Comprehensive General LUMI Course (February 14-17, 2023)

Location: Virtual

This four-day online course serves as a general comprehensive introduction to the LUMI architecture and programming environment. It will include lessons about compiling and using software, programming models (HIP and OpenMP offload), porting, executing jobs, and optimizing applications to run on AMD MI250X. After the course you will be able to work efficiently on both the CPU (LUMI-C) as well as GPU partitions (LUMI-G).

The course will be jointly conducted by the LUMI HPE Centre of Excellence (HPE CoE), AMD and the LUMI User Support Team (LUST).

The course is intended to users with ongoing projects on LUMI, users with project proposals in one of the national or EuroHPC channels, and support staff of local organisations of the LUMI consortium members.

Below is a tentative schedule of the course.

These are the main topics day by day:

- Day 1. Connecting to the system, building and executing applications and simple use of GPUs via libraries.
- Day 2. Programming GPUs via OpenACC and OpenMP, Optimizations techniques, Additional software on LUMI, LUMI support.
- Day 3. Debugging, I/O, HIP programming, ROCm tools.
- Day 4. Profiling, Advanced ROCm tools.

February 14 (all times CEST) – Day 1

- 09:00 Welcome, introduction to the course (Emmanuel/Jørn/Harvey) Course organisation. Demonstration on how to use HedgeDoc.
- 09:15 Introduction to the HPE Cray Hardware and Programming Environment (Harvey) Focus on the HPE Cray EX hardware architecture and software stack. Tutorial on the Cray module environment and compiler wrapper scripts.
- 10:30 break (20 minutes)
- 10:50 First steps for running on Cray EX Hardware (Harvey) Examples of using the Slurm Batch system, launching jobs on the front end and basic controls for job placement.

11:20 Exercises: about 40 minutes

- 12:00 lunch break (90 minutes)
- 13:30 Overview of compilers and Parallel Programming Models (Alfio) An introduction to the compiler suites available, including examples of how to get additional information about the compilation process. Special attention is given the Cray Compilation Environment (CCE) noting options relevant to porting and performance. CCE classic to Clang transition. Description of the Parallel Programming models.
- 14:30 Exercises: about 30 minutes
- 15:00 *break (30 minutes)*
- 16:00 Scientific Libraries (Alfio) Presentation of the Cray Scientific Libraries for CPU and GPU execution.
- 16:30 Exercises: about 30 minutes
- 17:00 Open Questions & Answers (participants are encouraged to continue with exercises in case there should be no questions)
- 17:30 End of the course day

February 15 (all times CEST) – Day 2

09:00 OpenACC and OpenMP offload with Cray Compilation Environment (Alfio) Directive-based approach for GPU offloading execution with the Cray Compilation Environment.

09:45 Exercises: about 30 minutes

- 10:15 break (30 minutes)
- 10:45 Advanced Application Placement (Jean) More detailed treatment of Slurm binding technology and OpenMP controls.
- 11:30 Exercises: about 30 minutes
- 12:00 lunch break (90 minutes)
- 13:15 Understanding Cray MPI on Slingshot, rank reordering and MPMD launch (Harvey) High level overview of Cray MPI on Slingshot, useful environment variable controls. Rank reordering and MPMD application launch.

14.10 Exercises: about 30 minutes

- 14:40 break (20 minutes)
- 15:00 Additional software on LUMI Software policy. Software environment on LUMI. Installing software with EasyBuild (concepts, contributed recipes). Containers for Python, R, VNC (container wrappers).
- 16:00 LUMI support *LUMI documentation. What can we help you with and what not? How to get help, how to write good support requests.* Some twice//frequent support questions of users on LUMI?

Some typical/frequent support questions of users on LUMI?

- 17:00 Open Questions & Answers (participants are encouraged to continue with exercises in case there should be no questions)
- 17:30 End of the course day

February 16 (all times CEST) – Day 3

- 09:00 Performance Optimization: Improving single-core efficiency (Jean)
- 09:30 Debugging at Scale gdb4hpc, valgrind4hpc, ATP, stat (Thierry)
- 09:50 Exercises: about 20 minutes
- 10:10 break (20 minutes)
- 10:30 I/O Optimisation Parallel I/O (Harvey) Introduction into the structure of the Lustre Parallel file system. Tips for optimising parallel bandwidth for a variety of parallel I/O schemes. Examples of using MPI-IO to improve overall application performance. Advanced Parallel I/O considerations Further considerations of parallel I/O and other APIs. Being nice to Lustre Consideration of how to avoid certain situations in I/O usage that don't specifically relate to data movement.
- 11:40 Exercises: about 20 minutes
- 12:00 *lunch break (90 minutes)*
- 13:30 Introduction to AMD ROCm ecosystem and HIP (George)
- 14:30 Exercises: about 30 minutes
- 15:00 break (30 minutes)
- 15:30 Debugging (George)
- 15:55 Exercises: about 20 minutes
- 16:15 Introduction to AMD Rocprof (George)
- 16:35 Exercises: about 25 minutes
- 17:00 Open Questions & Answers (participants are encouraged to continue with exercises in case there should be no questions)
- 17:30 End of the course day

February 17 (all times CEST) – Day 4

09:00 Introduction to Perftools - Perftools-lite modules (Alfio) Overview of the Cray Performance and Analysis toolkit for profiling applications. Demo: Visualization of performance data with Apprentice2.

09:40 Exercises: about 30 minutes

- 10:10 *break (20 minutes)*
- 10:30 Advanced performance analysis (Thierry) Automatic performance analysis and loop work estimated with perftools. Communication Imbalance, Hardware Counters, Perftools API, OpenMP. Compiler feedback and variable scoping with Reveal.
- 11:30 Exercises: about 30 minutes
- 12:00 lunch break (90 minutes)
- 13:30 Introduction to AMD Omnitrace (George)
- 13:55 Exercises: about 20 minutes
- 14:15 Introduction do AMD Omniperf (George)
- 14:40 Exercises: about 20 minutes
- 15:00 break (30 minutes)
- 15:30 Best practices: GPU Optimization, tips & tricks / demo
- 16:30 Exercises: about 30 minutes
- 17:00 Open Questions & Answers (participants are encouraged to continue with exercises in case there should be no questions)
- 17:30 End of the course day