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SC2002 – NAS Demo Abstracts

1. HyperWall

POC: Chris Henze

The hyperwall is a new concept in visual supercomputing, conceived and developed by the NAS Exploratory Computing Group. The hyperwall will allow simultaneous and coordinated visualization and interaction of an array of processes, such as a the computations of a parameter study or the parallel evolutions of a genetic algorithm population. Making over 65 million pixels available to the user, the hyperwall will enable and elicit qualitatively new ways of leveraging computers to accomplish science.

It is currently still unclear whether we will be able to transport the hyperwall to SC02. The crucial display frame still has not been completed by the metal fabrication shop, although they promised an August delivery. Also, we are still working the fragile node issue, which may require transplantation of the compute nodes from the present 2U cases into 3U cases. This modification will increase the present 3-rack configuration to 5 racks.

IF the hyperwall can be conveyed to Baltimore, we will be able to show a number of examples of parallel scientific visualization and computation. Applications we have running now include:

Parallel visualization of parametric CFD studies of an RLV (reusable launch vehicle), using gel (a sophisticated scalar/vector field visualization tool that is similar in spirit to FAST, but a lot more powerful). This allows direct visualization of features in CFD parameter landscapes, including the onset of vortex bursting, the transition to turbulence, bifurcations in separation/attachement, etc.

High-dimensional mutlivariate visualization of CFD datasets. This allows simultaneous views of various projections of high-dimensional data. We will almost certainly have these multiple views "linked" by SC02, allowing the user to interactively select subsets of the data in any space while viewing the selections in all other spaces. By combining the selections with boolean operators, we can support arbitrary condition queries on the dataset.

Parallel displays of the multiple dynamic variables from the Goddard Cumulus Ensemble Model (the "cloud model"). We may have multiple simultaneous live runs of the GCEM implemented by SC02, showing for example a direct ongoing comparison between different versions of cloud microphysics. This kind of "sensitivity analysis" (in serial) is primarily how the model is deployed by the Goddard scientists.

Live navigation through the 2-parameter family of carbon nanotubes. We will certainly have multiple live steerable molecular dynamics simulations wired into this by SC02 (probably by nest week). This will essentially be 49 copies of Virtual Mechanosynthesis, all controllable by a single user, who can for example apply the same physical input to a collection of different nanotubes to explore the profound electronic and mechanical effects of chirality.

Browsing of candidate protein docking complexes produced by high-end caluclations on the 1024. The browser also supports the application of various heuristic filters that are used by protein scientists to assign biological importance to the candidates. The parallel visualization allows one to explore clustering in a 6-dimensional configuration space, which is really what this sort of simulation is all about. The particular application here represents an investigation with Jonathan Trent into engineering protein nanotubes.

We will probably have other applications as well by SC02.

It is unlikely that the live interface to the cricket neuron will be available by SC02.

Note: The hyperwall will require substantial real estate in a demo booth. The display wall is about 10' wide by 9' high. The PC linux cluster driving the displays is contained in 4 racks which sit behind the display wall. The hyperwall requires about 20KW of power.

2. Real Time Ray Tracing with University of Utah

POC: Chris Henze

This looks like a go. After much discussion with the Utah folks, Ames network folks, and SGI, we've decided that constructing a very high bandwidth connection between chapman and the SC02 showfloor is infeasible in the current timeframe. Therefore, we will attempt to establish an optimized gig-E connection and focus our efforts on compressing the datastream. The demo will show the results of a highly optimized volume renderer running interactively on chapman. We are currently working to identify extremely large datasets that will show off the power of chapman and the renderer, and that are relevant to the kind of science that such high-end computing enables.

3. Stanford University Simulation Based Medical Planning Demo

POC: Nathan Wilson – Stanford University

The current paradigm for surgery planning for the treatment of cardiovascular disease relies exclusively on diagnostic imaging data to define the present state of the patient, empirical data to evaluate the efficacy of prior treatments for similar patients, and the judgment of the surgeon to decide on a preferred treatment. The objective of this work is to create a simulation-based medical planning system for cardiovascular disease that uses computational methods to evaluate alternative surgical options prior to treatment using patient-specific models of the vascular system.

The interactive demo will show the major steps in going from diagnostic medical imaging data to hemodynamic simulation. An example of creating a pre-operative geometric model from magnetic resonance imaging (MRI) data will be shown. The subsequent steps to prepare for analysis of mesh generation and boundary condition specification will be demonstrated. Finally, the simulation results will be visualized along with the imaging data to evaluate the surgical procedure.

4. Cart3D: A Package for Automated Grid Generation and Aerodynamic Database Creation

POC: Michael Aftosmis

This demo will highlight various aspects of NASA's Cart3D software for fully automated geometry processing and CFD simulation. Attendees will be able to reposition components of several pre-built vehicle geometries and watch while meshes suitable for CFD analysis are automatically generated on-demand. An entire suite of CFD runs for the chosen configuration can then be submitted for processing on the Information Power Grid. Animations, images, and other results from previously computed simulation suites will also be availible for demonstration.

5. Multiscale Quantum-Mechanical/Classical Atomistic Simulations Using Globus on a Grid of Distributed PC Clusters in the US and Japan

POC: Subhash Saini

Subhash Saini (NASA Ames Research Center, USA)
Hideaki Kikuchi, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta
(University of Southern California and Louisiana State University, USA)
Hiroshi Iyetomi (Niigata University, Japan)
Shuji Ogata, Takahisa Kouno (Yamaguchi University, Japan)
Fuyuki Shimojo (Kumamoto University and Hiroshima University, Japan)
Kenji Tsuruta (Okayama University, Japan)

We will demonstrate results from multiscale quantum-mechanical/classical atomistic simulations on a Grid of geographically distributed PC clusters, to study environmental effects of water molecules on fracture in silicon. The multiscale simulation approach seamlessly combines i) atomistic simulation based on the molecular dynamics (MD) method and ii) quantum mechanical (QM) calculation based on the density functional theory (DFT). The multiscale MD/QM simulation code has been Grid-enabled using:

a modular, additive hybridization scheme,
multiple QM clustering, and
computation/communication overlapping.

A preliminary run of the code has achieved a parallel efficiency of 94% on 25 PCs distributed over 3 PC clusters in the US and Japan, and a larger test involving 154 processors on 5 distributed PC clusters will be demonstrated. We will show a movie that walks through a silicon crack tip, showing water-silicon reactions.

6. Visualizing Active Remote Sensing Data

POC: Pat Moran

We would demonstrate how we can use a Field Model module for HDF-EOS data to interface with a Distributed Active Archive Center (DAAC). We would couple a graphics display to the data model to enable interactive visualizaiton of the data. The demonstration should be of particular interest to NASA GSFC attendees.

7. IPG Services Architecture

POC: Tony Lisotta

1. IPG Job Manager
2. IPG Broker
3. IPG Information Abstraction.
4. Accounting/Accountless Prototype
5. IPG Monitoring & Mgmt. Systems Prototype
6. Performance Prediction – W. Smith

Performance Prediction

A computational grid, such as the IPG, offers a large variety of computer systems to users. To assist users in selecting which computer system to use, we have developed techniques to predict the execution time of applications on space shared computers and predict when applications will begin executing on these systems. We will demonstrate how users can use our techniques to select the IPG system that will complete their applications at the earliest time.

8. Multi-level Parallelization and Optimization Environment

POC: Rupak Biswas

In this demo, we show three tools working together to transform serial codes into multi-level parallel versions. We will demonstrate a typical parallelization scenario where a user starts with a serial climate modeling code and uses CAPO, a tool for assisting in parallelization, to produce an OpenMP version of the code. In the demo scenario, we will be overly aggressive in parallelization and the resulting program will not produce the same answers as the serial code we started with. We will then use an automatic debugging tool, which uses information from CAPO, to isolate the cause of the execution differences. Once we have fixed the problem, we will use Paraver to demonstrate how performance of the parallel program can be analyzed. The scenario will conclude with a visualization of the data computed by the program. In addition to the integrated parallelization scenario, we will do in-depth demonstrations of the individual tools to show their multi-level parallel capabilities.

Traveler List (tentative): Henry Jin
Gabriele Jost (CSC)
Greg Matthews (CSC)
Rupak Biswas

9. Static Poster and Video viewing area.

We will have Poster Wall – "hall of fame" area in the booth. This area will be used for high profile project posters as well as the Projects that have received NASA awards over the past year. We will invite the Program offices to create a poster for this area also.

We will also create a looping video presentation discussing the posters shown on the walls. This area is still in the planning stages.

SGI 1024 System and Performance
IBM Star Cluster
Program posters (CICT, CNIS, CoSMO)
VAD Heart Model – Invention of the Year
HiMAP – Space Act of the Year
CART3D – ARC Software of the Year