Introduction to HPC2N, Kebnekaise and HPC

Birgitte Brydsö, Pedro Ojeda May, and others at HPC2N

> HPC2N Umeå University

21. September 2023







 High Performance Computing Center North (HPC2N) is a competence center for Scientific and Parallel Computing







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 A part of National Academic Infrastructure for Supercomputing in Sweden (NAISS)









Provides state-of-the-art resources and expertise:

Scalable and parallel HPC







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- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)





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- Software for e-Science applications
- All levels of user support
 - Primary, advanced, dedicated
 - Application Experts (AEs)







HPC2N

Primary objective: to raise the national and local level of HPC competence and transfer HPC knowledge and technology to new users in academia and industry.







HPC2N (partners)

HPC2N is hosted by



UMEÅ UNIVERSITY

Partners:















HPC2N (funding and collaborations)

 Funded mainly by Umeå University, with contributions from the other HPC2N partners





HPC2N (funding and collaborations)

- Funded mainly by Umeå University, with contributions from the other HPC2N partners
- Involved in several projects and collaborations























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 - Research group meetings @ UmU
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- User training and education program
 - 0.5 3 days; ready-to-run exercises
 - Introduction to HPC2N and Kebnekaise
 - Parallel programming and tools (OpenMP, MPI, debugging, perf. analyzers, Matlab, R, MD simulation, ML, GPU, ...)
 - Using Python in an HPC environment, 1 December 2023
 - Introduction to Git, 13-17 November 2023
 - Introduction to running R, Python, and Julia in HPC, 17-19 October 2023
 - Workshop: Matlab in HPC, 11, 18, 25/26 September 2023
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- NGSSC / SeSE & university courses







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- Björn Torkelsson, deputy director
- Lena Hellman, administrator





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- Research Engineers under DDLS, HPC2N/SciLifeLab
 - System Developer, IT
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 - Data Steward







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System and support

- Erik Andersson
- Birgitte Brydsö
- Niklas Edmundsson (Tape coord)
- Ingemar Fällman
- Magnus Jonsson
- Roger Oscarsson
- Åke Sandgren
- Mattias Wadenstein (NeIC, Tier1)
- Lars Viklund







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- Contact through regular support
 - If you have a specific problem/question and/or need consultation







HPC2N (users by discipline)

- Users from several scientific disciplines:
 - Biosciences and medicine
 - Chemistry
 - Computing science
 - Engineering
 - Materials science
 - Mathematics and statistics
 - Physics including space physics
 - ML, DL, and other AI







HPC2N (users by discipline, largest users)

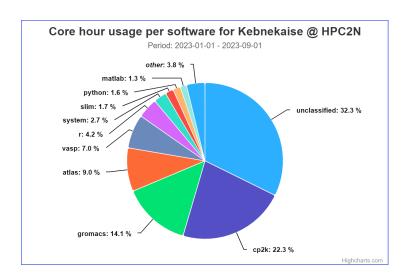
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 - Physics including space physics
 - Machine learning and artificial intelligence (several new projects)







HPC2N (users by software)









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- In 2023, Kebnekaise was extended with
 - 2 dual NVIDIA A100 GPU nodes
 - one many-core AMD Zen3 CPU node







Kebnekaise (compute nodes)

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Large Memory	20	Intel Xeon E7-8860v4, 4 x 18 cores, 3072 GB, EDR Infiniband







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		AMD Zen3 (AMD EPYC 7413), 2 x 24 cores,
		512 GB, EDR Infiniband,
2 × A100	2	2 x NVidia A100,
		2 x 6912 CUDA cores,
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GPU-volta	10	2 x NVidia V100,
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2xGPU !!! Being phased out !!!	32	Intel Xeon E5-2690v4, 2 x 14 cores,
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- Also SweStore disk based (dCache)
 - Research Data Storage Infrastructure, for active research data and operated by NAISS, WLCG







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- I will cover more details in the next section, where we go more into detail about HPC2N and Kebnekaise.







HPC

What is HPC?







High Performance Computing (definition)

"High Performance Computing most generally refers to the practice of **aggregating computing power** in a way that delivers much **higher performance** than one could get out of a typical desktop computer or workstation in order to **solve large problems** in science, engineering, or business." ¹

¹https://insidehpc.com/hpc-basic-training/what-is-hpc/







High Performance Computing (opening the definition)

- Aggregating computing power
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 - Compared to 4 cores in a modern laptop

³200 billion (milliard)







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Solve large problems

- When does a problem become large enough for HPC?
- Are there other reasons for using HPC resources? (Memory, software, support, etc.)

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High Performance Computing (large problems)

- A problem can be large for two main reasons:
 - Execution time: The time required to form a solution to the problem is very long
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 - More cores, more nodes, GPUs, . . .





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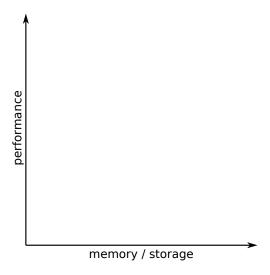
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- The latter by adding more memory / storage
 - More memory per node (including large memory nodes), more nodes, . . .
 - Kebnekaise: 128GB 192GB, 512GB, 3TB
 - Large storage solutions, . . .







High Performance Computing (what counts as HPC)

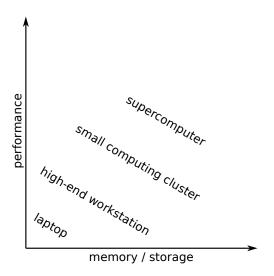








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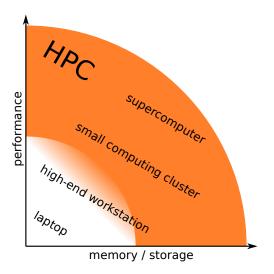








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- Support and documentation





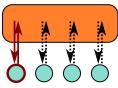


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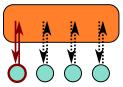


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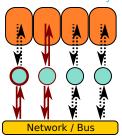




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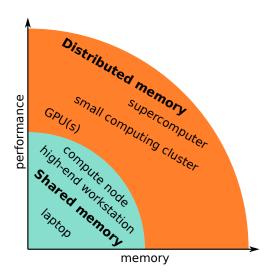
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- Distributed memory: Multiple distinct memory spaces.



- Everyone has direct access only to the local data
- Requires communication













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- GPUs: CUDA, OpenCL, OpenACC, OpenMP, ...







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 - Many lightweight streams of operations





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 - Single stream of operations
 - Multi-core: Vectorized Matlab, pthreads, OpenMP
 - Multiple streams of operations
 - Work distribution, coordination (synchronization, etc), . . .
 - 3 Distributed memory: MPI, ...
 - Multiple streams of operations
 - Work distribution, coordination (synchronization, etc), ...
 - Data distribution and communication
- GPUs: CUDA, OpenCL, OpenACC, OpenMP, . . .
 - Many lightweight streams of operations
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- GPUs: CUDA, OpenCL, OpenACC, OpenMP, . . .
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 - Data distribution across memory spaces and movement







 Complexity grows when we aim for extra performance and/or memory/storage:





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 - Single-core: LAPACK, ...
 - Load correct toolchain etc





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 - 2 Multi-core: LAPACK + parallel BLAS, ...
 - Load correct toolchain etc
 - Allocate correct number of cores, configure software to use correct number of cores, . . .
 - Oistributed memory: ScaLAPACK, ...
 - Load correct toolchain etc
 - Allocate correct number of nodes and cores, configure software to use correct number of nodes and cores, . . .







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 - Allocate correct number of nodes and cores, configure software to use correct number of nodes and cores, . . .
 - Data distribution, storage, ...
- GPUs: MAGMA, TensorFlow, . . .
 - Load correct toolchain etc
 - Allocate correct number of cores and GPUs, configure software to use correct number of cores and GPUs, . . .







End (questions?)

Questions?





