

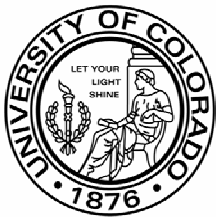
Grid-BGC: A Grid-Enabled Terrestrial Carbon Cycle Modeling System

Jason Cope

Ph.D. Candidate

Department of Computer Science

University of Colorado, Boulder



NCAR

Outline

- ❑ Introduction
- ❑ Carbon Cycle Simulation – Daymet and BiomeBGC
- ❑ Motivation
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- ❑ Conclusions / Future Work

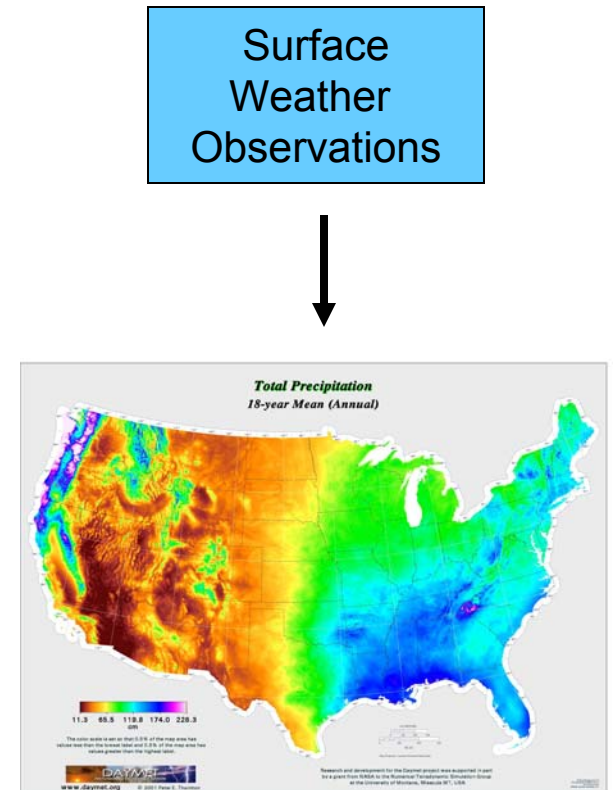
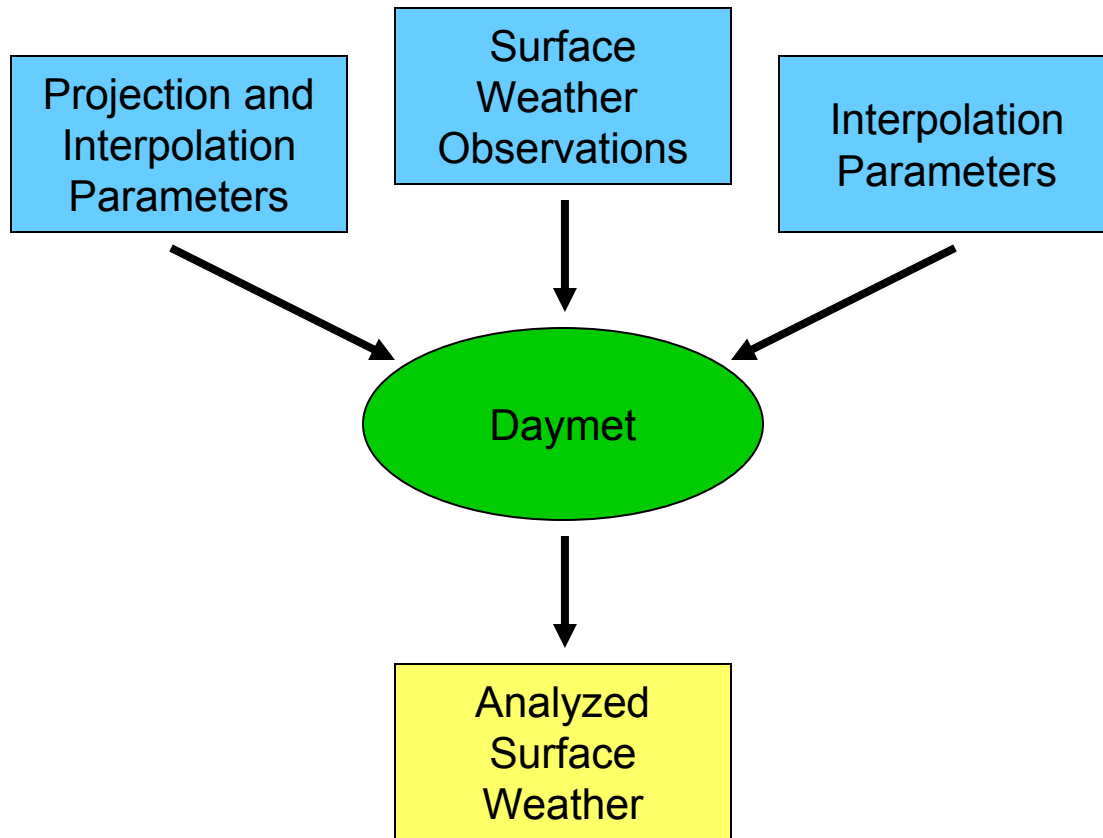
Introduction - Participants

- ❑ 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) and the Terrestrial Ecology programs
- ❑ 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

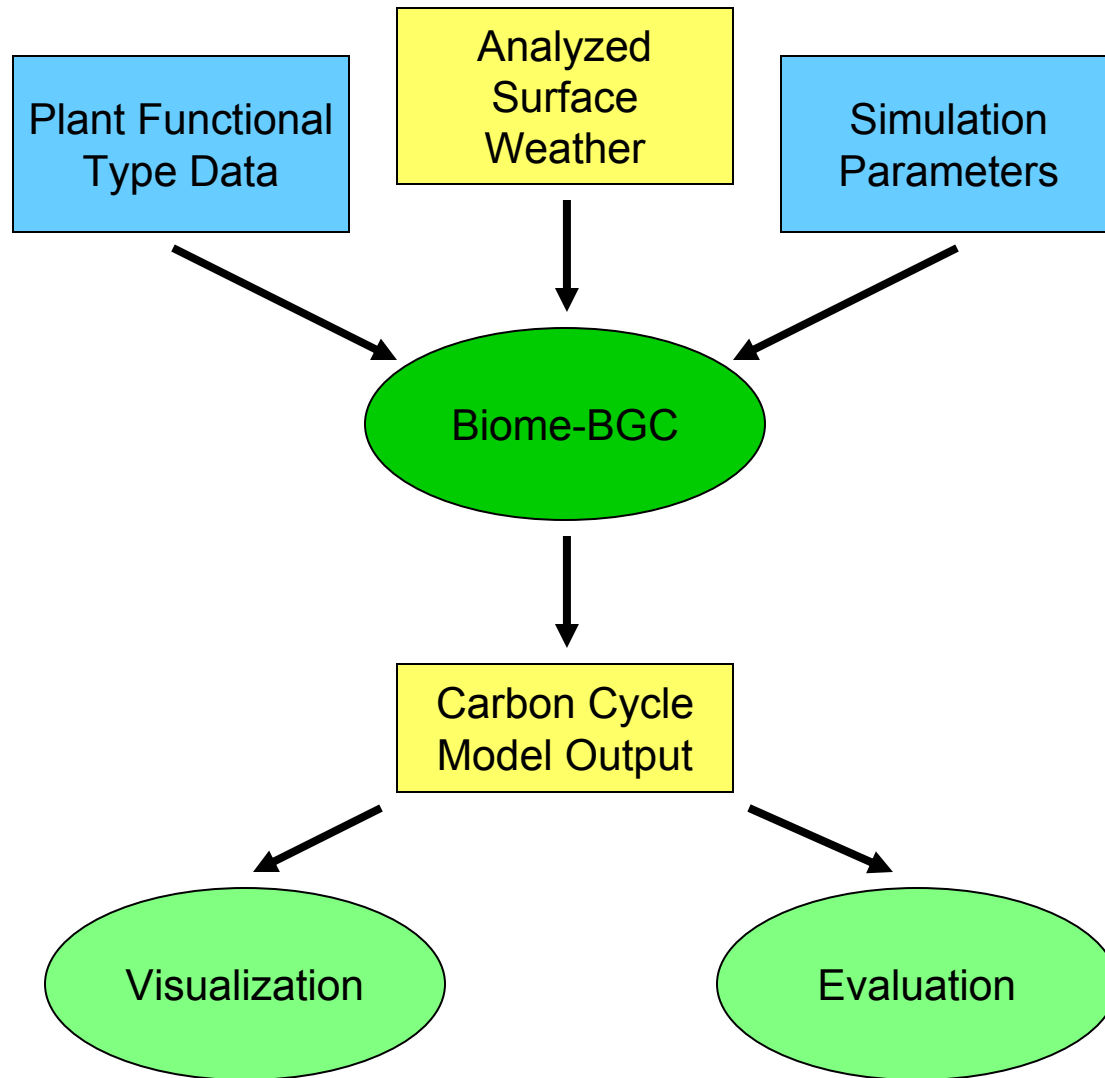
Introduction - Project Objectives

- ❑ 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 design objective of this projects is to allow scientists to easily configure and run simulations of the global carbon cycle.
- ❑ In production, the system should be able to model the carbon cycle for large spatial domains across the globe

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

Motivation – Design Solution

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 other data intensive, distributed applications
- ❑ Grid-BGC is a perfect fit for this design

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

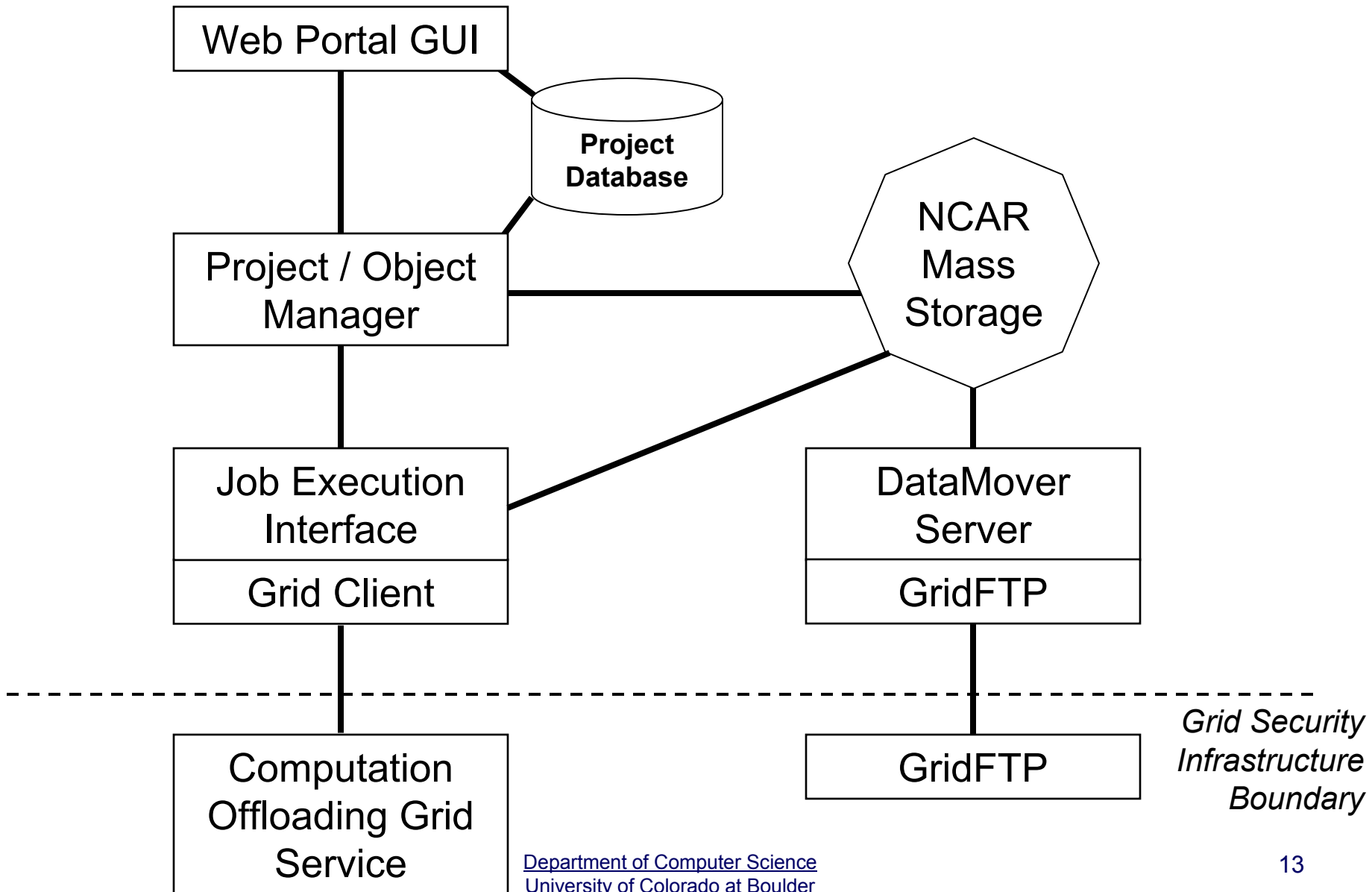
Grid-BGC System Architecture – Solution Components

- ❑ 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



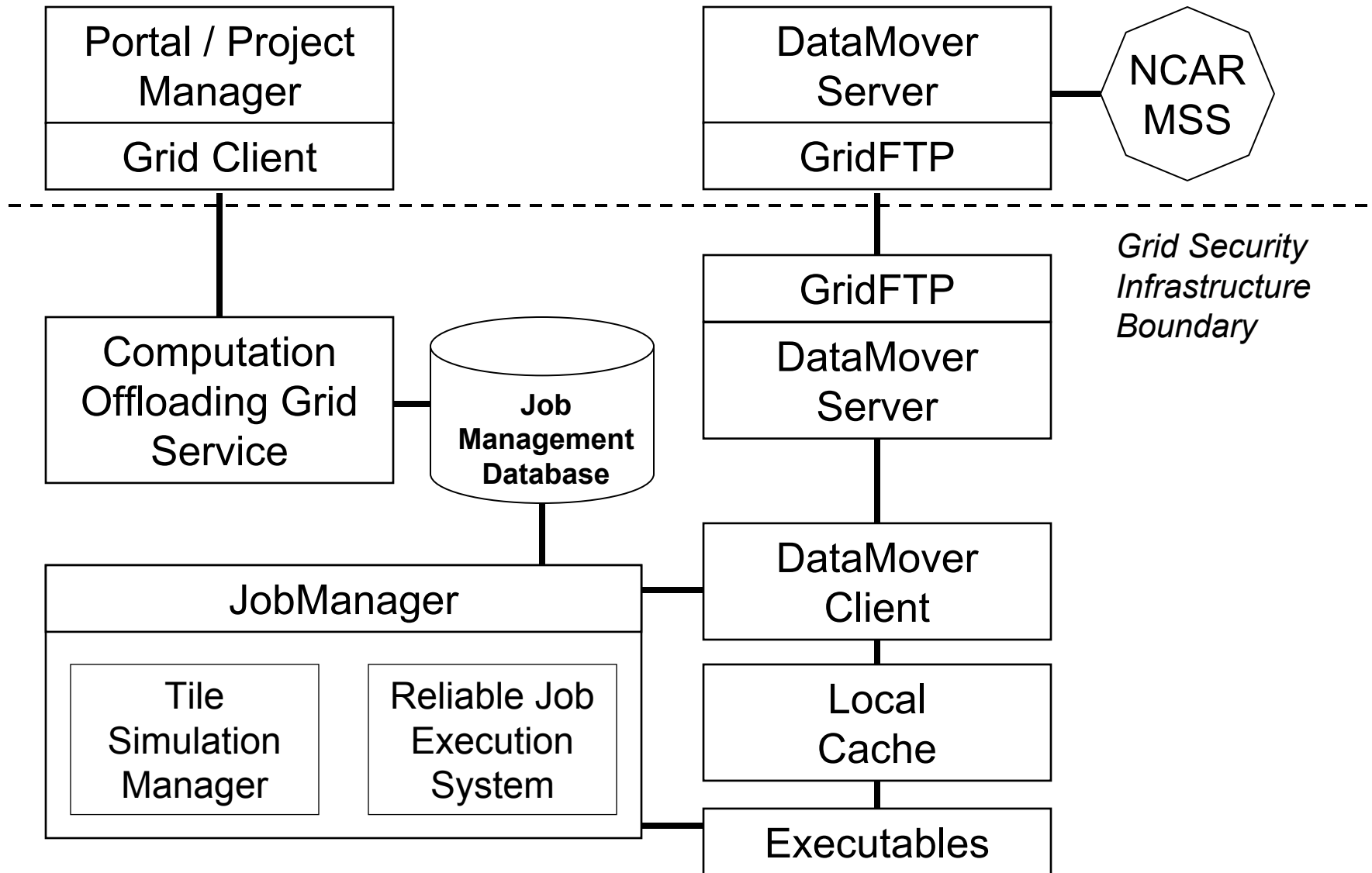
Grid-BGC System Architecture – Web Portal GUI

- ❑ 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 other computations 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

Grid-BGC System Architecture – File Transfers Through DataMover

- ❑ DataMover provides a set of command line utilities to perform file transfers and operations in a grid environment
 - ❑ srm-copy
 - ❑ srm-ls
 - ❑ srm-mkdir
 - ❑ srm-status

- ❑ The JobManager executes these utilities to transfer files to and from
 - ❑ Computational resource storage caches
 - ❑ NCAR Mass Storage System

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

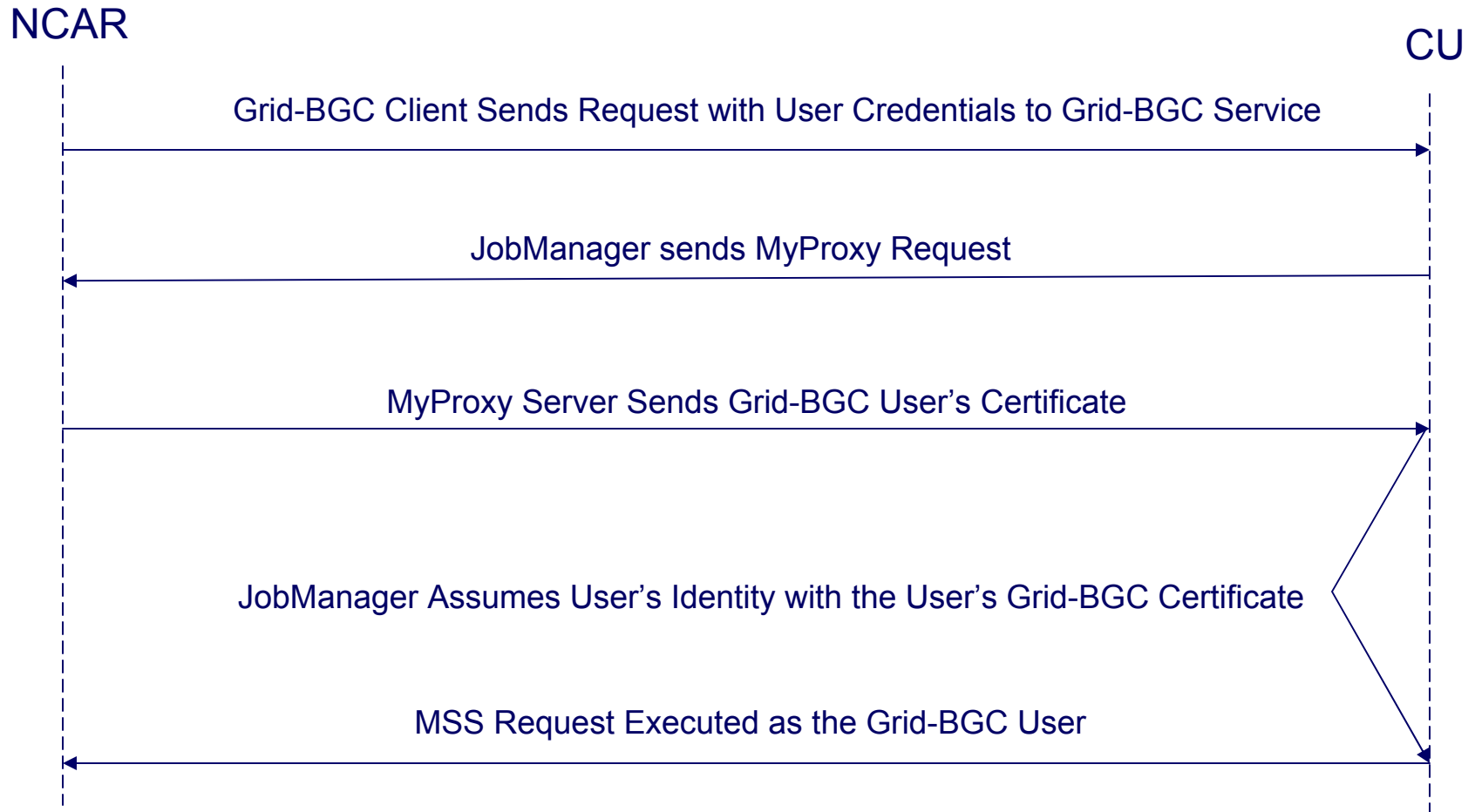
Experiences – Security

- ❑ 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



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

- ❑ 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
 - ❑ Bouncy Castle CA / Java APIs

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

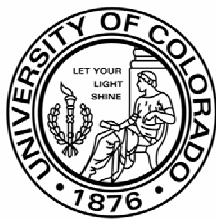
Acknowledgements

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Questions?
Ideas? Comments?
Suggestions?

<http://www.gridbgc.ucar.edu>
Jason.Cope@colorado.edu



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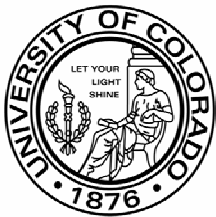
Appendix

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Globus Toolkit 4 and Grid-BGC

- ❑ We are closely watching progress and developments with GT4, especially in the areas of
 - ❑ Security – Integration of MyProxy into GT4
 - ❑ GridFTP – Performance Improvements, Data Storage Interface (DSI)

- ❑ We will proceed with respect for the past (GT3) and a bold vision for the future (GT4)

Installing the Grid-BGC Framework

- ❑ Currently, the following components are required
 - ❑ Java SDK 1.4.2_05
 - ❑ Globus Toolkit 3.2
 - ❑ DataMover 1.2.0
 - ❑ MyProxy 1.4
 - ❑ Postgres 7.4.5
 - ❑ Grid-BGC service
 - ❑ Daymet and Biome-BGC models