

Cherry L. Emerson Center for Scientific Computation

THE CENTER'S BILLING SCHEME and RATES

BASIC SERVICE: Emerson Center Monthly Computational Access Fee

ALL user groups are charged \$300 per month for access to the benefits outlined below.

- 1. Provided group-based account with individual user ID's for group members
- 2. Allocated 50GB of disc space for group /home, 50 GB storage space, and 50 GB checkpoint directories.
- 3. Provided with access to licensed software products
 - a. Gaussian-2016 (or latest version)
 - b. GaussView 6.0 (or latest version)
 - c. Molpro-2016 (or latest version)
 - d. Molcas-10.0 (or latest version)
 - e. Amber-16 (or latest version)
 - f. DFTB+ 2.0 (or latest version)
 - g. VASP 6.5 (or latest version)
 - h. Turbomole 8.1 (or latest version)
 - ORCA 4.0 (or latest version)
 - Tinker (or latest version)
 - j. k. GROMACS, (or latest version)
 - Matlab, Mathematica, and many others (pls check the Center's Software Library)
- 4. Allowed to run up to two (2) computational job on the Emerson Center's computer cluster at any time
- 5. Provided with the basic technical support required to utilize Emerson Center's computational resources (update of OS, system libraries, backup of /home directory, and more).
- 6. Provided with the basic scientific and consulting support required to utilize Emerson Center's computational resources

Additional Computational Resource Allocations

For users that require more than 50GB of disc spaces (total of 150 GB) and need to run more than two (2) computational jobs at any time, the Emerson Center will provide additional computational resources in increments of 150GB and two (2) computational jobs at a cost of \$300 per month.

Emerson Center Scientific Consulting Fee

In addition to basic technical support, users can solicit additional scientific support from Dr. Jamal Musaev and Dr. Alex Kaledin at rates of \$100/hr and \$42/hr, respectively. Drs. Musaev and Kaledin will document their respective hours on a monthly basis.