Outline

● Applications Already Available at NERSC
● Available Compilers
● Available Libraries

● Fix the problem Game
Did you know that NERSC offers precompiled executables for more than 100 applications?
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Example, Materials Science:

Quantum ESPRESSO, NAMD, LAMMPS, NWChem, VASP, BerkeleyGW, SIESTA, Abinit, Gamess, GROMACS, GPAW MEEP, cpmd, libxc, etsf_io, atompaw, Wiek2K, Gaussian, PARATEC, cp2k, Wannier90, Amber, Yambo, XCrysdan, Q-Chem
Applications Already Available

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

The NERSC Software Database on the web shows all of our available pre-compiled applications for Hopper, Edison, Carver.
Applications
Already Available

Many application pages contain compilation instructions
e.g. Abinit

Compilation Instructions

Some advanced users may be interested in tweaking the Abinit build parameters and building Abinit themselves in their own directory. In order to aid in this process, and to provide a greater degree of transparency, the build instructions for the Abinit module are listed below. The following procedure was used to build Abinit 6.8.2 on Hopper.

```
% module swap PrgEnv-pgi PrgEnv-gnu

% module swap gcc gcc/4.5.2

% module load netcdf atompaw etsf_io wannier90 libxc

% ./configure --prefix="pwd"/.. FC=f77 CC=CC CXX=CC FCFLAGS="-O3" CFLAGS="-O3" CXXFLAGS="-O3" --with-fc-vendor=gnu

% make

% make install
```
Available Compilers

Compilers vs. Compiler Wrappers

pgf90, pgcc, pgCC (ifort, icc) vs ftn, cc, CC (mpif90, mpicc, mpiCC)

The compiler wrappers are the same as the underlying compilers with the addition of flags included by default and libraries linked by default (like MPI libraries for example)

The same compiler wrapper command (.e.g. ftn) can refer to any underlying compiler available on the system (e.g. pgi, gnu, intel etc...
## Available Compilers

### Available Compilers Across Machines:

<table>
<thead>
<tr>
<th></th>
<th>Edison</th>
<th>Hopper</th>
<th>Carver</th>
</tr>
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<tbody>
<tr>
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<td>✗</td>
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<tr>
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<td></td>
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**Hopper/Edison Module Access:**

```
% module swap PrgEnv-intel PrgEnv-gnu
```

**Carver Module Access:**

```
% module swap pgi gcc
% module swap openmpi openmpi-gcc
```
### Available Compilers

#### Useful Compiler Options on Hopper:

<table>
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<tr>
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<td>-fast</td>
<td>-O3 -fast-math</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>OpenMP</strong></td>
<td>-mp=nonuma</td>
<td>-fopenmp</td>
<td>-openmp</td>
<td></td>
</tr>
<tr>
<td><strong>Version</strong></td>
<td>-V</td>
<td>--version</td>
<td>-V</td>
<td>-V</td>
</tr>
<tr>
<td><strong>Verbose</strong></td>
<td>-v</td>
<td>-v</td>
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</tr>
<tr>
<td><strong>Debugging</strong></td>
<td>-g -C -WI,- ydgemm_</td>
<td>-g -fbounds-check</td>
<td>-g -warn all - CB</td>
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- The "-v" option displays the complete link and compile line unwrapped from ftn
- The "-WI,-y<symbol_name>" reports which library the linker is currently using for the symbol <symbol_name>"
**Available Compilers**

**Useful Compiler Options on Edison:**

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- The "-v" option displays the complete link and compile line unwrapped from ftn.

- The "-Wl,-y<symbol_name>" reports which library the linker is currently using for the symbol <symbol_name>.
Available Compilers

Tips for using compilers:

- Use the compiler wrappers for parallel programs:
  hopper/edison: **ftn, cc, CC** not **gcc, gfortran, pgf90, ifort** ...
  carver: **mpif90, mpicc, mpiCC**
Available Compilers

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- Use the compiler wrappers for parallel programs:
  - hopper/edison: ftn, cc, CC not gcc, gfortran, pgf90, ifort ...
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- ftn links libraries (blas etc...) by default on Hopper (need -mkl=cluster on edison with intel). mpif90 does not.
Available Compilers

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- Use the compiler wrappers for parallel programs:
  
  hopper/edison: ftn, cc, CC not gcc, gfortran, pgf90, ifort ...
  
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- Hopper/Edison statically link by default, but Carver dynamically links by default.
Available Compilers

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- Use the compiler wrappers for parallel programs:
  - hopper/edison: ftn, cc, CC not gcc, gfortran, pgf90, ifort ...
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- ftn links libraries (blas etc...) by default on Hopper (need -mkl=cluster on edison with intel). mpif90 does not.

- Hopper/Edison statically link by default, but Carver dynamically link by default.

You can dynamically link on Hopper by adding -dynamic flag to compilation and "setenv CRAY_ROOTFS DSL" in batch script and/or use CCM.
Available Compilers

Tips for using compilers:

To show libraries linked automatically with ftn

```
% ftn -v test.f90 -o test.x
...
Using built-in specs.
...
```

To show which library "dgemm" is used from:

```
% ftn -Wl,-ydgemm_ test.f90 -o test.x
/scratch/scratchdirs/jdeslip/cc8lmteH.o: reference to dgemm_
/opt/xt-libsci/11.0.03/gnu/46/mc12/lib/libsci_gnu_mp.a(dgemm.o): definition of dgemm_
```
Software libraries at NERSC are managed in modules.

Modules add and remove executables and libraries from your $PATH and $LD_LIBRARY_PATH as well as define environment variables.

They are used by doing "module load" command

e.g. "% module load fftw"
Available Libraries

Most math and science libraries are available

e.g. Carver:

```bash
% module avail fftw

------------------------------------------- /usr/common/usg/Modules/modulefiles -------------------------------------------
fftw/2.1.5(default) fftw/3.2.2 fftw-Intel/2.1.5 fftw-gnu/2.1.5
fftw/2.1.5-gnu fftw/3.2.2-gnu fftw-Intel/3.2.2 fftw-gnu/3.2.2

% module show fftw/2.1.5

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
```
Jack is having trouble building and running some of his favorite applications at NERSC.

Can you help fix the problem?

Rules:  No looking ahead.
Prizes:  Eternal glory in the minds of those around you.
Quantum ESPRESSO on Hopper:

% cat README
...
Quick installation instructions for the impatient:
./configure [options]
make all
...
...
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% cat README
...
Quick installation instructions for the impatient:
./configure [options]
make all
...

That seems easy enough...

% ./configure ... (Success!)
% make all ... come back in 20 minutes ... (Success!)

% aprun -n 5 ~/PresentationDir/espresso-4.3.2/bin/pw.x -in ./in

Program PWSCF v.4.3.2 starts on 25Jan2012 at 15:19:44
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The output looks weird and repeated....
Solution

Use the compiler wrappers, ftn, cc, CC. They can often be specified in configure:

./configure FC=ftn CC=CC CXX=CC or in make.sys file
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./configure FC=ftn CC=CC CXX=CC or in make.sys file

```bash
% cat make.sys
.....
DFLAGS = -D__PGI -D__ACML
FDFLAGS = $(DFLAGS)
MPIF90 = pgf90
#F90 = pgf90
CC = pgcc
F77 = pgf77
.....
```

```bash
% cat make.sys_fixed
.....
DFLAGS = -D__PGI -D__ACML -D__MPI
FDFLAGS = $(DFLAGS)
MPIF90 = ftn
#F90 = ftn
CC = cc
F77 = ftn
.....
```
% cat arch.mk
...
FCPP   = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK   = ftn

LAPACKLIB =
FFTWLIB   =

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...
Round 2

BerkeleyGW on Hopper

% cat arch.mk
...
FCPP = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK = ftn

FOPTS = -fast
FNOOPTS = $(FOPTS)
...

% make
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:270: undefined reference to `fftwnd_f77_create_plan_
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:270: undefined reference to `fftwnd_f77_create_plan_
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:285: undefined reference to `fftwnd_f77_one_
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:287: undefined reference to `fftwnd_f77_one_
Solution

"undefined reference" errors usually mean you are missing a library at link time. In this case, we are missing the fftw library. Note that ftn links lapack/blas equivalents automatically.
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```plaintext
% cat arch.mk
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F90free = ftn -Mfree
LINK   = ftn

LAPACKLIB =
FFTWLIB   =

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...

% module load fftw
% cat arch.mk -fixed
...
FCPP   = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK   = ftn

LAPACKLIB =
FFTWLIB   = -L$(FFTW_DIR) -ldfftw

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...
% module load fftw mkl
% cat arch.mk
...
F90free = mpif90 -Mfree
LINK   = mpif90
FOPTS  = -fast

FFTWPATH  = $(FFTW_ROOT)
FFTWLIB   = -L$(FFTW_LIBDIR) -ldfftw
FFTWINCLUDE = $(FFTW_INC)

LAPACKLIB = $(MKL)
SCALAPACKLIB = -L$(MKL_LIBDIR) -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64
...

% make (SUCCESS!)
Round 3

BerkeleyGW on Carver

```
% module load fftw mkl
% cat arch.mk
...
F90free = mpi90 -Mfree
LINK   = mpi90
FOPTS  = -fast

FFTWPATH   = $(FFTW_ROOT)
FFTWLIB     = -L$(FFTW_LIBDIR) -ldfftw
FFTWINCLUDE = $(FFTW_INC)

LAPACKLIB   = $(MKL)
SCALAPACKLIB = -L$(MKL_LIBDIR) -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64
...

% make (SUCCESS!)
```

(later that day...)

```
% mpirun -np 2 xi0.cplx.x
xi0.cplx.x: error while loading shared libraries: libmkl_scalapack_lp64.so: cannot open shared object file: No such file
xi0.cplx.x: error while loading shared libraries: libmkl_scalapack_lp64.so: cannot open shared object file: No such file
```
Round 3

Solution

On carver, we link against shared object files. These need to be present at runtime.

These need to be in your $LD_LIBRARY_PATH
Solution

On carver, we link against shared object files. These need to be present at runtime.

These need to be in your $LD_LIBRARY_PATH

% module load mkl fftw

(or)

% export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/common/usg/mkl/10.2.2.025/lib/em64t:/usr/common/usg/fftw/2.1.5/lib
etsf_io on Hopper

% module swap PrgEnv-pgi PrgEnv-gnu
% module load netcdf
% ./configure --prefix="`pwd`/../" CC=cc CXX=cc FC=ftn F77=ftn FCFLAGS="-O3" F77FLAGS="-O3" CFLAGS="-O3" CXXFLAGS="-O3" --with-netcdf-module-path="$CRAY_NETCDF_DIR/gnu/45/include" --enable-fortran

checking for module extension for compiler 'gcc'... mod
checking for ranlib... ranlib
checking for ar... ar
checking for /opt/cray/netcdf/4.1.3/gnu/45/include/netcdf.mod... yes
checking for netcdf library... no
Action: install NetCDF and set the library link path with --with-netcdf-ldflags.
configure: error: "No 'NetCDF' library found."

But... This worked for me one month ago just fine!?!?!?
Round 4

Solution

To debug ./configure errors. Look at generated config.log.

```
% cat config.log
....
configure:3866: ftn -o conftest -O3 -I/opt/cray/netcdf/4.1.3/gnu/45/include conftest.f90 -lnetcdf >&5
conftest.f90:3.12:
  use netcdf
    1
Fatal Error: Wrong module version '4' (expected '6') for file 'netcdf.mod' opened at (1)
configure:3872: $? = 1
configure: failed program was:
    | program main
    | use netcdf
    | integer :: s, ncid
    | s = nf90_open(path = "", mode = NF90_NOWRITE, ncid = ncid)
    | end program main
....
```

ftn --version shows gcc 4.6, but netcdf module was compiled with gcc 4.5.
Summary of Good Practices

- Use developer recommended compiler and compiler options
- Use compiler wrappers
- Test your application against lower optimization levels and included tests
- Use system provided libraries
NERSC Website:
- http://www.nersc.gov/nusers/systems/carver/
  programming/index.php
- http://www.nersc.gov/users/computational-systems/
hopper/programming/

Man Pages:
% man pgf90

eMail Us:
consult@nersc.gov

Presentation URL: http://goo.gl/zXcDz
% cat jobscript.e3250732

Initial temperature 500.0000000000002 500.0000000000001
Application 5341714 exit signals: Floating point exception

% cat Makefile
...
FC = ftn #mpif90 -fpp  # Modified
DEFINES = -DMPI
FILESF77= mdheff.F readinput.f readepqr3ndonsite.f ran1.f timer.f
OBJSF77= $(FILESF77:.F=.f)
OBF77= $(FILESF77:.f=.o)
.f.o:
   $(FC) -c $(FFLAGS) $(DEFINES) $<
....

do ia=rank+1,nsites,nprocs
Round 2

User MPI Code

% cat jobscript.e3250732

Initial temperature 500.0000000000002 500.0000000000001
Application 5341714 exit signals: Floating point exception

% cat Makefile

...  
FC = ftn #mpif90 -fpp  # Modified  
DEFINES = -DMPI  
FILESF77= mdheff.F readinput.f readepqr3ndonsite.f ran1.f timer.f  
OBJSF77= $(FILESF77:.f=.o)  
.f.o:  
   $(FC) -c $(FFLAGS) $(DEFINES) $<  
....  

do ia=rank+1,nsites,nprocs  
nprocs=0
Solution

The $(DEFINES)$ was not included in the compilation of the .F files.

% cat Makefile
...
FC = ftn #mpif90 -fpp       # Modified
FLAGSOPM = #-O2 -march=pentium3 -mtune=core2 -assume byterecl -funroll-loops -fp-model precise -pc64 # Modified
DEFINES = -DMPI

FILESF77= mdheff.F readinput.f readepqr3ndonsite.f ran1.f timer.f
OBJSF77= $(FILESF77:.f=.o)
  .f.o:
      $(FC) -c $(FFLAGS) $(DEFINES) $<
  .F.o:
      $(FC) -c $(FFLAGS) $(DEFINES) $<
  ....