Proper use of a Computing Cluster

A look at 3 generations of linux based clusters and their usage, in an opensource environment.

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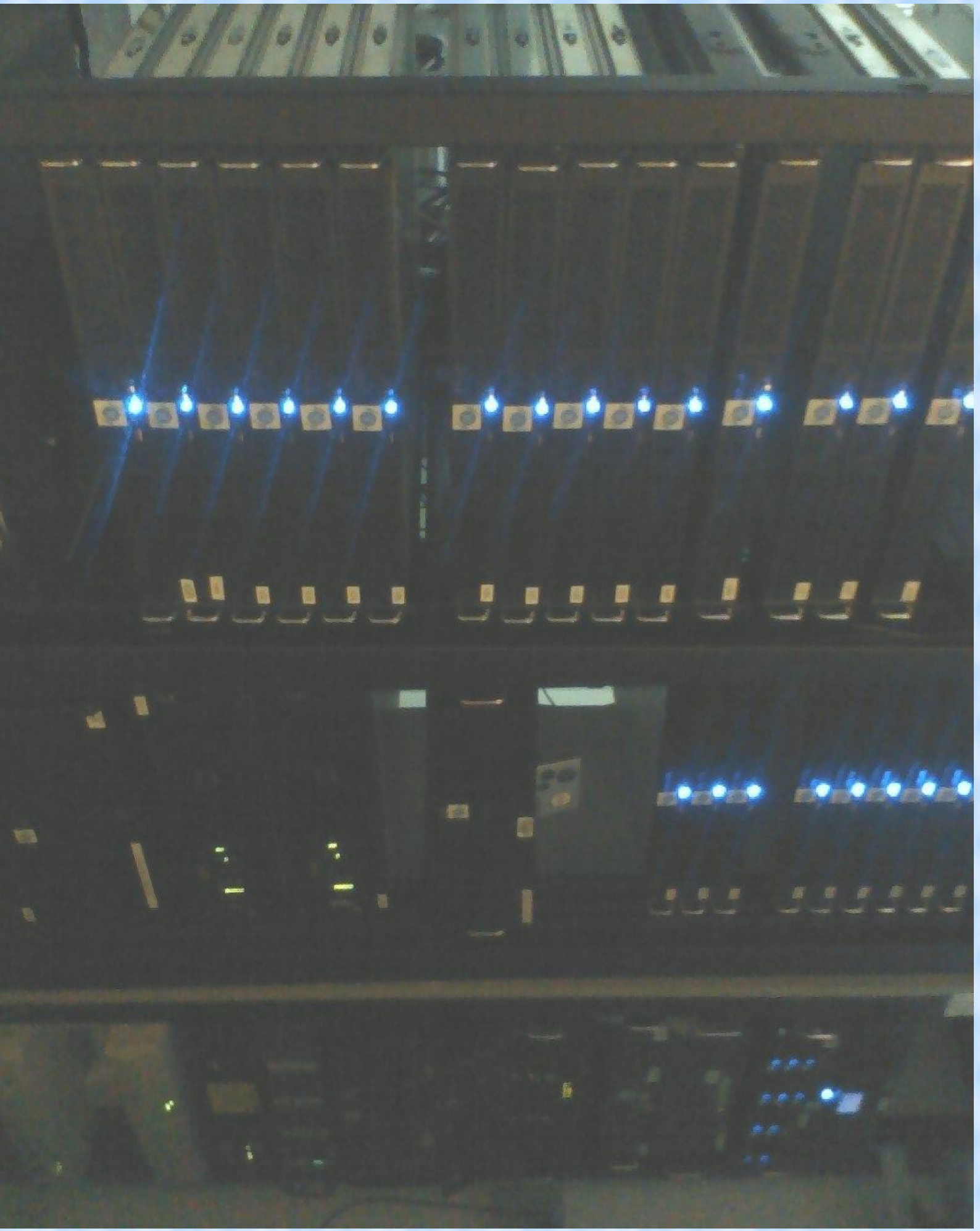
- Overview of the 3 clusters:
  - 3 clusters: 10 node 20 cpu Redhat Linux 7
    13 node 52 cpu Fedora 3 (pre-configured)
    16 node 128 cpu Fedora 7 (pre-configured)
    10 node 20 cpu Fedora 10
  - Ganglia 3.0.1 / 3.0.4 / 3.1.1 (3.1.2)
  - Torque 1.2.0 / 2.1.8 / 2.1.10 (2.4.0)
  - Openmpi - / 1.2.5 / 1.2.4 (1.3.3)
  - Lam - / 7.1.2 / 7.1.4 (7.1.4)
  - Mpich2 1.0.2 / 1.0.6 / 1.1.1 (1.1.1)
- Primary applications are scientific

- The environment:
  - 6 x 12' room
  - Big air conditioner (~ 72° / clusters idle)
  - 4 racks
  - 37 nodes (8 servers, 29 cluster (227 cpus))
  - Gigabit backend network (NFS, MPI, backup, scientific equipment). Network extends throughout the building
  - 9 UPSs



- 1st impressions of the Redhat 7/FC3 clusters
  - Primarily used as batch environment for access to high performance hardware. (similar to the batch environment of the 70s mainframe days)
  - MPI libraries were not utilized
  - ~ 90% of the jobs are generated from weekend/nightly database processing and web applications. These jobs are supported by scientists-developers.
  - An 8 core Xeon server exists to support experiments and data analysis.
- Clusters use Torque to support the coordination and execution of hundreds of jobs.

- 1st impression of the 'new' FC7 cluster
  - Initially no difference in usage
  - New software package arrives; requires many cpus but does not support MPI. A run is designed and setup, broken into separate parts, and submitted as many individual jobs -> with data created for each job. When complete the scientist collates the data and processes the results.
  - Compatible with taking an ordinary password/shadow file and submitting individual 'john the ripper' jobs, one for each line. The administrator would examine the results and identify weak passwords.

- FC7 cluster goes into production
- Redhat 7 cluster is reinstalled as development environment with FC10
  - Ganglia
  - Torque
  - Lam-devel, mpich2-devel, Openmpi-devel
  - Compat-gcc, Intel Fortran/C compilers
  - Gsh, pdsh
- Cluster is isolated from network via iptables.
- 1 simple ssh script to manage nodes.

- MPI version of 'hello world' using openmpi
  - Setup ssh
    - Ssh-keyscan to update known_hosts with all node keys
    - Ssh-keygen to update authorized_keys with key of headnode
  - Compile and run:

    mpicc whello.c
    mpirun -n 20 ./a.out
- MPI version of 'hello world' using mpich2:

  mpicc whello.c
  mpdboot -v -n 16 -f ~/mpd.hosts
  mpiexec -n 128 ./a.out

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```
#include <stdio.h>  /* printf and BUFSIZ defined there */
#include <stdlib.h> /* exit defined there */
#include <mpi.h>    /* all MPI-2 functions defined there */

int main(argc, argv)
int argc;
char *argv[];
{
   int rank, size, length;
   char name[BUFSIZ];

   MPI_Init(&argc, &argv);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   MPI_Comm_size(MPI_COMM_WORLD, &size);
   MPI_Get_processor_name(name, &length);

   printf("%s: hello world from process %d of %d\n", name, rank, size);

   MPI_Finalize();

   exit(0);
}

[kostenba@master3 ~/test]$
```

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```
[kostenba@n00 whello]$ mpirun.openmpi -n 20 ./a.out | sort
n00: hello world from process 0 of 20
n00: hello world from process 10 of 20
n01: hello world from process 11 of 20
n01: hello world from process 1 of 20
n02: hello world from process 12 of 20
n02: hello world from process 2 of 20
n03: hello world from process 13 of 20
n03: hello world from process 3 of 20
n04: hello world from process 14 of 20
n04: hello world from process 4 of 20
n05: hello world from process 15 of 20
n05: hello world from process 5 of 20
n06: hello world from process 16 of 20
n06: hello world from process 6 of 20
n07: hello world from process 17 of 20
n07: hello world from process 7 of 20
n08: hello world from process 18 of 20
n08: hello world from process 8 of 20
n09: hello world from process 19 of 20
n09: hello world from process 9 of 20
[kostenba@n00 whello]$
```

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```
kostenba  8348  8345  0 12:54 ?        00:00:00 sshd: kostenba@notty
kostenba  8428  8349  0 12:54 ?        00:00:00 ps -ef
DONE for n02
root     28137  2469  7 12:54 ?        00:00:00 sshd: kostenba [priv]
kostenba 28162 28137  0 12:54 ?        00:00:00 sshd: kostenba@notty
kostenba 28276     1  0 12:54 ?        00:00:00 orted --bootproxy 1 --name 0.0.4
 --num_procs 11 --vpid_start 0 --nodename n03 --universe kostenba@n00:default-un
iverse-24967 --nsreplica 0.0.0;tcp://192.168.0.10:51339 --gprreplica 0.0.0;tcp:/
/192.168.0.10:51339
kostenba 28290 28276  0 12:54 ?        00:00:00 ./a.out
kostenba 28292 28276  0 12:54 ?        00:00:00 ./a.out
kostenba 28298 28163  0 12:54 ?        00:00:00 ps -ef
DONE for n03
kostenba  3449     1  3 12:54 ?        00:00:00 orted --bootproxy 1 --name 0.0.5
 --num_procs 11 --vpid_start 0 --nodename n04 --universe kostenba@n00:default-un
iverse-24967 --nsreplica 0.0.0;tcp://192.168.0.10:51339 --gprreplica 0.0.0;tcp:/
/192.168.0.10:51339
kostenba  3450  3449  5 12:54 ?        00:00:00 ./a.out
kostenba  3451  3449  5 12:54 ?        00:00:00 ./a.out
root      3452  2182  6 12:54 ?        00:00:00 sshd: kostenba [priv]
kostenba  3455  3452  0 12:54 ?        00:00:00 sshd: kostenba@notty
kostenba  3532  3456  3 12:54 ?        00:00:00 ps -ef
DONE for n04
root      4216  2101  6 12:54 ?        00:00:00 sshd: kostenba [priv]
```

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```
[kostenba@master3 ~]$ /opt/mpich2/ch3_sock-gnu/bin/mpdboot -v -n 16 -f ~/mpd.hos
ts
running mpdallexit on master3.bw03.cabm.rutgers.edu
LAUNCHED mpd on master3.bw03.cabm.rutgers.edu  via
RUNNING: mpd on master3.bw03.cabm.rutgers.edu
LAUNCHED mpd on n001.bw03.cabm.rutgers.edu  via  master3.bw03.cabm.rutgers.edu
LAUNCHED mpd on n002.bw03.cabm.rutgers.edu  via  master3.bw03.cabm.rutgers.edu
LAUNCHED mpd on n003.bw03.cabm.rutgers.edu  via  master3.bw03.cabm.rutgers.edu
LAUNCHED mpd on n004.bw03.cabm.rutgers.edu  via  master3.bw03.cabm.rutgers.edu
RUNNING: mpd on n001.bw03.cabm.rutgers.edu
RUNNING: mpd on n002.bw03.cabm.rutgers.edu
LAUNCHED mpd on n005.bw03.cabm.rutgers.edu  via  n001.bw03.cabm.rutgers.edu
RUNNING: mpd on n003.bw03.cabm.rutgers.edu
LAUNCHED mpd on n006.bw03.cabm.rutgers.edu  via  n001.bw03.cabm.rutgers.edu
RUNNING: mpd on n004.bw03.cabm.rutgers.edu
LAUNCHED mpd on n007.bw03.cabm.rutgers.edu  via  n001.bw03.cabm.rutgers.edu
LAUNCHED mpd on n008.bw03.cabm.rutgers.edu  via  n001.bw03.cabm.rutgers.edu
LAUNCHED mpd on n009.bw03.cabm.rutgers.edu  via  n004.bw03.cabm.rutgers.edu
LAUNCHED mpd on n010.bw03.cabm.rutgers.edu  via  n004.bw03.cabm.rutgers.edu
LAUNCHED mpd on n011.bw03.cabm.rutgers.edu  via  n004.bw03.cabm.rutgers.edu
LAUNCHED mpd on n012.bw03.cabm.rutgers.edu  via  n004.bw03.cabm.rutgers.edu
LAUNCHED mpd on n013.bw03.cabm.rutgers.edu  via  n003.bw03.cabm.rutgers.edu
LAUNCHED mpd on n014.bw03.cabm.rutgers.edu  via  n003.bw03.cabm.rutgers.edu
LAUNCHED mpd on n015.bw03.cabm.rutgers.edu  via  n003.bw03.cabm.rutgers.edu
RUNNING: mpd on n005.bw03.cabm.rutgers.edu
RUNNING: mpd on n006.bw03.cabm.rutgers.edu
RUNNING: mpd on n007.bw03.cabm.rutgers.edu
RUNNING: mpd on n008.bw03.cabm.rutgers.edu
RUNNING: mpd on n009.bw03.cabm.rutgers.edu
RUNNING: mpd on n010.bw03.cabm.rutgers.edu
RUNNING: mpd on n011.bw03.cabm.rutgers.edu
RUNNING: mpd on n012.bw03.cabm.rutgers.edu
RUNNING: mpd on n013.bw03.cabm.rutgers.edu
RUNNING: mpd on n014.bw03.cabm.rutgers.edu
RUNNING: mpd on n015.bw03.cabm.rutgers.edu
```

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```
n013.bw03.cabm.rutgers.edu: hello world from process 105 of 128
n002.bw03.cabm.rutgers.edu: hello world from process 106 of 128
n001.bw03.cabm.rutgers.edu: hello world from process 107 of 128
n008.bw03.cabm.rutgers.edu: hello world from process 108 of 128
n007.bw03.cabm.rutgers.edu: hello world from process 109 of 128
n006.bw03.cabm.rutgers.edu: hello world from process 110 of 128
n005.bw03.cabm.rutgers.edu: hello world from process 111 of 128
master3.bw03.cabm.rutgers.edu: hello world from process 112 of 128
n004.bw03.cabm.rutgers.edu: hello world from process 113 of 128
n012.bw03.cabm.rutgers.edu: hello world from process 114 of 128
n011.bw03.cabm.rutgers.edu: hello world from process 115 of 128
n010.bw03.cabm.rutgers.edu: hello world from process 116 of 128
n009.bw03.cabm.rutgers.edu: hello world from process 117 of 128
n003.bw03.cabm.rutgers.edu: hello world from process 118 of 128
n014.bw03.cabm.rutgers.edu: hello world from process 120 of 128
n013.bw03.cabm.rutgers.edu: hello world from process 121 of 128
n015.bw03.cabm.rutgers.edu: hello world from process 119 of 128
n002.bw03.cabm.rutgers.edu: hello world from process 122 of 128
n001.bw03.cabm.rutgers.edu: hello world from process 123 of 128
n008.bw03.cabm.rutgers.edu: hello world from process 124 of 128
n007.bw03.cabm.rutgers.edu: hello world from process 125 of 128
n006.bw03.cabm.rutgers.edu: hello world from process 126 of 128
n005.bw03.cabm.rutgers.edu: hello world from process 127 of 128
[kostenba@master3 ~/test]$
```

File Edit View Terminal Help

```
kostenba 19322     1  0 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19356 19322  5 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19357 19322  5 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19358 19322  6 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19359 19322  6 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19360 19322  7 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19361 19322  6 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19362 19322  5 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19363 19322  5 11:27 ?        00:00:00 python2.5 /opt/mpich2/ch3_sock-g
nu/bin/mpd.py -h n004.bw03.cabm.rutgers.edu -p 30817 --ncpus=1 -e -d
kostenba 19364 19356  0 11:27 ?        00:00:00 ./a.out
kostenba 19365 19357  0 11:27 ?        00:00:00 ./a.out
kostenba 19366 19358  0 11:27 ?        00:00:00 ./a.out
kostenba 19367 19359  0 11:27 ?        00:00:00 ./a.out
kostenba 19368 19360  0 11:27 ?        00:00:00 ./a.out
kostenba 19369 19361  0 11:27 ?        00:00:00 ./a.out
kostenba 19370 19362  0 11:27 ?        00:00:00 ./a.out
kostenba 19371 19363  0 11:27 ?        00:00:00 ./a.out
root     19372  2500  0 11:27 ?        00:00:00 sshd: kostenba [priv]
kostenba 19377 19372  0 11:27 ?        00:00:00 sshd: kostenba@notty
kostenba 19378 19377  2 11:27 ?        00:00:00 tcsh -c ps -ef | grep kostenba
kostenba 19399 19378  0 11:27 ?        00:00:00 ps -ef
kostenba 19400 19378  0 11:27 ?        00:00:00 grep kostenba
DONE for n009
```

Automated NMR Protein Structure Calculation with CYANA

1 Resonance frequencies: Depending on its local environment, each atom (nuclear spin) has a characteristic resonance frequency that can be detected by NMR.

2 Through-space interactions: Hydrogen atoms that are less than 5 Å (5×10^{-10} m) apart from each other in the protein interact by the Nuclear Overhauser Effect (NOE).

3 Peaks: The NOE interaction between nearby atoms gives rise to signals ("peaks") in NMR spectra with 2, 3 or 4 frequency dimensions.

4 NOESY NMR spectrum: A NOESY spectrum provides information on a network of thousands of short distances between hydrogen atoms in the protein.

5 Assignment: To make this information useful, it is necessary to identify for each peak in the spectrum the pair of atoms in the protein that is responsible for it.

6 Overlap problem: Usually several hydrogen atoms share almost the same resonance frequencies. This "overlap" makes it difficult and very cumbersome to assign manually each peak to a unique hydrogen atom pair.

7 Automated NOE assignment: The assignment of NOESY peaks is performed fully automatically with the program CYANA. Automation is essential for the overall efficiency of NMR protein structure determination.

8 Structure calculation: From the knowledge of short atom-atom distances and the amino acid sequence of the protein, the arrangement of the atoms in space is calculated using CYANA.

9 High-performance computing: The structure calculation requires a large amount of computation power. Up to 128 processors are used in parallel for CYANA.

10 Protein structure: The final result of the NMR structure determination is the three-dimensional structure of the protein in solution.

11 Structure-function relationship: The protein structure can reveal the function of the protein and form a basis for the development of drugs against human diseases.

- The new version of software uses MPI
- The software is compiled using GCC and the LAM libraries
- The need for resource management becomes more obvious
- Cyana jobs run 3 to 4 hours, typically configured for 56 CPUs.

File Edit View Terminal Help

```
[kostenba@master3 ~]$ do.it "ps -ef | grep orted | grep -v grep"
kostenba 17171  2958  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.2 --num_procs 8 --vpid_start 0 --nodenam
 n001 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n001
DONE for n002
kostenba 31253  2925  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.3 --num_procs 8 --vpid_start 0 --nodenam
 n003 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n003
DONE for n004
kostenba  7886  2925  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.1 --num_procs 8 --vpid_start 0 --nodenam
 n005 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n005
DONE for n006
kostenba 10819  2921  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.7 --num_procs 8 --vpid_start 0 --nodenam
 n007 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n007
kostenba 20755  2927  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.4 --num_procs 8 --vpid_start 0 --nodenam
 n008 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n008
kostenba 22330  2923  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.5 --num_procs 8 --vpid_start 0 --nodenam
 n009 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n009
DONE for n010
DONE for n011
DONE for n012
DONE for n013
kostenba  8498  2918  0 08:32 ?        00:00:00 orted --no-daemonize --bootproxy 1 --name 0.0.6 --num_procs 8 --vpid_start 0 --nodenam
 n014 --universe kostenba@n005.bw03.cabm.rutgers.edu:default-universe-7882 --nsreplica "0.0.0;tcp://172.16.0.5:62971" --gprreplica "0.
.0;tcp://172.16.0.5:62971"
DONE for n014
DONE for n015
```

```
e  Edit  View  Terminal  Help
rep 28121 lsof.out
naexe. 7887  kostenba    7u     IPv4          2617120                TCP *:28121 (LISTEN)
naexe. 7887  kostenba    8u     IPv4          2617251                TCP n005.bw03.cabm.rutgers.edu:28121->n007.bw03.cabm.rutger
du:21602 (ESTABLISHED)
naexe. 7887  kostenba   16u     IPv4          2617252                TCP n005.bw03.cabm.rutgers.edu:28121->n007.bw03.cabm.rutger
du:21603 (ESTABLISHED)
naexe. 7887  kostenba   17u     IPv4          2617253                TCP n005.bw03.cabm.rutgers.edu:28121->n007.bw03.cabm.rutger
du:21606 (ESTABLISHED)
naexe. 7887  kostenba   19u     IPv4          2617285                TCP n005.bw03.cabm.rutgers.edu:28121->n014.bw03.cabm.rutger
du:17952 (ESTABLISHED)
naexe. 7887  kostenba   20u     IPv4          2617289                TCP n005.bw03.cabm.rutgers.edu:28121->n008.bw03.cabm.rutger
du:50483 (ESTABLISHED)
naexe. 7887  kostenba   21u     IPv4          2617315                TCP n005.bw03.cabm.rutgers.edu:28121->n007.bw03.cabm.rutger
du:21618 (ESTABLISHED)
naexe. 7887  kostenba   24u     IPv4          2617333                TCP n005.bw03.cabm.rutgers.edu:28121->n001.bw03.cabm.rutger
du:60712 (ESTABLISHED)
naexe. 7887  kostenba   25u     IPv4          2617334                TCP n005.bw03.cabm.rutgers.edu:28121->n008.bw03.cabm.rutger
du:50493 (ESTABLISHED)
naexe. 7887  kostenba   26u     IPv4          2617335                TCP n005.bw03.cabm.rutgers.edu:28121->n003.bw03.cabm.rutger
du:41017 (ESTABLISHED)
naexe. 7887  kostenba   27u     IPv4          2617336                TCP n005.bw03.cabm.rutgers.edu:28121->n014.bw03.cabm.rutger
du:17974 (ESTABLISHED)
naexe. 7887  kostenba   28u     IPv4          2617337                TCP n005.bw03.cabm.rutgers.edu:28121->n008.bw03.cabm.rutger
du:50494 (ESTABLISHED)
naexe. 7887  kostenba   29u     IPv4          2617338                TCP n005.bw03.cabm.rutgers.edu:28121->n009.bw03.cabm.rutger
du:37318 (ESTABLISHED)
naexe. 7887  kostenba   30u     IPv4          2617339                TCP n005.bw03.cabm.rutgers.edu:28121->n003.bw03.cabm.rutger
du:41018 (ESTABLISHED)
naexe. 7887  kostenba   31u     IPv4          2617340                TCP n005.bw03.cabm.rutgers.edu:28121->n001.bw03.cabm.rutger
du:60713 (ESTABLISHED)
naexe. 7887  kostenba   32u     IPv4          2617341                TCP n005.bw03.cabm.rutgers.edu:28121->n014.bw03.cabm.rutger
du:17975 (ESTABLISHED)
naexe. 7887  kostenba   33u     IPv4          2617342                TCP n005.bw03.cabm.rutgers.edu:28121->n007.bw03.cabm.rutger
du:21633 (ESTABLISHED)
naexe. 7887  kostenba   34u     IPv4          2617343                TCP n005.bw03.cabm.rutgers.edu:28121->n003.bw03.cabm.rutger
du:41019 (ESTABLISHED)
naexe. 7887  kostenba   35u     IPv4          2617344                TCP n005.bw03.cabm.rutgers.edu:28121->n001.bw03.cabm.rutger
du:60714 (ESTABLISHED)
```

File Edit View Terminal Help

```
=>cat tcp.txt
tcpdump -i eth0 -w tcp.out net 172.16.0.0/24 and not udp port 8649 and not port 123 and not icmp and not host falcon
tcpdump -r tcp.out | wc -l
reading from file tcp.out, link-type EN10MB (Ethernet)
116667
tcpdump -r tcp.out port nfs | wc -l   (81%)
reading from file tcp.out, link-type EN10MB (Ethernet)
94953
tcpdump -r tcp.out port 28121 | wc -l (10%)
reading from file tcp.out, link-type EN10MB (Ethernet)
11949
tcpdump -r tcp.out port 62971 | wc -l  (2%)
reading from file tcp.out, link-type EN10MB (Ethernet)
3367
tcpdump -r tcp.out port ssh | wc -l   (1%)
reading from file tcp.out, link-type EN10MB (Ethernet)
1422

=>
```

Security

- Follow basic unix guidelines
- Torque allows configuration for job submission from other servers or desktops. Encryption and authentication are not supported, a UID check is done. (not recommended)
- There are no restrictions on the jobs, they can execute any unix command and will assume the privilages of the user.
- By default root can not submit jobs
- Treat all nodes as a single unit, not much can be done to restrict access from the cluster head to the nodes.

- Use iptables to restrict access to cluster
- Torque logging is good but cumbersome
- There is no logging of MPI.
- Configure use of NTP and central syslog host.
- If a separate NFS server is used, access must be enabled on the cluster nodes too.
- Best scenario, configure cluster as a 'dead end' using outbound firewall restrictions. Cluster nodes on backend network only, restrict access to backend and use firewall to block all non-backend traffic.
- Audit key config files on entire cluster to be all the same (use cron to sync files)

Accounting

- PBSACCT – available from sourceforge
  - Author: Ole Holm Nielsen

Department of Physics, University of Denmark

- Collates Torque logs from the head node
- Generate and store reports once a month via cron
- May need to tweek depending on Torque version – possible changes in log format.

File Edit View Terminal Help

```
=>cat Report.August_2009

Portable Batch System USER accounting statistics
------------------------------------------------

A total of 25 accounting files will be processed.
The first record is dated 08/01/2009, last record is dated 08/28/2009.

                          Wallclock          Average Average
Username    Group   #jobs      days  Percent  #nodes  q-days  Full name
--------    -----   ----- ---------  ------- ------- -------  ---------
   TOTAL        -  137054    413.17   100.00    1.45    0.00
 binchen      nmr   82995     10.89     2.64    1.00    0.00  Mao Binchen
   spine   apache   41241    268.08    64.88    1.00    0.00
 yphuang      nmr   11801      1.40     0.34    1.00    0.00
    mani      nmr     756      0.36     0.09    1.00    0.00  Rajeswari Mani
    psvs   nobody     216      0.64     0.15    1.00    0.00
kostenba      nmr      23     14.22     3.44   11.60    0.00
  prossi      nmr      17    103.70    25.10   48.00    0.00
    guan      nmr       5     13.88     3.36   15.90    0.00

Portable Batch System NODE accounting statistics
------------------------------------------------

A total of 25 accounting files will be processed.
The first record is dated 08/01/2009, last record is dated 08/28/2009.

Total number of nodes is 483, and the accounting period is 25 days.
Average number of busy nodes=  11.91 which is  2.47 percent of total.
Average number of busy cpus=  16.53.
=>
```

- Monitoring the 3 clusters using Ganglia
- Provides a simple drill down graphical view of cluster resources.
- Client processes run on cluster nodes and report to a master process running on the cluster head node.
- Master processes from other clusters report to a central master process running on a cluster head node.

Ganglia .sourceforge.net

The CABM Grid Report for Tue, 22 Sep 2009 07:00:22 -0400

Get Fresh Data

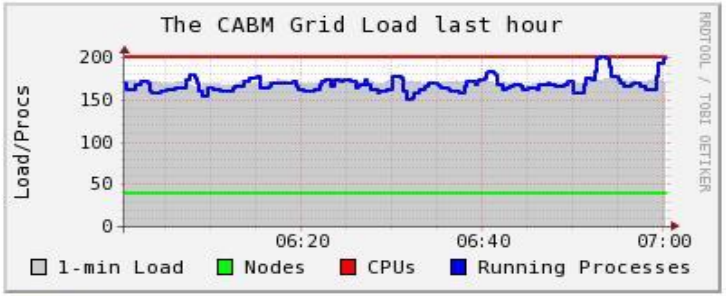
Last hour **Sorted** descending

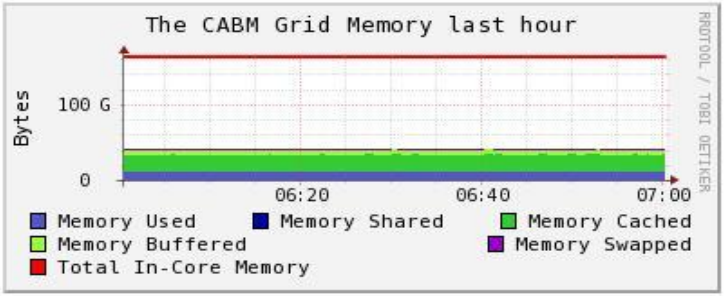
The CABM Grid > --Choose a Source

The CABM Grid (3 sources) (tree view)

CPUs Total: **200**
Hosts up: **39**
Hosts down: **0**

Avg Load (15, 5, 1m):
85%, 85%, 85%
Localtime:
2009-09-22 07:00

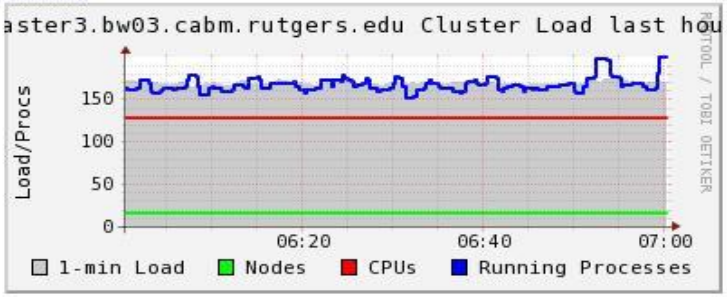


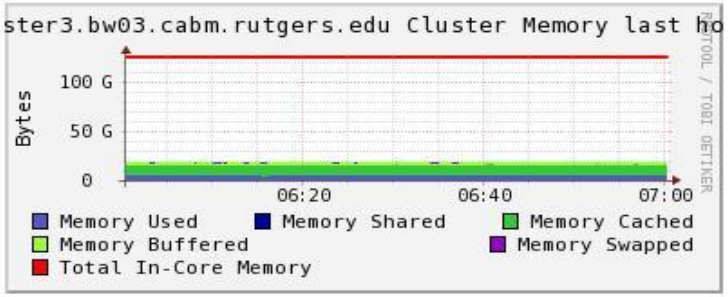


master3.bw03.cabm.rutgers.edu (physical view)

CPUs Total: **128**
Hosts up: **16**
Hosts down: **0**

Avg Load (15, 5, 1m):
132%, 132%, 132%
Localtime:
2009-09-22 07:00

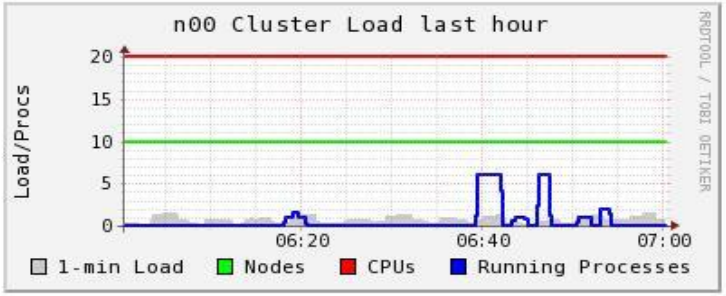


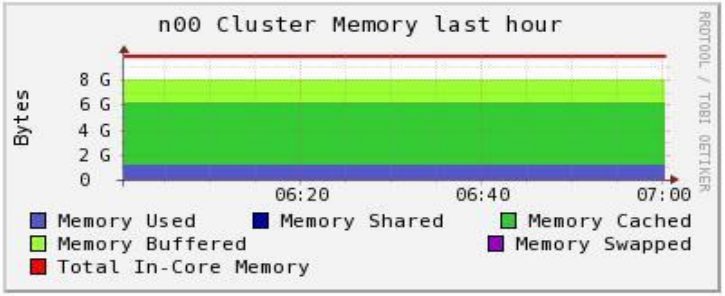


n00 (physical view)

CPUs Total: **20**
Hosts up: **10**
Hosts down: **0**

Avg Load (15, 5, 1m):
4%, 5%, 4%
Localtime:
2009-09-22 07:00





m30.cabm.rutgers.edu (physical view)

Ganglia:: master3.bw03.cabm.rutgers.edu Cluster Report - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://n00/?c=master3.bw03.cabm.rutgers.edu&m=load_one&r=hour&s=descending&hc=4

nbtscan

Most Visited Smart Bookmarks Red Hat, Inc. Red Hat Network Support Shop Products Training

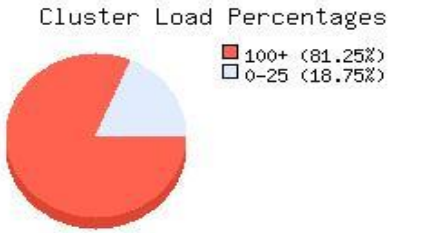
Ganglia:: master3.bw03.ca... | Phil and Karen's future "catc... | PSI Structural Genomics Kno... | NESG NMR Blind Data

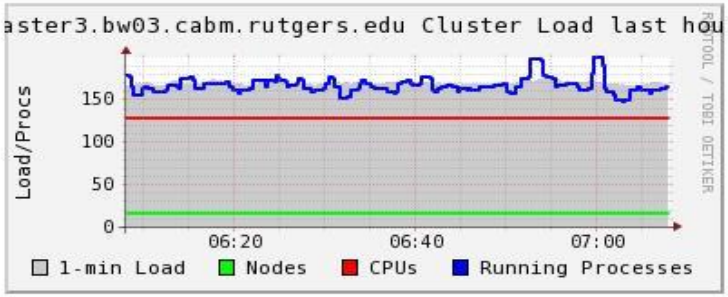
The CABM Grid > master3.bw03.cabm.rutgers.edu > --Choose a Node

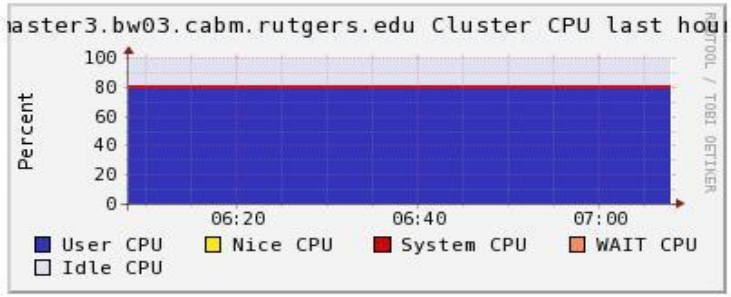
Overview of master3.bw03.cabm.rutgers.edu

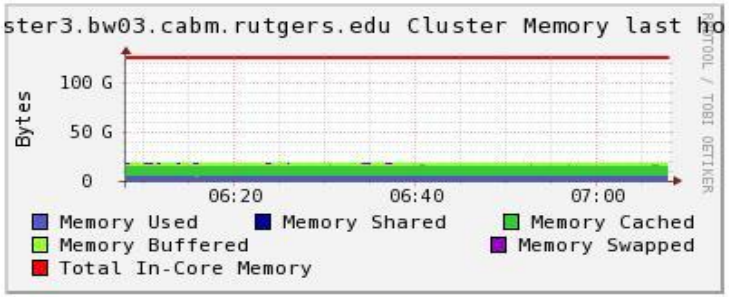
CPUs Total: **128**
Hosts up: **16**
Hosts down: **0**

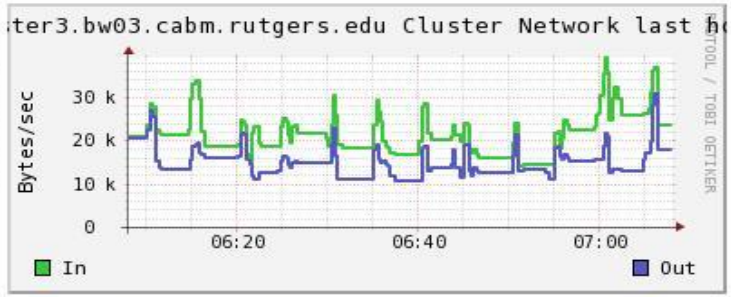
Avg Load (15, 5, 1m):
131%, 131%, 131%
Localtime:
2009-09-22 07:07



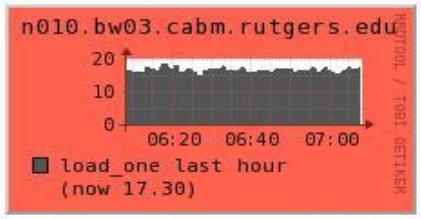


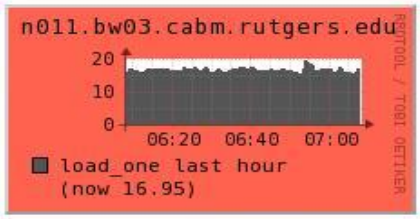


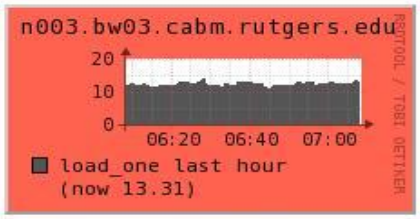


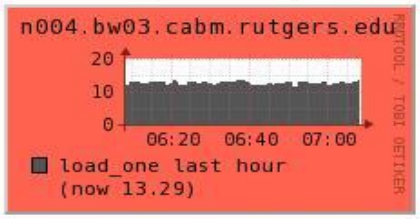


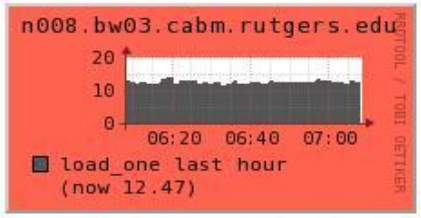
Show Hosts: yes no | master3.bw03.cabm.rutgers.edu **load_one** last **hour** sorted **descending** | Columns 4 Size small

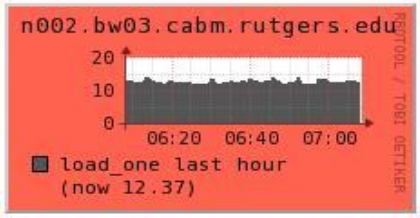


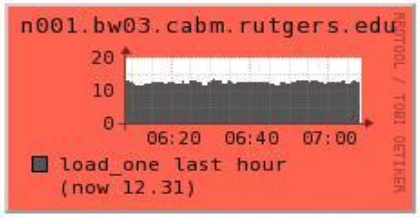


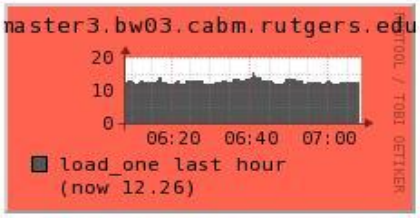


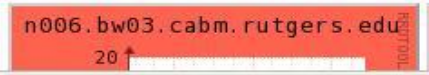


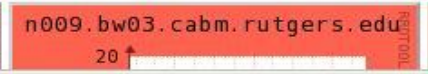


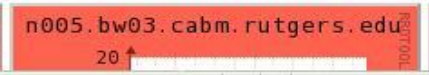


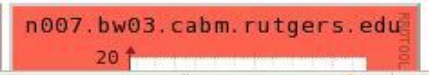












Done

Now: Cloudy, 60 °F | Tue: 76 °F | Wed: 81 °F

master3.bw03.cabm.rutgers.edu cluster - Physical View | Columns 2

Verbosity level (Lower is more compact):
3 2 1

Total CPUs: **128**
Total Memory: **125.1 GB**

Total Disk: **1226.6 GB**
Most Full Disk:
master3.bw03.cabm.rutgers.edu (92.5% Used)

n015.bw03.cabm.rutgers.edu	Last heartbeat 3s	0.00
n014.bw03.cabm.rutgers.edu	Last heartbeat 20s	0.00
n013.bw03.cabm.rutgers.edu	Last heartbeat 3s	0.00
n012.bw03.cabm.rutgers.edu	Last heartbeat 21s	3.64
n011.bw03.cabm.rutgers.edu	Last heartbeat 20s	0.00
n010.bw03.cabm.rutgers.edu	Last heartbeat 10s	0.00
n009.bw03.cabm.rutgers.edu	Last heartbeat 15s	0.00
n008.bw03.cabm.rutgers.edu	Last heartbeat 5s	0.00
n007.bw03.cabm.rutgers.edu	Last heartbeat 2s	0.00
n006.bw03.cabm.rutgers.edu	Last heartbeat 19s	0.00

cpu: 2.43G (8) mem: 7.82G

Ganglia .sourceforge.net

n012.bw03.cabm.rutgers.edu Node View for Thu, 24 Sep 2009 08:02:46 -0400

Get Fresh Data

Host View

The CABM Grid > master3.bw03.cabm.rutgers.edu > n012.bw03.cabm.rutgers.edu

n012.bw03.cabm.rutgers.edu Info

n012.bw03.cabm.rutgers.edu

Load: 4.33 4.08 4.01
1m 5m 15m

Location: Unknown

Cluster local time Thu Sep 24 08:02:40 2009
Last heartbeat received 13 seconds ago.
Uptime 2 days, 17:33:03

CPU Utilization: 44.7 0.9 54.4
user sys idle

Hardware
CPUs: 8 x 2.43 GHz
Memory (RAM): 7.82 GB
Local Disk: Using 9.764 of 66.144 GB
Most Full Disk Partition: 60.4% used.

Software
OS: Linux 2.6.23.1-21.fc7 (x86_64)
Booted: September 21, 2009, 2:29 pm
Uptime: 2 days, 17:33:03
Swap: Using 0.0 of 12229.2 MB swap.

Physical View | Reload

Look at a large European grid

- Provides access world wide for the scientific community.
- Clusters located throughout the Europe
- Rigorous registration process.
- Uses 2 factor authentication using key and user/pass.
- Job submission can use gLite/linux or web based front end.

GridICE the eyes of the Grid

is monitoring e-nmr

XML

You need to install the Macromedia Flash Player in order to see the Geo view.

Click on the icon and follow the instructions.

After that, you can be back on this page, reload and enjoy the geographycal view.

Get macromedia FLASH PLAYER

File Edit View History Bookmarks Tools Help

http://gridice-enmr.cerm.unifi.it/geo/geo.php

pbsacct

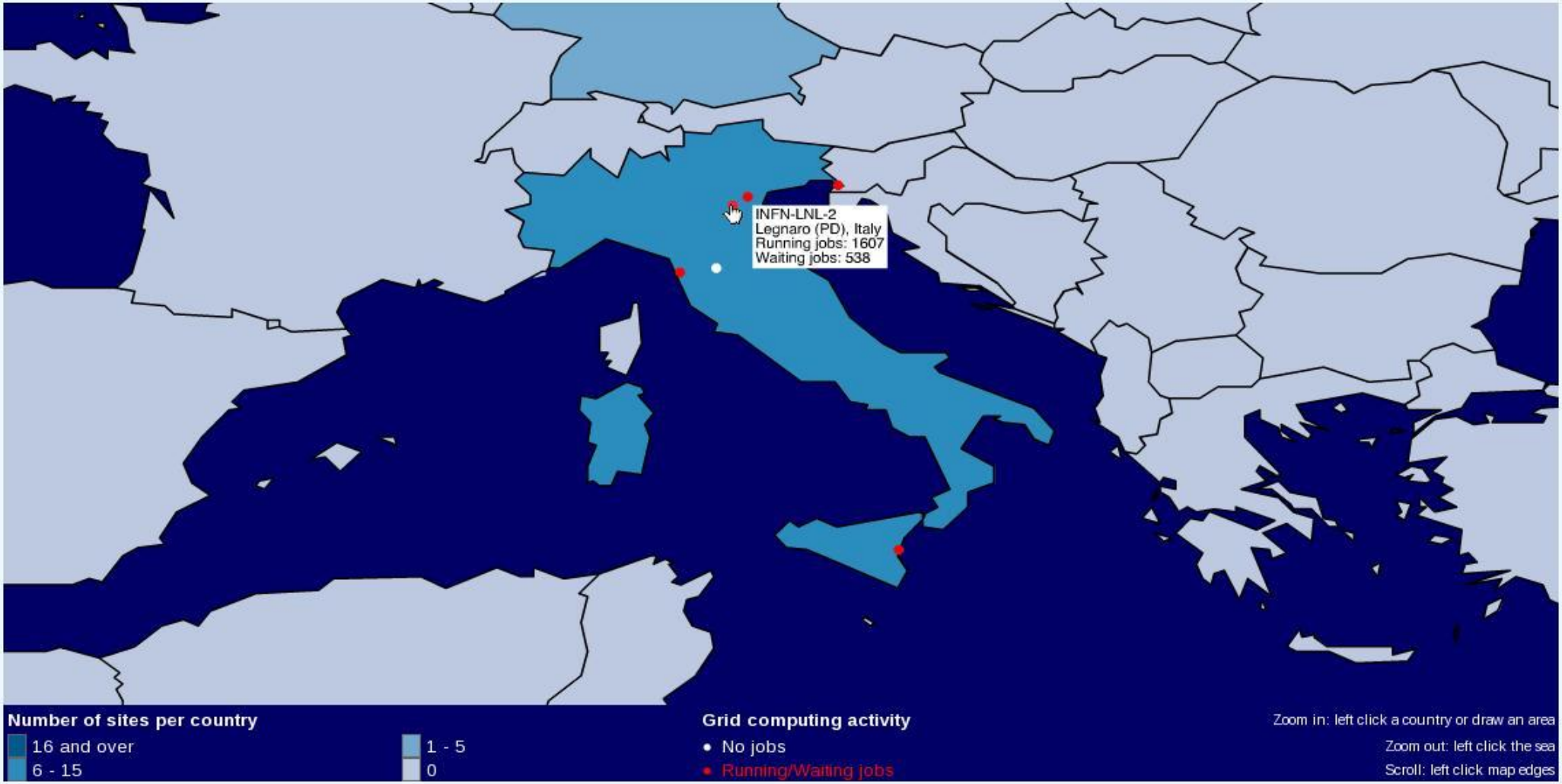
Most Visited Smart Bookmarks Red Hat, Inc. Red Hat Network Support Shop Products Training

Nagios | CNN.com - Breaking Ne... | http://www....l#resources | INFN - GridICE - Grid Mon... | WebHome < MonitoringI...

Click on the icon and follow the instructions.

After that, you can be back on this page, reload and enjoy the geographycal view.

Get macromedia FLASH PLAYER



Generated: Thu, 24 Sep 2009 16:31:31 +0200 GridICE Homepage

× Find: tew-441 Previous Next Highlight all Match case

GridICE — the eyes of the Grid

is monitoring e-nmr

Site ▼		Region	GK#	Q#	RunJob	WaitJob	Computing Resources: JobLoad	Power	WN#	CPU#	CPULoad	Storage Resources: Available	Total	%	MH#
BCBR		NorthEu	1	5	0	5	-	-	-	-	-	-	-	-	-
BMRZ-FRANKFURT		Ger/Swi	1	5	0	1	0%	67K	6	20	0%	-	-	-	10
CIRMMP		Italy	1	5	0	0	66%	89K	4	32	66%	-	-	-	11
CNR-ILC-PISA		Italy	1	5	3	22	-	-	-	-	-	-	-	-	-
HTC-BIGGRID		NorthEu	1	2	880	0	-	-	-	-	-	-	-	-	-
INFN-CATANIA		Italy	1	16	124	135	87%	603K	90	287	70%	-	-	-	138
INFN-LNL-2		Italy	3	24	1607	626	100%	3M	313	1588	94%	-	-	-	135
INFN-PADOVA		Italy	2	14	140	1554	87%	85K	27	82	65%	-	-	-	41
INFN-TRIESTE		Italy	1	7	132	25	-	-	-	-	-	42 MB	98 MB	57%	73
NIKHEF-ELPROD		NorthEu	2	16	1862	132	-	-	-	-	-	-	-	-	-
TOTAL: 10	**3**	**3**	**14**	**99**	**4748**	**2500**	67%	**4M**	**440**	**2009**	59%	**42 MB**	**98 MB**	57%	**408**

Generated: Thu, 24 Sep 2009 16:28:50 +0200 GridICE Homepage

CYANA STRUCTURE CALCULATIONS

Input Files and Parameters

Job name (One word): demo

Files Upload

Amino acid sequence (3 letter code) file : Browse...

File with upper distance bound restraints : Browse...

File with torsion angle restraints : Browse...

Enter Structure calculation parameters

Number of structures : Initial (Range 20 - 100) 50 Final (Max 50) 10

Number of torsion angle dynamics steps (Range 1000 - 10000) : 5000

Residue number range for RMSD calculation : From 10 To 100

Choose the type of Structure calculation

- (•) Default {Without Peak list(s)}
- ( ) Using assigned Peak list(s)
- ( ) Using unassigned Peak list(s)

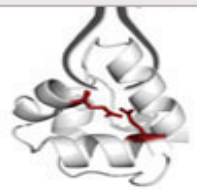
Peak list(s) Parameters

Additional Parameters & Files

Job Submission

Username :

Password :



PSVS

Protein Structure Validation Software suite

One structure, rich report

The protein structure validation software suite (PSVS) is used for assessment of protein structures generated from NMR, X-ray crystallographic and homology modeling methods.

(Welcome)

(About PSVS)

(Run PSVS)

(PSVS manual)

Please enter the required information. (You must complete the options marked with *)
Residue selection applies for Procheck analysis,RMSD calculation and structure superimposition

1. Other Options:(more) ○ Input More Infor ◉ Don't Input

2. Project name:* my project

3. Your name: kostenba

3.1 Email address:* kostenba@cabm.rutgers.edu

4. Type of structure:* ○ X-ray crystal ◉ NMR (Solution/Solid State) ○ Homology model

5. Atomic coordinates file:* Browse...

5.1 Naming convention for atoms in coordinates file:* ◉ Protein Data Bank ○ Dyana or Cyana ○ CNS or Xplor

5.2 Filter-in only standard amino acid