment