Using CRI's Computational Infrastructure for Bioinformatics Analysis

Instructors: Mike Jarsulic, Olumide Kehinde, Kyle Hernandez

CRI SYSTEMS RESOURCES OVERVIEW

HPC

Tarbell Cluster: High Performance Computation Cluster

for Data Analysis

Large Memory Server: (SAS/STATA/X-Windows)

Web Portals

Galaxy: Integrates with the HPC & provides a suite of tools for data analysis

•

REDCap: for building online surveys and databases.

Research data can be exported to statistical

packages (SPSS, SAS, Stata, R)

Data Storage

Home Data: 10GB Limit

Lab Shares: From 100GB

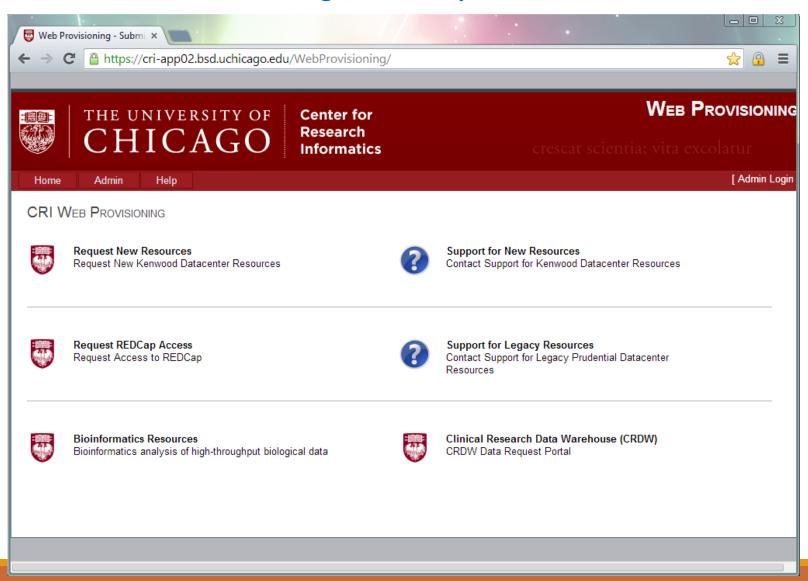
Fast Scratch Space: Shared 60TB

Virtualization

Virtual Machines: Hosted Windows & Linux Servers for building web applications and databases

HOW TO REQUEST CRI RESOURCES/SUPPORT

Visit: cri.uchicago.edu > Request Resources



ONLINE FORMS

Admin Help Home CRI WEB PROVISIONING - NEW SERVICE REQUEST Request IBI User Account for REDCap Request IBI User Account (REDCap) Request IBI Collaborator Account for REDCap Request Collaborator Account (REDCap, IBICluster, Storage) Request Lab Share Creation Request creation of a Lab Share to store research data in a highly secure clustered storage system with tape library backup. Request User Access to Lab Share Request user access to an existing Lab Share Request Access to HPC Resources Request Access to Galaxy, the High Performance Computing Cluster or Large Memory Server Request Software Installation on HPC or LMEM Request installation of software on the 1024 Core High Performance Cluster or the Large Memory Super Computer Request Virtual Machine Creation Request creation of a virtual machine instance Request Collaborator Account Creation Request creation of an account for a collaborator Request Firewall Access Request firewall access Request Collaborator Account Deactivation Request deactivation of an account for a collaborator





Revoke Resource Access

Request removal of user access to the HPC Biocluster, Large Memory Server, Galaxy, or Lab Share

REQUESTING SUPPORT

- 1) For BSD Account issues, please contact CBIS help@bsd.uchicago.edu or call 773-702-3456
- 2) Use appropriate form on the Request Site to create a support ticket;

Visit: cri.uchicago.edu, Request Resources Link

- -Trouble with installed software/ modules
- -Job submission issues
- -Questions
- 1) Call the CRI Help Desk to follow up on tickets 773-834-8475

DATA MANAGEMENT

-Home Directories: /home/<username>
Limited to 10GB. Single user access to data
Check your current working directory with command #pwd

-Lab Shares: /group/<share-name>
Group access to backed-up data
Changing directory: #cd /group/share-name

-Scratch Space: /scratch/<share-name>
60TB Space for staging input used in analysis jobs and for temp files from job execution.

Data in scratch is purged periodically.

-Remote Access to Data
Login to the Campus VPN (cvpn.uchicago.edu)

DATA TRANSFER TO/FROM CRI STORAGE

Accessing Share From a Windows PC:

Option 1:

Click the Start Button > Type "run" in the Search Box and press "Enter" > In the run window, type \\bulkstorage.uchicago.edu\<Lab-share-name>, press "Enter"

Login with your BSD Account, format "BSDAD\
bsd-username>"

Option 2:

From "My Computer" > "Map Network Drive"

Folder name: \\bulkstorage.uchicago.edu\<Lab-share-name>

*If you are not logged in to the BSDAD Domain, Check "Connect using different credentials"

Login with your BSDAD Account, format "BSDAD\<bsd-username>"

Accessing Share From a Mac:

From "Finder" > "Go"

Server Address: smb://bulkstorage.uchicago.edu/<Lab-share-name> Login with your BSDAD Account, format "BSDAD\<bsd-username>"

DATA TRANSFER TO/FROM CRI STORAGE (Cont'd)

Using Rsync, SCP or SFTP to transfer large data:

Host: cri-syncmon.cri.uchicago.edu

Login: BSD Account/Password

Path: /group/<share-name>

Port: 22

Examples of Free SFTP Graphical Clients:

WinSCP, CoreFTP (Windows Only) or

FileZilla, Cyberduck (Windows & Mac)

HOW TO USE ANALYSIS RESOURCES

High Performance Computing (HPC) Cluster:

Execute analysis in batch mode
Execute analysis in interactive mode
X Window System

Large Memory Server:

Execute SAS or Stata analysis X Window System

SPECIFICATIONS

Interactive Nodes:

2 Nodes

2 AMD Opteron 6274 processors (32 cores)

128 GB RAM

Scientific Linux 6 Update 4

Compute Nodes:

34 Nodes

4 AMD Opteron 6274 processors (64 cores)

256 GB RAM

Scientific Linux 6 Update 4

SPECIFICATIONS (Cont'd)

Large Compute Nodes:

2 Nodes

4 Intel Xeon E7-4860 processors (40 cores)

Hyper-threaded

1 TB RAM

Scientific Linux 6 Update 4

Large Memory Server:

8 Intel Xeon E7-8870 processors (80 cores)

Hyper-threaded

1 TB RAM

Redhat Linux 6 Update 4

PRODUCTION ENVIRONMENT

Complete:

TORQUE Resource Manager MOAB Scheduler Galaxy Scratch Space (60 TB)

Coming Soon:

Web services
Simplified Parametric Submission
Job portability
Trickled submission
More Scratch Space

SOFTWARE ENVIRONMENT

Compilers:

GNU Compilers Intel Compilers PGI Compilers

Language Support:

C/C++

FORTRAN

Perl

Python

R

BEST PRACTICES

- DO NOT Install Software into your home directory/lab share
- DO NOT Write your job scripts using MS Word
- DO NOT Copy/Paste from MS Word documents into your jobs
- DO Contact ME (<u>mjarsulic@bsd.uchicago.edu</u>)
 if you are planning on running a large analysis
- DO Understand that Java programs grow in memory
- DO NOT Run analysis on the interactive nodes