High Performance Computing Center

IT Division, Texas Tech University

Mission

Our mission is to promote research and education by integrating leading-edge computing, storage and visualization capabilities in higher education, and support advancing disciplinary diversity, partnerships, and service excellence through high performance computing.

Vision

Our vision is to facilitate, foster and integrate disciplinary capabilities and high performance computing with a goal to create new research and educational opportunities, interdisciplinary collaborations, and knowledge expansion in disciplinary and cross-disciplinary areas of science, engineering and medicine.

Our Commitment

- Manage research computing equipment and train non-HPCC cluster administrators
- Install and maintain application software and routine system management
- Support research computing needs and foster new disciplinary and interdisciplinary collaborations
- Provide training with a goal to improve user efficiency in computational sciences through HPCC • Facilitate and support collaborations for computing grants
- Collaborate with research users in developing new grant opportunities

Services

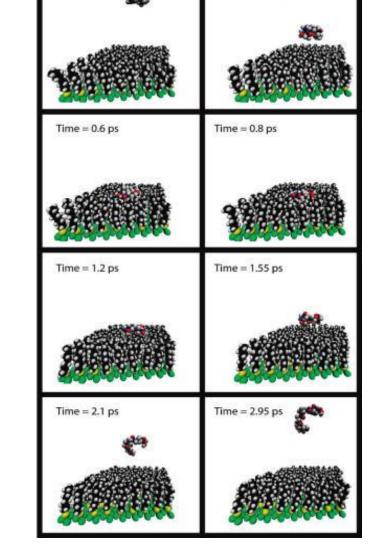
- We install, configure, and maintain application specific software packages
- Migrating computer programs from PC to Linux
- User training
- Licensed software packages are to be handled directly by the requesting user
- Write to hpccsupport@ttu.edu for additional information

Major Users

Atmospheric Sciences **Biological Sciences** Chemistry Molecular Dynamics Mathematics Computer Science Petroleum Engineering

Biomedical Engineering Cancer Radiotherapy Modeling High Energy Physics Mechanical Engineering Electrical and Computer Engineering Industrial Engineering

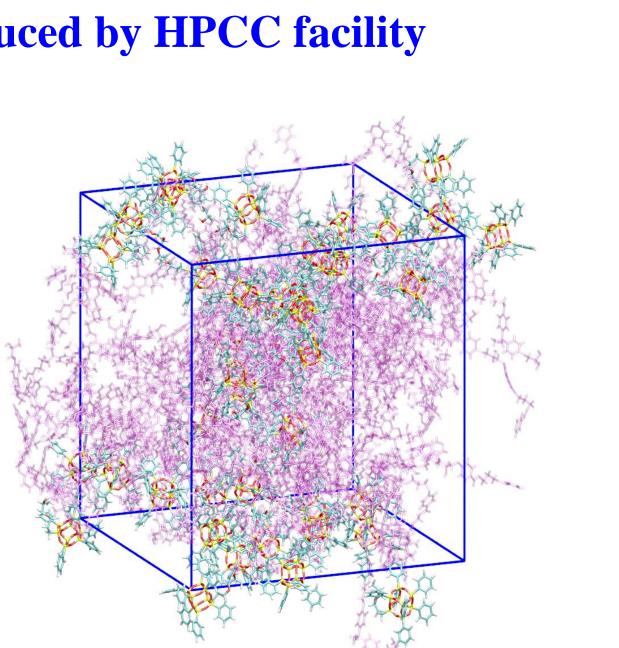
Researchers provided images produced by HPCC facility



Time = 0.35 ps

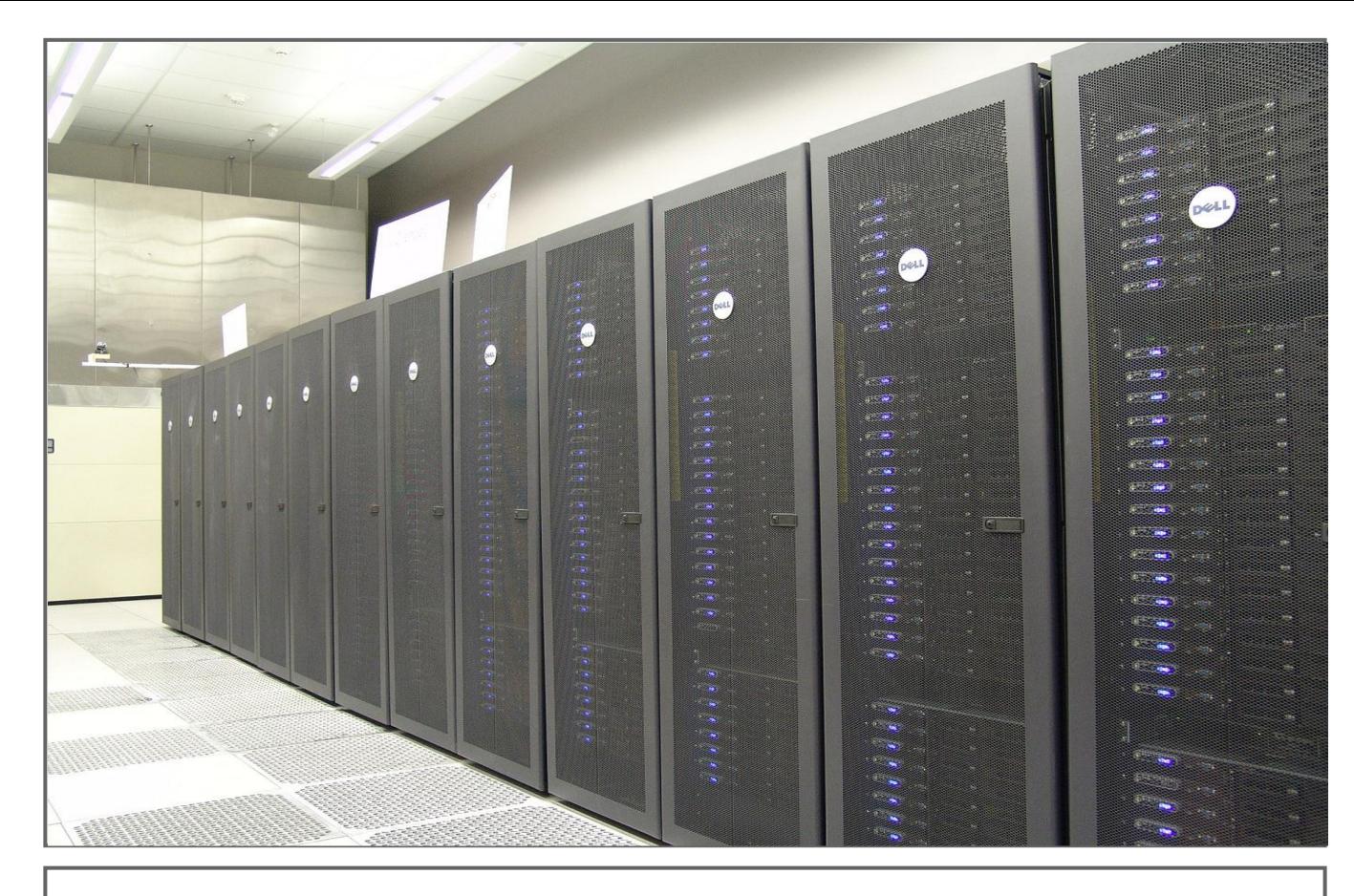
Snap-shots of a trajectory with a collision energy of 90 eV which illustrates the unfolding process.

Curtsey Drs. George L. Barnes and William L. Hase Departments of Chemistry and Biochemistry, Texas Tech University



A built cross-linked epoxy-POSS nanocomposite structure at a density of 1.188 g/cm³

Curtsey Po-Han Lin and Dr. Rajesh Department of Chemical Engineering, Texas Tech University



Research Infrastructure

•Hrothgar (installed in '10)

- 640 nodes (7680 cores) for parallel jobs
- 128 nodes (1024 cores) for serial jobs
- 86 teraflops peak over 7680 2.8 GHz cores and 12.3 teraflops over 1024 3.0 GHz cores
- 17 terabytes of memory and 1.2 petabytes of storage
- DDR Infiniband for connecting parallel nodes and storage
- Gigabit Ethernet for connecting serial nodes and storage
- Additional 46 nodes part of a community cluster

Antaeus (upgraded in '10)

- Community cluster for grid work and high energy physics
- 6.2 teraflops over 512 3.0 GHz cores
- 48 2.4 GHz cores
- 1 terabyte of memory and 280 terabytes of storage
- Gigabit Ethernet (GigE)

• TechGrid

- 1000 desktop machines in a Condor grid
- Used during times that machines would otherwise be inactive
- single jobs can run hundreds of iterations simultaneously
- Weland (installed in '10) Cluster for grid work • 1.295 teraflops over 128 2.63 GHz cores
 - 384 gigabytes of memory and mounts 106 terabyte antaeus storage system
 - 16 nodes with 8 capable of DDR Infiniband

•Janus (upgraded in '10) – Windows cluster

• One Dell PowerEdge R510 login server, with eight 2.4 GHz cores, 24 gigabytes of memory and 20 terabytes of shared storage

- 18 compute nodes, each node is a Dell PowerEdge 1950 server, with eight 3 GHz cores and 16 gigabytes memory each node
- GigE only

• TACC Lonestar (became operational in '11)

- 9,000,000 core hours per year have been purchased by TTU IT for TTU researchers
- 302 teraflops over 22,656 3.33 GHz cores
- 44 terabytes of memory and 1276 terabytes of storage
- Five large memory nodes, six cores each, each node has 1TB of memory
- Eight GPU nodes each node has two NVIDIA M2070 GPUs
- ODR infinband for MPI communications

Grid Computing Services

•On-campus computing grids

- TechGrid: Desktop computer cycles are donated during inactive times.
- 1000 3.0GHz processors running Windows operating system in a Condor grid
- Single jobs can run hundreds of iterations simultaneously
- and statistical modeling; and genomic analysis (biology).

• Distributed, National and International Grid Activities HPCC personnel maintain the tools and services necessary to participate in these organizations:

- The Open Science Grid (OSG) • HPCC staff maintain the tools and services necessary to participate in OSG
- projects
- SURAgrid

• A regional grid that encompasses more than 20 universities in the Southeastern United States

• PEGrid

• A Petroleum Engineering-specific grid called PEGrid co-founded by TTU, three other Texas universities, several software companies and four oil companies to pursue bestpractices exchange and interchange between industry and academics in this area

NSF Teragrid

• The largest single system on Teragrid in Texas is the 400 teraflop system called Ranger at UT Austin's Texas Advanced Computing Center, which has a 5% Texas allocation for researchers from Texas universities • Assist researchers in preparing their proposals and/or benchmarking their scientific applications in preparation for applying for allocations on Ranger or on other Teragrid computing facilities

Other HPCC Services

- Consulting services for a variety of applications
- Code optimization and parallelization strategies
- Organizing seminars and meeting with various research groups on campus
- Helping in bidding a system either for a proposal or to purchase on a grant
- Introducing campus researchers to national scale resources

Contact Us

- Support: <u>hpccsupport@ttu.edu</u>
- HPCC website: <u>http://www.hpcc.ttu.edu</u>
- New account: <u>http://www.hpcc.ttu.edu/php/AccountRequest.php</u>
- Contact our office at (806) 742-4350



• 128 core Nehalem Linux cluster (Weland) with 24GB per node (each node has 8 cores)

• 3-D rendering, physics modeling; computational chemistry electro nuclear dynamics simulations; mathematics prime number research and statistical analysis; business financial

• A national grid that gathers and allocates resources to virtual organizations – collaborative organizations consisting of individuals and researchers from different home organizations and/or physical locations linked together through technology and common purpose • Support a multi-faculty TTU research team with its participation in the Large Hadron Collider at CERN laboratory near Geneva, Switzerland and with its work in other related

• New software request: <u>http://www.hpcc.ttu.edu/php/RequestSoftware.php</u>

