

Parallel Programming Environments: HPC, Grid, Cloud and Hybrid Computing

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4/23/12



Presentation Outline

- C-DAC Mission
- > HPC Mission
 - **Program Development Environments**
 - GARUDA Grid
 - C-DAC Scientific Cloud
 - Multicore-Accelerators Roadmap
 - Hybrid Computing
 - Petascale Computing

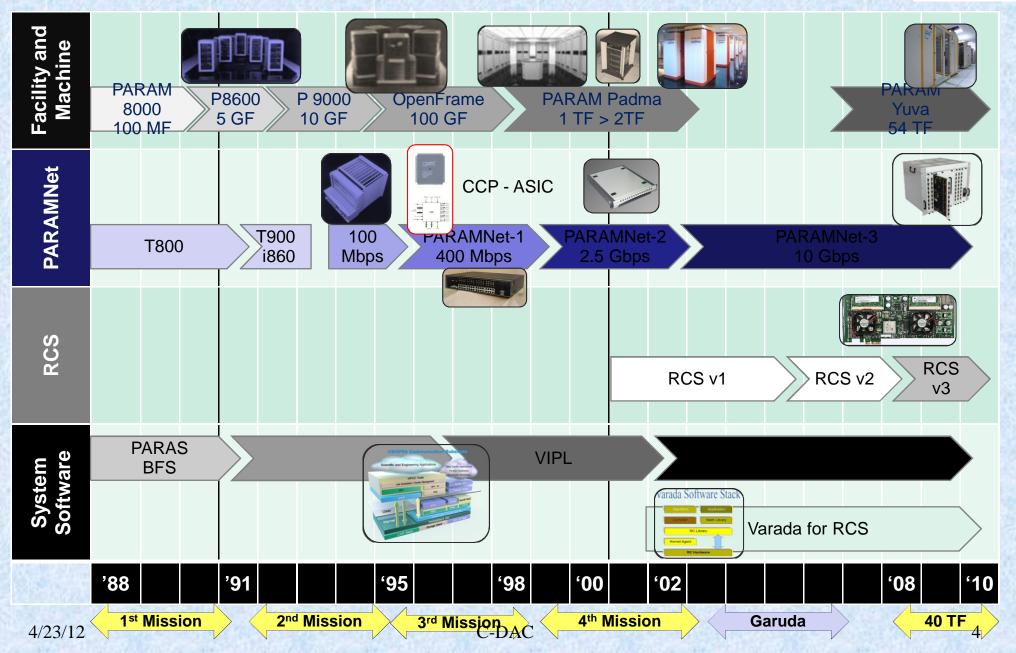
C-DAC Mission



- CDAC was launched as India's initiative to Design & Develop Indigenous High Performance Computers.
- C-DAC engaged in Thematic Research in HPC, Grid Cloud, Hybrid Computing, and PARAM Series of HPC Machines.

Application Enablers – 1988 to 2011





C-DAC's PARAM Systems





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PARAM Yuva at C-DAC Pune



- 54 TF peak performance
 - 37.8 TF max HPL-LINPAC (70%).
 - *PARAMNet* + *Kshipra* SAN (48 nodes).
 - RCS + Avatar(s) + Varada (16 nodes).
 - Infiniband and Ethernet networks.
 - 200 TB Storage and 10 Gbps. *PFS* over SAN.
 - Tools for system management and reporting
 - 2500 sq-ft facility.
 - ~ 1 MW at full load.
 - 19" Cabinets designed In-house.



PARAMNet-3 in PARAM Yuva



NIC



•Based on GEMINI: 4th Generation Communication Co-Processor Developed by C-DAC

Protocol Offload Engine in Hardware, supporting Send/Recv, RDMA and datagram communication protocols
Based on PCI-e (4X/8X) host interface and 10Gbps CX-4 physical link interface

16 MB onboard fast memory
User level access to 4096 hardware

•User level access to 4096 hardware endpoints

Virtual address support with protection

Switch



•Modular Chassis based Architecture

•48 Ports with each port working at 10Gbps full duplex

•Also a 16-port variant for smaller deployments

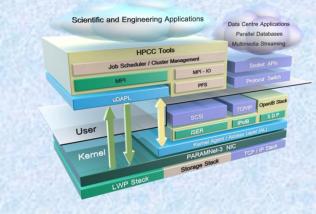
•Aggregate switching throughput of approx 1 Terabits/sec

•Low latency (1 us), near wire speed throughput for each port

•Support for large clusters through multi-staging C-DAC

Software Stack: Kshipra

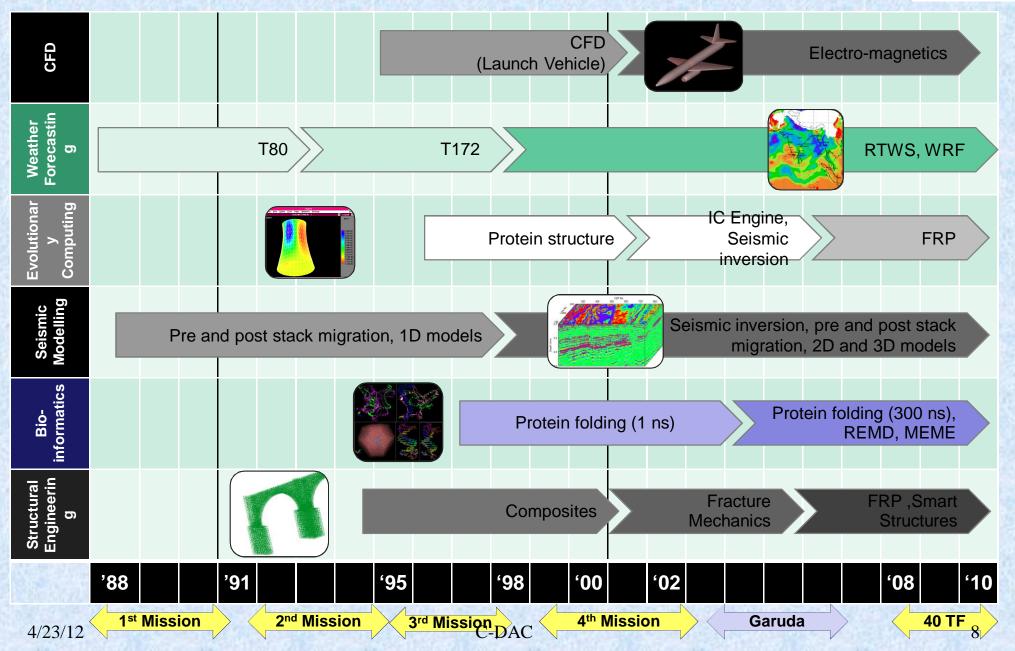
KSHIPRA Communication Substrate



- Program Development Environment (PdE) for PARAMNet-3
- upports two RDMA enabled Industry Standard Interfaces
 - Direct Access Provider Library (DAPL)
 - Open Fabrics Enterprise Distribution (OFED) stack
- Enables a whole gamut of networking applications from HPC / Enterprise computing areas

HPC Applications – 1988 to 2011





Weather and Climate Research



- Weather forecast Modeling Operational sponsored projects from INDG and Kerala State Planning Board for daily Village/local level weather information
 - Simulations using 40 nodes of PARAM Yuva
- Aerosol Modeling for Climate Change Study Study of Sulphate & carbon aerosol effects using global and regional aerosol models.
 - Joint R&D project with Chemical Engineering Department, IITB, sponsored by Indo-US Forum and ISRO-GBP and University of Iowa, USA
 - Development of coupled WRF-STEM modeling system
- Forecast Improvement R&D project in progress for research using assimilation of observational data

Earthquake Engineering Research



- The Earthquake Simulation study on PARAM Yuva includes:
 - Dynamic simulations of fault ruptures and study of earthquake time histories.
 - Structural response to high frequency ground motion.
 - Probabilistic seismic hazard calculations and Risk Analysis.
- OpenSees software has been ported on PARAM Yuva



Bioinformatics Resources & Applications Facility

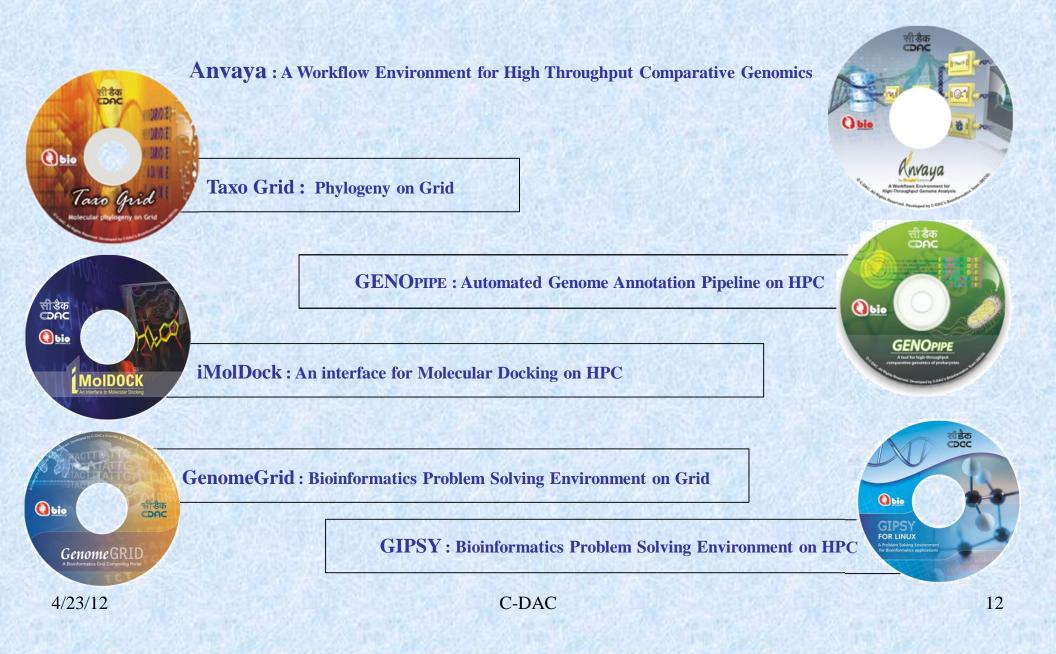
- Facility exclusive for bioinformatics research
- Funded by the Department of Information Technology (DIT), Ministry of Communications and Information Technology
- An enabling platform for collaborative research

Biogene: RCS Enabled Cluster

- 1TF cluster enabled with AMD processor 2.6Ghz, RCS cards, 50TB storage, 378GB RAM and Infiniband connectivity
- Total 16 RCS cards
- RCS enabled SW
- Multiple Bioinformatics software Grid enabled
- Web-computing portals 4/23/12



Bioinformatics Application Software for High-End Clusters and Grid





Computer Aided Engineering

Computational Structure Mechanics (CSM)

OpenSees software Framework on PARAM YUVA.

Existing bridge on Guhagar-Karad-Jat-Vijapur, S.H. 78, 315.5 m length across Krishna River near Karad, Mahrashtra.

Earthquake Simulation for the entire bridge on Param Yuva with 560000 quad elements.

Complete strength analysis of the Bridge using OpenSees

Computational Fluid Dynamics (CFD)

Tarang, Spectral based parallel CFD solver in public domain.

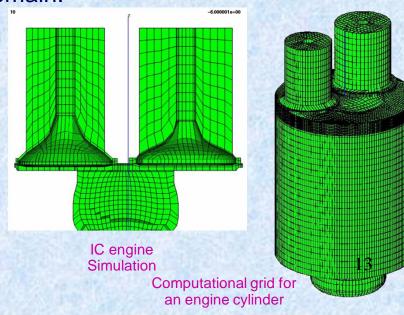
It is the most accurate compared to finite element and finite volume method.

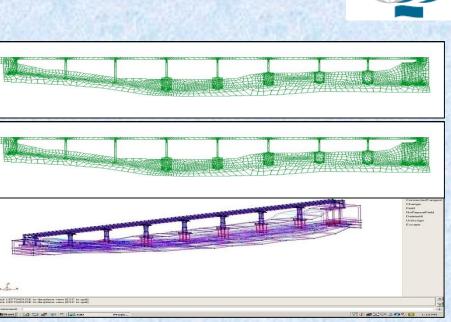
It can simulate turbulent fluid flow, convection, MHD flow, passive scalar turbulence, etc. in simple geometry.

Computations of energy spectrum, fluxes, shell-toshell energy transfer, structure functions and other 40 agnostics. C-DAC

Tested on 1024^3 (~ 10^9) grid points.









Reconfigurable Computing



Systems that dynamically modify their hardware for accelerating applications - Mainly based on FPGAs

10X-200X ... Acceleration

C-DAC 1414headed RC in India –

Accelerated Solutions for

Bioinformatics

Radio Astronomy

Fracture mechanics

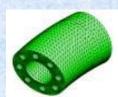
Scientific & engineering routines

Crypto analysis

And Many More...

C-DAC







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Reconfigurable Computing



Design & Development of Reconfigurable Computing (FPGA based) Solution for Application acceleration

RCS-V3 deployed in PARAM-Yuva 16 nodes
RCS-V4 deployed in 1TF BioGen cluster

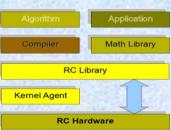
small form factor, CE & FCC compliance

Performance runs show 10-100X Acceleration
Eco-friendly HPC solution





Varada Software Stack



Avatars



System Software development Activities



- Development of System Software for the PARAM series of supercomputers
- Provide Tools and Solutions for performance and usability challenges of Supercomputers
- Provide Services, Technology Solutions, Consultancy and Training in the area of High Performance Computing (HPC), Grid, and Cloud Computing
- Research in enabling technologies

System Software Development - Profile



Engaged in R,D&D of System Software for HPC, Grid, Cloud & Hybrid Computing

Areas of Expertise

- Compilers for High Level Languages
- Assemblers, Linkers, Loaders
- Debuggers
- Profilers
- IDEs, PSEs and Portals
- Device Drivers
- Protocol Development
- File System Development
- Fine tuning and optimizations
- Simulators Embedded & MIL Std Processors

Products and Projects

- Compilers- Fortran90, Coral66, Parallelizing Compiler
- Fortran77to90 Converter
- Parallel Debugger
- Intg Development Env (IDE)
- System Mgmt Tools
- Problem Solving Env (PSE)
- Resource Brokers
- Parallel File System
- Message Passing Libraries

- * Simulators (MIL Std)
- * Assemblers
- * Profilers
- * Metric Advisor
- * Portals
- * Schedulers
- * Workflows
- * Installation Mgr

Platforms : Solaris, AIX, Linux

Providing Technology Solutions/Consultancy Services in HPC, Grid, Cloud Computing related tasks



HPCC Software Suite

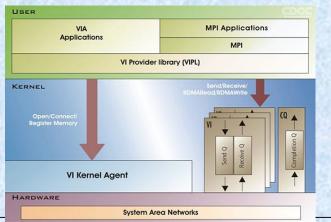
(High Performance Communication & Computation Software Suite)



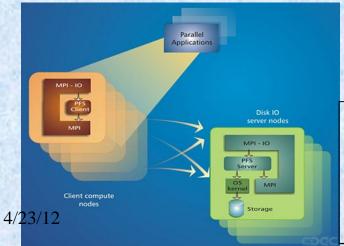
- **Base software** including lightweight communication substrate, optimized MPI, parallel file system
- Program Development Environment for complete program development and Problem Solving Environments
- System Management & Monitoring tools
- Software Engineering Tools C-DAC 18

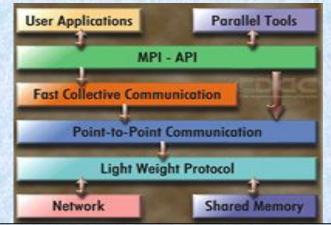
HPCC- Base Software





KSHIPRA – Scalable Communication substrate layered over PARAMNet and Gigabit Ethernet for UNIX clusters.





C-MPI - High Performance implementation of MPI on Cluster of Multi-Processors (CLUMPS).

•Supports Applications in Fortran and C.

- MultiProtocol support Applications can run
 - TCP/IP on Fast/Gigabit Ethernet or
 - VIA on PARAMNET

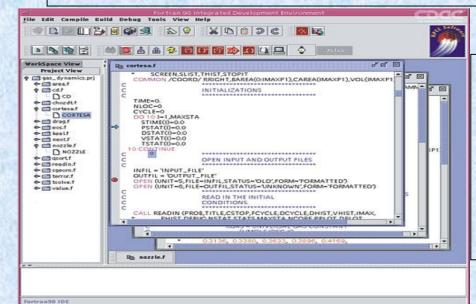
C-PFS – Parallel File System Provides MPI-IO file system interface to parallel applications



HPCC- Program Development Environment

CDF90 – Fortran 90 compiler compliant with ANSI 1537 E standard

- MPI based parallel programming
- Mixed language programming with C
- C77to90 FORTRAN77 to Fortran 90 source code converter



F90IDE - Integrated Development Environment for Fortran 77/90 containing a compiler, debugger, profiler, source code browser and Fortran 77 to F90 converter

> Map to multiple execution units

> > CDII

CDII

Result

SMP System

CDI

PCF90 – automatic parallelizing compiler Fortran90

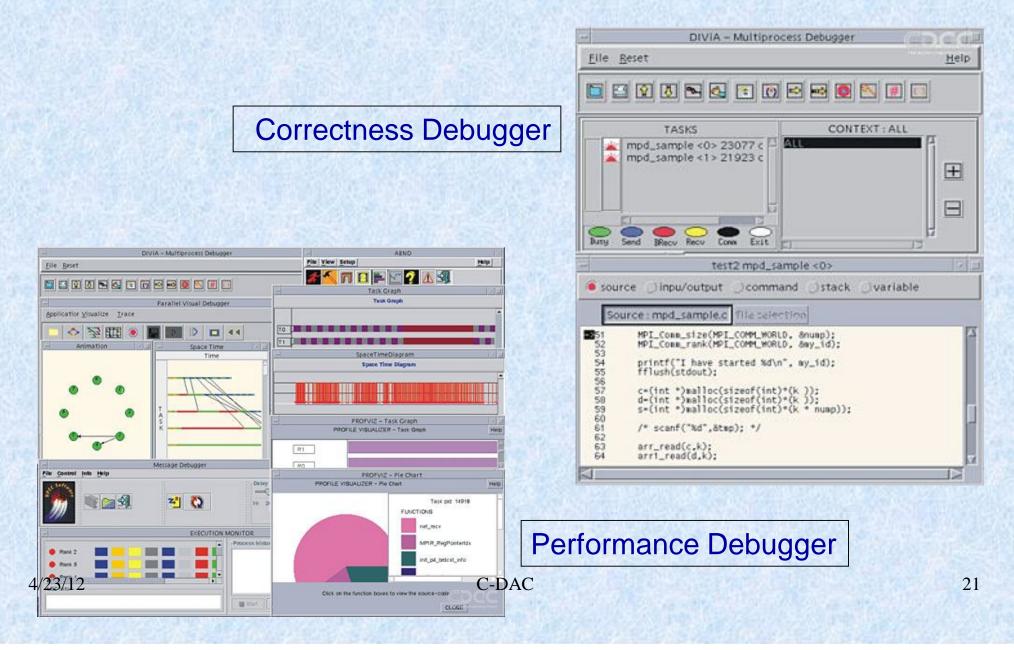


PCF90

HPCC- Program Development Environment

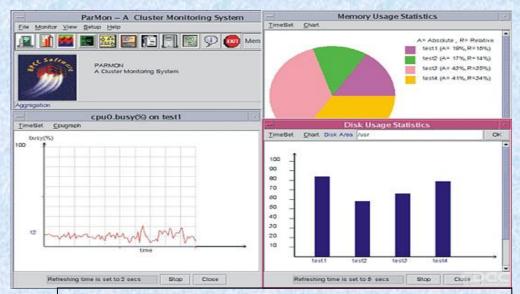


DIViA – Debugger Integrated with Visualizer and Analyzer



HPCC- System Management Tools

C-DAC



PARMON - Cluster monitoring: CPU, memory, Disk

JSAP – Job Submission Accounting Package for PARAM Padma



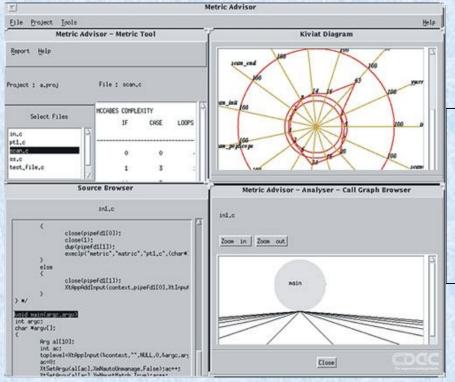
RMS - Resource Management Software for effective load balancing and load scheduling on clusters.

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cation: http://192.168.63.54:8080	0/examples/servlet/UserOptionServlet	
hat's New? What's Cool? Destinations	Net Search People Software	
CDCC		1 8 CL
	pment of Advanced Computing	
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CDA	AC \$ JUD SUBILISSION AND ACCOUNTING PACKAge 101 C 1 SP	
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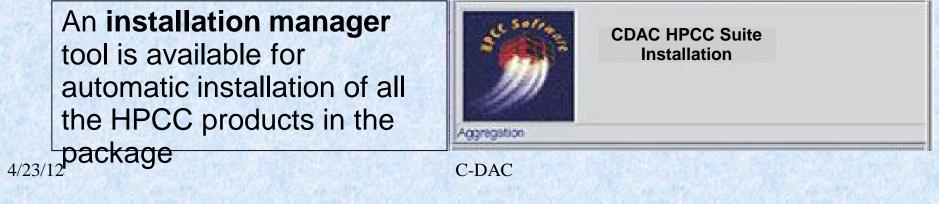
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HPCC-Software Engineering Tools



Metric Advisor -Software engineering tool for metrics. Evaluates Halstead, McCabe, Complexity Density,Fan-in and Fan-out metrics.



Upgrade of legacy COMED System



PC based cross compiler for CORAL66 language and simulator for an embedded system for defence.

- Software:
 - Coral Cross Compiler
 - Assembler
 - Linker, Relocator, Loader
 - System Libraries
 - Simulator

Hardware:

 EPROMing station with communication to PC and graphical interface

Successful flight testing for software developed with the CDAC system.

UNA (Ulyss Navi Attack) Development System

Two pass assembler (cross platform) for specific AT382 architecture

- Components
- UT382-50 assembler, linker, loader
- magnetic tape interface

CDAC achieved binary equivalence between the assembler generated executable and the HP1000 executable.

Ada95 Cross Compilation



Feasibility Study / Requirements Gathering for Ada95 Cross Compilation System for Target Intel 80960

Clients:

- Aeronautical Development Agency (ADA)
- Aeronautical Development Establishment (ADE)

Works:

- Proof of Concept Demonstration
- Feasibility Study, Requirements Gathering
- Detailed reports, approach & proposal



GARUDA – The Indian National Grid Computing Initiative

GARUDA

Global Access to Resources Using Distributed Architecture

GARUDA-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 - Overview





& INTEGRATIVE BIOLOGY

Genomics Knowledge Partner

Inter-University Centre for

Astronomy and Astrophysics

Connectivity Summary

Legend Connected

Lucknow

Chennai

Thiruy an anth apura m 🎑

Varanasi

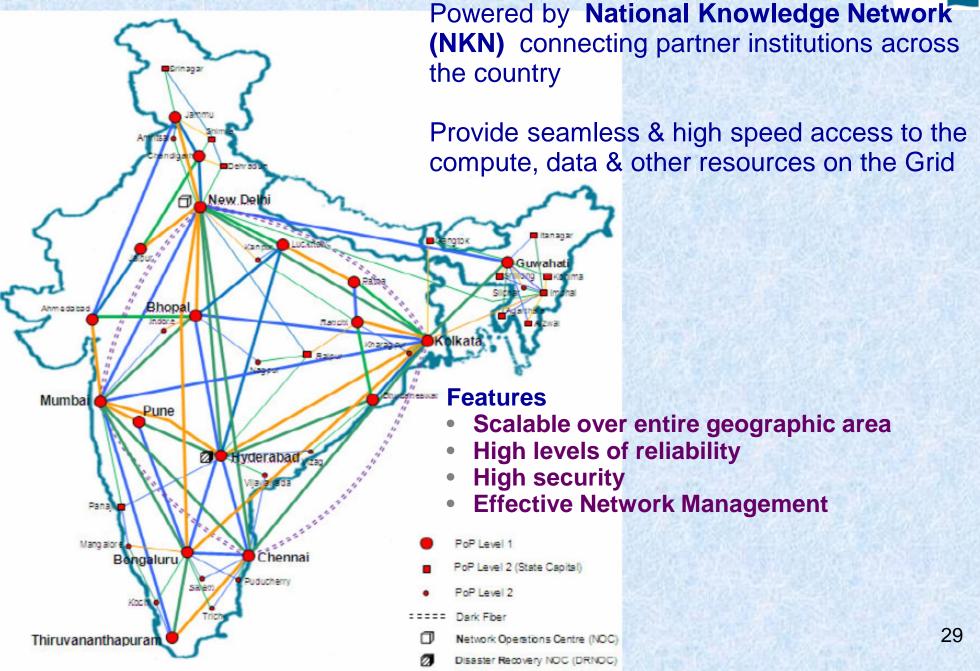
Kharagpur 🕘 🥥 Kolkata

Total number of Institutions: 45 Institutions Connected: 45

Guwahati

GARUDA Backbone





GARUDA Resources



- C-DAC centres at Bangalore, Pune, Hyderabad & Chennai are contributing a set percentage of their computing resources
- HPC Systems from Partner Institutions
- Total Processors : 6000+

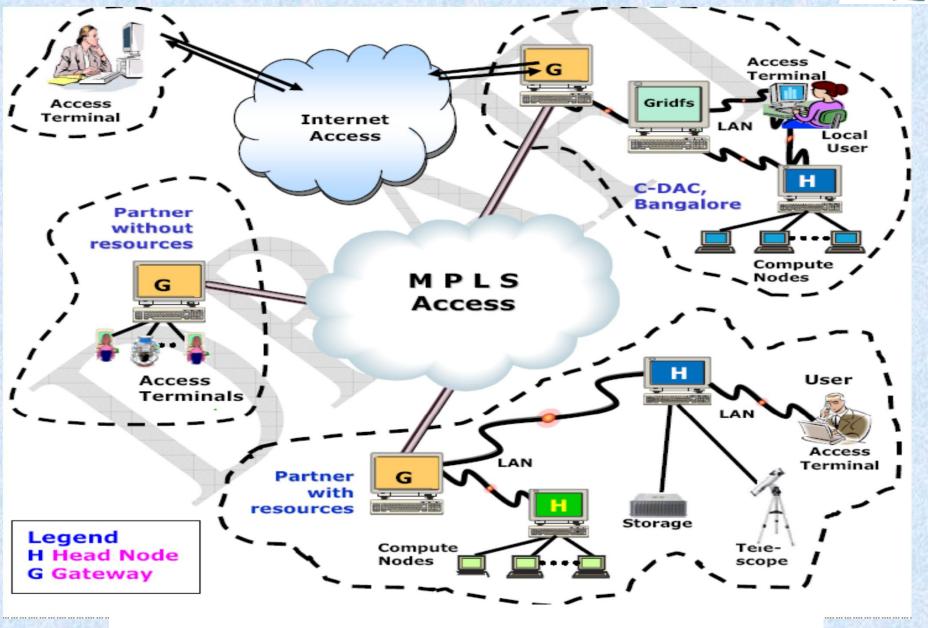




- Satellite Terminals and Bandwidth from SAC-Ahmedabad
- Grid Labs at C-DAC: Bangalore, Pune and Hyderabad
- Part of the PARAMYuva (54 TF) system of C-DAC

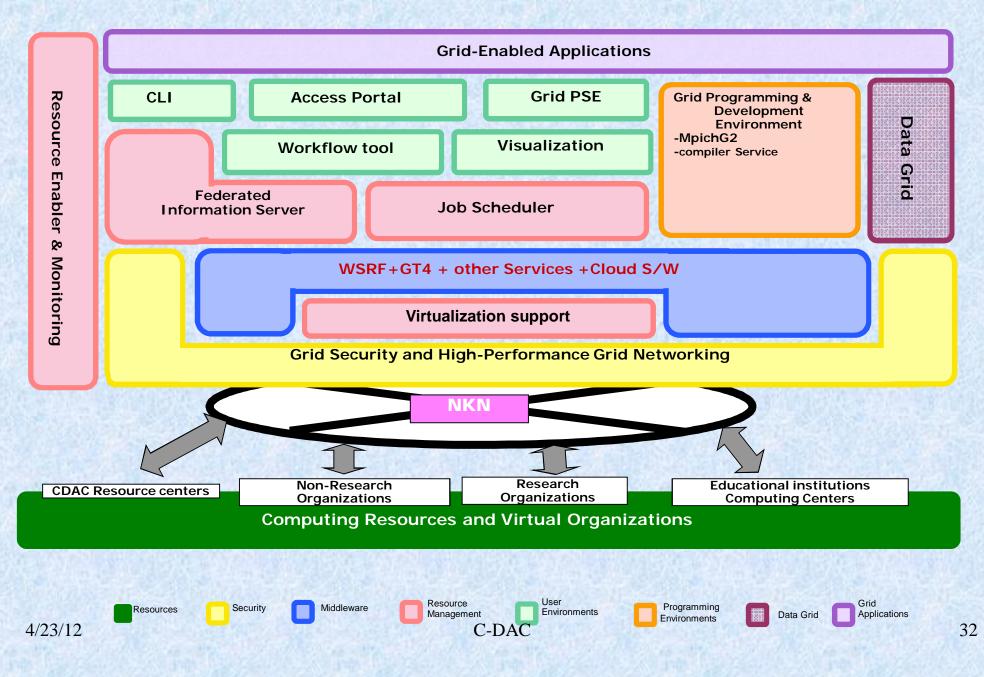
Garuda Architecture





Garuda High Level System Components





GARUDA-Component Architecture



Management, Monitoring

- & Accounting
- Paryaveekshanam
- Web MDS
- GARUDA Information Service
- GARUDA Accounting

GARUDA Resources

- Compute, Data, Storage,
- Scientific Instruments,
- Software,...



Resource Mgmt & Scheduling

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

Access Methods

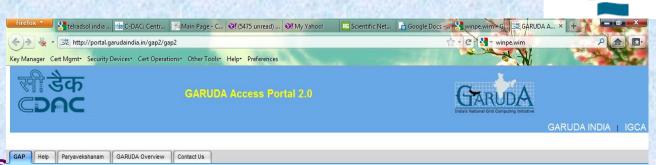
- Access Portal for SOA
- Problem Solving Environments

Security Framework

- IGCA Certificates
- MyProxy
- VOMS

Garuda Grid Portal - Features

- Basic / Advanced Job Submission
- Browse Avail. resources
- Provision to View:
 Status, Output, Error Files Welcome Page
- Addresses usability challenges of GARUDA
- GARUDA Access Methods include Access Portal & PSE for Applications.
- PSE for Bio-informatics has been released.
- Access through Satellite Grid under progress



 Welcome to GARUDA ACCESS PORTAL
 User

 About
 User

 GARUDA - India's National Grid Computing Initiative will unleash a comprehensive computational capabilility to enable the user community to participate in increasingly interdisciplinary scientific experiments and also conduct simulations on an unprecedented scale.
 Pass

 Image: Ima



GARUDA Ac...

 user Name subrata

 Password

 Password

 I accept Garuda User Policy

 I arccept Garuda User Policy

 I arccept Garuda User Policy

 I arm a First Time User of this page / Change of VO

 Login

 Sign Up?

 Forgot User Id or Password?

 Help

 Support & Latest News

 If any problems please report to Support team

 If new to portal . please contact IGCA to obtain certificates and login

 About GridWayand it's user Guide

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http://portal.garudaindia.in

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🔨 Garuda - ove... 🖳 Applications... 📲 Subrata-GTS...

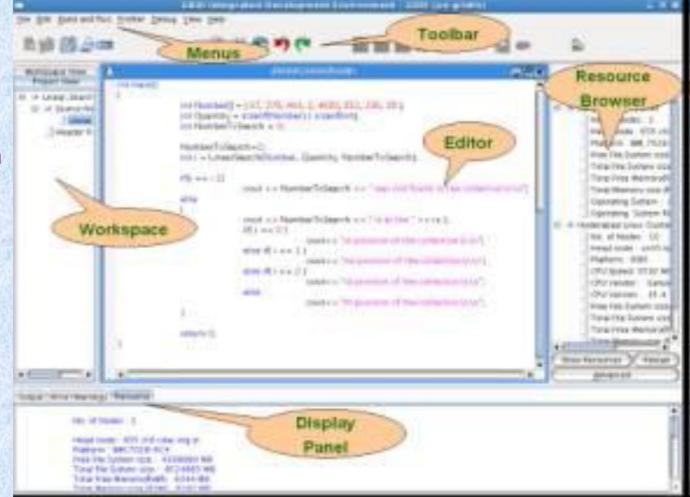


Integrated Program Development Enironment: Data Management & Collaborative Environments

GARUDA Integrated Development Environment (G-IDE)

Carry out entire program development life cycle for the Grid

Provides an Unified Interface- editors, compilers, debuggers, profilers, workflow environments





O Medium (26%-50%)

OLow (0%-25%)

O Not Operation

ID

100

101

Code

eLNK

eNOD

Priority

Normal

Normal

Status

Open

Open

Centr

C-DAC Chennai

C-DAC Chennai

- Support activities to provide a fault-tolerant and continuously available set of services
- Network Operation Centre has been set up with following components
 - High resolution, scalable display wall
 - Paryavekshanam Grid Monitoring software
 - Help Desk has been set up



GARUDA Statistics

- 70TF-15TB Compute-Storage Power
- 65 Partnering Institutes
- 20 cities across India
- 800+ users
- 14+ Virtual Organizations
- Past Year Usage:
 - Jan to June 2011 = 28990 jobs
 - July to Dec 2011 = 21684 jobs
- International Collaborations:
 - EU-India Grid
 - caBIG, USA
- IGCA established
- Successful Applications: Open Source Drug Discovery (OSDD), DMSAR, OpenEye Docking, Winglet Optimization, Aerosol Modeling, and many more
- 70+ Publications, 2 Indian Patents

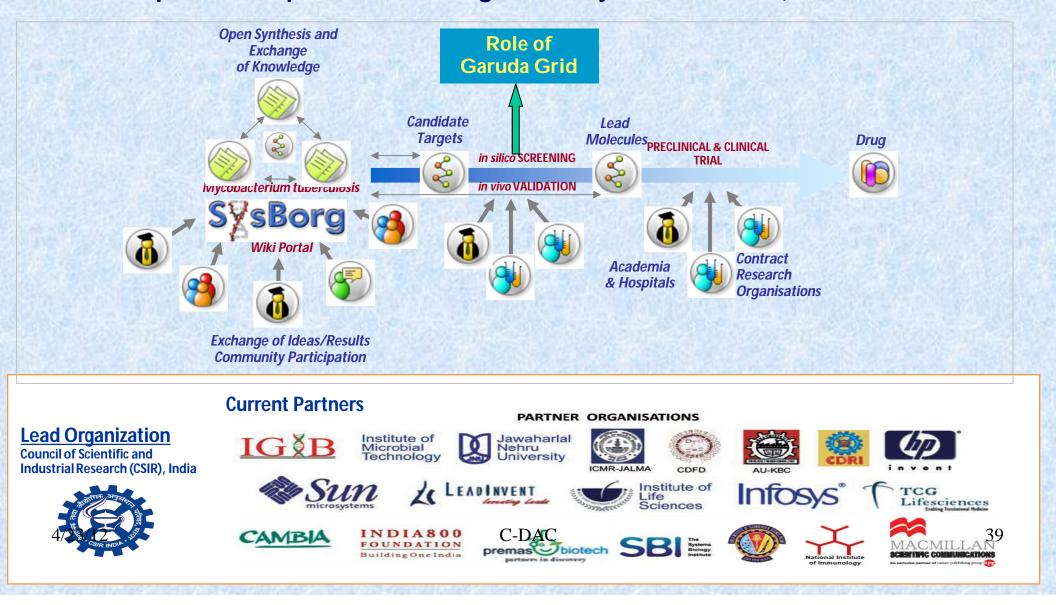


HPC & Grid Applications

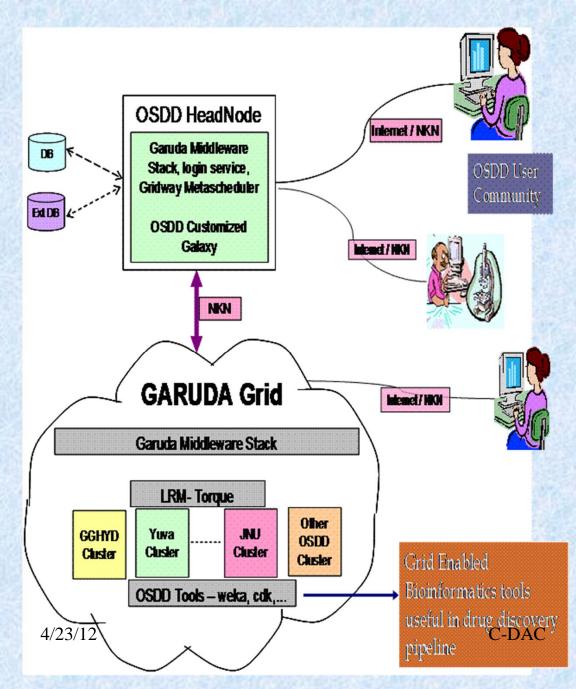


Open Source Drug Discovery (OSDD) A CSIR-led initiative for affordable healthcare

OSDD is a programme to find cures for neglected tropical diseases that affect for the entire spectrum of processes in drug discovery – tuberculosis, malaria



OSDD-GARUDA



- 70+ OSDD users given access to Garuda through a OSDD VO (Virtual Organization)
- Over 3500 jobs have been run on Garuda by OSDD members (consuming 4000+ hrs of CPU wall time)
- JNU, IGIB, UoH, IISc have NKN connection to GARUDA; - for remote locations like MCC, GARUDA has been made accessible through the Internet.
- Garuda provides HPC clusters to run drug discovery problems
- Galaxy Workflow for genomics proteomics applications
- Distributed job execution through Gridway (metascheduler)
- Parallelizing specific applications
- Supporting required bio-tools

Winglet Design

- Reduces aerodynamic drag by altering the flow field near tip
- Can convert some of the otherwise wasted energy in wing tip vortex to an apparent thrust
- Improved take-off characteristics (but design optimized for it may pay penalty for cruise conditions & may be vice versa)
- Can improve aircraft handling characteristics (increased roll rate & roll authority)
- Reduction in noise levels is also noticed

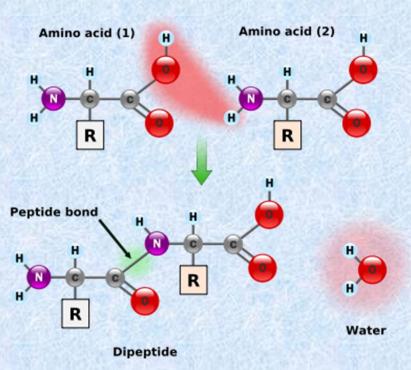
Present Design of Wing / Winglet Configuration

Objective of the Study:

"To design a blended winglet for RTA wing configuration with minimum drag at cruise C₁ of 0.55"

Protein Structuring

- Prediction of the 3D structure of proteins from their amino acid sequences
- Proteins are made up of 20 naturally occurring amino acids
- Applications of PSP
 - Understand function of proteins
 - Drug design
 - In the design of novel enzymes
- Genetic Algorithm is used to calculate the Energy of the molecule.
- Energy = non-bond energy + torsion angle interactions (AMBER force field)
- Lower the energy better is the fitness

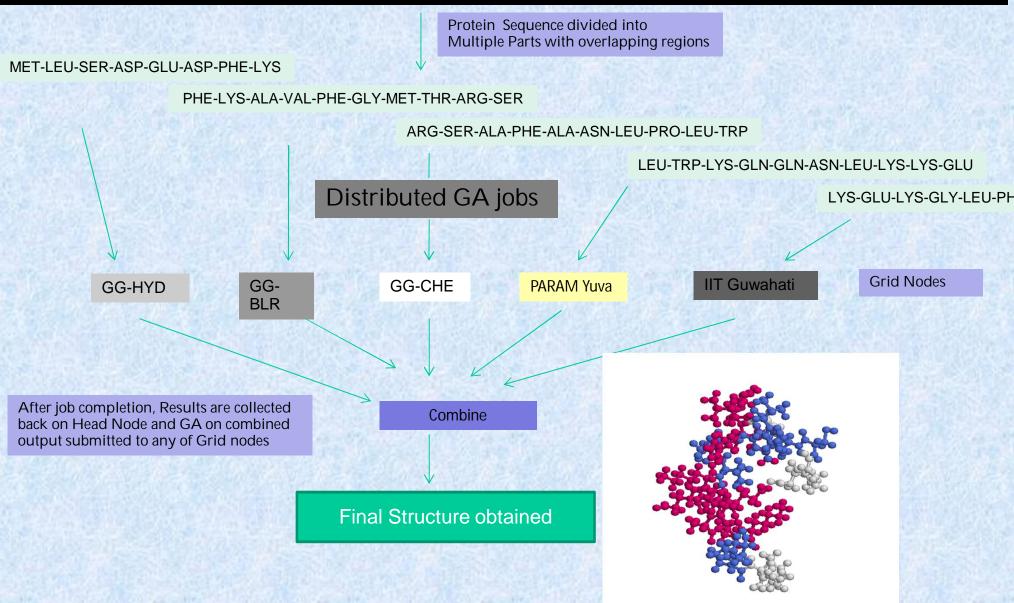


• The complexity of GA code increases with the increase in protein sequence size as it affects chromosome length and population size- potential grid application

Distributed GA Based Protein Structure Prediction



MET-LEU-SER-ASP-GLU-ASP-PHE-LYS-ALA-VAL-PHE-GLY-MET-THR-ARG-SER-ALA-PHE-ALA-ASN-LEU-PRO-LEU-TRP-LYS-GLN-GLN-ASN-LEU-LYS-GLU-LYS-GLY-LEU-PHE



Problem Solving Environment for PSP

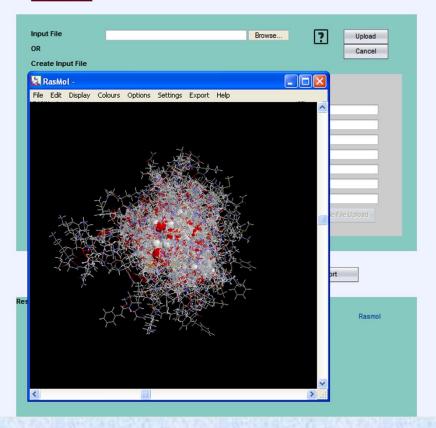


Held

- PSE for PSP
- PSP based on evolutionary computing (GA) method
- Functional modules of the PSP application implemented as services on Garuda
- Integrated with Login Service
- Released PSE-PSP v1.0 Feb 2010
- Used by IICT students Dec 2010



PROTEIN STRUCTURE PREDICTION





Grid Computing for Bioinformatics

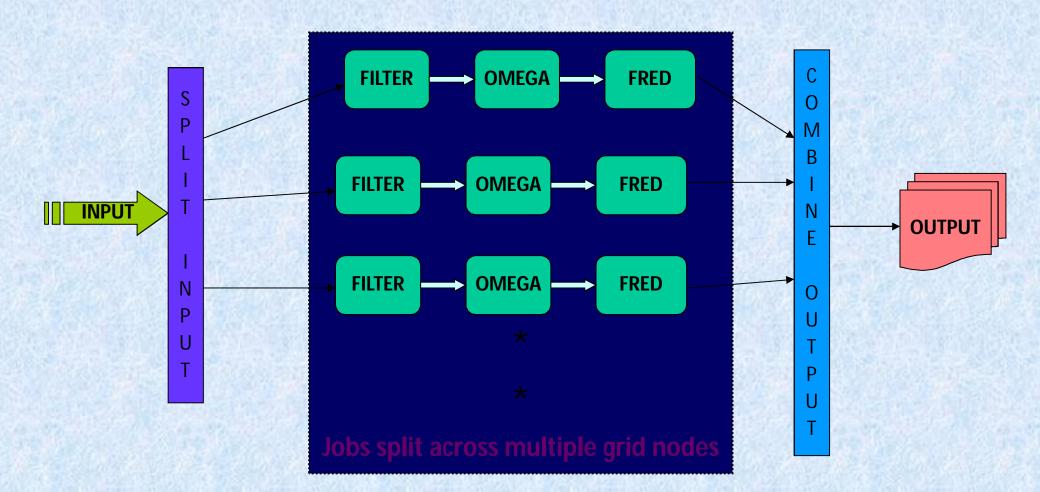
 Enable sharing of
 Bioinformatics data from different sites by creating a virtual organization of the data

Combining computational resources beyond those available to researchers at a single location.

> Depending on intensity of code and dataset, job can be submitted either on any of the grid nodes or across C-DAC



Grid-Based Docking Using OpenEye Modules



FILTER, OMEGA and FRED modules of Openeye Docking have been pipelined on multiple GARUDA GRID computational resources

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Patents & Publications



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INTERNATIONAL **CYBERINFRASTRUCTURE: ACTIVITIES AROUND THE GLOBE** GUEST EDITOR RADHA NANDKUMAR

- A National Grid Infrastructure for Australian Researchers John O'Callaghan, Australian Partnership for Advar
- Cyberinfrastructure for Multidisciplinary Science in Brazil
- 15 GARUDA: India's National Grid Computing Initiative

N. Mohan Ram, Chief Investigator - GARUDA S. Ramakrishnan, Director General - C-DAC

Cyber Science Infrastructure Initiative for Boosting Japan's Scientific Research Masao Sakuchi, Shigeki Yamada, Noboru Sonehara, Shigeo Urushidani, Jun Adachi, and Kazunobu Konishi, National Institute of Informatics (NII) Satoshi Matuoka, Tokyo Institute of Technology / NI

http://www.ctwatch.org/quarterly

THIS WEEK

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INTERNATIONAL SCIENCE GRID

Image of the Week - India's National Grid Computing Initiative

GARUDA-which takes its name from a large, bird-like creature in Hindu and Buddhist mythology-is a collaboration of researchers and experimenters aiming to establish a nation wide grid in India. Currently in its Proof of Concept phase, GARUDA will link centers for computation, mass storage and scientific instruments, to enable data and computing intensive science in India for the 21st century.

The GARUDA high-speed network will connect 45 institutions in 17 cities at 10-100 megabits per second bandwidth. To access an interactive version of this map visit the Garuda collaboration's Web site.

The GARUDA project is coordinated by Center for Development of Advanced Computing, C-DAC is a partner of EuIndiaGrid project. Interoperability between GARUDA and EGEE infrastructure is a main goal of Eundiagrid.



GARLDA will link 45 institutions in 17 cities via a high-speed network to promote science and computing in India. Image courtesy of GARUDA

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IGCA Gets Accreditation from APgridPMA



The Indian Grid Certification Authority (IGCA), a certification authority for grid, has received accreditation from Asia Pacific Grid Policy Management Authority (APgridPMA) to provide access of worldwide grids to Indian researchers.

CDAC

Indian researchers can now request user and host certificates to IGCA, part of the Centre for Development of Advanced Computing (C-DAC) and get access to worldwide grids. Indian researchers mainly constitute users of GARUDA grid,

foreign collaborators, or institutes related to grid research and scientific collaborations from India that allow researcher to access the grid.

Inaugurating IGCA, principal scientific adviser to Govt. of India said "The Indian Grid Certification Authority has been started by C-DAC at the most appropriate time for researchers to collaborate among international Grids using the multi gigabits per second network connectivity offered by National Knowledge Network (NKN). I congratulate C-DAC and encourage them to take the task forward."

Landra Cinch gravestages (department of IT) of Ministers of Communication and IT Cast of India said

GARUDA India web site http://www.garudaindia.in





Scientific Cloud Computing



- Gartner: "Cloud computing is a style of computing where massively scalable IT-related capabilities are provided as a service'across the Internet to multiple external customers"
- It is difficult and expensive for an organization to set up and maintain their own HPC infrastructure
- Grid Computing has a limitation to Scallability to outreach to large number of Users
- Accounting / Business processing is an integral part of Cloud Computing
- Scientific Cloud provide an alternative for HPC outreach
- Increased networked capacity and availability
- Virtualization: Increase System Utilization

Scientific Cloud - Activities



- Cloud computing for HPC and Scientific Applications
- Standardization & Interoperability between clouds
- Enabling technologies like Reconfigurable Computing System (RCS), ubiquitous devices etc. on Cloud
- Cloud middleware & System Software development
- Cloud Standards & Open SourceContributions
- Security Aspects of Scientific Cloud.
- Scientific Applications on Cloud
- Cloud Collaborations Framework s
- Cloud Excellence Centre: Research Participation from Academic institutes

Multicore-GPGPU Activities



Working on to provide a multicore GPGPU environment with complete software and enable key applications. Research on Nextgen tools & technologies to be taken up for smooth transition to Petascale.

Multicore-GPGPU Testbed

- Setup Testbed cluster @ BLR & HYD
- Extension to new architectures (APU/MIC/etc.)
- Enabling multicore-GPGPU on cluster/grid/cloud
- Deploy & Study open source / third party Tools and Libraries
- Challenges of system (h/w & s/w)

Programming Aspect

- Hybrid programming (MPI + OpenMP + CUDA/OpenCL) on diff environments
- Benchmarking (CUDA&OpenCL on diff env. multicore/GPU-cluster/grid/ cloud)
- Understanding behavior, threshold, other issues

Multicore-GPGPU





Application Aspect

- select applications from: DM, Bio, Climate, EADS, CFD, Viz, Img Processing, CIEMAT
- Optimizing libraries (manually
- Porting applications to new platform
- Benchmarking

Users/Application Developers

- Handholding for application porting
- Dissemination training(C-DAC CUDA Training Centre), Workshops, Conference
- Participation in Open Source / Standards activities

Development of System Software & Tools

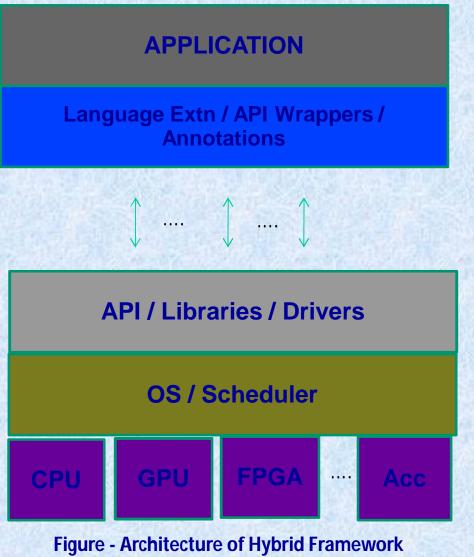
- Finetuning open source tools (PIPS conv, debugger, profiler, etc)
- Data Distribution advisor
- Monitoring & Checkpointing (Indo Spanish)
- Converters CUDA/OpenCL (moving towards hybrid paradigm)
- New programming paradigm like PGAS
- Autotuners & optimizers

Hybrid Computing for Scientific Applications



Hybrid Computing: Different types of computational units -CPU + GPU + FPGA + APU ...

- Establish Prototype Hybrid system
- Application specific optimized libraries on GPU & FPGA
- Design & Develop the system software stack for hybrid system:
 - Parallel code development framework
 - Target code generating driver
 - Flexible scheduler
 - Runtime libraries for diverse targets
 - Tools profiler, debugger, checkpoint, system management tools (monitoring, accounting)
- Test system software with select appln
- Dissemination & sharing with scientific labs

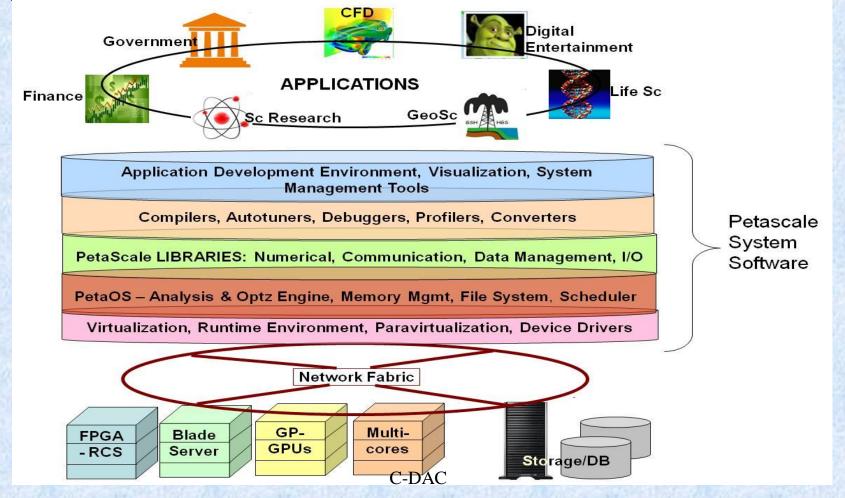


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System Software for Petascale



The System Software should provide support for building, debugging, running and finetuning applications on petascale systems handling the underlying challenges of concurrency, resiliency, energy, heterogeneity and performance

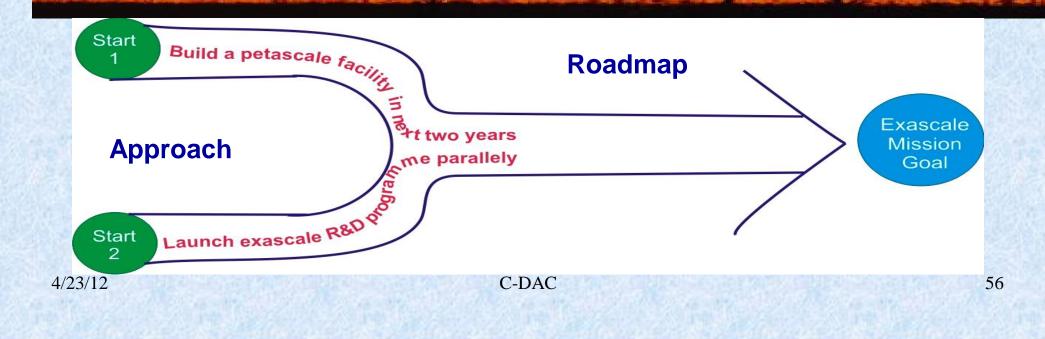




PetaScale Computing

Challeges to Address:

- Performance : Processor + Interconnect + Storage
- Programmability: Concurrency + Scalability + Locality
- Resiliency
- Energy
- : Hardware + Software
 - : Power Consumption + Heat Generation





Conclusion

- A National Research Society Engaged in HPC, Grid, Cloud, and Hybrid Computing
- Support Research Communities doing the state of Art technology research
- Support Open Source Research
- Participate in International Collaborative Research



Thank You