UABGrid - A campus-wide distributed computational infrastructure

Users:

UABgrid is a collaboration between academic and administrative IT units at the University of Alabama at Birmingham, including office of the Vice President for Information Technology, Computer and Information Sciences, Mechanical Engineering, Biostatistics, Microbiology, and Structural Biology. Additional computational scientists include mathematicians, physicists, and geologists. These users currently run jobs directly on one or more clusters and also a supercomputer managed by the Alabama Supercomputer Authority. We view UABgrid as an opportunity for our institution to maximize use of its investments in computational resources through shared access, and to minimize the administrative effort required in doing so.

At our institution, High Performance Computing for traditional application areas such as surface modeling and engineering simulations has recently coincided with the rapidly growing field of Bioinformatics. As one of the top research institutions in NIH funding (ranked 20th) and 4th in the SouthEast (behind Johns Hopkins, Duke, and UNC Chapel Hill) UAB's research administration is highly attuned to supporting biomedical research requirements and has recently begun a concerted effort to build up the computational resources available for campus use. We view grid computing as a means of aggregating centrally funded and department-owned computational cycles for the benefit of all participants.

Numbers: approximately 25 computational/engineering scientists; 35 bioinformaticists and a community of over 100 faculty/staff who use the BLAST application. Approximately 100 PhD/grad students are working on some aspect of these applications and up to 150 students/semester use for coursework. This amounts to 2-5% of faculty (depending on whether you include BLAST users) and 1.5% of students. [Note: there is a larger amount of computation occurring in department owned computer labs; it is feasible to consider porting these applications to the campus grid at some future point in time].

Training:

Almost all of these users are trained in their specific application field, and have learned how to use one or another cluster or parallel supercomputer by logging in and submitting a job file. The staff from the central IT Academic Computing department have been working with Globus and condor software through the NMI TestBed program and have become quite familiar with it; these staff people have a combined 30 years of Unix system experience, scientific application programming and support, and experience developing web applications. One computer science faculty member focuses on grid computing as his research area and has taught a graduate level course in grid computing once per year for each of the past two years. Together, the IT and CIS grid people constitute the core of trained personnel, and about 8 graduate students work half time under their supervision.

As we have only recently completed our mastery of the grid components and portal implementation, we have written very little documentation to date. Our goal for this coming academic year is to move into operational mode, which will of necessity include some training and documentation.

User Access:

We have developed a customized portal, based on OGCE. Its front door is located at http://uabgrid.uab.edu/. Details involved in creating, using, and managing certificates are hidden from end users. The key features of UABgridCA are its use of authoritative identity management, its ability to hide certificate management from end-users, and its function as gateway from username and password-based to digital certificate-based identity. The UABgridCA has been cross-certified with University of Virginia's NMI Testbed Bridge CA, a stand in bridge CA for the planned integration with Higher Education Bridge Certification Authority (HEBCA) [1]. The Testbed Bridge CA can be used for inter-institutional collaboration and resource sharing on the SURAGrid [2]. A detailed description of our implementation can be found in [3, 4]. A key feature is that users access the grid via the campus single sign on, called the 'BlazerID'. The UAB 'BlazerID', named for the university mascot, serves as the user's identity for many network services on campus and is integral to UAB's central, authoritative LDAP-based directory and authentication infrastructure.

Currently, our portal provides access to the one-time registration, web-enabled grid-login, and basic workspace (proxy manager with GRAM job launch fields, GridFTP, and Ganglia view. Most of the students use a command line interface and manage their own private keys, as this is part of their learning process. We are planning for computational students (*e.g.*, math, physics, chemistry) to be able to use this web interface. For applications in common use, like BLAST, we are building an application-specific interface for ease of use; our first such endeavor was GridBlast. The user needs only to browse to their input file, set a few parameters (mostly from drop-down list) and go.

We expect students working on grid technology to use command line interface, and we expect most users of the grid to employ the web interface. We believe a portal or other web interface is a necessity for this class of users.

Applications actually run:

BLAST (with and without MPI libraries)
PovRAY
Genomics matching program from Ga State
G-BLAST – A GT4.0 based Grid Service for BLAST

This year we will be adding at least one surface modeling application and also a structural biology application. We may also be looking at running a distributed version of a commercial statistics application.

Job scheduling:

Since we are still in early development, current job scheduling is available at the specific resource. The Collaborative Computing Lab (CCL) in the Department of Computer and Information Sciences is involved in developing a resource broker and metascheduler to determine which machine to selecting for submitting a job.

Resource requirements:

Overall, the biggest problem identified has been long queue waits for access to individual clusters (i.e., not enough nodes). The performance of the bioinformatics applications tends to be dependent on the staging of large data repositories involved. The engineering simulations run on clusters tend to be storage bound (in terms of what is available within the cluster).

Infrastructure:

Globus Toolkit Versions 2.X, 3.X and 4.X Condor (NMI release) Pubcookie (will be replaced by Shibboleth this year) MyProxy OGCE PHPki LDAP campus authentication service & directory

Software needed: C, C++, Fortran, Java compilers; BLAS and LAPACK libraries, MPI and Pthread libraries, BLAST Program, R Package.

Resources: heterogeneous (although there is a pair of homogeneous clusters). We have not yet addressed synchronizing software resources; however, we are interested in the UMICH model that introduces a grid "head node" so that the grid stack is installed in front of a cluster rather than on every node. This approach also provides a clean administrative border between grid admin and cluster admin.

Specialized components: we are building a general-purpose, highly configurable collaboration environment where the grid portal interface is just one of several applications sharing a common system environment (including identity and user attributes) by using Shibboleth in a VO Service Provider model. This implementation is called myVOC, developed under NSF grant [] and that has been demonstrated at [].

Account Management:

UAB's central IT organization provides a BlazerID Central service as part of the campus architecture, a single management point for password resets, email account creation or deactivation, and user-authoritative attribute management. There is also a centralized Help Desk called AskIT that has a trouble ticket system. We will leverage AskIT and their trouble ticket system. Therefore, UABgrid does not need to determine who is a member of the UAB community; in addition, attributes such as "STUDENT", currently enrolled course numbers, department affiliation are readily available to us using

Shibboleth. It is possible for application-specific attributes or VO-specific role information to be made available, either by adding new attributes to the central LDAP directory or through our VO Service.

Authorization is currently managed by contents of the grid mapfile. Each system administrator can make use of that information to implement their respective usage policies. For the systems available campus-wide, we temporarily map the BlazerID provided in the grid map file to one of 20 accounts that have been pre-established on the system. In the Department of Computer and Information Sciences, individual accounts are created for users based on the BlazerID and the corresponding entries are added to the grid map file manually.

Our overall architecture does application-specific account provisioning and it is worth noting that it would be possible to apply this same approach to automatically provision a permanent account for a particular BlazerID. There are multiple usage policies in place: systems managed by ITAC are available to anyone with a valid BlazerID. Systems managed by the Enabling Technologies Lab give first priority to engineering faculty, then other faculty, then students. Systems available through the Department of Computer and Information Sciences are made available to any UAB faculty and staff whenever the cluster is available and students in the department are given the highest priority. We consider the ability to support multiple policies to be a plus in our campus culture.

Usage Tracking:
We are just beginning to think about this, but we believe it may be central to the success or failure of a campus grid. We will definitely track both users and jobs. We will be accountable to owners of the participating systems; to be determined is whether that information would be public, available to respective owners, or available to all participating sysadmins. There has been a user committee advising the Enabling Technologies Lab on usage policies; that process will be expanded to include campus-owned clusters and our job will be to implement those policies. Especially for "frequently run jobs" where we would be developing a customized web interface we will monitor the job itself in order to optimize performance. This type of job monitoring will also be necessary at a later phase when we are attempting to run a single job on multiple resources.

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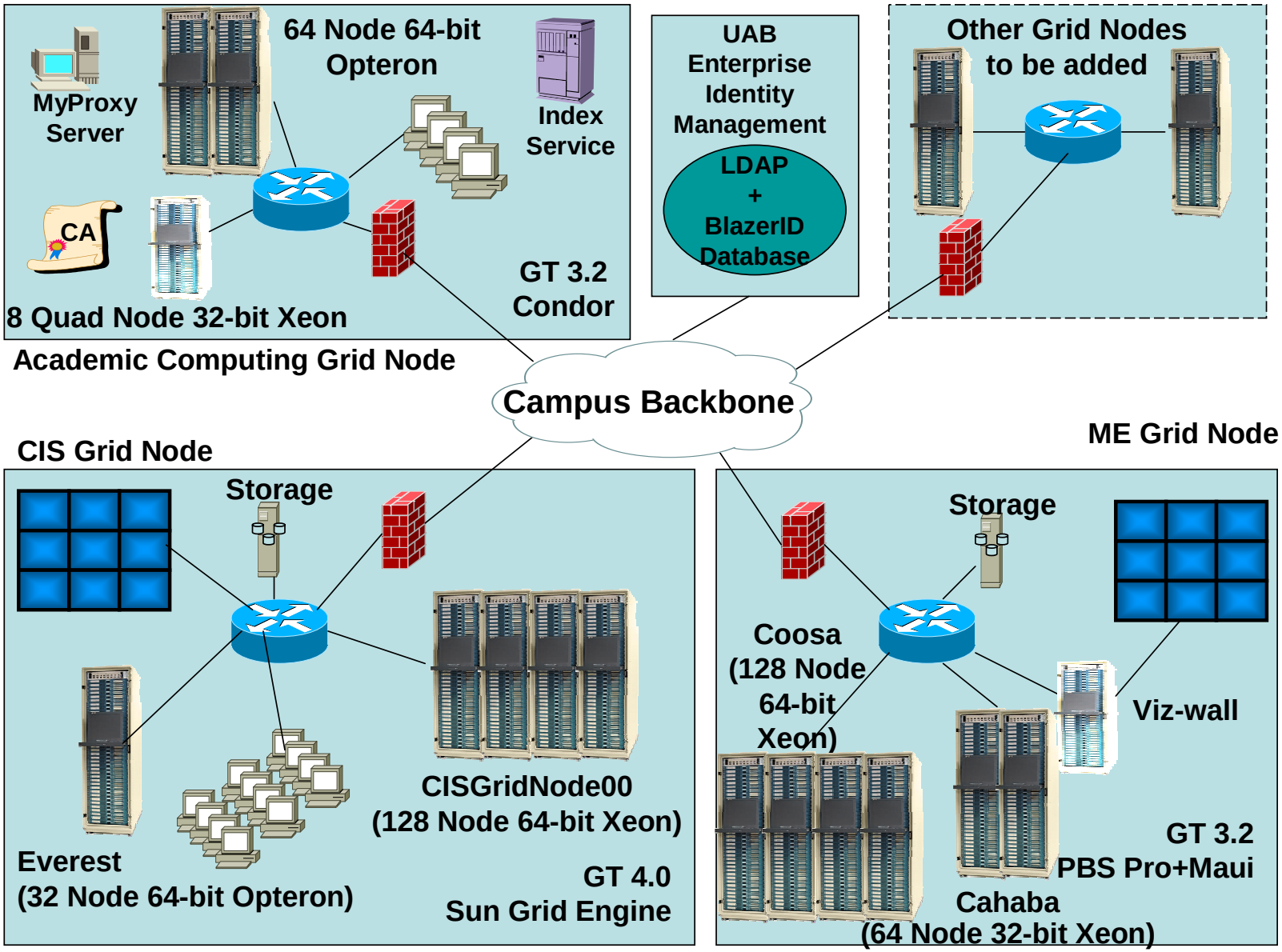
64 Node 64-bit Opteron
MyProxy Server
Index Service
CA
GT 3.2 Condor
8 Quad Node 32-bit Xeon
Academic Computing Grid Node
UAB Enterprise Identity Management
LDAP + BlazerID Database
Other Grid Nodes to be added
Campus Backbone
CIS Grid Node
Storage
CISGridNode00 (128 Node 64-bit Xeon)
Everest (32 Node 64-bit Opteron)
GT 4.0 Sun Grid Engine
ME Grid Node
Storage
Coosa (128 Node 64-bit Xeon)
Viz-wall
GT 3.2 PBS Pro+Maui
Cahaba (64 Node 32-bit Xeon)