Applications
National Institute for Computational Sciences (NICS): NSF and ORNL 2011 Model Problems

Presented by

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Scientific Computing and Workflows
National Institute for Computational Sciences

Enabling Transformational Science

SC07

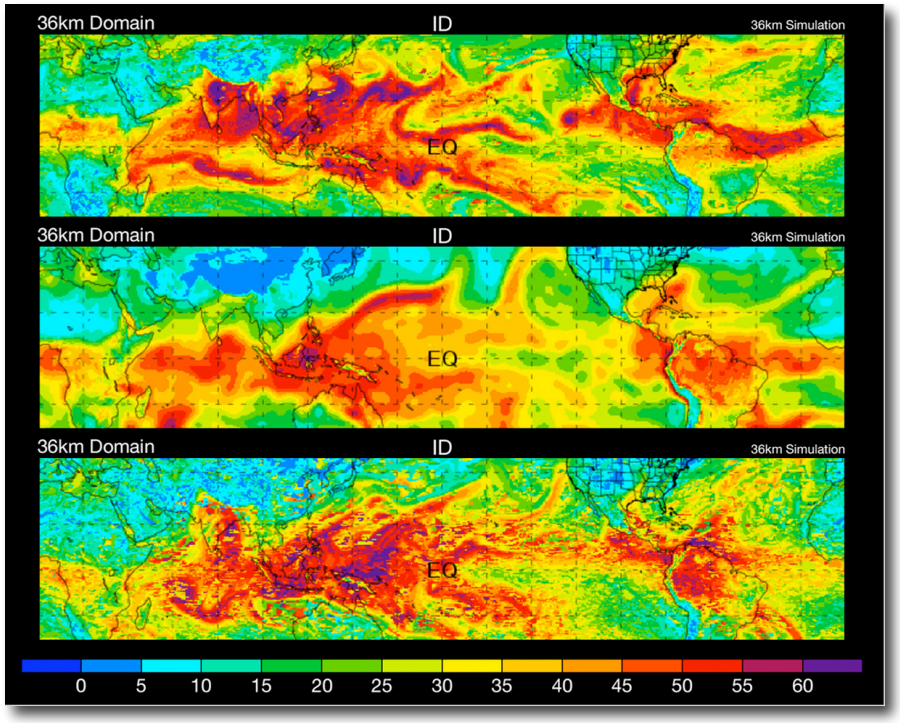
NSF

OAK RIDGE National Laboratory

WRF
Climate

Current Benchmark: 4-km horizontal resolution, 100 levels, 2.2 billion cell WRF global channel model representing one element of global WRF composite grid, periodic in longitudinal extent and 40N-40S in latitudinal extent.

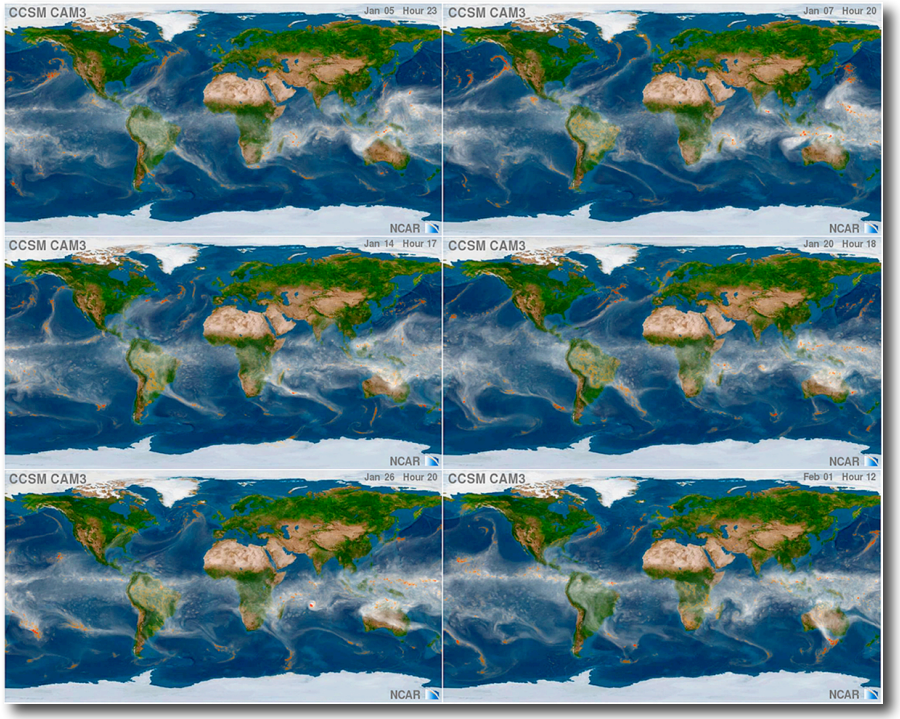
Model Problem: Global WRF cloud-resolving model (WCRM) for 0.1-1 km nature and real-data simulations of global atmosphere at all relevant scales to provide breakthrough understanding of convective organization at tropics and mid-latitudes and other climatological and meteorological processes.



POP, CICE, HOMME
Climate

Current Benchmark: 6912 cores, 1/10 degree grid, standard 12-day Baroclinic instability simulation with 30 km spatial resolution in the horizontal dimension at the equator, 1,328 spectral elements, 64 points per spectral element, and 96 vertical levels.

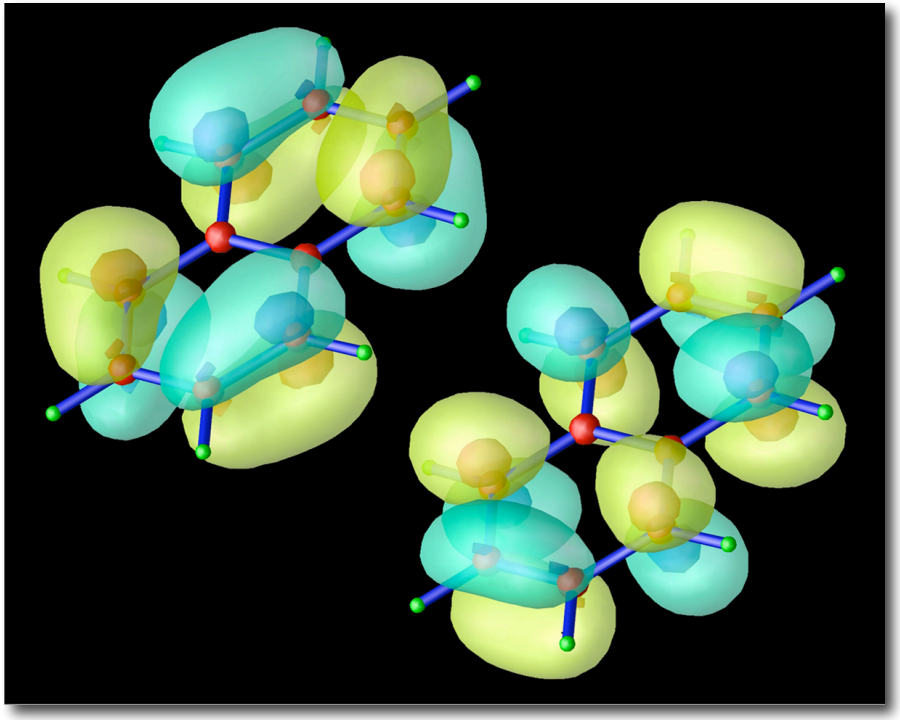
Model Problem: An ensemble of ten 200-year simulations with ultra-high resolution applied to high-emission and low-emission scenarios will be performed. These simulations will consist of HOMME (with extensions) at 30 km, the Parallel Ocean Program (POP), Community ICE Model (CICE), and a newly developed land model at 0.1 degrees of 10 km resolution.



PARSEC
Materials

Current Benchmark: 1,173 atom run using 1536 processors

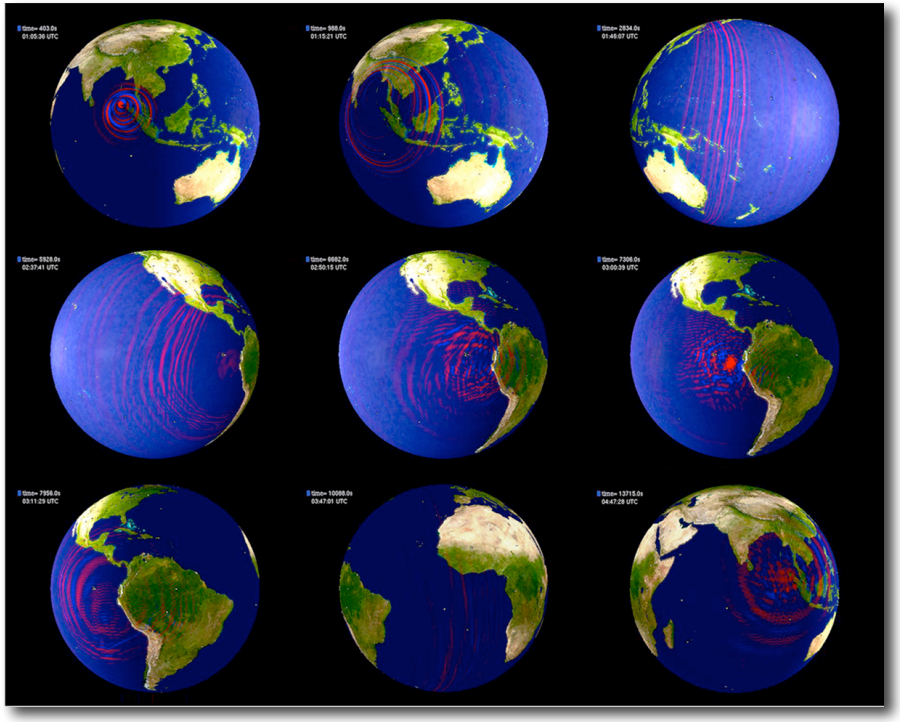
Model Problem: To improve our understanding of the magnetic properties of clusters of atoms, we will model 30,500 transition-metal atoms, defined within spherical clusters of diameter of 9 nm, with a density of 80 atoms/nm3. The mesh size, in real space, will be 1.28 • 108 grid points with a spacing of 0.3 a.u. = 0.016 nm.



DNS/CFD
Climate

Current Benchmark: 4,056 processors

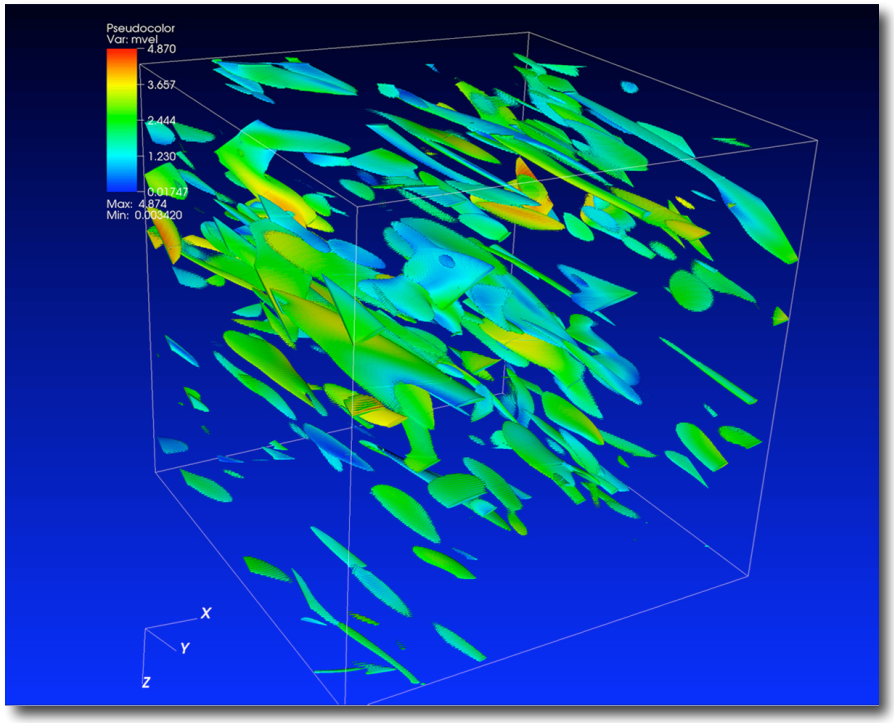
Model Problem: Reach a shortest period of 1 s in a simulation requiring 4,320 elements along one side of one chunk of the cubed sphere, consuming 120 TB of memory.



DNS/CFD
Combustion

Current Benchmark: 4,0963 grid on 8192 cores

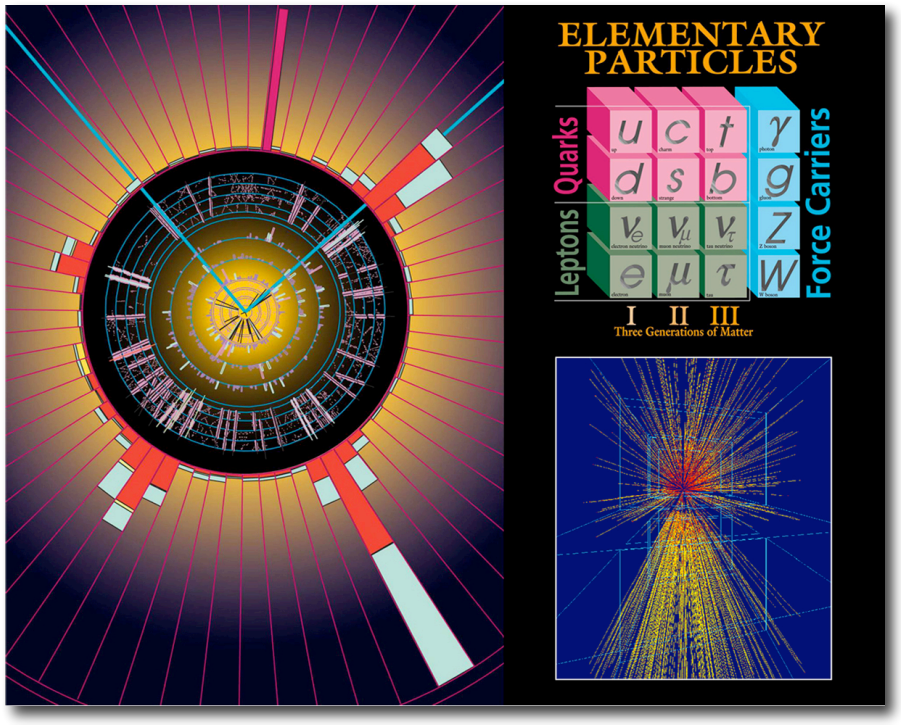
2011 Model Problem: 12,2883-mesh resolution simulation of fully developed homogeneous turbulence in a period domain for one eddy turnover time at a value of RI of order 2000, using a de-aliased, pseudo-spectral algorithm, a fourth-order explicit Runge-Kutta time-stepping scheme, with a time-step of 0.0001 eddy turnaround times.



MILC
High Energy Physics

Current Benchmark: 11,000 cores of XT4

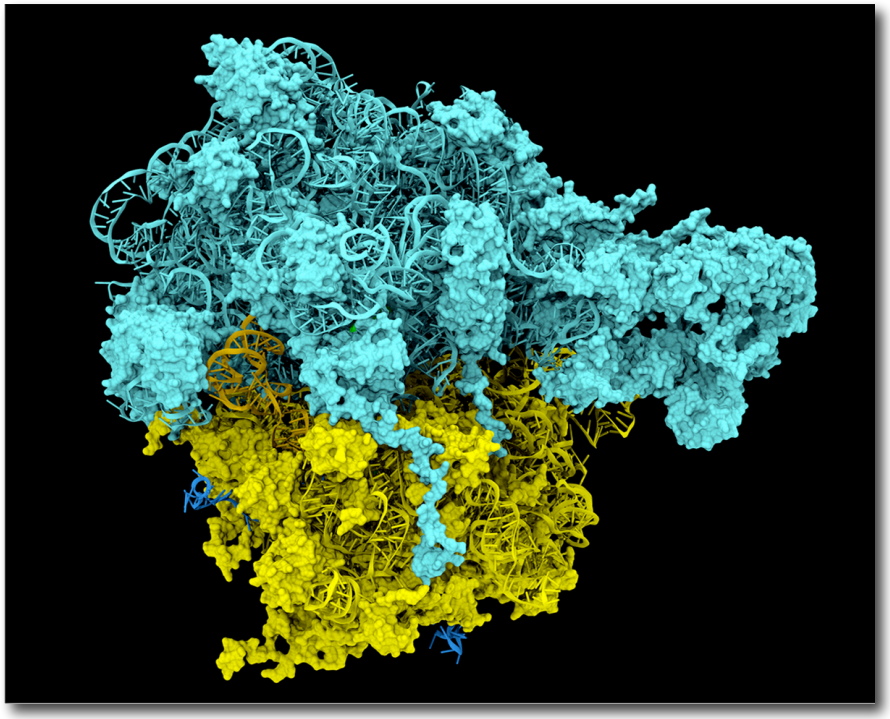
2011 Model Problem: A lattice-gauge QCD calculation in which 50 gauge configurations are generated on a 843 • 144 lattice with a lattice spacing of 0.06 fermi, the strange quark mass set to its physical value, and the light quark mass set to 5% of the strange quark mass.



NAMD
Biology

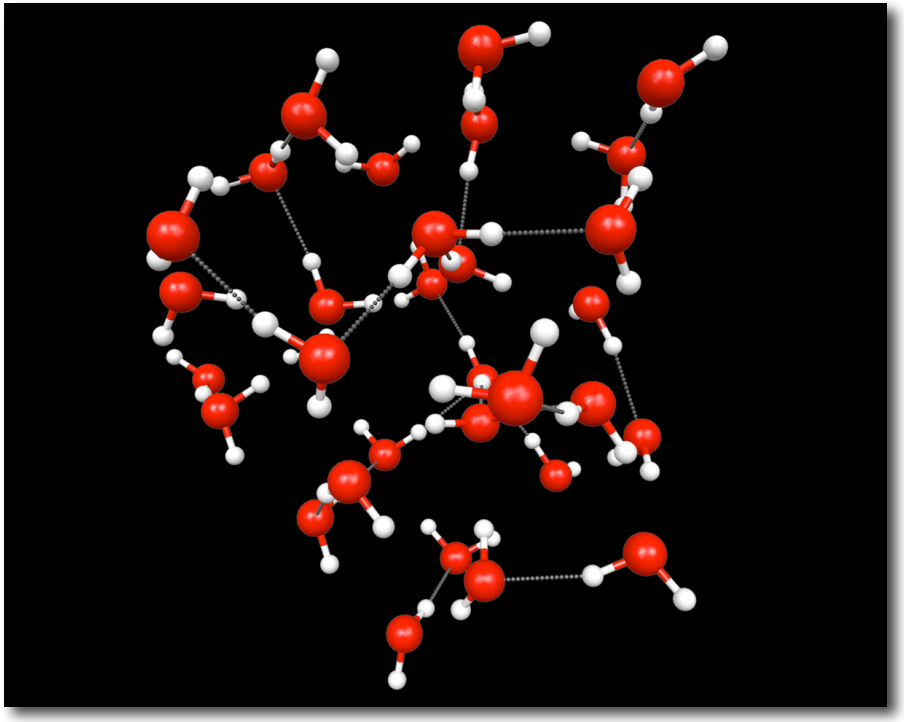
Current Benchmark: 5 million atoms

2011 Model Problem: We will simulate curvature- inducing protein BAR domains binding to a charged phospholipid vesicle over 10 ns of simulation time under periodic boundary conditions. The vesicle, 100nm in diameter, will consist of a 2:1 mixture of DOPC and DOPS. The system consists of 100 million atoms, including 100,000 lipids and 1,000 BAR domains solvated in 30 million water molecules, with NaCl included at a concentration of 0.15M.



GAMESS
Chemistry

Molecular dynamics of liquid water using high-accuracy first-principles calculations



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