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# Powering Statistical Genetics with the Grid: Using GridWay to Automate R Workflows

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# Outline

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- Overview
- Our Plan
- Problems
- Solutions
- Project Status
- Future Directions



# Statistical Genetics

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- One area of study is the application of statistical methods to understand gene expression and how it relates to expressed traits
- Uses statistical analysis to determine the distribution of traits
- Attempts to build a mapping between general genetic traits and an individual's expression of those traits
- For example, which genes control the expression of diabetes?



# UAB Statistical Genetics

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- Section on Statistical Genetics (SSG) is part of the Department of Biostatistics in the School of Public Health
- Provide graduate programs in statistical genetics
- Support research use of statistical methods
- Conduct statistical methodology research
- Lead by Dr. David Allison



# Statistical Genetics Workflow

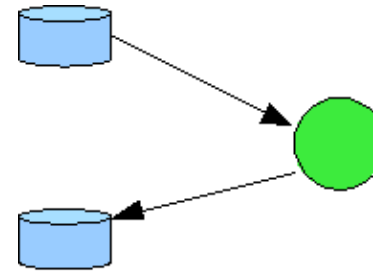
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- Applied Analysis
  - Real data from experimental results
  - Variables are regions of genome and may vary from 10K to 100K
  - Ex. identify region association with a disease
  - Occurs when experimental data is available
- Methodological Analysis
  - Random data generated for simulated analysis
  - Understand behavior of statistical methods used in real data analysis
  - 2k - 5k variables analyzed (maximum practical for existing, traditional 2 cluster resource pool)
  - Occurs repeatedly when methods are studied

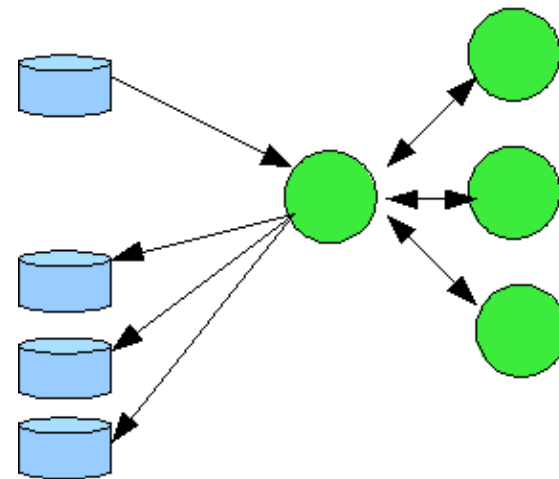
# Statistical Genetics Workflow Characteristics



- Data analysis code written in R
- Process level and MPI granularity
- Embarrassingly (obvious) parallel (workflow)
- Already benefits from cluster-scale computing (384 CPUs, ~3Tflops)



Single Process



MPI-Based Process



# Statistical Genetics Workflow Issues

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- Methodological analysis limited by available compute power
  - Accuracy improves when simulated data is same size as real data
  - Currently 2k-5k variables, ideally 10k-20k (two to ten times the current scale!)
- Manual, multi-cluster job management is problematic and inefficient
- Manual, multi-cluster R environment management does not scale
- Many inexperienced users excluded



# Can “the Grid” Help?

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- The workflow characteristics are ideal for grid migration – 1000's of isolated computations
- More compute power readily increases workflow throughput
- Management issues are not computation problems but scaling problems
- Signs point to Yes





# R-Group Goals

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- Assess feasibility of grid-based workflow
- Build larger computational pool to increase R program workflow throughput
- Expand accessibility of workflow leveraging web-based user interface to grid via GridSphere
- Migrate workflow as a test of UABgrid infrastructure



# UABgrid Overview

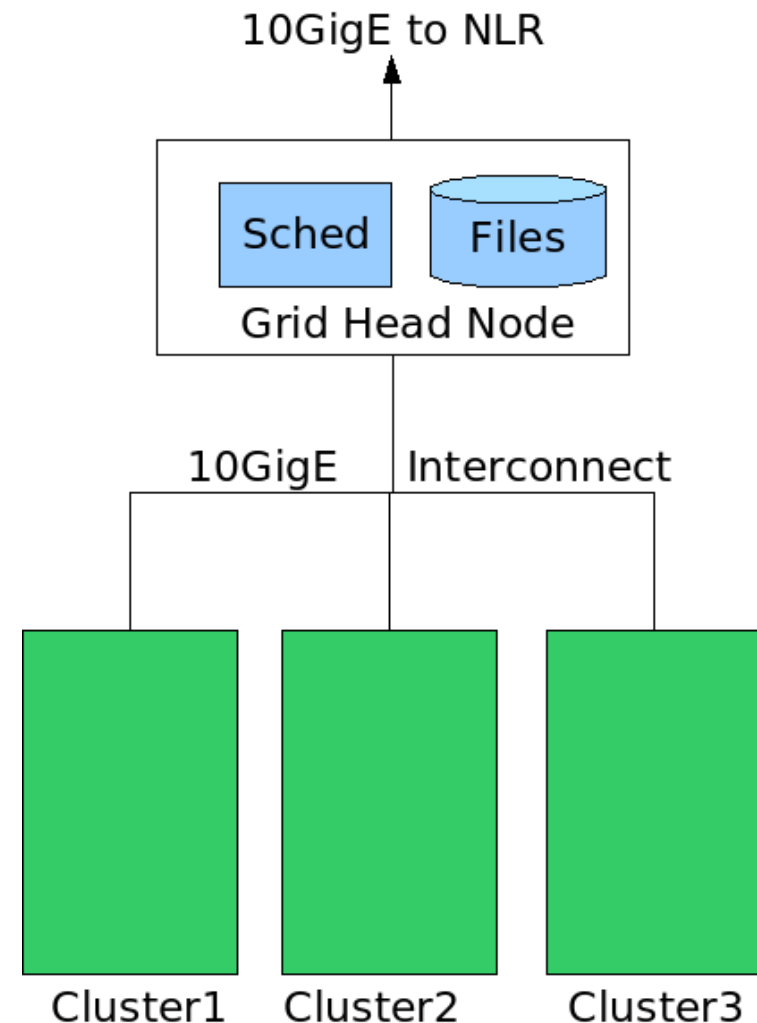
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- UABgrid Pilot launched at campus HPC Boot-Camp September 2007
- User-driven collaboration environment supports web and grid applications
- Leverages InCommon for user identification
  - SSO for web applications
  - Self-service certificate generation for Globus users
- Provides meta-cluster to harness on- and off-campus compute power using GridWay

# UABgrid Meta-Cluster Design



- Grid head node for job and data staging
- On-campus ROCKS clusters supply compute power via Globus interface
- Additional compute power supplied by SURAgrid, OSG, or TeraGrid



# UABgrid Meta-Cluster Specs

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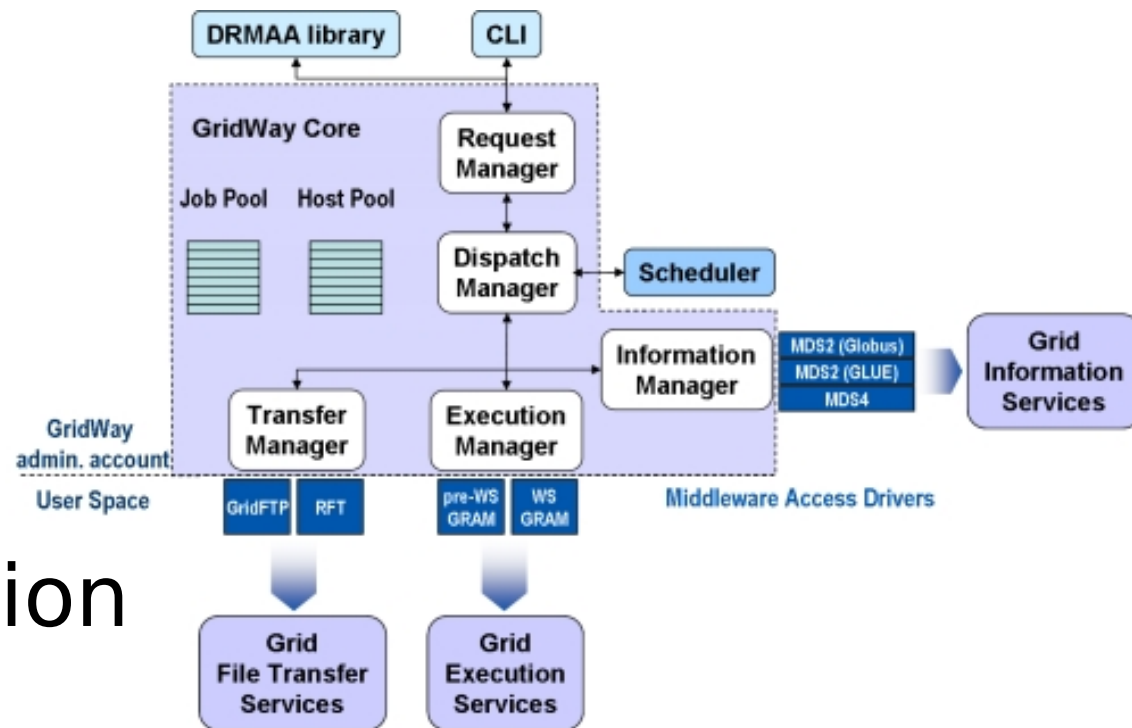


- Today
  - 3 campus clusters, 448 processors, 3+Tflops of power
- 2008 Q2 Targets
  - 5 campus clusters, 960 processors, ~8Tflops of power
  - Large-memory system at state super-computing center
- On Going
  - Engage SURAggrid, TeraGrid, and other suppliers for more compute power
  - Local expansion through campus HPC investments



# GridWay Overview

- Grid meta-scheduler
- Manages job and data staging to clusters using Globus interfaces
- Familiar job template abstraction
- Pluggable schedulers and providers





# Initial Solution

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- It's an ideal grid use case
- R application already works on target cluster
- UABgrid meta-cluster already has working GridWay job submission to target cluster
- Should be straight forward migration of cluster (SGE) job scripts to GridWay job scripts
- What could possibly go wrong?

# What Could Possibly Go Right?

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- GridWay Issues
- Globus Issues
- MPI Issues
- R Issues
- Configuration Management Issues



# GridWay Issues

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- GridWay job templates stage the data and the executable
- Executable staging controlled with path naming
  - Relative path names cause staging
  - Fully qualified path names avoid it
- Fully qualified executable names are not portable - different cluster, different path
- Easily solved with shell script wrappers - delay executable name resolution until runtime





# Globus Issues

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- SGE is not a native job manager in Globus
- Requires error-prone post-install configuration on ROCKS clusters
- Job Type definitions (single, multiple, MPI) are not well defined and vary across sites and schedulers
  - SGE treats single jobs with CPU>1 as array job
  - PBS treats it as a single job that reserved x CPUs



# MPI Issues

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- MPI job type in Globus has been the most challenging
- Globus SGE JobManager assume MPICH (MPIv1)
- R MPI codes assume MPIv2 support, prefer LAM/MPI or OpenMPI
- Exploring two solutions
  - Globus LAM/OpenMPI support
  - Rmpi MPICH support
- Simply does not work out of the box



# R Issues

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- Development is active with regular release cycles
- Feature rich environment for developing and using statistical methods
- It does for statistics what Perl does for text processing
- Large public library of tools and methods CRAN (akin to Perl's CPAN)
- Many jobs have compatibility matrix
- Not bad, just complex



# Configuration Management Issues

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- Compatibility matrix for R scripts hard to maintain
- Many clusters with identical configurations not available (not even with 2 clusters)
- Need solution that keeps configuration in the hands of those most interested
- Look to options that empower application specialists with configuration management framework...



# Containerization

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- Types of Containers
  - User Accounts
  - Virtual Machines
  - Java Boxes
- Account Container
  - Initial target because most common and addresses R application configuration
  - Allows for library dependency and site dependency configuration
  - Full continuum of deployment options from fully staged for each job to statically cached on resources



# Reflections on Progress

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- Would have liked to focus on workflow migration issues, instead we had to focus on component compatibility issues
- Initial goal was intentionally simplistic but provide surprisingly challenging
- Don't be surprised when infrastructure is not ready
- Problems can be solved individually, but all will need to be solved before it will work – *this is a production application*



# R-Group Update

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- Lifecycle Model
  - Feasibility Study
  - Requirements Analysis
  - Design Application Framework
  - Implementation by mid-2008
  - Maintenance
- Status
  - Feasibility study reasonably complete: definitely possible even with technology glitches to work out
  - Requirements for existing resources are known
  - Will continue to follow open source model: release early and release often



# Future Plans

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- ASA Resources
  - Add large memory resource via grid to address some R job requirements for large data structures
- SURAgrid and OtherGrid Resources
  - What resources are available for reliable or predictable compute power generation?
  - Explore NIH Biowulf “swarm” model
- Explore custom resources like BlueGene
  - Are there statistical computations that could benefit from porting to a massively parallel processor?
  - Could web-service provide R-level abstractions?





# Addition Information

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- UABgrid R-Group Project
  - <http://projects.uabgrid.uab.edu/r-group>
- UAB Section on Statistical Genetics (SSG)
  - <http://www.ssg.uab.edu>
- UABgrid
  - <http://docs.uabgrid.uab.edu>
- UAB
  - <http://www.uab.edu>



# Contacts

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