TIGRE: The Texas Grid Computing Infrastructure Project

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Grids are “Hot”

Data - Computation - Information - Access - Knowledge
But What Are They?

Collection of heterogeneous computing resources

- Computers, data repositories, networks, and tools
- Varying in power, architectures, and purpose

Distributed

- Across the room, campus, city, state, nation, globe

Complex (Today)

- Hard to program
- Hard to manage
- Interconnected by networks
  - Links may vary in bandwidth
  - Load may vary dynamically
  - Reliability and security concerns

BUT – The platform for next generation computational science and engineering!
Texas Internet Grid for Research and Education (TIGRE)

- TIGRE is a state funded project of the HiPCAT consortium.
- TIGRE is a construction project primarily between Rice, A&M, TTU, UH, and UT Austin.
- TIGRE is an “application driven” project targeted primarily to extend the computational scope in
  - Bioscience and medicine
  - Energy and
  - Environment
TIGRE Vision

Design and deploy state-of-the-art grid computing infrastructure to

- Enhance the research and educational capabilities
- Facilitate new modalities for Academic-government-private research partnerships.
- Foster advanced computing technology transfer to Texas companies/industry.
- Become national model for organizations serving higher education
- Competitive model for external funding.
<table>
<thead>
<tr>
<th>Application Users</th>
<th>Resource Providers</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Compile &amp; Debug codes</td>
<td>• GSI OpenSSH</td>
</tr>
<tr>
<td>• Resource Selection</td>
<td>• Web Portal</td>
</tr>
<tr>
<td>• Who to contact?</td>
<td>• TTS, CSM</td>
</tr>
<tr>
<td>• Stage In/Out Data</td>
<td>• Grid/UberFTP, GridSCP</td>
</tr>
<tr>
<td>• Job submission &amp; Exec.</td>
<td>• WS-GRAM, Condor-G</td>
</tr>
<tr>
<td>• Is my data secure?</td>
<td>• AuthZ/AuthN (MyProxy)</td>
</tr>
<tr>
<td>• Application Mgmt. &amp; Collaborations</td>
<td>• Application VOs?</td>
</tr>
<tr>
<td></td>
<td>• Outreach/Tutorials, etc.</td>
</tr>
</tbody>
</table>
TIGRE: “Activity Driven”

Steering Committee:
- PIs from TIGRE Institutions.
- Defined Quarterly Milestones.
- Planning & Driving the Project direction.
- Meets periodically via F2F or teleconference.

Developers Team:
- Personnel funded through the TIGRE project.
- Milestones are divided into a set of project deliverables.
- The deliverables constitute one or more activities/sub-activities depending on the granularity of the task.
TIGRE: “Milestones & Deliverables”

YEAR 1
Project start date: Dec 1, 2005
Q1: Project plan ✔
Web site ✔
Certificate Authority ✔
Minimum testbed requirements ✔
Select 3 driving applications ✔
Q2: Alpha portal ✔
Q3: Define software stack ✔
Distribution Mechanism ✔
Simple demo of UltraScan from UTHSCSA (TIGRE app) ✔
Q4: IN PROGRESS …
Alpha client software distributed

YEAR 2
Q1: Alpha customer management services system deployed & demonstrated
Q2: Global grid scheduler deployed
Q3: Stable software available (only bug fixes after this)
Required services TIGRE specified
Q4: Complete hardening of software
Complete documentation
Finalized procedures and policies to join TIGRE & document
Demonstrate TIGRE at SC2007

... Making excellent progress!!
TIGRE Grid Middleware

Consists of two initial stacks – client stack and server stack, drawn from the VDT – web service based.

- **Contents of the cluster/compute server stack**
  - *Globus Toolkit 4.0 (Servers and clients)*
  - *Grid Proxy programs for obtaining TIGRE credentials*
  - *GSI OpenSSH, UberFTP, MyProxy, and Gondor-G*
  - *GPIR monitoring (added manually after the VDT pieces)*

- **Contents of the client only software stack**
  - *Globus Toolkit 4.0 clients (Grid Proxy programs, WS-GRAM client, and GridFTP client for secure, and high-bandwidth file transfers)*
  - *GSI OpenSSH client for compiling and debugging programs*
  - *UberFTP, MyProxy client for obtaining TIGRE credentials, and*
  - *Condor-G job scheduling and management*

- **Grid Storage (Not resolved for TIGRE yet)**
Sever Stack: VDT 1.3.10 based TIGRE stack is wrapped in the customized PacMan for TIGRE.

- Host and user grid certificates were issued by TACC.
- TIGRE Developers are provided with login accounts.
- User credentials are mapped manually to their login accounts.
- TIGRE Institutions contributed resources for TIGRE testbed.
- Grid Portal Information Repository (GPIR) service from TACC reports cluster status at the TIGRE portal [http://tigreportal.hipcat.net](http://tigreportal.hipcat.net)
- TIGRE server stack is fully web-service based. XML is used to create job submission scripts.
- WS-GRAM interface for local job scheduler prepares the job submission script and launches the job on the scheduler.
## Parallel Computing Resources

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Department</th>
<th>System</th>
<th>CPUs</th>
<th>Peak GFlops</th>
<th>Memory GBytes</th>
<th>Disk GBytes</th>
<th>Status</th>
<th>Load</th>
<th>Jobs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandera</td>
<td>The University of Texas at Austin</td>
<td>Texas Advanced Computing Center</td>
<td>TACC DGO Cluster</td>
<td>8</td>
<td>48</td>
<td>8</td>
<td>144</td>
<td></td>
<td></td>
<td>OR-CQ-00</td>
</tr>
<tr>
<td>Calclab</td>
<td>Texas A&amp;M University</td>
<td>Department of Mathematics</td>
<td>Calclab Optplex Cluster</td>
<td>223</td>
<td>1200</td>
<td>224</td>
<td>765</td>
<td></td>
<td></td>
<td>OR-CQ-00</td>
</tr>
<tr>
<td>Cosmos</td>
<td>Texas A&amp;M University</td>
<td>Texas A&amp;M Supercomputing Facility</td>
<td>SGI Altix</td>
<td>128</td>
<td>656</td>
<td>256</td>
<td>4096</td>
<td></td>
<td></td>
<td>600-00</td>
</tr>
<tr>
<td>Lonestar</td>
<td>The University of Texas at Austin</td>
<td>Texas Advanced Computing Center</td>
<td>Dell Linux Cluster</td>
<td>1024</td>
<td>8291</td>
<td>1984</td>
<td>33736</td>
<td></td>
<td></td>
<td>500-00</td>
</tr>
<tr>
<td>RTC</td>
<td>Rice University</td>
<td>Computer and Information Technology Institute</td>
<td>HP Itanium II Linux Cluster</td>
<td>230</td>
<td>1044</td>
<td>596</td>
<td>7000</td>
<td></td>
<td></td>
<td>OR-CQ-00</td>
</tr>
</tbody>
</table>

Total: 1677 CPUs, 9249 GFlops, 3068 GBytes, 45741 GBytes

## High Throughput Computing Resources

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Department</th>
<th>System</th>
<th>Active PCs</th>
<th>Active CPUs</th>
<th>Memory GBytes</th>
<th>Disk GBytes</th>
<th>Resource Details</th>
<th>Jobs</th>
</tr>
</thead>
<tbody>
<tr>
<td>all-test</td>
<td>Texas Tech University</td>
<td>High Performance Computing Center</td>
<td>Condor</td>
<td>0 / 0</td>
<td>0 / 0</td>
<td>0</td>
<td>0</td>
<td>Q</td>
<td>Q</td>
</tr>
<tr>
<td>Redeo</td>
<td>The University of Texas at Austin</td>
<td>Texas Advanced Computing Center</td>
<td>Condor</td>
<td>387 / 764</td>
<td>62 / 65</td>
<td>1241</td>
<td>5299</td>
<td>Q</td>
<td>Q</td>
</tr>
</tbody>
</table>

Total: 387 / 764, 62 / 65, 1241, 5299

*Jobs Key: #R - Number of Jobs Running, #Q - Number of Jobs Queued, #O - Number of Jobs in an Other State*
<job>
  <executable>binary</executable>
  <directory>${GLOBUS_USER_HOME}/DEST-DIR</directory>
  <argument>-f</argument>
  <argument>input file</argument>
  <argument>output file</argument>
  <fileStageIn>
    <transfer>
      <sourceUrl>gsiftp://submission-hostname:2811/input file</sourceUrl>
      <destinationUrl>file:///${GLOBUS_USER_HOME}/inputfile</destinationUrl>
    </transfer>
  </fileStageIn>
  <fileStageOut>
    <transfer>
      <sourceUrl>file:///${GLOBUS_USER_HOME}/output file</sourceUrl>
      <destinationUrl>gsiftp://hostname:2811/output file</destinationUrl>
    </transfer>
  </fileStageOut>
</job>
Proth's Theorem (1878): Let $N = h.2^k+1$ with $2^k > h$. If there is an integer $a$ such that
\[ a^{(N-1)/2} = -1 \pmod{N}, \]
then $N$ is prime. “$a$” is called the witness.

The goal of Proth code is to find largest prime in a given $[h_i:h_f, k]$ domain.

Importance: Large primes are of great importance in data encryption standards, and computer security. More info on Proth can be found at [http://www.prothsearch.net](http://www.prothsearch.net)

Proth is an ideally “grid suitable” application.

Algorithm:
1. Submit $(h_i, k)$ pair to a processor,
2. Collect all results into a DEST-DIR.
3. Search for primes in the list.
Bioscience & Medicine

1. UltraScan (TACC & UTHSCSA)

2. Computational Radiotherapy (TTHSC, JACC, SWCC, and MDACC)
Radiological Use of Fast Protons

ROBERT R WILSON
Research Laboratory of Physics, Harvard University Cambridge, Massachusetts
Accepted for publication in July 1945.

Except for electrons, the particles which have been accelerated to high energies by machines such as cyclotrons or Van de Graaff generators have not been directly used therapeutically. Rather, the neutrons, gamma rays, or artificial radioactivities produced in various reactions of the primary particles have been applied to medical problems. This has, in large part, been due to the very short penetration in tissue of protons, deuterons, and alpha particles from present accelerators.

Higher-energy machines are now under construction, however, and the ions from them will in general be energetic enough to have a range in tissue comparable to body dimensions. It must have occurred to many people that the particles themselves now become of considerable therapeutic interest. The object of this paper is to acquaint medical and biological workers with some of the physical properties and possibilities of such rays.

To be as simple as possible, let us consider only high-energy protons: later we can generalize to other particles. The accelerators now being constructed or planned will yield protons of energies above 125 MeV (million electron volts) and perhaps as high as 400 MeV. The range of a 125 MeV proton in tissue is 12 cm, while that of a 200 MeV proton is 27 cm. It is clear that such protons can penetrate to any part of the body.
Proton Depth Doses

From MGH Website
Proton v. Photon Therapy

SOBP: Spread-out Bragg Peak

From MGH Website
Represent **stochastic processes** probabilistically using random number generators…

Simulate the motion of the particles through matter using known microscopic **physics processes**…

Require accurate knowledge of the physical **geometry** and **material composition** of the matter traversed…

“**Score**” energy deposited and calculate **dose** endpoints statistically for designated volumes within the geometry by running many incident trial particles.
Justification

Benchmark runs @ MD Anderson

- Monte Carlo simulation of water phantom using 250 MeV proton beams.
- A 60 3.0 GHz Pentium 4 processor cluster, 200 M particle histories, 2D geometry.
- Runtime: eight hours, 2% - 4% uncertainty.

Simple Math

- Facility cost: $125 M. Cost effective treatment requires 300-350 patients day.
- Less than half-an-hour per patient (assuming 5 gantries).

Target

- 1000 Pentium 4 processors are required for 2D simulations.
Pilot Project: HDR Branchy Vs. Proton

Code sets: FLUKA, GEANT4, MCNP.

Collaboration: MDACC, UH, JACC, and TTU.

Future Directions

- Software toolkit for treatment planning.
- Potential industrial collaborations.
- Data security.
- Classroom demonstrations & educational outreach.
- Medical Physics program.
TIGRE is an “application driven” grid computing infrastructure development project.

TIGRE is targeted to mitigate computational challenges in three driving application areas of interest to the state of Texas. They are (1) Bioscience and medicine (2) energy and (3) environment.

TIGRE adopted “activity driven” top-down approach to meet the milestones determined by the project PIs (the Steering Committee).

The ultimate goal of TIGRE is to connect with the national grid projects such as TeraGrid, and OSG. Its future directions include

- Expansion to involve other Texas institutions beyond the primary five.
- Identify new applications and their grid suitability, and explore setting up of application VOs (OSG approach).
- Extend scientific scope by recruiting interdisciplinary applications.
- Competitive model for advanced computing in institutions primarily engaged in higher education.