### 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** 





- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)





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  - Application Experts (AEs)







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  - Primary, advanced, dedicated
  - 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 mainly by **Umeå University**, with contributions from the **other HPC2N partners** 









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- Involved in several projects and collaborations
  - DDLS, EGI, EISCAT, eSSENCE, NOSEG, Swedish Science Cloud, . . .







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







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- Workshops and seminars







#### Management

- Paolo Bientinesi, director
- Björn Torkelsson, deputy director
- Lena Hellman, administrator





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- Research Engineers under DDLS, HPC2N/SciLifeLab
  - System Developer, IT
  - Data Engineer
  - 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 (up to 100 h)







### 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)

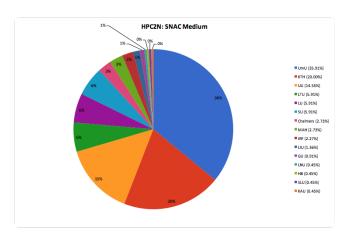
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## HPC2N (medium users by university)



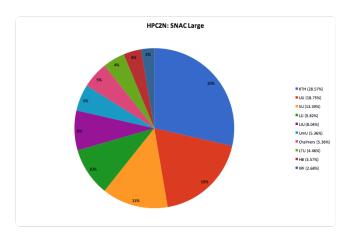
Projects with allocations at HPC2N: 2014-01-01 to 2016-05-30







## HPC2N (large users by university)



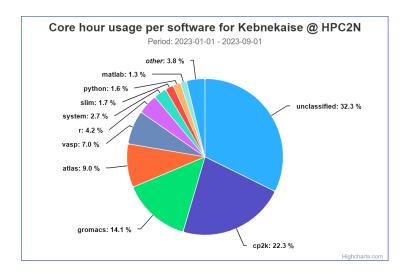
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### HPC2N (users by software)









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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)

	,,	Description
Compute	432	Intel Xeon E5-2690v4, 2 x 14 cores
!!! Will "soon" be retired !!!		128 GB, FDR Infiniband







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Compute-skylake	52	Intel Xeon Gold 6132, 2 x 14 cores, 192 GB, EDR Infiniband, AVX-512







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Compute-AMD Zen3		1 TB, EDR Infiniband







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	I ID, EDR Infinidand
20	Intel Xeon E7-8860v4, <b>4 x 18 cores</b> , <b>3072 GB</b> , EDR Infiniband
	<b>432 52</b> 1







Name	#	Description
2xGPU ! Will "soon" be retired!	32	Intel Xeon E5-2690v4, 2 x 14 cores, 128 GB, FDR Infiniband, 2 x NVidia K80
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2xGPU 20		Intel Xeon E5-2690v4, $2 \times 14$ cores,
	20	128 GB, FDR Infiniband,
! Will "soon" be retired !	32	2 x NVidia K80
	$4 \times 2496$ CUDA cores, $4 \times 12$ GB VRAM	
4xGPU 4		Intel Xeon E5-2690v4, 2 x 14 cores,
	4	128 GB, FDR Infiniband,
	4	4 x NVidia K80
		8 x 2496 CUDA cores, 8 x 12 GB VRAM





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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 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." <sup>1</sup>

<sup>&</sup>lt;sup>1</sup>https://insidehpc.com/hpc-basic-training/what-is-hpc/







### High Performance Computing (opening the definition)

- Aggregating computing power
  - ▶ 533 nodes in 15 racks totalling 16504 cores
  - Compared to 4 cores in a modern laptop

<sup>&</sup>lt;sup>3</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? (Memory, software, support, etc.)

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  - ► More cores, more nodes, GPUs, ...





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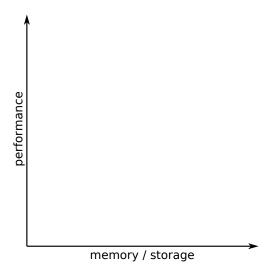
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- The latter by adding more memory / storage
  - More memory per node (including large memory nodes), more nodes, . . .
  - Kebnekaise: 128GB 192GB, 512GB, 3TB
  - Large storage solutions, . . .







# High Performance Computing (what counts as HPC)

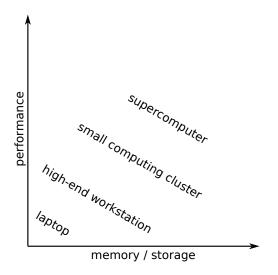








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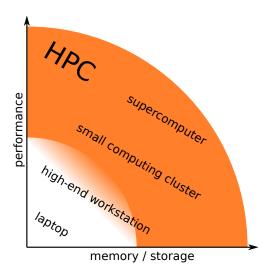








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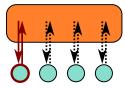
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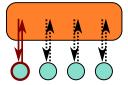


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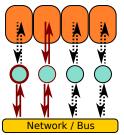




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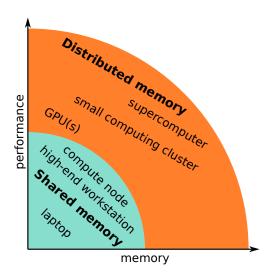
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- Distributed memory: Multiple distinct memory spaces.



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













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







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    - Multiple streams of operations
    - ▶ Work distribution, coordination (synchronization, etc), ...
    - Data distribution and communication
- GPUs: CUDA, OpenCL, OpenACC, OpenMP, . . .
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  - 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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    - Load correct toolchain etc







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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?



