

BASIC SERVICE: Emerson Center Monthly Computational Access Fee

For September 2024, half share subscription fee has been set to be **\$375 per month** allowing to access 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

Gaussian-2016 (or latest version)

GaussView 6.0 (or latest version)

Molpro-2016 (or latest version)

Molcas-10.0 (or latest version)

Amber-16 (or latest version)

DFTB+ 2.0 (or latest version)

VASP_6.5 (or latest version)

Turbomole_8.1 (or latest version)

ORCA_6.0 (or latest version)

Tinker (or latest version)

GROMACS, (or latest version)

Matlab, Mathematica, and many others (pls check the Center's Software Library)

4. Allowed to run up to four (4) computational jobs on the Emerson Center's computer clusters **star**, and **spark** each, and three (3) jobs on the fire 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 space (total of 150 GB) and need to run more computational jobs (see point-4, above) at any time, the Emerson Center will provide additional computational resources in increments of 150GB, and additional computational jobs (allocated exactly in same way as that provided in point-4, above) for additional \$375 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 **\$125/hr** and **\$75/hr**, respectively. Drs. Musaev and Kaledin will document their respective hours on a monthly basis.