Integrating HPC Resources, Services, and Cyberinfrastructure to Develop Science Applications

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NSF XSEDE: An Example of the Scale of the Challenge

- US NSF XSEDE: 11+ resource partners
- 40/100 GigE backbone
- PetaFlops (aggregate), Multi PByte storage
- Gateways: 100’ s of large projects, 1000’ s of users
- Future Grid Project: cloud computing resources
Smaller Scale CI: SDSU Science DMZ

Legend:
- 10G LR
- 10G CX4
- 1G

CENIC
CalREN-HPR
ESnet and Internet2
CalREN-DC

EWDM MUX-8 at SDSU Administration Building
sdcsu-sw-3

periSONAR Measurement Point (MP)

10GBASE CU SFP+ Transceiver

LAN handoff for XD Circuit
#4931

CSRCnet

LAN handoff for DC Circuit
#2602

Cisco 1002 Aggregation Services Routers (ASRs)

Juniper Networks ISG 2000

Campus Core Switch

Science DMZ Hosts in CSL-120 SDSU VizCenter

Science DMZ Hosts in EBA-111 University Computer Operations

3xOS10K-8XLU/32S
(32 port SFP+ Line Card)
1x8 port SFP+ 40GE Line Card

9x10GBASE CU SFP+ Transceiver

periSONAR MP and MA Service Host

periSONAR Measurement Point (MP)

OS10K8

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The SDSU Cyberinfrastructure
Web Application Framework (CyberWeb)

• CyberWeb simplifies the utilization of heterogeneous, computational environments required by high-performance computing applications

• Part of an ongoing NSF project, the Open Grid Computing Environments (OGCE) project, which has a focus on XSEDE Gateway projects
  – Evolved from Grid Portal (GridPort) Toolkit Project

• Team effort:
  – PI: Mary Thomas (CS & CSRC Departments)
  – M.S. students Hetang Shah, Smita More, and Carny Cheng working on distinctly different aspects
CyberWeb: Support Computational Environments

Provide a bridge between generalized users and high-end resources, emerging technologies and cyberinfrastructure.

Simplify HPC resource usage by using common/familiar Web and emerging technologies.

Facilitate access to, and utilization of, a variety of science applications.

Develop Applications that can operate within heterogeneous computing environments.
CyberWeb Architecture & Technologies: Classic 3-Tier Design

- **Clients:**
  - remote applications, Web services
  - Web portals.
  - Command line interface (CLI)

- **Services Oriented Architecture:**
  - capable of hosting/exposing any functionality as a service.

- **Web Service Gateway Interface (WSGI):**
  - Pylons: Web 2.0 WSGI application framework
  - Relational databases
  - XML, JavaScript, AJAX,
  - Google Gadgets, social networks

- **Security & Authentication**
  - Automatic and integrated
  - Support multiple protocols

- **Dynamic Database:**
  - admin Web pages, for configuring CyberWeb installations, applications, users, remote resources and services.

- **Job Execution:**
  - Job distribution Web service framework for task execution and management.

- **Data Management:**
  - distributed

- **Connectivity:**
  - Heterogeneous resources and services (remote or local).
  - Any network (TCP/IP, 10GigE)
CyberWeb Architecture

![Diagram of CyberWeb Architecture]

- Pylons WebApp Server
  - Router
  - Controllers
  - Templates
- Auth/Act Services
  - Accts, MyGW, ...
  - Authentication
  - SSH/GSI/SSH Condor, SGE...
- Cyberweb Database
- Jodis Services (Job Management & Distribution)
  - Execution: Interactive, Batch
  - Data: FTP, View, Vis
- Misc Tasks: Events, Mses...

Connections:
- GCOM Application Clients
- Users
- Cyberweb: Web Service, Portal, Google App, ...
- Archival
- Workstations
- Applications & Services
- Compute Clouds/Grids
- Web 2.0 Services
CyberWeb: Features & Capabilities

- **Dynamic Database**
  - core to everything

- **Security/Authentication:**
  - HTTPS/SSH/GSI Users
  - Access Control List (ACL)
  - Validated authentication information visible to all modules and components being used by the portal.
  - Map CyberWeb users to accounts on remote resources

- **Supports multiple applications:**
  - Configurable in DB

- **Heterogeneous:**
  - Accesses multiple hosts and queuing systems
  - Distributed environment
  - New systems added via database admin

- **Job Execution:**
  - Dynamically build & deploy jobs
  - Moves and stages I/O files
  - Interactive unix cmds
  - Queing/batch jobs
  - Job Monitoring

- **Data Management:**
  - 3rd party file transfer
  - Job staging & history
  - “Plug-n-play” approach for resource configuration and its use

- **Post Processing Services:**
  - Visualization, Analysis
CyberWeb Database

• Implemented using
  – Pylons/SQLAlchemy (API to multiple databases)
  – MySQL and SQLite + JSON

• Design based on major existing grid databases
  – TeraGrid; Open Grid Forum; FutureGrid/Cyberaide

• Database is core to everything:
  – Resource configuration (add/remove hosts, queues,
  – Accounts: map CW account to users remote host account on TG, workstations, Condor, SGE, etc.
  – Authentication: ssh, gsi, condor, srb, sge, ...
  – File management; input/output; move files
  – Dynamic project/task naming
CyberWeb: Database Admin

- Design based on existing grid RDB’s:
  - XSEDE/TeraGrid
  - Open Grid Forum FutureGrid
  - Cyberaide

- Technologies:
  - Pylons/SQLAlchemy (API to multiple databases)
  - MySQL and SQLite + JSON
  - JavaScript and Ajax

- Dynamic admin functions:
  ① add and configure resources;
  ② define services running on them;
  ③ create and validate users, and accounts for access.

- “Live” machines: available for use immediately by other services.
CyberWeb App: GCEM Coastal Simulation Portal

- Automatic Data Archival
- 3rd Party File Transfer & Data Management
- Security Services (SSH, Grid Security Infrastructure)
- User Account Management and Customization
- Database Driven Accounts, Resources, Services
- Simple Visualization Services
- Choose from Multiple Applications and Test Cases
- Dynamic Job Execution Builder
- Run Jobs Using Multiple Resources
- Job Tracking, Management and History
CyberWeb: Home Page

- Customized Home Page
- Dynamic view of available resources and services
  - Tested by job distribution service
- News/Events/Messaging
- Account creation, customize, set preferences
- HTTPS
GCEM Portal: File Transfer and Data Management

• Big Data Support: working with GlobusOnline project (paper at XSEDE’13*)
• 3rd party file transfer between resources, local host.
• View file contents
• Quick viz views
CyberWeb: Job Management

- **Select Jobs:**
  - Pulled from DB

- **Build and submit job**
  - “Live” resources pulled from db
  - store in historical database

- **Monitor jobs and status**

- **Resources & Services monitor**
CyberWeb Visualization (CyberViz)

• Based on Python & Gnuplot lib
• View interim or final data
• Set parameters such as job, plot type, scale
• Requests trigger data transfer from compute host to archival system
• Generate images or movies
CyberWeb App: Running Parallel UCOAM Applications

- parUCOAM code integrated in CE
- Application deployed to remote resources
- CA/CyberWeb
  - builds and deploys test cases
  - Manages results
  - Performs simple visualization
CyberWeb App: CyberCHEQS Project

- Combustion simulations to model chemical reactive flows.
- Uses Web service to update chemical composition
- CyberWeb services used to run jobs in parallel
- Scales to millions of jobs on hundreds of node - EP
- Collaboration with S. Bhattacharji and C. Paolini (SDSU)
Future Work

• Job execution/task management:
  – History
  – Job builder & compiler
  – Auto scheduler, interrupt/kill/steering

• Data & visualization
  – Access to larger archival resources
  – “Big Data:” Integrate GlobusOnline & other tools

• Automate application deployment

• Expand post processing capabilities

• Add Cloud resources

• Simplify installation
  – Unit Test System
  – Installation via Python egg

• Develop large scale gateways on XSEDE
Thank You

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• References: