### Introduction to HPC2N

HPC2N, Umeå University

September 14, 2023







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



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



 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)

- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- Grid and cloud computing (WLCG NT1, Swedish Science Cloud)

- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- Grid and cloud computing (WLCG NT1, Swedish Science Cloud)
- National Data Science Node in "Epidemiology and Biology of Infections" (DDLS)

- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- Grid and cloud computing (WLCG NT1, Swedish Science Cloud)
- National Data Science Node in "Epidemiology and Biology of Infections" (DDLS)
- Software for e-Science applications

- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- Grid and cloud computing (WLCG NT1, Swedish Science Cloud)
- National Data Science Node in "Epidemiology and Biology of Infections" (DDLS)
- 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



#### 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

















## HPC2N (training and other services)

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

### HPC2N (training and other services)

- User support (primary, advanced, dedicated)
  - Research group meetings @ UmU
  - Also at the partner sites
- 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
    - Introduction to Kebnekaise, 21 September 2023

### HPC2N (training and other services)

- User support (primary, advanced, dedicated)
  - Research group meetings @ UmU
  - Also at the partner sites
- 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
    - Introduction to Kebnekaise, 21 September 2023
- Workshops and seminars

### Management

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

#### Management

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

#### **Application experts**

- Jerry Eriksson
- Pedro Ojeda May

### Management

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

#### Application experts

- Jerry Eriksson
- Pedro Ojeda May

#### Others

- Mikael Rännar (WLCG coord)
- Research Engineers under DDLS, HPC2N/SciLifeLab
  - System Developer, IT
  - Data Engineer
  - Data Steward

#### Management

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

#### Application experts

- Jerry Eriksson
- Pedro Ojeda May

#### Others

- Mikael Rännar (WLCG coord)
- Research Engineers under DDLS, HPC2N/SciLifeLab
  - System Developer, IT
  - Data Engineer
  - Data Steward

### 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):

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

Jerry Eriksson Profiling, Machine learning (DNN), MPI, OpenMP, OpenACC

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

Jerry Eriksson Profiling, Machine learning (DNN), MPI, OpenMP, OpenACC

Pedro Ojeda May

Molecular dynamics, Profiling, QM/MM, NAMD, Amber, Gromacs, GAUSSIAN, R

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

Jerry Eriksson Profiling, Machine learning (DNN), MPI, OpenMP, OpenACC

Pedro Ojeda May

Molecular dynamics, Profiling, QM/MM, NAMD, Amber, Gromacs, GAUSSIAN, R

Åke Sandgren General high level programming assistance, VASP. Gromacs. Amber

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

Jerry Eriksson Profiling, Machine learning (DNN), MPI,

OpenMP, OpenACC

Pedro Ojeda May Molecular dynamics, Profiling, QM/MM, NAMD, Amber, Gromacs, GAUSSIAN, R

Åke Sandgren General high level programming assistance,

VASP, Gromacs, Amber

Contact through regular support

If you have a specific problem/question and/or need consultation

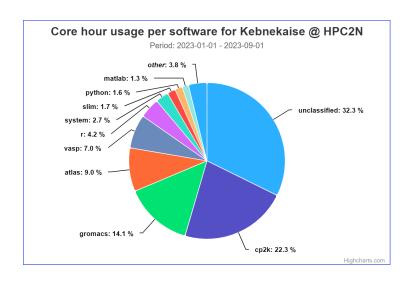
## HPC2N (users by discipline)

- 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)

- Users from several scientific disciplines:
  - Biosciences and medicine
  - Chemistry
  - Computing science
  - Engineering
  - Materials science
  - Mathematics and statistics
  - Physics including space physics
  - Machine learning and artificial intelligence (several new projects)

### HPC2N (users by software)



• The current supercomputer at HPC2N

- The current supercomputer at HPC2N
- Named after a massif (contains some of Sweden's highest mountain peaks)

- The current supercomputer at HPC2N
- Named after a massif (contains some of Sweden's highest mountain peaks)
- Kebnekaise was
  - delivered by Lenovo and
  - installed during the summer 2016

- The current supercomputer at HPC2N
- Named after a massif (contains some of Sweden's highest mountain peaks)
- Kebnekaise was
  - delivered by Lenovo and
  - installed during the summer 2016
- Opened up for general availability on November 7, 2016

- The current supercomputer at HPC2N
- Named after a massif (contains some of Sweden's highest mountain peaks)
- Kebnekaise was
  - · 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

- The current supercomputer at HPC2N
- Named after a massif (contains some of Sweden's highest mountain peaks)
- Kebnekaise was
  - 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
- In 2023, Kebnekaise was extended with
  - 2 dual NVIDIA A100 GPU nodes
  - one many-core AMD Zen3 CPU node

# Kebnekaise (compute nodes)

Name	#	Description
Compute-AMD Zen3	1	AMD Zen3 (EPYC 7762), 2 x 64 cores, <b>1 TB</b> , EDR Infiniband

# Kebnekaise (compute nodes)

Name	#	Description
Compute-AMD Zen3	1	AMD Zen3 (EPYC 7762), 2 x 64 cores, <b>1 TB</b> , EDR Infiniband
Compute-skylake	52	Intel Xeon Gold 6132, 2 x 14 cores, 192 GB, EDR Infiniband, AVX-512

# Kebnekaise (compute nodes)

Name	#	Description
Compute-AMD Zen3	1	AMD Zen3 (EPYC 7762), 2 x 64 cores, <b>1 TB</b> , EDR Infiniband
Compute-skylake	<b>52</b>	Intel Xeon Gold 6132, 2 x 14 cores, 192 GB, EDR Infiniband, AVX-512
Compute !!! Being phased out !!!	432	Intel Xeon E5-2690v4, 2 x 14 cores, 128 GB, FDR Infiniband

# Kebnekaise (compute nodes)

Name	#	Description
Compute-AMD Zen3	1	AMD Zen3 (EPYC 7762), 2 x 64 cores, <b>1 TB</b> , EDR Infiniband
Compute-skylake	52	Intel Xeon Gold 6132, 2 x 14 cores, 192 GB, EDR Infiniband, AVX-512
Compute !!! Being phased out !!!	432	Intel Xeon E5-2690v4, 2 x 14 cores, 128 GB, FDR Infiniband
Large Memory	20	Intel Xeon E7-8860v4, 4 x 18 cores, 3072 GB, EDR Infiniband

Name $\#$ Description	
AMD Zen3 (AMD EPYC 7413), 2 x 24 core	S,
512 GB, EDR Infiniband,	
$2 \times A100$ 2 <b>2</b> x <b>NVidia A100</b> ,	
$2 \times 6912$ CUDA cores,	
2 x 432 Tensor cores	

Name	#	Description
		AMD Zen3 (AMD EPYC 7413), 2 x 24 cores,
		512 GB, EDR Infiniband,
2 × A100	2	2 x NVidia A100,
		$2 \times 6912$ CUDA cores,
		2 x 432 Tensor cores
		Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband,
GPU-volta	10	2 x NVidia V100,
		$2 \times 5120$ CUDA cores, $2 \times 16$ GB VRAM,
		2 x 640 Tensor cores

Name	#	Description
2 × A100	2	AMD Zen3 (AMD EPYC 7413), 2 x 24 cores,
		512 GB, EDR Infiniband,
		2 x NVidia A100,
		2 x 6912 CUDA cores,
		2 x 432 Tensor cores
GPU-volta	10	Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband,
		2 x NVidia V100,
		$2 \times 5120$ CUDA cores, $2 \times 16$ GB VRAM,
		2 x 640 Tensor cores
		Intel Xeon E5-2690v4, 2 x 14 cores,
4xGPU	4	128 GB, FDR Infiniband,
!!! Being phased out !!!	4	4 x NVidia K80
		$8 \times 2496$ CUDA cores, $8 \times 12$ GB VRAM

Name	#	Description
	2	AMD Zen3 (AMD EPYC 7413), 2 x 24 cores,
		512 GB, EDR Infiniband,
2 × A100		2 x NVidia A100,
		2 x 6912 CUDA cores,
		2 x 432 Tensor cores
GPU-volta	10	Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband,
		2 x NVidia V100,
		$2 \times 5120$ CUDA cores, $2 \times 16$ GB VRAM,
		2 x 640 Tensor cores
		Intel Xeon E5-2690v4, 2 x 14 cores,
4×GPU	1	128 GB, FDR Infiniband,
!!! Being phased out !!!	4	4 x NVidia K80
		8 x 2496 CUDA cores, 8 x 12 GB VRAM
2xGPU !!! Being phased out !!!	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

• 553 nodes in 15 racks

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs
- More than 135 TB memory

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs
- More than 135 TB memory
- 71 switches (Infiniband, Access and Management networks)

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs
- More than 135 TB memory
- 71 switches (Infiniband, Access and Management networks)
- 16504 CPU cores

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs
- More than 135 TB memory
- 71 switches (Infiniband, Access and Management networks)
- 16504 CPU cores
- 501760 CUDA cores

- 553 nodes in 15 racks
- Intel Broadwell and Skylake, AMD Zen3
- NVidia A100, V100, K80 GPUs
- More than 135 TB memory
- 71 switches (Infiniband, Access and Management networks)
- 16504 CPU cores
- 501760 CUDA cores
- 12800 Tensor cores

• Basically four types of storage are available at HPC2N:

- Basically four types of storage are available at HPC2N:
  - Home directory
    - $\bullet$  /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB, user owned

- Basically four types of storage are available at HPC2N:
  - Home directory
    - /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB, user owned
  - Project storage
    - /proj/nobackup/abc
    - Shared among project members

- Basically four types of storage are available at HPC2N:
  - Home directory
    - ullet /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB, user owned
  - Project storage
    - /proj/nobackup/abc
    - Shared among project members
  - Local scratch space
    - \$SNIC\_TMP
    - SSD (170GB), per job, per node, "volatile"

- Basically four types of storage are available at HPC2N:
  - Home directory
    - ullet /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB, user owned
  - Project storage
    - /proj/nobackup/abc
    - Shared among project members
  - Local scratch space
    - \$SNIC\_TMP
    - SSD (170GB), per job, per node, "volatile"
  - Tape Storage
    - Backup
    - Long term storage

- Basically four types of storage are available at HPC2N:
  - Home directory
    - ullet /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB, user owned
  - Project storage
    - /proj/nobackup/abc
    - Shared among project members
  - Local scratch space
    - \$SNIC\_TMP
    - SSD (170GB), per job, per node, "volatile"
  - Tape Storage
    - Backup
    - Long term storage
- Also SweStore disk based (dCache)
  - Research Data Storage Infrastructure, for active research data and operated by NAISS, WLCG

 In order to use Kebnekaise, you must be a member of a compute project

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month
  - A regular CPU core cost 1 core hour per hour, other resources (e.g., GPUs) cost more

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month
  - A regular CPU core cost 1 core hour per hour, other resources (e.g., GPUs) cost more
  - Not a hard limit but projects that go over the allocation get lower priority

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month
  - A regular CPU core cost 1 core hour per hour, other resources (e.g., GPUs) cost more
  - Not a hard limit but projects that go over the allocation get lower priority
- A compute project contains a certain amount of storage
  - If more storage is required, you must be a member of a storage project

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month
  - A regular CPU core cost 1 core hour per hour, other resources (e.g., GPUs) cost more
  - Not a hard limit but projects that go over the allocation get lower priority
- A compute project contains a certain amount of storage
  - If more storage is required, you must be a member of a storage project
- As Kebnekaise is a local cluster, you need to be affiliated with UmU, IRF, SLU, Miun, or LTU to use it

- In order to use Kebnekaise, you must be a member of a compute project
  - A compute project has a certain number of core hours allocated for it per month
  - A regular CPU core cost 1 core hour per hour, other resources (e.g., GPUs) cost more
  - Not a hard limit but projects that go over the allocation get lower priority
- A compute project contains a certain amount of storage
  - If more storage is required, you must be a member of a storage project
- As Kebnekaise is a local cluster, you need to be affiliated with UmU, IRF, SLU, Miun, or LTU to use it
- Projects are applied for through SUPR (https://supr.naiss.se)