### Introduction to HPC2N, Kebnekaise and HPC

Birgitte Brydsö, Pedro Ojeda May, and others at HPC2N

> HPC2N Umeå University

19. January 2022







► 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





- 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, SNIC Cloud)



- Scalable and parallel HPC
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- ► **Grid and cloud** computing (WLCG NT1, SNIC Cloud)
- Support
  - Primary, advanced, dedicated
  - Application Experts (AEs)



- ► Scalable and parallel **HPC**
- Large-scale storage facilities (Project storage (Lustre), SweStore, Tape)
- ► **Grid and cloud** computing (WLCG NT1, SNIC Cloud)
- Support
  - 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 by Swedish Research Council (VR), SNIC and various partners









# HPC2N (funding)

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





- 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



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



- 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 (e.g., OpenMP, MPI, debugging, performance analyzers, Matlab, R, MD simulation, Deep Learning, GPU, ...)
- NGSSC / SeSE & university courses



- 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 (e.g., OpenMP, MPI, debugging, performance analyzers, Matlab, R, MD simulation, Deep Learning, GPU, ...)
- NGSSC / SeSE & university courses
- 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

- Bo Kågström
- Mikael Rännar (WLCG coord)
- Anders Backman
- Kenneth Bodin
- Claude Lacoursière (Algoryx)







#### Management

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

#### Application experts

- Jerry Eriksson
- Pedro Ojeda May

#### Others

- Bo Kågström
- Mikael Rännar (WLCG coord)
- Anders Backman
- Kenneth Bodin
- Claude Lacoursière (Algoryx)

#### System and support

- Frik 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)**:

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



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

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

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







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

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

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

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







► 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

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



► 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 or dedicated support form<sup>1</sup>
  - ► If you have a specific problem/question and/or need consultation (up to 100 h)

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



# 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



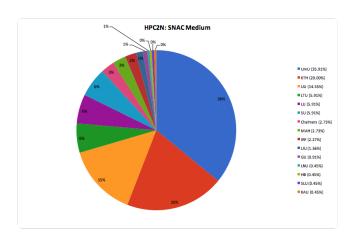


### HPC2N (users by discipline, largest users)

- 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 (several new projects)



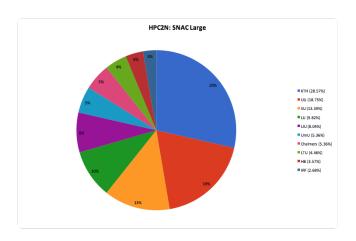
# HPC2N (medium users by university)



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



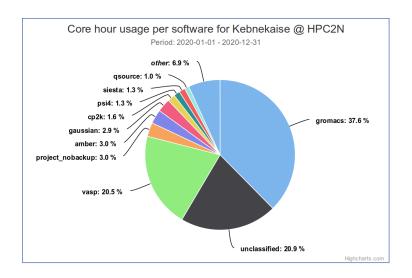
# HPC2N (large users by university)



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



### HPC2N (users by software)







### Kebnekaise

► Latest supercomputer at HPC2N





#### Kebnekaise

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



#### Kehnekaise

- Latest 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



### Kehnekaise

- Latest 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



#### Kebnekaise

- Latest 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

# Kebnekaise (compute nodes)

Name	#	Description
Compute	432	Intel Xeon E5-2690v4, 2 x 14 cores,
		128 GB, FDR Infiniband



# Kebnekaise (compute nodes)

Name	#	Description
Compute	432	Intel Xeon E5-2690v4, 2 x 14 cores,
		128 GB, FDR Infiniband
Compute-skylake	52	Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband, AVX-512



# Kebnekaise (compute nodes)

#	Description
432	Intel Xeon E5-2690v4, 2 x 14 cores,
	128 GB, FDR Infiniband
52	Intel Xeon Gold 6132, 2 x 14 cores,
	192 GB, EDR Infiniband, AVX-512
20	Intel Xeon E7-8860v4, 4 x 18 cores,
	3072 GB, EDR Infiniband
	<b>432</b> 52



# Kebnekaise (compute nodes)

Name	#	Description
Compute	432	Intel Xeon E5-2690v4, 2 x 14 cores,
		128 GB, FDR Infiniband
Compute-skylake	52	Intel Xeon Gold 6132, 2 x 14 cores,
		192 GB, EDR Infiniband, AVX-512
Large Memory	20	Intel Xeon E7-8860v4, <b>4 x 18 cores</b> ,
		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
	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	





# Kebnekaise (GPU nodes)

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





# Kebnekaise (GPU nodes)

Name	#	Description
2xGPU	32	Intel Xeon E5-2690v4, 2 x 14 cores,
		128 GB, FDR Infiniband,
		2 x NVidia K80
		$4 \times 2496$ CUDA cores, $4 \times 12$ GB VRAM
4xGPU		Intel Xeon E5-2690v4, 2 x 14 cores,
	4	128 GB, FDR Infiniband,
		4 x NVidia K80
		$8 \times 2496$ CUDA cores, $8 \times 12$ GB VRAM
GPU-volta		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



▶ 602 nodes in 15 racks





- ▶ 602 nodes in 15 racks
- ▶ 19288 cores (of which 2448 cores are KNL-cores)
  - ▶ 18840 available for users (the rest are for managing the cluster)



- 602 nodes in 15 racks
- ▶ **19288 cores** (of which 2448 cores are KNL-cores)
  - ▶ 18840 available for users (the rest are for managing the cluster)
- More than 136 TB memory



- 602 nodes in 15 racks
- ▶ **19288 cores** (of which 2448 cores are KNL-cores)
  - ▶ 18840 available for users (the rest are for managing the cluster)
- More than 136 TB memory
- ▶ 71 switches (Infiniband, Access and Managment networks)



- 602 nodes in 15 racks
- ▶ **19288 cores** (of which 2448 cores are KNL-cores)
  - ▶ 18840 available for users (the rest are for managing the cluster)
- More than 136 TB memory
- 71 switches (Infiniband, Access and Managment networks)
- 728 TFlops/s Peak performance (expansion not included)



- ▶ 602 nodes in 15 racks
- ▶ 19288 cores (of which 2448 cores are KNL-cores)
  - ▶ 18840 available for users (the rest are for managing the cluster)
- More than 136 TB memory
- > 71 switches (Infiniband, Access and Managment networks)
- ▶ 728 TFlops/s Peak performance (expansion not included)
- 629 TFlops/s Linpack (all parts, except expansion)
  - 86% of Peak performance

▶ Basically five types of storage are available at HPC2N:





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



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



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



- Basically five types of storage are available at HPC2N:
  - Home directory
    - ightharpoonup /home/X/Xyz, \$HOME,  $\sim$
    - 25 GB. user owned
  - Project storage
    - /proj/nobackup/abc
    - Shared among project members
  - Local scratch space
    - \$SNTC TMP
    - SSD (170GB), per job, per node, "volatile"
  - SweStore disk based (dCache)
    - part of SNIC Storage, nationally accessible storage



- Basically five types of storage are available at HPC2N:
  - Home directory
    - ► /home/X/Xyz, \$HOME, ~
    - 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"
  - SweStore disk based (dCache)
    - part of SNIC Storage, nationally accessible storage
  - ► Tape Storage
    - Backup
    - Long term storage



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
- ▶ 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."<sup>2</sup>

<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)



<sup>&</sup>lt;sup>3</sup>728 trillion (billion)

#### 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
- Higher performance
  - 728 000 000 000 000 arithmetical operations per second<sup>3</sup>
  - Compared to 200 000 000 000 Flops in a modern laptop<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>200 billion (milliard)







<sup>&</sup>lt;sup>3</sup>728 trillion (billion)

#### 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

#### ► Higher performance

- ▶ 728 000 000 000 000 arithmetical operations per second<sup>3</sup>
- ► Compared to 200 000 000 000 Flops in a modern laptop<sup>4</sup>

#### Solve large problems

- When does a problem become large enough for HPC?
- ► Are there other reasons for using HPC resources? (Memory, software, support, etc.)

<sup>&</sup>lt;sup>4</sup>200 billion (milliard)



<sup>&</sup>lt;sup>3</sup>728 trillion (billion)

# High Performance Computing (large problems)

- A problem can be large for two main reasons:
  - 1. Execution time: The time required to form a solution to the problem is very long
  - 2. Memory / storage use: The solution of the problem requires a lot of memory and/or storage



#### High Performance Computing (large problems)

- A problem can be large for two main reasons:
  - 1. Execution time: The time required to form a solution to the problem is very long
  - 2. Memory / storage use: The solution of the problem requires a lot of memory and/or storage
- The former can be remedied by increasing the performance
  - ► More cores, more nodes, GPUs, ...

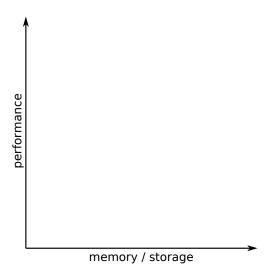


#### High Performance Computing (large problems)

- A problem can be large for two main reasons:
  - 1. Execution time: The time required to form a solution to the problem is very long
  - 2. Memory / storage use: The solution of the problem requires a lot of memory and/or storage
- ► 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, . . .

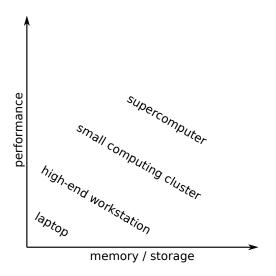


# High Performance Computing (what counts as HPC)





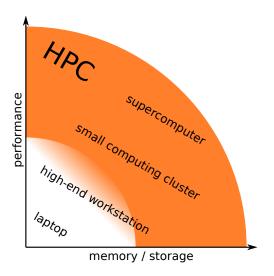
## High Performance Computing (what counts as HPC)







#### High Performance Computing (what counts as HPC)





# High Performance Computing (other reasons)

Specialized (expensive) hardware





# High Performance Computing (other reasons)

- Specialized (expensive) hardware
  - ► GPUs, Nvidia Tesla V100 GPUs are optimized for Al



# High Performance Computing (other reasons)

- Specialized (expensive) hardware
  - ► GPUs, **Nvidia Tesla V100 GPUs** are optimized for Al
  - Intel Xeon Phi



# High Performance Computing (other reasons)

- Specialized (expensive) hardware
  - ► GPUs, Nvidia Tesla V100 GPUs are optimized for Al
  - Intel Xeon Phi
  - High-end CPUs (AVX-512 etc) and ECC memory



# High Performance Computing (other reasons)

- Specialized (expensive) hardware
  - ► GPUs, **Nvidia Tesla V100 GPUs** are optimized for Al
  - Intel Xeon Phi
  - High-end CPUs (AVX-512 etc) and ECC memory
- Software
  - ► HPC2N holds **licenses** for several softwares
  - Software is pre-configured and ready-to-use



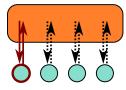
# High Performance Computing (other reasons)

- Specialized (expensive) hardware
  - ► GPUs, **Nvidia Tesla V100 GPUs** are optimized for Al
  - ▶ Intel Xeon Phi
  - High-end CPUs (AVX-512 etc) and ECC memory
- Software
  - ► HPC2N holds **licenses** for several softwares
  - Software is pre-configured and ready-to-use
- Support and documentation

Two memory models are relevant for HPC:



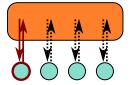
- Two memory models are relevant for HPC:
  - Shared memory: Single memory space for all data.



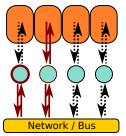
- Everyone can access the same data
- Straightforward to use



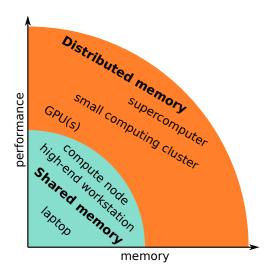
- Two memory models are relevant for HPC:
  - ► Shared memory: Single memory space for all data.



- 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





The programming model changes when we aim for extra performance and/or memory:



- ▶ The programming model changes when we aim for extra performance and/or memory:
  - 1. Single-core: Matlab, Python, C, Fortran, ...
    - Single stream of operations



- ▶ 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



- 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), . . .



- 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
    - ▶ Work distribution, coordination (synchronization, etc), ...



- 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
    - Work distribution, coordination (synchronization, etc), . . .
    - Data distribution and communication



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

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



- ► 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
    - ▶ Work distribution, coordination (synchronization, etc), ...
    - 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:



- Complexity grows when we aim for extra performance and/or memory/storage:
  - 1. Single-core: LAPACK, ...
    - 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



- 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, ...



- 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, ...
  - 3. Distributed memory: ScaLAPACK, ...
    - 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, ...
  - 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, ...





- 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, . . .
  - 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, . . .

- 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, . . .
  - 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?

