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)**

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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

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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, . . .

HPC2N (training and other services)

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- Workshops and seminars

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HPC2N (personnel)

Management

- ► Paolo Bientinesi, **new** director
- ► Björn Torkelsson, deputy director
- ► Lena Hellman, administrator

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

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

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► Contact through regular support or dedicated support form[1]
  ► If you have a specific problem/question and/or need consultation (up to 100 h)

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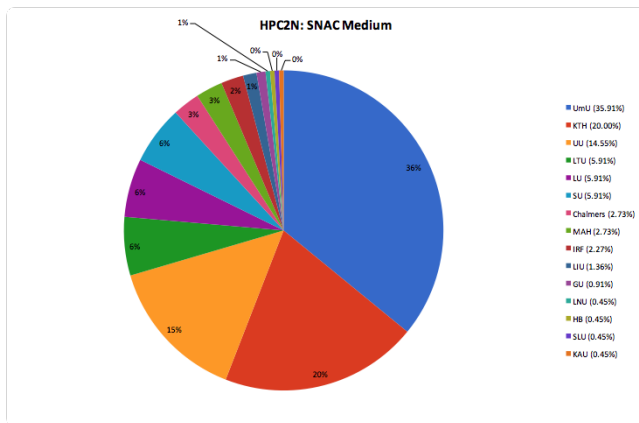
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HPC2N (users by discipline)

- 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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HPC2N (users by discipline, largest users)
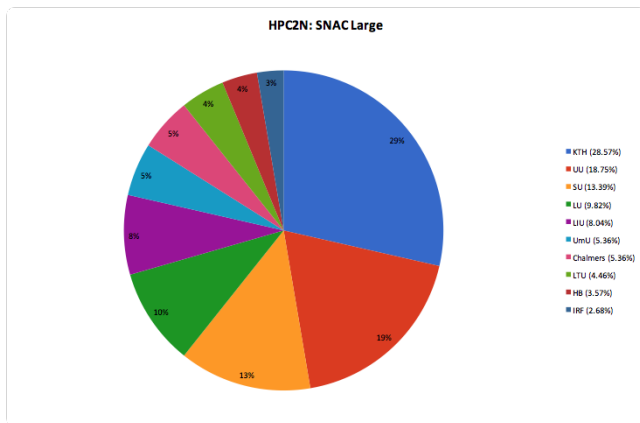
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  - Deep learning and artificial intelligence (several new projects)
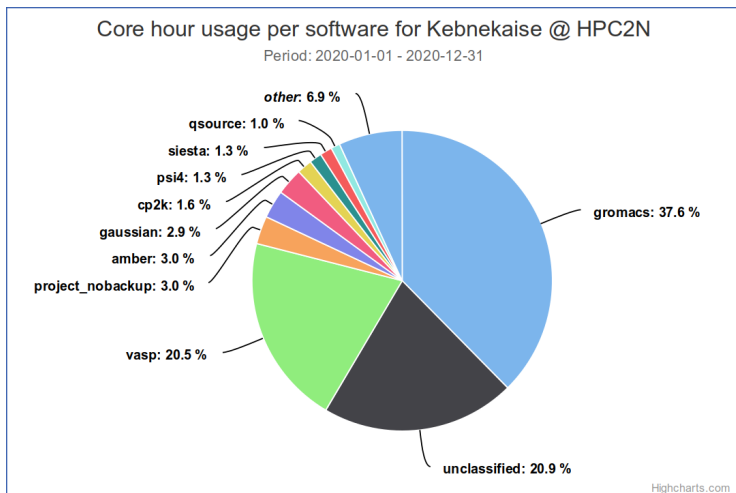
HPC2N (medium users by university)

HPC2N: SNAC Medium

- UmU (35.91%)
- KTH (20.00%)
- UU (14.55%)
- LTU (5.91%)
- LU (5.91%)
- SU (5.91%)
- Chalmers (2.73%)
- MAH (2.73%)
- IRF (2.27%)
- LiU (1.36%)
- GU (0.91%)
- LNU (0.45%)
- HB (0.45%)
- SLU (0.45%)
- KAU (0.45%)

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

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HPC2N (large users by university)

HPC2N: SNAC Large

- KTH (28.57%)
- UU (18.75%)
- SU (13.39%)
- LU (9.82%)
- LIU (8.04%)
- UmU (5.36%)
- Chalmers (5.36%)
- LTU (4.46%)
- HB (3.57%)
- IRF (2.68%)

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

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HPC2N (users by software)

Core hour usage per software for Kebnekaise @ HPC2N

Period: 2020-01-01 - 2020-12-31

other: 6.9 %
qsource: 1.0 %
siesta: 1.3 %
psi4: 1.3 %
cp2k: 1.6 %
gaussian: 2.9 %
amber: 3.0 %
project_nobackup: 3.0 %
vasp: 20.5 %
unclassified: 20.9 %
gromacs: 37.6 %

Highcharts.com

Kebnekaise

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    - delivered by Lenovo and
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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
Compute	**432**	Intel Xeon E5-2690v4, **2 x 14 cores**, **128 GB**, FDR Infiniband

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KNL	36	Intel **Xeon Phi** 7250 (Knight's Landing), 68 cores, 192 GB, 16 GB MCDRAM, FDR Infiniband

Kebnekaise (GPU nodes)

Name	#	Description
2xGPU	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	10	Intel Xeon Gold 6132, 2 x 14 cores, 192 GB, EDR Infiniband, **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]

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[2]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

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[3]728 trillion (billion)
[4]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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High Performance Computing (large problems)

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1. Execution time: The time required to form a solution to the problem is very long
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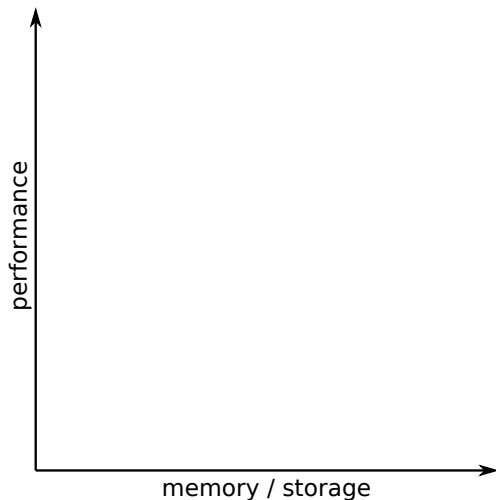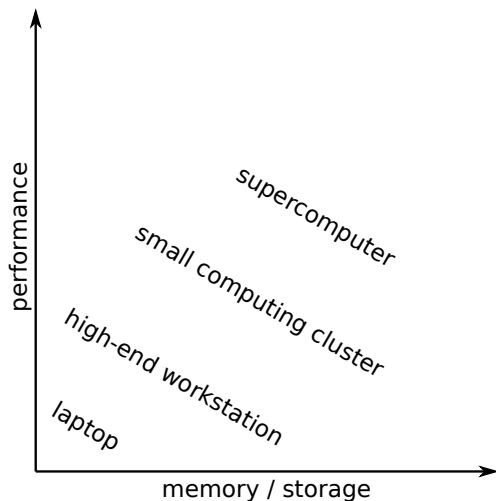# High Performance Computing (large problems)

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- The former can be remedied by **increasing the performance**
  - More cores, more nodes, GPUs, . . .
- The latter by **adding more memory / storage**
  - More memory per node (including large memory nodes), more nodes, . . .
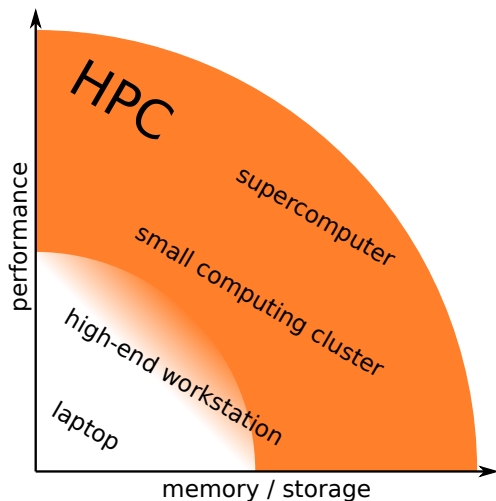 - Large storage solutions, . . .

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High Performance Computing (what counts as HPC)

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  - ▶ High-end CPUs (AVX-512 etc) and ECC memory

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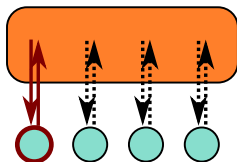# High Performance Computing (other reasons)

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

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- ▶ **Support and documentation**

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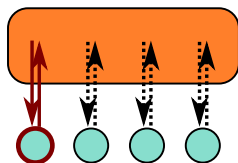
▶ Two memory models are relevant for HPC:

    ▶ Shared memory: Single memory space for all data.

        ▶ **Everyone can access the same data**

        ▶ Straightforward to use

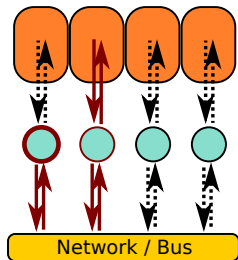# High Performance Computing (memory models)

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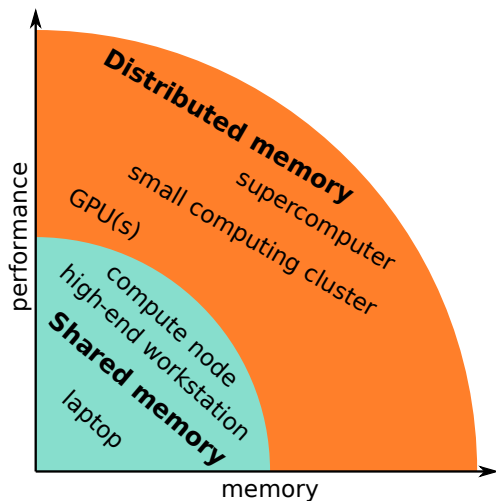

      - **Everyone can access the same data**
      - Straightforward to use

    - Distributed memory: Multiple **distinct** memory spaces.

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

Network / Bus

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High Performance Computing (memory models)

High Performance Computing (programming models)

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  3. Distributed memory: **MPI**, . . .
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     - Work distribution, coordination (synchronization, etc), . . .

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   ▶ **Data distribution and communication**

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

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   ▶ **Data distribution across memory spaces and movement**

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High Performance Computing (software)

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        - ► 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**, . . .

Questions?