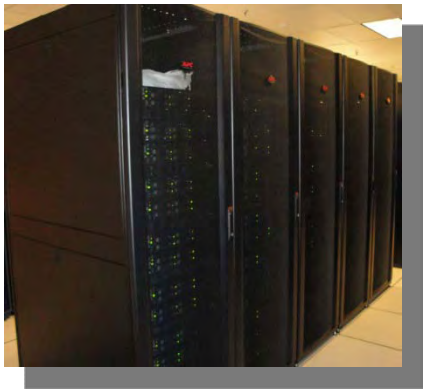
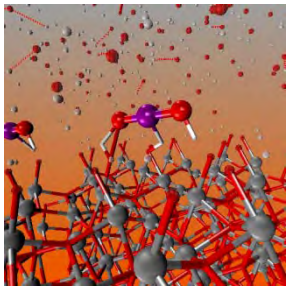
NWChem New Technology Development Cluster

Capability/Need

- Computing cluster named "Barracuda"
- Leading edge hardware technologies including processors, GPGPUs and networks
- **Ensures readiness** for HPCS-4
- Enables EMSL's NWChem software advancements to access new science at the **extreme scales**

Barracuda





Extreme-scale computing will enable the realistic modeling of molecules interacting with a reactive surface

Science/Users

- Bringing NWChem to the **extreme scale** will enable EMSL users to tackle new scientific questions by:
  - Obtaining results with a **faster** time-to-solution on large computing platforms, **moving toward real-time simulation**
  - Tackling scientific problems with **greater accuracy and precision**
  - **Integrating** complex methods and dynamics to tackle new scientific questions.

EMSL Strategy Alignment; Specifics

- Science themes: Biological Interactions/Dynamics; Geochemistry/Biogeochemistry and Subsurface Science; Science of Interfacial Phenomena
- Cross-cutting challenges: Static-Dynamics; Design/Synthesis of Complex Materials; Linking Theory/Experiment; Bridging Scales
- EMSL capability area: Molecular Science Computing
- Anticipated availability: EMSL staff access since October 2009
- Technical POC: Bert de Jong

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