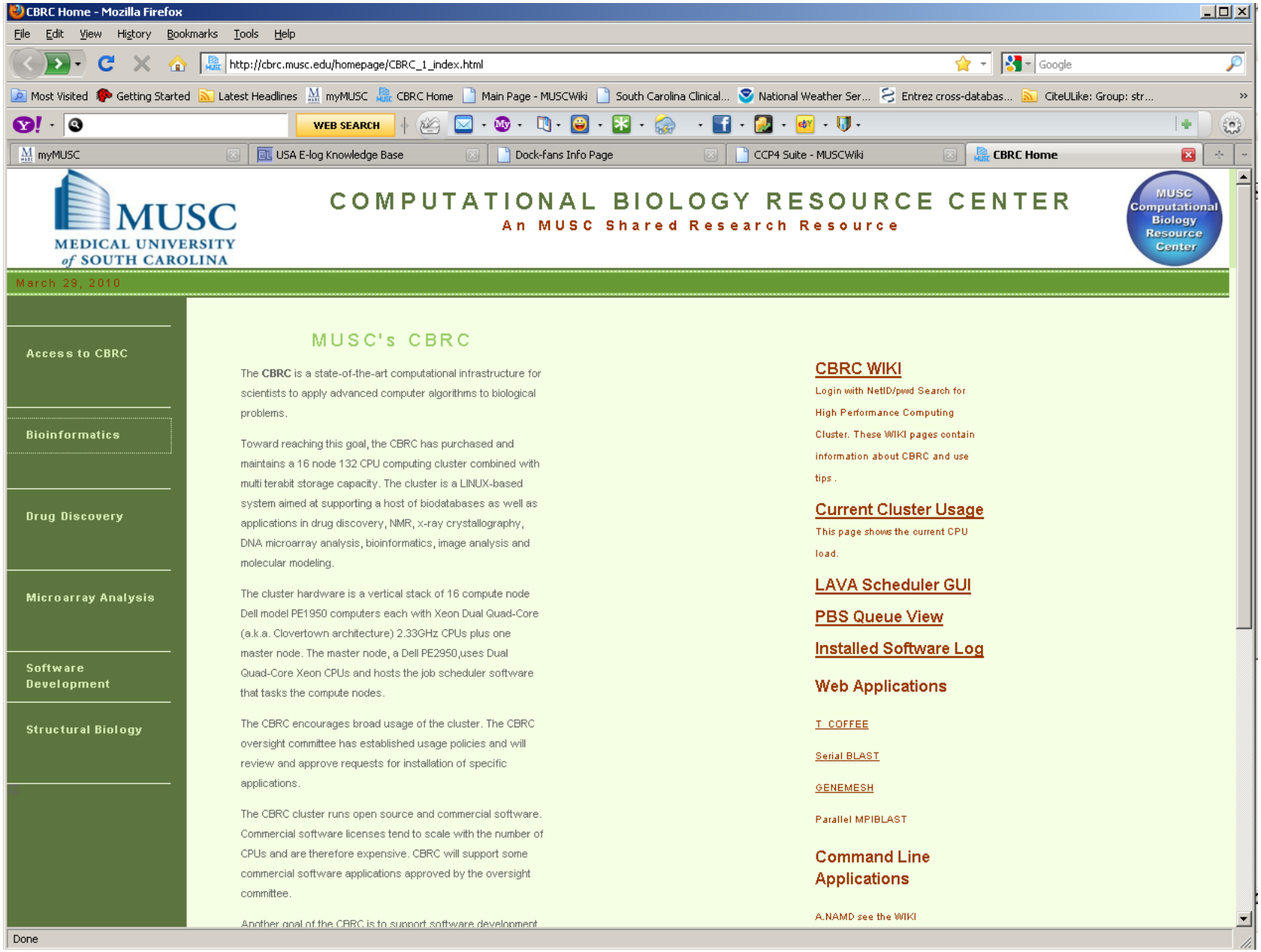
CBRC Home - Mozilla Firefox
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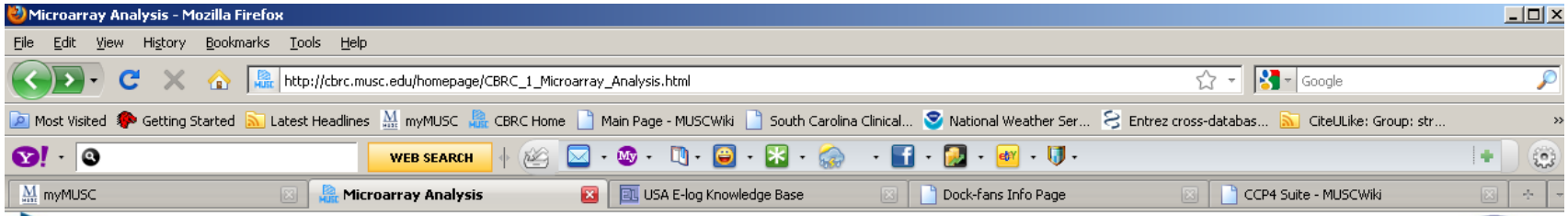
MUSC
MEDICAL UNIVERSITY of SOUTH CAROLINA
COMPUTATIONAL BIOLOGY RESOURCE CENTER
An MUSC Shared Research Resource
MUSC Computational Biology Resource Center
March 29, 2010
Access to CBRC
Bioinformatics
Drug Discovery
Microarray Analysis
Software Development
Structural Biology
MUSC's CBRC
The CBRC is a state-of-the-art computational infrastructure for scientists to apply advanced computer algorithms to biological problems.
Toward reaching this goal, the CBRC has purchased and maintains a 16 node 132 CPU computing cluster combined with multi terabit storage capacity. The cluster is a LINUX-based system aimed at supporting a host of biodatabases as well as applications in drug discovery, NMR, x-ray crystallography, DNA microarray analysis, bioinformatics, image analysis and molecular modeling.
The cluster hardware is a vertical stack of 16 compute node Dell model PE1950 computers each with Xeon Dual Quad-Core (a.k.a. Clovertown architecture) 2.33GHz CPUs plus one master node. The master node, a Dell PE2950,uses Dual Quad-Core Xeon CPUs and hosts the job scheduler software that tasks the compute nodes.
The CBRC encourages broad usage of the cluster. The CBRC oversight committee has established usage policies and will review and approve requests for installation of specific applications.
The CBRC cluster runs open source and commercial software. Commercial software licenses tend to scale with the number of CPUs and are therefore expensive. CBRC will support some commercial software applications approved by the oversight committee.
Another goal of the CBRC is to support software development
CBRC WIKI
Login with NetID/pwd Search for High Performance Computing Cluster. These WIKI pages contain information about CBRC and use tips .
Current Cluster Usage
This page shows the current CPU load.
LAVA Scheduler GUI
PBS Queue View
Installed Software Log
Web Applications
T_COFFEE
Serial BLAST
GENEMESH
Parallel MPIBLAST
Command Line Applications
A.NAMD see the WIKI
Done



MUSC
MEDICAL UNIVERSITY of SOUTH CAROLINA

COMPUTATIONAL BIOLOGY RESOURCE CENTER

An MUSC Shared Research Resource

MUSC Computational Biology Resource Center

Microarray Analysis

The CBRC cluster computer runs a number of DNA microarray analysis applications including:

GeneMesh:

GeneMesh is a web-based program designed to relate genes in a query set to descriptors making up the hierarchical structure of the U.S. National Library of Medicine's (NLM) controlled vocabulary thesaurus, Medical Subject Headings (MeSH). GeneMesh accomplishes this by referring to the GeneMesh Database, a unique database of genes associated with MeSH terms.

Other DNA microarray analysis tools developed at MUSC include the following:

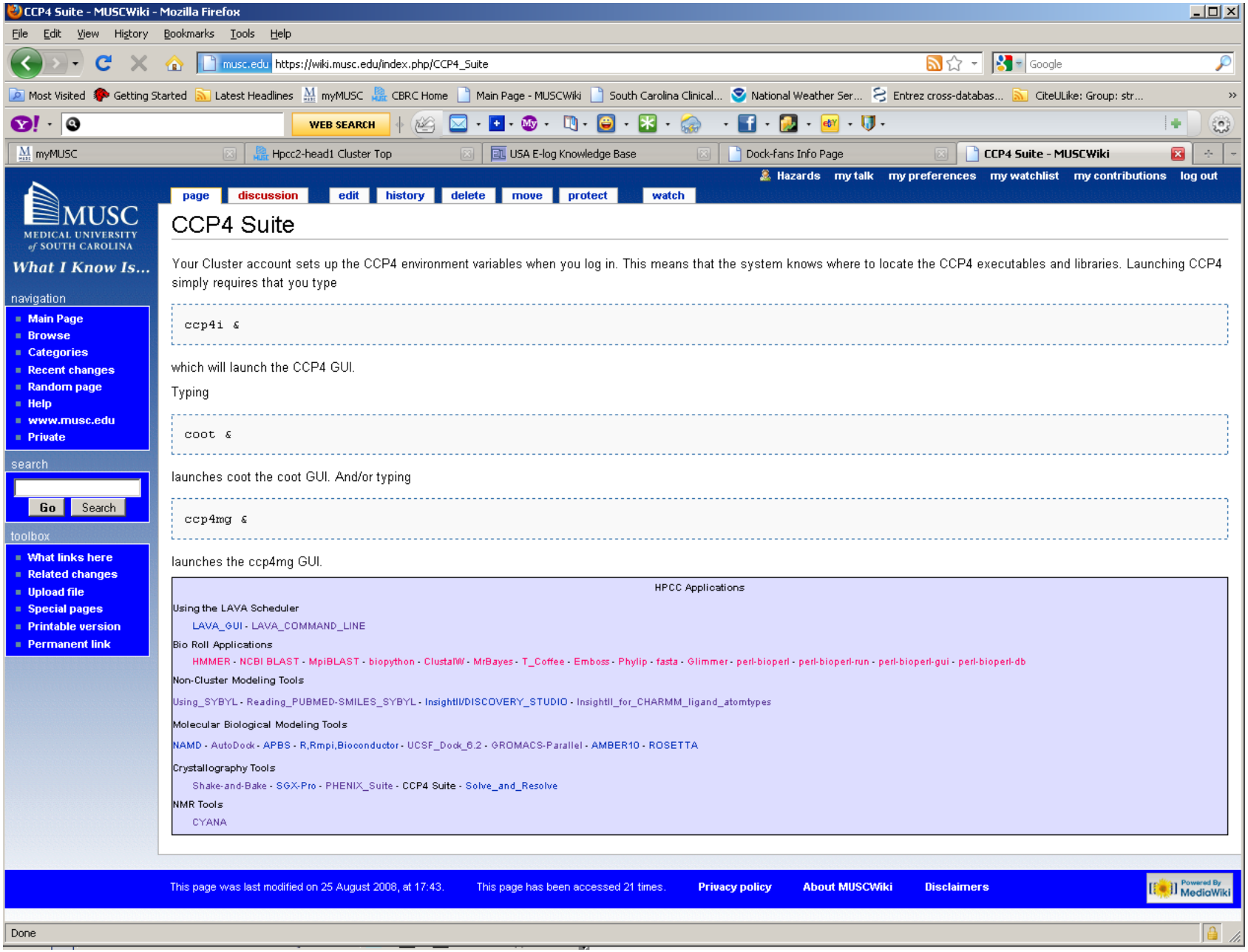
ArrayQuest:

ArrayQuest is a web-based program for the analysis of DNA microarray data. ArrayQuest is designed to apply various types of analysis scripts including those written in R to microarray data stored in the MUSC DNA Microarray Database, the Gene Expression Omnibus (GEO) or data uploaded to the ArrayQuest center-point web server in a password-protected area. ArrayQuest has been described in an article published in the journal BMC Bioinformatics (Argraves et al., 2005)

MUSC DNA Microarray Database:

The MUSC DNA Microarray Database is a web-based relational database system for archiving DNA microarray hybridization data (raw and normalized) derived experimentation performed through the MUSC DNA Microarray Facility. The database was designed using microArrayDB and uses MySQL server to store microarray hybridization data and metadata such as project information (i.e., investigator contact information, experimental design), cRNA target information and process controlling information. The MUSC DNA Microarray Database has been described in an article published in the journal Bioinformatics (Argraves et al., 2003).


Structural Biology at MUSC
Center for Structural Biology | X-ray Crystallography | NMR | Protein Production Lab | Molecular Modeling
Center for Structural Biology
X-ray Crystallography
NMR
Protein Production Lab
Molecular Modeling
Welcome to Structural Biology at MUSC
Click here to email Webmaster
173 Ashley Avenue, BSB501 PO Box 250509 Charleston, SC 29425
Tel (843) 792-4321 Fax (843) 792-4322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Hazards my talk my preferences my watchlist my contributions log out
page discussion edit history delete move protect watch
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What I Know Is...
navigation
Main Page
Browse
Categories
Recent changes
Random page
Help
www.musc.edu
Private
search
Go Search
toolbox
What links here
Related changes
Upload file
Special pages
Printable version
Permanent link
CCP4 Suite
Your Cluster account sets up the CCP4 environment variables when you log in. This means that the system knows where to locate the CCP4 executables and libraries. Launching CCP4 simply requires that you type
ccp4i &
which will launch the CCP4 GUI.
Typing
coot &
launches coot the coot GUI. And/or typing
ccp4mg &
launches the ccp4mg GUI.
HPCC Applications
Using the LAVA Scheduler
LAVA_GUI - LAVA_COMMAND_LINE
Bio Roll Applications
HMMER - NCBI BLAST - MpiBLAST - biopython - ClustalW - MrBayes - T_Coffee - Emboss - Phylip - fasta - Glimmer - perl-bioperl - perl-bioperl-run - perl-bioperl-gui - perl-bioperl-db
Non-Cluster Modeling Tools
Using_SYBYL - Reading_PUBMED-SMILES_SYBYL - InsightII/DISCOVERY_STUDIO - InsightII_for_CHARMM_ligand_atomtypes
Molecular Biological Modeling Tools
NAMD - AutoDock - APBS - R,Rmpi,Bioconductor - UCSF_Dock_6.2 - GROMACS-Parallel - AMBER10 - ROSETTA
Crystallography Tools
Shake-and-Bake - SGX-Pro - PHENIX_Suite - CCP4 Suite - Solve_and_Resolve
NMR Tools
CYANA
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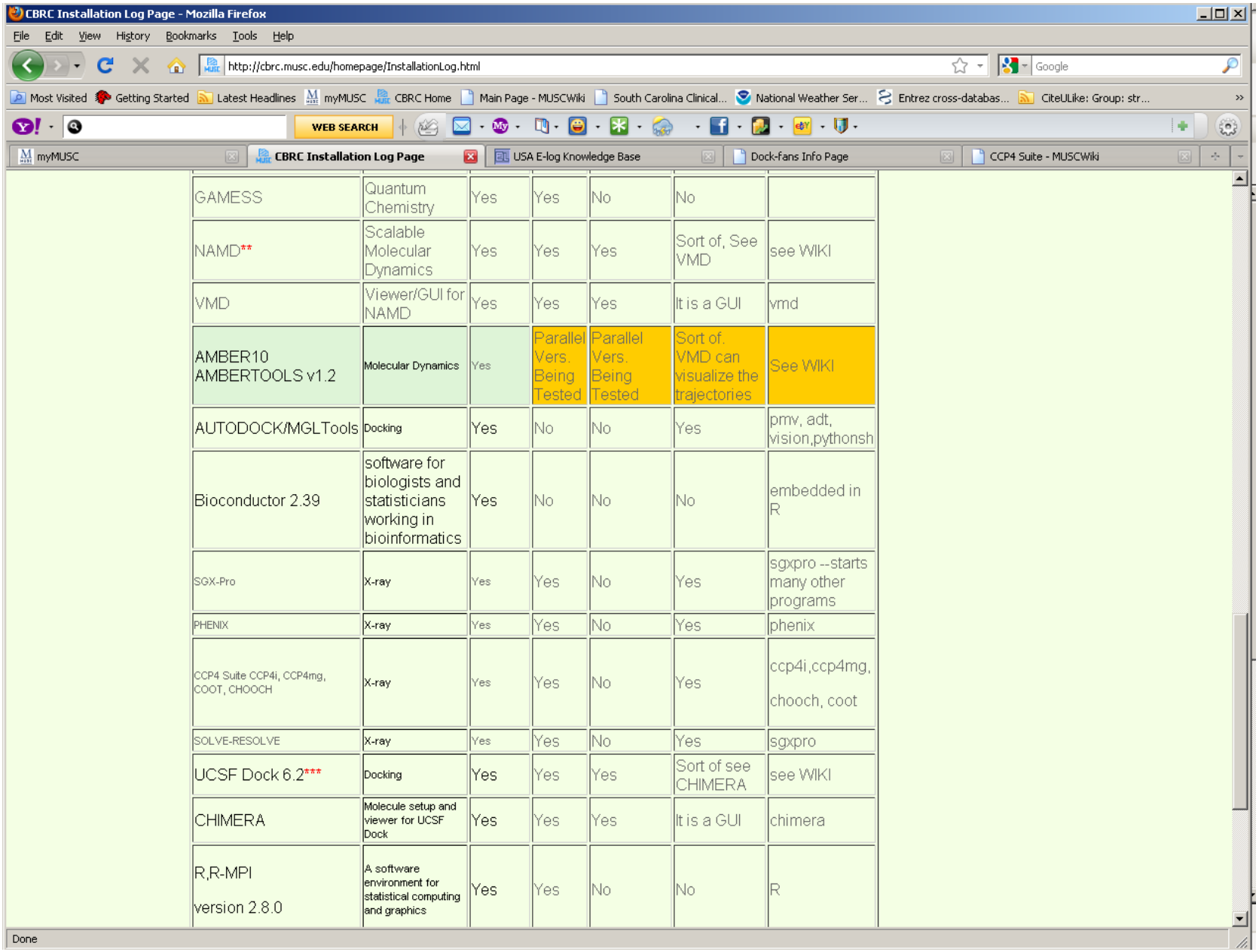
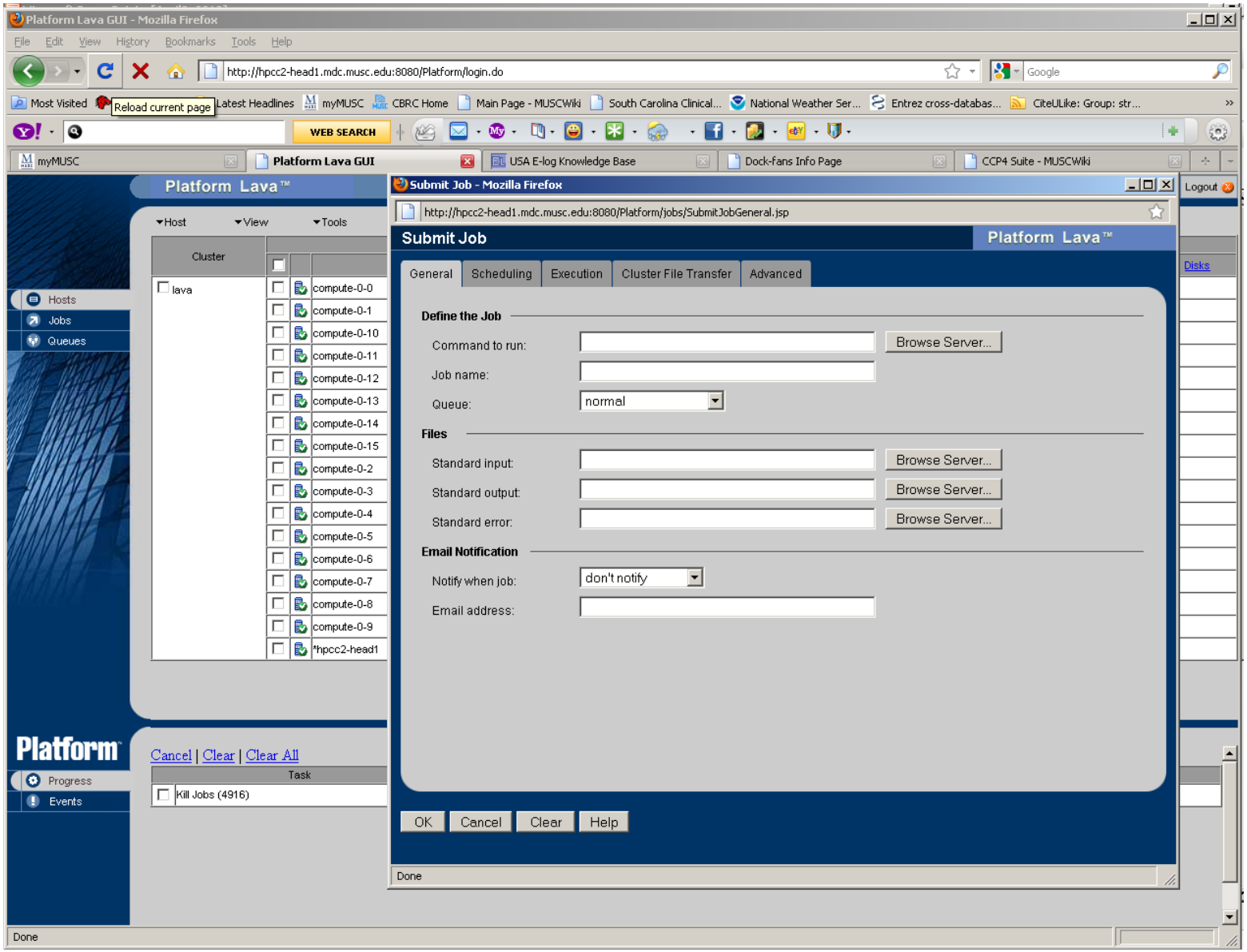


GAMESS	Quantum Chemistry	Yes	Yes	No	No	
NAMD**	Scalable Molecular Dynamics	Yes	Yes	Yes	Sort of, See VMD	see WIKI
VMD	Viewer/GUI for NAMD	Yes	Yes	Yes	It is a GUI	vmd
AMBER10 AMBERTOOLS v1.2	Molecular Dynamics	Yes	Parallel Vers. Being Tested	Parallel Vers. Being Tested	Sort of. VMD can visualize the trajectories	See WIKI
AUTODOCK/MGLTools	Docking	Yes	No	No	Yes	pmv, adt, vision,pythonsh
Bioconductor 2.39	software for biologists and statisticians working in bioinformatics	Yes	No	No	No	embedded in R
SGX-Pro	X-ray	Yes	Yes	No	Yes	sgxpro --starts many other programs
PHENIX	X-ray	Yes	Yes	No	Yes	phenix
CCP4 Suite CCP4i, CCP4mg, COOT, CHOOCH	X-ray	Yes	Yes	No	Yes	ccp4i,ccp4mg, chooch, coot
SOLVE-RESOLVE	X-ray	Yes	Yes	No	Yes	sgxpro
UCSF Dock 6.2***	Docking	Yes	Yes	Yes	Sort of see CHIMERA	see WIKI
CHIMERA	Molecule setup and viewer for UCSF Dock	Yes	Yes	Yes	It is a GUI	chimera
R,R-MPI version 2.8.0	A software environment for statistical computing and graphics	Yes	Yes	No	No	R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WEB SEARCH
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Platform Lava GUI
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CCP4 Suite - MUSCWiki
Platform Lava™
Host View Tools
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Hosts
Jobs
Queues
Platform
Progress
Events
Cancel | Clear | Clear All
Task
Kill Jobs (4916)
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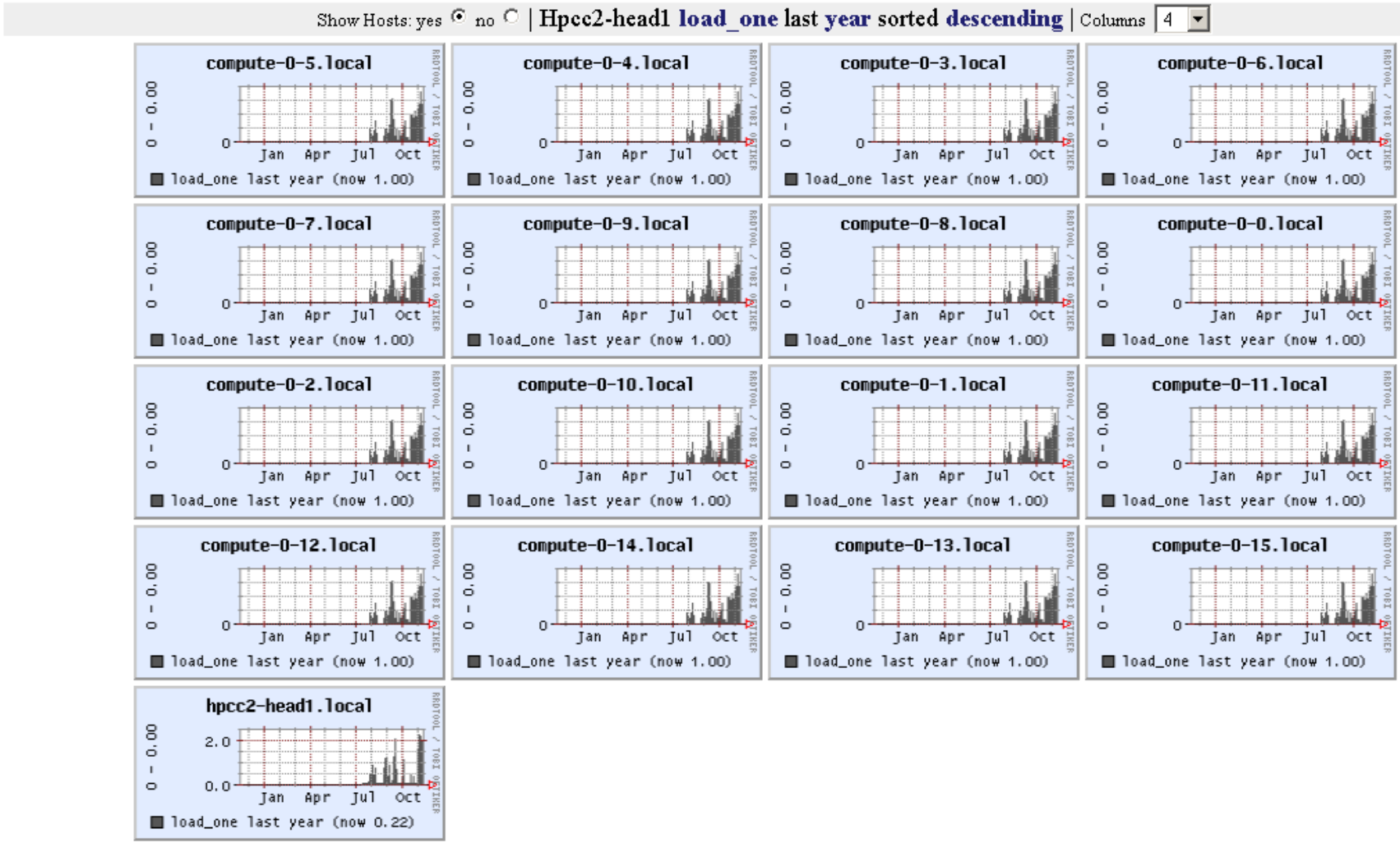
Submit Job
Platform Lava™
General Scheduling Execution Cluster File Transfer Advanced
Define the Job
Command to run:
Browse Server...
Job name:
Queue:
normal
Files
Standard input:
Standard output:
Standard error:
Email Notification
Notify when job:
don't notify
Email address:
OK Cancel Clear Help
Done
Disks



(Nodes colored by 1-minute load) | Legend

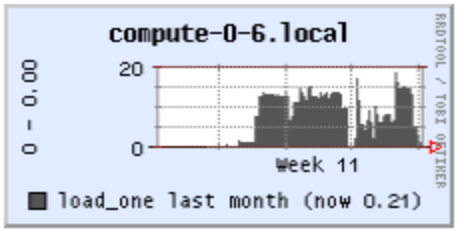
November 2009 usage trend by month

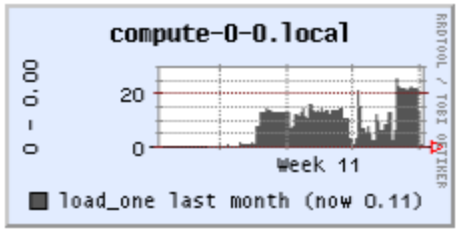
Tue Mar 16 16:39:45 EDT 2010

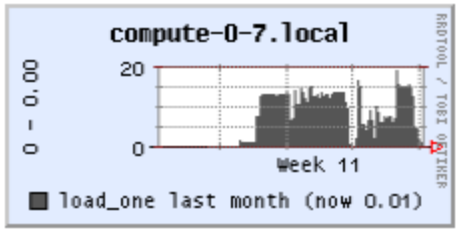
User	#jobs	Task description
1	8	bayesian evolution
2	75	cheminformatics
3	52	R bioinformatics
4	15	NMR analysis
5	1	User bioinformatics
6	46	User bioinformatics

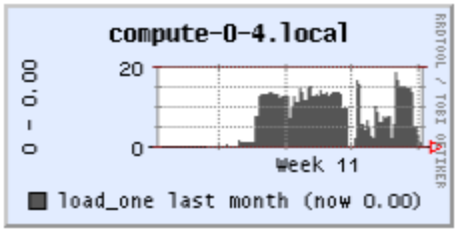
Tue Mar 16 16:39:45 EDT 2010

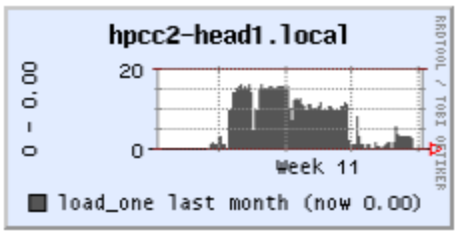
Show Hosts: yes ◉ no ○ | Hpcc2-head1 **load_one** last **month** sorted **descending** | Columns 4

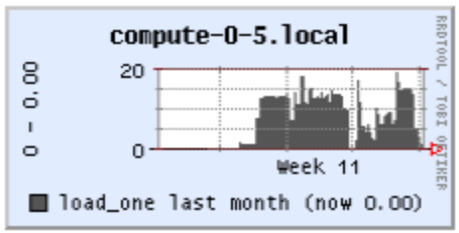


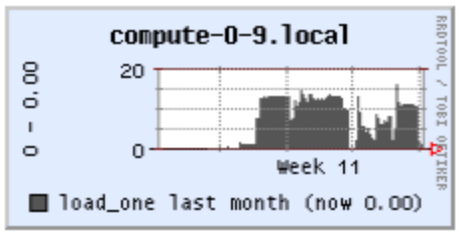


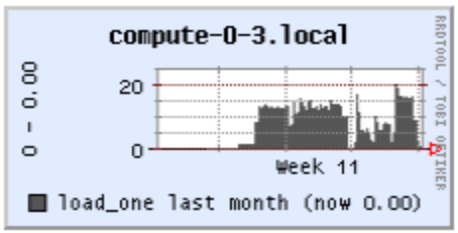


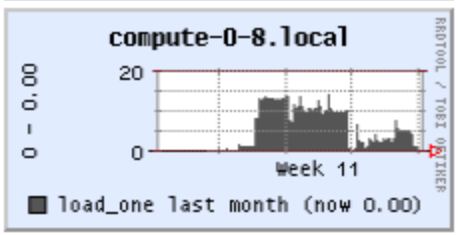


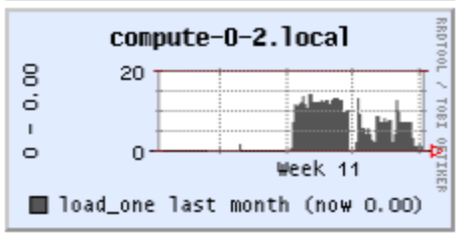


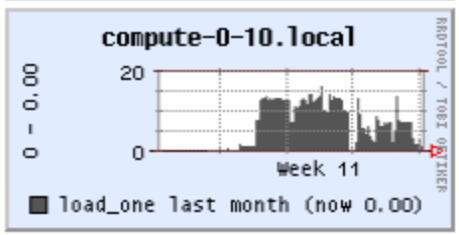


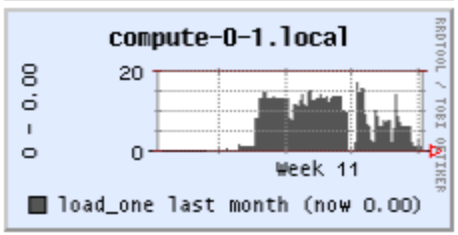


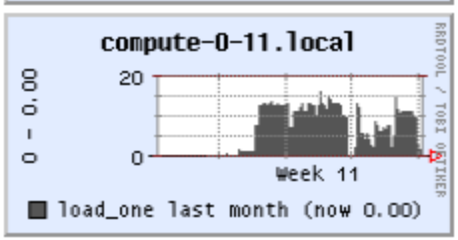


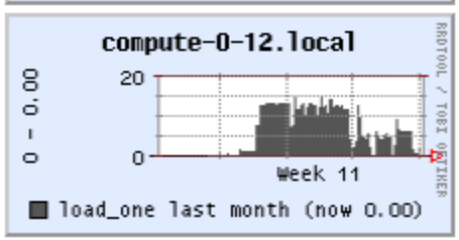


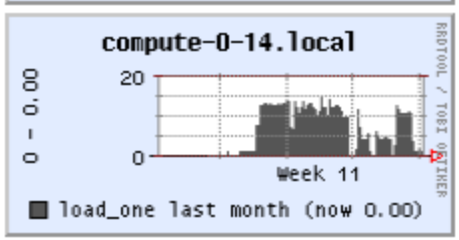


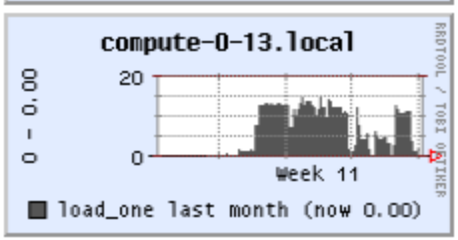


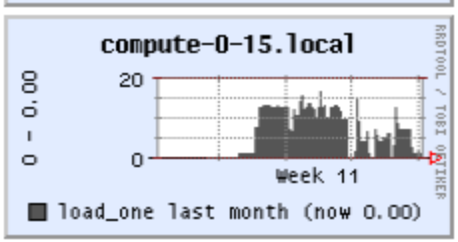


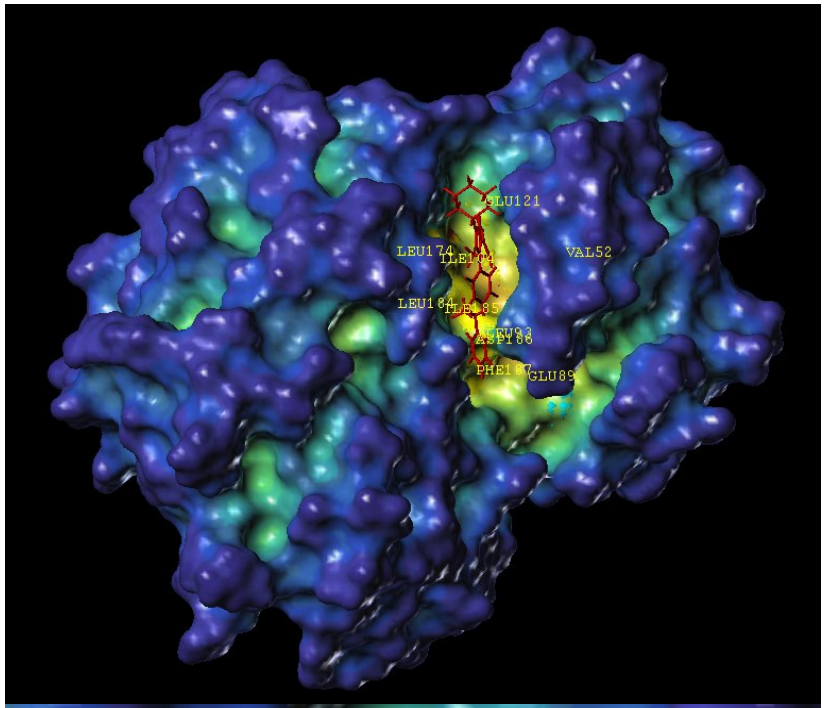


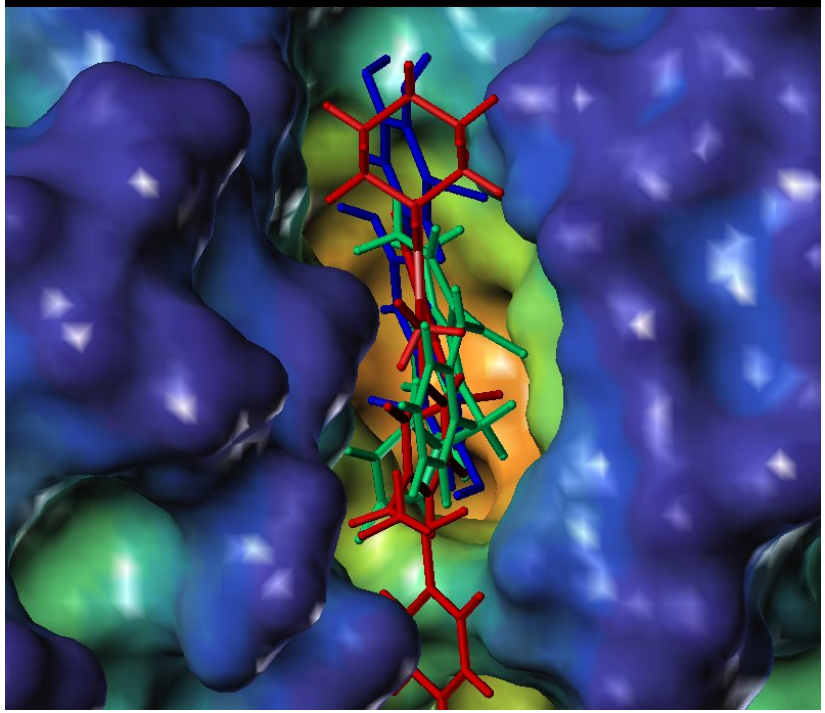












In silico docking for Drug Discovery

Databases:

Several million compounds from 14 publically available/locally derived databases ZINC, NCI, Chembridge.

Software:

AUTODOCK

UCSF DOCK 6.3

User issues
Project proposals
Storage Space
CPU use
Software
Site Design
In house growth
EPSCOR usage growth

Getting an Account

- HPC Allocation Request Form

The Palmetto Cluster

- Introduction
- Conventions, plugins
- The palmetto architecture
- Getting an account
- Accessing the machine
- Finding software and documentation
- Compiling your code
- Compiling your parallel code
- Running your job
- Debugging your code
- Using application software and libraries
- Using storage

High Performance Computing

High-performance computing (HPC) refers to large jobs with more or less tightly coupled subprocesses that can run in parallel and communicate with each other by sharing memory locations or by passing messages across a specialized network. *Computing clusters* are collections of processors (often mounted in racks) coupled together by a shared-memory buss or a high-speed network.

Clemson is in the process of developing several cluster resources:

- CCIT has pooled resources with several researchers on campus to purchase a large HPC cluster. This is known as **palmetto** or "The Condo Cluster." The guide shown in the menu to your left describes the cluster along with how to access and use it.
- CCIT manages and/or houses independent clusters for several researchers on campus. In return, spare cycles on these machines are available for use by the Clemson community.
  - **axiom** is the Mathematical Sciences Department's IBM OpenPower cluster.
    - 48 compute nodes, 4 interactive nodes, and a head node, each with dual-core Power5 64-bit processors, 4GB of memory and 80GB of disk
    - 550GB of shared RAID10 disk
    - Red Hat Enterprise Linux 5 Advanced Server, GNU and IBM XL compilers, torque and maui queue manager
    - Documentation
  - **wcnitc** is an Electrical and Computer Engineering Intel cluster.
    - 70 compute nodes, each with 4 Intel x86_64, 12GB of memory

News and Updates

- Palmetto Phase 4 Expansion
- Cyberinfrastructure Seminar Series
- Recent posts
- CITI News Aggregator
- July 27, 2009 - Website update
- CCIT News Aggregator
- June 2 Conversion of the /lustre file system to PVFS.
- Our booth
- Presentations
- Posters
- SC3

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COMPUTING RESOURCES

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- Verne
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- Software

USER SUPPORT

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- Kraken User Guide
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- Request Software
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Kraken XT5

Jan 28, 2009

NICS has taken delivery of a new Cray XT5. The new machine, which replaces the Cray XT4, will be called by the same name, 'Kraken'. The new Kraken XT5 will be available starting Monday February 2. Over the next two months, until March 30, both machines will be available to facilitate the transition from the XT4 to the XT5.

Do **NOT** run executables which had been compiled on the XT4 on the XT5. This may cause serious system problems. It should be possible to transfer the source and use the same make procedure.

Currently, to access Kraken XT4 using OTP authentication, SSH to `kraken`, for example:

```
ssh kraken.nics.tennessee.edu
```

To use password authentication, replace `kraken` with `kraken-pwd`. These names will continue to connect to Kraken XT4 until March 2, after which the names will connect to Kraken XT5.

During the transition period (February 2 – March 30), each system may also be reached unambiguously. To connect to the XT5, SSH to `kraken-xt5`, to connect to the XT4, SSH to `kraken-xt4`. To use password authentication, simply append `-pwd` to the machine name. For example, the following connects to the new XT5 using password authentication.

```
ssh kraken-xt5-pwd.nics.tennessee.edu
```

Tags: News NICS

TERAGRID

NICS User Support

9:00 am - 6:00 pm ET
1.865.241.1504

TeraGrid

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1.866.907.2383

- Submit a Ticket via web
- Submit a Ticket via email
- TeraGrid Knowledge Base