The European flagship supercomputer of the North – a status update

Dr. Pekka Manninen

Director, LUMI Leadership Computing Facility CSC – IT Center for Science, Finland

Adjunct Professor, University of Helsinki

LUMI Consortium

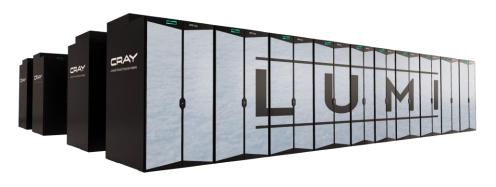
• Unique consortium of 10 countries with strong national HPC centers

Countries which have signed the EuroHPC Declaration LUMI Consortium countries

CSC Datacenter in Kajaan

- The resources of LUMI will be allocated per the investments
- The share of the EuroHPC JU (50%) will be allocated by a peer-review process (cf. PRACE Tier-o access) and available for all European researchers
- The shares of the LUMI partner countries will be allocated by local considerations and policies – seen and handled as extensions to national resources

LUMI: one of the fastest supercomputers in the world



- LUMI will be an HPE Cray EX supercomputer manufactured by Hewlett Packard Enterprise
- Peak performance over **550 petaflop/s** makes the system one of the world's fastest
 - Fastest today is Fugaku supercomputer in Japan with 513 petaflop/s, second fastest Summit in USA with 200 petaflop/s)

1 system550550Pflop/sPeak PerformanceModern laptop computers



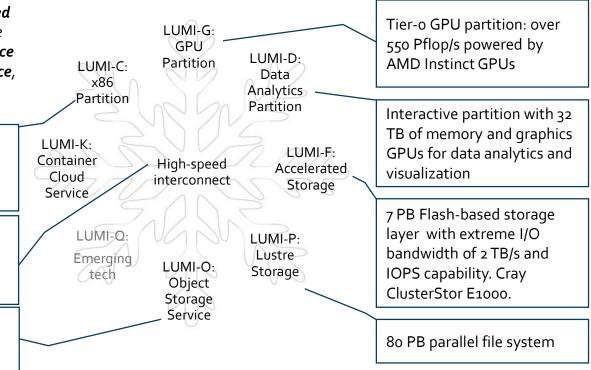
LUMI, the Queen of the North

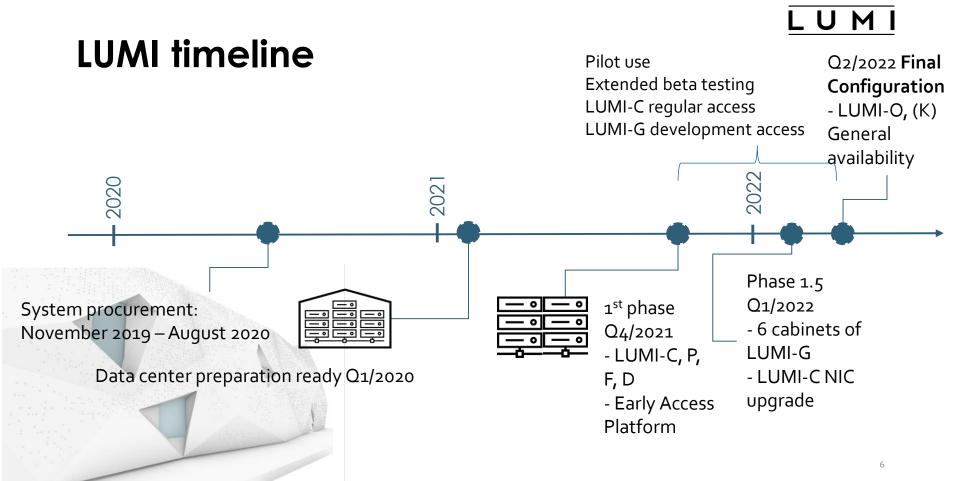
LUMI is a Tier-o GPU-accelerated supercomputer that enables the convergence of high-performance computing, artificial intelligence, and high-performance data analytics.

- Supplementary CPU
 partition
- ~200,000 AMD EPYC CPU cores

Possibility for combining different resources within a single run. HPE Slingshot technology.

30 PB encrypted object storage (Ceph) for storing, sharing and staging data





Enhanced user experience

- In addition to traditional CLI, we wish to support high-level interfaces on LUMI, i.e. seamlessly integrate Jupyter Notebooks, Rstudio and such to back-end to LUMI
 - Open OnDemand piloted, deployment on Lumi Q2/22
- Large software budget will enable a rich stack of pre-installed software
 - ISV applications is being procured and software being installed at the moment
- Datasets as a Service: curated large reference datasets available and maintained
- Support for handling sensitive (GDPR subjected, IP-closed, etc) data
 - Progressing in collaboration with the Elixir community

LUMI

LUMI user support

- LUMI user support and a centralized helpdesk by the distributed LUMI User Support Team
 - The model is based on a network of **dedicated LUMI experts**: each partner will provide one full-time person for the task
 - User Support Team will also provide end-user training, maintain the software portfolio and user documentation of the system
- Helpdesk open, see https://www.lumi-supercomputer.eu/user-support/
- "Level 3" support (e.g. application enabling, methodology support) via local centers as well as the EuroHPC Competence Centers

LUMI

LUMI Phase 1 pilot projects

https://www.lumi-supercomputer.eu/lumi-pilot-projects-selected/

- Belgium: **M. Rasquin, T. Toulorge** and **K. Hillewaert**, Direct Numerical Simulations of a Smoothed Backward Facing Step Featuring Incipient Separation
- Belgium: **G. Lapenta**, LIFTHRASIR: LumI First Tests of the HaRdware Architecture by Simulations of Interplanetary Regions
- Czech Republic: **D. Legut**, Understanding the Physics of Phonons utilizing electronic structure and atomistic calculations employing state-of-the-art methods
- Czech Republic: **D. Biriukov**, Interaction network in extracellular space: an all-atom simulation model of the glycocalyx and cell membrane
- Denmark: **O. Christiansen** and **J. Elm:** High Performance Computing Quantum Chemistry on LUMI
- Denmark: **G. Frølund Pedersen** and **O. Franek** : Perfect Antennas for Reconfigurable Intelligent Surfaces
- Estonia: **T. Laisk** and **R. Mägi:** Genetic Susceptibility Factors of Different Traits

- Estonia: G. Väli, High-Resolution Ocean Model for Main Basins of The Baltic Sea
- Finland: M. Palmroth, LUmi Carrington Kinetic simulations
- Finland: S. Kaptan, Molecular Basis of Intelligence
- Iceland: H. Jónsson, Computational Chemistry
- Iceland: H. Úlfarsson, Algorithmic Mathematics
- Norway: M. Carlsson, Solar Atmospheric Modelling
- Norway: **M. Bentsen**, Computing for nationally coordinated NorESM experiments
- Poland: G. Wlazłowski, Supersolidity in ultracold Fermi gas
- Poland: J. M. Bujnicki, Drugging the genomic RNA of SARS-CoV-2 with small molecules
- Sweden: **O. Agertz** and **F. Renaud**, The baryon cycle in colliding galaxies
- Sweden: **P. Schlatter** and **J. Vincent** and **J. Gong**, Turbulence data generation on Boeing hump
- Switzerland: N. Marzari, High-throughput computing

Getting LUMI resources

- LUMI resources are allocated in terms of GPU-hours, CPU-core-hours, and storage hours
 - Each project applies and gets a combination of this
 - No dedicated hardware all users can access the whole system within the batch job policies
 - All countries receive shares of these pools per their share of the TCO
- Resources brokered in terms of
 - Preparatory access projects (XS) single-PI
 - Development access projects (S) single-PI
 - General access (Tier-1) projects (M) single-PI
 - Extreme scale (Tier-o) projects (L) single-PI, should be mostly GPU hours
- Researchers affiliated to Danish institutions can apply from the EuroHPC allocation or from Denmark's own allocation

LUMI programming environment

- ROCm (Radeon Open Compute)
 - Usual set of accelerated scientific libraries (BLAS, FFT etc)
 - Usual machine learning frameworks and libraries (Tensorflow, PyTorch etc)
 - Compilers for the GPUs
- Cray Programming Environment (CPE) stack
 - Cray Compiling Environment, LibSci libraries, CrayPAT, Reveal, debuggers,...
 - CPE Deep Learning Plugin
- More information:

https://www.lumi-supercomputer.eu/may-we-introduce-lumi/

Preparing applications and workflows LUM for LUMI

- Remember the possibility of combining CPU and GPU nodes within one job perhaps only part of the application needs to be GPU-enabled
- Consider writing your application on top of modern frameworks and libraries
 - Kokkos, Alpaka etc, or domain-specific frameworks
- Convert CUDA codes to HIP, OpenACC codes to OpenMP5
 - HIPify tools can automatize the effort
 - We have observed this to be very straightforward, more so than we expected
- LUMI 1st phase features a code porting platform (MI100 GPUs)

Concluding remarks

- EuroHPC era: Unprecendent amount of computational resources and capabilities available for European research & innovation
 - Complemented by competence building and user support activities
- LUMI, the Queen of the North: leadership-class resource designed for a broad range of user communities and workloads, with an enhanced user experience
 - LUMI will be a GPU system, which needs some preparatory work but it will be a robust production system, and not experimental or esoteric in any manner
 - Modernizing HPC applications for harnessing the largest systems is not trivial, and needs a lot of focused effort but it will pay off
 - We are getting there! LUMI-C in production soon, LUMI-G in Q2/22