THE UNIVERSITY OF CHICAGO

BIOLOGICAL SCIENCES

Computing with the CRI: Storage, HPC, and Virtual Servers

November 2nd, 2017

Introduction

- IT Operations & Infrastructure team
- Three main service lines
  - Storage (Lab shares)
  - Virtual servers and system administration
  - HPC and other compute services (e.g. Stats, WinStats)

- Procedures following the BSD's Information Security Policies to be able to store and process ePHI (HIPAA) data for research use

- All primary resources are behind firewalls in 6045 Kenwood datacenter

- Data is backed up to tape in the 1155 (E 60th St.) datacenter

Resource Access

REDCap

HPC Cluster

Lab Shares

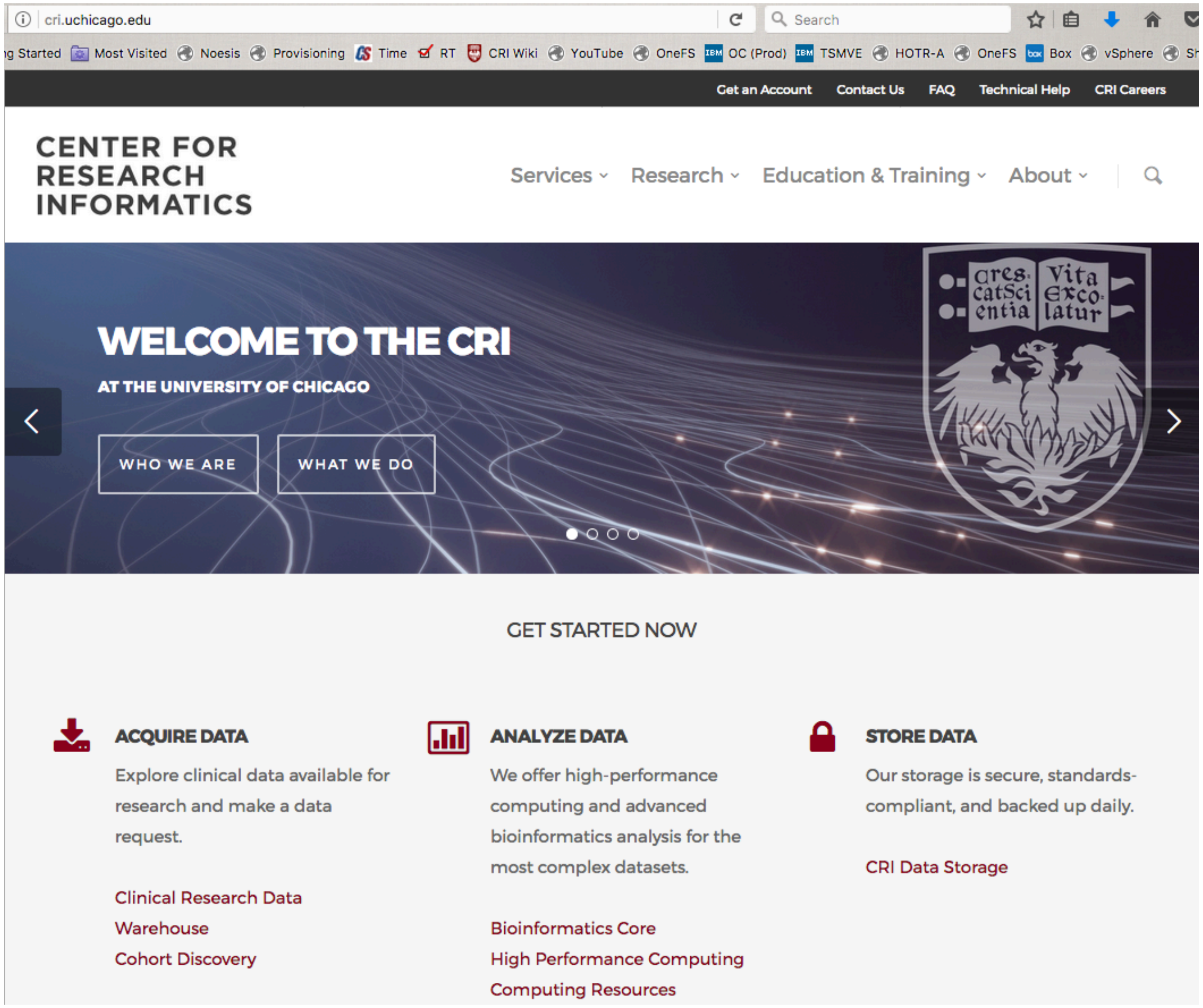
VMs

WinStats

In order to access CRI resources:

- You need to have an active BSD account
- You need to request access using our Web Provisioning Forms
- A ticket will be created and you will be sent access instructions

Requesting Access to CRI Resources



CENTER FOR RESEARCH INFORMATICS

WELCOME TO THE CRI

AT THE UNIVERSITY OF CHICAGO

GET STARTED NOW

ACQUIRE DATA

Explore clinical data available for research and make a data request.

Clinical Research Data Warehouse
Cohort Discovery

ANALYZE DATA

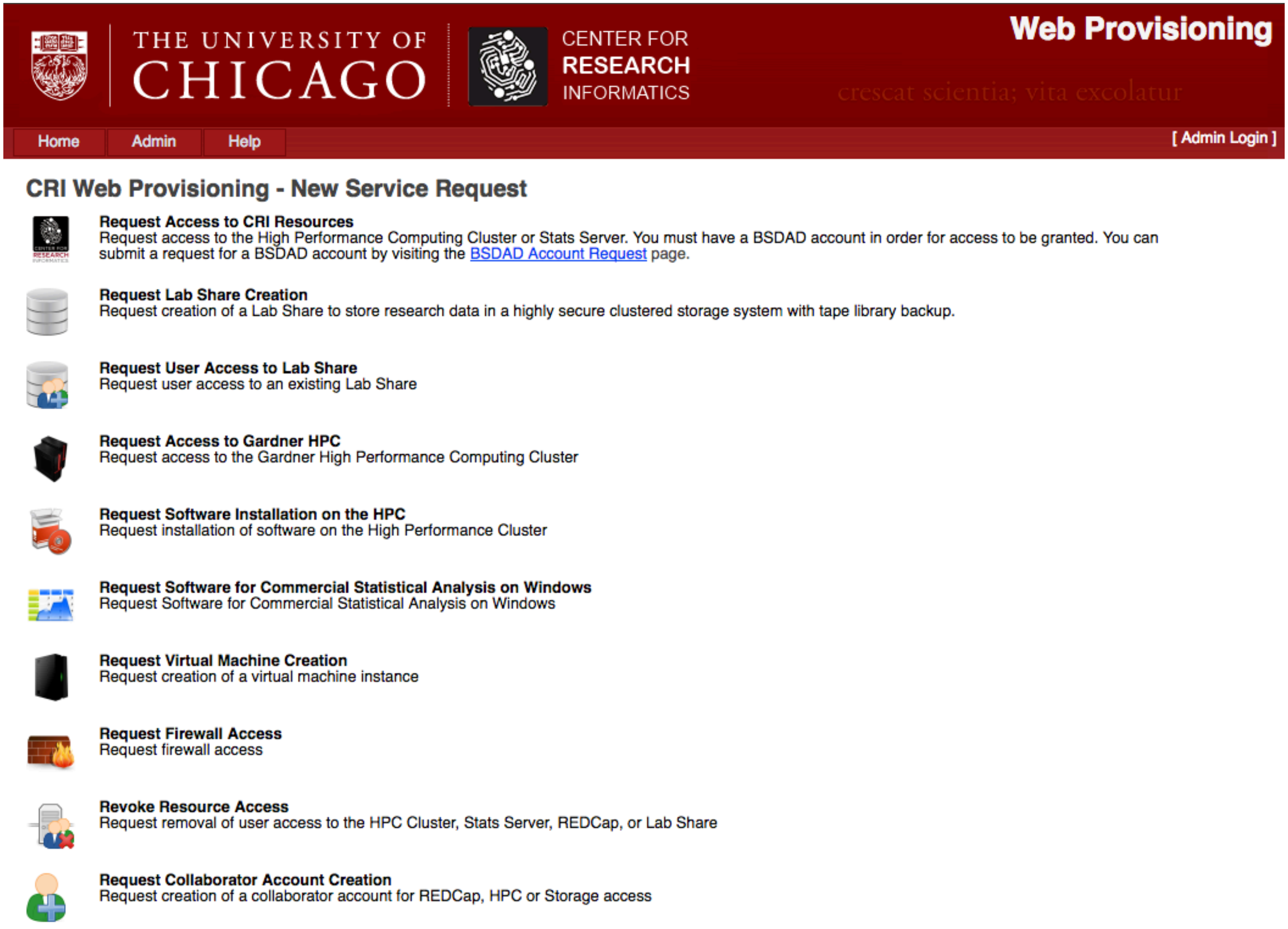
We offer high-performance computing and advanced bioinformatics analysis for the most complex datasets.

Bioinformatics Core
High Performance Computing
Computing Resources

STORE DATA

Our storage is secure, standards-compliant, and backed up daily.

CRI Data Storage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CENTER FOR RESEARCH INFORMATICS
Web Provisioning
crescat scientia; vita excolatur
Home
Admin
Help
[Admin Login]

CRI Web Provisioning - New Service Request

Request Access to CRI Resources
Request access to the High Performance Computing Cluster or Stats Server. You must have a BSDAD account in order for access to be granted. You can submit a request for a BSDAD account by visiting the BSDAD Account Request page.

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 Gardner HPC
Request access to the Gardner High Performance Computing Cluster

Request Software Installation on the HPC
Request installation of software on the High Performance Cluster

Request Software for Commercial Statistical Analysis on Windows
Request Software for Commercial Statistical Analysis on Windows

Request Virtual Machine Creation
Request creation of a virtual machine instance

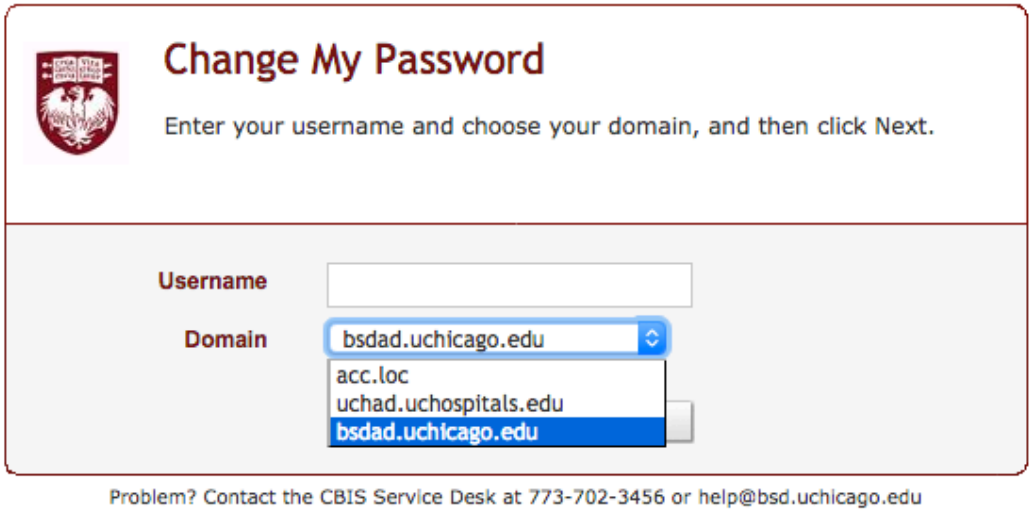
Request Firewall Access
Request firewall access

Revoke Resource Access
Request removal of user access to the HPC Cluster, Stats Server, REDCap, or Lab Share

Request Collaborator Account Creation
Request creation of a collaborator account for REDCap, HPC or Storage access

Changing your Temporary Password

https://mail.uchospitals.edu/changemypassword/



Change My Password

Enter your username and choose your domain, and then click Next.

Username

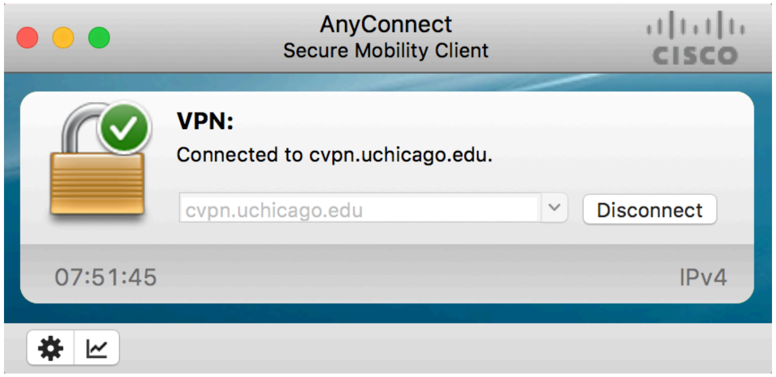
Domain bsdad.uchicago.edu

Problem? Contact the CBIS Service Desk at 773-702-3456 or help@bsd.uchicago.edu

- Make sure you change your temporary password quickly.
- Do not write down your password; you can write down a clue to help you remember the password instead and keep in a secure location.
- Do not share your password or account access with anyone else.
- When choosing a new password, you will be required to use at least one capital letter, one lowercase, one number, and one symbol.
- In addition to these requirements, it is good practice to refrain from using personal information like a birthday or name.

VPN Access

- Needed if you want to access CRI resources from outside campus
- Collaborator accounts are enabled for BSDVPN access
- Download and install the Cisco AnyConnect Secure Mobility Client
  - https://cvpn.uchicago.edu
  - https://bsdvpn.uchicago.edu
- You can setup two factor authentication for your account
  - https://2fa.bsd.uchicago.edu

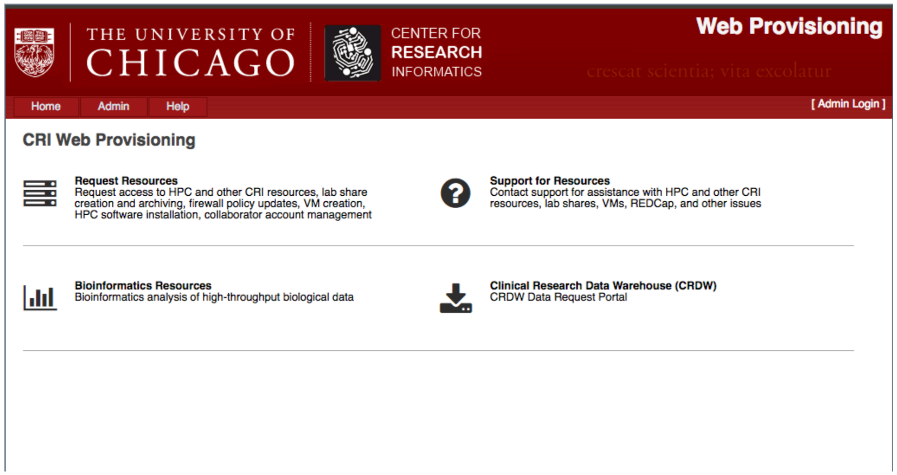


VPN:
Connected to cvpn.uchicago.edu.

Getting Help

- Contact the CRI using our Support Portal:
  - cri.uchicago.edu > Technical Help > Support for Resources

  - This will create a ticket in the appropriate queue for faster processing
  - Ensures we collect information necessary to start processing the ticket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CRI Web Provisioning

Request Resources
Request access to HPC and other CRI resources, lab share creation and archiving, firewall policy updates, VM creation, HPC software installation, collaborator account management

Support for Resources
Contact support for assistance with HPC and other CRI resources, lab shares, VMs, REDCap, and other issues

Bioinformatics Resources
Bioinformatics analysis of high-throughput biological data

Clinical Research Data Warehouse (CRDW)
CRDW Data Request Portal

Getting Help (CBIS)

If you have a non-CRI managed account, please contact the CBIS Service Desk at help@bsd.uchicago.edu or call 773-702-3456.

- *For BSD email issues*
- *BSD account password reset*

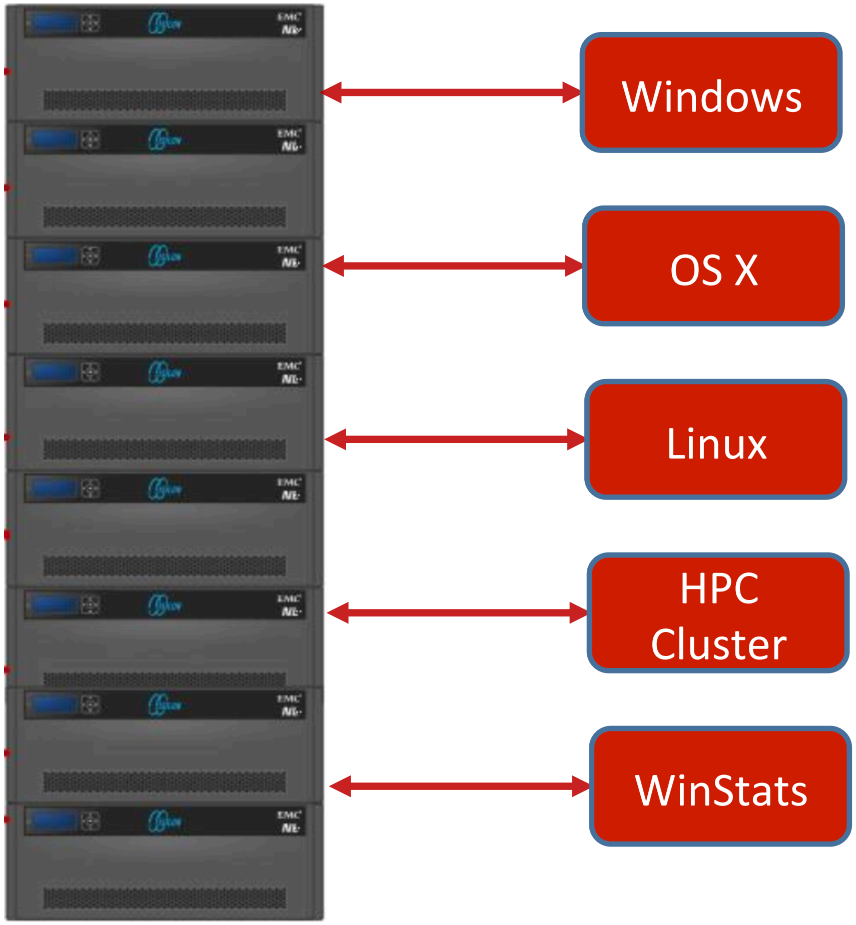
THE UNIVERSITY OF CHICAGO MEDICINE & BIOLOGICAL SCIENCES
Chicago Biomedicine Information Services

For immediate service, call us at **(773)702-3456** *anytime! We are here to assist you* **24/7!**

How can we help you?

CRI Data Storage Infrastructure

- 1.8PB Capacity
- High performance Nodes
- Archive Tier Nodes
- Backed up nightly
- Connected to the HPC cluster
- Easy and flexible share access
- Extended access controls
- Quota notifications



CRI Storage Shares

- Home Directories
- Lab Shares
- Departmental Shares
- Group Shares
- Scratch Space
  - Accessible only from the HPC Cluster
  - Temporary space for staging input for analysis jobs and temp files from job execution.

Storage Access Methods

- SMB/CIFS
- NFS (Servers Only)
- SCP/SFTP

  You can use graphical SFTP clients such as:
  - WinSCP, CoreFTP (Windows Only) or
  - FileZilla, Cyberduck (Windows & Mac)
- Rsync (use cri-syncmon.cri.uchicago.edu)

Virtual Server Environment

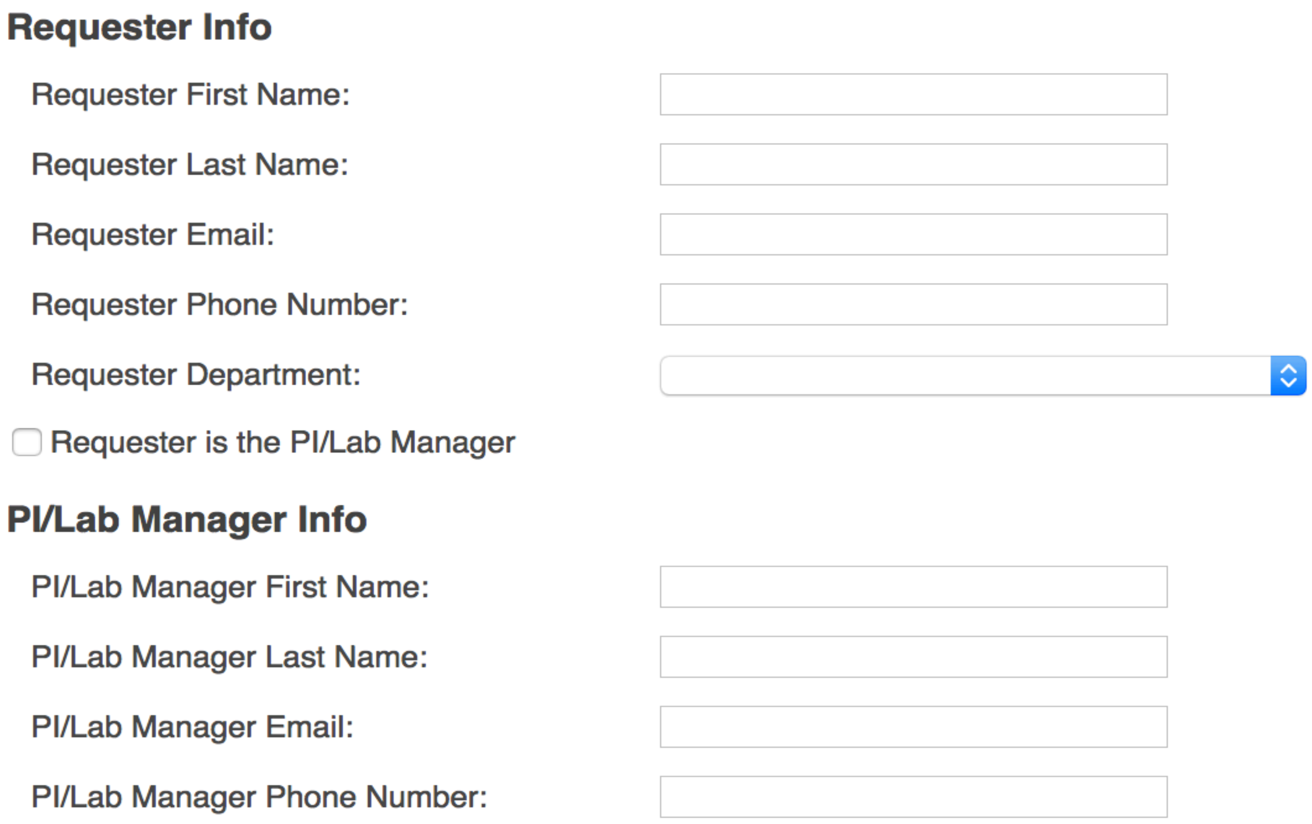
- Current Environment
  - 2 servers for management and CRI systems
    - Currently using 8% of CPU
    - Currently using 37% of memory
  - 6 servers for all other servers
    - Currently using 6% of CPU
    - Currently using 49% of memory
  - Each server:
    - 2 sockets – each socket with 20 cores
    - 512GB Memory
    - No hard drive – only dual SD card
  - Data Storage:
    - Compellent
    - SSD layer – All writes happen here
    - 7K Layer – Less used data moved here overnight

Request a Virtual Machine

- Fill out form
- We will read the answers and respond to the ticket with questions
- Our Process:
    1. Create VM
    2. Configure server with needed space
    3. Configure security settings
    4. Install main software
    5. Give over VM to customer to install/configure the rest of the server
    6. After configuration, we will run security scans
    7. Get firewall configured for final network
    8. Move server out of staging network
    9. Setup basic monitoring of system: disk, CPU, memory, known applications
    10. Setup backups – Nightly snapshot of VM and exports of known databases

Request Form

- People Information



Requester Info

Requester First Name:

Requester Last Name:

Requester Email:

Requester Phone Number:

Requester Department:

□ Requester is the PI/Lab Manager

PI/Lab Manager Info

PI/Lab Manager First Name:

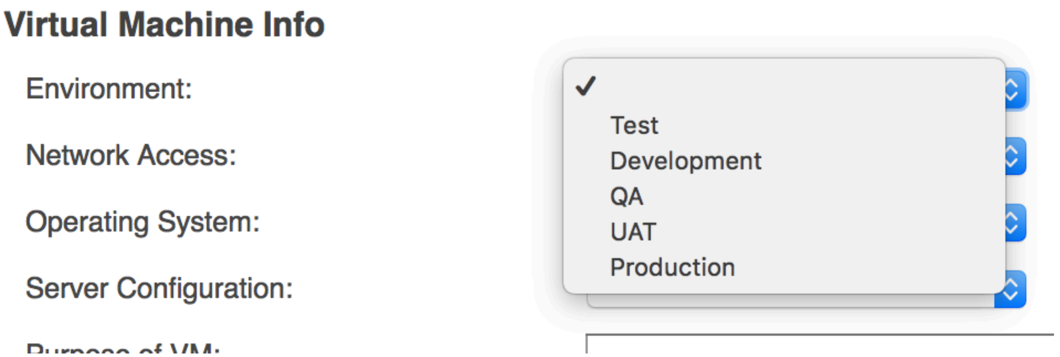
PI/Lab Manager Last Name:

PI/Lab Manager Email:

PI/Lab Manager Phone Number:

Request Form

- Environment



Virtual Machine Info

Environment:

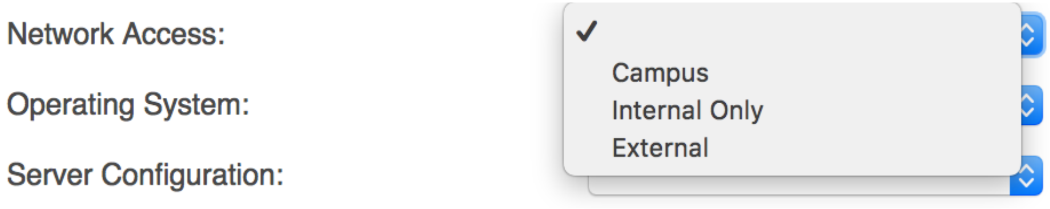
Network Access:

Operating System:

Server Configuration:

Purpose of VM:

- Network

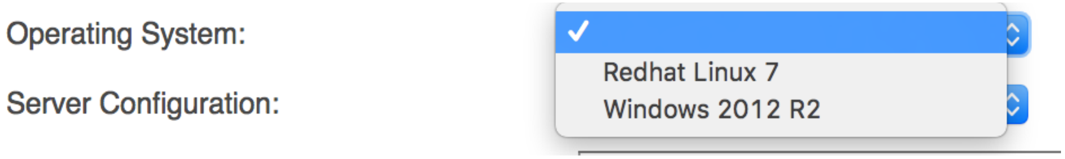


Network Access:

Operating System:

Server Configuration:

- OS

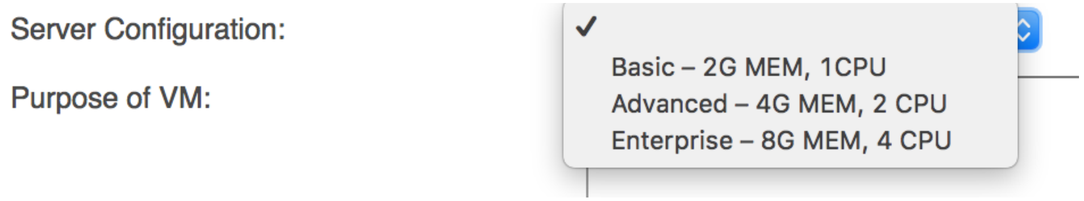


Operating System:

Server Configuration:

Request Form

- Size of server



Server Configuration:

Purpose of VM:

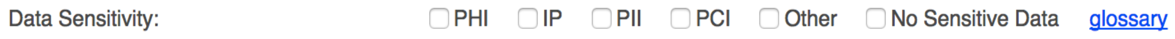
✓

Basic – 2G MEM, 1CPU
Advanced – 4G MEM, 2 CPU
Enterprise – 8G MEM, 4 CPU

- Purpose

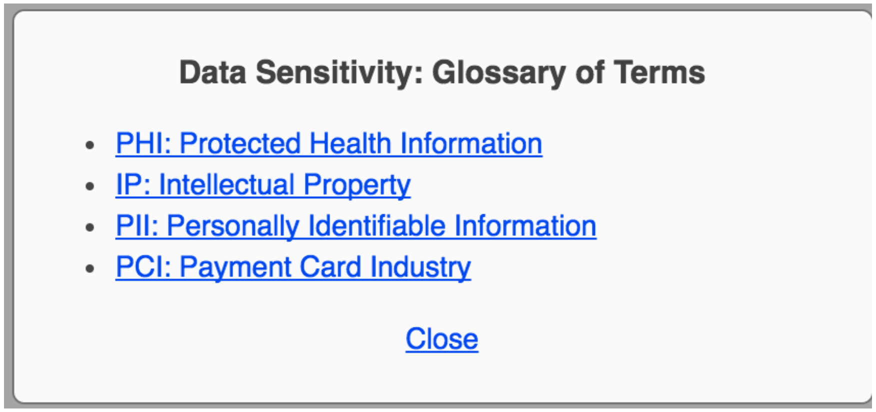
Purpose of VM:

- Data Sensitivity



Data Sensitivity: □ PHI □ IP □ PII □ PCI □ Other □ No Sensitive Data glossary

- Definition of Types of Data



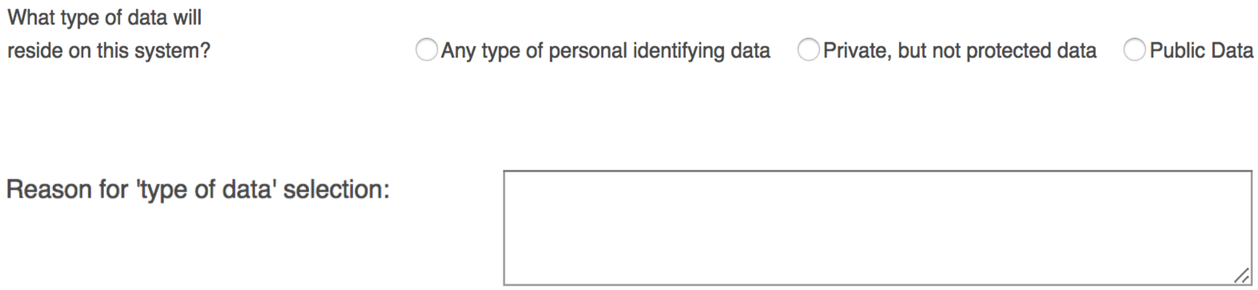
Data Sensitivity: Glossary of Terms

- PHI: Protected Health Information
- IP: Intellectual Property
- PII: Personally Identifiable Information
- PCI: Payment Card Industry

Close

Request Form

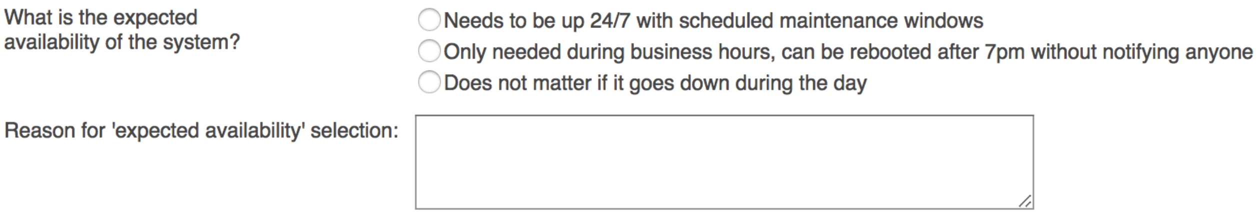
- **C** onfidentiality



What type of data will reside on this system? ○ Any type of personal identifying data ○ Private, but not protected data ○ Public Data

Reason for 'type of data' selection:

- **A** vailability

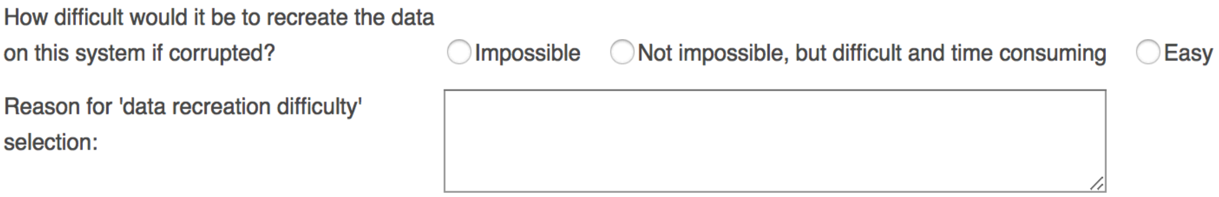


What is the expected availability of the system?

○ Needs to be up 24/7 with scheduled maintenance windows
○ Only needed during business hours, can be rebooted after 7pm without notifying anyone
○ Does not matter if it goes down during the day

Reason for 'expected availability' selection:

- **I** ntegrity

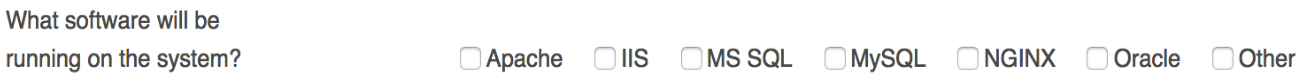


How difficult would it be to recreate the data on this system if corrupted? ○ Impossible ○ Not impossible, but difficult and time consuming ○ Easy

Reason for 'data recreation difficulty' selection:

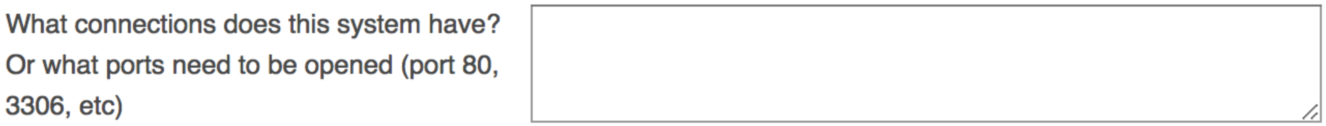
Request Form

- Other Software



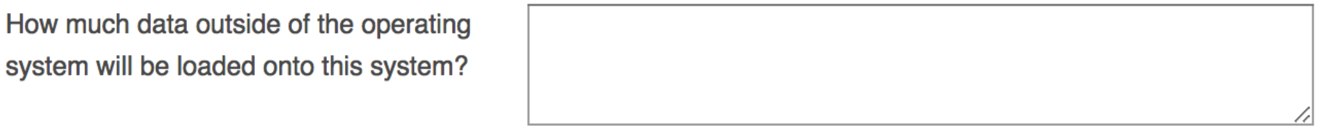
What software will be running on the system? □ Apache □ IIS □ MS SQL □ MySQL □ NGINX □ Oracle □ Other

- Firewall Rules



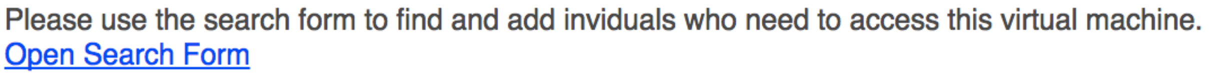
What connections does this system have? Or what ports need to be opened (port 80, 3306, etc)

- Disk Space Needs



How much data outside of the operating system will be loaded onto this system?

- Other Users



Please use the search form to find and add inviduals who need to access this virtual machine.
Open Search Form

Other Software used by CRI

- SaltStack – Configuration Management
- IPA Server – Redhat's Identity Policy Audit Linux Domain
  - Trust with BSDAD to provide BSDAD Accounts to Linux servers and bulkstorage
- Device 42 – Inventory System with API
- Nagios – Monitoring/Alerting - Can have custom setup
- RequestTracker (RT) – Ticketing System from Best Practical – Can provide ticket queues for other groups
- GitLab – https://git.cri.uchicago.edu - Can provide git, and other development tools (code review, wiki, issue tracking), to other groups

Commercial Software - Winstats

- Specifications
  - 2 CPUs: 2.4GHz Intel Xeon E7-8870
  - 10 cores per CPU
  - 512 GB of RAM
  - 1.18 TB of dedicated SSD storage

Commercial Software – Stats (Linux)

- Specifications
  - 2 servers
    - 2 Intel Xeon E5-2698 v3 CPUs
    - 2.3 GHz
    - 16 ops/cycle
    - 16 cores per CPU
    - 768 GB RAM per server

Commercial Software - Software

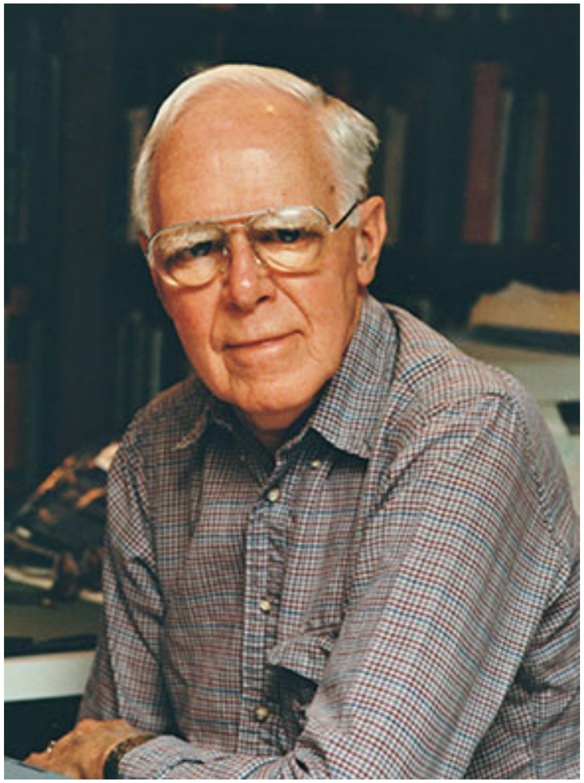
- SPSS (Winstats)
- Stata
- SAS
- R (not really commercial but...)
- Matlab (Linux)
- Mathematica

High Performance Computing - Staff

- Mike Jarsulic (Sr. HPC Administrator)
  - Lived in Pittsburgh for about 32 years
  - Attended the University of Pittsburgh (at Johnstown)
  - Bettis Atomic Power Laboratory (2004-2012)
    - Scientific Programmer (Thermal/Hydraulic Design)
    - Thermal/Hydraulic Analyst - USS Gerald R. Ford
    - High Performance Computing
  - University of Chicago (2012-present)
  - Dislikes Mimes

- Qiannan Miao (Student HPC Administrator)
  - Current UChicago MPCS Student
  - Lots of coursework focusing on machine learning
  - Graduates 12/2017
  - Dislikes Mimes

High Performance Computing – Martin Gardner



- Graduate of the University of Chicago (1936)
- Yeoman on the USS Pope during WWII
- Amateur Magician
- Mathematical Games
- Skepticism
- Literature
- Art

High Performance Computing – What is a HPC Cluster?

- Storage
- Login Nodes
- Scheduler Node
- Compute Nodes
- GPUs
- Xeon Phi

High Performance Computing – Storage

- Isilon Storage Cluster
  - Home Directories (/home/<userid>)
  - Lab Shares (/group/<labid>)
  - Applications (/apps/software)
  - Total Size: 1.8 PB
  - Bandwidth: 1 Gb/s
  - Permanent, Quota'd, Backed Up
  - Available everywhere

- Scratch Space
  - Total Size: 175 TB
  - Bandwidth: 56 Gb/s
  - Purged, Private, Not Quota'd, Not Backed Up
  - Limited availability

High Performance Computing – Login Nodes

- Purpose
  - User interface for the HPC cluster
  - Composing editing jobs
  - Submitting jobs
  - Tracking/Managing jobs
  - Writing source code
  - Compiling source code
- DO NOT RUN ANALYSIS ON THE LOGIN NODES!!!

High Performance Computing – Scheduler Node

- Purpose
  - Keeps track of which resources are available on each compute node of the cluster
  - Schedules jobs based on available resources
  - Maintains historical metrics on jobs

High Performance Computing – Compute Nodes

- Specifications
  - Nodes:
    - 88 standard
    - 28 mid-tier
    - 4 high-tier
  - Processors (2 per node):
    - Intel Xeon E5-2683 v3
    - 14 cores
    - 2.0 GHz
    - 16 ops/cycle
  - Memory
    - Standard: 4 GB/core
    - Mid-tier: 16 GB/core
    - High-tier: 45 GB/core

High Performance Computing – Accelerator Nodes

- GPUs
  - 5 Nodes
  - 1 NVidia Tesla K80 per node
    - Contains 2 NVidia Tesla GK210 GPUs
    - 2496 CUDA cores
    - 24 GB memory
- Xeon Phi
  - 1 node
  - 2 Intel Xeon Phi P5110 coprocessors
    - 60 Cores per coprocessor
    - 8 GB RAM

High Performance Computing – Software

- Compilers
  - GNU
  - Intel
  - PGI
  - Java JDK

- Scripting Languages
  - Perl
  - Python
  - R

- Software Environment
  - LMod

High Performance Computing – Obtaining an Account

- Prerequisites: BSD Account
- Sign up for and account
  - http://cri.uchicago.edu
  - Experience Level
  - Software Requests
  - Email Address for Job Output
  - Emergency Phone Number
- Collaborator Accounts

High Performance Computing - Support

- How to get help?
  - Email: hpc@rt.cri.uchicago.edu
  - Support form on the CRI Website
  - Documentation: Coming Soon
  - Ask a friend
  - Office Hours (Tuesday/Thursday)
  - Bioinformatics Core
  - CRI Seminar Series

- How not to get help?
  - Calling me (unless it's an emergency)
  - Email me directly

Future: New Storage System

- Problems with Isilon Cluster
  - Enterprise solution; not designed for research environments
  - High expansion cost
  - High maintenance cost
  - Ethernet requirement
  - Not POSIX-compliant (parallel file access)
  - Low read iops

- Problems with Scratch Storage
  - Glusterfs
  - Poor performance on small files
  - Poor metadata performance
  - Stability

Future: New Storage System

- Goals
  - Combine scratch and permanent storage into one system
  - Lower costs
  - Increase performance
  - Utilize Infiniband network
  - POSIX-compliant
  - Maintain stability and security of the Isilon

- Options
  - Lustre (Intel)
  - GPFS (IBM)

Future: New Storage System – Metadata Ops

Values are in operations per second

All operations are file operations

Operation	Isilon	Scratch	Lustre	GPFS
Creation	3188	884	22025	30665
Stat	80940	5684	96346	39247
Read	6474	6176	50557	88245
Removal	210	209	16521	11736

Future: New Storage System – Multiple Files

All Values in MB/s

8 processes; 1 file per process

API	Operation	Isilon	Scratch	Lustre	GPFS
POSIX	Read	110	347	31949	22430
POSIX	Write	108	106	3459	11292
MPI-IO	Read	9	370	N/A	22212
MPI-IO	Write	10	138	N/A	7522

Future: New Storage System – Single File

All Values in MB/s

8 processes; single shared file

API	Operation	Isilon	Scratch	Lustre	GPFS
POSIX	Read	109	119	24980	18447
POSIX	Write	94	112	4503	9176
MPI-IO	Read	5	110	N/A	17439
MPI-IO	Write	3	65	N/A	8467

Future: Current Projects

- Globus Online for data transfers (being set up now)
- Deep Learning / Machine Learning (exploring needs and options)
- Container-based computing for both HPC and applications (exploring needs, options w/ tests)
- Visualization (exploring and testing)

Questions?