

The Research Computing Center

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THE UNIVERSITY OF
CHICAGO

**Research
Computing
Center**

info@rcc.uchicago.edu

Advance research and scholarship at the University of Chicago by providing research computing resources, support, education, training, and advanced technologies.

Office of the Vice President for Research
and for National Laboratories

Research Development
(Arete)

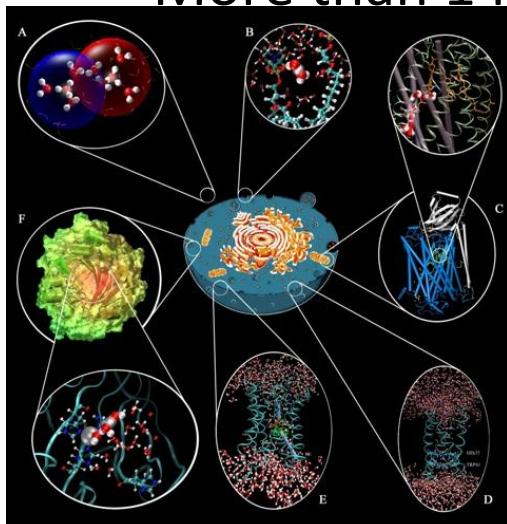
University Research
Administration (URA)

Research Computing
Center (RCC)

Center for Technology
Development and
Ventures (UChicago
Tech)

UChicago

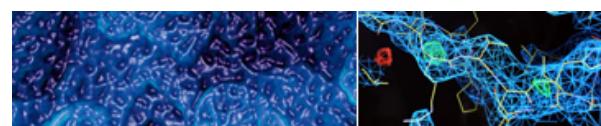
- 4 major graduate divisions: (1) Physical Sciences, (2) Biological Sciences, (3) Social Sciences, (4) Humanities
- 8 major schools (Booth, Pritzker, SSA)
- More than 140 institutes and centers



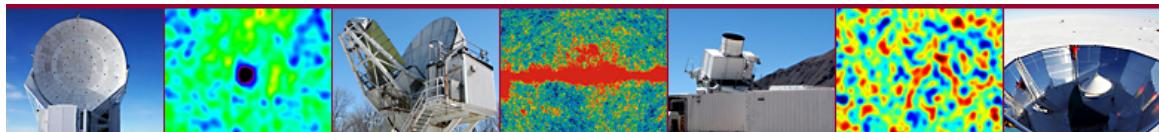
Institute for
Biophysical Dynamics



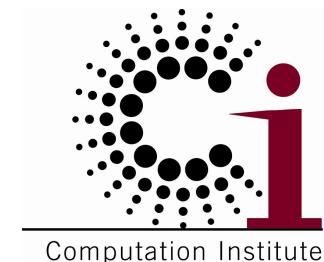
Enrico Fermi Institute



Institute for Molecular Engineering



Kavli Institute for Cosmological Physics



Computation Institute



The University of Chicago Booth School of Business



Institute for
Genomics &
Systems Biology



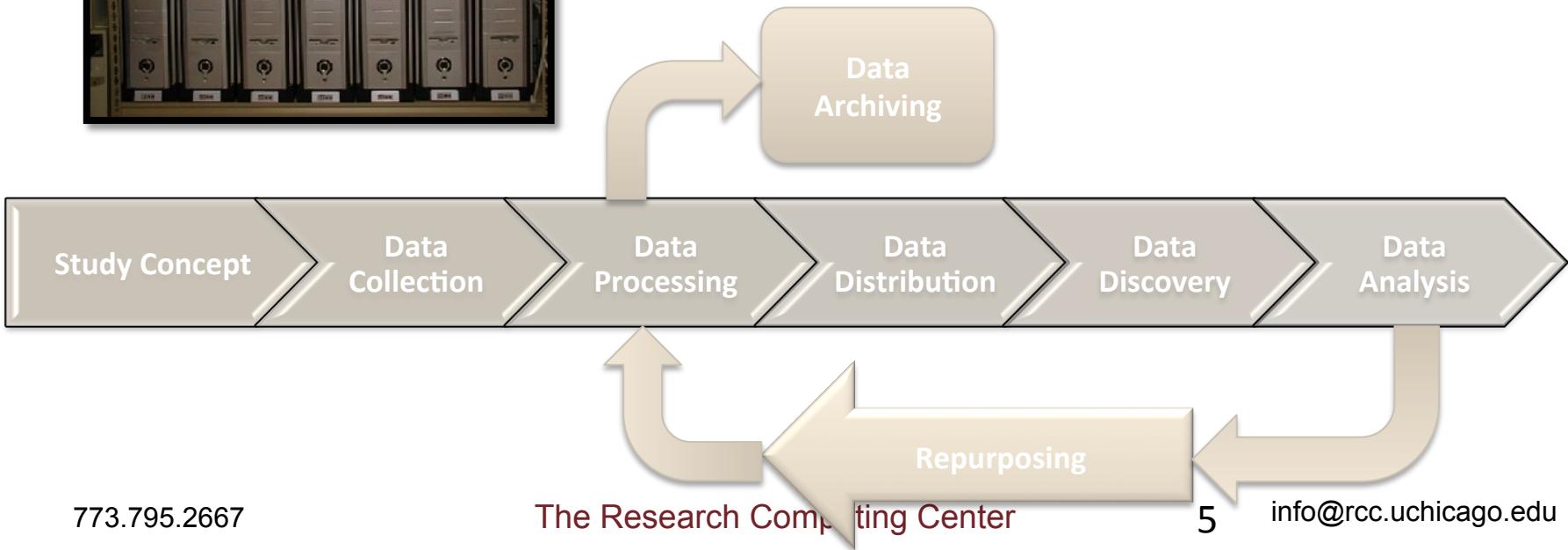
An array of research disciplines with widely varying computation and data management needs

Astronomy & Astrophysics
Biochemistry & Molecular Biology
Chemistry
Chicago Booth, Instruction & Research
Computational Institute
Computer Science
Ecology & Evolutionary Biology
Economics
Enrico Fermi Institute
Geophysical Sciences
Health Studies
Linguistics
Mathematics
Medicine
Molecular Engineering, Institute for Organismal Biology & Anatomy
Pediatrics
Physics
Psychiatry and Behavioral Neuroscience
Psychology
Radiation & Cellular Oncology
Radiology
Statistics

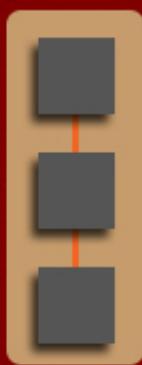
What issues are researchers facing?



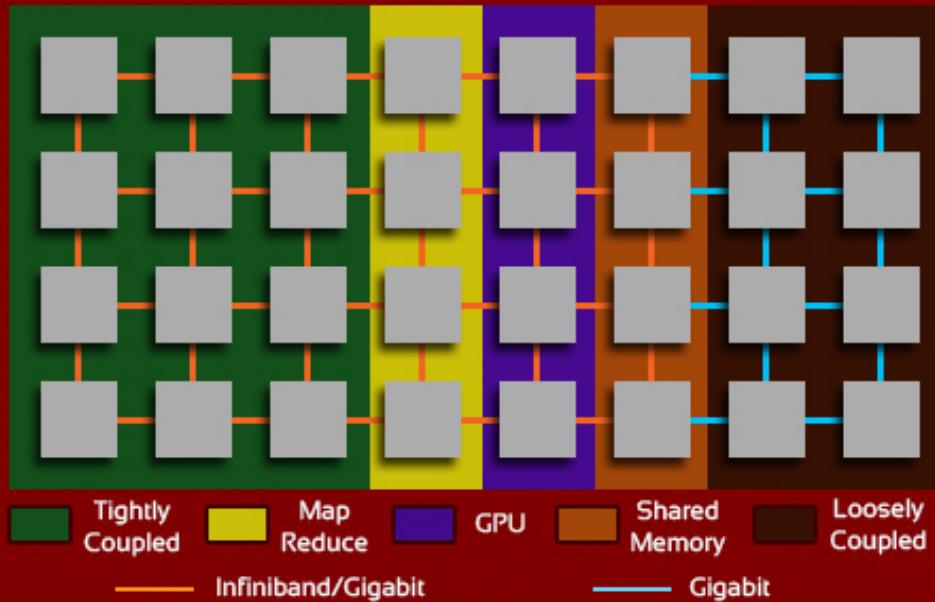
Lack of data management know-how
Complexity of computing/storage hardware
Ad hoc solutions
Poor performance, excessive cost



6045 Data Center



Login
Pool



Tape Backup
and Storage

Crerar Library
Zar Room



Data Visualization Laboratory

Regenstein 216



Walk-in User Lab

Edelstone

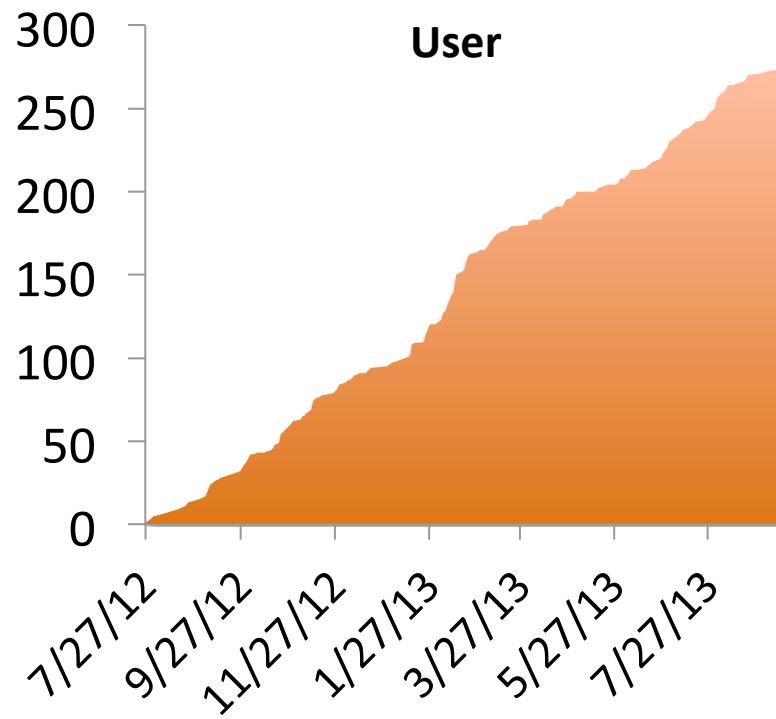
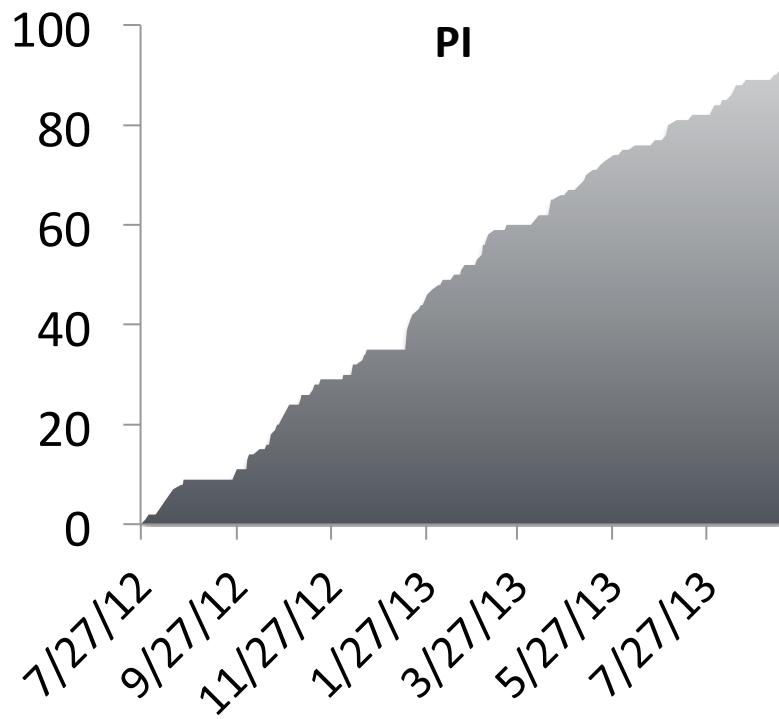


RCC Staff

Programs and Services

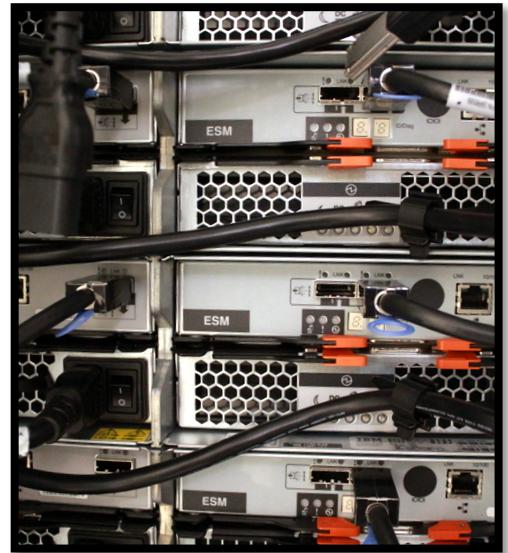
- Campus Resource Allocations
- Cluster Partnership
 - Special CPP: Cluster Management
- Computing Tools
- Consultant Partnership
- Workshops and Training
- Education
- Outreach
- New Faculty Support
- Grant Support (letter of commit, data management)

Research Account Requests



Cluster Partnership Program

- Allows researchers to augment RCC HPC and storage infrastructure
 - Tightly-coupled nodes
 - Loosely-coupled nodes
 - GPU accelerators
 - Shared memory nodes
 - High performance storage
 - Capacity storage
 - Tape backup
- Partner hardware is similar to the hardware of the RCC cluster
- Contact info@rcc.uchicago.edu for system requests with requirements outside the RCC CPP



Faculty Support

Assistance in the recruitment process

Early access to RCC resources and help transitioning to UChicago

Evaluation and acquisition of hardware

Commitments to funding agency

Data management plans

The screenshot shows the homepage of the Office of Science and Technology Policy (OSTP). At the top, there is a blue header bar with the OSTP logo on the left and the text "Office of Science and Technology Policy" in white. Below the header, there is a navigation menu with links: "About OSTP", "OSTP Blog", "Pressroom", "Divisions", "R&D Budgets", "Resource Library", and "Newsletter".

Expanding Public Access to the Results of Federally Funded Research

[Subscribe](#)

Posted by Michael Stebbins on February 22, 2013 at 12:04 PM EDT



The Obama Administration is committed to the proposition that citizens deserve easy access to the results of scientific research their tax dollars have paid for. That's why, in a policy memorandum released today, OSTP Director John Holdren has directed Federal agencies with more than \$100M in R&D expenditures to develop plans to make the published results of federally funded research freely available to the public within one year of

Development of Computing Tools



Fast easy parallel scripting -
on multicores, clusters,
clouds and supercomputers

Secure, reliable, high-
performance data transfer

Access to distributed high
throughput computing
resources

Globus Online RCC Implementation

The screenshot shows the RCC Globus Online interface. At the top, there's a header with the RCC logo and 'THE UNIVERSITY OF CHICAGO'. Below it, a navigation bar includes 'Manage Data', 'Groups', 'labello's Profile', and 'Sign Out'. The main area is titled 'Transfer Files'.

On the left, a window titled 'Endpoint: ucrrcc#sharing' shows a list of files and folders, including '20130416.gofls.parsed', 'benchmark', 'bin', 'bosco', 'build-software', 'docs.mystuff', 'exercise-system', 'games', 'gaussian', 'gitwork', 'goflperftest', 'intel', 'lib', 'mcmc', 'mdanalysis', 'meeting', 'namd.rcc-docs', 'notes', 'oneoffs', and 'privatemodules'. On the right, another window titled 'Endpoint: labello@Labello-Mac' shows a similar list of files and folders, including 'Desktop', 'Documents', 'Downloads', 'Dropbox', 'Google Drive', 'Movies', 'Music', 'Pictures', 'Public', 'Sites', 'bin', 'gitwork', 'install', 'projects', 'sandbox', 'simpIemm', 'simpIemm.backup', 'software', 'svrwork', 'workshops', and 'Intel.Call.Notes'. Both windows have 'select all' checkboxes and 'refresh list' buttons.

At the bottom, there are buttons for 'more options', 'Label This Transfer' (with a text input field), and a note: 'This will be displayed in your transfer activity.' The footer contains the University of Chicago logo, address '600 S. Ellis Ave, Suite 126 Chicago IL 60637', phone number '773-705-2967', 'Contact Us', and the 'globus online' logo.

- Use UChicago authentication
- Available with each RCC account
- Easy install of Globus Connect
- Branded/Site entry
- Stats/monitoring of RCC use

```
[labello@midway-login1 .ssh]$ ssh labello@cli.globusonline.org scp go#ep1:/share/godata/file1.txt ucrrcc#midway:~/  
Task ID: 72e14746-a210-11e2-97d0-123139404f2e  
Type <CTRL-C> to cancel or bg<ENTER> to background  
[XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX] 1/1 0.00 mbps
```


[Manage Data](#)
[Groups](#)
[labello's Profile](#)
[Sign Out](#)

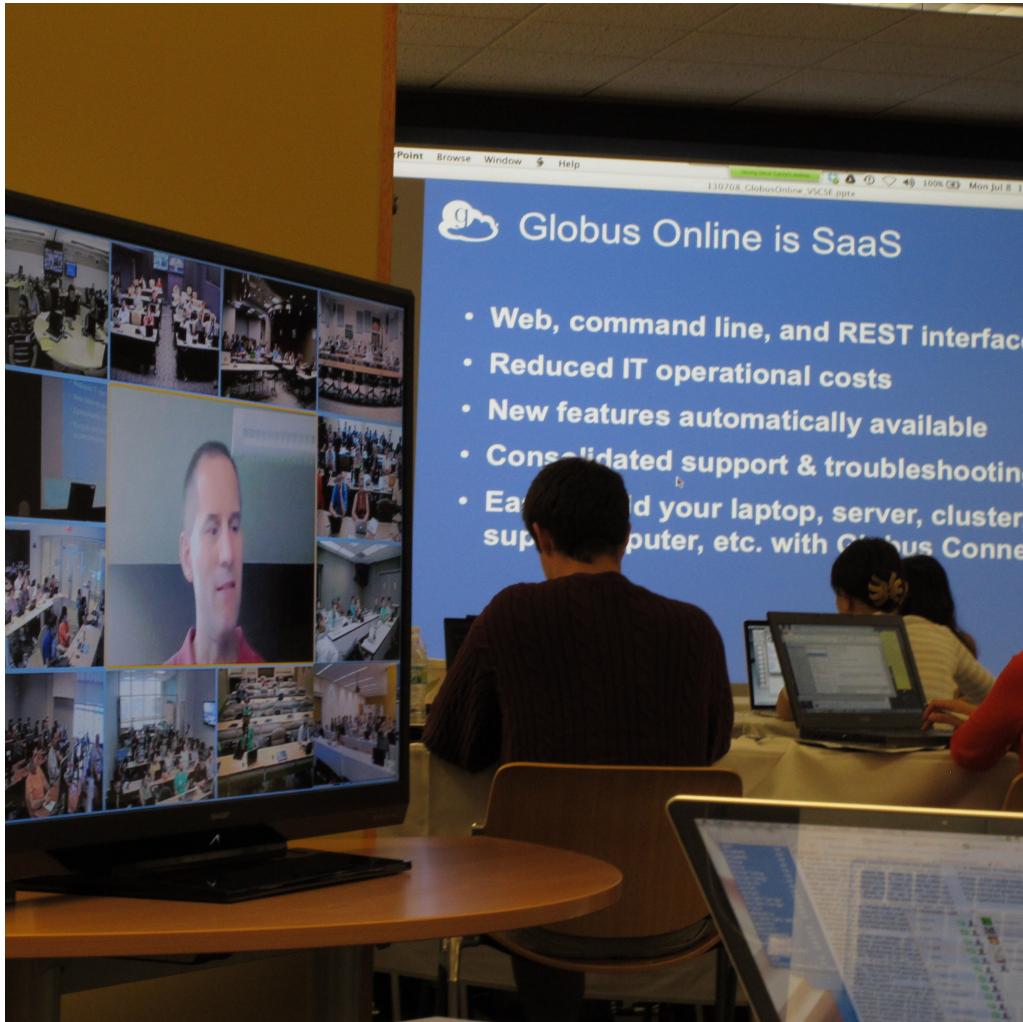
Transfer Activity

Cancel

◀◀ ◀ 1 of 1 ▶ ▶▶

View 25 Records

	Status	Label	Task Progress	Completion Time	Request Time
<input type="checkbox"/>		Task Id:ce7fb13c-a77e-11e2-97d0-123139404f2e	<div style="width: 100%;">38 / 38</div>	04/17/2013 11:49 AM	04/17/2013 11:49 AM
<input type="checkbox"/>		Task Id:7ccf0e3e-a439-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/13/2013 07:56 AM	04/13/2013 07:55 AM
<input type="checkbox"/>		Task Id:595fcad4-a438-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/13/2013 07:47 AM	04/13/2013 07:47 AM
<input type="checkbox"/>		Task Id:bde7299e-a437-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/13/2013 07:43 AM	04/13/2013 07:43 AM
<input type="checkbox"/>		Task Id:ea56bf7c-a38c-11e2-97d0-123139404f2e	<div style="width: 100%;">430 / 430</div>	04/12/2013 11:24 AM	04/12/2013 11:20 AM
<input type="checkbox"/>		Task Id:72e14746-a210-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/10/2013 01:57 PM	04/10/2013 01:57 PM
<input type="checkbox"/>		Task Id:363e91b8-a210-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/10/2013 01:55 PM	04/10/2013 01:55 PM
<input type="checkbox"/>		Task Id:26319a9a-a210-11e2-97d0-123139404f2e	<div style="width: 100%;">1 / 1</div>	04/10/2013 01:55 PM	04/10/2013 01:55 PM
<input type="checkbox"/>		Task Id:dbce26c8-0430-11e2-bf56-1231380b8963	<div style="width: 100%;">254 / 254</div>	09/21/2012 04:15 PM	09/21/2012 04:11 PM
<input type="checkbox"/>		Task Id:23bbbd3c-0430-11e2-bf56-1231380b8963	<div style="width: 100%;">9 / 9</div>	09/21/2012 04:07 PM	09/21/2012 04:05 PM
<input type="checkbox"/>		Task Id:e46de40c-042f-11e2-bf56-1231380b8963	<div style="width: 100%;">2 / 2</div>	09/21/2012 04:04 PM	09/21/2012 04:04 PM
<input type="checkbox"/>		Task Id:cecd4d68-042f-11e2-bf56-1231380b8963	<div style="width: 100%;">4 / 4</div>	09/21/2012 04:04 PM	09/21/2012 04:03 PM
<input type="checkbox"/>		Task Id:031d46c8-042f-11e2-bf56-1231380b8963	<div style="width: 100%;">1 / 1</div>	09/21/2012 03:58 PM	09/21/2012 03:57 PM
<input type="checkbox"/>		Task Id:e3f674c2-042e-11e2-bf56-1231380b8963	<div style="width: 100%;">1 / 1</div>	09/21/2012 03:57 PM	09/21/2012 03:57 PM
<input type="checkbox"/>		Task Id:fcab8ad6-e31b-11e1-bf56-1231380b8963	<div style="width: 100%;">2 / 2</div>	08/10/2012 01:48 PM	08/10/2012 01:48 PM
<input type="checkbox"/>		Task Id:df7ea564-dc19-11e1-bf56-1231380b8963	<div style="width: 100%;">26 / 26</div>	08/01/2012 03:53 PM	08/01/2012 03:45 PM



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A screenshot of a web-based interface for Globus Online SaaS. The top navigation bar includes 'Point', 'Browse', 'Window', 'Help', and a timestamp 'Mon Jul 8 13:07:08, 2013'. The main content area features a blue header 'Globus Online is SaaS' with a cloud icon. Below it is a bulleted list of benefits: 'Web, command line, and REST interfaces', 'Reduced IT operational costs', 'New features automatically available', 'Consolidated support & troubleshooting', and 'Easily add your laptop, server, cluster, supercomputer, etc. with Globus Connect'. The bottom half of the page shows two transfer windows. The left window has an 'Endpoint' field set to 'enter endpoint name' and a 'Path' field set to '/'. It displays the message 'Please select an endpoint above.' The right window also has an 'Endpoint' field set to 'uchicago.vault' and a 'Path' field set to '/'. It displays the message 'Could not access . Please check the path and try again.' There are buttons for 'View Transfer Activity', 'Get Globus Connect', and 'Turn your computer into an endpoint'. Other buttons include 'Manage Data', 'Groups', 'Labello's Profile', and 'Sign Out'.

info@rcc.uchicago.edu



Welcome to OSG Connect

Efficiently connect your science to cycles and data.

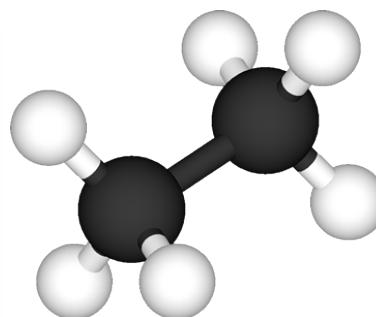
~mml

Molecular Modeling Lite: Lightweight molecular mechanics, geometry optimizations, and molecular dynamics code for teaching.

```
25 18 hc hc 4.38 Angs 0.000 kcal/mol
25 19 hc hc 2.56 Angs 0.001 kcal/mol
25 20 hc hc 3.11 Angs 0.000 kcal/mol
25 21 hc hc 3.07 Angs 0.000 kcal/mol
25 22 hc hc 2.50 Angs 0.000 kcal/mol

E(BONDS)      0.301604 kcal/mol
E(ANGLES)      0.320023 kcal/mol
E(TORSIONS)    0.324661 kcal/mol
E(VDW)         3.324425 kcal/mol
E(EL)          0.005795 kcal/mol

E(TOTAL): 4.276508 kcal/mol
```



Executable

```
#!/bin/bash

source /cvmfs/oasis.opensciencegrid.org/osg/palms/setup
palmsdosetup anaconda
python mml/mml/energy.py --molfile mml/tests/ethane.mol.ac
~
```

- No local software installation
- cNet authentication (Local cluster, Globus, email)
- Leverage global application software stack (palms/oasis)
- Time to first job submission measured in minutes

Submit

```
Universe = vanilla
Executable = mml.sh
transfer_input_files = /home/labello/mml

Error = job.error
Output = job.output
Log = job.log
requirements = (HAS_CVMFS_oasis_opensciencegrid_org == TRUE) && (CVMFS_oasis_opensciencegrid_org_REVISION >= 729)
+ProjectName="UChicago-RCC"
Queue 1
```

```
/* C source code is found in dgemm_example.c */

#define min(x,y) (((x) < (y)) ? (x) : (y))

#include <stdio.h>
#include <stdlib.h>
#include "mkl.h"

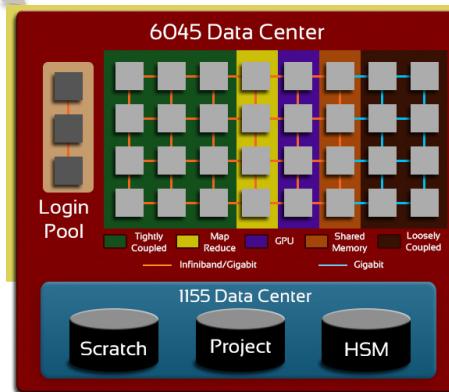
int main()
{
    double *A, *B, *C;
    int m, n, p, i, j;
    double alpha, beta;

    printf ("\n This example computes real matrix C=alpha*A*B+beta*C using \n"
           " Intel® MKL function dgemm, where A, B, and C are matrices and \n"
           " alpha and beta are double precision scalars\n\n");
}
```

- proprietary compiler
- Intel Math Kernel Library (MKL)
- `icc -mkl -static eg.c`

```
[labello@login01 osg-quickstart]$ condor_submit job-to-midway
Submitting job(s).
1 job(s) submitted to cluster 31260.
```

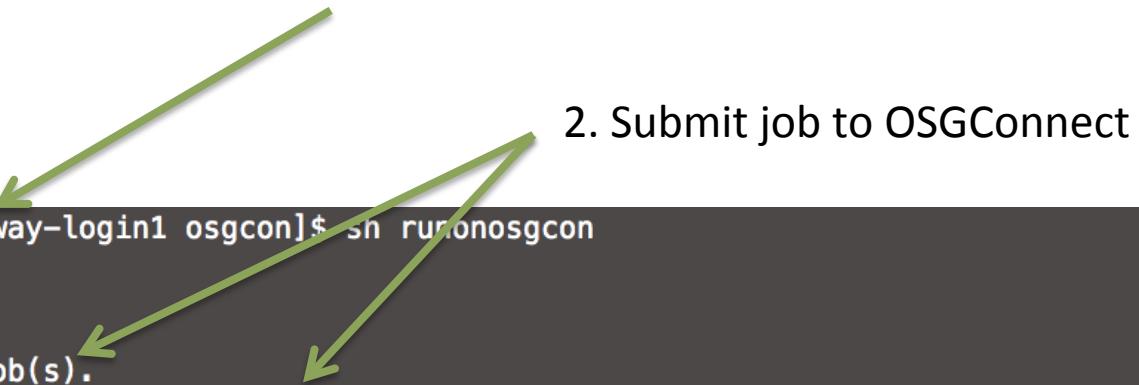
From osgconnect to Midway



1. From Midway (local resource)

2. Submit job to OSGConnect

```
[labello@midway-login1 osgcon]$ sh runonosgcon
a.out
run.condor
runjob.sh
Submitting job(s).
1 job(s) submitted to cluster 31257.
[labello@midway-login1 osgcon]$ cat runonosgcon | wc -l
8
```



The diagram illustrates the workflow for submitting a job to OSGConnect. It consists of two main steps: 1. From Midway (local resource), which points to the local files listed in the terminal output (a.out, run.condor, runjob.sh). 2. Submit job to OSGConnect, which points to the submission command 'sh runonosgcon' and its output indicating the job has been submitted to cluster 31257.

- Internal Evaluation
- Identify need and use cases
- Determine appropriate implementation
- Training & community
- Beta testing new features

Research Computing Center

Transfer Files

Endpoint ucrc#sharing Path /~/

select all | none up one folder refresh list

- 20130416.gpfs.parsed
- 20130909.gpfs.parsed
- benchmark
- bin
- bosco
- build_software

new folder show hidden files delete selected files share

The screenshot shows the "Transfer Files" interface from the Research Computing Center. It displays two separate file transfer windows. The left window is titled "Transfer Files" and has an endpoint of "labeledo@Labelo-wac". The right window is titled "ucrcc#midway" and also has an endpoint of "labeledo@Labelo-wac". Both windows show a list of files and folders, with the right window showing a larger list including "CompToolsForBioChem", "benchmark", "bin", "bosco", "build_software", "exercise-system", "gaussian", "goldperfest", "log", "montee", "molecular", "oneofs", "privatemodules", "public_html", "scratch", "scratch-midway", "avwork", and "tutorial". A "Label This Transfer" input field is visible at the bottom of the right window.

Research Computing Center

Workshop Series

Intro to the Research Computing Center
Birali Runesha
Crerar Library | Zar Room
Tuesday, October 8, 2013 | 1-3 p.m.

Intro to GPU Computing with CUDA
Robin Weiss
Crerar Library | Zar Room
Thursday, October 24, 2013 | 1-3 p.m.

Research Data Management Resources at UChicago
Nicholas Labello and Elisabeth Long
Crerar Library | Zar Room
Wednesday, November 13, 2013 | 1-3 p.m.

Programming with SWIFT Scripts
Michael Wilde
Crerar Library | Computer Classroom
Tuesday, December 3, 2013 | 1-4 p.m.

Big-Data Movement with Globus-Online
Steve Tuecke
Crerar Library | Kathleen A. Zar Room
Wednesday, January 15, 2014 | 1-3 p.m.

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