



Local HPC

Software and sw development

UNIVERSITY OF BERGEN





Outline

- Changes
- Details
- Documentation





Changes

- EasyBuild to provision new software
 - Naming
 - Stricter intermodule dependencies
- Some old SW will be removed





Basics

- Modules
 - module av
 - module load / unload
 - module switch
 - module list
- Only /work and /shared are available on computes
- aprun - to launch on compute nodes





Compiling specifics

- PrgEnv-*compiler*
 - Cray
 - PGI
 - GNU
- Default is PrgEnv-cray
 - module switch PrgEnv-cray PrgEnv-gnu





Compiler wrappers

- ftn - Fortran 90/95 programs
- cc - C programs
- CC - C++ programs
- module notur
- Will automatically include libs & includes from loaded modules
 - gcc -L/loaded_lib_path -lmodulelib ... ->
 - cc myprog.c -o myprog





Linking specifics

- Default is static
- If you need dynamic:
 - Compiling
 - `export CRAYPE_LINK_TYPE=dynamic`
 - Running
 - `export CRAY_ROOTFS=DSL`





Default optimisations

- craype-interlagos - Compute node optimised build
- craype-istanbul - Login node optimised





AMD Interlagos specifics

- 1 FPU per 2 Cores





Computes

- 2 CPUs:
 - 32 cores (16FPUs)
 - 32 GB RAM
 - /work and /shared





Optimisation continued

- Bulldozer / Interlagos
 - FMA and AVX
 - Cray compiler: with -hfp3 or -hfp2
 - PGI: is default when you have -tp=bulldozer
 - GNU(set of optimizations): -march=bdver1 -Ofast -mprefer-avx128 -funroll-all-loops -ftree-vectorize
- cray-libsci - BLAS, LAPACK, ScaLAPACK, BLACS, IRT, SuperLU, CRAFFT
- petsc - MUMPS, SuperLU, ParMETIS, HYPRE





Debugging

- Totalview
 - `totalview -newUI`
- Coredumps
 - `ulimit -c unlimited`
 - `gdb exe core`
 - Totalview





Profiling

- CrayPat
- ARM Performance reports





Resources

- [https://docs.hpc.uib.no/wiki/
Application_development_\(Hexagon\)](https://docs.hpc.uib.no/wiki/Application_development_(Hexagon))
- support@hpc.uib.no





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