Collaborative Analysis of Petabyte-Scale Scientific Data

Jordan Raddick
Johns Hopkins University
Motivation

- Much of the scientific process is about data
  - collect, clean, archive, organize, analyze, publish, mirror, distribute, curate...

- Jim Gray: “Often it turns out to be more efficient to move the questions than the data.”
Motivation

- Helen Shen: “Brown's students write explanatory text and intersperse it with raw code and the charts and Sitting in the airplane... Brown can interact with the work..”

*Nature, 5 November 2014*
Collaborative data-driven science

History

- Started with the SDSS SkyServer (2001)
- Goal: instant access to rich content
- 2012: NSF DIBBS to extend/reengineer SkyServer
Collaborative data-driven science

SkyServer in 2001
Collaborative data-driven science

SkyServer today
Collaborative data-driven science

Data from HPC Simulations

- HPC is an instrument in its own right
- Need public access to the best and latest
  - Largest simulations approach/exceed petabytes
  - Also need ensembles of simulations
- Creates new challenges
  - Access?
  - Data lifecycle?
  - Analysis patterns?
  - Architectural support?
- Our total science data: ~2.5PB
  - Everything is a Big Data problem!
Collaborative data-driven science

Cosmological Simulations

- Mirror of Millennium DB (universe sim)

  Raw data:
  - Particles
  - FOF groups
  - Subhalos
  - Density fields
  - Halo merger trees
  - Synthetic galaxies
  - Mock catalogs
  - Mock images
Turbulence databases (JHUTB)

- http://turbulence.pha.jhu.edu/
Next step: Numerical Laboratories

- From data retrieval to data analysis
  - No need to download entire datasets
  - Analysis is server-side through web services
- Use virtual sensor metaphor ("the cow in the tornado")
  - Many access patterns are local in space and/or time
- turbulence.pha.jhu.edu:
  19 trillion points delivered!
Hydrostatic and non-hydrostatic simulations of dense waters cascading off a shelf: The East Greenland case Marcello G. Magaldi; Thomas W.N. Haine
Collaborative data-driven science

Genomics

Building a DB of a trillion short reads from Next Gen Sequencing
Materials Science

Daphalapurkar, Brady, Ramesh, Molinari. JMPS (2011)
SciServer Project Objectives

- Extend infrastructure to support additional science domains
- Host and serve Petabyte datasets
- Support custom user datasets
- Provide access and query services
- Provide scalable compute services
- Support analyses and data sets too large to handle locally
- Provide collaborative tools for shared analysis

*Computations stay CLOSE to the DATA...*
## SciServer Project Components

<table>
<thead>
<tr>
<th>Major Components</th>
<th>Supporting Technologies</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Core</strong></td>
<td>Microsoft SQL Server</td>
</tr>
<tr>
<td>• Login Portal</td>
<td>Open Stack</td>
</tr>
<tr>
<td>• CASJobs</td>
<td>Docker</td>
</tr>
<tr>
<td>• SciServer Compute</td>
<td>Jupyter</td>
</tr>
<tr>
<td>• SciDrive</td>
<td></td>
</tr>
<tr>
<td><strong>Applications</strong></td>
<td></td>
</tr>
<tr>
<td>• SkyQuery</td>
<td></td>
</tr>
<tr>
<td>• SkyServer</td>
<td></td>
</tr>
<tr>
<td>• GLUSEEN</td>
<td></td>
</tr>
<tr>
<td>• Turbulence</td>
<td></td>
</tr>
</tbody>
</table>
## SciServer Project Timeline

### Timelines

<table>
<thead>
<tr>
<th>Year 1</th>
<th>(2013-2014)</th>
<th>Project Setup, Scoping, Planning, Begin Refactoring, SDSS Unification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Year 2</td>
<td>(2013-2014)</td>
<td>Architectural Refactoring – API, Single Sign-on, prototype Compute</td>
</tr>
<tr>
<td>Year 3</td>
<td>(2013-2014)</td>
<td><strong>SciServer System Release, Interactive Compute, Scalable Job Management, Basic Dashboard, Initial Collaborative capabilities</strong></td>
</tr>
<tr>
<td>Year 4</td>
<td>(2013-2014)</td>
<td>Implementation in Science Domains, Educational workbooks</td>
</tr>
<tr>
<td>Year 5</td>
<td>(2013-2014)</td>
<td>System Scale out, Data Analytics, Advanced Deployment Scenarios</td>
</tr>
</tbody>
</table>
# SciServer Project Current Plans

## Timelines – Year 3

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Apr 2016</td>
<td>• SciServer System Release</td>
</tr>
</tbody>
</table>
| May 2016 | • Interactive Compute  
            • SkyQuery  
            • Gluseen                                                 |
| August 2016 | • Prototype Scalable Job Management  
            • Basic Dashboard  
            • Initial Collaborative capabilities                     |
| October 2016 | • Scalable Job Management  
            • Turbulence  
            • Cosmology                                                 |
| November 2016 | • Project 3 year Review                                         |
Login Portal
Collaborative data-driven science

SkyServer

Welcome to the new SkyServer!

We are proud to announce that SkyServer now connects to the new SciServer® science framework! If you have a login through SciServer, you can log in using the control on the top right. Logins on allow you to connect seamlessly with the updated CasJobs and the brand-new SciServer database management tool.


These new features come from the first release of the SciServer framework, which we call SciServer Altair. For more information about the new features of SciServer Altair, please see our New Features in section on the SciServer website.

Welcome to the DR12 site!!!

This website contains data from the Sloan Digital Sky Survey, a project to make a map of a large part of the universe. We would like to show you the beauty of the universe, and share with you our excitement as we build the largest map in the history of the world.

Data Access

Navigáte
Quick Links | Explore
Finding Chart
Image List
Search
1Q9 | 2Q9 | 3Q9
SQL Search
Cross-3D
CasJobs

Education

For Educators
Lesson Plans
Middle School
High School
College Lab Activities
Interactor Guides
Student/Public Research
Galaxy Zoo
Zooniverse

Links

sdss.org
Data Release 12
SDSS-III Science
Science Archive Server
About Astronomy
About the SDSS
About SkyServer
VAD
Credits

Help

Start Here | FAQ
Glossary
Tool User Guides
Cooking with Sloan
SQL Tutorial
About the Database
Schema Browser
Sample SQL Queries
Data Release Papers

News

Data from data from data release 12 (DR12). What’s new in DR12, what’s new on this site and known problems. Here...
CasJobs: Query
CasJobs: MyDB
What is SciServer Compute?

- Interactive Jupyter notebooks hosted inside Docker containers.

- Pre-configured images to create new containers from (R, Python, MATLAB, ...).

- High-bandwidth, low-latency access to other SciServer services and data sources through the notebooks.

- Users manage their own containers.
What are Docker Containers?

Type 1 Hypervisor

Type 2 Hypervisor

Linux Containers

- Hypervisor
- Operating System
- Hardware

- Hypervisor
- Operating System
- Hardware

- Container
- Bins / Libs

- Container
- Bins / Libs

Docker

CLI

REST API

Dockerfile
Collaborative data-driven science
Collaborative data-driven science

Data Storage Configuration

Docker Container

/home/idies
workspace
persistent
sdss_das

Notebook Server

Persistent Storage

User

SDSS DAS
Run asynchronous non-interactive jobs in separate Docker containers. It’s meant to be more than just Jupyter notebooks!

Create new VM nodes on-demand to accommodate growing number of users.

Provide scratch (temporary) storage space for working with large amounts of data.

Improve resource management.
Questions?
Architectural Challenges

- Define tradeoffs
  - Data Analytics system is different from supercomputer
  - What is the right balance between I/O and compute?

- Need high bandwidth to big data
  - Computations/visualizations must be on top of the data
  - Must support at least few 100TB per server
  - Petascale: 3 copies for production (or erasure code?)
  - Wide area data movement/backbone is hard

- Lessons from the database world:
  - It is nontrivial to schedule complex I/O patterns
  - For subsets we must use indexing, cache resilient storage