GARUDA: Pan-Indian distributed e-infrastructure for compute-data intensive collaborative science

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Abstract GARUDA is a nation-wide grid of computational nodes, mass storage and scientific instruments with an aim to provide technological advancements required to enable compute-data intensive, collaborative applications for the twenty-first century. From a Proof-of-Concept, the GARUDA has evolved to an operational grid, aggregating nearly 70TF-15TB compute-storage power, via high-speed National Knowledge Network and hosts a stack of middleware and tools to enable hundreds of users from diverse communities like life science, earth science, computer aided engineering, material science, etc. Evolution and confluence of research and technologies has led to the maturity of GARUDA grid: there have been addition of several hundred CPUs, large data stores, standardization of grid middleware, research on interoperability between grids and participation from varied application communities that have made significant impact to GARUDA. The GARUDA partner institutes are using this e-infrastructure to grid enable applications of societal and national importance. The authors in this paper present the manner of

building a nation-wide operational grid and its evolution, its deliverables, architecture and applications.

Keywords Grid computing · e-Infrastructure · e-Science · Virtual communities · Networking · Grid enable

1 Introduction

The revolutionary changes in technologies brought the scientific and engineering communities to embrace grid technology [1], and new e-infrastructures. The new scientific applications are having challenging demands of data, computing power, instrumentation intensive science and importance for collaborations.

Analysis of multi-Petabyte archives are required in fields as diverse as astronomy, biology, medicine, environment engineering and high-energy physics [2] to gain insights into the nature of matter, life or other aspects of the physical world. The Large Hadron Collider [2] is the world's largest high-energy particle accelerator and collider, located at CERN to search for the key to generation of matter. Similar challenges beckon the environment and earth observation, disaster management [3, 4], astronomy, bio-informatics [5], Human Genome project [6], and human health care monitoring. Grid is a type of parallel and distributed system that enables the sharing, selection, and aggregation of heterogeneous geographically distributed autonomous resources dynamically depending on their availability, capability, performance, cost, and users quality-of-service (QoS) requirements.

Major initiatives are underway worldwide, aimed variously, at supporting major science and grid research projects, developing and facilitating grid technologies. The Japan's 'Grid Consortium Japan' [7], China's 'CNGrid'

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[8], Korea's 'K*Grid' [9], and Italy 'INFN Grid' [10], are indicative of the global awakening to the potential of grid computing.

2 GARUDA grid

National governments are realizing the importance of new e-infrastructures to enable scientific progress and enhance research competitiveness. Making e-infrastructures available to the research community is crucial and is important to the researchers and the development teams in India. Similar to the international scenario the Indian Government also realized the strategic importance of grid computing. The Department of Electronics and Information Technology [11], Government of India, supported CDAC [12], to develop and deploy a nation-wide computational grid-GARUDA [13, 14].

The GARUDA is a Pan-Indian grid connecting 71 research/academic institutions spread over 30 cities of the country via high speed (multi-gigabit), highly reliable and available National Knowledge Network (NKN) [15].

The GARUDA grid aggregates over 70TF-15TB compute-storage power of heterogeneous HPC resources from 16 resource provider sites. All the participating institutes of GARUDA are connected on the NKN.

The authors in this paper try to highlight the architecture of the Indian national grid—GARUDA; readers can get more details from [3–5, 13, 14, 16–21].

2.1 GARUDA architecture

GARUDA has a hybrid architecture as it supports both centralized and peer-to-peer; for the grid administration it is centralized, while from the end users' perspective the GARUDA works in peer-to-peer mode. It offers Service Oriented Architecture based on Globus 4.0.7 middleware [22]. The participating institutes may be partners contributing resources or partners without resources. Figure 1 depicts the overall architecture of GARUDA built on the NKN backbone.

2.2 GARUDA network

The NKN [15, 23] is the Indian National Initiative of state-of-the-art multi-gigabit Pan-India network for providing a unified high-speed network backbone for all knowledge related institutions in the country. The NKN enables scientists, researchers and academicians from different backgrounds and diverse geographies to work closely in critical and emerging areas. The design of NKN comprises of an ultra-high-speed CORE (multiples of 10 Gbps),

Fig. 1 GARUDA architecture

Fig. 2 GARUDA partners on NKN backbone

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complimented with a distribution layer at appropriate speeds; participating institutions at the edge connect to the NKN seamlessly at speeds of 1 Gbps or higher. Design and performance [24] details can be referred International Journal of Computer Applications (0975-888) Volume 48, No. 13, June 2012. The network is designed to support Overlay-, Dedicated-, and Virtual Networks. It is highly reliable, scalable and highly available by design and provides strict QoS and security. Figure 2 shows the NKN backbone connecting the GARUDA resources and partners. Users can access the grid either from NKN or Internet.

The GARUDA partner institutes are connected on Layer 2/3 Multi-Protocol Label Switching Virtual Private Network (VPN) [25] on NKN backbone. The backbone of GARUDA VPN is NKN with bandwidth of 1 Gbps, and provisions of QoS and security.

NKN had a Point-of-Presence in most cities where GARUDA partner institutes were located. The NKN

network end point was made available to these institute premises. The last mile cable extension to the Laboratory/ Computer Centre was done in cooperation with the partner institute. The GARUDA team jointly with NKN and administrators of the partner institutes configured the Customer Premise Equipment (routers) as shown in Fig. 3, thereby connecting the institutes over NKN.

2.3 GARUDA resources

GARUDA has a pragmatic approach of augmenting resources through resource initiatives and collaborations—the PARAM Yuva [26] supercomputer at CDAC Pune, and GSAT-3 satellite terminals [27] for satellite communication of Space Application Centre (SAC) [28], ISRO.

With growing popularity of grid computing several partner institutes also volunteered to contribute compute resources to the project. Host certificates [29] were issued

Fig. 3 Partners connectivity to NKN

Fig. 4 GARUDA software stack

for these clusters and the grid middleware (described in next section) was deployed on them.

A utility (GARUDA Sigma) for automated installation and configuration of the core middleware components was

developed; the GARUDA administrators were able to remotely login, download and configure the newly added resources.

2.4 GARUDA stack

The GARUDA grid hosts a stack of middleware and tools for secure access, program development, problem solving environments, scientific visualization, storage grid solutions, metascheduler, and grid monitoring and management system, to help developers and application users to utilize the system effectively. The Fig. 4 shows components of the software stack—consisting of GARUDA Access Portal [16], monitoring tool—Paryavekshanam [17], GARUDA integrated development environment [18], automatic grid service generator [19], PSE for protein structure prediction [5], Kepler and Galaxy [30] workflows, and GARUDA visualization gateway.

GARUDA Access Portal (Fig. 5) is a web portal for submitting and monitoring jobs and accounting. Secure access to GARUDA is enabled through Indian Grid Certification Authority (IGCA) [31] certificates and authentication using MyProxy [32]. Grouping users into virtual communities is supported through Virtual Organization Membership Service (VOMS) [33]. The GARUDA portal allows reservation of computational nodes for guaranteed availability of resources. The jobs are scheduled on grid resources by Gridway [34] and GT4 web services. The portal supports data management through GARUDA-storage resource manager (G-SRM) [35].

Globus 4.0.7 is the core of GARUDA middleware. Several (middleware-level) services like the login service,

Fig. 5 GARUDA access portal **Fig. 6** GARUDA storage resource manager

compiler service, accounting service, and reservation service have been developed in-house to facilitate building of applications and tools. The Gridway metascheduler deployed on the grid headnode talks to the local resource managers (such as PBS/Torque [36, 37] and Loadleveler [38]) to manage the job submission (execution). Gridway (v5.6.1) has been customized to survive the failures of computing resources and information systems in GARUDA, with a failover module in Middleware Access Driver for information management. Gridway is well integrated with GARUDA Reservation System to take care of jobs with prior resource reservation. We have also introduced a custom stage in pre- and post-processing mechanisms for

serving jobs large number of input and output files. Gridway was also further customized to schedule and run OpenMP parallel jobs considering the specific job requirements. Gridway is integrated with the GARUDA Storage Grid to service data staging requirements of jobs and there is provision introduced for adding user specific job wall time for long running jobs.

The G-SRM has been engineered based on open source Disk Pool Manager [39], supports Grid Security Infrastructure (GSI) [40] and VOMS security mechanisms, dynamic space management, provides direct data transfer from compute cluster to GSRM storage, and has interoperability with other SRM implementations like Bestman

Fig. 7 Grid enabled flood assessment system

Table 1 DMSAR execution time on GARUDA resources

Date set size (GB)	Serial processing (h)	With 272 procs on GG-BLR (min)	With 368 processes on PARAM Yuva (min)
9	30	64	26

[41] and StoRM [42]. Figure 6 reveals the integration of compute- and data grids.

In the GARUDA architecture the grid headnode is centralized point of access to GARUDA, and hosting the portal and Gridway. This creates concerns of load and bottleneck for multiple simultaneous user accesses, in addition to making the headnode a critical point of failure. To alleviate this concern failover for headnode and the hybrid architecture were planned.

The software deployment architecture was well thought out to prevent load issues. For example, probes (information providers) are run on the different clusters for monitoring the resource; the time interval for running these scripts and data transferred have been carefully selected to avoid overloading the system.

2.5 GARUDA security

For enhanced security and international compliance, GARUDA established the IGCA, in addition to the basic GSI and VOMS. It is the first Indian Certificate Authority established to address security issues of grids and interoperability between international grids. The IGCA received accreditation from Asia Pacific Grid Policy Management

Fig. 8 GARUDA for OSDD

Authority [43] to provide access of worldwide grids to Indian researchers. The IGCA will help scientists, users and collaborative community in India and neighboring countries, to obtain an internationally recognized passport to interoperate with worldwide grids. Details of IGCA can be obtained at <http://ca.garudaindia.in/>.

2.6 GARUDA communities

Scientists collaborating for common problem, felt the need for secure and controlled sharing of resources. For this purpose, the VOMS [33] developed by European Datagrid project and publicly available in Globus Alliance, was customized and deployed on GARUDA. Domain specific virtual communities have been created under GARUDA such as atmospheric science, life science, computer aided engineering, material science, geophysics, health

Fig. 9 OSDD–GARUDA interface

informatics, etc. and special virtual organization (VO) for Open Source Drug Discovery (OSDD) community.

3 GARUDA applications

Application enablement involves understanding the nature of application and executing it suitably in the grid environment to take advantage of the virtualized grid infrastructure to improve processing speed and/or increase collaboration. The GARUDA has successfully demonstrated compute-collaboration intensive applications such as synthetic aperture radar (SAR) raw data processing for flood assessment [3, 4], PSE, molecular docking, OSDD [20, 44], Collaborative Classroom [45], etc.

3.1 Flood assessment

For assessing the extent of inundation during a flood, SAR is employed to capture the raw data of the flood affected region [3, 4]. This raw data is voluminous and processing it is a compute intensive/time consuming task involving processing several blocks of data, by using FFTs, data compression, mosaicing, etc. This program has been effectively parallelized at two levels—the code has inherent iterative constructs performing large matrix manipulations, which are parallelized using MPI and OpenMP to work on a cluster of SMPs (CLUMPs). Secondly, the voluminous data (typically ~35 GB) itself can be split and processed on separate CLUMPs in almost same time. The

partial results obtained by processing each partition is merged to obtain the complete resultant image. The application flow is depicted in Fig. 7 and the execution time for typical data set is shown in Table 1.

The benefits of grid enabling the SAR based flood assessment application is evident in both improved processing speed as well as increased collaboration. Collaborative analysis of the resultant image by experts at different geographic locations is possible by using a visualization software called Leica Virtual Explorer which enables remote sharing of visualization. This project was done in partnership with SAC, ISRO [28].

3.2 OSDD

GARUDA is facilitating the OSDD [44]—a CSIR initiative funded by Government of India, to develop drugs for tropical infectious diseases like malaria, tuberculosis, etc. Drug discovery involves characterizing a disease on a molecular level like—identifying the target and its structure, identifying potential ligand binding sites and applying docking methods, identifying the lead and lead optimization. Considering the number of possibilities of drug-to-target interactions, it is evident that this process is exhaustive requiring enormous data and compute power offered by grid computing.

GARUDA is facilitating the OSDD applications [20, 21] which have enormous data and complex algorithms demanding tremendous computational cycles beyond those available at any single location. Running drug design on

grid computing also enhanced the collaboration between bio- and chemoinformatics researchers. Figure 8 shows the compute-data intensive phases of drug discovery, where grid GARUDA is utilized.

The users of OSDD community required Galaxy workflow [30] to compose their applications and then execute it on the GARUDA infrastructure. In order to facilitate their requirements, an interface architecture as shown in Fig. 9 was designed. Gridway job-runner was developed for Galaxy, GARUDA Login Service was integrated, specific bio-tools were deployed and parallelized, and separate VO was created. Currently, about 79 OSDD users have successfully run their jobs on GARUDA (about 3,500 jobs consuming approximately 5,000 CPU hours wall time). Access to GARUDA grid via Internet has been enabled to help OSDD users not having NKN connectivity.

3.3 Winglet design

An optimal winglet design requires large number of Computational Fluid Dynamics (CFD) simulations for parametric and optimization studies. Genetic Algorithms using cross-breeding and local mutations run iteratively on large population size to yield potential winglet designs. A winglet optimization application by Zeus Numerix Private Limited, simulating 6,000 winglets taking nearly 30 days sequential computing time was able to complete in about 3 hours by running concurrently over large computing resource of GARUDA grid.

4 GARUDA usage and operation

4.1 Awareness/dissemination

The agreed mode of communication from GARUDA to the partnering institutes was at the management level. As a result, information about GARUDA, had not percolated to the researchers level in some organizations. This issue came to light during interactions at different levels. To overcome this shortfall, GARUDA organized thematic workshops, partner meets [46] and periodic telephonic interactions with scientists in the partner institutes. The project website [47] was populated with technical reports, publications and news letters to serve as a mechanism for the GARUDA community to exchange and disseminate information easily.

4.2 Grid enablement

Domain researchers working on compute-data intensive scientific problems were eager to use the new grid computing infrastructure but one of the problems in grid

enabling applications was the complexity involved in knowing about the GARUDA tools and their usage. As a result application developers find it difficult to grid enable their applications.

This issue was solved by handholding the application developers. An in-house grid application enablement team was formed with a mandate to interact with the application/domain experts to find out problems faced by the application developers and provide on-site support to them. Issues faced by application developers ranged from understanding grid computing, understanding their application characteristics, parallelizing codes, managing configuration settings, libraries, and use of third party software, etc.

The main objective of application developers was to get significant improvement in speed/execution time by exploiting the vast grid resources. However, the problem in most cases was that the application itself was not parallelized. The application enablement team studied the codes and parallelized them into hybrid MPI + OpenMP code which could run multiple threads on GARUDA's CLUMPS. Further, in applications such as the flood assessment by processing SAR raw data, it was observed that the voluminous data need to be divided thoughtfully and sent for processing on different clusters of the grid, to concurrently process the vast data thereby improving the processing time. Scalability and benchmarking was carried out for several applications (like flood assessment, PSE, winglet design).

4.3 Help desk/customer support (GGOA and RT)

Complexity of managing the grid increased as the number of grid users increased, and as the number of resources and software tools were added. A well trained group called

Fig. 10 GARUDA-EGI interoperability

Table 2 GARUDA resource usage

Location	2010		2011		Mid 2012	
	Jobs submitted	CPU hours utilized	Jobs submitted	CPU hours utilized	Jobs submitted	CPU hours utilized
C-DAC, Bangalore	8648	48699	16430	112018	7168	194852
C-DAC, Chennai	6087	29484	9307	58091	2538	101380
C-DAC, Hyderabad	5357	15717	10075	72419	4843	68424
C-DAC, Pune	12565	144119	5905	74254	2136	54612
IISc	9	0	2002	4	1602	56
IIT, Delhi	554	1	554	239	624	2
IIT, Guwahati	1104	8113	1879	9463	1186	7780
IMSC	50	2486	0	0	0	0
JNU	0	0	2096	1	614	0
MIT, Chennai	0	0	125	0	168	28
PRL	0	0	361	0	916	14
Total	34374	248619	48734	326489	21795	427148

GARUDA Grid Operations and Administration (GGOA) was formed to front end the customer support to GARUDA affiliates. Any problem or query was recorded and tracked with a unique identification number using the Request Tracker (RT) [48] software. The RT has a mechanism to report and resolve problem/request; if the problem remains unsolved for a long time, the RT automatically escalates the case to the reporting officers.

The GGOA team conducts weekly tele-meetings with local system administrators to effectively resolve issues at different locations of GARUDA grid.

Table 2 shows the utilization of various GARUDA resource by different users.

5 Interoperability with international grids

Interoperability between grids is an important research issue. As each nation has grid infrastructure, it is essential to work out mechanisms to collaborate between these grids. The EU–India Grid project [49] was setup in early 2007 to identify mechanism for interoperability between grids. It is supporting and linking grid community in Europe and India and to promote research in both regions. GARUDA grid has GT4 and Gridway metascheduler while EGI (European Grid Initiative) with CREAM CE [50, 51] and Gridway. To facilitate interoperability between the grids the Gridway has been tweaked to recognize the target grid and do job submission-management accordingly, as shown in Fig. 10.

Presently the interface between the two grids has been completed and job submission from either grid to any resource belonging to EGI or GARUDA has been successfully demonstrated. In fact the key part of interoperability between grids is unified job submission (resource usage) [52].

Fig. 11 Satellite grid–GARUDA interface

6 SATGrid–GARUDA interface

Combining Satellite technology and grid computing concepts, SAC, ISRO designed a satellite grid (SATGrid). Based on security, authentication, monitoring and discovery and data transfer (GridFTP) of Globus Toolkit 2.4.3 and SAC developed scheduler GANESH [53], a prototype satellite based grid was established. It was desired to submit compute intensive jobs from this grid to GARUDA's unprecedented resource. For this a SATGrid–GARUDA interface was developed to using certificate chaining for authentication of SATGrid users to GARUDA and job execution was supported through GARUDA portal APIs, as shown in Fig. 11.

Table 3 Components evolution in GARUDA project phases

Features	Phase		
	GARUDA PoC (2004–2008)	GARUDA Foundation (2008–2009)	GARUDA Operational (2009–2013)
Architecture	Centralized	Centralized	Hybrid: centralized—P2P
Network	Private	Private	NKN
Resource	5TF-2TB	16TF-8TB	70TF-15TB
Middleware	Globus 2.4.3 (stable release)	Globus 4.0.7 (stable release)	Globus + clouds
Web compliance	Pre WS	Web service based	Web service based
SOA support	Not supported	Service oriented grid	Supported
Grid metascheduler	Moab	Gridway	Gridway-tuned
QoS compliance	Rudimentary	Advanced reservation	Support for resources and services
Storage solutions	SRB—commercial	SRM—open source S/W	SRM—Gridway integrated for seamless job submission
Virtual community support	Virtual community groups formed	Enabling virtual communities thru VOMS	Fully supported

7 GARUDA evolution

In 2004, GARUDA started with an ambitious plan for Pan-Indian computing grid with an aim to provide the technology required to enable data and compute intensive science for the twenty-first century. The Research and Development organizations having data-compute intensive problems were approached as collaborating partners. The key objectives of Proof-of-Concept (PoC) GARUDA were—resource aggregation, establishing nation-wide communication network, provisioning grid tools and services, and grid enablement and deployment of select applications. Considering the enormity of task, PoC GARUDA adopted a pragmatic approach to setting up the grid by using a judicious mix of open source and in-house developed and industry components.

In 2006–2007 it was observed that grid technology was fast converging with web services architecture with the invention of Web Services Resource Framework (WSRF) [54]. SOA [55]—a combination of the principles of object orientation and web services led to formulation of Open Grid Standards Infrastructure (OGSI) [56]. In compliance to the OGSI, Globus released the GT 4.x in 2008. Also successful demonstration of PoC prompted us to think about turning the research investment into tangible commercial opportunities. Hence the GARUDA evolved to a service oriented grid with stable GT 4.x middleware during the Foundation Phase in 2008–2009. The Table 3 gives the details of the Proof-of-Concept (PoC), Foundation and Operational phases of GARUDA.

Many grand projects like the TeraGrid [57], NAREGI [58], and Distributed European Infrastructure for Supercomputing Applications (DEISAs) [59] have had their quota of achievements as well as learning. As mentioned by Peter H. Beckman, in the article ‘Building the

TeraGrid’—one of the most important learning is to have a precise definition of the word ‘grid’ specifying the architecture, application and policies, differentiating it from general distributed computing. DEISA had to cope with issues of dynamic, heterogeneous and geographically distributed resources, manpower and operation issues. NAREGI had to cope with finetuning the middleware for coexistence of multi-type jobs, production level loads and interoperability with other grids. Operational issues was a common issue faced by all grids.

GARUDA also encountered several technical, administrative and managerial issues—in terms of interface for diverse users, parallelizing and optimizing users’ applications, interoperation, standards [60] and security, usage policies, etc.

8 Conclusion

GARUDA has become a successful Indian nation-wide operational grid and helped to build the grid community in the country. With various research and academic institutes actively participating in GARUDA, it has created awareness in parallel and distributed computing in the country starting at the Graduate Engineering levels. Many of the research and academic institutes are participating in collaborative projects using aggregated resources of the grid. GARUDA teams are working on next generation technologies such as interoperability of grid and cloud, workflows and PSEs for various application areas, and on mobile interfaces for GARUDA that will significantly improve the ease of access to this critical e-infrastructure.

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