Introduction to HPC2N, Kebnekaise and HPC

Birgitte Brydsö, Pedro Ojeda May, and others at HPC2N

> HPC2N Umeå University

8. September 2021







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





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A part of Swedish National Infrastructure for Computing (SNIC)





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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- Support
 - Primary, advanced, dedicated
 - Application Experts (AEs)



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 - Application Experts (AEs)
- International network for research and development

HPC2N (partners)

HPC2N has five partners:

- ► Luleå University of Technology
- ► Mid Sweden University
- Swedish Institute of Space Physics
- Swedish University of Agricultural Sciences (SLU)
- Umeå University



HPC2N (funding)

Funded by Swedish Research Council (VR), SNIC and various partners









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- Involved in several projects and collaborations
 - EGI, PRACE, EISCAT, eSSENCE, NOSEG, SNIC Science Cloud, ...



- User support (primary, advanced, dedicated)
 - Research group meetings @ UmU
 - Also at the partner sites



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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 (e.g., OpenMP, MPI, debugging, performance analyzers, Matlab, R, MD simulation, Deep Learning, GPU, ...)



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- Workshops and seminars



Management

- Paolo Bientinesi, new director
- ► Björn Torkelsson, deputy director
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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



► HPC2N provides advanced and dedicated support in the form of **Application Experts (AEs)**:

¹https://www.snic.se/support/dedicated-user-support/



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- Contact through regular support or dedicated support form¹
 - ► If you have a specific problem/question and/or need consultation (up to 100 h)

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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
 - Deep learning and artificial intelligence





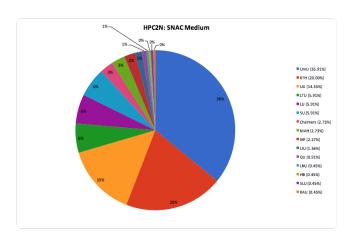
HPC2N (users by discipline, largest users)

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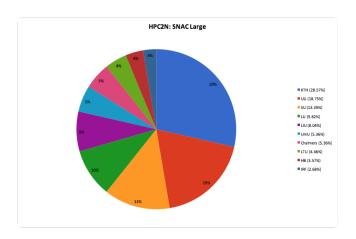
HPC2N (medium users by university)



Projects with allocations at HPC2N: 2014-01-01 to 2016-05-30



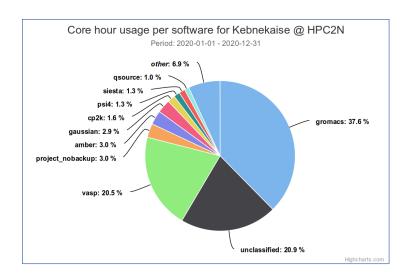
HPC2N (large users by university)



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HPC2N (users by software)







Kebnekaise

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- Opened up for general availability on November 7, 2016
- ▶ In 2018, Kebnekaise was **extended** with
 - 52 Intel Xeon Gold 6132 (Skylake) nodes, as well as
 - 10 NVidian V100 (Volta) GPU nodes



Kebnekaise (compute nodes)

Name	#	Description
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Large Memory	20	Intel Xeon E7-8860v4, 4 x 18 cores ,
		3072 GB, EDR Infiniband
KNL		Intel Xeon Phi 7250 (Knight's Landing),
	36	68 cores, 192 GB, 16 GB MCDRAM,
		FDR Infiniband



Kebnekaise (GPU nodes)

Name	#	Description
2×GPU	32	Intel Xeon E5-2690v4, 2 x 14 cores, 128 GB, FDR Infiniband, 2 x NVidia K80 4 x 2496 CUDA cores, 4 x 12 GB VRAM





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GPU-volta		Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband,
	10	2 x NVidia V100,
		2 x 5120 CUDA cores, 2 x 16 GB VRAM,
		2 x 640 Tensor cores



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- 629 TFlops/s Linpack (all parts, except expansion)
 - 86% of Peak performance



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 - ► Tape Storage
 - Backup
 - Long term storage



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



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." 2

²https://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

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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:
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- The former can be remedied by increasing the performance
 - ► More cores, more nodes, GPUs, ...

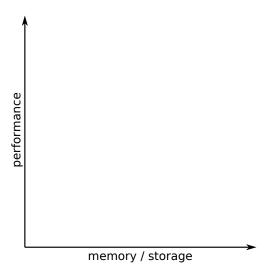


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- The latter by adding more memory / storage
 - More memory per node (including large memory nodes), more nodes, . . .
 - Large storage solutions, . . .

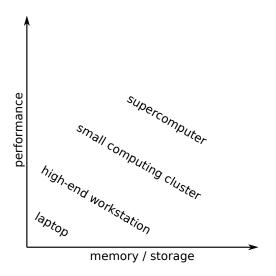


High Performance Computing (what counts as HPC)



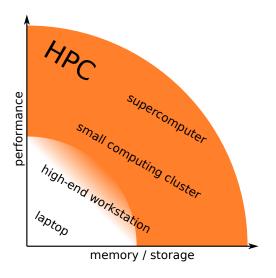


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High Performance Computing (other reasons)

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 - Software is pre-configured and ready-to-use



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- Support and documentation

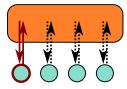


► Two memory models are relevant for HPC:





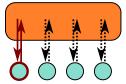
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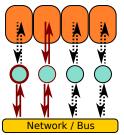
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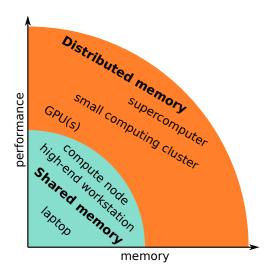
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- Distributed memory: Multiple distinct memory spaces.



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









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 - 3. Distributed memory: **MPI**, ...
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- ► GPUs: CUDA, OpenCL, OpenACC, OpenMP, . . .



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 - Multiple streams of operations
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 - Data distribution and communication
- GPUs: CUDA, OpenCL, OpenACC, OpenMP, . . .
 - ► Many lightweight streams of operations
 - Work distribution, coordination (synchronization, etc), . . .
 - Data distribution across memory spaces and movement



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





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 - 2. Multi-core: LAPACK + parallel BLAS, ...
 - Load correct toolchain etc



- Complexity grows when we aim for extra performance and/or memory/storage:
 - 1. Single-core: LAPACK, ...
 - Load correct toolchain etc.
 - 2. Multi-core: LAPACK + parallel BLAS, ...
 - Load correct toolchain etc
 - ▶ Allocate correct number of cores, configure software to use correct number of cores, ...



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 - 3. Distributed memory: ScaLAPACK, ...
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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, . . .
 - 3. Distributed 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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 - 1. Single-core: LAPACK, ...
 - Load correct toolchain etc
 - 2. Multi-core: LAPACK + parallel BLAS, ...
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 - ▶ Allocate correct number of cores, configure software to use correct number of cores, . . .
 - 3. Distributed memory: ScaLAPACK, ...
 - Load correct toolchain etc
 - Allocate correct number of nodes and cores, configure software to use correct number of nodes and cores, . . .
 - Data distribution, storage, . . .

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 - 1. Single-core: LAPACK, ...
 - Load correct toolchain etc
 - 2. Multi-core: LAPACK + parallel BLAS, ...
 - Load correct toolchain etc
 - ▶ Allocate correct number of cores, configure software to use correct number of cores, . . .
 - 3. Distributed memory: ScaLAPACK, ...
 - Load correct toolchain etc
 - 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?

