Grid-BGC: A Grid-Enabled Terrestrial Carbon Cycle Modeling System

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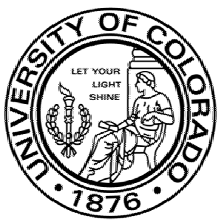


NCAR

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
  - Don Middleton, NCAR
  - Nate Wilhelmi, NCAR
  - Matthew Woitaszek, CU

Project Objectives

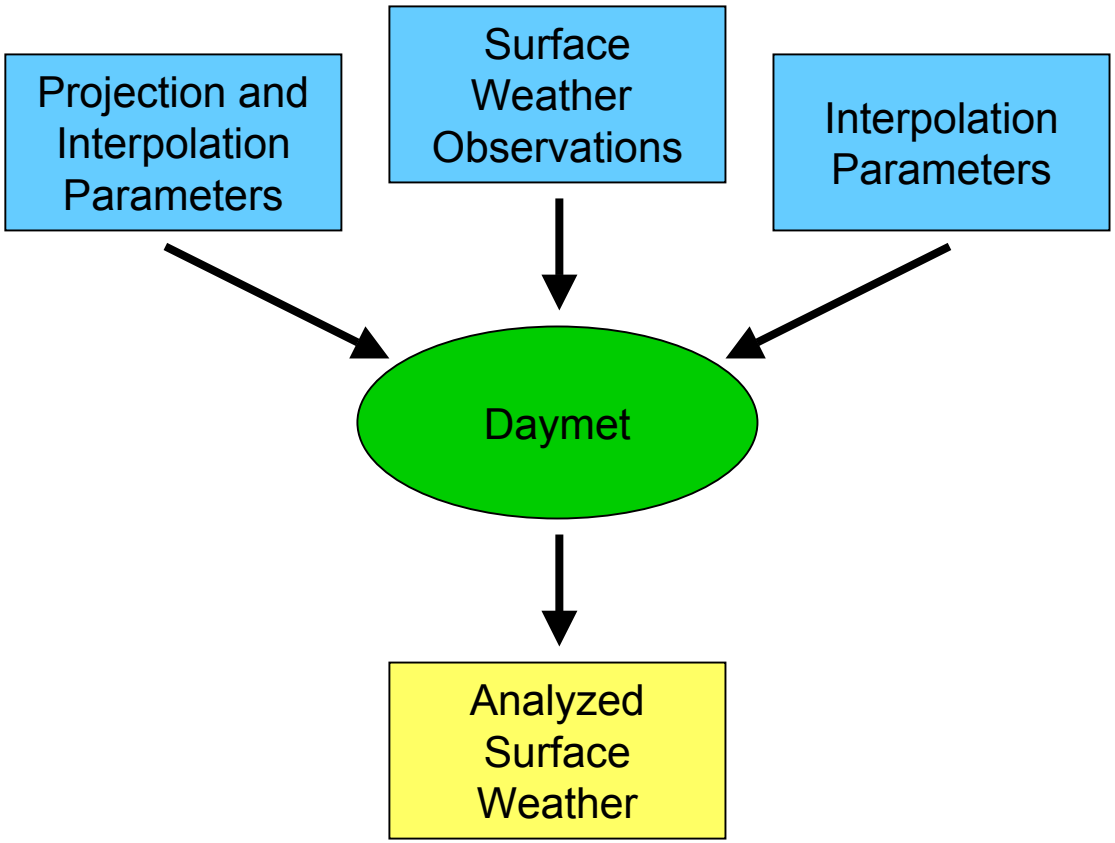
- The objective of the Grid-BGC project is to create an end-to-end technological solution for high-end Earth system modeling that will reduce the costs and risks associated with research on the global carbon cycle and its coupling to climate.

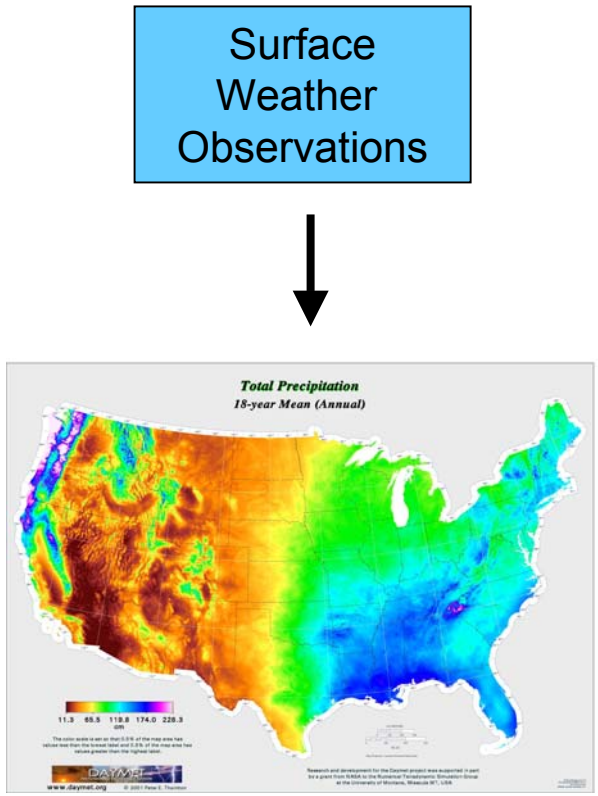
- The prime objective of this projects is to allow scientists to easily configure and run simulations of the global carbon cycle.

Outline

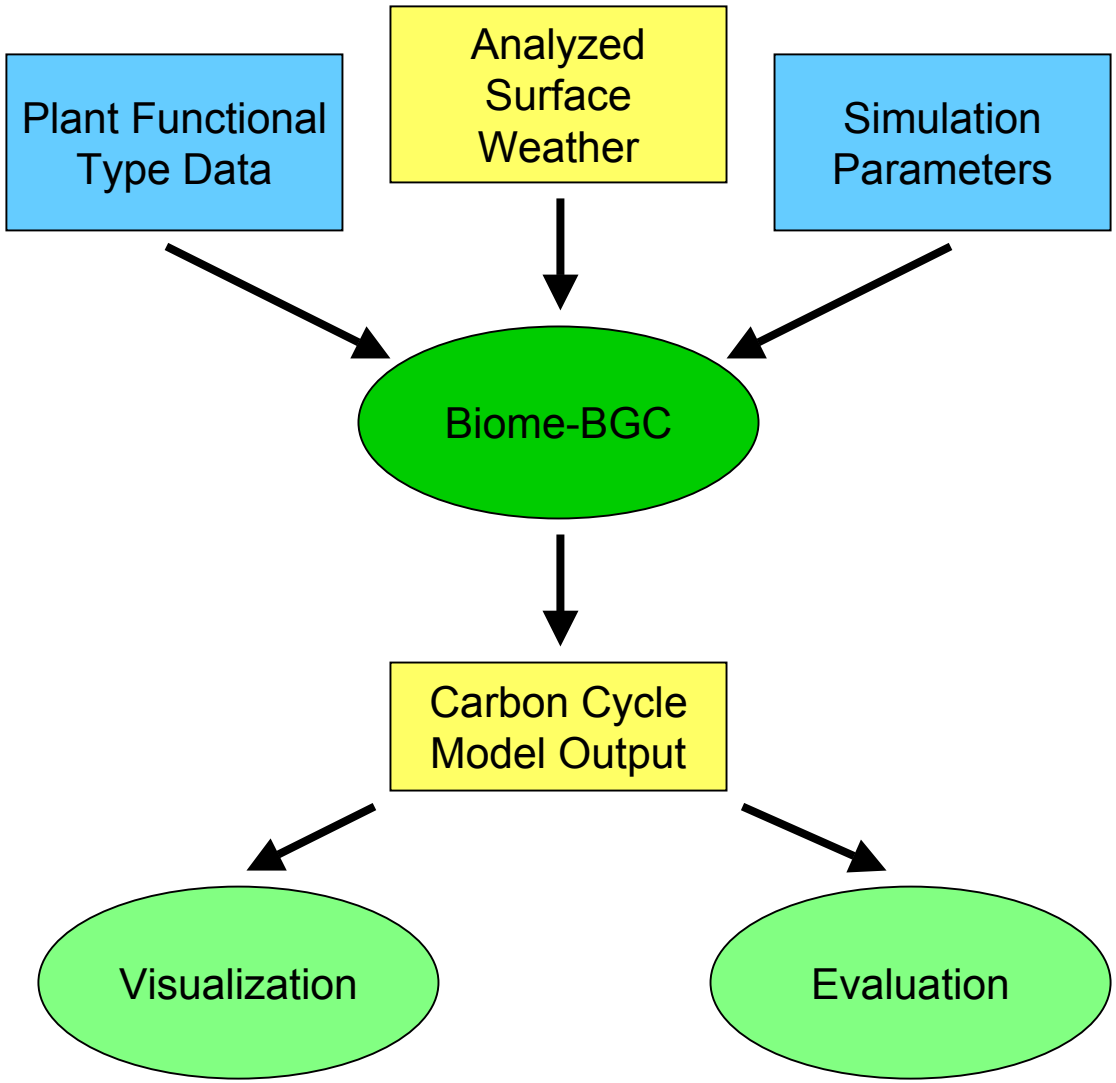
- Introduction
- Carbon Cycle Simulation – Daymet and BiomeBGC
- Motivation
- Grid-BGC System Architecture
- Implementation Experiences
- Conclusions / Future Work

Carbon Cycle Simulations – Part 1





Carbon Cycle Simulations – Part 2



Carbon Cycle Simulations – Spatial Simulations

- Moving towards spatial simulations
  - Biome-BGC was originally intended as a point-based terrestrial carbon cycle model
  - The model can be extended to a spatial model by executing the model for every individual point in the spatial domain
  - Spatial model is embarrassingly parallel
  - Each point requires appropriate configuration files
- Grid-BGC spatial model terminology
  - Tile = a single point-based model
  - Job = a model run for a single tile
  - Simulation = all point-based models in the analyzed spatial domain

Motivation – Problems With The Old Execution Pipeline

- High operational costs
  - Required significant amount of overhead from scientists to setup and execute the simulations
  - No model failure detection or correction available
- Complex execution pipeline
  - Configuration complexity increased with the size of the simulations
  - Very little automation available
  - Many different system components were required to perform the simulations
- Distributed design
  - Allocated computational resources are located at distributed locations
  - Execution pipeline did not support security and file transfers needs between distributed locations

Motivation – Grid-BGC Project Requirements

- In order to create a high-end earth modeling system, the Grid-BGC system design should
  - Limit the costs of global carbon cycle modeling
    - Decrease modeling complexity
    - Use alternative computational resources
  - Reduce the risks and increase reliability of the models
    - Task automation
    - Fault tolerance
    - Provide a secure and accountable operating environment
  - Ease the simulation process for scientists
    - Provide an easy to understand user interface to simplify modeling tasks
    - Limit user interactions with the models and other system related tasks
  - Use grid computing technologies to easily enable a distributed computing environment

- The Grid-BGC system design can adequately fulfill most of these requirements if treated as a case of the Data Grid Application problem

Motivation – Data Grid Application Problem

- Data Grid – A grid computing system that deals with controlled sharing and management of distributed data

- Data Grid Application Problem
  - Computationally expensive model exists that does not completely utilize the computational resources at a single site
  - Partial utilization of resources is viewed as waste or misappropriation
  - Model can be distributed to other computational sites that better suit the models computational requirements
  - Along with other grid computing tools, this model requires data grid technologies to help transfer large data sets required by the computations

Motivation – Data Grid Application Problem

General Solution: Create an offloading compute service deployable at remote grid compute sites.

- Targets resources at a collaborating grid computation site to run or support a specific application
- Supports basic data grid application requirements through grid computing tools
- Make compute service generic and extensible so that it can execute any application that fits the Data Grid Application model
- Grid-BGC is a perfect fit for this design pattern.

Motivation – Grid-BGC Design Goal

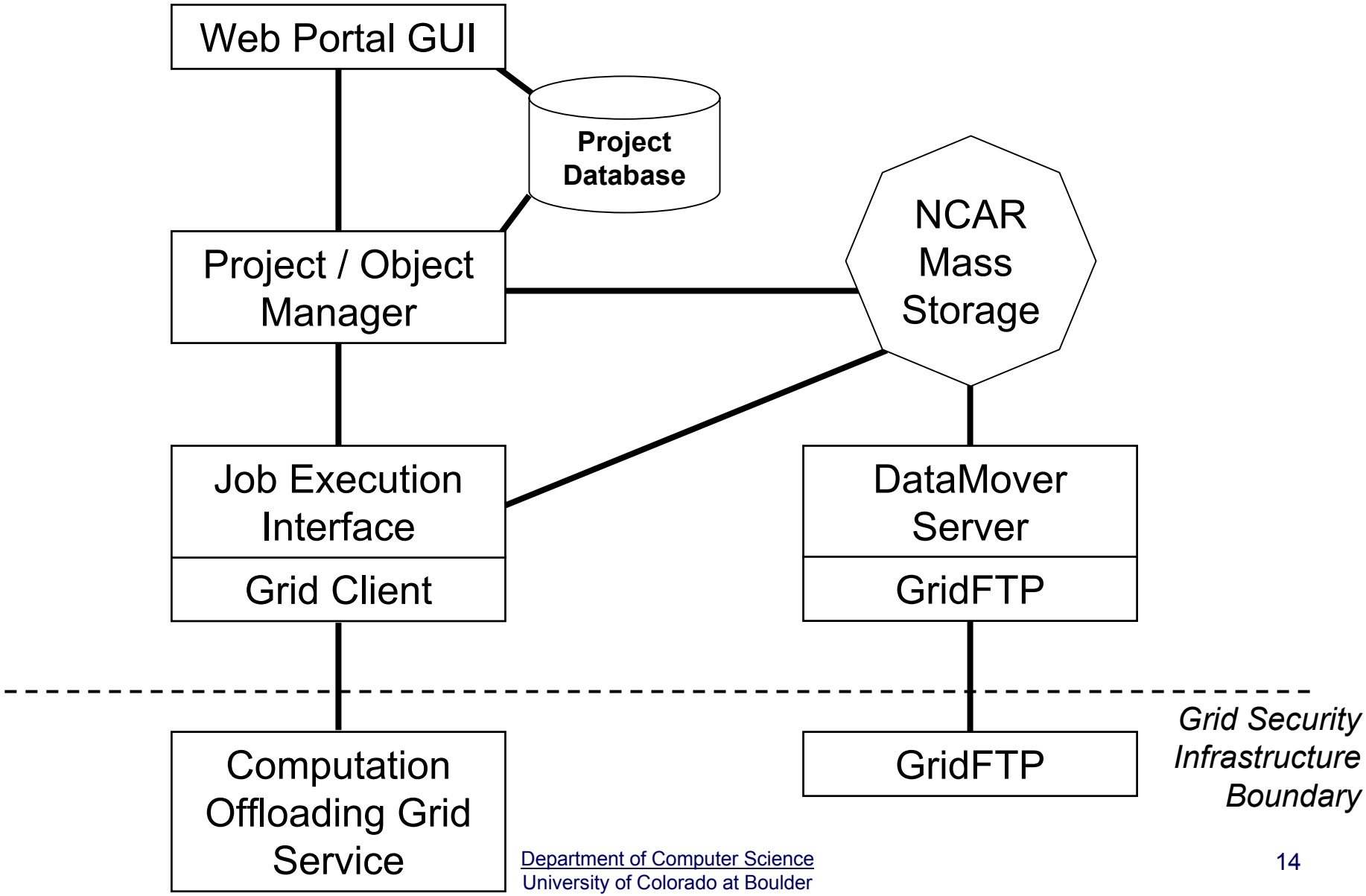
Design Goal: Allow scientists to easily configure and run simulations of the global carbon cycle.

- Minimize the scientists interaction with the models and the distributed nature of the system
- Automate complex configuration tasks
- Provide failure detection and correction support for the scientific models

Grid-BGC System Architecture – Solution Components

- Web Portal GUI
  - Organize complicated workflows
  - Support collaboration recognizing data object dependencies
- Computational Offloading Grid Service
  - Automate job execution on remote platforms
  - Eliminate user interaction with computational resources
  - Reliable execution of a task
- Data Transfer Facilities
  - Grid-FTP
  - DataMover

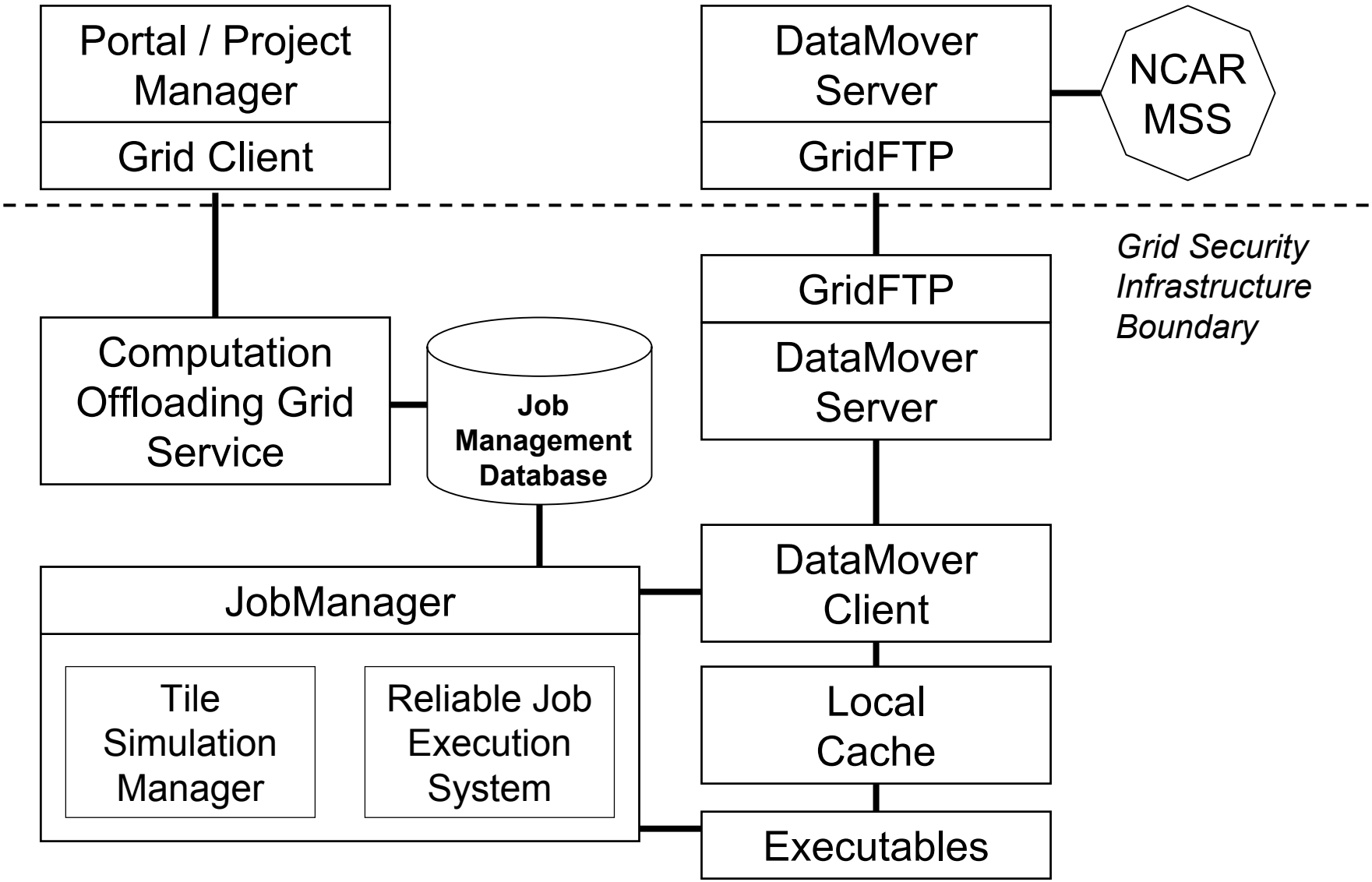
Grid-BGC System Architecture – Top Down



Grid-BGC System Architecture – Web Portal GUI

- Portal provides high-level management capabilities to the user base, including:
  - Workflow management
  - Data sharing
  - Collaboration
- Distributed thin-client implementation
- Currently under development

Grid-BGC System Architecture – Bottom Up



Grid-BGC System Architecture – Computation Offloading Grid Service

- Globus Grid Service interprets and logs user requests to the Grid-BGC computational infrastructure
  - Exposes methods to request for the system to start, stop, and query Grid-BGC jobs
  - Stores all requests to the Job Management Database
- All requests and responses to and from the service are written in an XML based specification language
  - Details how a method will act upon a Grid-BGC job or the Grid-BGC system
  - Generic language definition can be used for DataGrid problems beyond Grid-BGC

Grid-BGC System Architecture – JobManager, A Reliable Execution Engine

- Daemon executing on the computational infrastructure at CU
- Composed of two separate components
  - Reliable Job Execution Service (RJES)
  - Tile Simulation Manager
- Provides reliable and secure job management functionality, including:
  - Starting, stopping, and monitoring of scientific models and other portions of the Grid-BGC software framework
  - Guarantees fault tolerant execution of Grid-BGC jobs
  - Stateless design allows the daemon to easily recover from a crash
  - Can only start Grid-BGC related jobs

Grid-BGC System Architecture – File Transfers Through DataMover

- DataMover
  - Under development by Alex Sim, et al.
  - Lawrence Berkeley National Laboratory
  - Project Website: http://sdm.lbl.gov/cgi-bin/srm-dist-index.pl
- DataMover provides reliable file transfers and replication for applications with large data sets
  - GSI Authentication
  - Reliable file transfers
  - File caching
  - NCAR Mass Storage System Interface
- Who else is using it?
  - Earth Systems Grid (NCAR)
  - Visual Data Toolkit (University of Wisconsin)
- Software is still under development

Experiences – Reliability

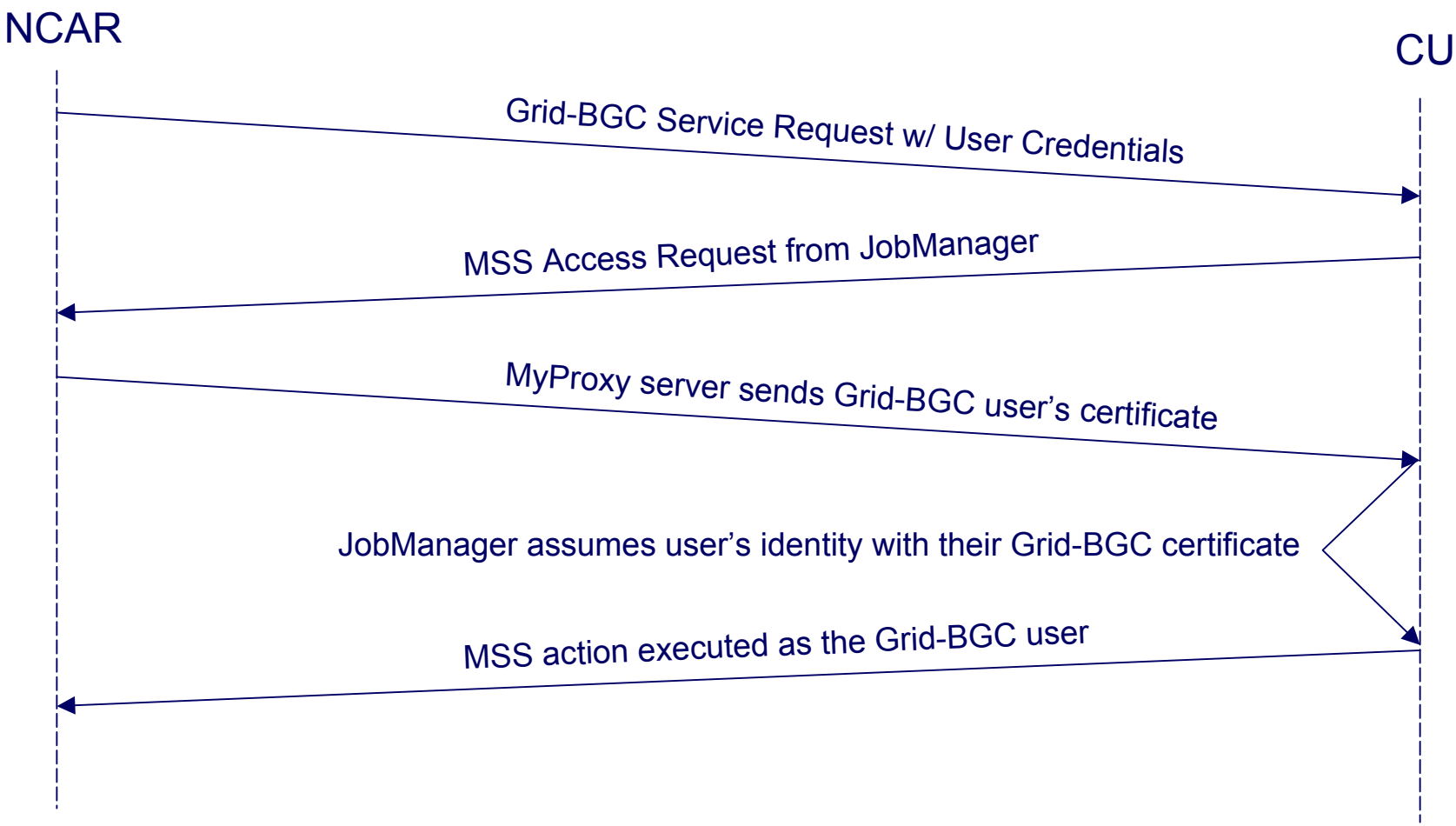
- Reliable Job Execution Service (RJES)
  - Execution service for Grid-BGC
  - Tracks execution of Biome-BGC, Daymet, and DataMover file transfers
- All Grid-BGC jobs tracked by RJES are arbitrarily restartable
  - Job metadata stored in a persistent database and monitored by Tile Simulation Manager
  - RJES polls database for changes in a jobs state and executes an appropriate task if necessary

Experiences – Security

- NCAR Security and Auditing Requirements
  - Resource usage must be accounted for
  - Mass storage system (MSS) access is restricted
- MyProxy Solution - Description
  - Each Grid-BGC account is issued an internally managed grid certificate
  - All certificates are managed by a MyProxy server
  - As MSS access is needed, the certificate is requested from the MyProxy server and the JobManager assumes the identity of the user using the certificate

Experiences – Security

- MyProxy Solution - Animation



Experiences – System Testing

- End-to-end tests
  - Test execution of Grid-BGC software framework
  - Testing environment
    - Client on NCAR's Dataportal Server
    - JobManager on CU's Hemipshere Cluster
    - New job request every 15 minutes for seven days
  - Successfully ran all jobs
- Successful fault tolerance tests
  - JobManager: shutdown, restart, invalid requests, kill running models
  - DataMover: network failures, invalid file requests, low disk space

Future Work

Reconcile our project with the definition of **workflow**:

> Workflow: A collection of tasks that are processed on distributed resources in a well defined order.

- By definition, we seem to have a workflow
  - Globus middleware is starting to provide workflow support
  - As it matures, we should probably try to use it
- We don't have portable executables
- Our portal interface supports modifiable shared data with dependencies

- Workflow initiatives: partial match with our project

Future Work

- Integrated testing
  - Full connect portal workflow management to Grid service
  - Run end-to-end simulation jobs to produce impressive maps
- Model performance testing
  - Appropriately target available clusters
- Multiple compute cluster support
  - Static selection by researchers with their own clusters
  - Dynamic selection among available clusters by load
- More security enhancements
  - Integrate our own CA with the NCAR login service

Conclusions

- The Grid-BGC system design provides
  - A cost effective solution for global carbon cycle modeling
  - A simplified approach to high-end earth system modeling
- The Grid-BGC design solution to the data grid application problem can be used to execute similar applications in a distributed environment

Acknowledgements

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Questions?
Ideas? Comments?
Suggestions?

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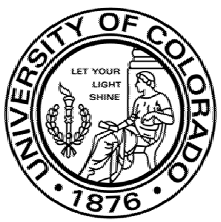

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