EMSL

Scientific Innovation Through Integration

NWChem - Computational Chemistry at Scale

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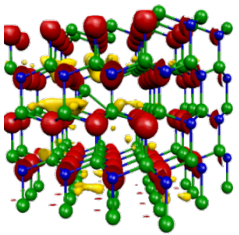
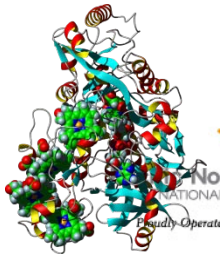
Delivering Computational Chemistry

EMSL

- DOE's Premier Computational Chemistry Software
- Provides one-of-a-kind computational chemistry modeling solutions for molecular science that are scalable with respect to scientific challenge and hardware
- Provides major integrated modeling and simulation capability
  - Broad range of molecules, including biomolecules, nanoparticles and heavy elements
  - Electronic structure of molecules
  - Extensive solid state capability (DFT plane-wave, CPMD)
  - Molecular dynamics, molecular mechanics





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Computational Chemistry at Scale

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- Computational chemistry solutions scalable with chemical system and computing capability
- Massively parallel computational chemistry software designed to take advantage of large computing resources
- Scalability demonstrated to tens of thousands of processors
- World-wide distribution (>2400 groups and computing centers)

MS^3
MOLECULAR SCIENCE SOFTWARE SUITE

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

GA TOOLS
PARALLEL COMPUTING LIBRARIES AND SOFTWARE TOOLS

ECCE
EXTENSIBLE COMPUTATIONAL CHEMISTRY ENVIRONMENT

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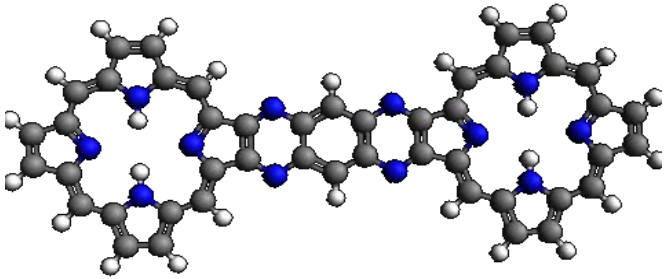
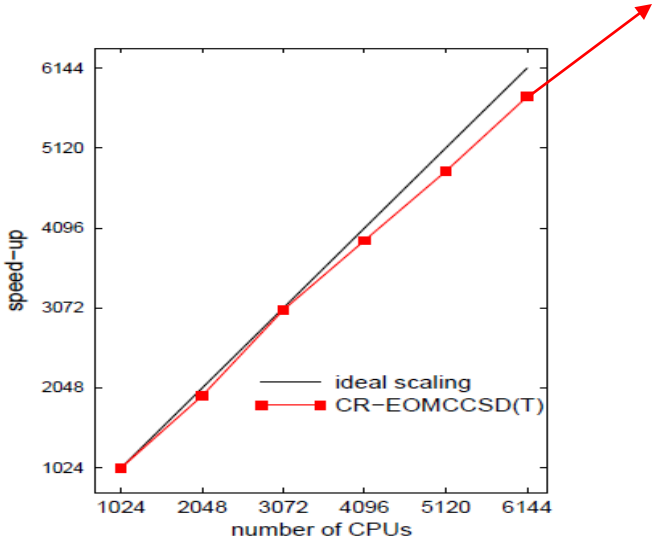
New Science with High Accuracy Methods

- Designing light harvesting systems and molecular switches requires a highly accurate and comprehensive understanding of the behavior of electrons in the system.



P_2TA molecule forms a basis for molecular switches and wires in nanoelectronics

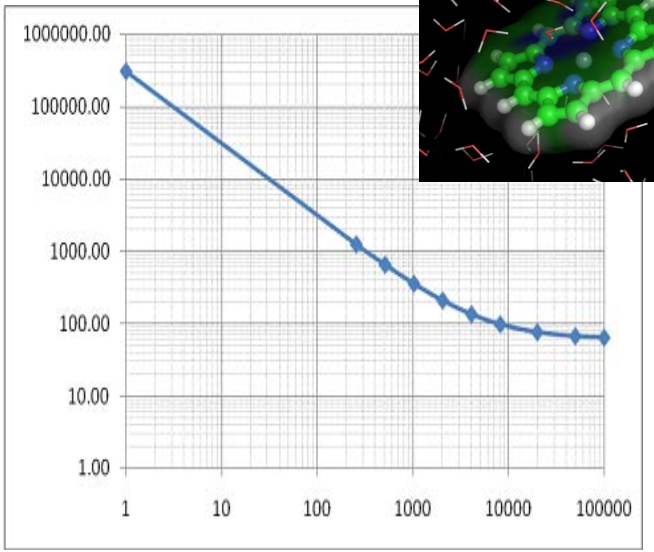


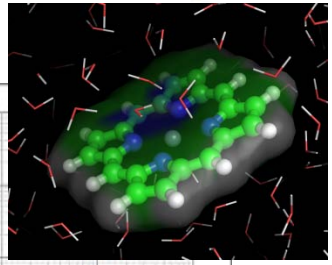
Ideal scaling of high accuracy CR-EOMCCSD(T) tripes for the P_2TA molecule

High Accuracy to the Petascale

EMSL

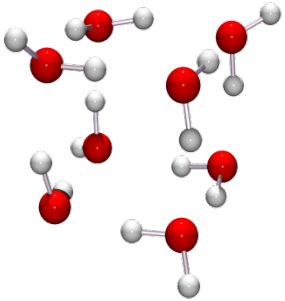
- Improving the parallel efficiency for coupled cluster algorithms
  - Balancing communication and operations
  - Better task scheduling based on knowledge of computational costs and overhead
  - Heterogeneous computing using processor groups
  - Improving data-localization reduces communication





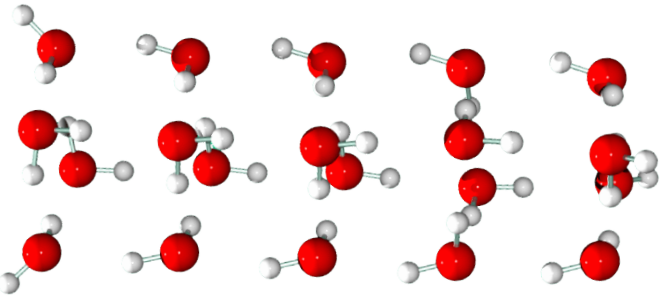
Performance model for the light harvesting Zn-porphyrine molecule

NWChem - Gordon Bell Finalist



2007

2009



8 water molecules on EMSL's MPP2 achieve 7 TFlops (63% of peak) on 1,840 processors

24 water molecules on ORNL's Jaguar achieve 1.31 PFlops (57% of peak) on 224,196 processors

ORNL – PNNL Collaboration

Improving our understanding of water's properties

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Chemistry at Interfaces Needs Petascale

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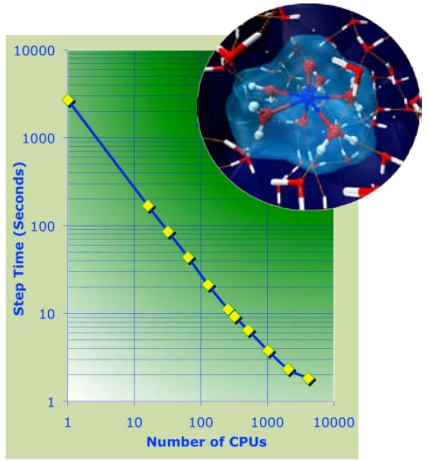
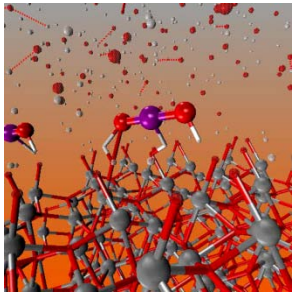
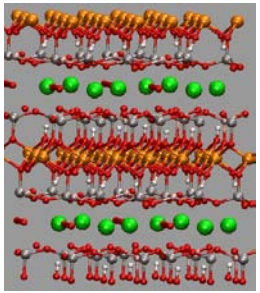
- Catalysis, hydrogen production, environmental remediation driven by chemistry at interfaces
- Chemistry at interfaces involves dynamical processes of complex chemical transformations



Car-Parrinello plane wave simulation of uranium oxide behavior in solution.



Molecules interacting with a reactive surface



Complex materials and interfaces

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Hard Petaflop Scaling of Plane Waves

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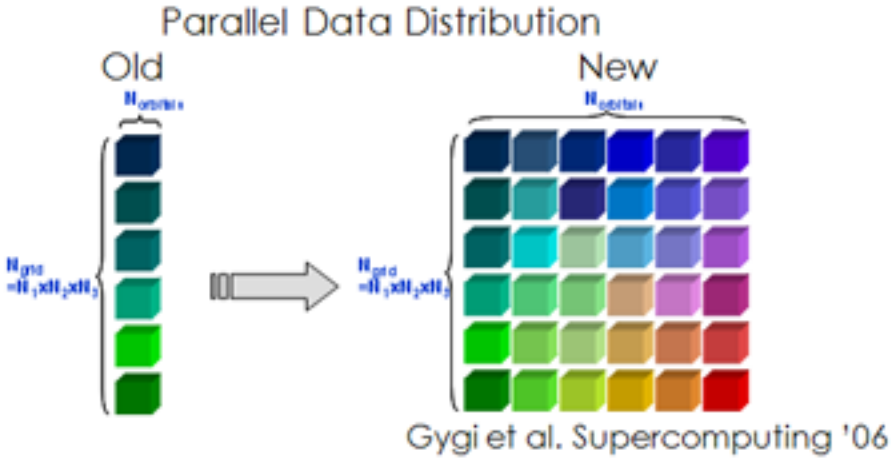
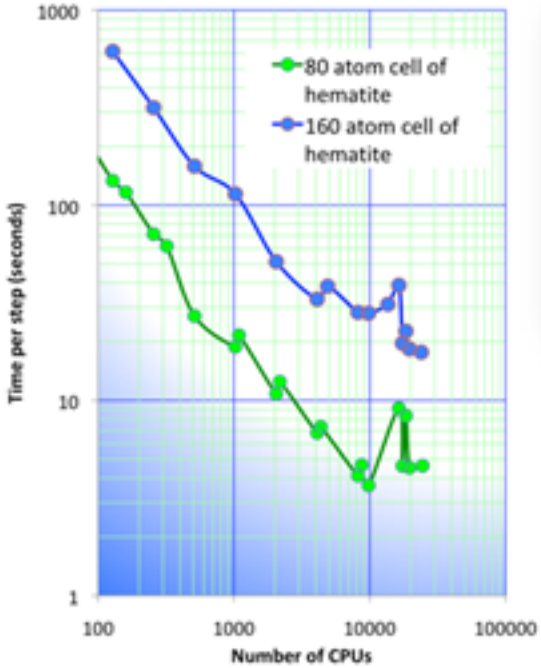
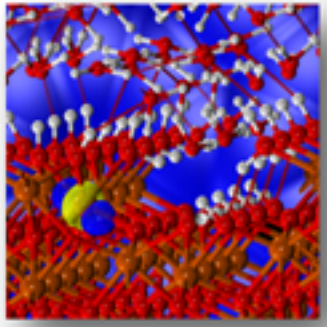
- Smart data distribution and smart communication algorithms enable hybrid-density functional theory to scale to large numbers of processors



Gygi et al. Supercomputing '06





Hybrid density functional theory plane wave calculation on hematite scaling on NERSC's Franklin

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Getting Ready for Extreme Scale Chemistry

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- Efficient NWChem on extreme scale platform enables our users to
  - Tackle larger molecular complexes with greater accuracy
  - Integrate of methods and dynamics
  - Obtain their results with a faster time-to-solution on large computing platforms
- Goal is to enable NWChem to run effectively on extreme scale platforms
  - Mitigating scalability issues in computational chemistry
  - Software infrastructure and architecture (re)design
    - 10,000s to 100,000s processors
    - Computing paradigm is changing drastically
    - Actor based models for efficient load balancing
    - Applications need fault resilience and/or tolerance

NWChem - Chemistry on New Architectures

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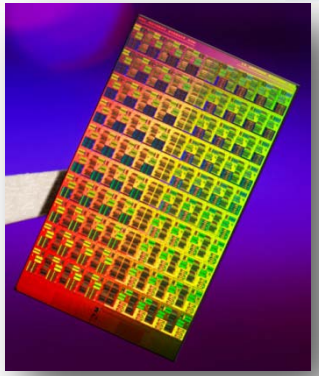
- Large multicore compute nodes
  - Heterogeneous nodes and/or heterogeneous computing in a node
- GPGPU
  - Rapidly evolving field
- Heterogeneous networks
  - Align data movement with network topology/bandwidth



Intel's Teraflop Research Chip has 80 cores and 1 TFlops performance

Barracuda: NWChem development cluster funded by Recovery Act

NVIDIA Tesla S1070
4 TFlops in 1U

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Achieving Scalability Takes a Team

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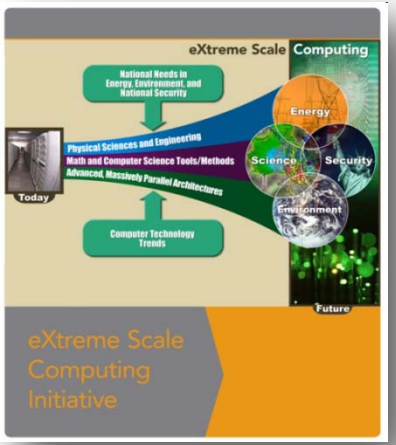
- Extreme scaling requires a collaborative multidisciplinary development team
  - Computational chemists
  - Mathematicians
  - Computer scientists

- PNNL's eXtreme Scale Computing Initiative leads the way
  - Scalable computational chemistry methods
  - Scalable software infrastructure
  - Fault tolerance at the application level



NWChem Is Going Open-Source

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- NWChem Consortium to deliver code and infrastructure for computational chemistry community to build upon
- Greatly expands user base through ease of access by students
- Expanding developers base by leveraging development and resources of universities and national labs
- Establish more collaborative development environment

NWChem - Delivering Computational Chemistry at Scale

Questions?

NWChem brochures available.