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

Mary P. Thomas

Department of Computer Science, and
Computational Sciences Research Center, San Diego State University

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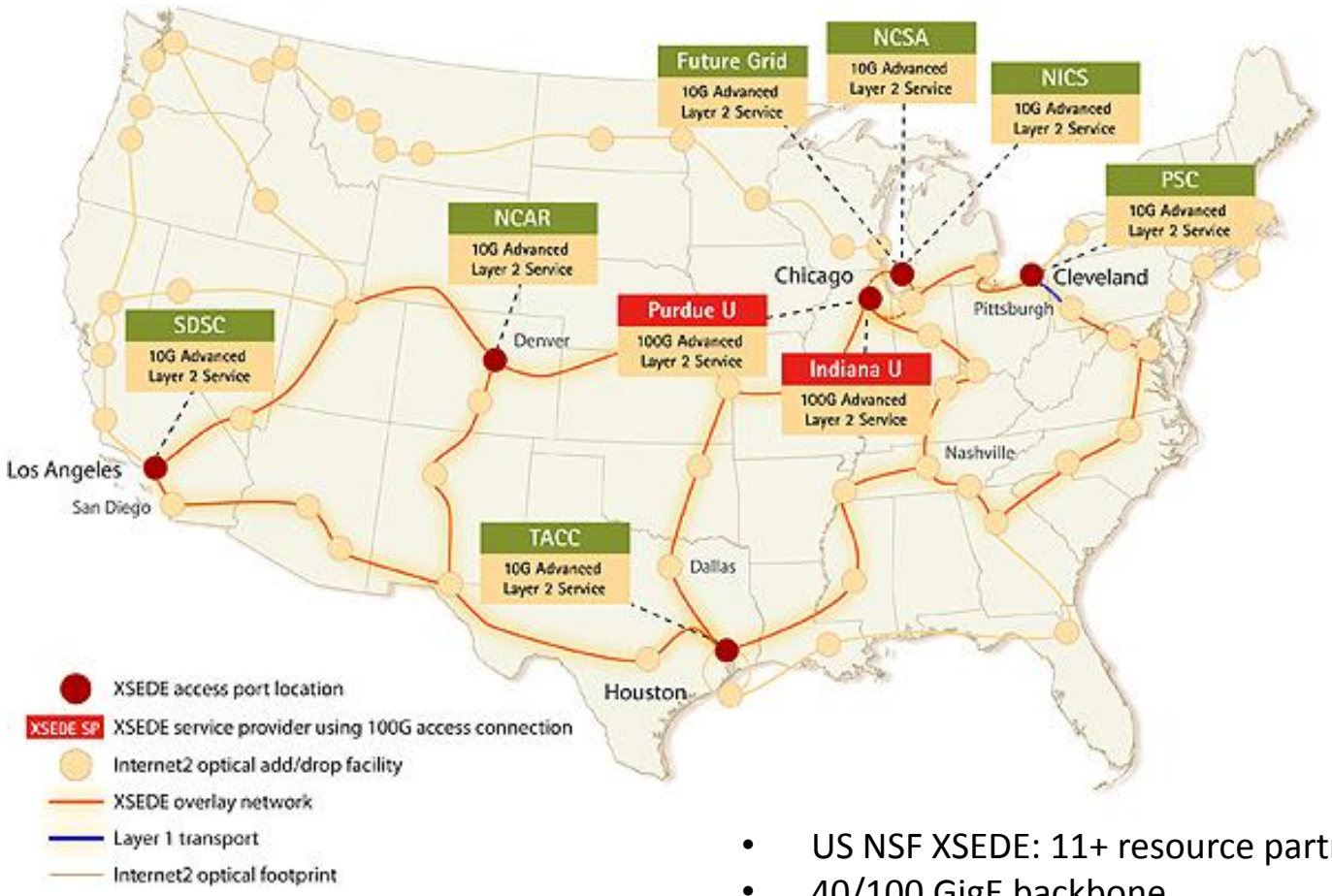
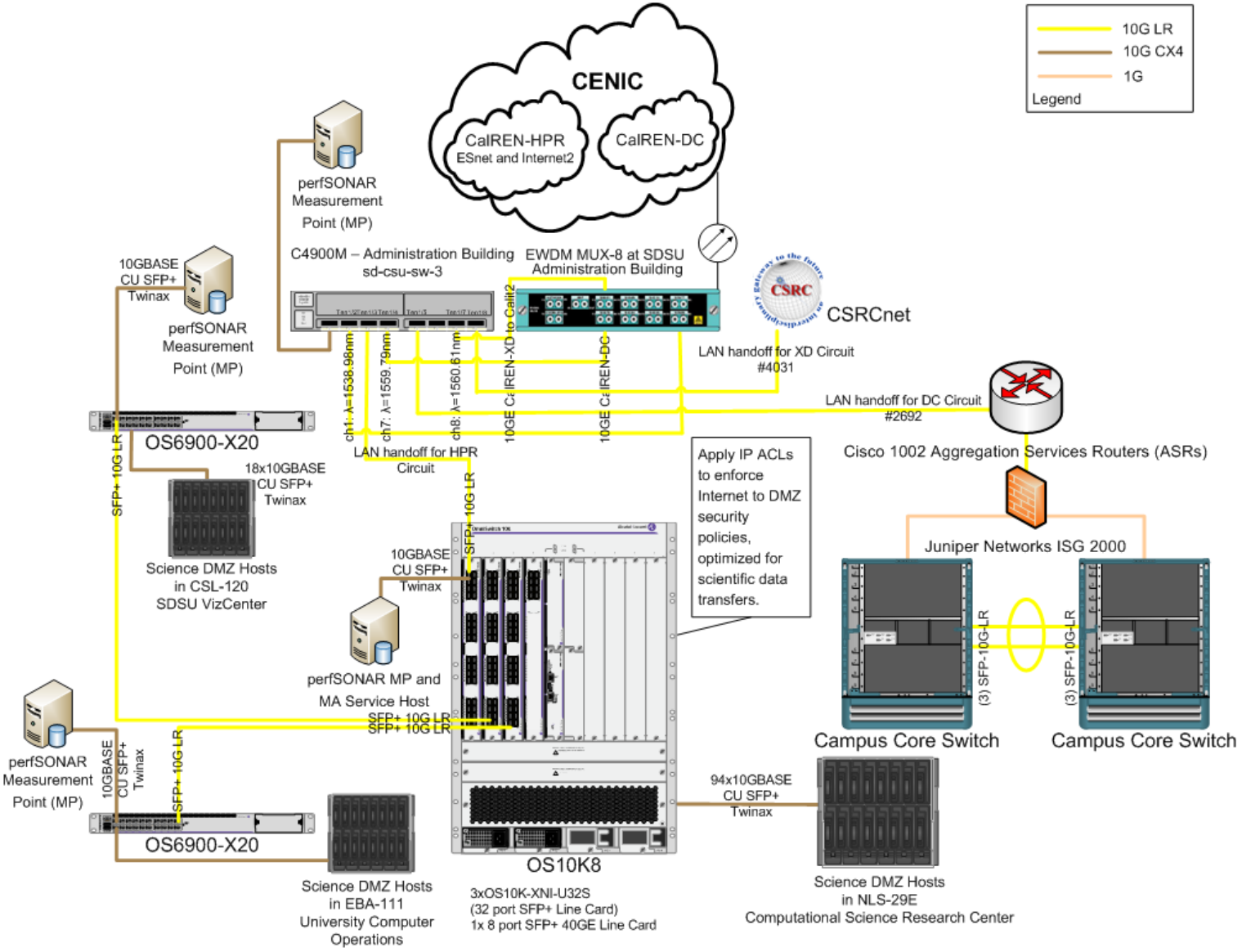
NSF XSEDE: An Example of the Scale of the Challenge



- 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

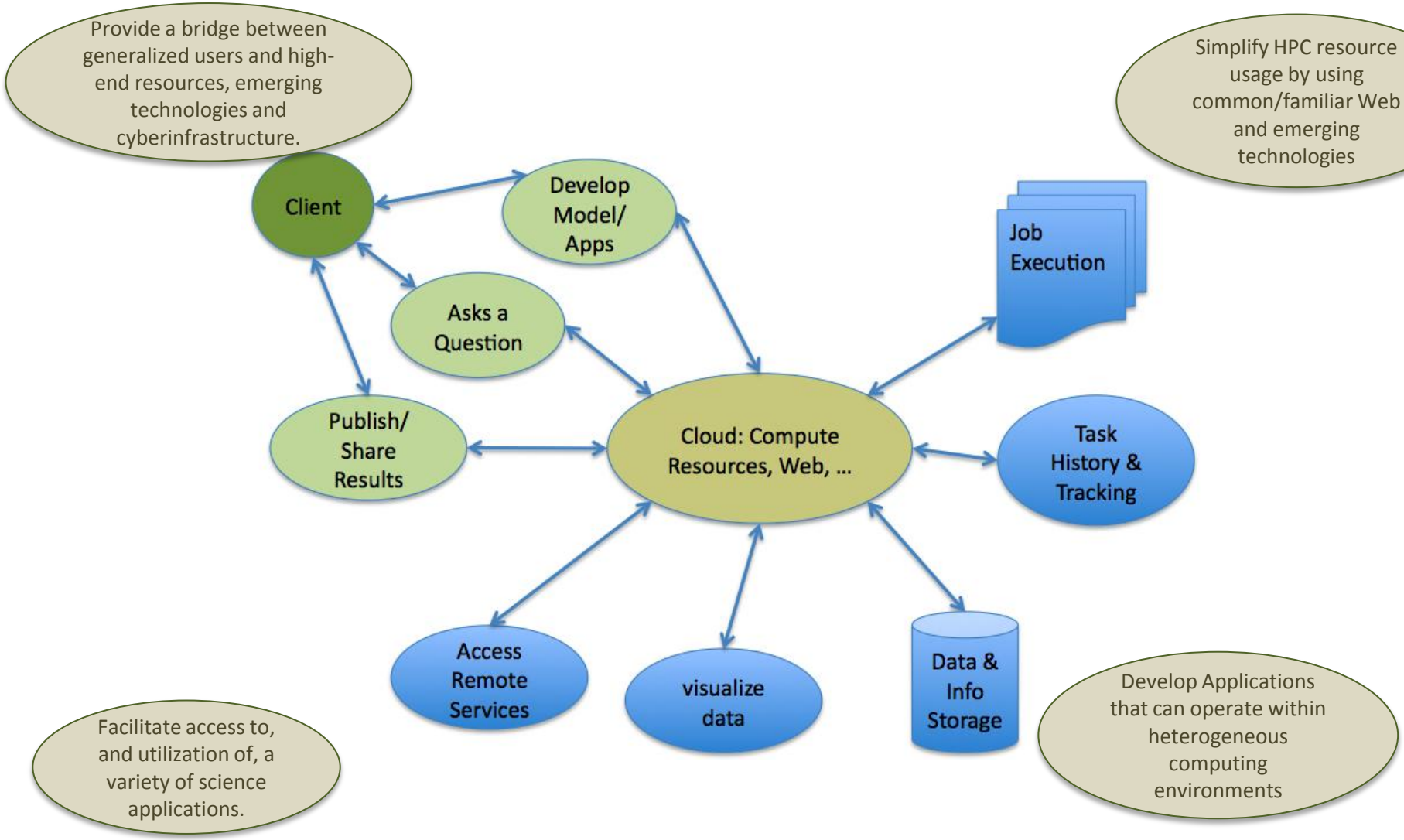


NSF Office of CyberInfrastructure CC-NIE Grant 1245312

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

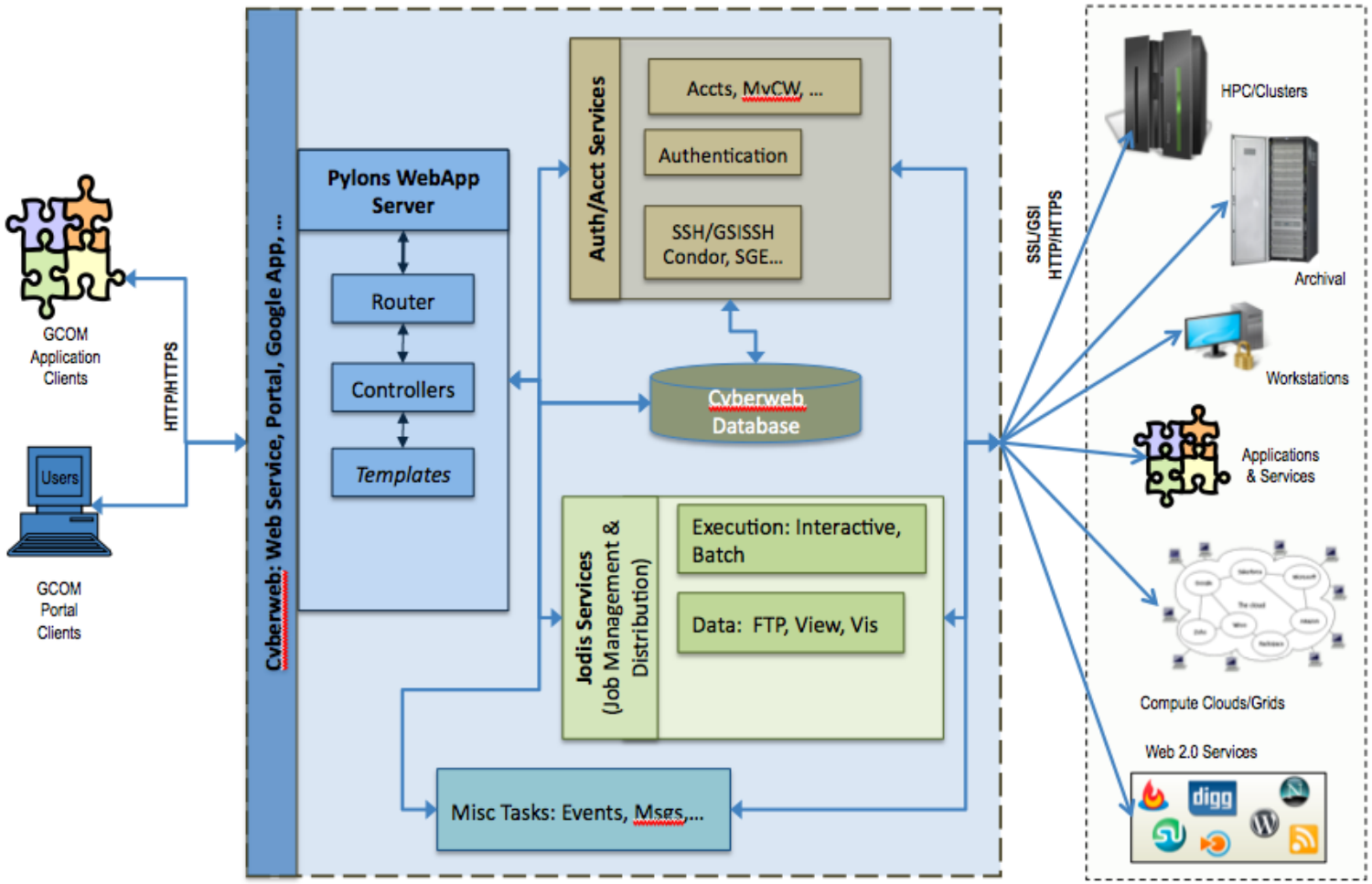
CyberWeb: Support Computational Environments



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



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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

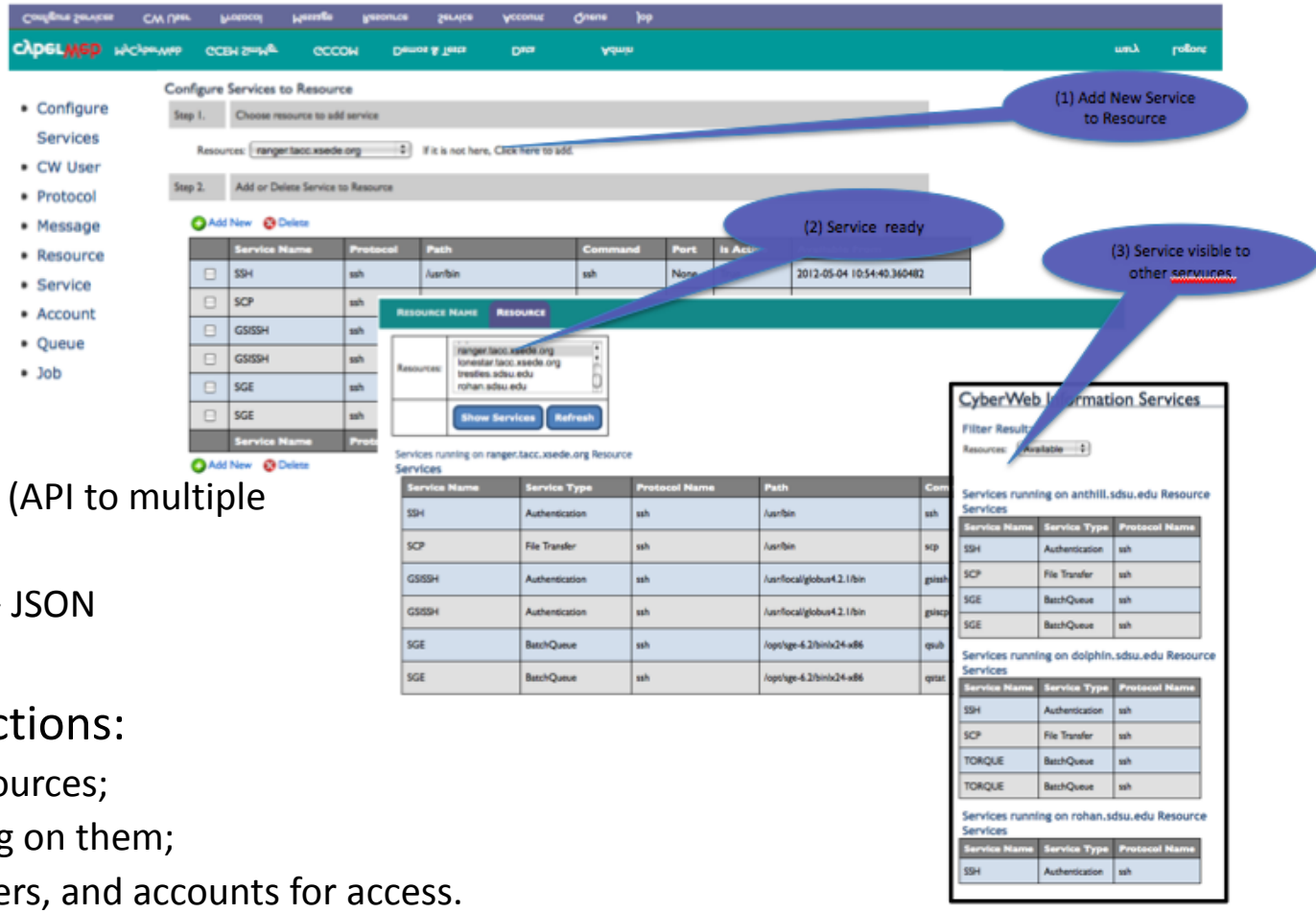
CyberWeb: Database Admin

- 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:

  ①add and configure resources;

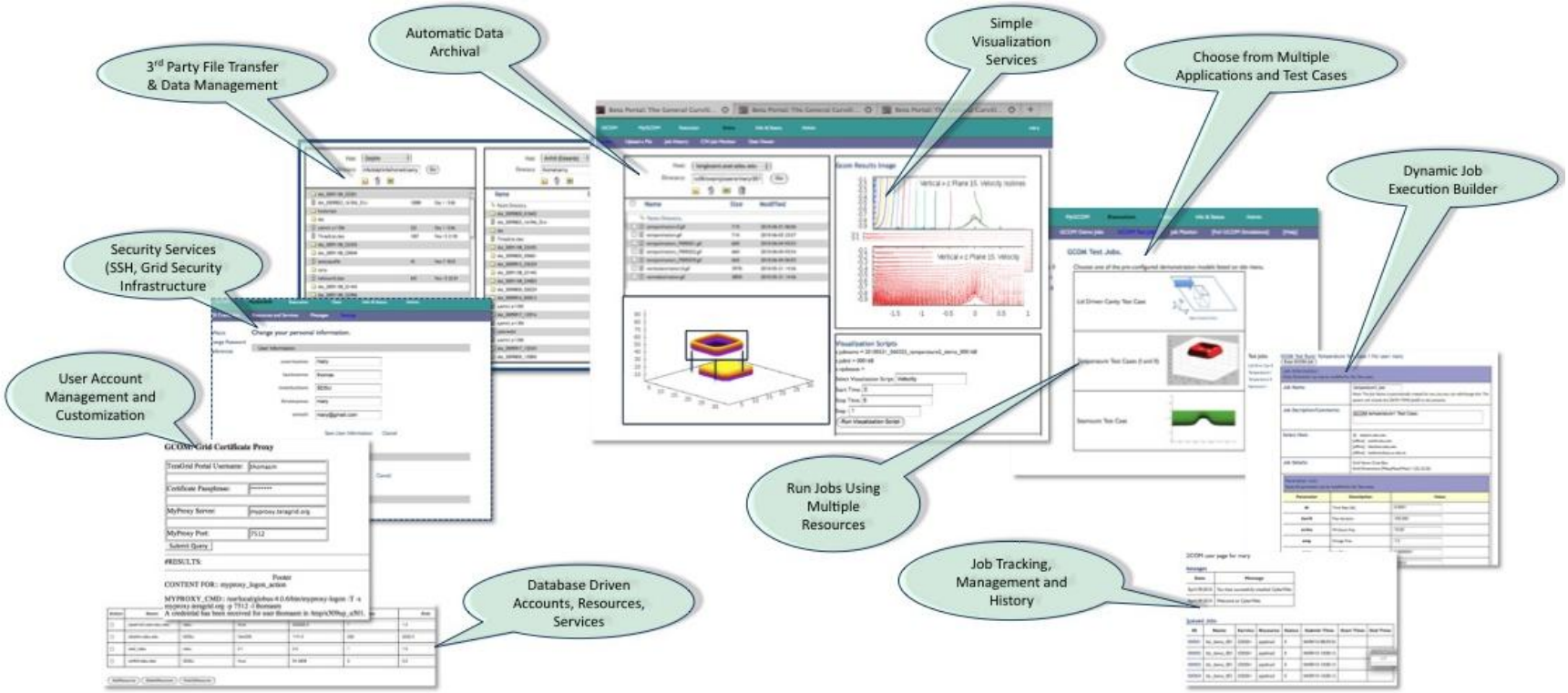
  ②define services running on them;

  ③create and validate users, and accounts for access.



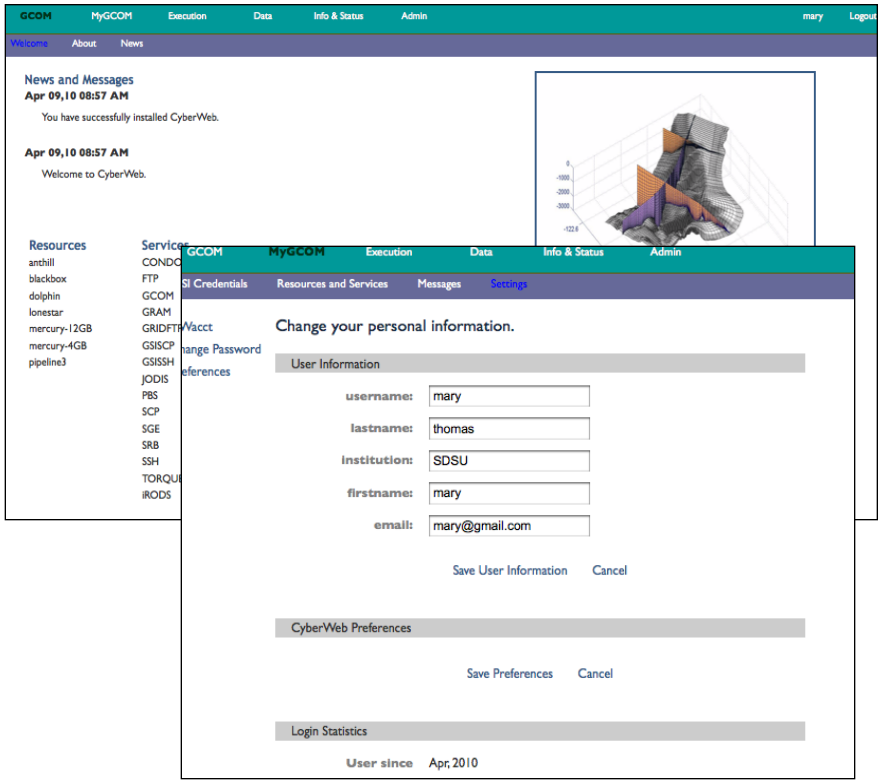
- "Live" machines: available for use immediately by other services.

CyberWeb App: GCEM Coastal Simulation Portal



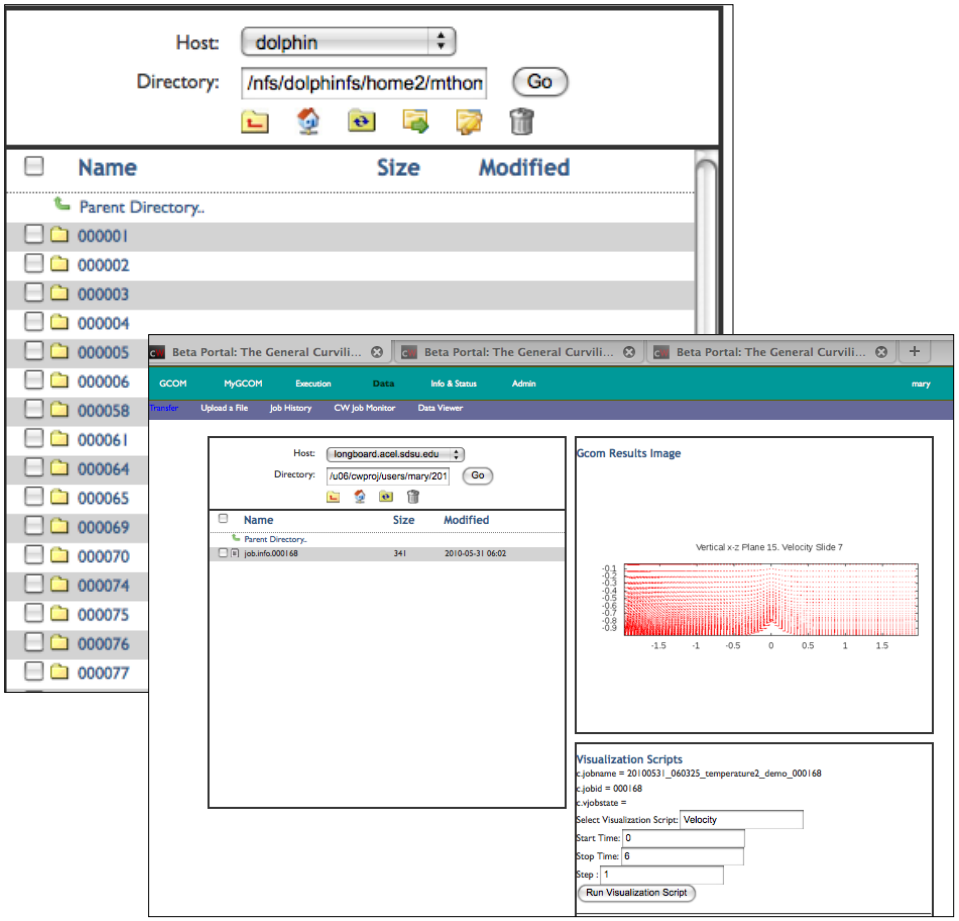
CyberWeb: Home Page

- 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

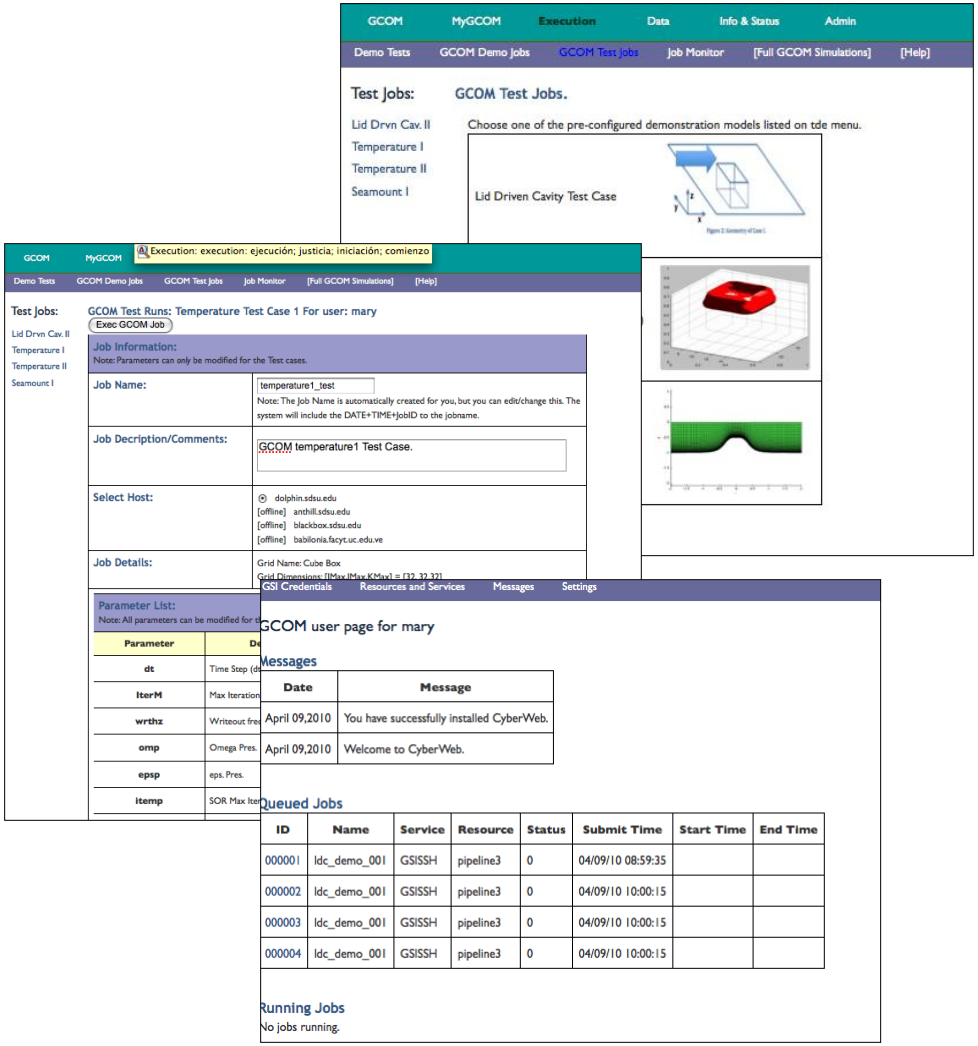
- Big Data Support: working with GlobusOnline project (paper at XSEDE'13*)
- 3rd party file transfer between resources, local host.
- View file contents
- Quick viz views



XSEDE'13 Conference, July 20-24, San Diego, CA. , http://www.xsede.org

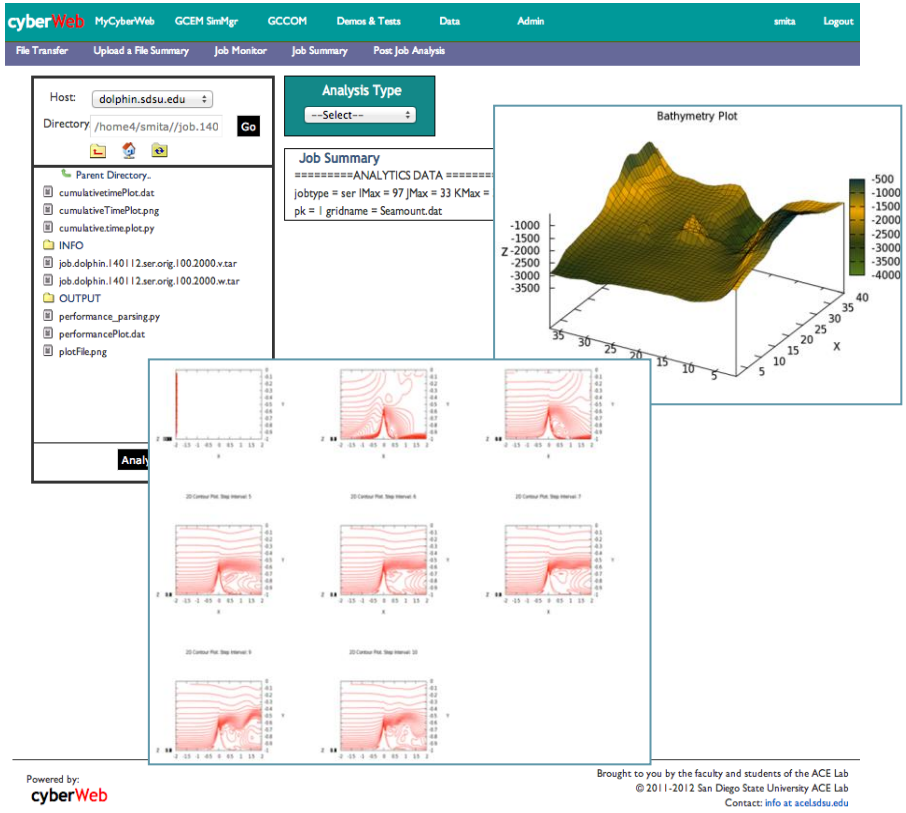
CyberWeb: Job Management

- 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



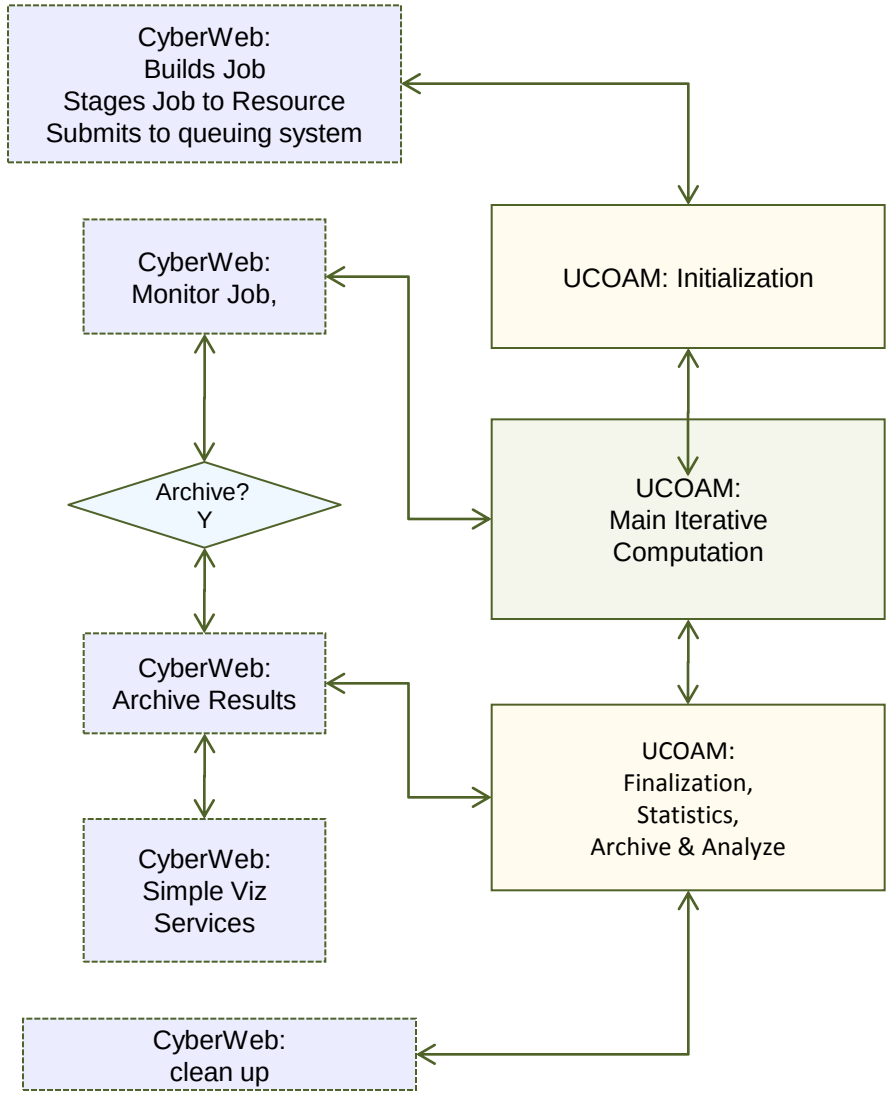
CyberWeb Visualization (CyberViz)

- 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



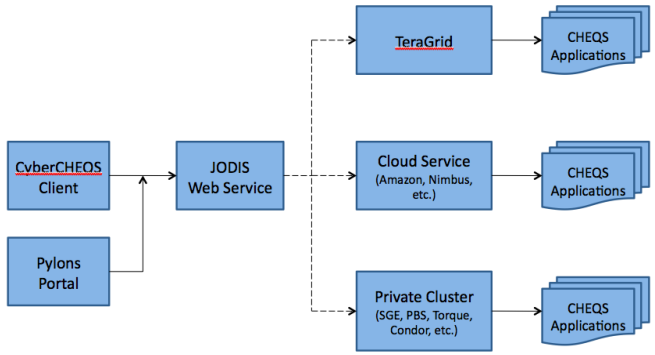
CyberWeb App: Running Parallel UCOAM Applications

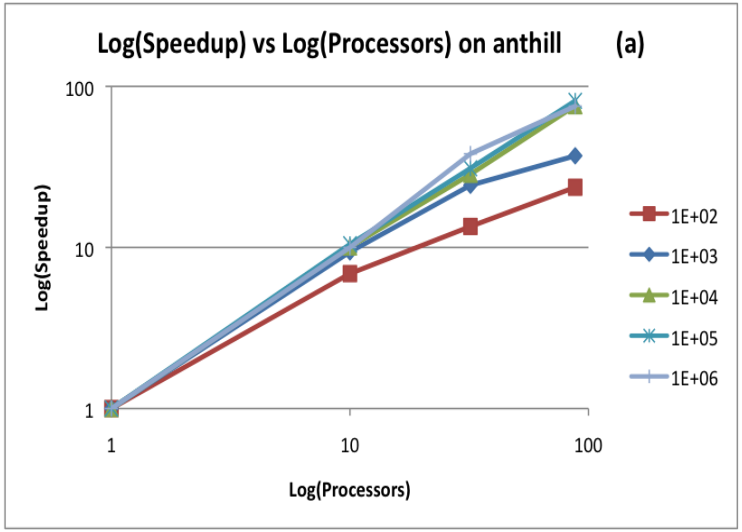
- parUCOAM code integrated in CE
- Application deployed to remote resources
- CA/CyberWeb
  - builds and deploys test cases
  - Manages results
  - Performs simple visualization



CyberWeb App: CyberCHEQS Project

- Combustion simulations to model chemical reacive 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

- Questions:
  - mthomas@mail.sdsu.edu
  - http://acel.sdsu.edu
- References:

  - M P Thomas, C Cheng, S More, and H Shah. Integrating HPC Resources , Services , and Cyberinfrastructure to Develop Science Applications Using Web Application Frameworks. In *Int. Conf. Parallel Distrib. Process. Tech. Appl.*, volume 2, pages 421–427, Las Vegas, NV, 2012.
  - Mary Thomas and Jose Castillo. A Cyberinfrastructure-Based Computational Environment for Unified Curvilinear Ocean Atmospheric Model (UCOAM). In *4th Int. Congr. Comput. Eng. Sci.*, 2013.
  - [21] Mary P Thomas and Jose E Castillo. Development of a Computational Environment for the General Curvilinear Ocean Model (GCOM). *J. Phys. Conf. Ser.*, 180(1), 2012.