

# LUMI

A white wolf is the central focus, standing in a futuristic, blue-toned digital environment. The background is filled with vertical light beams, floating particles, and a grid-like pattern, creating a high-tech, data-driven atmosphere. The wolf is looking slightly to the right of the camera.

## HPE Cray Programming Environment

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Evolving version

# Why do I need to know this?

- **Q:** “I only want to run some programs, why do I need to know about programming environments?”
- **A:** They are an intrinsic part of an HPC system
  - The middleware essential for parallel computing is often part of the PE
  - Programs are preferably installed from sources to generate binaries optimised for the system. When running, the build environment needs to be at least partially recreated.
    - Less relevant on HPE Cray systems though as they do something that is unusual on most HPC systems
  - Even when installing from prebuilt binaries, some modules from the programming environment might still be needed
    - Inject an optimised MPI library
    - But sometimes a prebuilt binary will not work due to middleware incompatibilities

# The Operating System

- The login nodes run SUSE Linux Enterprise Server 15 SP4
  - Subtle differences with Red Hat derivatives and Debian derivatives
- The compute nodes run Cray OS, a restricted version of SUSE with some daemons inactive or configured differently and Cray's way of accessing file systems.
  - Goal is to limit OS jitter for better scalability of large applications
  - On the GPU nodes there was still the need to reserve 1 core for OS and drivers
  - This also implies that some software may not be able to run on the compute nodes
    - E.g., no /run/user/\$UID
- Small system image, don't expect everything you find on a workstation
  - Smaller than most tier-2 systems

# Low-noise mode

- Can mean different things
- Cray OS already reduces noise by disabling some daemons on the compute nodes
  - Reduces compatibility with regular applications
  - So some Cray systems had 2 modes
    - “Emulation mode”, “Cluster Compatibility Mode” where those daemons were enabled
    - “Scalability mode” also often called “low-noise” mode with the regular Cray OS
- Disabling some daemons is not always enough for extreme scalability
  - LUMI-GPUs have a more extreme form of “low-noise” mode: OS processes restricted to a reserved core that is not available for applications (core 0)
  - Assymetry in the node: 1 CCD with 7 available cores and 7 with 8 available cores
  - Additional headache for proper setup of efficient GPU applications
    - So LUMI now actually reserves 1 core per CCD

# Programming models

- C/C++ and Fortran provided by several compilers in the PE
- MPI and OpenSHMEM for distributed memory, RCCL
- OpenMP, also for GPU programming
- OpenACC only in Cray Fortran
- HIP, AMD alternative for CUDA
- Commitment to OpenCL unclear
- Not part of the regular PE, but we try to provide SYCL also
- Users reported success running Julia
- **NO CUDA!!!!**
  - And there will never be as this is NVIDIA proprietary technology

# Development environment on LUMI

- Compilers: Cray Compiling Environment (CCE), GNU compiler collection (AMD GPU support not enabled), AMD AOCC and ROCm compilers
- Cray Scientific and Math Libraries: FFTW, BLAS+Lapack, ...
- Cray Message Passing Toolkit
- Additional tools to integrate everything and offer hugepages support
- Cray Performance Measurement and Analysis Tools
- Cray Debugging Support Tools
- Python and R
- A number of AMD tools (not always pre-installed)
- 3rd party: Linaro (ARM) Forge, Vampir, ...
- But no Intel oneAPI HPC Toolkit...

# Cray Compiling Environment

- Default compiler on most Cray systems
  - Designed for scientific software in an HPC environment
  - LLVM-based with extensions by HPE Cray for vectorization and shared memory parallelization
- Standards support:
  - C/C++ compiler essentially Clang/LLVM with Cray extensions for optimization
  - Fortran is HPE Cray's own frontend and optimizer, supporting most of Fortran 2018 (and strict about it)
  - OpenMP support including offload: Full 5.0, partial 5.1/5.2 and working on more, see `man intro_openmp`
  - OpenACC support only in Fortran: 2.0, partial 2.x/3.x, see `man intro_openacc`
  - PGAS: UPC 1.2 and Fortran 2008 coarray support
  - MPI bindings

# Scientific and math libraries

- LibSci
  - BLAS (Basic Linear Algebra Subroutines) and CBLAS (C interface wrappers)
  - LAPACK and LAPACKE (C interface to LAPACK)
  - IRT (Iterative Refinement Toolkit)
  - BLACS (Basic Linear Algebra Communication Subprograms) and ScaLAPACK
- LibSci\_ACC: A subset of GPU-optimized routines from LibSci
- FFTW<sub>3</sub>: Fastest Fourier Transforms in the West
- Data libraries: netCDF and HDF<sub>5</sub>
- Cray TPSL does no longer exist as a product



# Cray MPI

- Derived from ANL MPICH 3.4
- With tweaks for Cray
  - Improved algorithms for many collectives
  - Asynchronous progress engine for overlap of computation and communications
  - Customizable collective buffering when using MPI-IO
  - Optimized Remote Memory Access (one-sided) fully supported including passive RMA
- GPU-aware communications
- Support for Fortran 2008 bindings
- Full MPI 3.1 support except for dynamic process management and `MPI_LONG_DOUBLE/MPI_C_LONG_DOUBLE_COMPLEX` for CCE
- No mpirun/mpiexec, but Slurm `srun` as the process starter
- Layered on libfabric with the Cassini provider, and a GPU Transfer Library

# GPU-aware MPI

- Cray MPICH supports
  - GPU-attached communication buffers, can use device pointers
  - GPU-NIC RDMA for inter-node MPI transfers
  - GPU Peer2Peer IPC for intra-node transfers (but with restrictions, see later)
- Enable: `export MPICH_GPU_SUPPORT_ENABLED=1`
- If the GPU code uses MPI operations that access GPU-attached memory regions:  
`export MPICH_OFI_NIC_POLICY=GPU`  
If only CPU buffers are used, is better `export MPICH_OFI_NIC_POLICY=NUMA`.
- See also later: Depending on how Slurm is used, Peer2Peer IPC might not work.  
Turn off: `export MPICH_GPU_IPC_ENABLED=0`.
  - Or alternatively: `export MPICH_SMP_SINGLE_COPY_MODE=NONE`
  - Both have severe consequences for performance

# Lmod

- The HPE Cray PE is configured through modules
  - On LUMI we use Lmod
- Basic module commands are similar in all 3 implementations of modules:
  - `module avail` : List available modules
  - `module list` : Show loaded modules
  - `module load` : To load a module
- Lmod supports a hierarchical module system: Distinguishes between available modules and installed modules
  - Some modules only become available after loading another module
  - Can be used to support multiple configurations with a single module name and version
  - Used extensively in the programming environment

# Compiler wrappers

- The HPE Cray PE compilers are usually used through compiler wrappers:
  - `cc` for C
  - `CC` for C++
  - `ftn` for Fortran
- Compiler selected based on the modules loaded
- Wrappers select the target CPU and GPU architectures based on target modules
- Some libraries are linked in automatically when the corresponding module is loaded
  - MPI: There is no `mpicc`, `mpiCC`, `mpif90`, etc.
  - LibSci and FFTW
  - netCDF and HDF5
- You can see what the wrapper does by adding `-craype-verbose`
- Wrappers are provided by the `craype` module

# Selecting the version of the CPE

- Release numbers are of the type yy.dd, e.g., 23.09 for the release made in September 2023.
- There is always a system default version assigned by the sysadmins
- The cpe module allows to change the default version
  - `module load cpe/23.09`
    - This module will try to switch loaded PE modules to the version corresponding to that PE version, but it sometimes fails due to bugs in that module. Loading it twice in separate `module load` commands fixes the issue.
    - Will produce a warning when unloading, but this is only a warning.
- Not needed when using the LUMI stacks, see later.

# The target modules

- CPU:
  - `craype-x86-rome`: Works everywhere, CPU in the login nodes and data and visualisation partition
  - `craype-x86-milan`: LUMI-C compute nodes
  - `craype-x86-trento`: LUMI-G CPU
- GPU:
  - `craype-accel-host`: Will tell some compilers to compile for the host instead
  - `craype-accel-amd-gfx90a`: The MI200 series used in LUMI-G
- Network:
  - `craype-network-ofi`: Needed for the Slingshot 11 interconnect
  - `craype-network-none`: Omits network-specific libraries
- Compiler wrappers have corresponding options to overwrite these settings

# PrgEnv and compiler modules

- The PrgEnv-\* modules load compiler, MPI and LibSci (and some other stuff)

PrgEnv	Description	Comp. mod.	Compilers
PrgEnv-cray	Cray Compiling Environment	cce	craycc, crayCC, crayftn
PrgEnv-gnu	GNU Compiler Collection	gcc gcc-native	gcc, g++, gfortran gcc-12, g++-12, gfortran-12
PrgEnv-aocc	AMD Optimizing Compilers (CPU only)	aocc	clang, clang++, flang
PrgEnv-amd	AMD ROCm LLVM compilers (GPU support)	amd	amdclang, amdclang++, amdflang

- rocm module needed when using PrgEnv-cray or PrgEnv-gnu on the GPUs

# Getting help

PrgEnv	C	C++	Fortran
PrgEnv-cray	man craycc	man crayCC	man crayftn
PrgEnv-gnu	man gcc	man g++	man gfortran
PrgEnv-aocc/PrgEnv-amd	-	-	-

- [Web-based documentation from HPE Cray: cpe.ext.hpe.com/docs](http://cpe.ext.hpe.com/docs)
- `--craype-help` for the compiler wrapper-specific help
- `--help` flag, e.g., for compilers
- `-dumpversion` (wrappers), `--version` (many compiler commands) for version information
- The `explain` command for Cray Fortran compiler error messages
- [LUMI documentation for developers: docs.lumi-supercomputer.eu/development](http://docs.lumi-supercomputer.eu/development)



# Google, ChatGPT and LUMI

- Google may not be your best friend to find information about the HPE Cray Programming Environment or error messages on LUMI
  - As it is currently mostly used on a few rather large systems
  - And as even HPE had little information available until May 2023
- ChatGPT won't do much better
  - Little data on the internet
  - And currently trained with data from 2 or 3 years ago
- HPE Cray has a command line alternative to Google: `man -K`
  - Example: Try  
`man -K FI_CXI_RX_MATCH_MODE`
- Or try the search box on [cpe.ext.hpe.com/docs](https://cpe.ext.hpe.com/docs)

# Other modules

- `cray-mpich` for MPI
- `cray-libsci` for LibSci
- `cray-fftw` for the Cray FFTW library
- `cray-netcdf`, `cray-netcdf-hdf5parallel`, `cray-parallel-netcdf`, `cray-hdf5`, `cray-hdf5-parallel`
- `cray-python` with a selection of packages including `mpi4py`, `NumPy`, `SciPy` and `pandas`
- `cray-R`

# Warning 1: You do not always get what you expect...

- The default behaviour of the Cray PE is to use system default versions of libraries at runtime
  - The versions of these libraries do not correspond to the modules loaded
  - In fact, many applications will run without reconstructing the compile environment
  - BUT: If the default version on the system changes, the behaviour of your application might change...
- Solution: Prepend `LD_LIBRARY_PATH` with `CRAY_LD_LIBRARY_PATH`:  
`export LD_LIBRARY_PATH=${CRAY_LD_LIBRARY_PATH}:$LD_LIBRARY_PATH`
  - Automated via module `lumi-CrayPath`
- Or use rpath linking of the CPE components when building:  
`export CRAY_ADD_RPATH=yes`

# Warning 2: Order matters

- Some modules are only available when others are loaded first
- Some examples
  - `cray-fftw` only available when a processor target module is loaded
  - `cray-mpich` requires both `craype-network-ofi` and a compiler to be loaded
  - `cray-hdf5` requires a compiler module to be loaded and `cray-netcdf` in turn requires `cray-hdf5`
  - And there are several other examples
- See next presentation to learn how to find modules (though it doesn't always work well for the PE modules)

# Note: Working without wrappers

- It is now possible to work without the HPE Cray PE compiler wrappers
  - Use the compilers from the “PrgEnv and compilers” slide
  - With `cray-mpich` loaded you can then use the traditional MPI compiler wrappers `mpicc`, `mpiCC`, `mpif90`, etc.
  - You’ll have to manually link all other libraries (BLAS, FFTW, netCDF, ...) even if you use those provided in the HPE Cray PE environment
- Tip: Most modules define environment variables that point to the bin and lib subdirectories
  - `CRAY_MPICH`
  - `CRAY_LIBSCI_PREFIX_DIR` / `CRAY_PE_LIBSCI_PREFIX_DIR`
  - `FFTW_ROOT`, `FFTW_INC` and `FFTW_DIR`

A wide-angle photograph of a snowy mountain range under a cloudy sky. The mountains are covered in snow, with some rocky outcrops visible. The sky is filled with soft, grey clouds. The word "Questions?" is written in a bold, black, sans-serif font in the center of the image.

**Questions?**