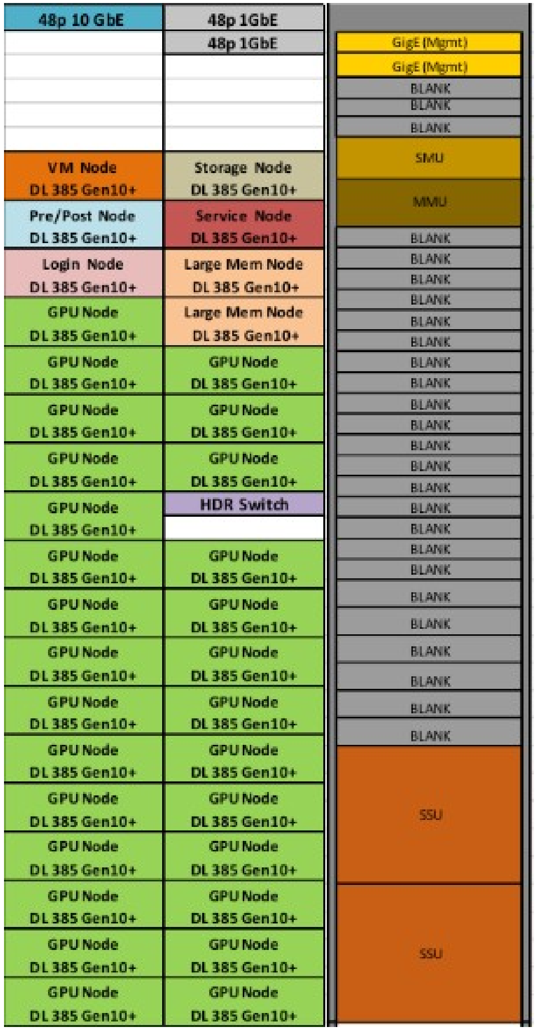
High Performance Computing at NIU

METIS



48p 10 GbE	48p 1GbE
	48p 1GbE
VM Node DL 385 Gen10+	Storage Node DL 385 Gen10+
Pre/Post Node DL 385 Gen10+	Service Node DL 385 Gen10+
Login Node DL 385 Gen10+	Large Mem Node DL 385 Gen10+
GPU Node DL 385 Gen10+	Large Mem Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	HDR Switch
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
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GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+
GPU Node DL 385 Gen10+	GPU Node DL 385 Gen10+

GigE (Mgmt)
GigE (Mgmt)
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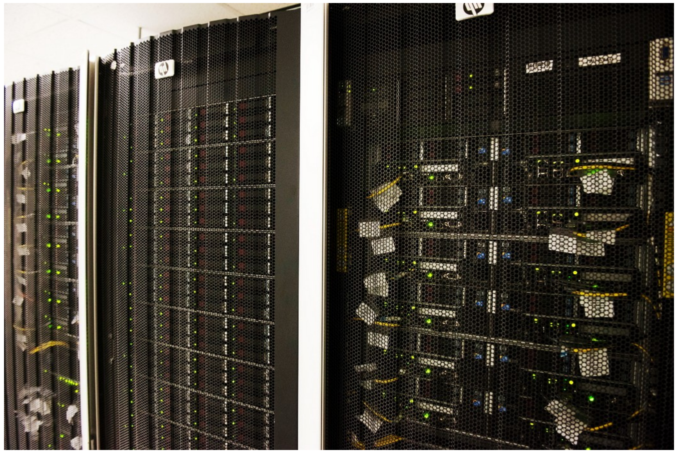
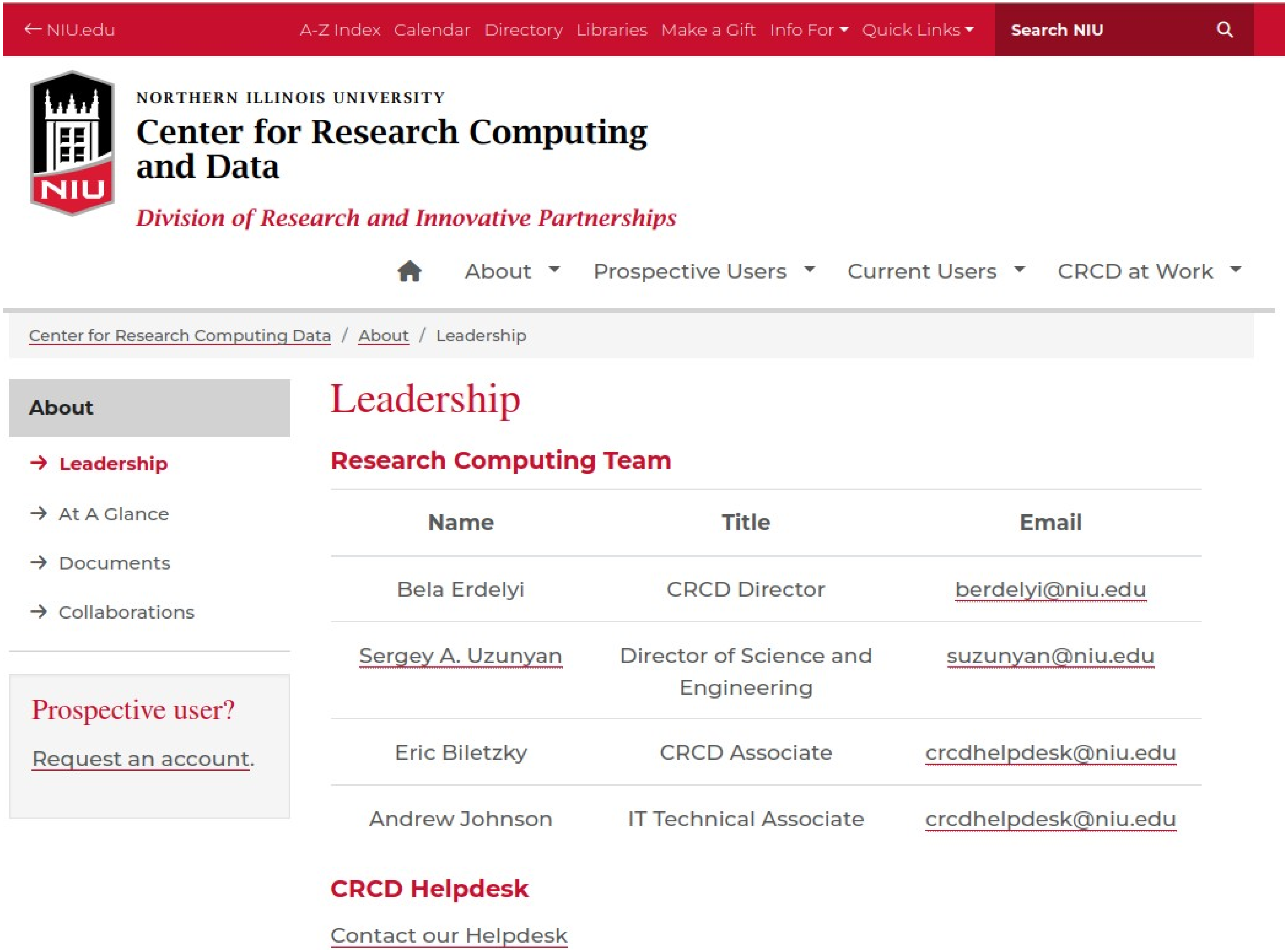
SSU

GAEA



NICADD

CRCD team



NORTHERN ILLINOIS UNIVERSITY

Center for Research Computing and Data

Division of Research and Innovative Partnerships

Leadership

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CRCD Helpdesk

Contact our Helpdesk

Prospective user?

Request an account.

Small team, efficient HPC management!

The origin of modern HPC

HPC cluster @ 1994 == Beowulf cluster: a number of computers (nodes) assembled to run as a single system

HPC cluster today:

- **An assembly of compute nodes designed to run as single system**

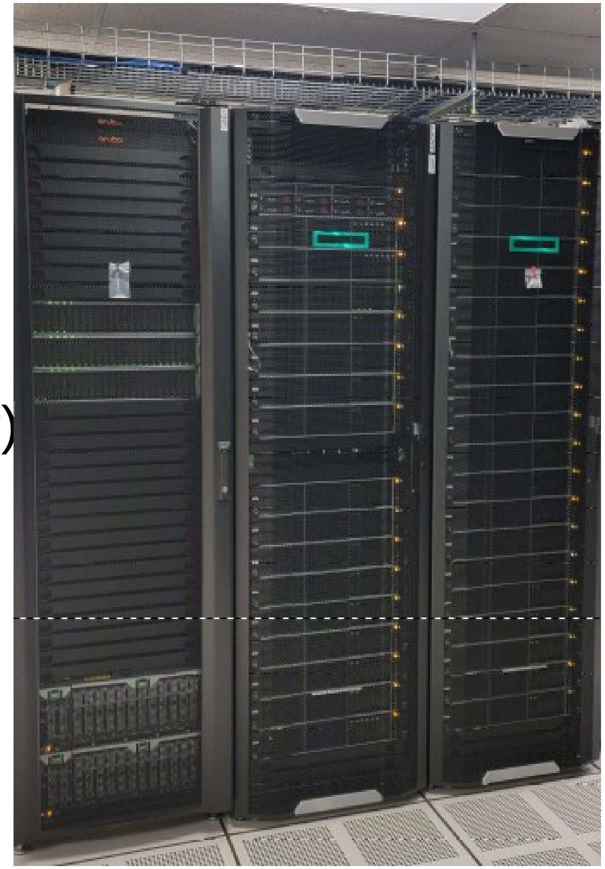
- A powerful compute nodes (desktops in a rack friendly form-factor)

+

- Fast interconnect (200 GBit/s)

+

- Large (1 PB+) parallel shared disk system



Becker, Donald J; Sterling, Thomas; Savarese, Daniel; Dorband, John E; Ranawak Udaya A; Packer, Charles V (1995). "BEOWULF: A parallel workstation for scientific computation". Proceedings, International Conference on Parallel Processing. 95.

National Aeronautics and Space Administration

HPC applications

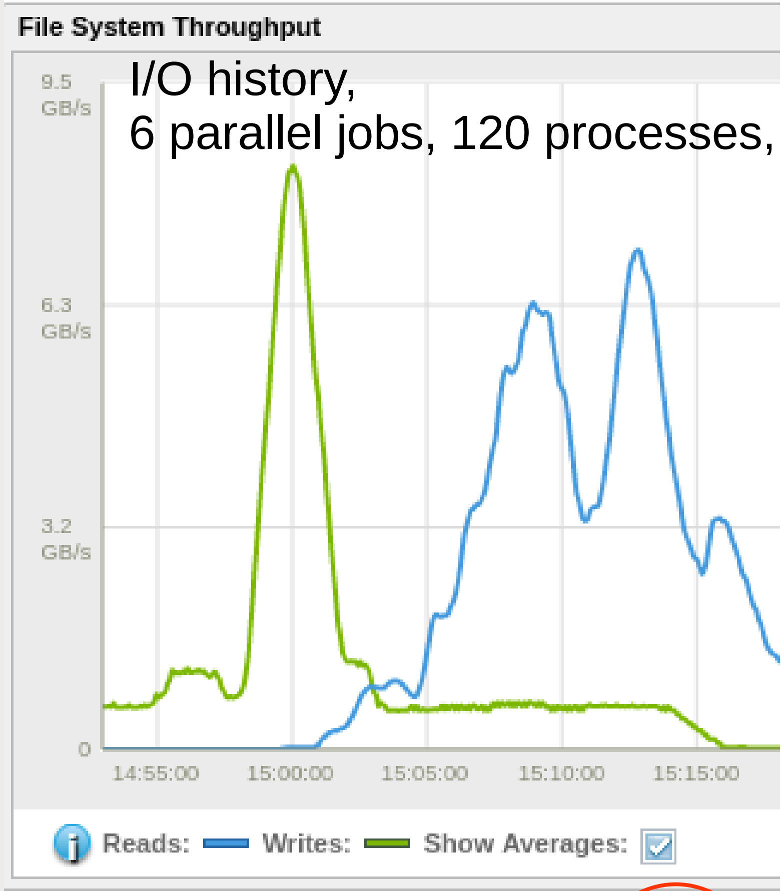
When to use HPC systems at NIU?

- a personal system (laptop or desktop) is “too slow”
- an application benefits from parallelization
- an application needs to be run multiple times
- an application needs extra memory
- an application needs a powerful GPU
- an application requires Linux OS to run

(and a different OS is needed on a personal system)

- fast access to large input data
- the results have to be easy accessible
- convenience: access to shared software libraries

and CRCD team support

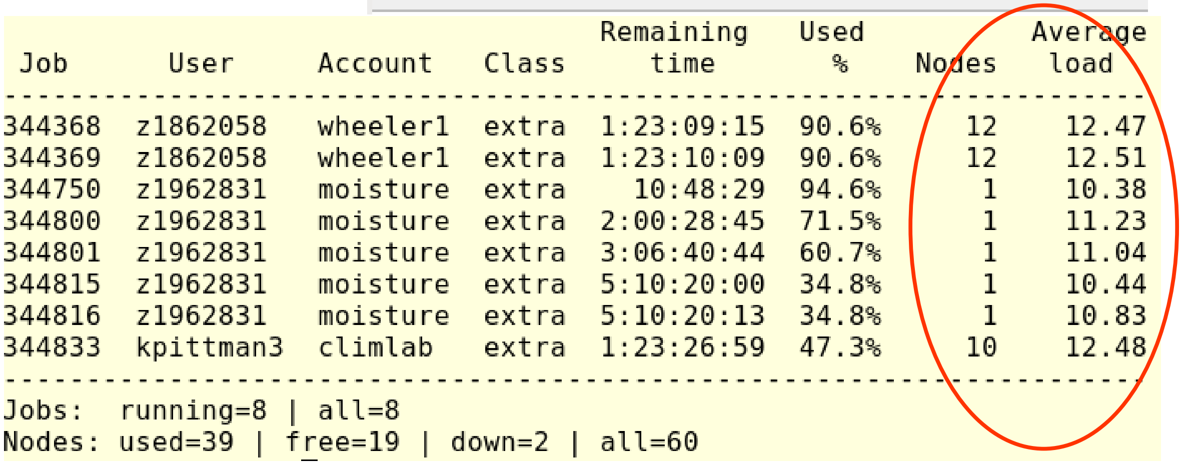

File System Throughput

I/O history,
6 parallel jobs, 120 processes,

Minimal requirements

- **read the CRCD documentation**
- **beginners knowledge of Linux**

Efficiency of shared HPC system depends on users accuracy


```
                                     Remaining   Used          Average
 Job      User      Account   Class    time        %    Nodes    load
-------------------------------------------------------------------------
344368  z1862058  wheeler1  extra  1:23:09:15  90.6%     12     12.47
344369  z1862058  wheeler1  extra  1:23:10:09  90.6%     12     12.51
344750  z1962831  moisture  extra    10:48:29  94.6%      1     10.38
344800  z1962831  moisture  extra  2:00:28:45  71.5%      1     11.23
344801  z1962831  moisture  extra  3:06:40:44  60.7%      1     11.04
344815  z1962831  moisture  extra  5:10:20:00  34.8%      1     10.44
344816  z1962831  moisture  extra  5:10:20:13  34.8%      1     10.83
344833  kpittman3 climlab   extra  1:23:26:59  47.3%     10     12.48
-------------------------------------------------------------------------
Jobs:   running=8 | all=8
Nodes:  used=39 | free=19 | down=2 | all=60
```

Why we use Linux?

Administrators

- Stability
- Security
- Assess to OpenSource
- Built for development
- Customizable
- Supported by the hardware vendors
- Easy to administer

Users

- Community support
- A lot of free distributions
- Can run on older hardware
- Easy to install
- Tons of applications
- A decent skill in resume (if you plan to work in Fortune 500 list)
- Fun to use

Recommended desktop Operating systems to work with NIU HPC

AlmaLinux™

Rocky Linux™

fedora

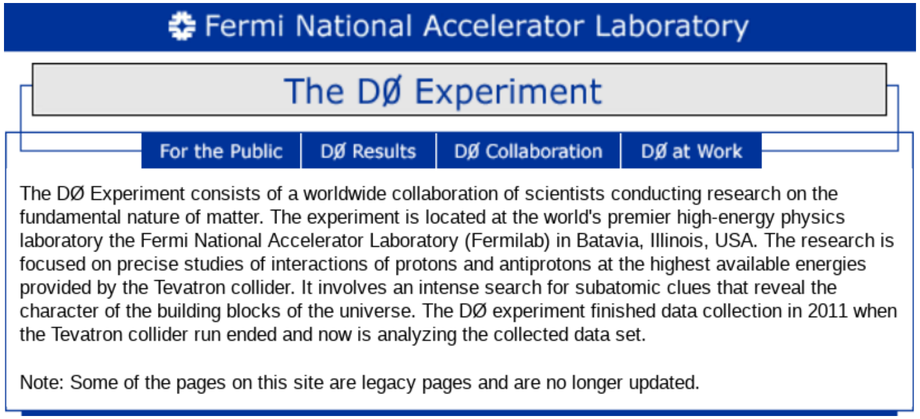
ubuntu

Mac™ OS

+More than 600 supported Linux distributions

The beginning of HPC at NIU

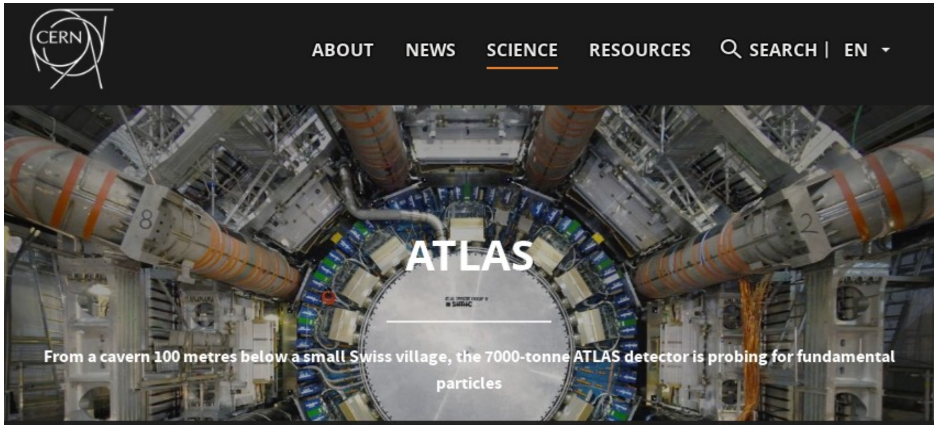
Year 2000 – 2 NIU Phys. Dep. Servers - niuhep.niu.edu and nicadd.niu.edu



The DØ Experiment

The DØ Experiment consists of a worldwide collaboration of scientists conducting research on the fundamental nature of matter. The experiment is located at the world's premier high-energy physics laboratory the Fermi National Accelerator Laboratory (Fermilab) in Batavia, Illinois, USA. The research is focused on precise studies of interactions of protons and antiprotons at the highest available energies provided by the Tevatron collider. It involves an intense search for subatomic clues that reveal the character of the building blocks of the universe. The DØ experiment finished data collection in 2011 when the Tevatron collider run ended and now is analyzing the collected data set.

Note: Some of the pages on this site are legacy pages and are no longer updated.



From a cavern 100 metres below a small Swiss village, the 7000-tonne ATLAS detector is probing for fundamental particles

ClueD0 desktop cluster
~400 desktops in 2004
D0 NICADD group

BEAM NICADD group

ATLAS Tier T3 clusters
ATLAS collaborators
ATLAS NICADD group

ClueD0 design

•Current copy of D0 software.

•Access to cluster-wide batch queues.

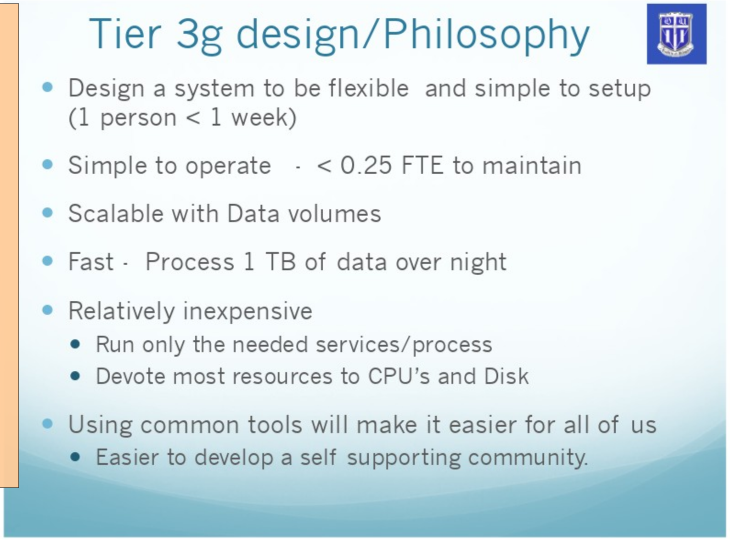
•Security patches and updates for your machines

•Local root access available on your machines...
Sys-admins available during the day to fix "supported" features

•Home directory backup every night...

•Centralized account management.

NICADD HPC
~20 nodes
700 processor slots (1.8-2.6 GHz) cluster under
the HT CONDOR batch system
running Scientific Linux OS
+
desktops and data servers



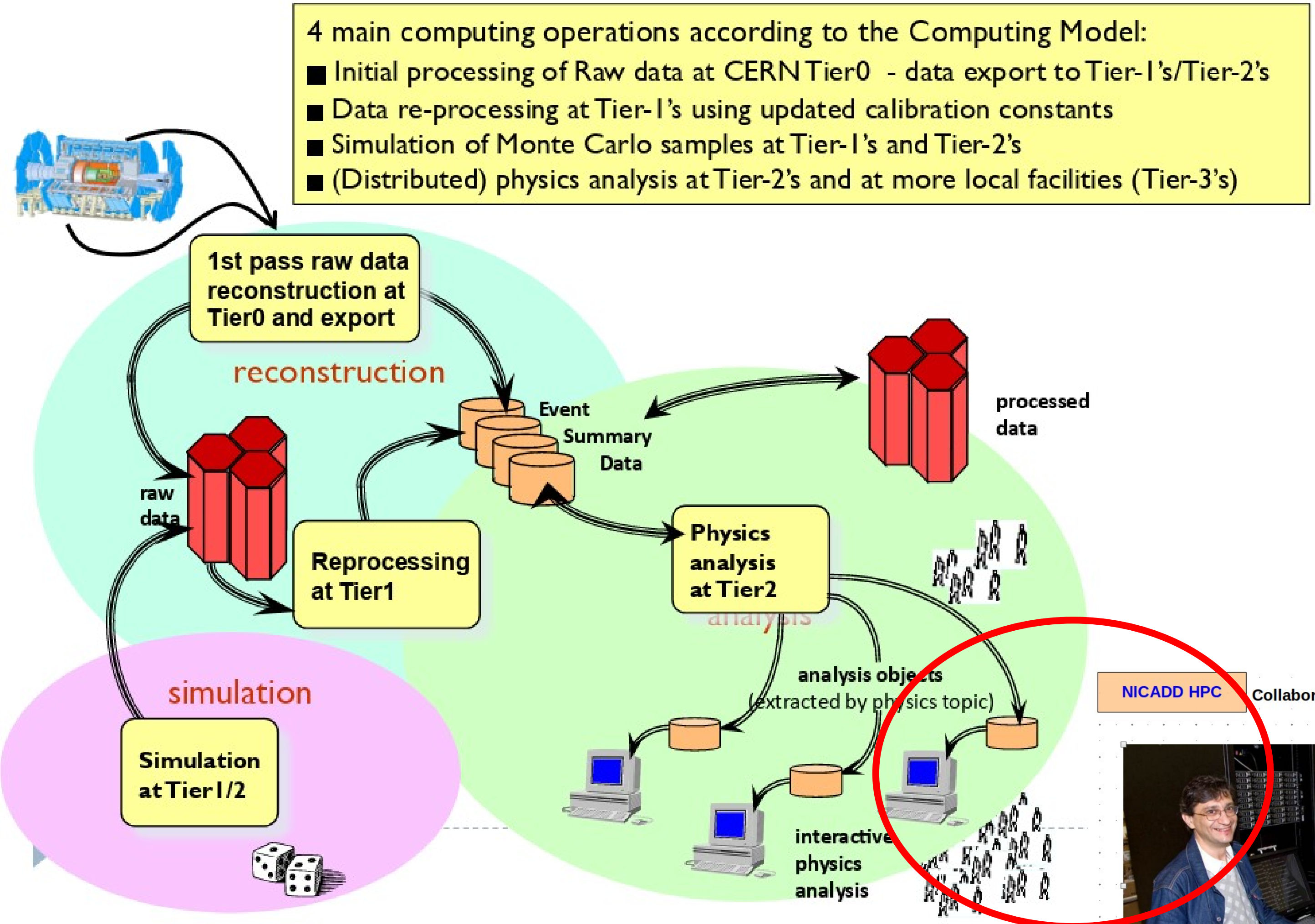
Tier 3g design/Philosophy

- Design a system to be flexible and simple to setup (1 person < 1 week)
- Simple to operate - < 0.25 FTE to maintain
- Scalable with Data volumes
- Fast - Process 1 TB of data over night
- Relatively inexpensive
  - Run only the needed services/process
  - Devote most resources to CPU's and Disk
- Using common tools will make it easier for all of us
  - Easier to develop a self supporting community.

ATLAS T3 project

Doug Benjamin, Duke University - T3 model at time of creation

Simplified View – Atlas Computing Model



4 main computing operations according to the Computing Model:

- Initial processing of Raw data at CERN Tier0 - data export to Tier-1's/Tier-2's
- Data re-processing at Tier-1's using updated calibration constants
- Simulation of Monte Carlo samples at Tier-1's and Tier-2's
- (Distributed) physics analysis at Tier-2's and at more local facilities (Tier-3's)

1st pass raw data reconstruction at Tier0 and export
reconstruction
raw data
Reprocessing at Tier1
Event Summary Data
processed data
Physics analysis at Tier2
analysis
analysis objects (extracted by physics topic)
interactive physics analysis
simulation
Simulation at Tier1/2

NICADD HPC

Fresno State Tier 3
CERN / Atlas Cluster
Hardware Overview

Cisco 6500 Series
Dell PowerConnect 6248

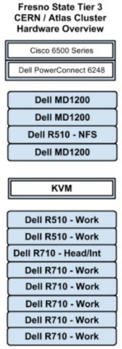
Dell MD1200
Dell MD1200
Dell R510 - NFS
Dell MD1200

KVM

Dell R510 - Work
Dell R510 - Work
Dell R710 - Head/Int
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work

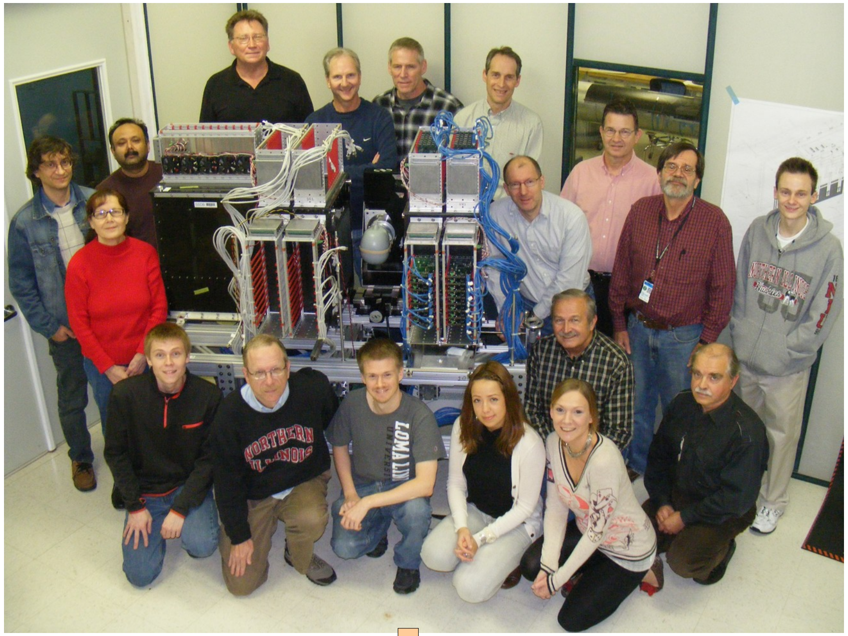
NICADD HPC

Collaboration with Fresno University Atlas Team, 2011-2013



Fresno State Tier 3
CERN / Atlas Cluster
Hardware Overview
Cisco 6500 Series
Dell PowerConnect 6248
Dell MD1200
Dell MD1200
Dell R510 - NFS
Dell MD1200
KVM
Dell R510 - Work
Dell R510 - Work
Dell R710 - Head/Int
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work
Dell R710 - Work

Proton Computed Tomography (pCT) project

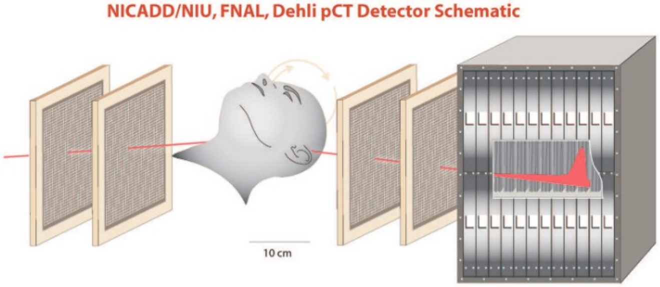


- Gaea built in 2012 as a GPU-based system to process 200 GB “images” in 10 min

pCT project PIs

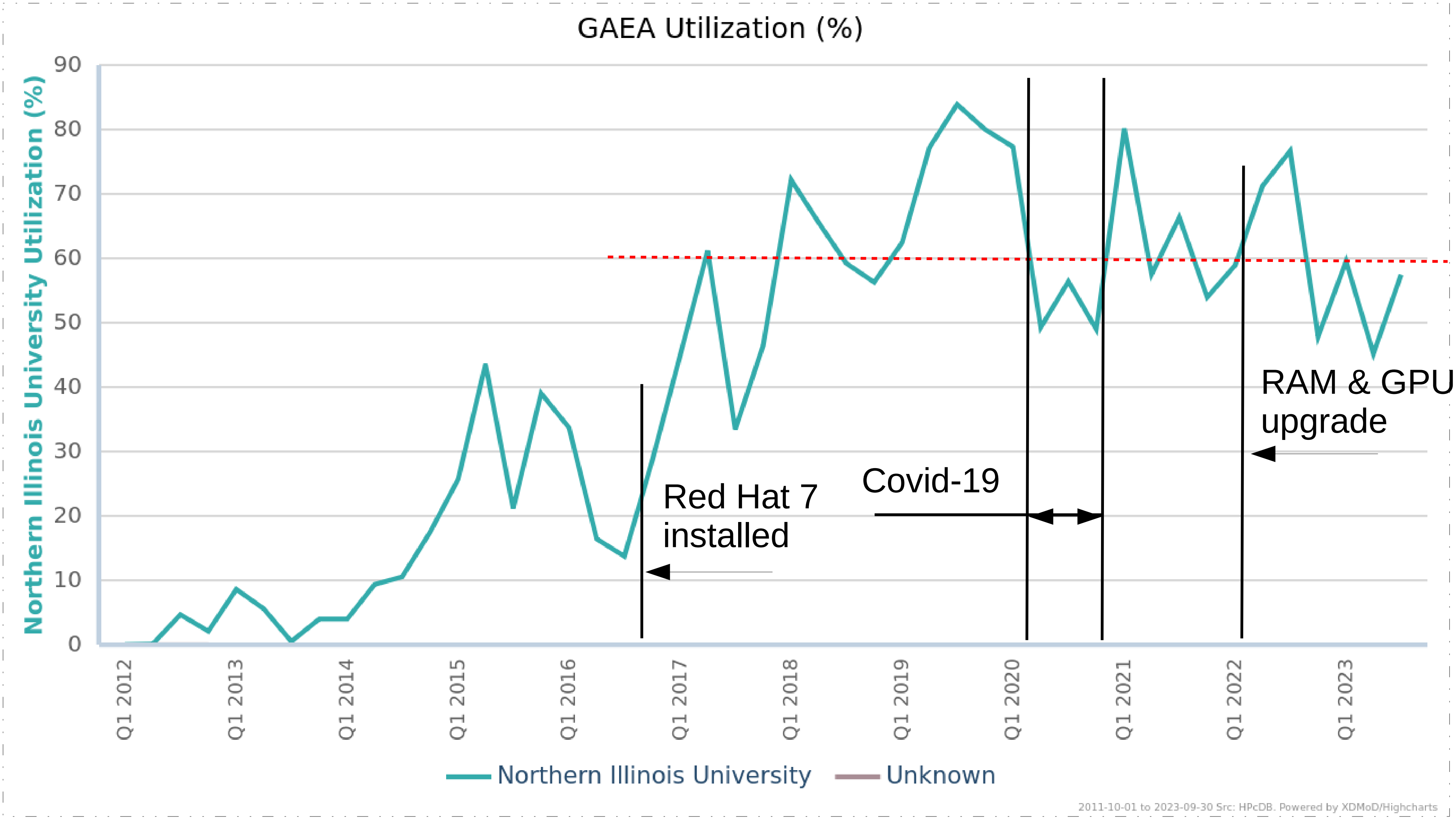
George Coutrakon and Nick Karonis

- Converted into a shared HPC system in 2014



GAEA HPC

GAEA utilization history

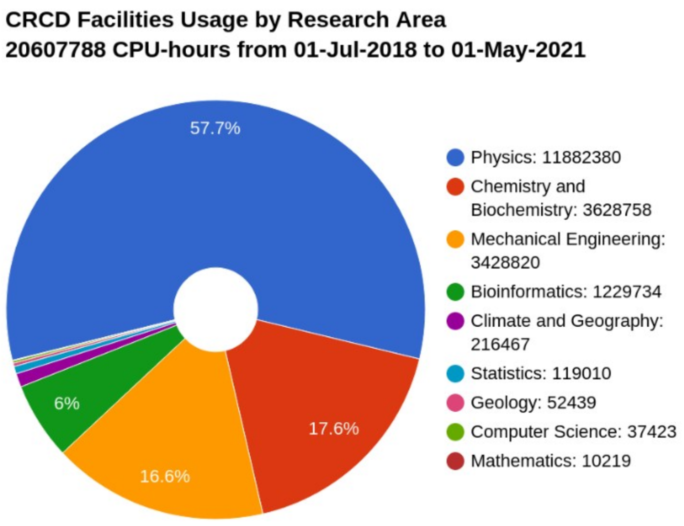


Red Hat 7 installed

Covid-19

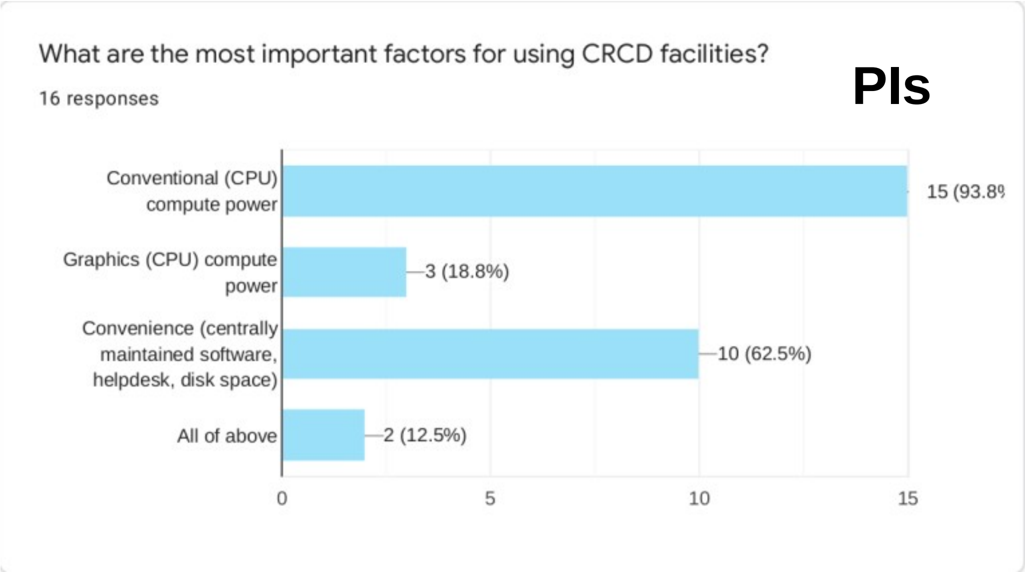
RAM & GPU upgrade

CRCD statistics (including NICADD), 2018-2021

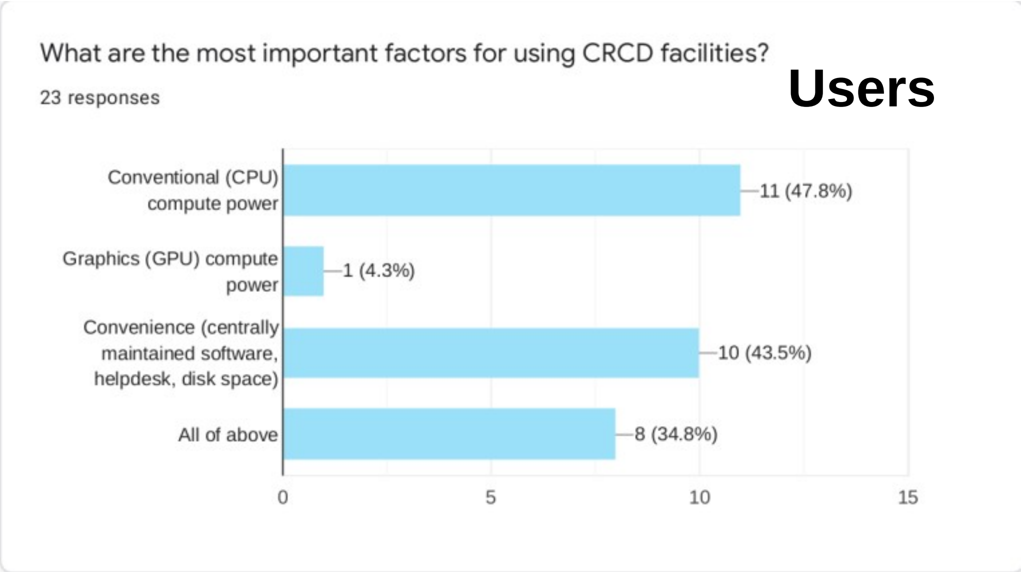


NIU total (Jul 2018 -Nov 2021)

1. Submitted research proposals: 50 requesting $20.5M
2. Funded research: 20 totaling $6.2M
3. Proposals still under review 3 totaling $3.1M
4. Journal papers: 71
5. Ph.D. thesis: 13 (10 completed/3 in progress)
6. Master thesis: 12 (10 completed/2 in progress)
7. Conference presentations: 38
8. External collaborations: 25



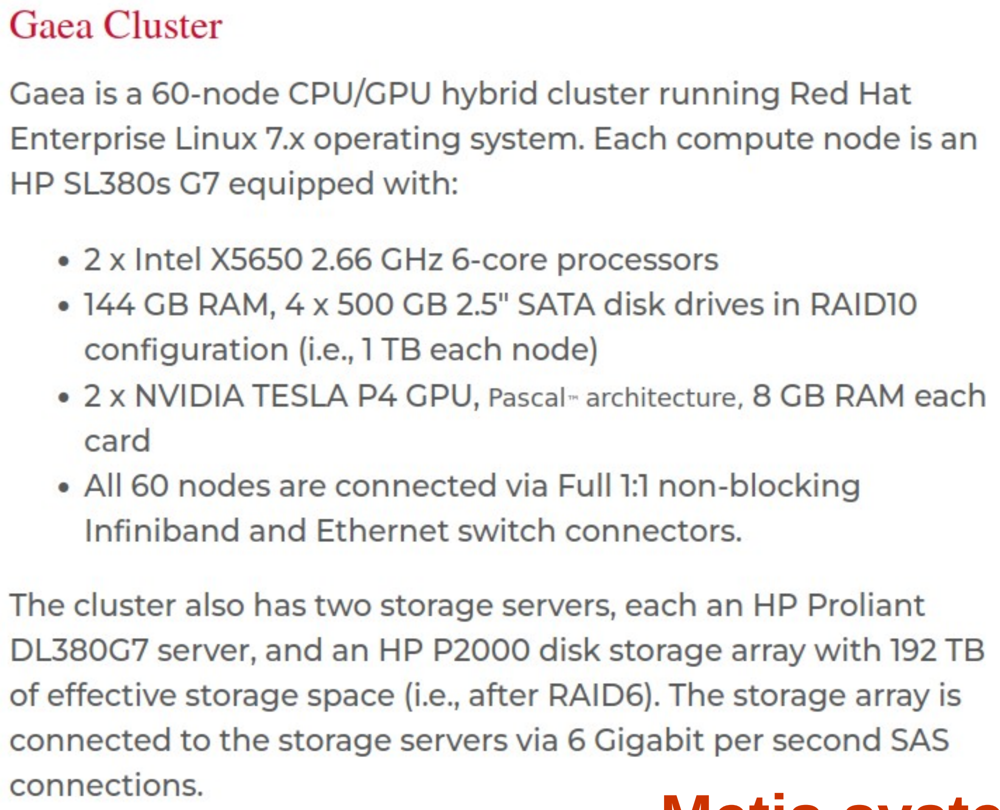
PIs



Users

The success of GAEA in attracting external funds allowed obtain NIU’s financing for the Metis system (Gerald Blazey, CRCD team, DoIT)

NIU HPC Systems specification

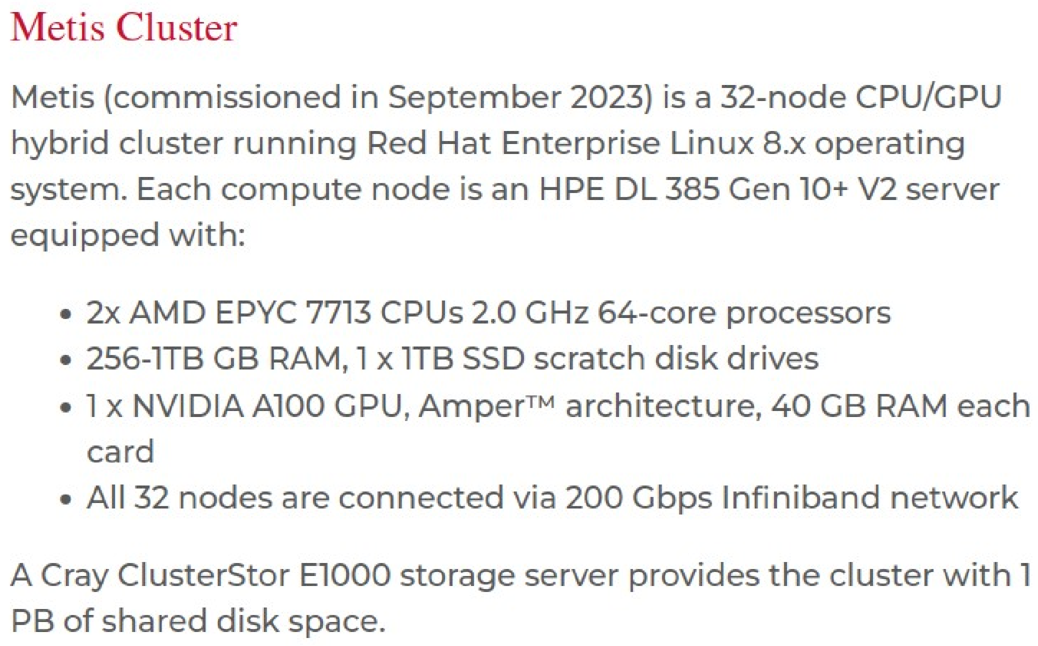


Gaea Cluster

Gaea is a 60-node CPU/GPU hybrid cluster running Red Hat Enterprise Linux 7.x operating system. Each compute node is an HP SL380s G7 equipped with:

- 2 x Intel X5650 2.66 GHz 6-core processors
- 144 GB RAM, 4 x 500 GB 2.5" SATA disk drives in RAID10 configuration (i.e., 1 TB each node)
- 2 x NVIDIA TESLA P4 GPU, Pascal™ architecture, 8 GB RAM each card
- All 60 nodes are connected via Full 1:1 non-blocking Infiniband and Ethernet switch connectors.

The cluster also has two storage servers, each an HP Proliant DL380G7 server, and an HP P2000 disk storage array with 192 TB of effective storage space (i.e., after RAID6). The storage array is connected to the storage servers via 6 Gigabit per second SAS connections.



Metis Cluster

Metis (commissioned in September 2023) is a 32-node CPU/GPU hybrid cluster running Red Hat Enterprise Linux 8.x operating system. Each compute node is an HPE DL 385 Gen 10+ V2 server equipped with:

- 2x AMD EPYC 7713 CPUs 2.0 GHz 64-core processors
- 256-1TB GB RAM, 1 x 1TB SSD scratch disk drives
- 1 x NVIDIA A100 GPU, Amper™ architecture, 40 GB RAM each card
- All 32 nodes are connected via 200 Gbps Infiniband network

A Cray ClusterStor E1000 storage server provides the cluster with 1 PB of shared disk space.

Metis system highlights

- 32 nodes, (128 2.0 GHz cores, A100 GPU, 256 GB RAM, 1 TB SSD scratch)/node
- RHEL 8.x Linux, PBSpro batch system, 1 PB Lustre scratch disk, 200 Gbps network
- Maximum theoretical performance in 64-bit TeraFlops (131 GPUs, 310 GPUs)
- For some applications be treated as a single computer with 4096 CPU cores

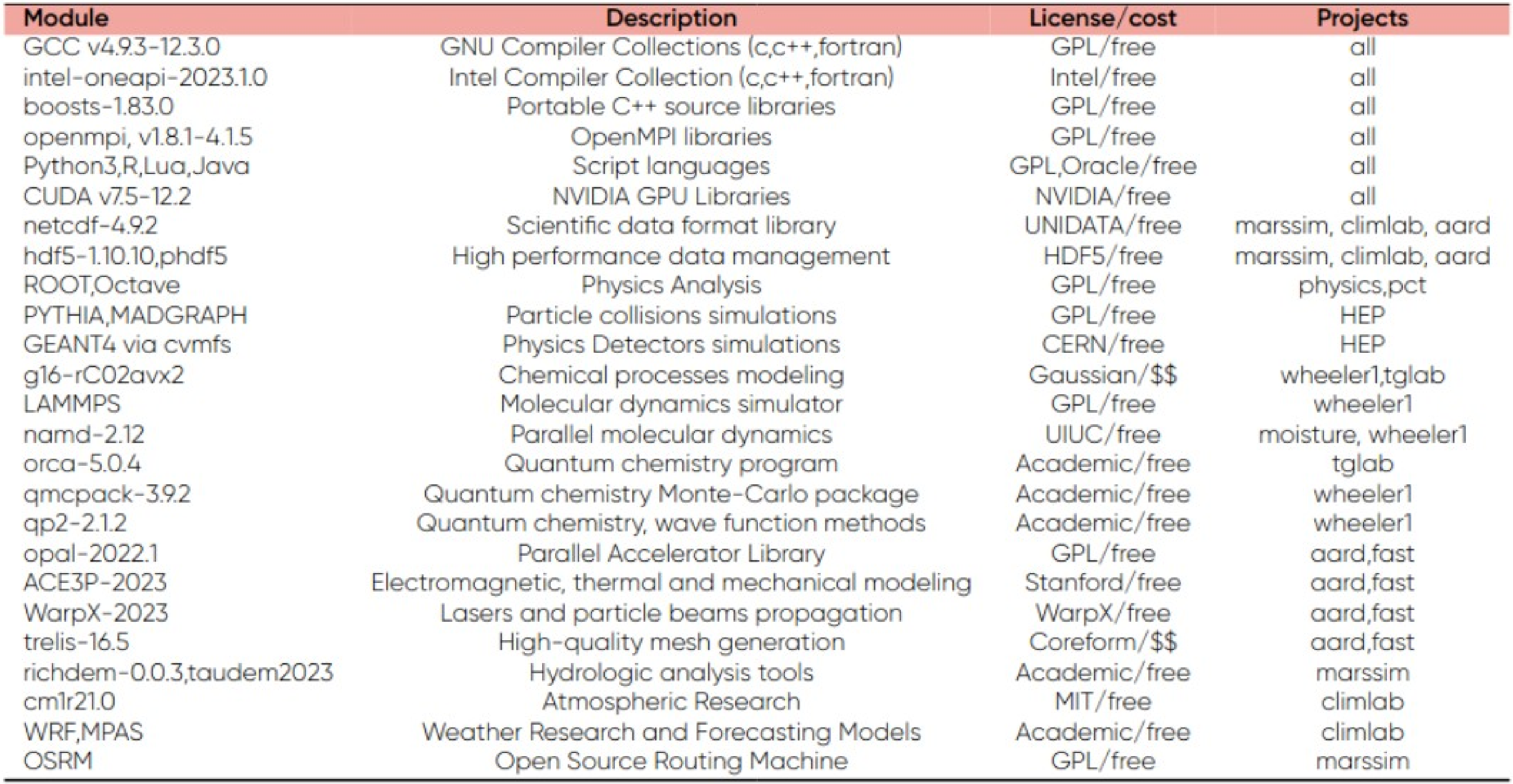
Metis favorites

- Tasks optimized OpenMPI-OpemMP-GPUs (can use all resources simultaneously)

- Single CPU instances of less than 2GB RAM running simultaneously

NIU HPC software installations

CRCD supported software at Metis, RHEL 8.x, October 2023



Module	Description	License/cost	Projects
GCC v4.9.3-12.3.0	GNU Compiler Collections (c,c++,fortran)	GPL/free	all
intel-oneapi-2023.1.0	Intel Compiler Collection (c,c++,fortran)	Intel/free	all
boosts-1.83.0	Portable C++ source libraries	GPL/free	all
openmpi, v1.8.1-4.1.5	OpenMPI libraries	GPL/free	all
Python3,R,Lua,Java	Script languages	GPL,Oracle/free	all
CUDA v7.5-12.2	NVIDIA GPU Libraries	NVIDIA/free	all
netcdf-4.9.2	Scientific data format library	UNIDATA/free	marssim, climlab, aard
hdf5-1.10.10,phdf5	High performance data management	HDF5/free	marssim, climlab, aard
ROOT,Octave	Physics Analysis	GPL/free	physics,pct
PYTHIA,MADGRAPH	Particle collisions simulations	GPL/free	HEP
GEANT4 via cvmfs	Physics Detectors simulations	CERN/free	HEP
g16-rC02avx2	Chemical processes modeling	Gaussian/$$	wheeler1,tglab
LAMMPS	Molecular dynamics simulator	GPL/free	wheeler1
namd-2.12	Parallel molecular dynamics	UIUC/free	moisture, wheeler1
orca-5.0.4	Quantum chemistry program	Academic/free	tglab
qmcpack-3.9.2	Quantum chemistry Monte-Carlo package	Academic/free	wheeler1
qp2-2.1.2	Quantum chemistry, wave function methods	Academic/free	wheeler1
opal-2022.1	Parallel Accelerator Library	GPL/free	aard,fast
ACE3P-2023	Electromagnetic, thermal and mechanical modeling	Stanford/free	aard,fast
WarpX-2023	Lasers and particle beams propagation	WarpX/free	aard,fast
trelis-16.5	High-quality mesh generation	Coreform/$$	aard,fast
richdem-0.0.3,taudem2023	Hydrologic analysis tools	Academic/free	marssim
cm1r21.0	Atmospheric Research	MIT/free	climlab
WRF,MPAS	Weather Research and Forecasting Models	Academic/free	climlab
OSRM	Open Source Routing Machine	GPL/free	marssim

Both CPU and GPU based packages supported up to the most recent versions (79 unique packages and 274 accounting for different versions).

HPC software use

https://www.niu.edu/crcd/current-users/crnt-users-software.shtml

CRCD installations

- Accessible via environment modules

```
module av; module load; module purge
```

Python modules

- pip3 manager

```
pip3 install pkgName
```

- conda manager
- conda create -name=p39tst python=3.9
- conda activate p39tst
- conda install pkgName

Personal installations

- Can be build from source under

/opt/metis/el8/ucontrib

Jupyter notebooks

- Install Jupyter notebook

```
pip3 install jupyter
pip3 install urllib3=1.26.6
```

- Launch a notebook at a port xxxxx

```
jupyter notebook –no-browser \
–port=xxxxx  -ip=0.0.0.0
```

- Connect via instructions at CRCD page

CVMFS based software libraries

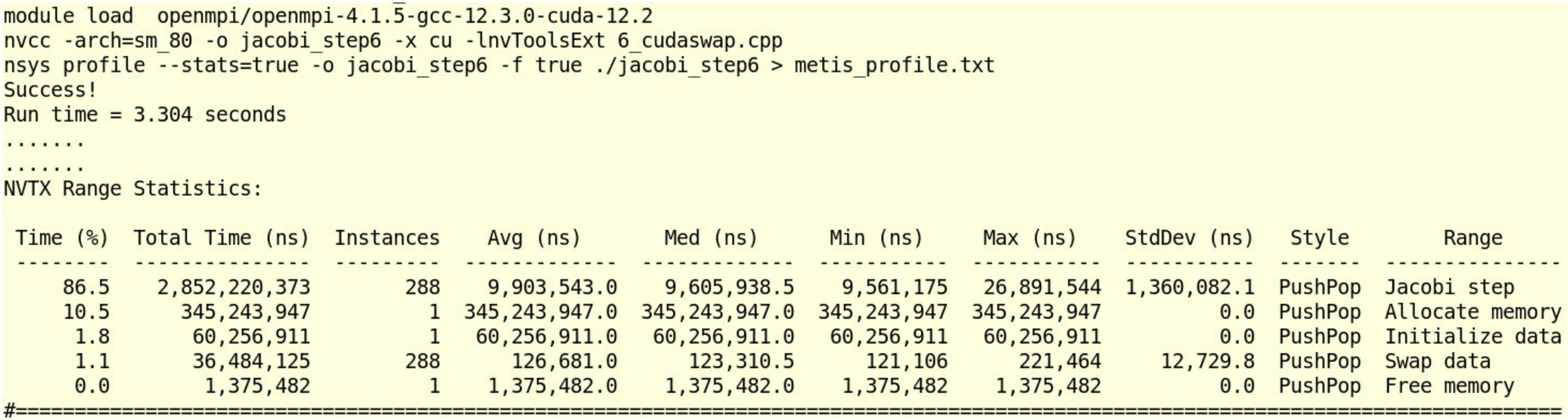
- Pre-mounted for ATLAS (/opt/atlas) and CMS (/opt/osg/cmssoft) repositories

CRCD installs and supports “tagged” versions
and provides resources for users applications under development

A note on a code quality

Nvidia A100 GPU on a Metis worker node, runtime 3.3 sec

(down from 23 sec for non-optimized code)

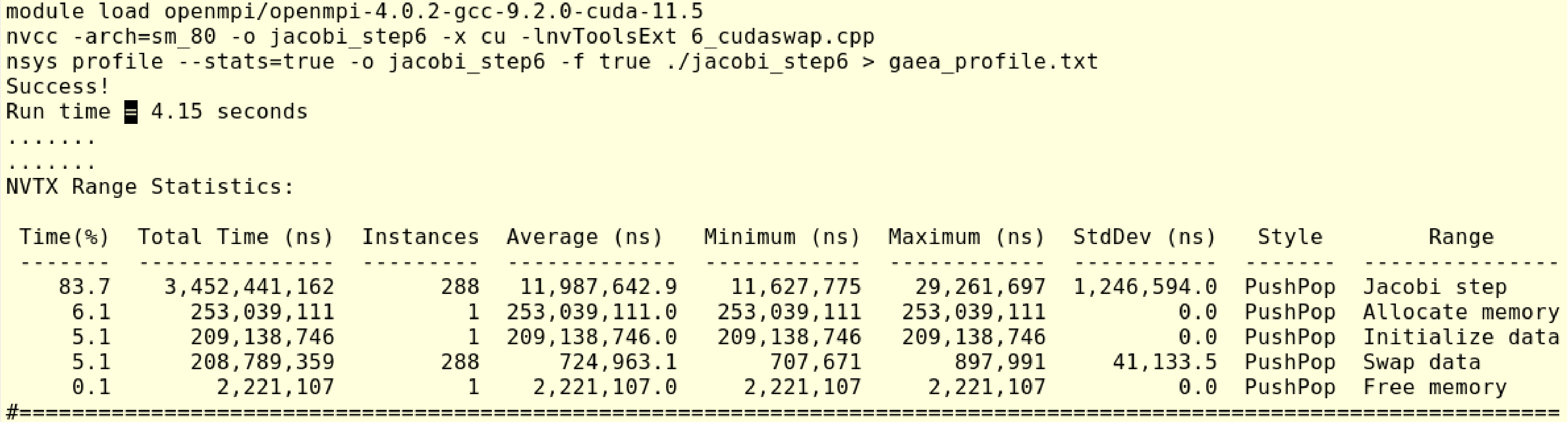


```
module load  openmpi/openmpi-4.1.5-gcc-12.3.0-cuda-12.2
nvcc -arch=sm_80 -o jacobi_step6 -x cu -lnvToolsExt 6_cudaswap.cpp
nsys profile --stats=true -o jacobi_step6 -f true ./jacobi_step6 > metis_profile.txt
Success!
Run time = 3.304 seconds
.......
.......
NVTX Range Statistics:

 Time (%)  Total Time (ns)  Instances    Avg (ns)       Med (ns)      Min (ns)     Max (ns)    StdDev (ns)   Style        Range
 --------  ---------------  ---------   -------------  -------------  -----------  -----------  -----------   -------  ---------------
     86.5    2,852,220,373        288     9,903,543.0    9,605,938.5    9,561,175   26,891,544  1,360,082.1   PushPop  Jacobi step
     10.5      345,243,947          1   345,243,947.0  345,243,947.0  345,243,947  345,243,947          0.0   PushPop  Allocate memory
      1.8       60,256,911          1    60,256,911.0   60,256,911.0   60,256,911   60,256,911          0.0   PushPop  Initialize data
      1.1       36,484,125        288       126,681.0      123,310.5      121,106      221,464     12,729.8   PushPop  Swap data
      0.0        1,375,482          1     1,375,482.0    1,375,482.0    1,375,482    1,375,482          0.0   PushPop  Free memory
#=====================================================================================================================================
```

Nvidia P4 GPU on Gaea worker node, runtime 4.2 sec

(down from 100 sec for non-optimized code)



```
module load openmpi/openmpi-4.0.2-gcc-9.2.0-cuda-11.5
nvcc -arch=sm_80 -o jacobi_step6 -x cu -lnvToolsExt 6_cudaswap.cpp
nsys profile --stats=true -o jacobi_step6 -f true ./jacobi_step6 > gaea_profile.txt
Success!
Run time = 4.15 seconds
.......
.......
NVTX Range Statistics:

 Time(%)  Total Time (ns)  Instances   Average (ns)   Minimum (ns)  Maximum (ns)  StdDev (ns)    Style        Range
 -------  ---------------  ---------   -------------  ------------  ------------  -----------  -------  ---------------
    83.7    3,452,441,162        288    11,987,642.9    11,627,775    29,261,697  1,246,594.0  PushPop  Jacobi step
     6.1      253,039,111          1   253,039,111.0   253,039,111   253,039,111          0.0  PushPop  Allocate memory
     5.1      209,138,746          1   209,138,746.0   209,138,746   209,138,746          0.0  PushPop  Initialize data
     5.1      208,789,359        288       724,963.1       707,671       897,991     41,133.5  PushPop  Swap data
     0.1        2,221,107          1     2,221,107.0     2,221,107     2,221,107          0.0  PushPop  Free memory
#=======================================================================================================================
```

Programming skills matter – a small run-time difference for a well optimized code

Metis policies

1. Default home directory quote is 25 GB; use /lstr/sahara/projectName/userName to store input and output (potentially large) data and to run batch jobs.

2. Only short test runs (<30 min) are allowed at the metis login node. Production jobs should be submitted via the batch system.

3. For each job the batch system reserves a requested set of resources: [(number of required CPUs, GPUs, amount of memory) x N_instances, the requested walltime]

4.Several instances can be dispatched to the same node. It is critical to estimate the required resources accurately.

5. We provide the batch system example with detailed explanations of the batch script language. Copy, test and modify /home/examples/examples-metis/cuda-mpi-pbs.

6. We only provide the previous day snapshot of the /home folder, /nfs/ihfs/home_yesterday. We recommend to use GitHub repositories for code development and frequently backup important data and results to remote locations.

7. Acknowledgment statement: **“This work used resources of the Center for Research Computing and Data at Northern Illinois University.”**

Metis is a shared system. Mutual accuracy is vital.

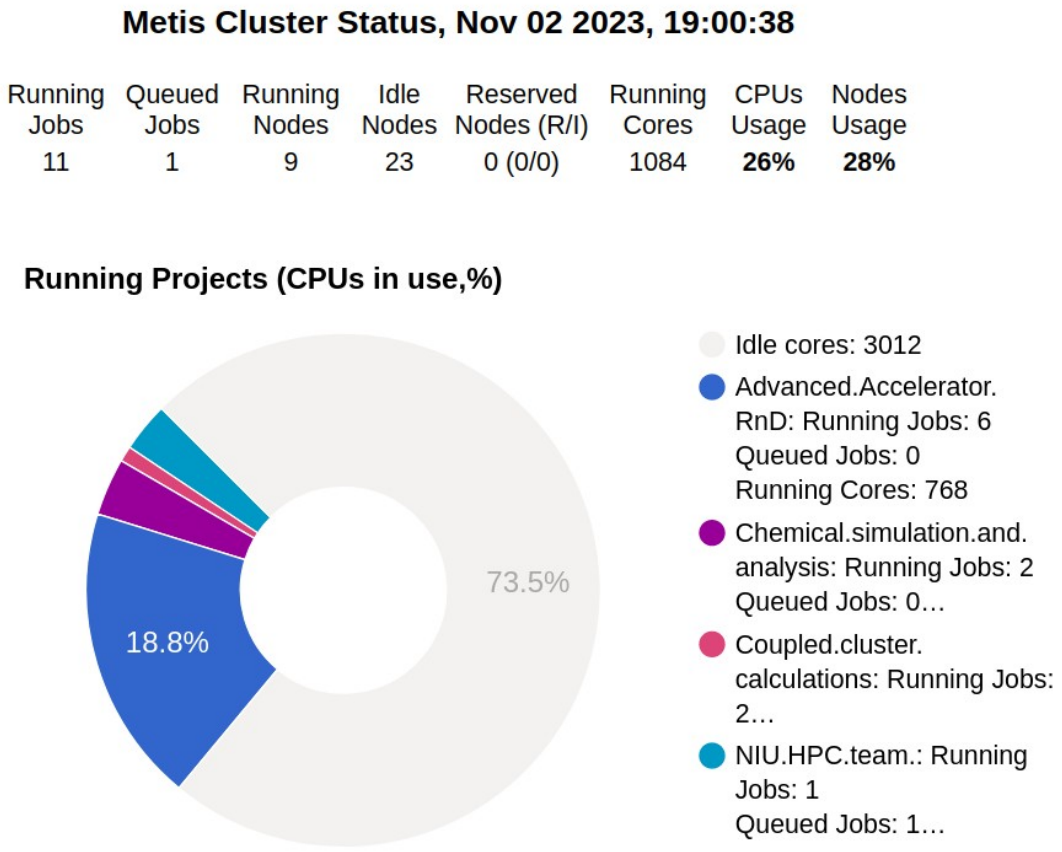
Current Operations - crcd.niu.edu

About ▾ Prospective Users ▾ Current Users ▾ CRCD at Work ▾

Center for Research Computing and Data

CRCD web site provides:

- real-time system status
- cluster usage policies
- detailed access instructions for beginners
- hardware and software documentation
- quick-start examples
- job monitoring tools
- contact information



Metis Cluster Status, Nov 02 2023, 19:00:38

Running Jobs	Queued Jobs	Running Nodes	Idle Nodes	Reserved Nodes (R/I)	Running Cores	CPUs Usage	Nodes Usage
11	1	9	23	0 (0/0)	1084	**26%**	**28%**

Running Projects (CPUs in use,%)

18.8%
73.5%
Idle cores: 3012
Advanced.Accelerator. RnD: Running Jobs: 6 Queued Jobs: 0 Running Cores: 768
Chemical.simulation.and. analysis: Running Jobs: 2 Queued Jobs: 0…
Coupled.cluster. calculations: Running Jobs: 2…
NIU.HPC.team.: Running Jobs: 1 Queued Jobs: 1…

The site accumulates the CRCD experience since its foundation; the first stop for new users.

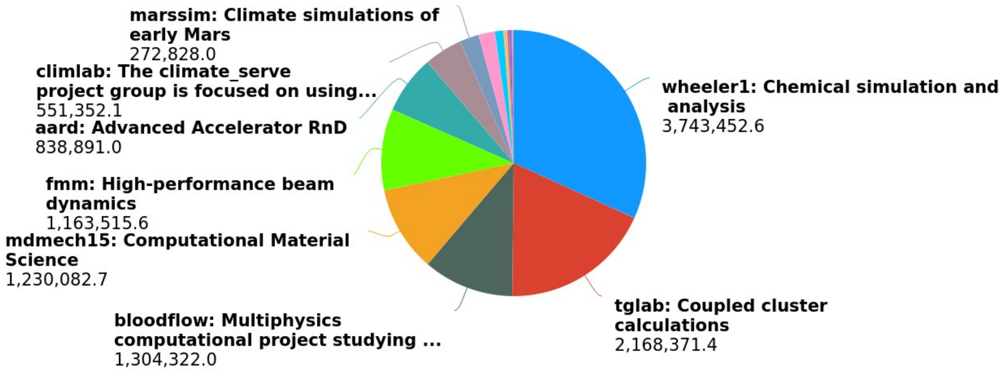
HPC usage metrics (Oct 2020 – Oct 2023)

- System availability ~100%
- Nodes availability 90 - 100%
- System load 57 – 88%
- Number of users/month 13 - 24
- Number of PIs/month 8 - 14

Gaea file systems:
used (total)
/home - 3 (10) TB
/data1 – 59 (85) TB
/data2 – 56 (80) TB

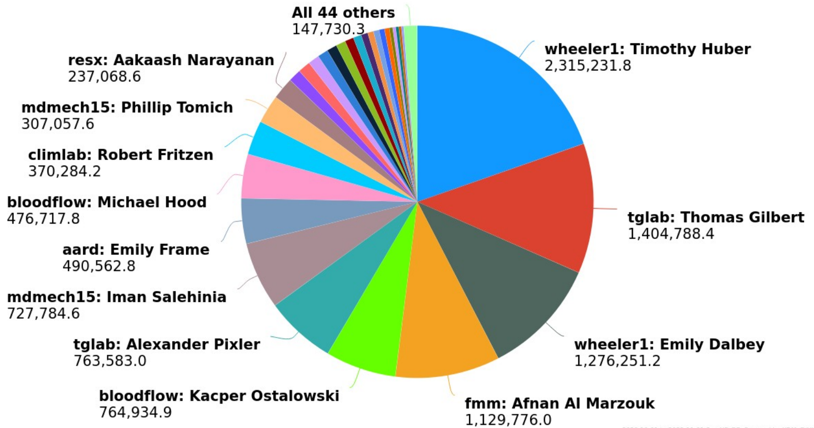
Mets file systems:
used (total)
/home - 2 (20) TB
/opt - 2 (15) TB
/lstr/sahara – 24 (848) TB

GAEA Job Wall Time by Project, CPU cores x Hours



2020-10-01 to 2023-11-01 Src: HPcDB. Powered by XDMoD/Highch

GAEA Job Wall Time by User, CPU cores x Hours



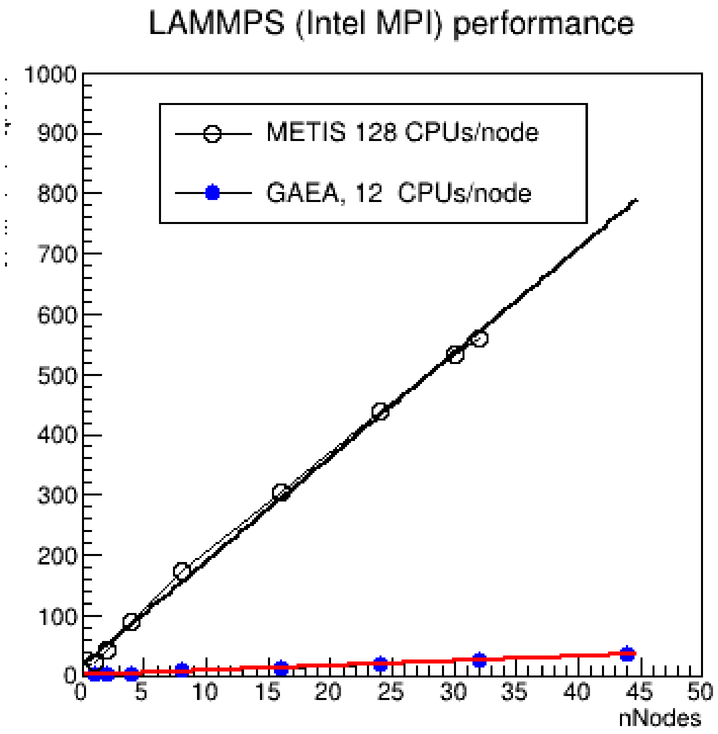
2020-10-01 to 2023-11-01 Src: HPcDB. Powered by XDMoD/Highcharts

We provide resources both for “large” and “small” projects.

Plans

Metis

- Study and tune up the system performance
- Possible nodes upgrade (memory and scratch drives)
- The base system for next years



Gaea

- System upgrade to Alma Linux8 in April (a long shutdown is expected)
- We may keep Gaea running after 2024 but only as a supporting system
- Please switch to Metis by Spring 2024

Nicadd

- Will continue maintain data servers and desktops
- Compute nodes will be eventually retired

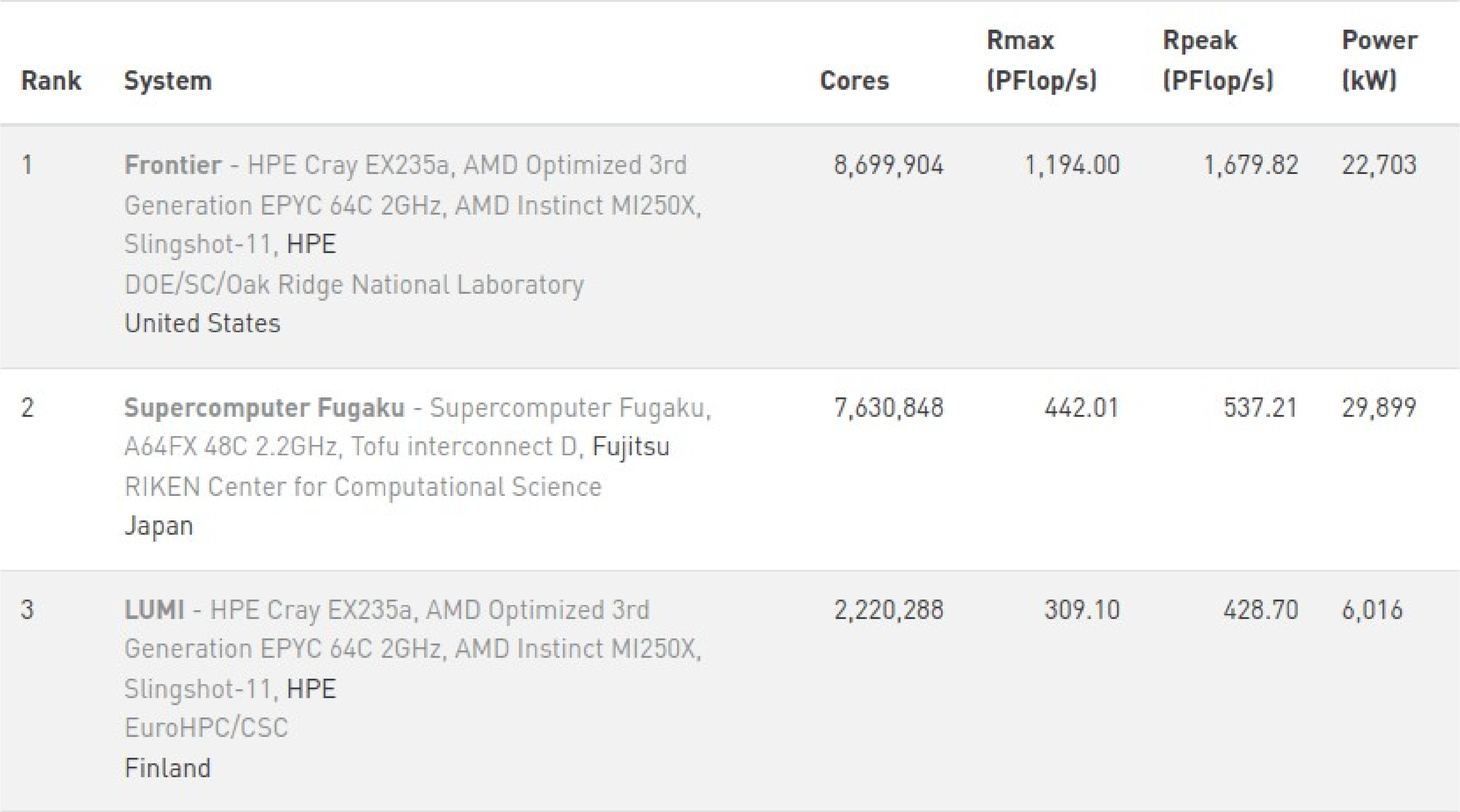
Summary

- Years of successful operations of CRCD facilities
- METIS system is up and running
- We are welcoming new users

Backup Slides

Top HPC systems

https://www.top500.org/lists/top500/2023/06/



Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016