## Cumulative HPC totals at Emerson Center:

**834 cores @ ~2.37GHz CPU**
**1.8TB RAM**
**48.9TB storage**

### Technical Details:

### 1. Front-end servers:

**euch6h** 43P 260 Power3 AIX5 200MHz 1-core 1GB RAM 25GB SCSI LL router
**wombat** 44P 170 Power3 AIX5 333MHz 1-core 0.5GB RAM 35GB SCSI LL server
**euch4e** 28P 6E4 Power3 AIX5 333MHz 1-core 2GB RAM 136GB SCSI NFS file server + user account sever + Mail and job submission front-end server + default login + LL alternative server
**euch3f** 44P 170 Power3 AIX5 333MHz 1-core 2GB RAM 17GB SCSI LL router + IBM software server
**euch2c** 29P 6E3 Power AIX5 333MHz 1-core 1GB RAM 136GB SCSI LL router
**P710** IBM AIX6 Server 4-core 8GB RAM 570 GB SAS backup server
**P710** IBM AIX6 Server 4-core 8GB RAM 570 GB SAS backup server

### Compute Clusters:

### A. star

"Microway 2U Server" Opteron 6128 2.0GHz 8-core 16GB RAM 3.5TB SATA STAR user account and job submission server; SuSe 11 Enterprise, 64 bit Linux

**star-nodes:**

7 "Microway 2U chassis" Opteron 6174 2.2GHz 24-core 80GB RAM 600GB SAS STAR compute nodes for 24-way parallel jobs
24 "Microway 2U chassis" Opteron 6134 2.3GHz 16-core 32GB RAM 1.2TB SAS STAR compute nodes for 16-way parallel jobs
5 "Microway 2U chassis" Opteron 6174 2.3GHz 16-core 16GB RAM 1.2TB SAS STAR compute nodes for 8-way parallel jobs
**star totals: ~2.3 MHz CPU w/ 624 core + 1.4TB RAM + 41.3TB storage**

### B. wind

"Team HPC 2U Server" Opteron 2.8 GHz 4-core 8GB RAM 584GB SAS WIND user account and job submission server; SuSe 10 Enterprise, 64 bit Linux

**wind-nodes:**

1 - 32 "Team HPC 1U chassis" Opteron 3.0 GHz 4-core 8GB 146GB SAS compute nodes for parallel & sequential jobs
**wind totals: 3.0GHz CPU w/ 132 core + 264GB RAM + 5.2TB storage**

### C. fire

SUN Fire V40z Opteron 2.2 GHz 2-core 4GB RAM 146GB SAS FIRE user account and job submission server; PGI Fortran server; graphics; SuSe 9.1 Pro, 64 bit Linux

**fire-nodes:**

1-26 SUN Fire V20z Opteron 2.2 GHz 2-core 4GB RAM 73GB SAS Compute nodes for parallel sequential jobs; SuSe 9.1 64 bit Linux
**fire totals: 2.2GHz CPU w/ 54 core + 108GB RAM + 2TB storage**

## D. IBM P4 standalone servers

1-6, "SP4 3U node P4+" ~1.3 GHz 4-core 4GB RAM 68GB SCSI Compute nodes for parallel & sequential jobs
**P4 totals: ~1.3GHz IBM CPU w/ 24 core + 24GB RAM + 0.4TB storage**

### Emerson Center (Licensed) Software Collection as of March 2012

*System Software:*
AIX 5.1, 5.3, 6.0 + XLF Fortran; SuSe 11 Linux Professional; PGI 11.10 and Intel 12.0 Fortran + libraries

*Electronic structure:*

| | |
|---|---|
| GAUSSIAN 09 | MOLPRO 2010 |
| VASP 4.6 & 5.2 | TURBOMOLE 6.0 |
| DFTB+ 1.1 | DALTON 2.0 |
| GAMESS-US 6.0 | ORCA |
| ACES II M | NWCHEM 5.0 |
| OCTOPUS 1.3 | COLUMBUS |
| CPMD-3.7.2 | CADPAC |
| MOPAC 2002 | HONDO |

*Simulation and modeling software:*

| | |
|---|---|
| GROMACS 4.5.5 | AMBER 11 |
| NAMD 2.6 | VMD |
| ROSETTA | ReaxFF |
| deMon-1.1.0 | TINKER |
| MM3 | DL_POLY 2.13 |

*Kinetics, QM dynamics, statistics software:*

| | |
|---|---|
| POLYRATE 9.7 | MOLSCAT |
| GAUSS 6 | RIOTS |

*Graphics and programming software:*

| | |
|---|---|
| MATLAB R2010a (network-limited) | Mathematica 8.0 (workstation) |
| Molden | VMD |
| GaussView 5 | |

*Crystal Structure Software:*

| | |
|---|---|
| Mercury 2.4 | XtalView 4.0 |