Servers, HPC systems, NMR lab, CAC, and AWS

Public-facing inventory of servers and the like in CCB, most of which are managed by ChemIT.
For a snapshot inventory, and the costs to CCB if they were hosted elsewhere, see ChemIT's spreadsheet in <R:\Chem IT\Projects & Tracking>. The data and analysis is in spreadsheet, "Chem IT Support & Services", tab "Alternative server costs".

1) CCB High Performance Computers (HPC)

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

- 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.
    - Matrix end-user documentation
    - 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
- 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.
- 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.

2) CCB non-HPC servers in 248 Baker Lab and AWS

Inventory and summary notes regarding non-cluster systems in 248 and AWS, including computational stand-alone systems, web servers, and file servers.

- Chemistry IT's AWS servers — Test migration: License server, Stockroom Apps, etc.

3) CCB NMR instrumentation systems

NMR's instrument machines, both Linux and Windows.

Linux software

- Oliver's demo of TOC

Power outage records, procedures, and to-do's

Summer 2013 and winter 2014, there were an inordinate number of power outages in Baker Lab, and other Chem buildings!

- ChemIT's record of recent power outages
    - Power outage record for Monday, April 11th — The impact on Chemistry's IT of about 40 minutes of unexpected power outage.
- UPS inventory and status — A snapshot of the UPS's used to support servers, switches, and other equipment under ChemIT's management. Mostly within ChemIT's Baker 248 server room.

Server costs if to use non-ChemIT alternatives