Appendix
Background and Selected HECC Examples

Briefing to the Presidential Advisory Committee February 27, 1997

Co-Chairs:
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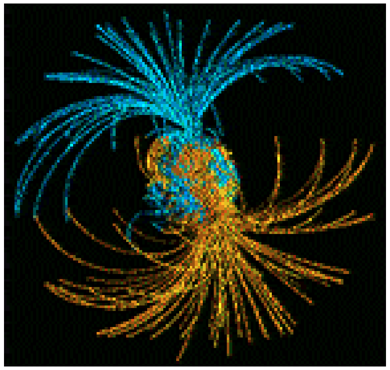
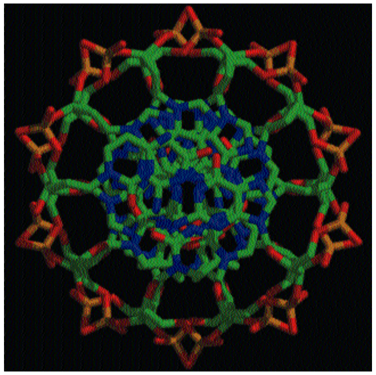
Participating HECC Agencies

- Department of Energy (DOE)
- National Aeronautics and Space Administration (NASA)
- National Security Agency (NSA)
- National Science Foundation (NSF)
- Defense Advanced Research Projects Agency (DARPA)
- National Institute of Standards and Technology (NIST)
- National Institutes of Health (NIH)
- National Oceanic and Atmospheric Administration (NOAA)
- Environmental Protection Agency (EPA)
- Department of Defense (DOD)

HECC FY1996-1997 Accomplishments



Complex computational modeling, pioneered by HECC R&D, was crucial to understanding why the inner core of the Earth rotates faster than the outer core. This explains the periodic reversal of the Earth's magnetic filed. *Science* magazine identified this as one of the "most significant scientific achievements" of the year.



HECC R&D provides the resources necessary to display and manipulate models of macromolecules such as proteins and nucleic acids. This axial view of DNA uses MIdasPlus, a molecule display and simulation system that is now available for use in university research programs.

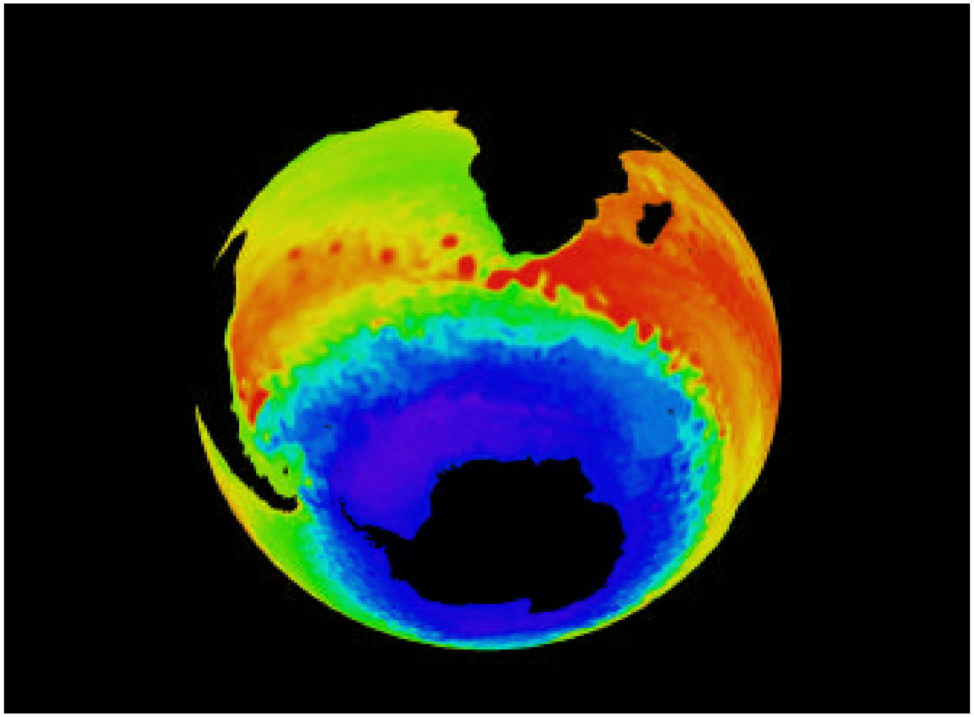
NSF's Partnerships for Advanced Computational Infrastructure, DOE's High Performance Computing Resource Providers, and NASA's Earth and Space Sciences testbeds provide access to parallel, scalable computing systems. Such systems further enhance researchers' ability to predict the dynamic interaction of physical, chemical, or biological processes, helping to protect and preserve our environment and improve the quality of life for future generations.

PETAFLOPS Workshops Findings

- PetaFLOPS systems possible:
  - in 20 years with COTS technology or
  - accelerate to 10 years with new technology
- Essential for many important applications
- Memory, cost, power & efficiency dominate
- New technology means paradigm shift - Innovation critical
- Fundamental systems software scaling problems
- Role of algorithms must improve
- Conduct point design studies
  - in hardware and software
- Develop engineering prototypes
  - multiple technology track demonstrations

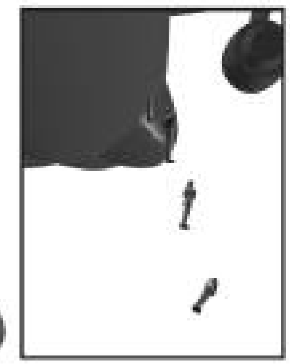
South Atlantic Eddies

- Understanding the processes that control the Earth's climate and predicting future changes in climate due to natural and anthropogenic influences will require computer models of the climate system that are more comprehensive and realistic than those we now have. Such models, known as general circulation models or global climate models, describe the time-evolving circulation and thermodynamics of the atmosphere and oceans, the two main components of the climate system. One of the principal impediments to the development of better models is the limited computational capacity of present-day supercomputers. The advent of parallel computers like the CM-5 and T3D provides an alternative approach with the promise of greatly increased computational power.
- Large eddies traversing the southern Atlantic Ocean are clearly visible in this figure of sea surface height (SSH) simulated with a three-dimensional global ocean model developed at Los Alamos National Laboratory for the massively parallel Connection Machine (CM-5) computer. The largest SSH values are shown in red, while the smallest values are shown in purple. Continents are islands are black. The eddies calculated by the model are spawned in the Agulhas Current at the tip of Africa and take about 2.5 years to reach the coast of South America, in agreement with satellite observations.



www.acl.lanl.gov/GrandChal/GCM/sa_eddies.html

DOD HPCMP Accomplishment
C-17 Paratrooper Drop Modeling

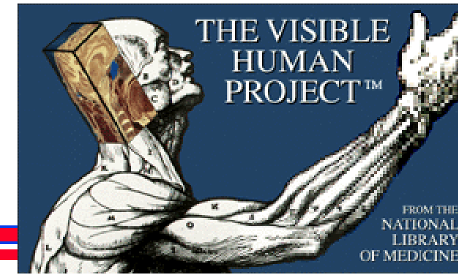


PROBLEM: Test jumps proved to be unsafe

SOLUTION:
- Jump airspeed changed
- Aircraft angle of attack changed
- Paratroop egress sequence changed from two simultaneous to alternating port, starboard, port...etc..

BENEFIT:
- HPC/CFD simulation provided major cost avoidance
  - eliminated need for redesign
- Saved program schedule

Visible Human Project



- The Visible Human Project is an outgrowth of the NLM's 1986 Long-Range Plan to create complete, anatomically detailed, three-dimensional representations of the male and female human body. The project collected transverse CT, MRI, and cryosection images of representative male and female cadavers The images form very large data sets—15 gigabytes for the male at 1 mm resolution, and 39 gigabytes for the female at 0.3 mm resolution. Projects are underway to convert pixel data to object data (such heart, brain, etc.) and provide rapid search and retrieval for the purposes of remote learning, 'virtual' surgery, and other medical efforts. Rendering and searching such large dataset requires the highest possible capabilities in computing and communications facilities. The long-term goal of the Visible Human Project is to transparently link the print library of functional-physiological knowledge with the image library of structural-anatomical knowledge into one unified resource of health information.
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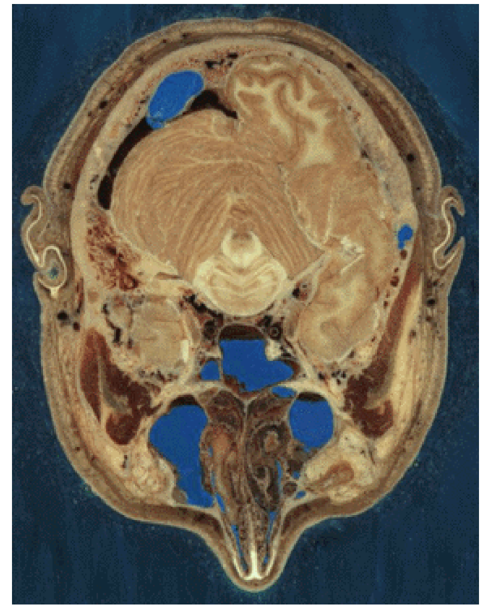
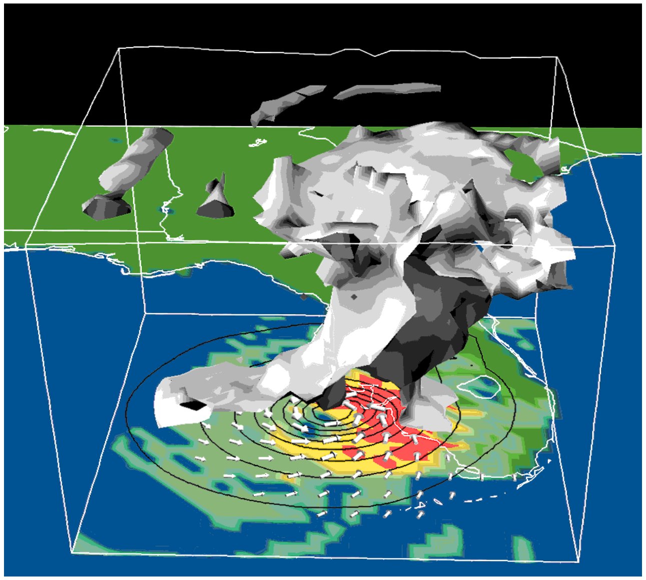
- The top image shows a section through head; including cerebellum, cerebal cortex, brainstem, nasal passages (from Head data subset).
- The bottom image shows a section through thorax, including heart (with muscular left ventricle), lungs, spinal column, major vessels, musculature (from Thorax data subset).



National Institutes of Health
National Library of Medicine
www.nlm.nih.gov/research/visible/visible_human.html

Examples of High End Computing and Computation Projects



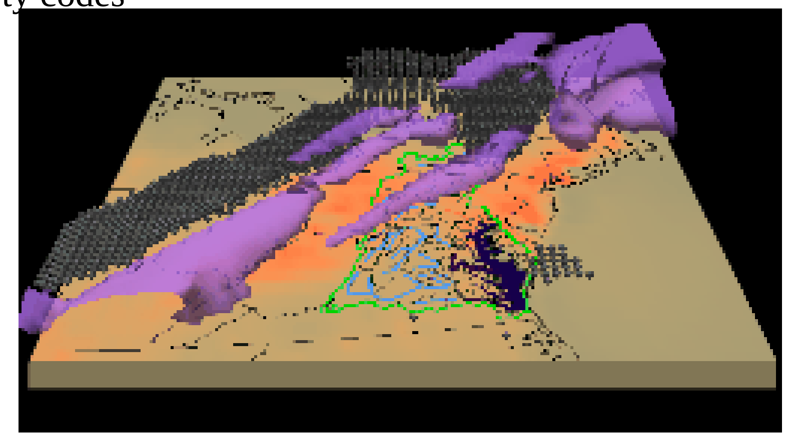
Tropical Storm Gordon, just before becoming a hurricane

GFDL/NOAA Hurricane Model

- Hurricane Prediction System
- 1993 - Run in semi-operational test mode
- 1994 - Part of National Centers for Environmental Prediction operational hurricane forecast suite
- 1995 -Model became fully operational
- 1996 - High resolution models run on highly parallel systems for the Centennial Olympics
- Run for tropical systems at all development stages
- Found to be in top performance group for forecasts out to 36 hours and superior to all other forecast models at 48 and 72 hours

Environmental Modeling

- Parallel logarithms used to model movement of groundwater contaminants
- Numerical simulations to estimate impact of decades of toxic pollution
- Research on nonlinear optimization and control techniques used to minimize groundwater cleanup costs
- Regional Particulate Model (RPM) developed to monitor air quality by region
- Parallel computing used to quantify potential effects of earthquakes on new construction and to assist in creating new safety codes



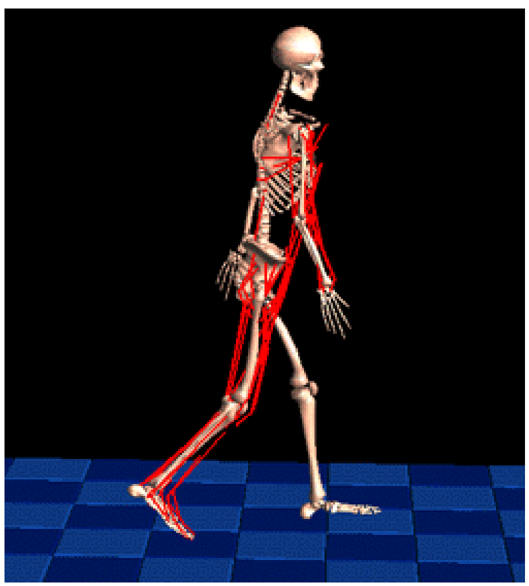
Simulation of nitrogen deposition to the Chesapeake Bay and surrounding areas during a rainstorm.

Biomedical Imaging, Biomedicine, Biomechanics, and Molecular Biology

HPCC Grand Challenge applications impacts all phases of biomedicine

- Simulates human motion on earth and in space
- Combines computer modeling with x-ray scattering
- Algorithm development to model and simulate DNA
- Searches and analyzes protein sequence data
- Determines energy profiles of important biological molecules

23-Degrees-of Freedom Model for Simulating Human Motion



Prototype Workstation Interface

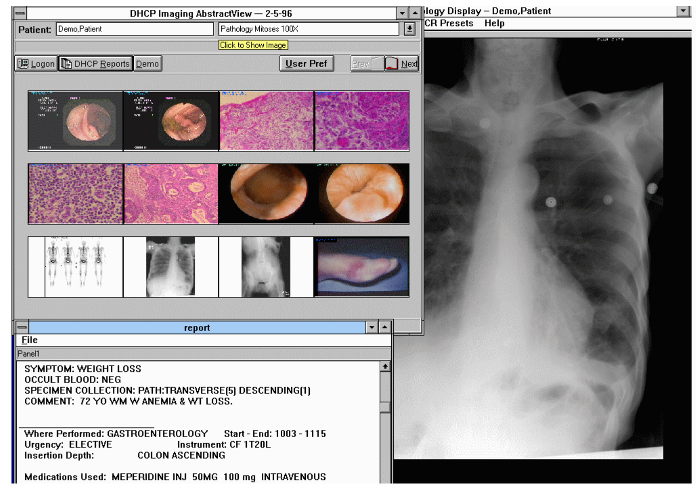
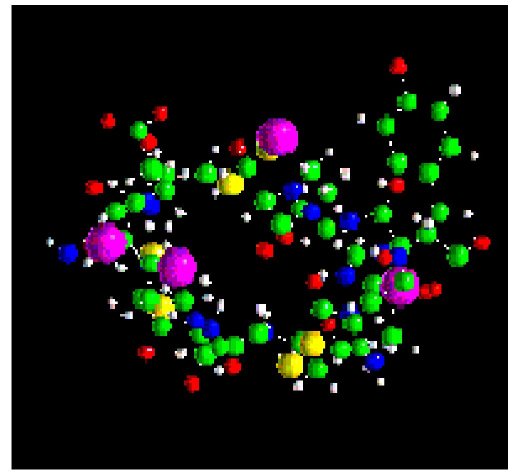


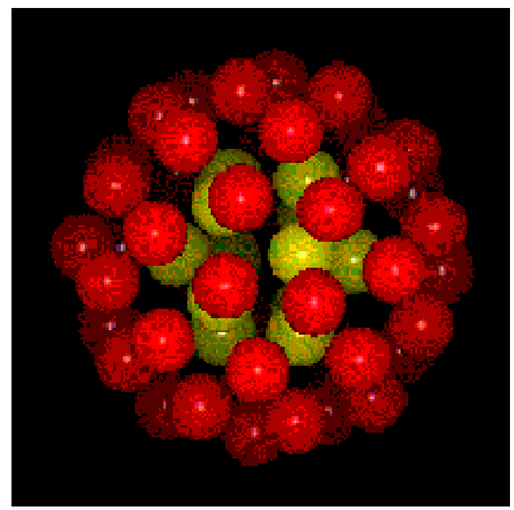
Image acquisition and storage technology

- Integrates medical images from diverse sources
- Securely stores and displays digital data and delivers information to physicians remotely
- Enables teleconsultation with top specialists even in remote or rural areas
- Supported by HPCC R&D investments

Global optimization in molecular dynamics

- Global optimization techniques are central to the solution of macromolecular modeling and simulation problems, since many fundamental problems in these areas are formulated as global optimization problems. The aim of our project is to develop a high-performance environment on the IBM SP at Argonne to support large scale global optimization algorithms and software for the solution of difficult global optimization problems arising in the modeling and simulation of large molecular systems. Currently, we are focusing on applications in protein conformation and modeling, ionic system configuration, and molecular cluster simulation.
- We are using optimization methods to find stable configurations of ionic systems. The stable configuration for an ionic system has the lowest energy, and therefore, can be found by minimizing the energy function for the system over the configuration space. Stable configurations for a set of small systems (< 100 ions) have been obtained by using global continuation algorithms on the IBM SP. We are now working on larger ionic systems. An important goal of this work is to find the stable configurations for very large systems, say, systems of 200,000 ions, from which a phase transition of the ionic system can be observed. The optimal structure with 60 ions is shown at right.

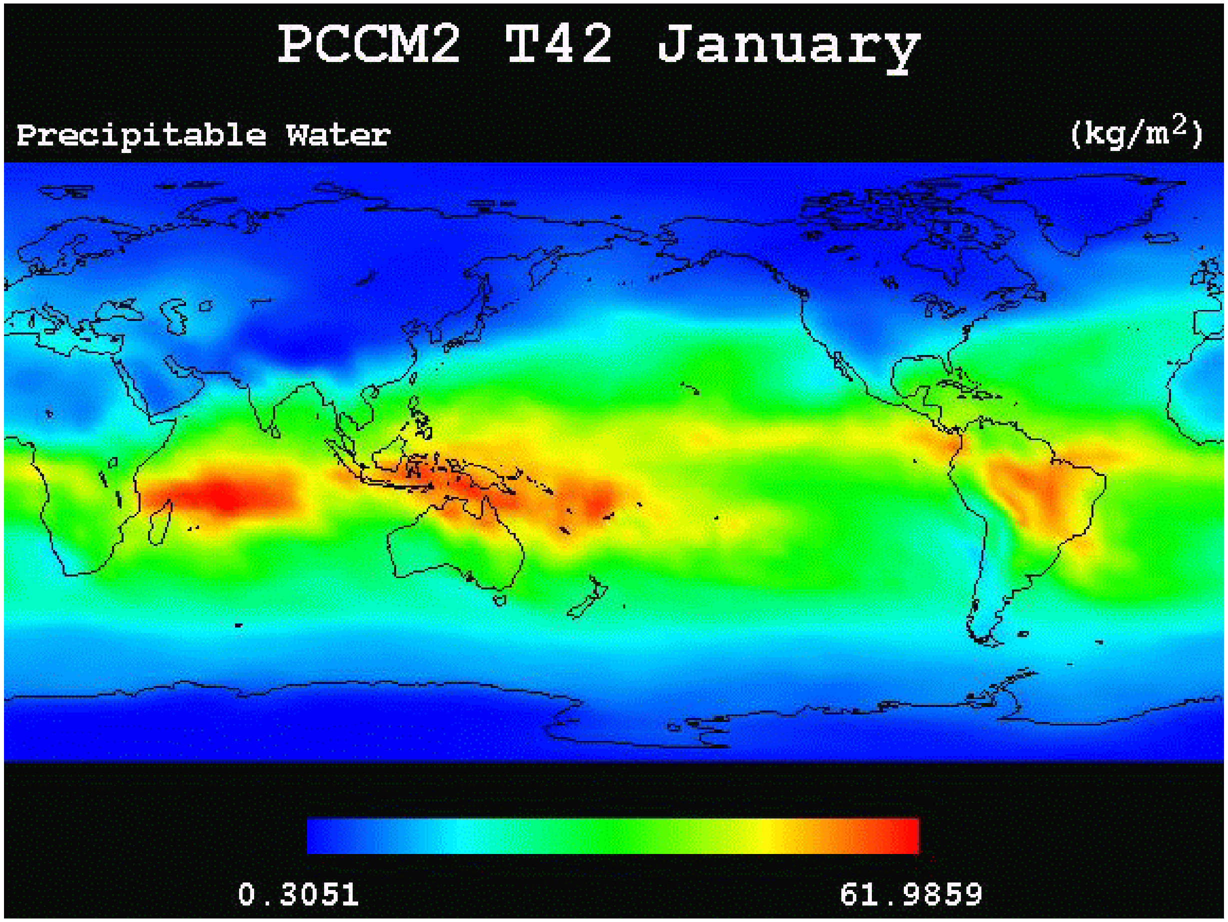




www.mcs.anl.gov/home/more/global/global.html

Global Climate Modeling

- The graphic above shows the average precipitable water in the atmosphere for January as calculated by the Parallel Community Climate Model (PCCM2).
- The calculation requires a 153 day simulation of the earth's weather and was performed on an Intel Paragon (XPS35) at Oak Ridge National Laboratory.
- The validation of this simulation by comparison with the NCAR CCM2 model output and with observations, have demonstrated the feasibility of use of massively parallel computers for climate modeling.



www.epm.ornl.gov/chammp/highlights.html

Large Scale Molecular Dynamics Simulation

- Condensed Matter and Statistical Physics A massively parallel MD simulation shows a 100x100x500-atom block of silicon 131 femtoseconds after bombardment by 11 silicon atoms hitting its 100x100 gray surface from above.
- Below the surface, for visual clarity only atoms displaced from their crystal position are shown. Colors represent different kinetic energies of the atoms. We observe both amorphization of the bulk material and channeling of implanted atoms.

www.acl.lanl.gov/96summer/Applications/lomdahl.html