#### Introduction to HPC2N, Kebnekaise and HPC

Mirko Myllykoski, Birgitte Brydsö, Pedro Ojeda May, and others at HPC2N

Department of Computing Science and HPC2N Umeå University

21. January 2021







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





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



▶ 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** (PFS-Lustre, SweStore, Tape)



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  - 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, ...





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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



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Contact through regular support or dedicated support form<sup>1</sup>

► 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



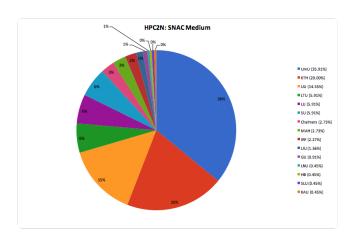


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  - Computing science
  - Engineering
  - Materials science
  - Mathematics and statistics
  - Physics including space physics
  - Deep learning and artificial intelligence (several new projects)



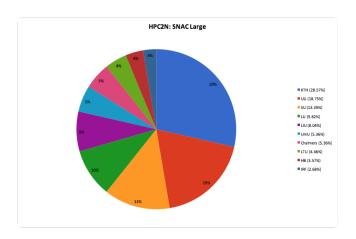
## HPC2N (medium users by university)



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



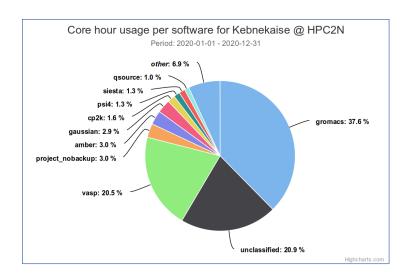
### HPC2N (large users by university)



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#### HPC2N (users by software)







#### Kebnekaise

► Latest supercomputer at HPC2N





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  - delivered by Lenovo and
  - installed during the summer 2016
- 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
Compute	432	Intel Xeon E5-2690v4, 2 x 14 cores,
		128 GB, FDR Infiniband



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52	Intel Xeon Gold 6132, 2 x 14 cores,
	192 GB, EDR Infiniband, AVX-512
20	Intel Xeon E7-8860v4, 4 x 18 cores,
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Large Memory	20	Intel Xeon E7-8860v4, <b>4 x 18 cores</b> ,
		3072 GB, EDR Infiniband
KNL	36	Intel Xeon Phi 7250 (Knight's Landing),
		68 cores, 192 GB, 16 GB MCDRAM,
		FDR Infiniband



## Kebnekaise (GPU nodes)

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





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2×GPU 32		Intel Xeon E5-2690v4, 2 x 14 cores,
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4×GPU 4		Intel Xeon E5-2690v4, 2 x 14 cores,
	4	128 GB, FDR Infiniband,
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GPU-volta 1		Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband,
	10	2 x NVidia V100,
		$2 \times 5120$ CUDA cores, $2 \times 16$ 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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- Birgitte will cover more details

## 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

<sup>&</sup>lt;sup>2</sup>https://insidehpc.com/hpc-basic-training/what-is-hpc/







### High Performance Computing (opening the definition)

- Aggregating computing power
  - ▶ 602 nodes in 15 racks totalling 19288 cores
  - ► Compared to 4 cores in a modern laptop

<sup>&</sup>lt;sup>4</sup>200 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?

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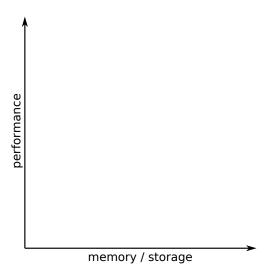


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- The latter by adding more memory / storage
  - More memory per node (including large memory nodes), more nodes, . . .
  - Large storage solutions, . . .



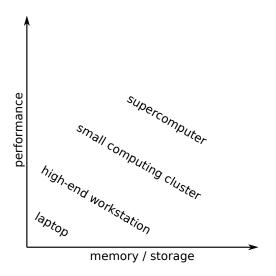
## High Performance Computing (what counts as HPC)







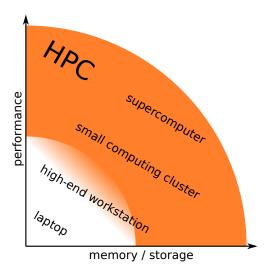
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# High Performance Computing (other reasons)

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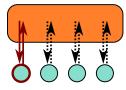


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- Support and documentation

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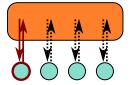
- Two memory models are relevant for HPC:
  - Shared memory: Single memory space for all data.



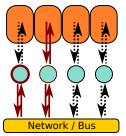
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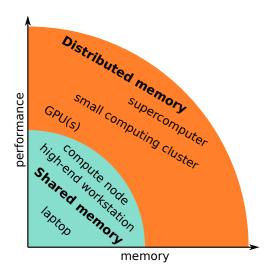
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- Straightforward to use
- Distributed memory: Multiple distinct memory spaces.



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





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  - 3. Distributed memory: **MPI**, ...
    - Multiple streams of operations
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- ► GPUs: CUDA, OpenCL, OpenACC, OpenMP, ...



- ► The programming model changes when we aim for extra performance and/or memory:
  - 1. Single-core: Matlab, Python, C, Fortran, ...
    - Single stream of operations
  - 2. Multi-core: Vectorized Matlab, pthreads, OpenMP
    - Multiple streams of operations
    - ► Work distribution, coordination (synchronization, etc), ...
  - 3. Distributed memory: MPI, ...
    - Multiple streams of operations
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  - 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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  - 1. Single-core: LAPACK, ...
    - Load correct toolchain etc.





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  - 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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    - 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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    - 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?

