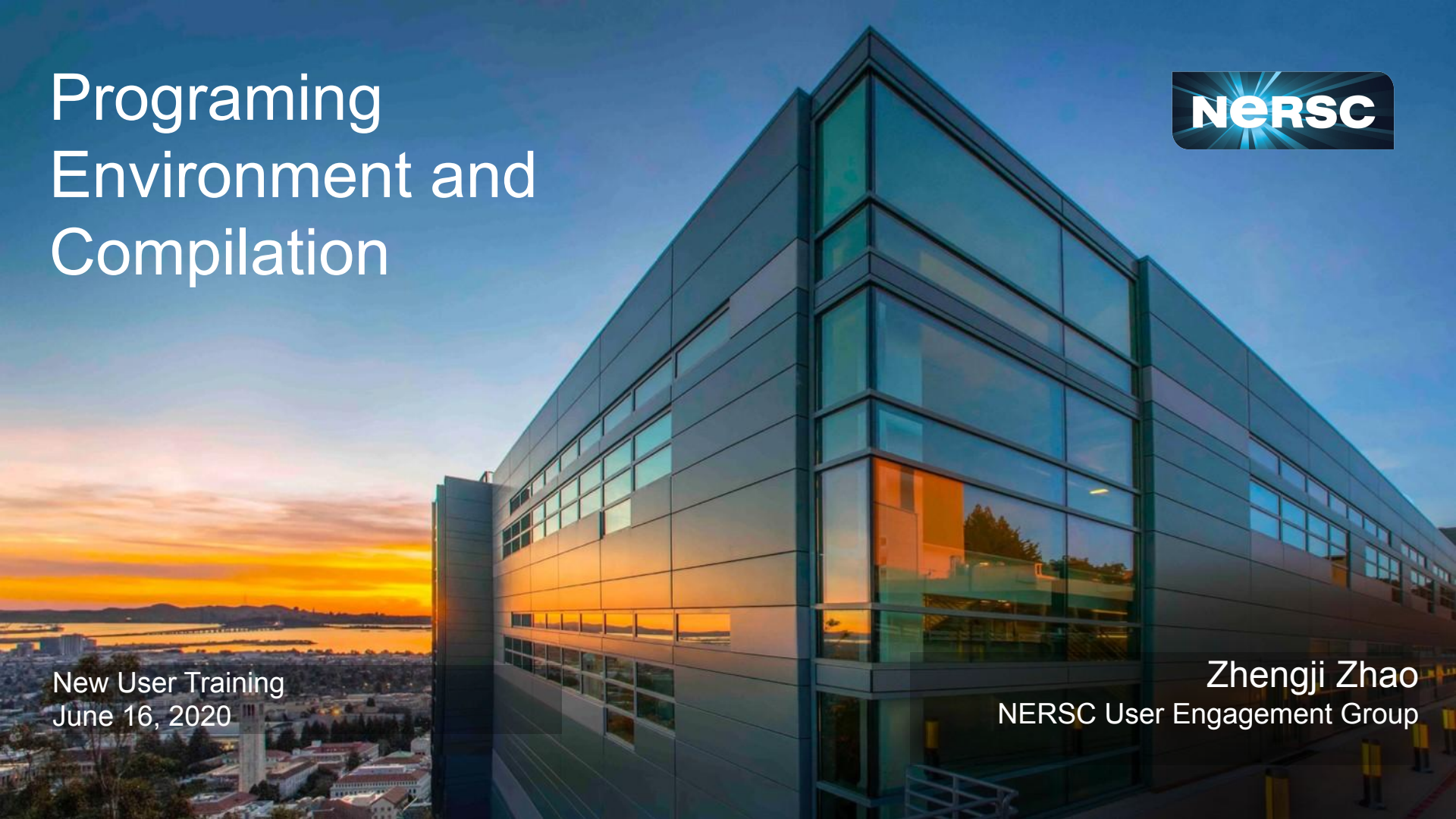
Programing Environment and Compilation



New User Training
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NERSC User Engagement Group

Outline

- Cori compilation overview
- Compile/link lines:

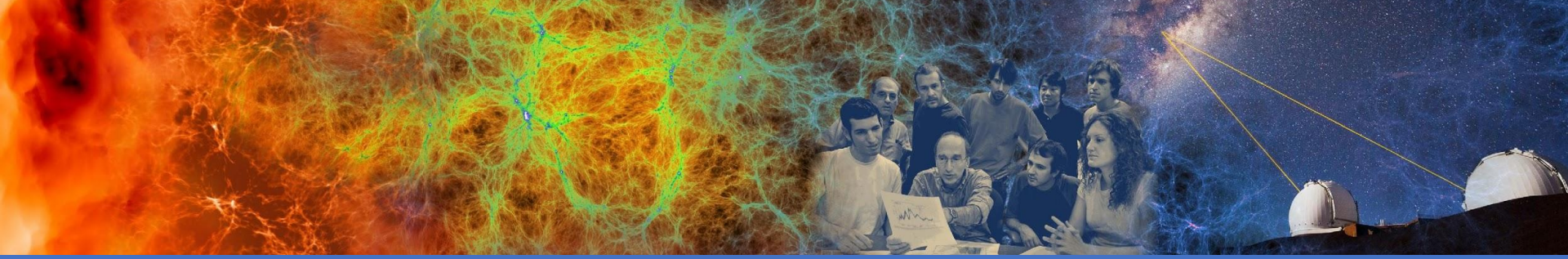
  Compiler +

  Compiler Flags +

  –I/path/to/headers +

  –L/path/to/library –l<library>

- Available libraries, and linking examples
- Spack - a package manager
- Summary



Cori Compilation Overview

Compilations on Cori

- Three programming environments are supported on Cori
  - Intel, GNU and Cray compilers are available; Intel is the default
- The programming environment modules, “PrgEnv-intel”, “PrgEnv-gnu”, and “PrgEnv-cray”, which include the compilers and matching libraries, provide user friendly programming environments
- Use “module swap PrgEnv-Intel PrgEnv-cray” to switch compilers
- Use the compiler wrappers provided by Cray, ftn, cc and CC for Fortran, C and C++ respectively, so that the header and library paths and libraries can be added on the compile/link lines automatically.

Cori System Configurations

- Cori KNL and Haswell – a Cray XC40
  - Cori has 9688 single-socket Intel® Xeon Phi™ Processor 7250 ("Knights Landing") nodes @1.4 GHz with 68 cores (272 threads) per node, two 512 bit vector units per core, and 16 GB high bandwidth on-package memory (MCDRAM) with 5X the bandwidth of DDR4 DRAM memory (>400 GB/sec) and 96 GB DDR4 2400 MHz memory per node
  - In addition, Cori has 2388 dual-socket 16-core Intel® Xeon™ Processor E5-2698 v3 ("Haswell") nodes @2.3GHz with 32 cores (64 threads) per node, two 256 bit vector units per core, 128 GB 2133 MHz DDR4 memory
  - Cori nodes are interconnected with Cray's Aries network with Dragonfly topology
- Binary compatibility: Haswell binaries run on KNL, but not vise versa, because KNL supports the extended instruction sets
- Separate builds for Haswell and KNL are recommended for optimal performance

Compilations on Cori (Cont.)

- Cross compilation: compiling for compute nodes from login nodes (Haswell)
- Default environment loads the craype-haswell module on Cori, which sets "CRAY_CPU_TARGET=haswell" for Cori. So, compilers build binaries that are optimized for Haswell processors by default when compiling with the compiler wrappers

Default programming environment on Cori:

```
zz217@cori06:~> module list
Currently Loaded Modulefiles:
  1) modules/3.2.11.4                 9) udreg/2.3.2-7.0.1.1_3.29__g8175d3d.ari          17) alps/6.6.57-7.0.1.1_5.10__g1b735148.ari
  2) nsg/1.2.0                       10) ugni/6.0.14.0-7.0.1.1_7.32__ge78e5b0.ari        18) rca/2.2.20-7.0.1.1_4.42__g8e3fb5b.ari
  3) altd/2.0                        11) pmi/5.0.14                                      19) atp/2.1.3
  4) darshan/3.1.7                   12) dmapp/7.1.1-7.0.1.1_4.43__g38cf134.ari          20) PrgEnv-intel/6.0.5
  5) intel/19.0.3.199                13) gni-headers/5.0.12.0-7.0.1.1_6.27__g3b1768f.ari 21) craype-haswell
  6) craype-network-aries            14) xpmem/2.2.20-7.0.1.1_4.8__g0475745.ari          22) cray-mpich/7.7.10
  7) craype/2.6.2                    15) job/2.2.4-7.0.1.1_3.34__g36b56f4.ari            23) craype-hugepages2M
  8) cray-libsci/19.06.1             16) dvs/2.12_2.2.156-7.0.1.1_8.6__g5aab709e
zz217@cori06:~>
```

To Compile for Cori Haswell

- Intel programing environment is the default

```
#to use Intel compilers
ftn -O3 mycode.f90        # Fortran
cc -O3 mycode.c           # for C
CC -O3 myC++code.C        # for C++
```

```
#to use GNU compilers
module swap PrgEnv-intel PrgEnv-gnu
ftn -O3 mycode.f90        # Fortran
cc -O3 mycode.c           # for C
CC -O3 myC++code.C        # for C++
```

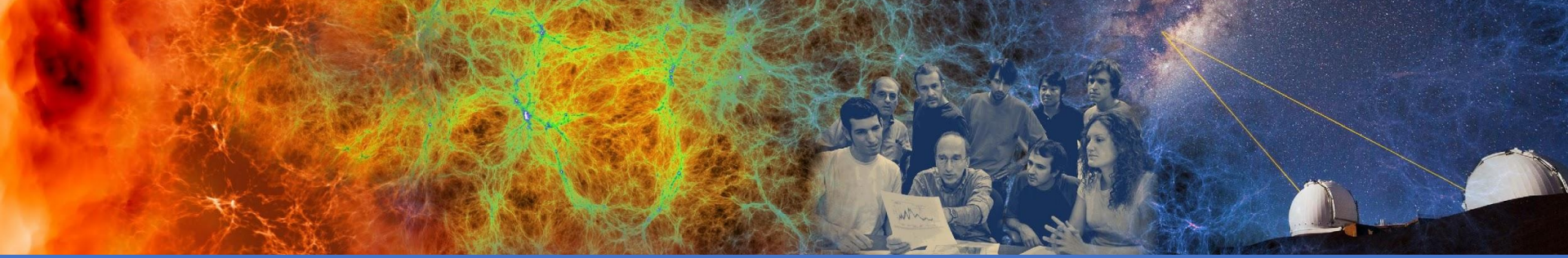
```
#to use Cray compilers
module swap PrgEnv-intel PrgEnv-cray
ftn -O3 mycode.f90         # Fortran
cc -O3 mycode.c            # for C
CC -O3 myC++code.C         # for C++
```

Note: the compiler wrappers, ftn, cc, and CC, are not Cray compilers; They invoke the Intel, GNU, or Cray compilers under the hood, depending on the loaded PE module (PrgEnv-<compiler>)

To Compile for Cori KNL

- Applications are cross compiled for KNL nodes from the login nodes (Haswell)
- Do "module swap craype-haswell craype-mic-knl" before compiling for KNL to build binaries that are optimized for the KNL architecture

```
module swap craype-haswell craype-mic-knl
ftn -O3 mycode.f90          # Fortran
cc -O3 mycode.c             # for C
CC -O3 myC++code.C          # for C++
```



Compile/Link Lines

Compiler Recommendations

- Will not recommend any specific compiler
  - Intel - better chance of getting processor specific optimizations, especially for KNL
  - Cray compiler – many new features and optimizations, especially with Fortran; useful tools like reveal work with Cray compiler only
  - GNU - widely used by open software
- Start with the compilers that vendor/code developers used so to minimize the chance to hit compiler and code bugs, then explore different compilers for optimal performance

Compiler Flags

Intel	GNU	Cray*	Description/ Comment
-O2	-O0	-O2	Default Optimization Level
default , or –O3	-O2 or -O3,-Ofast	default	Recommended Compiler Flags
-qopenmp	-fopenmp	–h omp for Fortran; -fopenmp for C/C++	OpenMP Flag
-g	-g	-g	Debug
-v	-v	-v	Verbose

*) Starting from CCE 9.0 version, Cray C/C++ compilers use LLVM as backend

- Validity check after compilation
- Compilers' default behavior could vary between compilers
  - Default number of OpenMP threads used is all CPU slots available for Intel and GNU compilers; 1 for Cray compiler
  - Use compiler man page for available compiler optimization flags, e.g., man ifort

Header and Library Paths and Libraries

- Manually:
  - Find out the paths to the headers, and libraries, then add

    “–I <header path> -L<library path> -l<libraries>” to your compile/link lines
- Automatically:
  - Using the compiler wrappers, which can do this for you
  - Compiler wrappers are strongly recommended

Compiler Wrappers, ftn, cc and CC

- Use ftn, cc, and CC to compile Fortran, C and C++ codes, respectively, instead of invoking the native compilers directly, such as `ifort, icc, icpc, gfortran, gcc, g++,` etc.
  - The compiler wrappers wraps the underlying compilers with additional compiler and linker flags depending on the modules loaded in the environment
  - The same compiler wrapper command (e.g. ftn) is used to invoke any compilers supported on the system (Intel, GNU, Cray)
- Compiler wrappers do cross compilations
  - Compiling applications on login nodes to run on compute nodes
  - For some applications, may need to set the `-host=x86_64` configure option (if available) when compiling for KNL from a login node
  - If compiling on a KNL node is needed, do "`salloc -N 1 -q interactive -C knl -t 4:00:00`" to get on to a compute node

Compiler Wrappers, ftn, cc and CC (Cont.)

- Compiler wrappers link dynamically by default on Cori
  - May need to load the same set of modules at run time or set the LD_LIBRARAY_PATH env so that shared libraries can be found. Alternatively, consider using the "`-Wl,-rpath=<library path>`" option when compiling
  - A dynamically linked executable may take some time to load shared libraries when running with a large number of processes
- Use the -static option of the compiler wrappers or set the environment variable "CRAYPE_LINK_TYPE=static" to link statically
  - Preferred for performance at scale

Why Compiler Wrappers?

- They include the architecture specific compiler flags into the compilation/link lines automatically

	Intel*	GNU	Cray	Required Module
Cori KNL	-xMIC-AVX512	-march=knl	-h cpu=mic-knl	craype-mic-knl
Cori Haswell	-xCORE-AVX2	-march=core-avx2	-h cpu=haswell	craype-haswell

*) for the latest Intel compilers, -march=knl,haswell can be used instead of -xcode.

- Automatically add header and library paths and libraries on the compilation/link lines
  - Compiler wrappers use the pkg-config tools to dynamically detect paths and libs from the environment (working with cray modules and some NERSC modules)
  - The architecture specific builds of libraries will be linked into
- Allow user provided options to take precedence

Verbose Output from Compiler Wrappers

- Depending on the modules loaded, compiler wrappers link to the MPI, LAPACK/BLAS/ScaLAPACK libraries, and more automatically
- Library names on Cori could be different from what you used before

```
zz217@cori06:~/tests/dgemm> module list
Currently Loaded Modulefiles:
  1) modules/3.2.11.4                                 9) udreg/2.3.2-7.0.1.1_3.29__g8175d3d.ari          17) alps/6.6.57-7.0.1.1_5.10__g1b735148.ari
  2) nsg/1.2.0                                       10) ugni/6.0.14.0-7.0.1.1_7.32__ge78e5b0.ari        18) rca/2.2.20-7.0.1.1_4.42__g8e3fb5b.ari
  3) altd/2.0                                        11) pmi/5.0.14                                      19) atp/2.1.3
  4) darshan/3.1.7                                   12) dmapp/7.1.1-7.0.1.1_4.43__g38cf134.ari          20) PrgEnv-intel/6.0.5
  5) intel/19.0.3.199                                13) gni-headers/5.0.12.0-7.0.1.1_6.27__g3b1768f.ari 21) craype-haswell
  6) craype-network-aries                            14) xpmem/2.2.20-7.0.1.1_4.8__g0475745.ari          22) cray-mpich/7.7.10
  7) craype/2.6.2                                    15) job/2.2.4-7.0.1.1_3.34__g36b56f4.ari            23) craype-hugepages2M
  8) cray-libsci/19.06.1                             16) dvs/2.12_2.2.156-7.0.1.1_8.6__g5aab709e

zz217@cori06:~/tests/dgemm> ftn -v dgemmx.f -Wl,-ydgemm_
...

/global/common/cori/software/altd/2.0/bin/ld    /usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/crt1.o /usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/crti.o /usr/lib64/gcc/x86_64-suse-linux/7/crtbegin.o --eh-frame-hdr --build-id -dynamic-linker /lib64/ld-linux-x86-64.so.2 -m elf_x86_64 -L/opt/cray/pe/libsci/19.06.1/INTEL/16.0/x86_64/lib -L/opt/cray/dmapp/default/lib64 -L/opt/cray/pe/mpt/7.7.10/gni/mpich-intel/16.0/lib -L/opt/cray/dmapp/default/lib64 -L/opt/cray/pe/mpt/7.7.10/gni/mpich-intel/16.0/lib -L/opt/cray/rca/2.2.20-7.0.1.1_4.42__g8e3fb5b.ari/lib64 -L/opt/cray/pe/atp/2.1.3/libApp -o a.out /opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64_lin/for_main.o -L/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mkl/lib/intel64 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64_lin -L/usr/lib64/gcc/x86_64-suse-linux/7/ -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64 -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/ -L/lib/../lib64 -L/lib/../lib64/ -L/usr/lib/../lib64 -L/usr/lib/../lib64/ -L/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64/ -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mkl/lib/intel64/ -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../../x86_64-suse-linux/lib/ -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../ -L/lib64 -L/lib/ -L/usr/lib64 -L/usr/lib /tmp/iforts9x6fo.o -ydgemm_ -rpath=/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64 -Ttext-segment=0x20000000 -zmax-page-size=0x20000000 --whole-archive -lhugetlbfs --no-whole-archive --no-as-needed -lAtpSigHandler -lAtpSigHCommData --undefined=_ATP_Data_Globals --undefined=__atpHandlerInstall -lrca -lz --as-needed -lmpich_intel --no-as-needed --as-needed -lmpichf90_intel --no-as-needed --as-needed -lsci_intel_mpi --no-as-needed --as-needed -lsci_intel --no-as-needed --as-needed -limf --no-as-needed --as-needed -lm --no-as-needed --as-needed -lpthread --no-as-needed -Bdynamic -Bstatic -lifport -lifcoremt -limf -lsvml -Bdynamic -lm -Bstatic -lipgo -lirc -Bdynamic -lpthread -Bstatic -lsvml -Bdynamic -lc -lgcc -lgcc_s -Bstatic -lirc_s -Bdynamic -ldl -lc /usr/lib64/gcc/x86_64-suse-linux/7/crtend.o /usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/crtn.o
/usr/bin/ld: /tmp/iforts9x6fo.o: reference to dgemm_
/usr/bin/ld: /opt/cray/pe/libsci/19.06.1/INTEL/16.0/x86_64/lib/libsci_intel_mpi.so: reference to dgemm_
/usr/bin/ld: /opt/cray/pe/libsci/19.06.1/INTEL/16.0/x86_64/lib/libsci_intel.so: definition of dgemm_
```

Verbose Output from Compiler Wrappers (Cont.)

```
zz217@cori06:~/tests/dgemm> ftn -v dgemmx.f -o dgemm.x -mkl -Wl,-ydgemm_
...

/global/common/cori/software/altd/2.0/bin/ld    /usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/crt1.o /usr/lib64/gcc/x86_64-suse-linux/7/.
./../../../lib64/crti.o /usr/lib64/gcc/x86_64-suse-linux/7/crtbegin.o --eh-frame-hdr --build-id -dynamic-linker /lib64/ld-linux-x86-64.so.2 -m e
lf_x86_64 -L/opt/cray/dmapp/default/lib64 -L/opt/cray/pe/mpt/7.7.10/gni/mpich-intel/16.0/lib -L/opt/cray/dmapp/default/lib64 -L/opt/cray/pe/mpt/
7.7.10/gni/mpich-intel/16.0/lib -L/opt/cray/rca/2.2.20-7.0.1.1_4.42__g8e3fb5b.ari/lib64 -L/opt/cray/pe/atp/2.1.3/libApp -o dgemm.x /opt/intel/co
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tel64 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mkl/lib/intel64 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/i
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64-suse-linux/7/../../../../lib64 -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib64/ -L/lib/../lib64 -L/lib/../lib64/ -L/usr/lib/../lib64 -
L/usr/lib/../lib64/ -L/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64/ -L/opt/intel/compilers_and_libraries_2019.3.199/
linux/mkl/lib/intel64/ -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../../x86_64-suse-linux/lib/ -L/usr/lib64/gcc/x86_64-suse-linux/7/../../../ -L
/lib64 -L/lib/ -L/usr/lib64 -L/usr/lib /tmp/ifortOJ86Zo.o --start-group -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 --end-group -Bdyn
amic -ydgemm_ -rpath=/opt/intel/compilers_and_libraries_2019.3.199/linux/compiler/lib/intel64 -Ttext-segment=0x20000000 -zmax-page-size=0x200000
00 --whole-archive -lhugetlbfs --no-whole-archive --no-as-needed -lAtpSigHandler -lAtpSigHCommData --undefined=_ATP_Data_Globals --undefined=__a
tpHandlerInstall -lrca -lz --as-needed -lmpich_intel --no-as-needed --as-needed -lmpichf90_intel --no-as-needed --as-needed -limf --no-as-needed
 --as-needed -lm --no-as-needed --as-needed -lpthread --no-as-needed --start-group -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 --end-
group -Bdynamic -Bstatic -lifport -lifcoremt -limf -lsvml -Bdynamic -lm -Bstatic -lipgo -lirc -Bdynamic -lpthread -Bstatic -lsvml -Bdynamic -lc
-lgcc -lgcc_s -Bstatic -lirc_s -Bdynamic -ldl -lc /usr/lib64/gcc/x86_64-suse-linux/7/crtend.o /usr/lib64/gcc/x86_64-suse-linux/7/../../../../lib
64/crtn.o
/usr/bin/ld: /tmp/ifortOJ86Zo.o: reference to dgemm_
/usr/bin/ld: /opt/intel/compilers_and_libraries_2019.3.199/linux/mkl/lib/intel64/libmkl_intel_lp64.so: definition of dgemm_
```
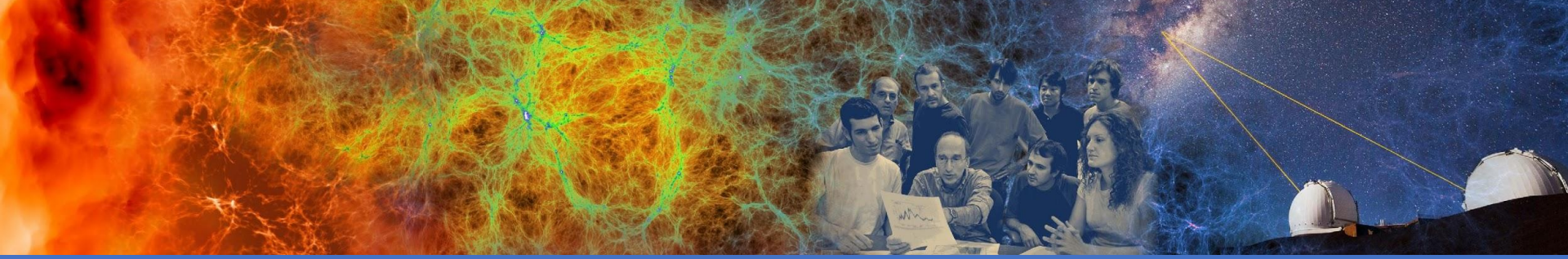



Available Libraries, and Linking Examples

Available Libraries

- Access via modules, type "`module avail`" or "`module avail -S <your string>`" to see the available modules
- Cray supports many software packages – Cray Developer Toolkits (CDT)
  - Modules from `/opt/cray/pe/modulefiles`, etc.
  - There are different builds for different compilers
  - Programming environment modules allow the libraries built with the matching compilers to be linked to
- NERSC staff also supports many libraries
  - Modules from `/usr/common/software/modulefiles`, etc.
  - Some of them interact with the Cray compiler wrappers while many of them do not

Available Libraries (Cont.)

- Where are the libraries and header files ?
  - Use "`module show <module name>`" to see the installation paths
  - Run "`ls -l <installation_path>/include`" and "`ls -l <installation_path>/lib`" to see the library files
  - e.g., Cray MPICH library:

```
zz217@cori06:~> module show cray-mpich
-------------------------------------------------------------------
/opt/cray/pe/modulefiles/cray-mpich/7.7.10:
…
setenv          CRAY_MPICH_DIR /opt/cray/pe/mpt/7.7.10/gni/mpich-intel/16.0
setenv          MPICH_DIR /opt/cray/pe/mpt/7.7.10/gni/mpich-intel/16.0
...
```

```
zz217@cori06:~> ls -l $CRAY_MPICH_DIR
total 0
drwxr-xr-x 2 root root  628 Nov 14  2019 include
drwxr-xr-x 3 root root 1239 Nov 14  2019 lib
```

Example: Linking to Cray Provided Libraries

- Linking to the Cray MPI and Cray Scientific libraries are automatic by default if compiler wrappers are used

```
CC parallel_hello.cpp   #or  ftn dgemmx1.f90
```

- Linking to HDF5 and NETCDF libraries are automatic, user just need to load the cray-hdf5 or cray-netcdf modules

```
module load cray-hdf5
cc h5write.c
```

- Note the library name could be different. Using the `-v` option to see the library names and other detail about the linking

Example: Linking to Cray Provided Libraries

- Linking to PETSc libraries are automatic, but users need to choose a proper module (e.g., real/complex, 32 or 64 bit integer builds)
  - E.g., “module load cray-petsc-complex-64”
  - Use “cc –v test1.c” to see the linking detail (test1.c can be any skeleton C code)
- Linking to fftw libraries
  - module load cray-fftw
  - Loading the cray-fftw module links to the pthread version of the library, “-lfftw3f_mpi -lfftw3f_threads -lfftw3f -lfftw3_mpi -lfftw3_threads -lfftw3”,
  - Use -qopenmp to link with the OpenMP version of FFTW

Linking to the NERSC Provided Libraries

- Some of the NERSC provided modulefiles are written to interact with the Cray compiler wrappers, e.g., elpa module on Cori

```
module load elpa
#automatically link to elpa and MKL ScaLAPACK libraries
ftn -qopenmp -v test2.f90
```

  - Type “module show <module name>” to check if the envs “<libname>_PKGCONFIG_LIBS”, “PE_PKGCONFIG_PRODUCTS”, and “PKG_CONFIG_PATH” are defined in the modulefiles, which compiler wrappers look for

- Most of the NERSC provided modulefiles do not interact with the compiler wrappers, user need to provide the include and library paths and libraries manually, e.g., GSL

```
module load gsl
ftn test3.f90 $GSL
#where GSL=-I/global/common/sw/cray/cnl7/haswell/gsl/2.5/intel/19.0.3.199/7twqxxq/include
-L/global/common/sw/cray/cnl7/haswell/gsl/2.5/intel/19.0.3.199/7twqxxq/lib -lgsl -lgslcblas
```

Linking to Intel MKL Library

- Resource:
  - Intel® Math Kernel Library Link Line Advisor, https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor/
  - Learn from Intel compiler verbose output using the "`-mkl={parallel,sequential,cluster}`" flag

- For intel compiler, use `-mkl` flag
  - `ftn test1.f90 -mkl` # default to parallel, the multi-threaded MKL
    # the cray-libsci will be ignored if -mkl is used.

Linking to Intel MKL Library (Cont.)

- For GNU compiler (e.g., to link to 32-bit integer build statically):
  - Save the `$MKLROOT` from the Intel compiler module, and then
  - Threaded: `"-L$MKLROOT/lib/intel64 -Wl,--start-group -lmkl_gf_lp64 -lmkl_gnu_thread -lmkl_core -lgomp -Wl,--end-group -lpthread -lm -ldl"`
  - ScaLAPACK: `"-L$MKLROOT/lib/intel64 -Wl,--start-group -lmkl_gf_lp64 -lmkl_gnu_thread -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64 -lmkl_core -Wl,--end-group -lgomp -lpthread -lm -ldl"`

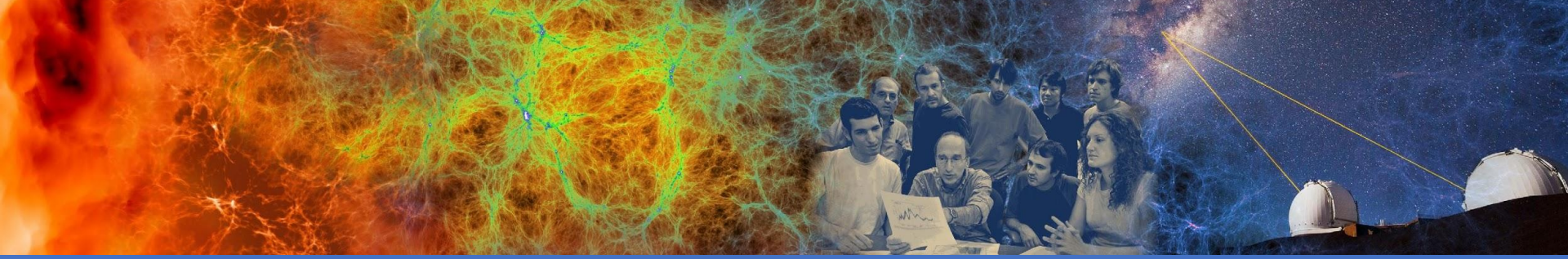
  Note, "`-Wl,--start-group`" … "`-Wl,--end-group`" for static linking

Linking to Intel MPI library

- Cray MPICH libraries are recommended for performance especially at scale
- Compiler wrappers link to Cray MPICH libraries by default
- However, if you need to link to Intel MPI library, do

```
module load impi
mpiifort test1.f90          #or mpiicpc test1.C
```

  - Note that the binaries linked to the Intel MPI need to run with srun instead of mpirun to get a proper process/thread affinity, https://docs.nersc.gov/jobs/examples/#intel-mpi



Spack - A Package Manager

Spack - A Package Manager

- Simple package installations
  - Spack installs the latest version of a package and its dependencies by default.
- Custom versions and configurations
  - Spack allows installation to be customized using a simple spec syntax to specify the version, build compiler, compile-time options, cross-compile platform, and dependencies, etc.
- Non-destructive installs
  - Uses hash from package/dependency configuration in the installation prefix
- Peaceful coexistence of packages
  - Uses RPATH to link dependencies; no need to manipulate LD_LIBRARY_PATH at runtime
- Easy package creation
  - package files are written in pure Python; one file for different builds

Spack Modules on Cori

- NERSC provides Spack modules for users
  - Allows access to NERSC's recommended, up-to-date configuration files
  - Configured to make use of the NERSC staff installed software, so no need to build each dependent package by themselves redundantly, saving compilation time and storage space
- To access, module load spack #currently spack 0.14.2 is made available
  - Create a directory (at the first time invocation only), `$HOME/sw`, and a few subdirectories under it on your account to build and install software on. E.g, software will be installed on your `$HOME/sw/opt/spack`directory, and the Spack generated modulefiles will be available at the `$HOME/sw/share/spack/modules`directory. You can create your own package files under the directory `$HOME/sw/var/spack/repos/$USER/packages`
- Users can overwrite these global setting with config files at ~/.spack

Building Software with Spack Modules

```
module load spack
spack list          # to see Spack supported packages
spack find -p       # to see the software installed by Spack

cd ~/sw/build
spack install <package name>   #to install a package

e.g.,
spack install wannier90@2.1.0 %intel@19.0.3.199 ^intel-mkl@19.0.3.199
spack install autoconf@2.69%intel@19.0.3.199 arch=cray-sles15-x86_64
spack install cp2k %intel blas=mkl +mpi ^intel-mkl
arch=cray-cnl7-haswell
```

Building Software with Spack Modules (Cont.)

```
train467@cori09:~/sw/build> spack install xerces-c
[+] /global/common/sw/cray/cnl7/haswell/libiconv/1.16/intel/19.0.3.199/vr7hfhz
[+] /global/common/sw/cray/cnl7/haswell/libiconv/1.16/intel/19.0.3.199/vr7hfhz
==> 41416: Installing xerces-c
==> Fetching https://archive.apache.org/dist/xerces/c/3/sources/xerces-c-3.2.2.tar.bz2
######################################################################################################################
################################### 100.0%
==> Staging archive:
/global/cscratch1/sd/train467/sw/spackbuild/spack-stage-xerces-c-3.2.2-ggdbuk52jm72rebq67s3ro2vxzaeozg4/xerce
s-c-3.2.2.tar.bz2
==> Created stage in
/global/cscratch1/sd/train467/sw/spackbuild/spack-stage-xerces-c-3.2.2-ggdbuk52jm72rebq67s3ro2vxzaeozg4
==> No patches needed for xerces-c
==> 41416: xerces-c: Building xerces-c [AutotoolsPackage]
==> 41416: xerces-c: Executing phase: 'autoreconf'
==> 41416: xerces-c: Executing phase: 'configure'
==> 41416: xerces-c: Executing phase: 'build'
==> 41416: xerces-c: Executing phase: 'install'
==> 41416: xerces-c: Successfully installed xerces-c
  Fetch: 2.30s.  Build: 2m 34.05s.  Total: 2m 36.35s.
[+] /global/homes/t/train467/sw/opt/spack/cray-cnl7-haswell/intel-19.0.3.199/xerces-c-3.2.2-ggdbuk5
```

If “spack install” fails

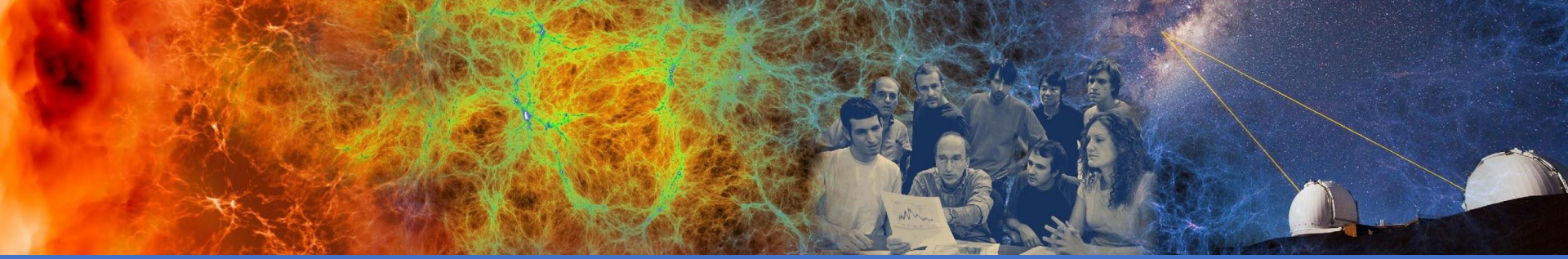
- Open an issue at https://github.com/spack/spack/issues
- Copy the failed package.py to your local repo to modify:

```
cp -pr $SPACK_ROOT/var/spack/repos/builtin/packages/<package name>
$HOME/sw/var/spack/repos/$USER/packages
spack edit <package name>
cd $HOME/sw/build
spack install <package name> ...
```

```
train467@cori02:~/sw/build> spack config get repos
repos:
- $HOME/sw/var/spack/repos/$USER
- /global/common/sw/spack/0.14.2/var/spack/repos/nersc
- /global/common/sw/spack/0.14.2d/var/spack/repos/builtin
```

Modify package.py files here

NERSC modified pakcage.py files are here



Summary

Summary

- Three supported programming environments: Intel, GNU, and Cray
- Use compiler wrappers where possible,
  - Add architecture specific optimization flags
  - Automatically add the header and library paths in to the compile/link lines, and link to the Cray MPI, LibSci and other Cray provided libraries if the modules are loaded
- To compile for Cori KNL, do
  - `module swap craype-haswell craype-mic-knl`

Summary (Cont.)

- There are many libraries available, use them where possible
  - Use "`module avail`" command to check available libraries
  - Use "`module show <module name>`" to see the installation paths if needed
- Most NERSC staff supported modules do not interact with the compiler wrappers
  - Users need to provide the header and library paths and libraries manually
- On Cori, applications are linked dynamically by default
  - Use of `rpath` is recommended
  - Use `/global/common/software/<project name>`directory to store your shared libraries and python modules as well as the dynamically linked applications

Summary (Cont.)

- To link applications statically, use the "`-static`" compiler wrapper option or set the env "`CRAYPE_LINK_TYPE=static`" before compiling
  - Static linking is recommended for large scale applications
- Learn from the compiler verbose output (`-v`)
- Spack is recommended to build your software

Recommended Readings

- NERSC website, especially,
  - Programming page at http://docs.nersc.gov,
  - https://docs.nersc.gov/programming/performance-debugging-tools/build-tools/#spack
- Compiler and linker man pages:
  - ifort, icc, icpc, crayftn, etc.
  - man ld (“`-Wl,-zmuldefs`”, “`-Wl,-y<symbol>`”)
- Spack
  - https://spack.readthedocs.io/en/latest/basic_usage.html#
  - https://docs.nersc.gov/development/build-tools/spack/


Thank You and
Welcome to
NERSC!
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