Impact of *Columbia* on NASA's Science and Engineering Applications

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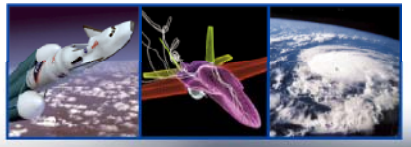
Integrated Support for Full Life-Cycle of High-Performance Modeling and Simulation

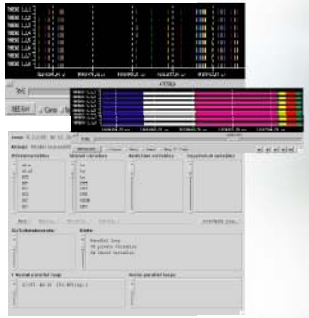
The Columbia supercomputer provides a peak of 62 teraflops to the user community

NASA Scientists and Engineers



Scientists and engineers set up computational problems, choosing effective codes and resources to solve NASA's complex mission problems.

Performance Optimization



NAS software experts utilize tools to parallelize and optimize codes, dramatically increasing simulation performance while decreasing turnaround time.

Data Analysis and Visualization

NAS experts apply advanced data analysis and visualization techniques to help scientists explore and understand large data sets.

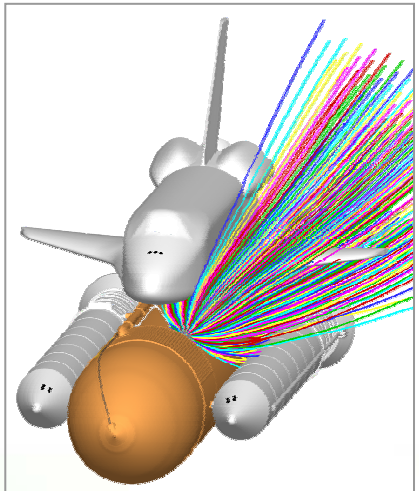
Supercomputers, Storage and Networks

The NAS supercomputer environment (hardware, software, network and storage) is used to execute the optimized code to solve NASA's large computational problems.

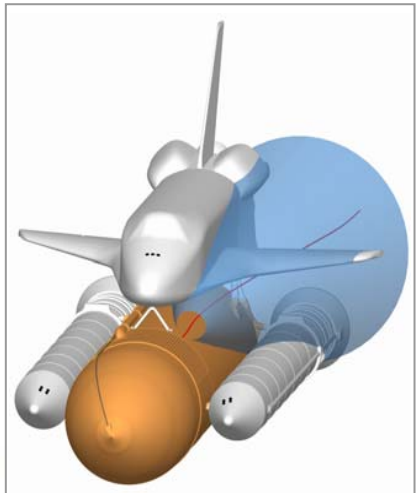
Space Shuttle Program: STS-107 Investigation and Debris Transport Analysis

Results from the computations on Columbia were a critical factor in returning the shuttle safely to flight

- Columbia was used to compute over 400 Overflow CFD solutions that have been used to quantify the airloads on specific components of the SSLV, including redesigned parts of the External Tank
- Columbia was used to compute unsteady moving-body 6-degree-of-freedom simulations of isolated pieces of debris with the Cart3D flow solver, which were used to develop models of the debris drag and cross-range in a supersonic flow
- Columbia was used to compute hundreds of millions of potential debris trajectories that were used to assess the threat from debris



Deterministic Zero Lift Trajectory + Range of Initial Velocities



Probabilistic Zero Lift Trajectory + Crossrange Cone

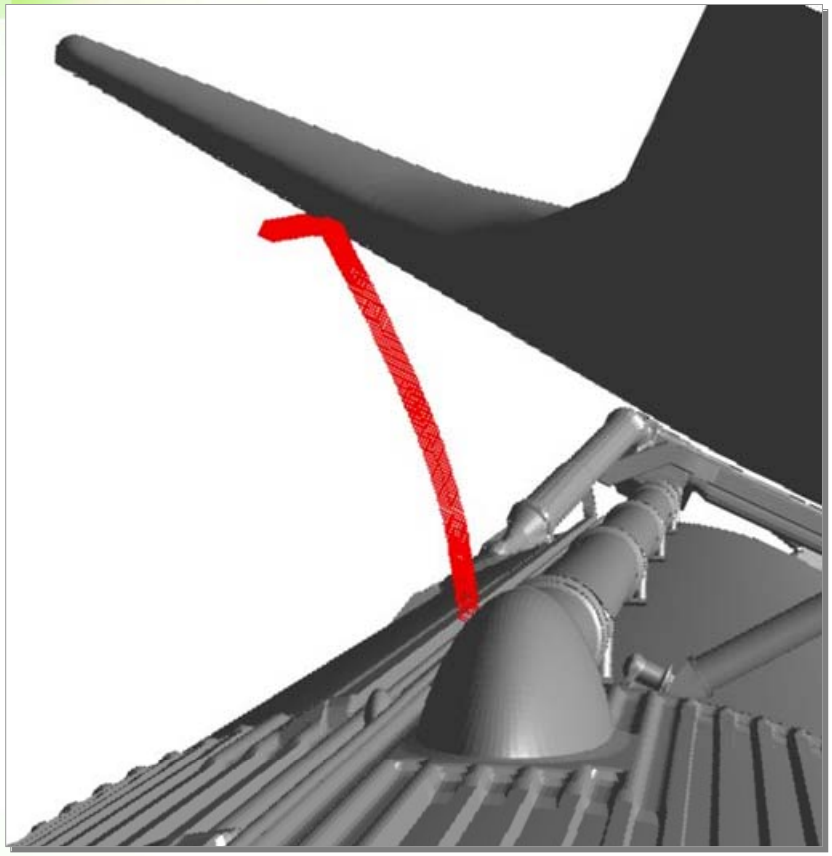
QuickTime™ and a Animation decompressor are needed to see this picture.

POC: *Reynaldo Gomez (NASA Johnson Space Center), Stuart Rogers, Michael Aftosmis (NASA Ames Research Center)*

Space Shuttle Program Return-to-Flight: STS-114 Immediate Analysis

Computed and enhanced video trajectories of ice/frost ramp foam debris

- Using Ames-developed debris-transport software running on *Columbia,* the NASA debris team provided support in several areas (ice/frost ramp foam was particularly critical)
- Enhanced video analysis (below) performed at end of day two showed foam may have hit the starboard wing



One of many debris simulations run on Columbia: Mass = 0.03 lbm, 30 ft/sec pop-off velocity

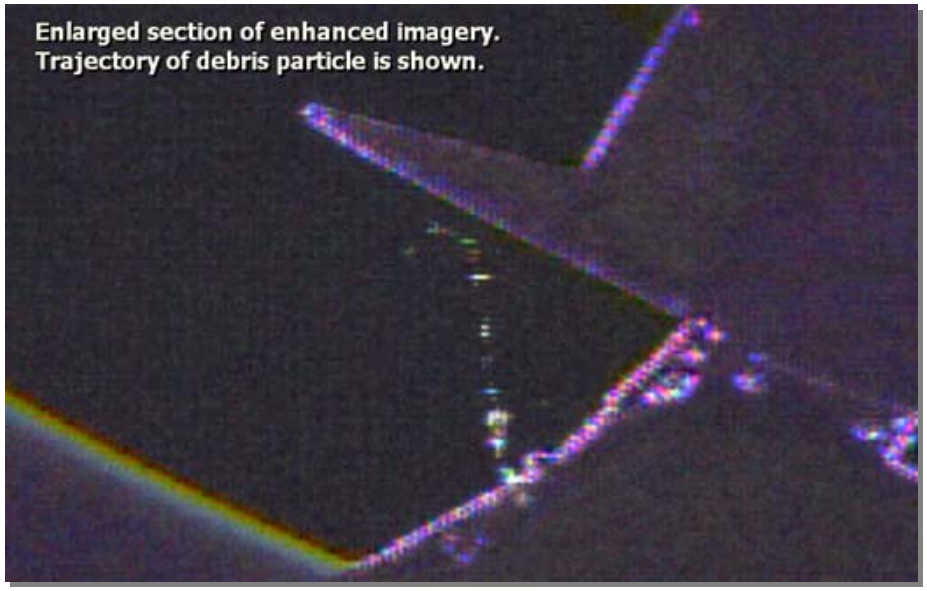


Image of ice/frost ramp foam debris captured from Umbilical Well Camera

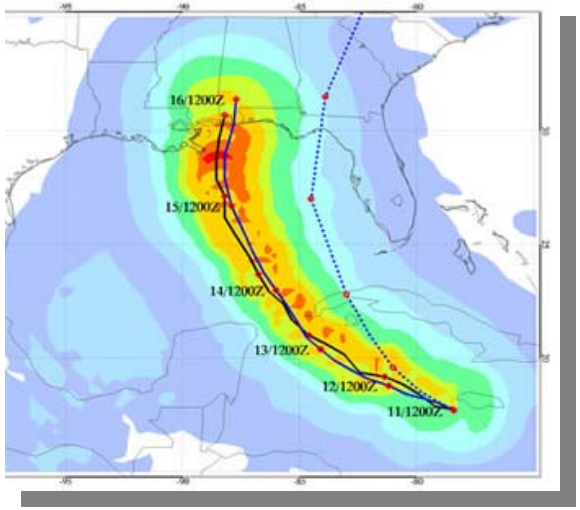
POC: *Reynaldo Gomez (NASA Johnson Space Center), Stuart Rogers, Michael Aftosmis (NASA Ames Research Center)*

Finite-Volume General Circulation Model (fvGCM)

Next-gen global climate & weather prediction modeling system to make ultra-high resolution apps a reality with high computational efficiency

- fvGCM has been running on *Columbia*, generating real-time, high-resolution (about 25 km) weather predictions focused on improving hurricane / snowstorm tracks / intensity forecasts.

Hurricane Ivan's track and intensity as forecasted by fvGCM 5 days before landfall (solid black), the official NHC forecast (dashed blue), and observed positions (solid blue)



Objectives:

- Bridge gap between weather and climate models, reduce uncertainties in climate change predictions, and assess regional impacts of global climate changes
- Real-time predictions of local and global long-range transport of unexpected releases of chemical, biological or radioactive gases (Homeland Security)
- Provide weather forecasts for the safety of astronauts and NASA assets on other planets (Space Exploration)

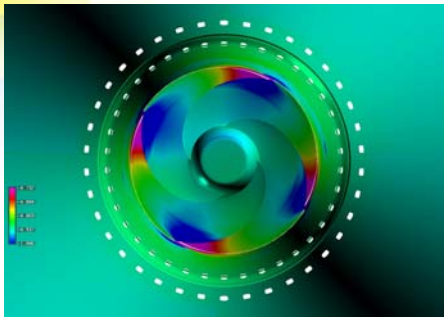
QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Total precipitable water in atmosphere

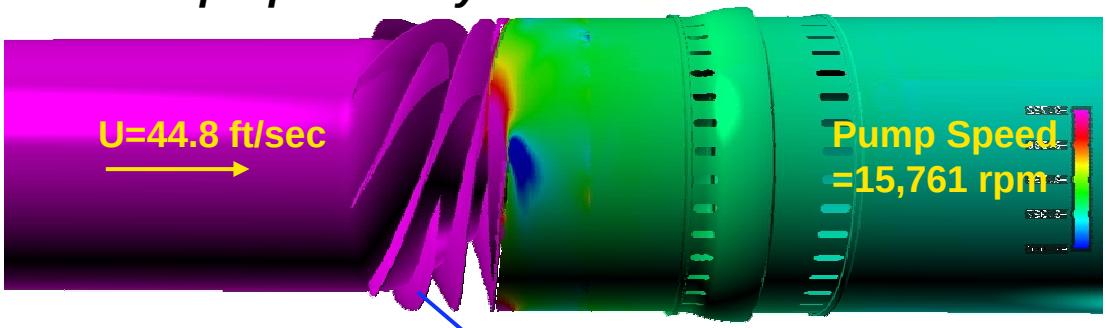
Partners: NASA/JPL, ARC, MSFC; NOAA/GFDL, NCAR, DOE/LLNL, and Universities

Unsteady Simulation of Space Shuttle Main Engine LH2 Flowliner

High-fidelity framework for design and analysis of fuel/oxidizer supply subsystem for liquid rocket propulsion systems



Strong backflow causing high-frequency pressure oscillations

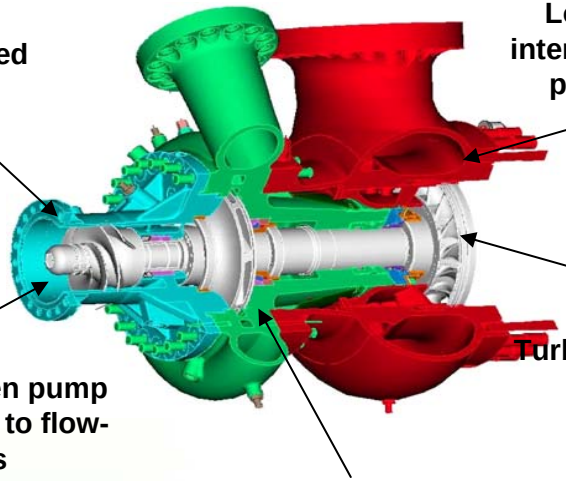


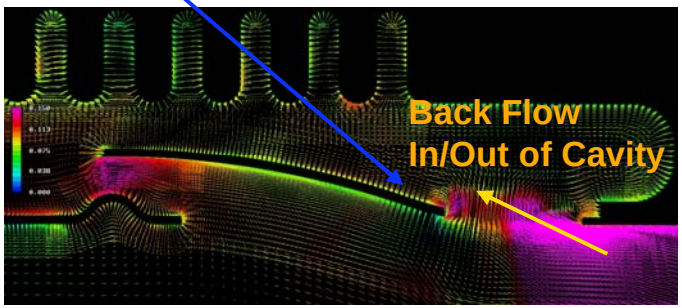
UPSTREAM LINER

DOWNSTREAM LINER

Pressure difference across inducer blades causes backflow near tip

UNSTEADY AND TRANSIENT FLOW IN LIQUID ROCKET ENGINE PUMP





Damaging frequency on flowliner due to LH2 pump backflow causes cyclic fatigue and cracks; these have been quantified in developing flight rationale for the flowliner

POC: *Cetin Kiris, Dochan Kwak (NASA Ames Research Center)*

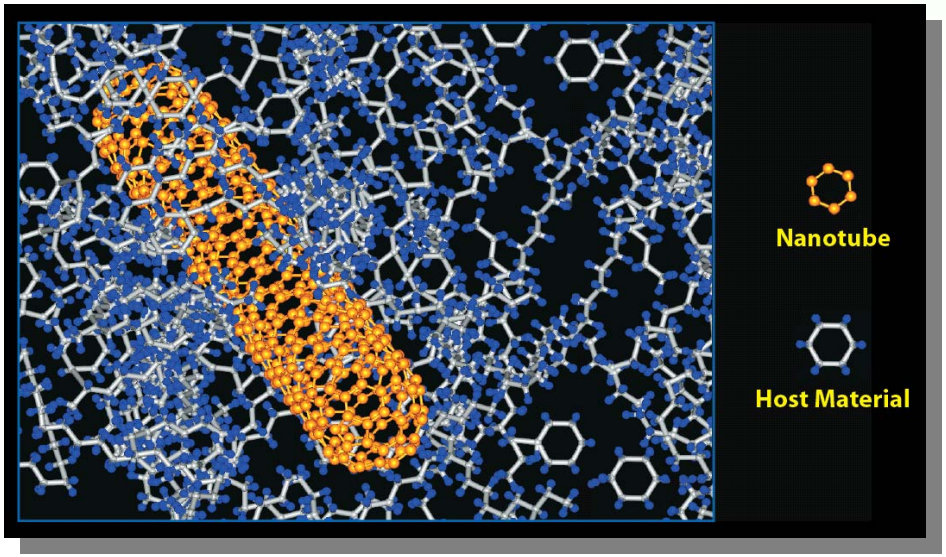
Computational Nanotechnology

Objectives:

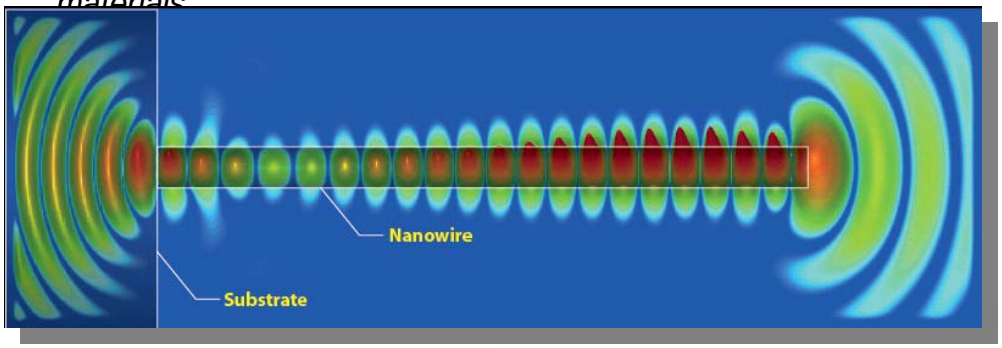
- Allow scientists to discover and explore phenomena in nanometer and molecular structures.
- Enable the design and fabrication of new materials and devices.
- Develop theory, models, and large scale simulations to establish the scientific basis and as cost-effective design tools.

Results:

- Running complex molecular dynamic simulations and models of various nano systems on supercomputers such as *Columbia* has lead to a variety scientific discovers and potential uses in:
  - Lightweight radiation shielding for astronauts and spacecraft
  - Communications and sensing
  - Astronaut health
  - Life detection
  - Decoding genomes



Like steel bars in concrete, carbon nanotubes embedded in a host material are expected to combine the best of both materials



The complex interaction between light and nanometer structures, like nanowires, has possibilities as new technology for devices and sensors. NASA researchers are studying light emission from a semiconductor nanowire — typically 10-100 nanometers wide and a few micrometers long—which functions as a laser.

POC: *Ioana Cozmuta (NASA Ames Research Ctr)*

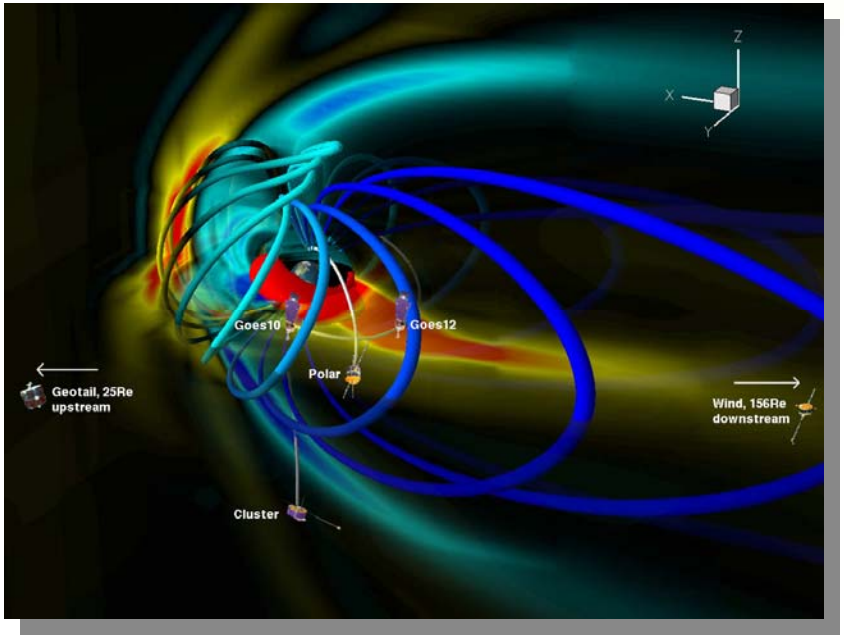
Solar Storm Simulations with the Space Weather Modeling Framework

Project Goals:

- Faster than real-time simulation of the entire Sun-Earth system following large geo-effective solar storms
- Long term goal is to create a space weather forecast capability to support NASA's missions

Objectives:

- To simulate the most geo-effective event of the Halloween solar storms of October-November 2003
- To simulate Saturn's space environment in support of the Cassini mission



For the first time, data from six satellites were matched with simulations

For the first time, the simultaneous observations of six satellites located at very different regions of the magnetosphere was achieved. This is a big qualitative leap in magnetospheric physics, made possible by the *Columbia* system. Scientists were able to explore the parameter space in the simulations and obtained excellent agreement with all six magnetospheric satellites.

POC: Tamas I. Gombosi (University of Michigan)

Peridynamic Modeling of Impact and Failure in Composite Materials

Helping understand material damage

- Recently, Ames Research Center, Sandia National Labs, and the Boeing company embarked upon a joint venture to explore the potential of a new technology for the investigation of impacts and failures in composite materials (peridynamics).
- The technique has been encoded as a computer model, EMU, by Sandia, with joint development work by Boeing. NAS Division provided application porting and scaling services as well as *Columbia* compute cycles for test and evaluation.
- To date, Boeing has completed a number of impact simulations on *Columbia* for V&V against actual test data. Total effort has consumed approximately 1 million CPU hours on *Columbia*. Results are promising.

Results on Columbia:

- *The failure mode is strongly influenced by the layup (fiber directions) of the composite material.*
- *The residual strength depends on the hidden damage caused by the previous impact.*

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

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POC: Abe Askari (Boeing), Stewart Silling (SNL), Jim Taft (NASA ARC)

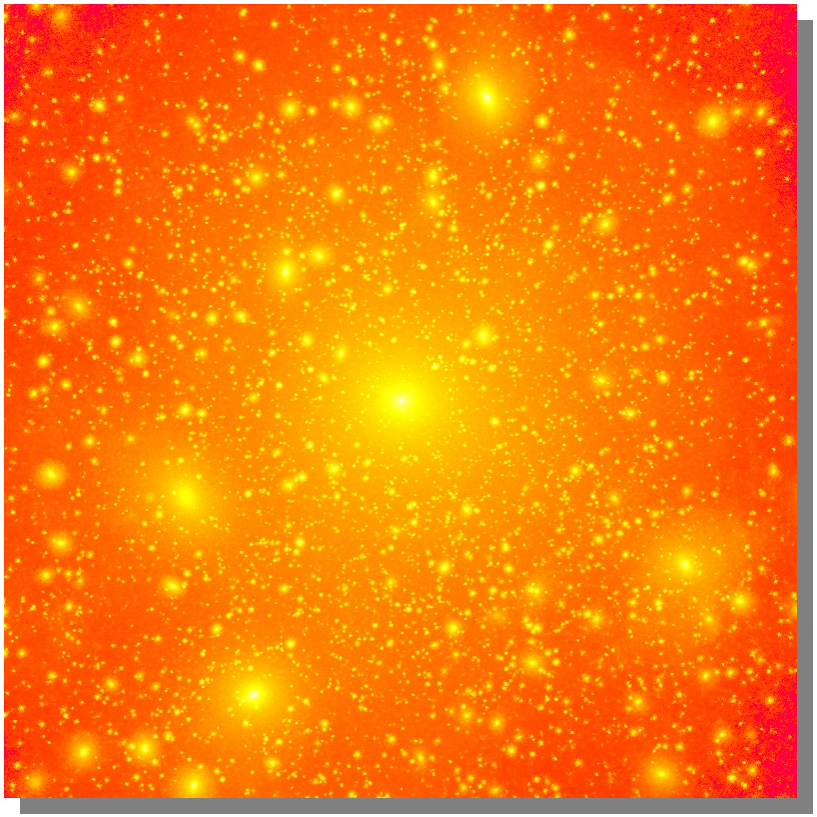
Hydro and N-Body Simulations of Early Structure Formation in the Universe

Objectives:

- To simulate the hydrodynamics of the feedback from the first luminous sources and their compact remnants.
- Use high-resolution N-body simulations to capture the evolution of the dark matter structures hosting the first stars and black holes from formation until today.
- To run the largest galaxy-scale simulation of dark matter structure to date. The final dark matter halo will incorporate 130 million particles within its virial radius.

Results:

- Columbia has enabled larger simulation runs with more mesh cells and particles than would have been possible with other systems.
- Able to run a greater number of simulations with varying parameters.



Dark matter density in the inner halo of a large galaxy. A wide range of sub-halo sizes is resolved and many of the larger substructures have their own sub-substructures bound to them.

POC: Piero Madau (University of California, Santa Cruz)

N-Body Simulation of Galaxy Dark Matter Halos

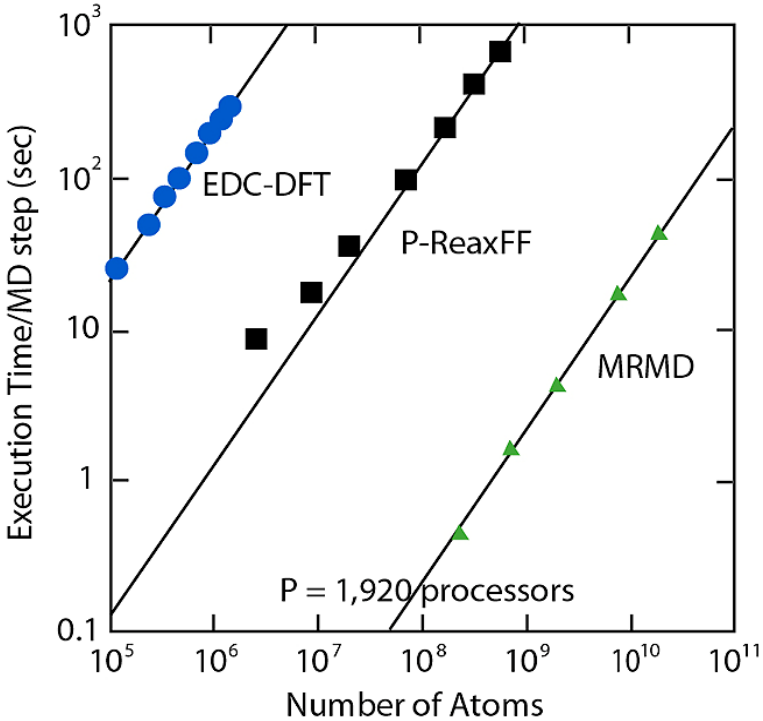
- Dark matter halos are the seeds for galaxies
- Current simulation is a multimass with 20 million particles in a Periodic 120Mpc box
- Completed in under a week using hybrid OpenMP/MPI code on 256 processors
- Multimass resolution used to resolve while preserving large-scale gravitational effects
- Cubic grid mesh adjusted at each time step based on evolution of particle distribution

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

POC: Joel Primack, Brandon Allgood (University of California, Santa Cruz)

Molecular Dynamics (MD) Performance

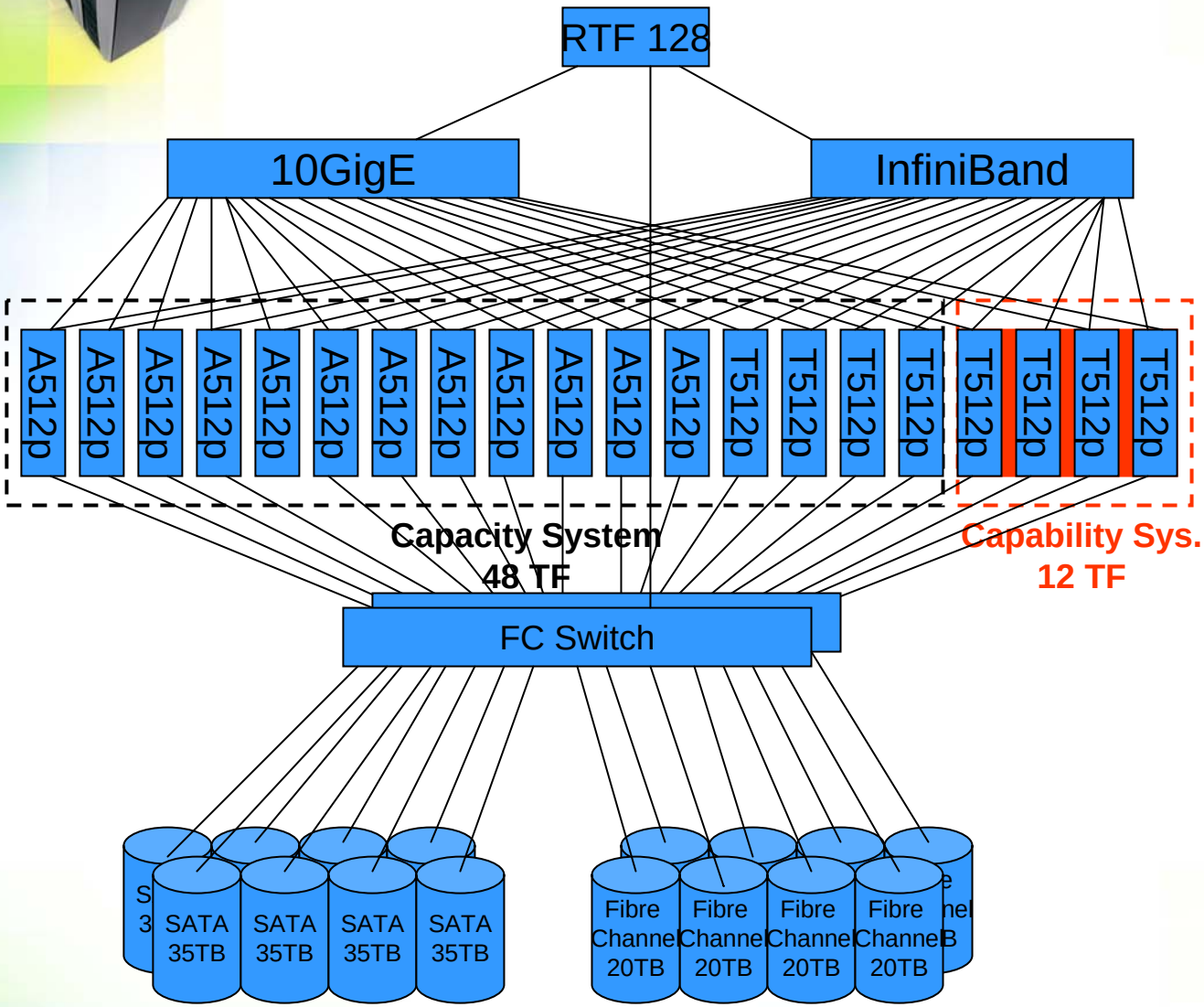
- Major design parameters for MD simulations of materials include the number of atoms in the simulated system and the methods to compute inter-atomic forces.
- Significant progress has been made in simulation methods, linear-scaling algorithms, and scalable parallel computing techniques.
- Currently performing larger performance tests o NASA Columbia, including 2.8 billion-atom reactive force-field and 6.9 million-atom density functional theory molecular dynamics simulations of chemical reactions.



Design-space diagram for MD simulations on 1,920 processors of Columbia. Total execution time per MD step is shown as a function of the number of atoms for three linear-scaling algorithms: Quantum-mechanical MD based on the embedded divide-and-conquer density functional theory (EDC-DFT, circles); parallel reactive force-field MD (P-ReaxFF, squares); and space-time multiresolution MD (MRMD, triangles).

POC: Aiichiro Nakano (University of Southern California), Deepak Srivastava (NASA Ames Research Center)

Columbia Configuration



Front End
- 128p Altix 3700 (RTF)

Networking
- 10GigE Switch 32-port
-10GigE Cards (1 Per 512p)
- InfiniBand Switch (288port)
- InfiniBand Cards (6 per 512p)
- Altix 3700 2BX 2048 Numalink Kits

Compute Node (Single Sys Image)
- Altix 3700 (A) 12x512p
- Altix 3700 BX2 (T) 8x512p

Storage Area Network
-Brocade Switch 2x128port

Storage (440 TB)
-FC RAID 8x20 TB (8 Racks)
-SATARAID 8x35TB (8 Racks)