

## Scientific Workspaces of the Future

The goal of this Argonne lead expedition is to form a partnership between technology developers and end users to deploy and further develop next generation high-end collaborative and network based scientific visualization tools and systems designed to meet the specific needs of distributed applications communities. The initial application foci will be the atmospheric modeling and simulation community and computational molecular biology community. The expedition will build on the Access Grid and the emerging suite of tools for large-format tiled displays and remote and parallel visualization of large-scale scientific data. A primary focus of the expedition is to develop and deploy user level tools that will enable significant use of the TeraGrid for collaborative science and distributed visualization.

ANL will lead the effort to deploy a number of discipline resources to the community via enhanced Virtual Venue services (e.g. persistent support for documents, locally hosted and remote applications, databases, and other tools). ANL will further develop the concept of Access Grid Virtual Venues to support Grid based access to domain-oriented problem solving environments. Virtual venues (VV) provide a mechanism to create associations of tools and data resources that are bound to virtual locations. The virtual venue server provides a point of contact for registering applications and services associated with a particular virtual location, which can be visited via an Access Grid node (e.g. group oriented node or the new personal interface node). This capability can be used to build virtual project rooms that make available to a user community persistence access to datasets, computational and analysis tools, shared documents and notebooks, access to remote sites via video, audio and text services and access to recorded sessions of previous interactions. Virtual venues can also provide persistent access to group oriented Grid Portals (IU). We propose to deploy two basic AG based collaborative problem-solving virtual venues by the end of year one.

- Virtual Computational Molecular Biology Laboratory – containing access to genomic and molecular biology databases and computational tools (e.g. BioCore, NAMD, GO, G-Whiz/WIT3, etc.) The computational biologists involved in the project will prioritize the specific selection of tools and databases. ANL will be responsible for managing this process and integrating these tools into the AG infrastructure. A major initial goal is to enable one or more existing distributed collaborations to begin working together via the Virtual CMB Laboratory on a regular basis and to incorporate this into teaching and training environments. (ANL, NCSA, ORNL)
- Virtual Atmospheric Modeling and Simulation Laboratory – will provide group access to Grid based simulation and modeling tools focused on climate and weather modeling, sample datasets useful for education and training. The Virtual AMS Laboratory will also provide a point of contact for collaborative analysis of large-scale output from climate simulations. ANL will work with the MEAD project to develop this capability.

Extend the concept of AG Virtual Venues to support access to high-performance remote visualization services. The idea here is to enable Tiled Displays to become active components of first class Access Grid nodes and exploit streaming visualization related services. Via the Virtual Venue services mechanism ANL will create several Grid services to support streaming high-end scientific visualization applications. These stream visualization services (e.g. Grid based versions of ParaView (LANL), ANL Volume Render (ANL), VisBench (NCSA), etc.) will enable remote coupling of visualization servers such as those being deployed as part of TeraGrid with network attached Tiled Displays and specially configured AG nodes (nodes that have graphics accelerators installed on the display nodes, ANL, EVL). An important idea to test here is the feasibility of using a Grid based version Chromium (ANL, LANL) to support network-based visualization.

- Grid Based Visualization Testbed -- Initial deployment and testing will be done between existing AG nodes, Tiled Displays and Grid based visualization servers located at ANL, NCSA and LANL. Additional deployments will be targeted at EVL, BU and other sites to be identified. These deployments will focus on the minimal development needed to port existing visualization tools to the Virtual Venue services model and demonstrate their utility.
- Application Specific Visualization Tools -- Deployment of application specific scientific visualization packages in Grid visualization mode. The applications partners will make specific selection of visualization tools to be ported to the Grid based visualization environment developed in this part of the expedition. Our goal will be to deploy one major visualization tool for each of the two virtual laboratories that use AG level graphics support and one each that can exploit high-resolution tiled displays. ANL will work closely with NCSA in this task.

Develop Grid based collaborative software infrastructure services address needed to provide APIs and related service interfaces for applications developers that will enable a variety of existing tools to be integrated into the collaborative framework defined by version 2.0 of the Access Grid. Current development directions for the Access Grid have targeted developing an OGSA compliant Virtual Venue server and associated collection of standard collaboration services. We propose to add to this set of collaboration services by developing several new capabilities by integrating existing tools. Since the Expedition process is not focused primarily on development we note that the approach taken here is mainly integration of existing tools with the Virtual Venue services model, not new development.

- Web Based Interface to Access Grid Sessions – to provide a lightweight communications conduit for Access Grid participants who are not able to use a full Access Grid node. This will enable incremental adoption of the Access Grid and the Virtual Venue based resources provided by the Access Grid. This work will also investigate Virtual Venue coupling and gateways to the Grid Portals efforts. ANL will work with the Portal Expedition to develop a robust Web based gateway to the Access Grid.
- 3D and Virtual Reality Interfaces to the Access Grid – there is substantial interest in supporting 3D and/or VR based visualization interface for the Access Grid. ANL will work with BU, LANL and EVL to incorporation advanced visualization services into the Access Grid and to develop backend access to the TeraGrid visualization infrastructure.

Management and Services Plan: The focus of this expedition is to improve the deployment and use of the Access Grid, Tiled Displays and remote and collaborative visualization tools in our two target communities. As expedition coordinator ANL will be responsible for developing an expedition management and services plan. Our preliminary plans include the following services activities. For the atmospheric sciences community Bob Wilhelmson will be responsible for community input, for the biosciences community Erik Jakobsson is responsible for community involvement with help from Natalia Maltsev. Ivan Judson will be responsible for product development, and coordinating the contributions from the technology development partners. Terry Disz will be responsible for coordinating between the applications groups and the technology groups and work in collaboration with Judson on product development. Jennifer Tieg von Hoffman will be responsible for coordinating technology transfer issues and interactions with PACS and EOT partners for the expedition. Rick Stevens will serve as overall coordinator and Mike Papka serve as deputy coordinator for the expedition. We expect to rely on ongoing support of documentation and training activities started by the PACS/EOT partners as part of the Access Grid Documentation Project and continued support of the Access Grid networking infrastructure via the PACS programs. We also plan to rely on some form of the X-in-a-box activities and support to continue to support the software that has been released to date, including improvements and updates.

### **Milestones 2003**

## Technology

### *Argonne National Laboratory*

- Hold initial face-to-face SWOF expedition planning meeting followed by quarterly meetings
- Design Virtual Venue based services for high-performance visualization, problem solving environments
- Select target visualization applications for atmospheric modeling and computational biology applications
- Release Virtual Venue services interface model
- Conduct AG based quarterly expedition meeting
- Deploy initial Grid based visualization services for applications communities
- Test initial web based interface to the Access Grid
- Test Chromium based network visualization service from TeraGrid visualization server
- Release virtual venue interface specification for collaboration services, modality translation and 3D/VR interfaces
- Deploy initial Tiled Display remote visualization testbed and test interfaces to TeraGrid visualization servers
- Begin testing initial modality translation services via Access Grid
- Demonstrate 3D and VR interfaces for the Access Grid
- Conduct AG based quarterly expedition meeting
- Deploy initial virtual computational molecular biology laboratory to target systems biology community including basic tools, directory services, initial databases and scientific datasets
- Deploy initial virtual atmospheric modeling and simulation laboratory to target UCAR community including basic tools, directory services, initial databases and scientific datasets
- Complete initial performance analysis of distributed visualization applications

### *Electronic Visualization Laboratory*

- Deployment/training for AGAVE systems; High speed reliable multicast for broadcasting full resolution graphics
- Deployment and Testing of TeraVision on a constrained number of sites to allow “walk-up and plug-in” distribution of laptop visuals; Deployment and Testing of voxel-based volume rendering on the AGAVE; Human factors experiments on use of tiled displays for increasing parallelism and group awareness between two sites
- Deployment of TeraVision for broadcasting tiled visualizations between a limited number of sites (2-3). Human factors experiments on the coordination of multiple workspace interfaces- e.g. AG, AGAVE, Digital Touch Screen white boards, Tiled Displays
- Remote volume rendering on the AGAVE. Testing of TeraVision for broadcasting tiled visualizations between a limited number of sites (2-3).

### *Boston University*

- Publish documentation for all major AG software releases, including new enhancements and advanced visualization services, in close collaboration with appropriate developers
- Coordinate technology transfer issues and interactions with PACS and EOT partners, participating in conference calls, meetings, and other activities
- Encourage deployment of new technologies through AG Users Seminar Series
- Provide AGDP overall vision and guidance
- Maintain and update existing AGDP documents, including the Authors' Guide
- Develop, edit, and contribute to new AGDP documents and AG-in-a-Box web-based tutorials

- Recruit members of appropriate development and target community groups to participate in the AGDP by authoring documents, and by serving on review and general support teams
- Participate in scientific workspaces planning meetings and virtual venue discussions
- Design 3D/VR navigation interface based on Virtual Venue interface specification; Participate in the visualization testbed
- Development of 3D/VR navigation interface with Virtual Venue support; Participate in deployment and testing of Tiled Wall visualization components
- Demonstrate integrated navigation and remote rendering using Virtual Venue service; Deploy end-to-end prototype of Grid-based data management, visualization and rendering

#### *Los Alamos National Laboratory*

- Develop initial version of tiled-display rendering service using Chromium
- Test and integrate Virtual Venue and Grid system services with rendering service; Develop initial versions of data management, visualization services using VTK, tailored to meet specific application community needs (Q2)
- Initial version of visualization and rendering prototypes complete
- Initial user testing and feedback

#### *NCSA*

- Move the VisBench application from a CORBA client/server application to a Grid services environment
- Create a cluster based parallel visualization server to handle large data visualization problems.
- Add collaborative capability to the VisBench application via the Grid based collaborative software infrastructure services that are being developed as part of this expedition.
- Work with the scientific community to adapt VisBench client software to particular application area needs.

#### *Brown University*

- Participation in service model design
- Incorporation of OpenAL under Chromium (CrOpenAL)
- Testing of CrOpenAL on TCASCV VR displays
- Install and test Grid-based visualization services on TCASCV rendering and display resources
- Design CrOpenAL server with OpenAL extensions, permitting compliance with Virtual Venue interface specification
- Participation in development of Virtual Venue specification for 3D/VR interfaces
- Implementation and testing of CrOpenAL server
- Installation and testing of Access Grid 3D and VR interface prototypes
- Installation and testing of virtual computational molecular biology laboratory
- Integration of CrOpenAL services with virtual computational molecular biology laboratory

### **Applications**

#### *Argonne National Laboratory (Biology)*

#### *Oak Ridge National Laboratory (Biology)*

- Streamline access to metabolic and regulatory networks databases (WIT3, EMP, KEGG), sequence databases (NCBI, SwissProt/Trembl, TIGR, JGI), protein structure databases (PDB, SCOP)
- Incorporate public genome sequence analysis tools, including genetic sequence analysis tools (Blast, FastA, Blocks, Pfam, etc.) and protein structure prediction tools (CATH, VAST, etc.). Develop teaching materials on using these visualization tools
- Develop teaching materials on using these tools and databases for genome annotations and metabolic reconstructions in the framework of WIT. Provide web-based user-friendly interface for navigation, interactive analysis and representation of genomic data to the scientific community through the Gwiz server
- Develop a prototype of new visualization tools for protein clusters and metabolic networks representation; integrate them into Genome analysis server framework. Develop and implement new tools for interactive analysis and display of metabolic and regulatory networks

*NCSA (Atmospheric)*

*UIUC (Biology)* Jakobsson and Schulten