

CCMR-ICSE Computer Cluster description & FAQ's

The Cornell Institute for Computational Science and Engineering (ICSE), in conjunction with the CCMR and a generous Intel donation, can now provide powerful research computing capabilities at a minimal charge. An Intel donation of 180 fast Xeon core processors (E5-2660v3 chip) form the CCMR-ICSE computer cluster, structured into nine 20-core systems. Each system has 96 GB of RAM and the cluster has over 200 TB of storage.

The CCMR-ICSE computer cluster will be housed in the ICSE computing facilities in Olin Hall at Cornell. This facility has extensive experience in high-performance computing and server management and will be available to students for software and programming support.

The ICSE Facilities operate on a fee-for-service basis. Any Cornell faculty who choose to use the cluster also have access to its software licenses (Matlab, Gaussian09, Materials Studio, *etc.*) as well as our large disk storage at no additional cost. More details on software, services and costs are covered below and on request *via* email (help@icse.cornell.edu).

The new CCMR-ICSE cluster consists of **nine 20-core systems**. Each of the 180 processors is a fast Intel Xeon E5-2660v3 chip. Each of the nine systems has 96 GB of RAM. The ICSE facilities have extensive disk storage (over 200 TB, compressed) available using the ZFS system.

We are expecting this cluster and use of the ICSE computing facilities to appeal to research groups in the following categories:

- Do *not* have, nor plan to have, their own computer cluster, but do have research computing needs.
- Need computing resources intermittently and want an 'easy in-easy out' arrangement.
- Would like to have access to software, such as Gaussian, Matlab, Materials Studio, *etc.*, without having to pay for the license(s).
- Do have their own cluster, but want access to software licenses that ICSE holds, or want access to extensive disk storage, or be part of a dynamic facility that keeps abreast of the latest advances in O/S and file services
- Enjoy the ability to get help with software, or programming support for graduate students, *etc.*
- Need to run extremely long jobs (our longest batch queue allows jobs to run for 90 days) that cannot be check-pointed (restarted from the end of the preceding run).
- Need to run jobs with large memory and/or have large storage needs, *e.g.*, for imaging.

A page of FAQs on using the new CCMR-ICSE cluster follows.

If you have questions on using the new cluster, contact Paulette Clancy; pc@icse.cornell.edu or Paulette.Clancy@cornell.edu

Frequently Asked Questions about the new CCMR-ICSE Computing Cluster

1. **Who has access to the cluster?** All Cornell faculty and researchers. Non-Cornell users should contact pc@icse.cornell.edu.
2. **What do you charge to use the cluster?** Unless you become a large user of the cluster, all groups will be charged \$250 per month to access the machines and take advantage of the existing ICSE infrastructure (firewalls, file servers, disk storage, etc.).
3. **Is that \$250/month charge per student?** **No.** The \$250/month covers *all* the students in a research group, whether that is 1 student or 10 students!
4. **Can post-docs, M.Eng., and undergraduate researchers use the cluster?** Yes, as long as they are members of a participating research group and faculty can vouch for them.
5. **How secure are the data?** We have a remote disaster recovery set-up in Rhodes Hall to which files are incrementally backed-up nightly. Backup of the Olin files is performed every night. We have duplicate disks that shadow each other's activity. The servers are also duplicated and protected by a UPS. There is one A/C unit in the facilities; if that failed, we would be down until it was fixed.
6. **I do imaging (or massive CFD calculations, or many other possible reasons) and need a lot of memory and storage capability. What resources do you have for that?** We have a file storage capability of over 200 TB of disk. To put this in context, most people's students use about 1 TB, but we have had users with needs of ~10 TB.
7. **Do I have to write a proposal to get an account on the CCMR-ICSE cluster?** **No.** Just send us a list of netIDs in your group and a start date and we can get you set up within 24 hours, typically. Our accounts person will then ask you for an account number.
8. **Prof. X and Prof. Y want to work on a joint project, do they each have to pay the usage fee?** **Probably.** We would make an exception if only one or two students are involved between the two groups. Typically we don't offer 'two for the price of one' deals—but feel free to ask.
9. **I have my own cluster; will you manage it?** Yes, we will manage your private cluster for you at a competitive price that scales non-linearly with increasing number of processors.
10. **I don't have my own computers, but I need access to computing resources. What can ICSE do to help?** We have a pool of shared computers that you can use, as and when you need it.
11. **What is your up-time and anti-hacking record like?** We have an outstanding uptime record. We have never been hacked in over 10 years (to our knowledge, at least).
12. **How is the ICSE Facility different from other Cornell facilities?** We share some common services with other computing facilities, but some are unique to ICSE.

Points of distinction include:

- ICSE's Facilities have a pool of shared computers for users to use. No need to buy your own machines. Most other facilities do not have this option in their business model.
- We offer the ability for research groups to join and leave easily, as their computing needs dictate.
- We do not charge for consulting on software or hardware issues.
- We employ a commercial batch queuing system, NBS (Network Batch System) that ensures "fair play" for users to prevent any one user or one group from dominating use of the facilities.
- ICSE continually advances the capabilities of the infrastructure. For example, we constantly search for better security, faster network communications, new file system capabilities (*e.g.*, ZFS), etc. In other facilities, your cluster's system typically remains static until you tell the system manager to change it. At ICSE, we are constantly looking

for ways to implement state-of-the-art system management to improve services for our clients.

- ICSE provides access to our software licenses at no additional charge. There is a shared pool of software licenses that we provide. This includes codes such as Gaussian 09, Matlab, Materials Studio, etc. We also provide access to freeware without you having the trouble of setting them up correctly; examples include LAMMPS, Quantum Espresso, etc. If your particular code/suite of programs is not mentioned, contact us to discuss.
- ICSE provides access to *a lot* of shared disk space, which is great for experimentalists and computational people alike. We have 200 TB of compressed storage; typical users have <1TB of disk storage, though we do have one user with over 10 TB of disk space.
- We are still a relatively small community, which allows us to tailor our policies to help our clients.

ICSE Facilities Software List: A partial list of the software on our facilities includes the following

Abinit	Boost	Charmm	Comsol	Cplex	Cplot
DFT	DL-Poly	Espresso**	Gromacs	gurobi	Intel fortran
LAMMPS	Matlab	mmts	mpich	MySQL	nMOLDYN
NWChem	octave	openMPI	PGI fortran*	plumed	python
Qchem	R	Schrodinger	TINKER		

*Portland Group fortran compiler (required for VASP)

** Including Quantum Espresso

Note- We do not yet have VASP, but are looking into its acquisition.