Overview of Grid computing and GARUDA grid

Ramesh Naidu Laveti
(rameshl@cdac.in)
CDAC Knowledge Park, Bangalore
www.garudaindia.in
Outline

- Grid Concepts
- Grid Middleware
- GARUDA Overview
- Tools and services on GARUDA
- Applications on GARUDA
Grid Concepts
What is Grid Computing?
The Internet

- The web allows you access to widely spread distributed information
- You need not know or care where it comes from
- You provide the processing power locally to put it on your computer screen.

The web is just content!
2nd analogy

Domestic Electricity

- When you need it, you access it
- You don’t know or care where it comes from
- A supplier company handles the delivery and control
- You only pay for what you use.

The Power Grid is just power!
Grid Computing

- Grid allows seamless access to information AND computing resources
- You need not know or care where either comes from
- Pay for CPU cycles you use!

The Grid is content and Power!
It means

- Grid allows users to share resources in a secure and seamless way.

- Grid also facilitates collaborative environment over the high speed communication Fabric.

- The Super Computing power is accessible to the end users without the need of huge investment on Super Computers.

- CPU cycles that would otherwise be wasted are put to good use.
How user connects to the grid?

User

Internet/NKN

Certificate

Grid Service

Grid Computing Resource
Concerns

• **Security**
  – Authentication & Authorization

• **Information**
  – Static and Dynamic information about available resources.

• **Job**
  – Submission and execution of Jobs

• **Data**
  – Storing and Replication of data available and generated
## Components of grid

<table>
<thead>
<tr>
<th>Category</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Network/Communication Fabric</td>
<td>NKN and Internet links</td>
</tr>
<tr>
<td>Computational Resources &amp; devices</td>
<td>CPU, Satellite terminals, Telescopes</td>
</tr>
<tr>
<td>Storage &amp; Visualization</td>
<td>SRB/SRM, Visualization, softwares</td>
</tr>
<tr>
<td>Program Development Environment</td>
<td>Debuggers, Compiler IDE, Profilers, Workflow tools</td>
</tr>
<tr>
<td>Access Methods</td>
<td>Grid Portals, PSE’s, CLIs</td>
</tr>
<tr>
<td>Applications</td>
<td>Bioinformatics, Climate Modeling</td>
</tr>
<tr>
<td>Monitoring &amp; Management</td>
<td>Ganglia, Nagios, Monalisa GridICE</td>
</tr>
</tbody>
</table>
Grid Middleware
What is a Grid Middleware

Grid Middleware is a layer between grid applications and low level functionality of grid:

- It provides **Scalability, Transparency, Heterogeneity, Fault Tolerance and Security** to the Grid.

- It provides an **uniform interface of the Grid to users** and handles all the complexity generated due to heterogeneous systems.

  - **Examples:** **GT** - Globus Toolkit (Argonne National Laboratory, Chicago)
    **Glite** - LightWeight Middleware for Grid computing (EGI)
Grid Middleware components

Security

Information Management

Job Management

Data Management

Grid Middleware
Grid Middleware: Security

• User/ Resource Authentication
• User/ Resource Authorization
• User and Resource Policies
• Virtual Organization (VO)
Grid Middleware: Job Management

• Submission, Status Query, Cancel & Destroy, Getting Output & Error
• Support an open Job Description Language
  – RSL, JDL
• Transferring input/output data from/to remote source/destination
• Support Serial/ Parallel Jobs (Heterogeneous & Homogeneous)
• Integration with all Local Resource Managers (LRM)
Grid Middleware: Data Management

- Two Basic Categories of Data Management
  - **Data Movement**
    - Secure
    - Robust
    - Efficient
    - Third party movement
  - **Data Replication**
    - One or more copies or replicas
    - Survive loss
    - Easy availability
      - Reduce access latency, increase robustness, scalability and performance for distributed applications.
Grid Middleware: Information Management

- System information is critical to operation of the grid and construction of applications
  - How does an application determine what resources are available?
  - What is the “state” of the computational grid?
  - How can we optimize an application based on configuration of the underlying system?
- We need a general information infrastructure to answer these questions
Popular Grids
Global Access to Resources Using Distributed Architecture
Motivation

- Sharing of high-end computational resources with the larger scientific and engineering community across the country
- Addressing the requirements of emerging HPC applications by integrating geographically distributed resources
- Creating a Collaborative Framework for solving applications which are interdisciplinary requiring experts from multiple domains and distributed locations
- Providing Universal access to resources
GARUDA – India’s national grid computing initiative bringing together academic, scientific and research communities for developing their data and compute intensive applications.

Partners – More than 60 institutes

International collaborations – EGI, CaBig
GARUDA Backbone
GARUDA Grid: Architecture

- Grid-Enabled Applications
  - CLI
  - Access Portal
  - Grid PSE
  - Workflow tool
  - Visualization
  - Federated Information Server
  - Job Scheduler
  - Grid Programming & Development Environment
  - WSRF+GT4 + other Services + Cloud S/W
  - Virtualization support

- Grid Security and High-Performance Grid Networking

- Computing Resources and Virtual Organizations
  - CDAC Resource centers
  - Non-Research Organizations
  - Research Organizations
  - Educational institutions Computing Centers

- Resources, Security, Middleware, Resource Management, User Environments, Programming Environments, Data Grid, Grid Applications

- NKN

- Grid Applications

- India’s National Grid Computing Initiative
GARUDA S/W Architecture

Management, Monitoring & Accounting
- Paryavekshanam
- GARUDA Information Service
- Ganglia
- Nagios
- GARUDA Accounting

GARUDA Resources
- Compute, Data, Storage,
- Scientific Instruments,
- Application Specific Software,

Access Methods
- Access Portal
- Problem Solving Environments
- Cmd line interface
- Visualization gateways
- workflows

Resource Mgmt & Scheduling
- GridWay Meta-scheduler
- Resource Reservation
- Torque, Load Leveler
- Globus 4.x (WS Components)

Security Framework
- IGCA Certificates
- MyProxy
- VOMS
<table>
<thead>
<tr>
<th><strong>Institution</strong></th>
<th><strong>Location</strong></th>
<th><strong>Resources</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Space Application Centre</td>
<td>Ahmedabad</td>
<td>VSAT Terminal - 2 Nos.</td>
</tr>
<tr>
<td>Indian Institute of Science</td>
<td>Bangalore</td>
<td>64 cpu; POWER5; Linux</td>
</tr>
<tr>
<td>Raman Research Institute</td>
<td>Bangalore</td>
<td>32 cpu; Opteron; Linux</td>
</tr>
<tr>
<td>Institute of Mathematical Sciences</td>
<td>Chennai</td>
<td>24 cpu; Opteron cluster</td>
</tr>
<tr>
<td>Madras Institute of Technology</td>
<td>Chennai</td>
<td>16 cpu; P4; Linux</td>
</tr>
<tr>
<td>Indian Institute of Technology</td>
<td>Delhi</td>
<td>32 cpu; Opteron; Linux</td>
</tr>
<tr>
<td>Jawaharlal Nehru University</td>
<td>Delhi</td>
<td>32+16+16 cpu; Opteron, Opteron, Itanium; Linux</td>
</tr>
<tr>
<td>Institute of Genomics and Integrative Biology</td>
<td>Delhi</td>
<td>48 cpu; Xeon; Linux</td>
</tr>
<tr>
<td>Indian Institute of Technology</td>
<td>Guwahati</td>
<td>128 cpu; Opteron; Linux</td>
</tr>
<tr>
<td>University of Hyderabad</td>
<td>Hyderabad</td>
<td>32 way SMP; POWER4, AIX</td>
</tr>
<tr>
<td>Indian Institute of Technology</td>
<td>Kharagapur</td>
<td>16+16 cpu; Power PC2, Xeon; AIX, Linux</td>
</tr>
<tr>
<td>Physical Research Laboratory</td>
<td>Ahmedabad</td>
<td>320cpus; 64bit AMD</td>
</tr>
<tr>
<td><strong>CDAC</strong></td>
<td><strong>Bangalore</strong></td>
<td>320 cpu Xeon Linux; 64 cpu Power 5 AIX</td>
</tr>
<tr>
<td><strong>CDAC</strong></td>
<td><strong>Hyderabad</strong></td>
<td>320 cpu Xeon Linux</td>
</tr>
<tr>
<td><strong>CDAC</strong></td>
<td><strong>chennai</strong></td>
<td>320 cpu Xeon Linux</td>
</tr>
<tr>
<td><strong>CDAC</strong></td>
<td><strong>Pune</strong></td>
<td>32 cpu Xeon Linux; 4068 CPU Linux</td>
</tr>
</tbody>
</table>
## Virtual User Community (VOMS)

<table>
<thead>
<tr>
<th>Group Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bioinformatics</strong></td>
<td>Application of statistics and computer science to the molecular biology</td>
</tr>
<tr>
<td><strong>ClimateModelling</strong></td>
<td>Deals with the dynamics of the climate system.</td>
</tr>
<tr>
<td><strong>OSDD</strong></td>
<td>Community dedicated to develop drugs for tropical infectious diseases like malaria, tuberculosis</td>
</tr>
<tr>
<td><strong>GeoPhysics</strong></td>
<td>Study related to physics of the Earth and its environment in space</td>
</tr>
<tr>
<td><strong>CAE</strong></td>
<td>usage of computer software to solve engineering problems</td>
</tr>
<tr>
<td><strong>IndianHeritage</strong></td>
<td>Focused on technology products for preserving &amp; processing Heritage texts</td>
</tr>
<tr>
<td><strong>HealthInformatics</strong></td>
<td>Focused on utilizing compute power for health informatics</td>
</tr>
<tr>
<td><strong>MaterialScience</strong></td>
<td>Interdisciplinary field applying the properties of matter to science and engineering</td>
</tr>
<tr>
<td><strong>Euindia</strong></td>
<td>The vision of a worldwide Grid for Research by both Europe and India</td>
</tr>
<tr>
<td><strong>ToolsDeveloper</strong></td>
<td>Forum to communicate and collaborate on developing Garuda Tools</td>
</tr>
<tr>
<td><strong>GarudaAdmin</strong></td>
<td>Meant for administrators from resource providers &amp; Garuda Operation team members</td>
</tr>
</tbody>
</table>
National Collaborations

Garuda - IIT, Mumbai

- CAE Application
- Winglet Modeling

Garuda - OSDD

- Drug discovery for common cause like tuberculosis and malaria.

Garuda – SAC, Ahmedabad

- Satellite terminals
- Ganesh Scheduler
- DMSAR
International Collaborations

**Garuda - EGI**
- Integrating technological components of Garuda and EGI
- Glite and Globus

**Garuda - CaBig**
- Interoperation of technological service among these grids
- Cancer Research application portability
- Contribution to standards for using distributed computing in Health care
Tools and services
– Indian Grid Certification Authority located at C-DAC, Knowledge Park, Bangalore, India.
– IGCA is the accredited member of APGridPMA.
– Issues X.509 Certificates to support the secure environment in Grid. (for GARUDA, institutes that do research in grid from India and foreign institutes that collaborates with GARUDA).
– http://ca.garudaindia.in
Garuda Grid Portal

- Basic Job Submission
- Advanced Job Submission
- Browse Available resources
- Provision to View Status, Output, Error Files

http://portal.garudaindia.in
GARUDA SLCS provides grid users an instant access to GARUDA grid for a trial period of 30 days.

**Highlights:**
- Hassle free registration
- Get an access in less than 5 mins
- Service over the internet

**Features:**
- GARUDA Job submission portal
- GARUDA Compiler Service

Website: http://labs.garudaindia.in
GARUDA Resources

- CDAC Resources
  - 4TF HPC clusters each at Bangalore, Chennai & Hyderabad
  - PARAM Yuva at Pune and PARAM Padma at Bangalore
- Fourteen of the partner institutions are also contributing resources
- Total computing power is more than 6200 CPUs equivalent to 70TF
- Storage space 220 TB
GARUDA Storage Resource Manager

- Storage service available on GARUDA to store any kind of file
  - More than 220 TB with a single access point
  - Storage space and Data sharing
- Prerequisites to access GSRM
  - IGCA certificate
  - GARUDA Account
  - VOMS registration
- Accessing GSRM
  - Web access using GARUDA portal
  - CLI
Grid Meta-Scheduler

Grid Middleware

Meta-Scheduler

Grid Middleware

Grid Middleware
Metascheduler - Gridway

- Open source lightweight meta-scheduler
- Enables large-scale, reliable and efficient sharing of computing resources managed by different LRM systems
- Simple scheduling mechanisms but extensible
- Allows job dependencies (workflow)
- Supports job migration
- Integrates seamlessly with Globus toolkit
- Portable
- Implements DRMAA (Distributed Resource Manager Application API)
How GARUDA Operates?

Grid monitoring server

MyProxy
Credential Management Service

RAT

IGCA

MyProxy
Credential Management Service

GridWay

GridWay

Primary

Secondary

Grid Information Services

Grid Information Services

WS

Grid-FTP

MDS

MDS4

PBS Cluster

Gridmap file

NKN

192.168.60.40

192.168.69.72

Internet

VOMS

14.1.139.72

14.1.139.72
Job Submission Flow for Garuda users

Garuda Grid User

Proxy credentials

GJT

Garuda Grid

GridWay

Garuda Info system

Match Requirements

Find suitable resource in Garuda

Submit job to the LRM of Matching node

Cluster

Gridway Job Template
Applications on GARUDA
OSDD Chemo-informatics

- OSDD has more than 5300 registered users from 130 countries
- Chemoinformatics - Community of about 400 people
• Around 70 OSDD users are accessing Garuda through **OSDD VO**

• **Galaxy Workflow** for genomics applications. Galaxy is an open-source genomics workbench framework.

• Distributed job execution through **Gridway**
OSDD - Garuda Interface

Internet/NKN

Results

GARUDA GRID

Garuda Middleware Stack

LRM- Torque

GGHYD Cluster

Yuva Cluster

JNU Cluster

Other OSDD Cluster

OSDD Tools – weka, cdk...

NKN

OSDD HeadNode

Garuda Middleware Stack, login service, Gridway Metascheduler

OSDD Customized Galaxy

Galaxy Workflow

Figure 1: Login page for OSDD-GARUDA Interface

log in

Galaxy

Analyze Data
Workflow
Data Libraries
Help
User

Galaxy

Analyze Data
Workflow
Data Libraries
Help
User

Log in

Open Source
Discovery

Figure 1: Login page for OSDD-GARUDA Interface
Bioinformatics: Protein Structure Prediction on Grid

• Genetic Algorithm for Protein Structure Prediction (PSP), an in-house developed code is Grid-enabled

• Concurrent jobs of PSP are done by splitting the protein molecule into multiple overlapping parts

• Uses *Divide-and-Construct* approach for
  – Reduction in Complexity
  – Possibility of Concurrency
  – To handle larger protein molecules
Collaborative Class Room

Supported Features:-

- Interface to Access grid
- GSRM based data storage for maintaining course repositories
- Indexing of course material based on key words

Website: http://ccr.garudaindia.in
Simulation of Safety for Nuclear Reactor

- Study of heat extraction from a nuclear reactor, is very important. Larger the heat extraction, cheaper will the electric power generation. But larger generation must be necessarily safe with temperature below specified limit.

- The simulations require machines such as Blue gene

- World over thermal hydraulics simulations are carried out using tens of fuel pins and the results are extrapolated for hundreds fuel pins

- We have simulated all the 217 fuel pins, which probably is world record

- Initial estimated simulation time was 24 days. CDAC and ZN have reduced this to mere 3 days

- A paper is being written for publication
Simulation of Safety for Nuclear Reactor

We also require specialized post processing capabilities to extract information from the simulations.
Astrophysics - Novel phases of ultra cold atoms

Superfluid

Mott insulator
Climate modeling on Garuda

- Seasonal Forecast Model (SFM) implemented on GARUDA to do ensemble forecasting
- A framework developed to do ensemble forecasting using the existing grid middleware services
- Several simulations were done
- Use GSRM for data storage
- Model resolution: 40 Km x 40 Km
- Needs 27 GB of disk space and 80hrs of wall clock time (If I use 64 processors – Intel Xeon, 3.16 GHZ, 16GB RAM, Infiniband connectivity) for 1 season of 1 year with 1 ensemble member
Thank You