1) CCB High Performance Computers (HPC)

Inventory counts and other details related to CCB's HPC clusters.

List does not include Linux file servers under ChemIT management. Add later?

See also

- aaClusters moving to CAC
- Cluster and HPC maintenance schedules

CCB Clusters, summary information

The following counts include **head nodes** and **compute nodes**.

- Details on our counts, including historical counts.

Columns needed - software installed / managed (do per cluster), Nodes/Cores, Age, storage (head/compute) and related (RAID: h/w or s/w?)

Cluster name	Number of node (HN and CN's)	ChemIT / other support	DNS name (may have CNAME)	Two-step (Duo) option for access NOTE: If so, still offers VPN alternative access	IP Gateway	Internal network	ChemIT Network	Headnode IPMI Network	Headnode OS	OS Version	Provisioning software	Provisioning software version
Ananth	41	CAC	astra.cac.cornell.edu		128.84.3.66		N/A	N/A	CentOS	6.2	Rocks	
Collum-Loring-Abruna-Widom "CLAW" Cluster	??	ChemIT	boltzmann.chem.cornell.edu	As of 1/18/17: Duo installed, NOT enabled	10.253.229.28	172.0.50.x	192.168.255.50	192.168.255.51	CentOS	6.6	Warewulf	
Hoffmann	28	ChemIT	sol.hoffmann.chem.cornell.edu		128.253.229.81	172.0.100.x	192.168.255.100	192.168.255.101	CentOS	6.4	Warewulf	3.4
Lancaster (w/ Crane)	11	ChemIT	revc.lancaster.chem.cornell.edu		128.253.229.213	172.0.60.x	none	192.168.255.61	CentOS	6.5	Warewulf	3.4
Scheraga	95	ChemIT	scheraga.chem.cornell.edu		128.253.229.65		192.168.255.1	192.168.255.5	Centos	6.5	Warewulf	
ChemIT (C4)	1	ChemIT	cluster.chem.cornell.edu		10.253.229.9		192.168.255.110	none	CentOS	6.4 from 6.2	Warewulf	
Totals:												

Deprecated Chemistry Clusters, summary info

Cluster name	Number of node (HN and CN's)	ChemIT / other support	DNS name (may have CNAME)	IP Gateway	Internal network	ChemIT Network	UPS for headnode See: UPS inventory and status	Upgrade status

Abruna (as stand-alone) (see Collum-Loring-Abruna-Widom "CLAW" Cluster)	10	ChemIT	Used to be: hartree.chem.cornell.edu	Used to be: 10.253.229.249		Used to be: 192.168.255.30		4/14: No h/w upgrades planned.
Collum (as stand-alone) (see Collum-Loring-Abruna-Widom "CLAW" Cluster)	9	ChemIT	Used to be: tera.collum.chem.cornell.edu	Used to be: 10.253.229.248	Used to be: 172.0.40.x	Used to be: none	Used to be: Yes (Where is this used now?!)	Fall'13: Upgraded OS and added 2 nodes

CCB non-cluster HPCs, summary information

Inventory and summary notes regarding non-cluster HPC systems in 248, including computational stand-alone systems.

Columns needed - software installed / managed (do per system; dedicated page?), Cores, Age, storage and related (RAID: h/w or s/w?)

Name of system, and purpose	ChemIT / other support	DNS name (may have CNAME)	IP Gateway	ChemIT Network	Headnode IPMI Network	OS	OS Version	UPS See: UPS inventory and status	Maintenance window	Upgrade status	
Baird: 1 rack-mounted computational computer	ChemIT	as-chm-bair-08.ad.cornell.edu compute.baird.chem.cornell.edu	10.253.229.178	192.168.255.120	192.168.255.121	Windows Server	2012R2	NONE			
Freed: Eldor	ChemIT	eldor.acert.chem.cornell.edu	10.253.229.96	192.168.255.87		CentOS	6.4	NONE			
Petersen: 2 rack-mounted computational computers	ChemIT	calc01.petersen.chem.cornell.edu calc02.petersen.chem.cornell.edu	10.253.229.196/192		192.168.255.54/55	Centos	7.2v1511	Yes			
Scheraga: 4 GPU rack-mounted computational computers	ChemIT	gpu.scheraga.chem.cornell.edu	10.253.229.70	192.168.255.139	192.168.255.138	CentOS	6.4	NONE			
								See: UPS inventory and status			

Index to the many children pages of this page

aaClusters moving to CAC

Documentation page place-holder for collecting information related to having current Chemistry IT-managed clusters (in 248 Baker Lab) moved to CAC.

- Why move Chemistry's clusters from Baker to CAC? — Printable PDF flyer (800px*2000px)

Abruna Cluster

ChemIT Cluster

Collum Cluster

8 compute nodes, 1 head node. Details on this page.

Collum-Loring-Abruna-Widom "CLAW" Cluster

Cluster built on Widom's headnode. 1 headnode and xx compute nodes.

Freed Acert Eldor HPC

Non-cluster HPC

Hoffmann Cluster

Lancaster Crane Cluster

Petersen Independent Nodes

Scheraga Cluster

Upgrading summer 2014.

- Matrix compute nodes — Table containing node numbers and hardware information.
    - Processor info and core counts — Matrix has 952 typical processor cores when all nodes are connected. It turns out Matrix can have as many as 9,144 cores if it could utilize 4 nodes with GPUs, which themselves contain yet another 8,192 cores! However, these additional GPU-based cores require specialized programming and have are not to-date been made available to researchers via the cluster. Those cores have only been accessible to researchers accessing these specialized nodes provisioned as workstations (and thus not attached
- Matrix end-user documentation
    - Matrix end-user application information — Details for end-users regarding their applications on Matrix, including who the group contact.
    - Matrix end-user documentation, from ChemIT — The new Matrix is faster, but it is different. Learn about the differences here to reduce your aggravation.
    - Matrix end-user documentation, from Group
    - Matrix user job limits
- Matrix users information (name, netid, status, quota) — On Matrix, researcher have both a quota for their home directory (keep as small as reasonable), and a quota for their storage directory.
- Scheraga Synology

zClarifying cluster responsibilities and ownership

Effective use of a cluster for research is enhanced with clarity of roles and responsibilities, along with shared conventions and procedures.

- Buying or adding to a cluster — Technical considerations when buying a new cluster, or adding to an existing cluster. Also applies to other high performance computing (HPC) systems.
- Lancaster and Crane's cluster — Lancaster and Crane share a headnode, so social conventions are required to ensure researchers are not negatively surprised.
- Roles and responsibilities for clusters managed by ChemIT
    - Cluster application software specifics — Various scientific applications are used on CCB clusters. In general, Research Groups are responsible for knowing their software. In many cases, ChemIT staff can assist researchers, but cannot take responsibility or expend unlimited effort.

zCluster backups and related considerations

Although there may be unique considerations regarding backups for high performance computer systems, including cluster, see first Backups and file storage options for research groups.

zCluster Computational Software

Computational software installed on CCB clusters, and who supports and manages which software.

zCluster counts details and history

Inventory counts of CCB's HPC computers, clusters only.

zConnecting to Clusters

zMaintenance and emergency procedures

Clusters and other high performance servers require maintenance. Documented procedures reduce surprises for both enabling scheduled maintenance and emergency work.

- Cluster and HPC maintenance schedules — Regular maintenance of clusters requires downtime. A maintenance schedule can reduce surprises and not unnecessarily delay required maintenance.
    - Cluster Maintenance SOP — This page includes a checklist for preparing any maintenance work, and a listing of the sequence of steps to take.
    - Templates of notification emails

zStorage for HPCs and other systems

Sometimes a local hard drive(s) is all you need. But often the right solution is something else. Look here for info. related to alternatives, some of which are successfully used in production and very cost-effective.

zUseful Linux HPC commands

- Linux commands — Commands Oliver wants to keep track of, at a minimum.