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Code IN – NAS Systems Division
Demos List – Code IN
SC2000 - Dallas, TX
November 6-9, 2000

Ilab-Parameter Study Creation and Submission on the IPG
POC: Maurice Yarrow, Karen M. McCann, with collaborators Rupak Biswas, Rob F. Van der Wijngaart.

Abstract:
The creation of parameter study suites has recently become a more challenging problem as the parameter studies have become multi-tiered and the computational environment has become a supercomputer grid. The parameter spaces are vast, the individual problem sizes are getting larger, and researchers are seeking to combine several successive stages of parameterization and computation. Simultaneously, grid-based computing offers immense resource opportunities but at the expense of great difficulty of use. We present ILab, an advanced graphical user interface approach to this problem. Our novel strategy stresses intuitive visual design tools for parameter study creation and complex process specification, and also offers programming-free access to grid-based supercomputer resources and process automation.

Large-Scale Parallel Distributed Computing
POC: M. Jahed Djomehri, CSC and Rupak Biswas

Abstract
The demo illustrates a parallel and distributed CFD simulation of a large scale memory and CPU intensive aerodynamic application on distributed multiple processors, aggregated via the Information Power Grid (IPG). The application is aimed toward obtaining a rigorous grid-independent solution around the hovering rotors of a helicopter in an effort to resolve important features of the vortical wakes. The approach is based on a parallel overset Navier-Stokes solver that was developed for tightly-coupled parallel machines, and is adapted to the distributed execution environment. The exchange of boundary data across resources is enabled by the Globus metacomputing toolkit. The load balancing mechanism is based on the near and off body grid partitioning and on a grouping strategy of the multi-zone overset meshes. The solution will be executed on NASA's IPG testbed, consisting of SGI Origin2000 machines.

Note: We (AAA group) are interested in hosting a demo at SC2000 for a large-scale distributed computing. Our group is hosting another demo at the same time for a different project, related to parametric studies via ILAB (POC, Maurice Yarrow). We would share resources for these projects.

Parallelization Toolkit in the Legacy Code Modernization Project
POC: Henry Jin, Michael Frumkin

Abstract:
As the rapid evolvement of high performance computing systems, porting legacy codes to the new environment becomes a very challenging task. Not only the process is costly and difficult but also error prone. As part of the Legacy Code Modernization project, we have evaluated and developed a set of tools to help ease the job of parallelization and performance tuning. These tools are aimed at automating the porting process as much as possible, reducing the porting cost and improving the development cycle. We will demonstrate the functionality of a prototype toolkit from program analysis to data distribution creation and parallel code generation. We will illustrate the generation of both message-passing (such as MPI) codes and directive-based (such as OpenMP and HPF) codes for a selected set of benchmarks and CFD applications. We will also demonstrate the capability of applying data distribution directives to OpenMP programs.

IPG Launch Pad
POC: George Meyers, Ext. 4-1338

Abstract:
The IPG Launch Pad is our version of what is often called a "user portal" to the Grid. The Launch Pad gives the user a web based access point to the IPG, allowing them to perform various functions from the web that they would otherwise be required to perform on their "home" system or one of the IPG hosts. The Launch Pad provides the ability to manipulate files, construct job specifications, submit jobs to the Grid, and get status on their jobs and Grid hosts. The Launch Pad provides security from any location via the "Myproxy" interface to their Globus PKI certificate. The ultimate goal is to provide an simplified interface to the IPG that users will want to use rather than having to learn a new set of complex commands required to access the Grid.

Support for Debugging Automatically Parallelized Programs

Point of Contact
Robert Hood, CSC
Gabriele Jost, CSC

Abstract
We will demonstrate a system that simplifies the process of debugging programs produced by computer-aided parallelization tools. The system uses relative debugging techniques to compare serial and parallel executions in order to show where the computations begin to differ. If the original serial code is correct, errors due to parallelization will be isolated by the comparison.

One of the primary goals of the system is to minimize the effort required of the user. To that end, the debugging system uses information produced by the parallelization tool to drive the comparison process. In particular, the debugging system relies on the parallelization tool to provide information about where variables may have been modified and how arrays are distributed across multiple processes. User effort is also reduced through the use of dynamic instrumentation. This allows us to modify the program execution without changing the way the user builds the executable.

The use of dynamic instrumentation also permits us to compare the executions in a fine-grained fashion and only involve the debugger when a difference has been detected. This reduces the overhead of executing instrumentation.

DeBakey Heart Assist Device
POC: Cetin Kiris, 4-4485

Approximately 20 million people worldwide suffer annually from heart failure, a quarter of them in America alone. In the United States, an alarmingly low 2,500 donor hearts are available each year. The DeBakey Ventricular Assist Device (VAD) prolongs life until a suitable transplant heart is available, and is used to boost blood flow in patients suffering from hemodynamic deterioration, that is, loss of blood pressure and lowered cardiac output.

The use of Computational Fluid Dynamics (CFD) technology lead to major design improvements on the heart assist device, enabling its human implantation. The DeBakey VAD is a miniaturized heart pump designed to increase blood circulation in heart failure patients awaiting a transplant. A ventricular assist device has to be small and efficient generating 5 liter per minute blood flow rate against 100 mm Hg pressure. Because blood is the operating fluid, the design of a VAD requires that it propel the blood gently; in other words it must minimize damage on red blood cells. In order to reduce red blood cell damage, the pumping device must be designed to prevent high shear stress regions and separated flow regions in the pump. In addition, the blood must be washed out properly since the formation of blood clots may appear within stagnation regions as a result of previously damaged blood cells. Since the size of the device is small and the operating condition is severe, instrumentation for flow measurements is extremely difficult. Therefore it became necessary to look at the flow by computational means. The detailed computational flow analysis now affords VAD designers with a view of the complicated fluid dynamic processes inside their devices.

Through the collaborative efforts of MicroMed Technology Inc., the NASA Ames Research Center, and NASA Johnson Space Center, the DeBakey VAD has evolved from early versions of the DeBakey VAD which caused thrombus formation (blood clotting) and hemolysis (red blood cell damage). To solve these problems, NASA Ames scientists employed NASA Shuttle main engine technology and NASA computational fluid dynamics (CFD) modeling capabilities, coupled with the NAS division's high performance computing technology, to make several design modifications that vastly improved the heart device's performance. A three-dimensional, viscous, incompressible Navier-Stokes code (INS3D) was used to analyze the flow through DeBakey VAD. Several design iterations were performed in order to increase hydrodynamic performances of this axial pump. The research team investigated seven different designs, altering cavity shapes, blade curvature, inlet cannula shapes, and impeller tip clearance size. They then suggested three major design modifications to solve the problems of cell damage resulting from exposure to high shear stress and interrupted regions of blood flow in the DeBakey VAD.

The first improvement was the addition of an inducer that spins with the impeller, drawing the blood in and out of the device, preventing a back flow. Additionally, the inducer provides enough pressure rise which eliminated back flow in the impeller hub region. The front edge of the blades was slanted forward, allowing blood to flow at the correct angle with the impeller, thereby increasing the efficiency of flow through the device. Second, CFD results suggested that the original design of the device caused clotting in the front bearing area where the blood passes over the flow straightener and meets the impeller blades. Expanding the hub area's width increased the circulation of blood, eliminating stagnant sections where clotting was known to occur. Additionally, they tapered the hub surface, accelerating blood flow, and thus creating good wall washing. Finally, the exiting flow angle of the blood is examined and the diffuser angle is repositioned. Changing the diffuser blade angle aligns it with the blood flowing through the device, creating a smoother transition of blood over surfaces, and reducing shear stress that causes cell damage. Clinical tests conducted by MicroMed Technology and Baylor College of Medicine have confirmed the improvement in performance — hemolysis was decreased tenfold. In collaboration with designers at MicroMed Technology, modifications made using CFD analysis have enabled the device to perform for more than 100 days. The longest successful trial period to date in a human was 120 days, after which a donor heart was transplanted. The team's ultimate goal is to make the VAD a permanent alternative to heart transplant surgery. Successful European trials of the device in human suggest its ability to provide long-term ventricular assistance.

Immersive Workbench Demos
Code INR

1. Growler.

POC: Chris Henze, Bryan Green
This is the new name for the generalized VMS, developed by Chris Henze and Bryan Green. The Brenner potential molecular dynamics code of the old VMS is now a module in a flexible multi-client-multi-server framework that can dynamically switch between different viewers/analysis tools and different physics simulation codes. In addition to old VMS, we will dynamically attach to COSMOS (Andrew Pohorille's biomolecular dynamics code), a PDB file viewer (showing various proteins, including protein nanotubes), and OVERFLOW (hopefully with haptic feedback). This demo will require the workbench and associated workstation.

At SC00 we will show biomolecules in VMS - i.e. proteins, DNA, membranes, etc. We will try to pick something dynamic to show, perhaps with the haptic - like an enzyme binding to its substrate, or an antibody binding to its antigen, etc. We are working with Andrew Pohorille about the science behind his code COSMOS, and with Jim Taft about his parallelized version for lomax.

We also plan on showing an interactive version of OVERFLOW. This will allow computational steering, like VMS does now. We plan on hooking up the haptic device to a simulated wing, so the user can move the wing, feel the resulting lift and drag, and also see realtime features (like vortex cores) developing in the flow.

We may also hook up several different visualization and analysis tools to the ongoing flow simulation - like Gel and PAT. Besides demonstrating concurrency of simulation and visualization/analysis, this will show the power of our component and framework architecture that makes all these permutations possible.

2. The Mars Landing Site Collaboration PSE

POC: Glenn Deardorff

The Mars Landing Site Collaboration PSE is a Web-based facility for Mars researchers to collaborate and share their ideas for landing sites for upcoming Mars missions. The resources available for perusal consist of images and abstracts for each landing site, as well as 3D VRML scenes incorporating Viking terrain data, Viking surface images, high-resolution Mars Orbiter Camera (MOC) images from the currently-orbiting Mars Global Surveyor (MGS), and elevation profiles from the MGS Mars Orbiter Laser Altimeter (MOLA).

Recent work has focused on the PSE's development as an interactive archive of global data returned by the MGS. Users can select regions on Mars for on-the-fly creation of VRML scenes, including texture-mapped Viking surface images, embedded MOC images, and embedded MOLA profiles. In addition, a MOC image archive consists of MOC images displayed contained within larger-scale Viking images for regional context. The MOC image archive allows for online Java-based image processing, and downloads of the MOC images at varying degrees of resolution. An interactive MOLA archive allows users to select regions for display of the MOLA elevation profiles contained therein. Selecting one of the region's MOLA tracks displays that track in profile, and allows users to query it for its coordinates and elevations.

Near-term work consists of allowing users to select arbitrary regions (as opposed to the current preset 5x10 degree regions) of Mars for MOLA interrogation, and incorporation of Thermal Emission Spectrometer (TES) data for rock and mineral distributions. Extension of this PSE to data from other planetary exploration missions in also planned.

3. AM/FM: Active Metadata / Field Model.
POC: Pat Moran
This demo will be showing the use of field model objects within in an interpreted environment. Each field model object will have associated metadata that will be used to control the data visualization.

NREN: Digital Sky Virtual Observatory
presented by Kevin Jones, Ken Freeman and Sally Miller

ARC SN1 Origin Performance
presented by James Taft

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Code IN Research Exhibits

Immersive Workbench Demos: 1) Growler, presented by Chris Henze, Bryan Green; 2) Web-Based Interactive Mars Data Archive, presented by, Glenn Deardorff 3) Active Metadata/Field Model, presented by Pat Moran

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