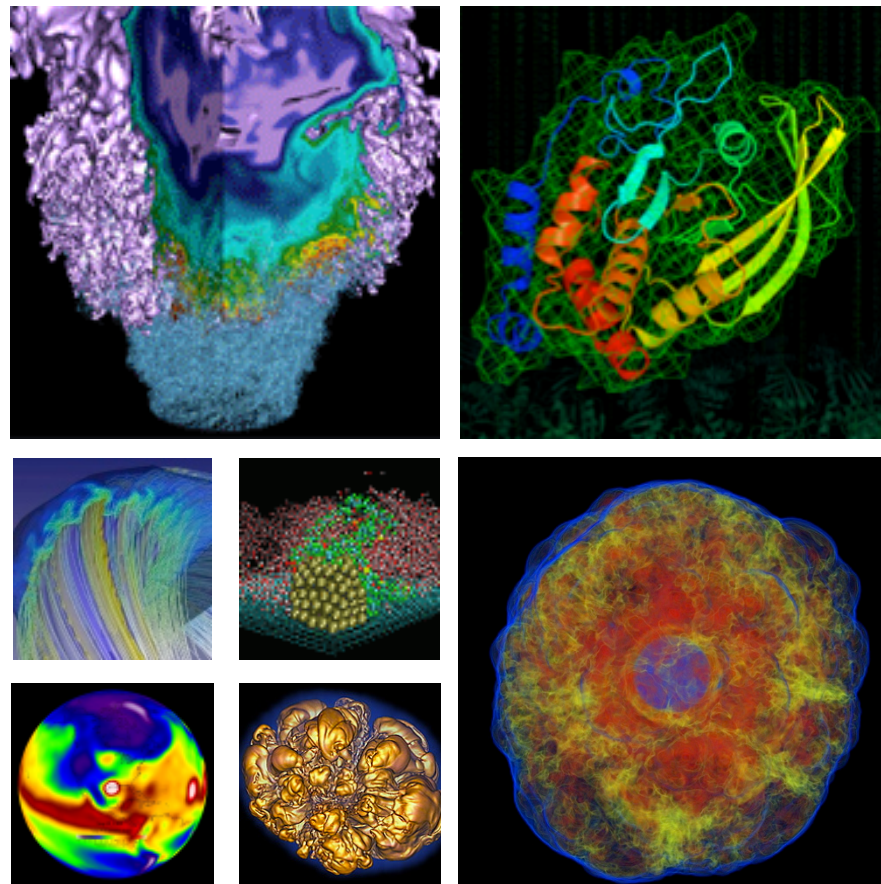


Available Software at NERSC



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Motivation



- **To introduce to users the availability of hundreds of software applications, libraries and tools on NERSC major computing platforms**
- **To recommend users to make use of them for improved scientific productivity and better performance.**

NERSC provides and supports hundreds of software packages



<http://www.nersc.gov/users/software/all-software-list/>

- **Compilers**
- **Libraries**
 - Math libraries
 - I/O libraries
- **Applications**
 - Development tools
 - Debuggers and profilers
 - Chemistry/Materials science applications
 - Visualization and analytics tools
- **Users are recommended to use them for good reasons**
- **This talk covers Edison, Hopper and Carver.**

Module approach is used to manage software packages at NERSC



- **Modules/Modulefiles**
 - defines shell environment variables and other functions, upon loading the modules, those environment are added to your shell environment
- **Commonly used module commands**
 - module list
 - module avail
 - module load
 - module show
 - module what_is
 - module help
- **MODULEPATH**
 - Vendor provided software
 - NERSC staff provided software

Module list –show modules loaded



Edison:

```
zz217@edison02:~> module list
Currently Loaded Modulefiles:
  1) modules/3.2.6.7
  2) nsg/1.2.0
  3) eswrap/1.0.20-1.010200.643.0
  4) switch/1.0-1.0501.47124.1.93.ari
  5) craype-network-aries
  6) craype/2.03
  7) intel/14.0.0.080
  8) cray-libsci/12.1.3
  9) udreg/2.3.2-1.0501.7914.1.13.ari
 10) ugni/5.0-1.0501.8253.10.22.ari
 11) pmi/5.0.1-1.0000.9799.94.6.ari
 12) dmapp/7.0.1-1.0501.8315.8.4.ari
 13) gni-headers/3.0-1.0501.8317.12.1.ari
 14) xpmem/0.1-2.0501.48424.3.3.ari
 15) job/1.5.5-0.1_2.0501.48066.2.43.ari
 16) csa/3.0.0-1_2.0501.47112.1.91.ari
 17) dvs/2.4_0.9.0-1.0501.1672.2.122.ari
 18) alps/5.1.1-2.0501.8471.1.1.ari
 19) rca/1.0.0-2.0501.48090.7.46.ari
 20) atp/1.7.1
 21) PrgEnv-intel/5.1.29
 22) craype-ivybridge
 23) cray-shmem/6.2.0
 24) cray-mpich/6.2.0
 25) torque/4.2.6
 26) moab/7.2.3-r19-b121-SUSE11
 27) altd/1.0
 28) usg-default-modules/1.0
zz217@edison02:~>
```

Carver:

```
zz217@cvrsvc01:~>module list
Currently Loaded Modulefiles:
  1) modules
  2) nsg/1.2.0
  3) moab/7.2.6-r12-b152
  4) torque/4.2.6
  5) pgi/12.9
  6) openmpi/1.4.5
  7) altd/1.0
  8) usg-default-modules/1.0
zz217@cvrsvc01:~>
```

Module avail – list modules available

```
zz217@edison11:~> module avail
```

```
----- /opt/cray/craype/default/modulefiles -----
craype-abudhabi          craype-hugepages128M    craype-hugepages512M    craype-ivybridge        craype-network-none     craype-xeon
craype-abudhabi-cu      craype-hugepages16M    craype-hugepages64M     craype-mc12             craype-sandybridge
```

```
----- /opt/cray/ari/modulefiles -----
alps/5.1.0-2.0501.8351.1.1.ari          job/1.5.5-0.1.2.0500.41368.1.92.ari          rca/1.0.0-2.0501.46504.10.20.ari
alps/5.1.1-2.0501.8471.1.1.ari          job/1.5.5-0.1.2.0501.45369.2.61.ari          rca/1.0.0-2.0501.48090.7.46.ari(default)
alps/5.1.1-2.0501.8507.1.1.ari(default)  job/1.5.5-0.1.2.0501.48066.2.43.ari(default)  sdb/1.0-1.0500.43793.6.11.ari
```

```
----- /opt/cray/modulefiles -----
PrgEnv-cray/5.0.41          cray-libsci/12.1.00          cray-petsc-complex/3.4.3.0(default)          hdf5/1.8.11(default)
PrgEnv-cray/5.1.18         cray-libsci/12.1.01          cray-shmem/5.6.1                             hdf5-parallel/1.8.11(default)
PrgEnv-cray/5.1.29(default)  cray-libsci/12.1.2          cray-shmem/5.6.5                             iobuf/2.0.4
PrgEnv-gnu/5.0.41          cray-libsci/12.1.3(default)  cray-shmem/6.0.0                             iobuf/2.0.5(default)
PrgEnv-gnu/5.1.18         cray-mpich/6.0.0            cray-shmem/6.0.2                             netcdf/4.3.0(default)
PrgEnv-gnu/5.1.29(default)  cray-mpich/6.0.2           cray-shmem/6.1.1                             netcdf-hdf5parallel/4.3.0(default)
PrgEnv-intel/5.0.41        cray-mpich/6.1.1           cray-shmem/6.2.0(default)                   ntk/1.5.0
PrgEnv-intel/5.1.18        cray-mpich/6.2.0(default)   cray-shmem/6.2.1                             onesided/1.5.0
PrgEnv-intel/5.1.29(default)  cray-mpich/6.2.1           cray-tpsl/1.3.01                             papi/5.0.1
atp/1.6.1                  cray-mpich2/5.6.1           cray-tpsl/1.3.04(default)                   papi/5.1.1
atp/1.6.3                  cray-mpich2/5.6.5           cray-trilinos/10.12.1.1                     papi/5.1.2
atp/1.7.0                  cray-mpich2/6.0.0           cray-trilinos/11.2.2.0                       papi/5.2.0(default)
atp/1.7.1(default)         cray-mpich2/6.0.2           cray-trilinos/11.4.1.0(default)             parallel-netcdf/1.3.1(default)
ccm/2.2.0-1.0500.43485.5.54  cray-mpich2/6.1.1           craype/1.01                                  parallel-netcdf/1.3.1.1
ccm/2.2.0-1.0501.46098.9.95  cray-mpich2/6.2.0(default)  craype/1.05                                  perftools/6.0.1
ccm/2.2.0-1.0501.48422.4.56(default)  cray-mpich2/6.2.1           craype/1.06                                  perftools/6.1.1
cray-ccdb/1.0.0(default)     cray-netcdf/4.2.1.1         craype/2.01                                  perftools/6.1.2
cray-ga/5.1.0.2(default)    cray-netcdf/4.3.0(default)  craype/2.03(default)                         perftools/6.1.3(default)
cray-hdf5/1.8.11(default)    cray-netcdf-hdf5parallel/4.2.1.1  craype/2.04                                  perftools-lite/6.1.1
cray-hdf5/1.8.9             cray-netcdf-hdf5parallel/4.3.0(default)  craypkg-gen/1.0.0(default)                   perftools-lite/6.1.2
cray-hdf5-parallel/1.8.11(default)  cray-parallel-netcdf/1.3.1.1(default)  craypkg-gen/1.0.0.6509                       perftools-lite/6.1.3(default)
cray-hdf5-parallel/1.8.9      cray-petsc/3.3.03           cudatoolkit/5.5.20-1.0501.7700.8.1         python3/3.3.2
cray-lgdb/2.0.1             cray-petsc/3.3.06           cudatoolkit/5.5.20-1.0501.7945.8.2(default)  stat/2.0.0.1(default)
cray-lgdb/2.1.0             cray-petsc/3.4.2.0          fftw/2.1.5.5                                  xt-mpich2/5.6.1
cray-lgdb/2.2.0             cray-petsc/3.4.3.0(default)  fftw/2.1.5.6                                  xt-mpich2/5.6.5(default)
cray-lgdb/2.2.2             cray-petsc-complex/3.3.03    fftw/3.3.0.1                                  xt-shmem/5.6.1
cray-lgdb/2.2.3(default)    cray-petsc-complex/3.3.06    fftw/3.3.0.3                                  xt-shmem/5.6.5(default)
cray-libsci/12.0.00         cray-petsc-complex/3.4.2.0    fftw/3.3.0.4(default)
```

```
----- /opt/modulefiles -----
cce/8.1.3                   gcc/4.7.2                   intel/14.0.1.106                       torque/4.2.6(default)
cce/8.1.9                   gcc/4.8.0                   java/jdk1.7.0_07                       xc-sysroot/5.0.15
cce/8.2.1                   gcc/4.8.1                   java/jdk1.7.0_45(default)              xc-sysroot/5.0.29
cce/8.2.2(default)         gcc/4.8.2(default)          moab/7.2.3-r19-b121-SUSE11(default)    xc-sysroot/5.0.41
cce/8.2.3                   intel/12.1.5.339            modules/3.2.6.6                         xc-sysroot/5.1.18
chapel/1.6.0                intel/13.0.1.117            modules/3.2.6.7                         xc-sysroot/5.1.29(default)
chapel/1.7.0.2(default)     intel/13.1.2.183            torque/4.2.3.1
eswrap/1.0.20-1.010200.643.0(default)  intel/13.1.3.192            torque/4.2.3.1_p1
fftw/2.1.5.4                intel/14.0.0.080(default)    torque/4.2.3.h5
```



Module avail – list modules available

--Continued



```
----- /usr/common/ug/Modules/modulefiles -----
abinit/7.0.5(default)      darshan/2.2.6             ipython/1.1.0(default)   numexpr/2.2.2(default)   taskfarmer/1.6.0(default)
adios/1.4.1(default)      darshan/2.2.7-105        jpeg/8d(default)         numpy/1.6.2              tc1/8.5.13(default)
adios/1.5.0                darshan/2.2.7-106(default) lammps/20130106          numpy/1.7.1(default)    totalview/8.11.0
adiosplain/1.4.1(default) ddt/3.2.1(default)       lammps/20130727(default) nwchem/6.1.1            totalview/8.12.0(default)
allineatools/4.1-33167    dfftpack/1.0(default)    latex/2012(default)     octave/3.6.4(default)   totalview/8.12.0-mem-debug
allineatools/4.2-34164(default) dlfm/1.4(default)        latex/2013              openmpi-ccm/1.6.3       totalview-support/1.1.4(default)
allineatools/4.2-34404    emacs/24.2(default)     matlab/R2011b           openmpi-ccm/1.6.5(default) training/2013
altd/1.0(default)         espresso/5.0.0           matlab/R2012a(default)  phonopy/1.6.2(default)  training/2014(default)
amber/12(default)         espresso/5.0.2(default)  matlab-nofonts/R2011b  pil/1.1.7(default)      udunits/2.1.24(default)
asciidoc/8.6.8(default)   espresso/5.0.2-2        matlab-nofonts/R2012a(default) pspline/nersc1.0       usg/1.1(default)
ase/3.6.0.2515            espresso/5.0.3          matplotlib/1.1.0       pycdf/0.6-3b           usg-default-modules/1.0(default)
ase/3.7.1.3184(default)  fftw-ccm/3.3.3          mercurial/2.2.1        pyhdf/0.8.3(default)   valgrind/3.9.0(default)
berkeleygw/1.0.4(default) g09/c1(default)         mercurial/2.4.2        pypmi/2.5b0(default)   vasp/4.6.35_vtst
berkeleygw/1.0.6        g09/d1                  mercurial/2.7.1(default) pymysqlite/2.6.3(default) vasp/5.3.2
boost/1.53                gamesss/1May2012R2      mkl/13.0.1             pytables/2.3.1         vasp/5.3.2_vtst
boost/1.54(default)      gdb/7.6.1(default)      mkl/13.0.3(default)    pytables/3.0.0(default) vasp/5.3.3(default)
bzip2/1.0.6(default)     git/1.8.1.1(default)    molpro/2010.1.26       python/2.7.3           vasp/5.3.3-ccce
cdat/5.2(default)        gnuplot/4.6.2          mpi4py/1.3.1(default)  python/2.7.5(default)  vasp/5.3.3-intel12
cdo/1.5.9(default)       htop/1.0.2(default)    mysql/5.1.63(default)  python_base/2.7.3      vasp/5.3.3-intel14
cfitsio/3.31(default)    gsl/1.15(default)      mysqlpython/1.2.3(default) python_base/2.7.5(default) vasp/5.3.3-pgi
cmake/2.8.10.2           gsl/1.16               namd/cvs_01032013      root/5.34(default)     vasp/5.3.3_vtst
cmake/2.8.11.2(default)  gw/3.7.3              namd/cvs_20130727     vasp/5.3.3_vtst-ccce   vasp/5.3.3_vtst-intel14
cp2k/2.3(default)        h4h5tools/2.2.1       nano/2.2.6(default)    vasp/5.3.3_vtst-pgi   virtualenv/1.10.1(default)
cp2k/2.4                  h5py/2.0.1             ncar/6.1.1(default)   virtualenv/1.8.2      virtualenvwrapper/3.6(default)
ctss/1.0(default)        hdf/4.2.8(default)     ncl/6.1.1(default)    siesta/3.1(default)   wannier90/1.2(default)
curl/7.28.1(default)     htop/1.0.2(default)    nco/4.2.5              silo/4.9.1(default)   wien2k-ccm/12.1(default)
cython/0.16              hwloc/1.7.2(default)   nco/4.3.1              slatec/4.1(default)   wien2k-ccm/13.1
cython/0.17.4            idl/8.0                nco/4.3.8(default)    sparsehash/2.0.2(default) zlib/1.2.7(default)
cython/0.19.1(default)  idl/8.2(default)       netcdf4-python/1.0.2  sprng/2.0              zlib/1.2.7(default)
darshan/2.2.4            intel/12.1.3           netcdf4-python/1.0.6(default) subversion/1.7.9(default)
darshan/2.2.4-oldd       ipm/2.00(default)      numexpr/2.0.1         superlu/2.5(default)
darshan/2.2.5-pre1      ipython/0.13.1        BerkeleyDB/5.1.19(default) cfengine/3.2.3(default) serial/1.0(default) serial/1.0_template  sudosh/3.2.0(default)
darshan/2.2.5-pre3
darshan/2.2.5-pre3-104

----- /usr/syscom/nsg/modulefiles -----
gpfs/1.1.0(default) nsg/1.2.0(default)

----- /usr/syscom/nsg/opt/modulefiles -----
BerkeleyDB/5.1.19(default) cfengine/3.2.3(default) serial/1.0(default) serial/1.0_template  sudosh/3.2.0(default)

----- /usr/common/ftg/Modules/modulefiles -----
bupc/2.16.2              bupc/2.16.2-5.0.41-gnu-4.8.0  bupc/2.18.0(default)   bupc/2.18.0-5.1.18-gnu-4.8.2
bupc/2.16.2-5.0.29-cray-8.1.4  bupc/2.16.2-5.0.41-gnu-4.8.1  bupc/2.18.0-5.0.41-cray-8.1.9  bupc/2.18.0-5.1.18-intel-13.1.3.192
bupc/2.16.2-5.0.29-cray-8.1.8  bupc/2.16.2-5.0.41-intel-13.1.2.183  bupc/2.18.0-5.0.41-gnu-4.8.1  bupc/2.18.0-5.1.18-intel-14.0.0.080
bupc/2.16.2-5.0.29-gnu-4.7.2  bupc/2.16.2-5.0.41-intel-13.1.3.192  bupc/2.18.0-5.0.41-intel-13.1.3.192  bupc/2.18.0-5.1.29-cray-8.2.2
bupc/2.16.2-5.0.29-gnu-4.7.3  bupc/2.16.2-rc1          bupc/2.18.0-5.1.18-cray-8.2.1  bupc/2.18.0-5.1.29-gnu-4.8.2
bupc/2.16.2-5.0.29-intel-13.0.1.117  bupc/2.16.2-rc1-5.0.29-gnu-4.7.2  bupc/2.18.0-5.1.18-cray-8.2.2  bupc/2.18.0-5.1.29-intel-14.0.0.080
bupc/2.16.2-5.0.41-cray-8.1.9  bupc/2.16.2-rc1-5.0.29-intel-13.0.1.117  bupc/2.18.0-5.1.18-gnu-4.8.1

----- /usr/common/graphics/Modules/modulefiles -----
ParaView/3.98.1          llvm/3.2-dso             mesa/9.2.2-classic-dso  uvcdat/1.2.0(default)  visit/2.6.3
VTK/5.10.1              mesa/9.2.0              mesa/9.2.2-llvmpipe(default) uvcdat/trunk          visit/2.7.1(default)
llvm/3.2                mesa/9.2.2-classic      mesa/9.2.2-llvmpipe-dso uvcdat/trunk-no-mpi
```



Compilers available

Compiler	Edison	Hopper	Carver
Intel	✓	✓	✓
PGI		✓	✓
GNU	✓	✓	✓
Cray	✓	✓	
Pathscale*		✓	
Bupc	✓	✓	✓
Default compiler	Intel	PGI	PGI

*) Newer versions of Pathscale compilers (> 4.0.13) are no longer supported on Hopper.

Libraries available

Library name	Description	Module name	Edison	Hopper	Carver
MPICH	MPI library	Cray-mpich	✓	✓	
Open MPI	MPI library	openmpi*	✓*	✓*	✓
LibSci	Cray Scientific libraries, including BLAS, BLACS, LAPACK, ScaLAPACK, FFT, FFTW	cray-libsci	✓	✓	
MKL	Intel Math Kernel library	intel	✓	✓	✓
ACML	AMD Core Math Library	acml		✓	
NAG	Mathematics and Statistical Library	nag;nag-intel;nag-gnu			✓
FFTW	Library for computing the discrete Fourier transform (DFT)	fftw	✓	✓	✓
GSL	GNU scientific libraries	gsl*	✓	✓	✓

*) Open MPI on Edison and Hopper are for Cluster Compatibility Mode (CCM) only

Libraries available

--Continued



Library name	Description	Module name	Edison	Hopper	Carver
PETSc	Portable, Extensible Toolkit for Scientific computation	cray-petsc; petsc	✓	✓	✓
Trilinos	Collections of building blocks for the development of scientific applications	cray-trilinos; trilinos	✓	✓	✓
TPSL	Cray third party scientific libraries include MUMPS, SuperLU, ParMETIS HYPRE, SCOTCH	cray-tpsl; mumps; hypre; superlu; ...	✓	✓	✓*
MPI-IO Library	Parallel IO library	Cray-mpich; openmpi*	✓	✓	✓
NETCDF	Library for portable data formats	Cray-netcdf; netcdf	✓	✓	✓
HDF5	Portable Library for extremely large and complex data	Cray-hdf5; hdf5	✓	✓	✓

*) They are separate modules on Carver

Debuggers and Performance Tools

Library name	Description	Module name	Edison	Hopper	Carver
DDT	Allinea parallel debugger	ddt	✓	✓	✓
Totalview	debugger	totalview	✓	✓	✓
GDB	GNU debugger		✓	✓	✓
LGDB	Cray Line Mode Parallel Debugger	Cray-igdb	✓	✓	
CCDB	Cray Comparative Debugger	Cray-ccdb	✓	✓	
ATP			✓	✓	
Perftools	craypat, reveal apprentice2,	perftools	✓	✓	
Perftools-lite	Light version of craypat	perftools-lite	✓	✓	
IPM	Profiling tool	ipm	✓	✓	✓
PAPI		papi	✓	✓	✓



Visualization and analytics applications



Application Name	Description	Module name	Edison	Hopper	Carver
Matlab	computing environment for numeric computation, graphics and visualization.	matlab	✓	✓	✓
mathematica	computational software program	mathematica	✓	✓	✓
R	Software environment for statistical computing and graphics	R		✓	✓
IDL	analysis and display of scientific data	idl	✓	✓	✓
VISIT	Visualization and analysis package.	visit	✓	✓	✓
ParaView	multiple-platform application for interactive, scientific visualization.	ParaView	✓	✓	✓

Chemistry/Materials science applications available



Application	Module name	Edison	Hopper	Carver
ABINIT	abinit	✓	✓	✓
AMBER	amber	✓	✓	✓
BerkeleyGW	gerkelygw	✓	✓	✓
CP2K	cp2k	✓	✓	✓
Quantum Espresso	espresso	✓	✓	✓
g09	g09	✓	✓	✓
GAMESS	gamess	✓	✓	✓
LAMMPS	lammps	✓	✓	✓
MOLPRO	molpro	✓	✓	✓
NAMD	namd	✓	✓	✓
NWCHEM	nwchem	✓	✓	✓
SIESTA	siesta	✓	✓	✓
VASP	vasp	✓	✓	✓
WIEN2k	wien2k;wien2k-ccm	✓	✓	✓

How to use available libraries on Edison and Hopper



- **Compiler wrappers, ftn, cc and CC are recommended to use on Edison and Hopper**
- **Upon loading the library modules, the compiler wrappers, ftn, cc and CC, can automatically include the include and library paths and libraries in the compile and link lines**
 - Bash shell scripts on Hopper
 - Uses pkg-config tools and .pc files on Edison
 - man pkg-config
- **Module load <module name>, that's it.**
 - To check, use the -v or --craype-verbose option to the compiler wrappers
- **Some exceptions, need to use manually.**

How to use available libraries on Edison and Hopper

--Continued



Compiler wrappers include mpich and libsci in the compile and link line by default

```
zz217@edison11:~> ftn -craype-verbose hello.f90
ifort -xAVX -static hello.f90 -I/opt/cray/mpt/6.2.0/gni/mpich2-intel/130/include -I/opt/cray/mpt/6.2.0/gni/sma/include -I/opt/cray/libsci/12.1.3/INTEL/130/sandybridge/include -I/opt/fftw/3.3.0.4/sandybridge/include -I/opt/cray/alps/5.1.1-2.0501.8471.1.1.ari/include -I/opt/cray/xpmmem/0.1-2.0501.48424.3.3.ari/include -I/opt/cray/gni-headers/3.0-1.0501.8317.12.1.ari/include -I/opt/cray/dmapp/7.0.1-1.0501.8315.8.4.ari/include -I/opt/cray/pmi/5.0.1-1.0000.9799.94.6.ari/include -I/opt/cray/ugni/5.0-1.0501.8253.10.22.ari/include -I/opt/cray/udreg/2.3.2-1.0501.7914.1.13.ari/include -I/opt/cray/rca/1.0.0-2.0501.48090.7.46.ari/include -I/opt/cray/wlm_detect/1.0-1.0501.47908.2.2.ari/include -I/opt/cray-hss-devel/7.1.0/include -I/opt/cray/krca/1.0.0-2.0501.47640.3.70.ari/include -Wl,--undefined=_ATP_Data_Globals -Wl,--undefined=__atpHandlerInstall -L/opt/cray/mpt/6.2.0/gni/mpich2-intel/130/lib -L/opt/cray/mpt/6.2.0/gni/sma/lib64 -L/opt/cray/libsci/12.1.3/INTEL/130/sandybridge/lib -L/opt/fftw/3.3.0.4/sandybridge/lib -L/opt/cray/alps/5.1.1-2.0501.8471.1.1.ari/lib64 -L/opt/cray/xpmmem/0.1-2.0501.48424.3.3.ari/lib64 -L/opt/cray/dmapp/7.0.1-1.0501.8315.8.4.ari/lib64 -L/opt/cray/pmi/5.0.1-1.0000.9799.94.6.ari/lib64 -L/opt/cray/ugni/5.0-1.0501.8253.10.22.ari/lib64 -L/opt/cray/udreg/2.3.2-1.0501.7914.1.13.ari/lib64 -L/opt/cray/atp/1.7.1/lib -L/opt/cray/rca/1.0.0-2.0501.48090.7.46.ari/lib64 -L/opt/cray/wlm_detect/1.0-1.0501.47908.2.2.ari/lib64 -lsma -lAtpSigHandler -lAtpSigHCommData -lsci_intel_mp -liomp5 -lfftw3 -lfftw3f -lcray_memcpy -lmpichf90_intel -lmpich_intel -lrt -lm -ldl -ldmapp -lmpi -lxpmmem -ludreg -lpmi -lalpslli -lalpsutil -lrca -lwlm_detect -lugni -lpthread -Wl,--as-needed,-limf,--no-as-needed -Wl,--as-needed,-lm,--no-as-needed
```

How to use available libraries on Edison and Hopper

--Continued



Compiler wrappers include netcdf libraries and paths in the compile and link line upon loading the cray-netcdf module

```
zz217@edison11:~> module load cray-netcdf
zz217@edison11:~> ftn -craype-verbose hello.f90
ifort -xAVX -static hello.f90 -I/opt/cray/netcdf/4.3.0/INTEL/130/include -I/opt/cray/mpt/6.2.0/gni/mpich2-
intel/130/include -I/opt/cray/hdf5/1.8.11/INTEL/130/include -I/opt/cray/mpt/6.2.0/gni/sma/include -I/opt/
cray/libsci/12.1.3/INTEL/130/sandybridge/include -I/opt/fftw/3.3.0.4/sandybridge/include -I/opt/cray/alps/
5.1.1-2.0501.8471.1.1.ari/include -I/opt/cray/xpmmem/0.1-2.0501.48424.3.3.ari/include -I/opt/cray/gni-
headers/3.0-1.0501.8317.12.1.ari/include -I/opt/cray/dmapp/7.0.1-1.0501.8315.8.4.ari/include -I/opt/cray/
pmi/5.0.1-1.0000.9799.94.6.ari/include -I/opt/cray/ugni/5.0-1.0501.8253.10.22.ari/include -I/opt/cray/udreg/
2.3.2-1.0501.7914.1.13.ari/include -I/opt/cray/rca/1.0.0-2.0501.48090.7.46.ari/include -I/opt/cray/
wlm_detect/1.0-1.0501.47908.2.2.ari/include -I/opt/cray-hss-devel/7.1.0/include -I/opt/cray/krca/
1.0.0-2.0501.47640.3.70.ari/include -Wl,--undefined=_ATP_Data_Globals -Wl,--undefined=__atpHandlerInstall -
L/opt/cray/netcdf/4.3.0/INTEL/130/lib -L/opt/cray/mpt/6.2.0/gni/mpich2-intel/130/lib -L/opt/cray/
hdf5/1.8.11/INTEL/130/lib -L/opt/cray/mpt/6.2.0/gni/sma/lib64 -L/opt/cray/libsci/12.1.3/INTEL/130/
sandybridge/lib -L/opt/fftw/3.3.0.4/sandybridge/lib -L/opt/cray/alps/5.1.1-2.0501.8471.1.1.ari/lib64 -L/opt/
cray/xpmmem/0.1-2.0501.48424.3.3.ari/lib64 -L/opt/cray/dmapp/7.0.1-1.0501.8315.8.4.ari/lib64 -L/opt/cray/
pmi/5.0.1-1.0000.9799.94.6.ari/lib64 -L/opt/cray/ugni/5.0-1.0501.8253.10.22.ari/lib64 -L/opt/cray/udreg/
2.3.2-1.0501.7914.1.13.ari/lib64 -L/opt/cray/atp/1.7.1/lib -L/opt/cray/rca/1.0.0-2.0501.48090.7.46.ari/lib64 -L/
opt/cray/wlm_detect/1.0-1.0501.47908.2.2.ari/lib64 -lsma -lAtpSigHandler -lAtpSigHCommData -lsci_intel_mp -
liomp5 -lfftw3 -lfftw3f -lcray_memcpy -lnetcdf -lnetcdf -lhdf5_hl -lhdf5 -lz -lmpich90_intel -lmpich_intel -lrt -
lm -ldl -ldmapp -lmpi -lxpmmem -ludreg -lpmi -lalpslli -lalpsutil -lrca -lwlm_detect -lugni -lpthread -Wl,--as-
needed,-limf,--no-as-needed -Wl,--as-needed,-lm,--no-as-needed
```



How to use available libraries on Edison and Hopper

--Continued



MKL example

```
zz217@edison11:~> ftn -v hello.f90 -mkl=cluster
```

```
...
```

```
ld /usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64/crt1.o /usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64/crti.o /usr/lib64/gcc/x86_64-suse-linux/4.3/crtbeginT.o --build-id -static -L/opt/cray/mpt/6.2.0/gni/mpich2-intel/130/lib -L/opt/cray/mpt/6.2.0/gni/sma/lib64 -L/opt/cray/libsci/12.1.3/INTEL/130/sandybridge/lib -L/opt/fftw/3.3.0.4/sandybridge/lib -L/opt/cray/rca/1.0.0-2.0501.48090.7.46.ari/lib64 -L/opt/cray/alps/5.1.1-2.0501.8471.1.1.ari/lib64 -L/opt/cray/xpmmem/0.1-2.0501.48424.3.3.ari/lib64 -L/opt/cray/dmapp/7.0.1-1.0501.8315.8.4.ari/lib64 -L/opt/cray/pmi/5.0.1-1.0000.9799.94.6.ari/lib64 -L/opt/cray/ugni/5.0-1.0501.8253.10.22.ari/lib64 -L/opt/cray/udreg/2.3.2-1.0501.7914.1.13.ari/lib64 -L/opt/cray/atp/1.7.1/lib -L/opt/cray/wlm_detect/1.0-1.0501.47908.2.2.ari/lib64 -o a.out /opt/intel/composer_xe_2013_sp1.0.080/compiler/lib/intel64/for_main.o -L/opt/intel/composer_xe_2013_sp1.0.080/compiler/lib/intel64 -L/opt/intel/composer_xe_2013_sp1.0.080/compiler/lib/intel64 -L/usr/lib64/gcc/x86_64-suse-linux/4.3/ -L/usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64 -L/usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64/ -L/lib/./lib64 -L/lib/./lib64/ -L/usr/lib/./lib64 -L/usr/lib/./lib64/ -L/opt/intel/composer_xe_2013_sp1.0.080/compiler/lib/intel64/ -L/usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../x86_64-suse-linux/lib/ -L/usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64 -L/lib/ -L/usr/lib64 -L/usr/lib /scratch1/scratchdirs/zz217/fortFkDPXn.o --start-group -lmkl_intel_lp64 -lmkl_cdft_core -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64 -lmkl_sequential -lmkl_core -liomp5 --end-group --undefined=_ATP_Data_Globals --undefined=__atpHandlerInstall -lsma -latpSigHandler -latpSigHCommData -lsci_intel_mp -liomp5 -lfftw3 -lfftw3f -lcray_memcpy -lmpichf90_intel -lmpich_intel -lrt -L/opt/intel/composer_xe_2013_sp1.0.080/compiler/lib/intel64 -limf -lm -ldl -ldmapp -lmpi -lxpmmem -ludreg -lpmi -lalpslli -lalpsutil -lrca -lwlm_detect -lugni -lpthread --as-needed -limf --no-as-needed --as-needed -lm --no-as-needed -L/opt/intel/composer_xe_2013_sp1.0.080/mkl/lib/intel64 -lifport -lifcore -limf -lsvml -lm -lipgo -lirc -lpthread -lsvml -lc -lgcc -lgcc_eh -lirc_s -ldl -lc /usr/lib64/gcc/x86_64-suse-linux/4.3/crtend.o /usr/lib64/gcc/x86_64-suse-linux/4.3/../../../../lib64/crtn.o
```

How to use these available libraries on Carver – provide the libraries and paths manually



1. Module show <module name> to see where the libraries reside

```
zz217@cvrsvc01:~>module show fftw
```

```
-----  
/usr/common/usg/Modules/modulefiles/fftw/2.1.5:
```

```
module-whatis  Loads the FFTW subroutine library for computing the discrete Fourier transform (DFT)  
setenv        FFTW_ROOT /usr/common/usg/fftw/2.1.5  
setenv        FFTW_LIBDIR /usr/common/usg/fftw/2.1.5/lib  
setenv        FFTW_INC /usr/common/usg/fftw/2.1.5/include  
setenv        FFTW -I/usr/common/usg/fftw/2.1.5/include -L/usr/common/usg/fftw/2.1.5/lib  
prepend-path  LD_LIBRARY_PATH /usr/common/usg/fftw/2.1.5/lib  
prepend-path  INFOPATH /usr/common/usg/fftw/2.1.5/info  
conflict     fftw/3.2.2
```

```
-----  
zz217@cvrsvc01:~>ls /usr/common/usg/fftw/2.1.5/lib
```

```
libdfft.a  libdrfft.a  libfftw.a  librfft.a  libsfft.a  libsrfft.a  libdfft.la  
libdrfft.la  libfftw.la  librfft.la  libsfft.la  libsrfft.la  libdfft_mpi.a  libdrfft_mpi.a  
libfftw_mpi.a  librfft_mpi.a  libsfft_mpi.a  libsrfft_mpi.a  libdfft_mpi.la  libdrfft_mpi.la  
libfftw_mpi.la  librfft_mpi.la  libsfft_mpi.la  libsrfft_mpi.la  libdfft_threads.a  
libdrfft_threads.a  libfftw_threads.a  librfft_threads.a  libsfft_threads.a  libsrfft_threads.a  
libdfft_threads.la  libdrfft_threads.la  libfftw_threads.la  librfft_threads.la  libsfft_threads.la  
libsrfft_threads.la
```


How to use these available libraries on Carver

--Continued



2. Then use `-l`, `-L` and `-I` to provide the libraries and paths in your compilation/link lines

```
mpicc test_fftw.c $FFTW -ldfftw_mpi -ldfftw  
Mpif90 test_fftw.f90 $FFTW -ldfftw_mpi -ldfftw
```

3. NERSC website for specific software packages

<https://www.nersc.gov/users/software/programming-libraries/math-libraries/fftw/>

How to use application software



- **Module avail <software name> to see available versions; module help <module name> to see the help info**
 - We recommend to use the default version or newer versions
 - Eg., module load vasp; module load vasp/5.3.3
- **Application specific website**
 - Access control, eg., VASP, G09, SIESTA
 - Job script and special execution rule, eg., Molpro, Wien2k
 - Some performance tips and common errors
- **Need to compile by yourself?**
 - Makefiles are available in the installation directories
 - If not, send emails to consult@nersc.gov

Application specific website



Browser address bar: <https://www.nersc.gov/users/software/applications/materials-science/vasp/>

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VASP

Description

VASP is a package for performing *ab initio* quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. The approach implemented in VASP is based on a finite-temperature local-density approximation (with the free energy as variational quantity) and an exact evaluation of the instantaneous electronic ground state at each MD step using efficient matrix diagonalization schemes and an efficient Pulay mixing.

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Access to VASP

VASP is available only to NERSC users who already have an existing VASP license. If you have a VASP license, send your license information to the VASP support at Vienna at vasp.materialphysik@univie.ac.at (and copy vasp_licensing@nersc.gov) requesting that they confirm your VASP license to NERSC staff at vasp_licensing@nersc.gov in order to gain access to the VASP binaries at NERSC. Please note, VASP 5 requires a separate license. The VASP 4.6 users will NOT be automatically upgraded to VASP 5. Therefore, you need to confirm your VASP 5 license separately if you are a VASP 4 user and just upgraded your license to VASP 5.

Modules

NERSC uses **modules** to manage access to software. To access VASP at NERSC you must first verify your VASP license via email. When your request has been processed you will be able to access the vasp executables.

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Available VASP modules –use the default or the latest versions



```
zz217@edison11:~> module avail vasp
----- /usr/common/usg/Modules/modulefiles -----
vasp/4.6.35_vtst      vasp/5.3.3(default)  vasp/5.3.3-intel14  vasp/5.3.3_vtst-cce
vasp/5.3.2           vasp/5.3.3-cce      vasp/5.3.3-pgi      vasp/5.3.3_vtst-intel14
vasp/5.3.2_vtst      vasp/5.3.3-intel12  vasp/5.3.3_vtst     vasp/5.3.3_vtst-pgi
```

```
zz217@hopper01:~> module avail vasp
----- /usr/common/usg/Modules/modulefiles -----
vasp/4.6.35          vasp/5.2.12          vasp/5.3.2-pgi      vasp/5.3.3-pgi
vasp/4.6.35.pkent    vasp/5.2.12-cce(default) vasp/5.3.2_vtst     vasp/5.3.3_vtst
vasp/5.2             vasp/5.2.12_vtst-pgi vasp/5.3.2_vtst-pgi vasp/5.3.3_vtst-pgi
vasp/5.2.11         vasp/5.3.2           vasp/5.3.3
```

```
zz217@cvrsvc01:~> module avail vasp
----- /usr/common/usg/Modules/modulefiles -----
vasp/4.6.35(default) vasp/5.2.11.tbdyn    vasp/5.2.matgen     vasp/5.3.2_vtst
vasp/5.2             vasp/5.2.12          vasp/5.3.3          vasp/5.2.11
vasp/5.2.12_vtst     vasp/5.2_ofed2      vasp/5.3.3_vtst     vasp/5.2.11.IKPTD
vasp/5.2.8           vasp/5.3.2           vasp/5.3.3_vtst.matgen
```

What does a VASP module define?

```
zz217@edison11:~> module show vasp
```

```
-----  
/usr/common/usg/Modules/modulefiles/vasp/5.3.3:
```

```
module-whatis      VASP: Vienna Ab-initio Simulation Package
```

Access to the vasp suite is allowed only for research groups with existing licenses for VASP. If you have a VASP license please email

vasp.Materialphysik@univie.ac.at and CC: vasp_licensing@nersc.gov

with the information on which research group your license derives from. The PI of the group as well as the institution and license number will help speed the process.

```
setenv      PSEUDOPOTENTIAL_DIR /usr/common/usg/vasp/pseudopotentials
```

```
setenv      VDW_KERNEL_DIR /usr/common/usg/vasp/vdw_kernel
```

```
setenv      NO_STOP_MESSAGE 1
```

```
prepend-path PATH /usr/common/usg/vasp/vtstscripts/default
```

```
prepend-path PATH /usr/common/usg/vasp/5.3.3/bin
```

Where are VASP binaries and where are the makefiles used?



```
zz217@edison11:~> ls -l /usr/common/usg/vasp/5.3.3/
total 8
drwxr-x--- 2 zz217 vasp5 2048 Jan 23 17:39 bin
drwxrwsr-x 2 zz217 usg  2048 Nov  9 07:16 makefiles
```

```
zz217@edison11:~> ls -l /usr/common/usg/vasp/5.3.3/bin
total 425780
-rwxrwxr-x 1 zz217 usg 67641916 Sep 17 14:48 gvasp
-rwxrwxr-x 1 zz217 usg 75191844 Sep 17 14:49 vasp
-rwxrwxr-x 1 zz217 usg 75163298 Sep 17 14:50 vasp_ncl
```

```
zz217@edison11:~> ls -l /usr/common/usg/vasp/5.3.3/makefiles
total 92
-rwxrwxr-x 1 zz217 usg  650 Apr 19  2013 build.sh
-rw-rw-r--+ 1 zz217 usg 14314 Jun 12  2013 makefile
-rw-rw-r--+ 1 zz217 usg 14327 Jul 16  2013 makefile.gamma
-rw-rw-r--+ 1 zz217 usg  1861 Jan 15  2013 makefile_lib
-rw-rw-r--+ 1 zz217 usg 14304 Jun 12  2013 makefile.ncl
zz217@edison11:~>
```

Take home message



- **NERSC supports hundreds of software packages, ranging from compilers, libraries and application packages, and users are recommended to use them.**
- **Use the module commands to interact with them.**
 - “**module avail**” command to see the available software
 - Use the **module load** <module name> to access
 - **Compiler wrappers on Edison and Hopper take care of the libraries and their paths for you most of the time**
 - If not, use **module show** <module name> to find out the installation directories
 - **Use the -v or -craype-verbose** option to the compiler wrappers to see detailed/exact compile/link lines on Hopper and Edison
- **Visit the software specific websites for software specific info**
- **Send your software requests to consult@nerisc.gov**



Thank you.