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Grid-BGC: A Grid Enabled Carbon Cycle Modeling Environment

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NCAR
Motivation: NCAR as an Integrator

- It is our position that NCAR must provide integrated solutions to the community.

- Scientific workflows are becoming too complicated for manual (or semi-manual) implementation.

- Not reasonable to expect a scientist to:
  - Design simulation solutions by chaining together application software packages
  - Manage the data lifecycle (check out, analysis, publishing, and check in)
  - Do this in an evolving computational and information environment

- NCAR must provide the software infrastructure to allow scientists to seamlessly (and painlessly) implement their workflows, thereby allowing them to concentrate on what they’re good at: SCIENCE!

- Goal is increased scientific productivity and requires an unprecedented level of integration of both systems and software.

- Long term investment: return to the organization won’t show up in the bottom line immediately.
Motivation: Robust Modeling Environments

- Our goal is to develop a simple, production quality modeling environment for NCAR and the geoscience community that insulates scientists from the technical details of the execution environment
  - Cyberinfrastructure
  - System and software integration
  - Data archiving

- Grid-BGC is an example of such an environment and is the first of these environments developed for NCAR
  - Learning as we develop and deploy
  - Tasked by the geoscience community, but developed services are applicable to other collaborative research projects
Outline

- Introduction
- Carbon Cycle Modeling
- Service Oriented Architecture for the Earth Sciences
- Grid-BGC System Architecture
- Re-tasking the services for other Earth Science applications
- Future Work
Introduction: Participants

- This is a collaborative project between the National Center for Atmospheric Research (NCAR) and the University of Colorado at Boulder (CU)

- NASA has provided funding for three years via the Advanced Information Systems Technology (AIST) program

- Researchers:
  - Peter Thornton (PI), NCAR
  - Henry Tufo (co-PI), CU
  - Luca Cinquini, NCAR
  - Jason Cope, CU
  - Craig Hartsough, NCAR
  - Rich Loft, NCAR
  - Sean McCreary, CU
  - Don Middleton, NCAR
  - Nate Wilhelmi, NCAR
  - Matthew Woitaszek, CU
Carbon Cycle Modeling: Workflow

Daymet inputs…

…Grid-BGC outputs
Carbon Cycle Modeling: Workflow

- Scientific models
  - Daymet
  - Biome-BGC
- Daymet interpolates a high resolution grid of weather observations for a region
- Biome BGC calculates carbon cycle parameters at the individual grid points for each region
- Models originally intended for analysis of small geographic regions.
- Analysis of larger regions is accomplished by simulating its composite regions
Goal: Create an easy to use computational environment for scientists running large scale carbon cycle simulations.

- Requires the management of multiple simultaneously executing workflows
  - Execution management
  - Data management
  - Task automation

- Distributed resources across multiple organizations
  - Data archive and front-end portal are located at NCAR
  - Execution resources are located at CU
# Choosing the Appropriate Architecture for Grid-BGC

<table>
<thead>
<tr>
<th>Description</th>
<th>Resource Oriented</th>
<th>Agent Oriented</th>
<th>Service Oriented</th>
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</thead>
<tbody>
<tr>
<td>Description</td>
<td>Homogenous hardware and software configuration</td>
<td>Intelligent software agents process tasks and goals</td>
<td>Heterogeneous hardware and software configuration possible</td>
</tr>
<tr>
<td></td>
<td>Infrastructure is exposed</td>
<td>Utilizes a resource or service oriented architecture</td>
<td>Functionality available to users and other systems as services with known interfaces</td>
</tr>
<tr>
<td>Pros</td>
<td>Large resource allocations across multiple virtual organizations possible</td>
<td>Automation</td>
<td>Provide abstract interfaces to functional components. Users and developers are not exposed to the underlying service implementation</td>
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<tr>
<td></td>
<td></td>
<td>Search large environments more effectively than a system user</td>
<td>Services become building blocks for more complicated services (code reuse)</td>
</tr>
<tr>
<td>Cons</td>
<td>Complex</td>
<td>A resource or service oriented architecture must be in place</td>
<td>Power is hidden</td>
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<tr>
<td></td>
<td>Security</td>
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9
Service Oriented Architecture for the Earth Sciences: Requirements

- Provide a simple and portable user interface to the services
- Support a variety of programming models (pthreads, MPI, …)
- Support wide range of computer architectures (IBM Power, AMD Opteron, Intel Xeon, …)
- Support management of simple scientific workflows
- Support large data sets (100 MB – 1 TB)
- Integrate wide range of distributed resources
  - NCAR Mass Storage System
  - Heterogeneous and distributed computational resources
Service Oriented Architecture for the Earth Sciences: Desired Services

- **User interface services**
  - Portal
  - GUI
  - Command line client

- **Data services**
  - Mass storage service
  - File transfer service
  - Data publishing service

- **Execution services**
  - Model execution service
  - Workflow control service
  - Resource allocation service

- **Metadata services**
  - Registry / index service
  - Resource brokerage service
Grid-BGC: System Overview

- **System goals**
  - Easy to use
  - Efficient and productive science

- **Development summary**
  - Prototype developed with GT 3.2
  - Current system redeveloped with GT4
  - Integrates resources from NCAR and CU

- **Architecture Implementation**
  - Not a pure service oriented architecture, but moving towards one
  - Currently more like a service oriented application
Service Oriented Architecture for the Earth Sciences: Implemented Services

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Grid-BGC: System Architecture

Web Portal User Interface

- Grid-BGC Model Web Service
- Daymet Model Web Service

Workflow Service

Workflow Manager

- Surfer Resource Broker
- WS-GRAM
- Globus RFT

MyProxy

GridFTP
Grid-BGC Portal

- Web interface to Grid-BGC
- JSP / Tomcat implementation using CoG Kit
- Composed of logical services
Grid-BGC Execution Services

- Execution service contains all functionality needed to run a model and is aware only of those models
- Provides interface to request and initialize a model run
  - Creates directory structure
  - Creates model initialization files
  - Registers file transfers and executables with the workflow manager
- Provides interfaces to query, terminate, and cleanup requested model runs
Workflow Control Service and Workflow Manager

- **Workflow Control Service**
  - Provides functions to register workflow tasks, model executions, and file transfers
  - Execution service uses the workflow control service functions to register its tasks
  - Workflow control service stores the workflow metadata in a persistent database

- **Workflow Manager**
  - Periodically queries the workflow metadata database for new tasks to execute
  - Delegates file transfers to the Reliable File Transfer service (RFT) and job executions to the Grid Resource and Allocation Management Service (GRAM)
Example Grid-BGC Workflow

Diagram:

- Grid-BGC Portal Clients
- Grid-BGC Service
- Workflow Control Service
- Job Data
- Workflow Manager
- Globus WS GRAM
- Globus Reliable File Transfer

Application Clients
Application Grid services
Workflow Manager Service
Globus Toolkit components
Current Grid Topology
Grid Enabling POP

- Parallel Ocean Program (POP)
  - Developed by the DOE at the Los Alamos National Laboratory
  - Component of NCAR’s Community Climate System Model (CCSM)

- Grid Enabling POP
  - Re-tasked the grid service and workflow subsystem to run POP
  - Required
    - New execution service
    - New client interface for accessing the service
    - No changes to the workflow subsystem
Future Work: Expansion of the Grid-BGC Environment

- Integrate new computational resources
  - Integrate NASA’s Columbia Supercomputer into the Grid-BGC environment
  - Integrate resources provided by the system’s users (University of Wisconsin, …)

- Continue to break out the desired services from current system components

- Visualization
Future Work: Grid Enabling More Earth Science Applications
Experiences from Simulating the Global Carbon Cycle in a Grid Computing Environment

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Questions?
Ideas? Comments?
Suggestions?
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NCAR