Home

Welcome to the knowledge pool for the Danish EuroHPC competence centre. Here you will find best practices, material about HPC, HPDA and AI software and hardware, Analysis of the Danish national HPCs infrastructure, relevant resources and literature. All the material can be found in pdf form for offline consultation by clicking on the symbol on the top-right corner of this page.

This knowledge pool is meant to be available both to completely new users and advanced/expert users. If you are a new user, visit the page *HPC 101* to learn the basics about High Performance Computing and get up to speed. Facilitation in accessing HPCs and dissemination activities are offered - if any is needed, feel free to contact eurocc@listserv.deic.dk.

If you desire a specific topic or material to be covered, or need any type of assistance related with the topics of the knowledge pool, contact the HPC facilitator at eurocc@listserv.deic.dk.

Basics of HPC

HPC (High Performance Computing) consists in clustering together a large amount of computing hardware, so that a large number of operations can be executed at once. A supercomputer consists of different types of hardware. In general, hardware is structured in this hierarchy:

- **CPU**, the unit that can execute a single sequence of instructions. A CPU can consists of multiple cores, so that multiple chains of instructions can be executed independently.
- **Node**, one of the computers that are installed into an HPC system.
- **Cluster**, a group of nodes that are connected together and therefore able to communicate and work together on a single task.

Moreover, a storage section connected all with one or more types of storage hardware is present in an HPC. A **node** can consists of only one or more CPUs and some RAM memory. There are other types of nodes containing different hardware combinations. The most common hardware that can be found in a node beyond RAM and CPUs is:

- **GPU**, a graphics card. This type of hardware was used for gaming and graphics software, but it has build up a lot of computational power capable of hundreds of parallel processes. This is particularly useful for specific types of linear algebra operations that require the same task to be performed repeatedly. Nvidia and AMD are the main GPU producers.
- **FPGA**, a programmable piece of hardware that can do specific operations many times faster than the other available solutions. It can be used to accelerate specific processes that are usually carried out using CPUs.

Access to HPC

HPC systems allow many users to log into the system at the same time and use part of those resources, usually after they are assigned by an administrator to each user (so that using more resources than assigned will result in stopping whatever software is executed at that time). In Denmark, you have two ways of logging into an HPC system: the first is through a user-friendly interactive interface (DeiC facility for interactive HPC), the second is through a classic command line, that requires some knowledge of the UNIX shell language (here is a good introduction to the Linux shell).

Usually, a user can access to a so-called *login node*: this has few computational resources allowing the user to login and perform basic operations (small code testing, file management). A user can get assigned

- a number of CPUs and eventually GPUs/FPGAs/...
- an amount of RAM
- a quantity of storage

- an amount of total time those resources need be used

When using DeiC's facility for interactive HPC, the user asks for resources directly through the dashboard once logged in. You will have the chance to exchange messages with the front office responsible for resource assignment, in case your resource demand is too low or too high. However, we suggest to contact first your local front office or eurocc@listserv.deic.dk (HPC facilitation responsible) to get help in submitting a request to obtain resources. For using non-interactive HPCs, you will need to contact the local front office and discuss the possibility of getting resources.

What can I use HPC for

HPC systems have a large amount of computational power, but this does not mean they are only to be used for large scale projects. You can indeed request entire nodes as well as a single CPU with some GB of RAM. The Danish HPCs are available for any academic application:

- research projects
- student projects
- student exercises in classroom teaching/lecturing

Students are not authorized to ask for resources. It will be responsibility of the lecturer/professor to obtain resources through the front office or facilitator. Any student can then be invited/ authorized in accessing the project whose resources have been allocated to.

Heavy focus of the Danish HPC ecosystem is on teaching and the training of new users, so applications for resources related to courses and students projects are very much welcomed.

Advantages of using HPC

Using HPC offers many advantages, not only limited to the resources available. In general, using HPC makes the difference in relation to

- getting a large amount of resources at a cost much lower than buying/owning your own powerful workstation
- sharing data and settings with other people in collaborative projects
- using software that is already installed or manageable through a package software: save time instead of configuring and adjusting things on your computer! This is an important aspect especially in teaching, where students have different OS, software versions, and problems with packages.
- getting technical support from the help desk without being on your own
- convenience in the sense that computations do not occupy resources on the user's personal computer that is then free to perform other tasks.

Best practices for HPC

This page lists some useful best practices to keep in mind when coding and running applications and pipelines on HPC systems.

Code coverage, testing, continuous integration

Every time we code, testing is a concern and is usually performed by the coder(s) regularly during the project. One can identify some basic main types of test:

Regression test	*Given an expected output from a specific input, the code is tested to reproduce that same output*
Unit test	*Tests the smallest units of the software (e.g. single functions) to identify bugs, especially in extreme cases of inputs and*
Continuous integration	*A set of tests the software runs automatically everytime the code is updated. This is useful to spot bugs before someone even uses the code.*

More things one might need to test are the performance/scalability of the code, usability, and response to all the intended types of input data.

Unit and regression test can be useful, but at some point not really feasible, since the code can scale to be quite large and complex, with a lot of things to control. It is thus a good practice to use continuous integration, and implement simple but representative tests that cover all the code, so that bugs can be spotted often before the final users do that. Code coverage tools to implement such tests exists for several programming languages, and also for testing code deployed on GitHub version control.

Links

Link	**Description**
pyTest	a package to test `python` code
Cmake	to test both `C`, `C++` and `Fortran code`

Link	Description
Travis CI	tool for continuous integration in most of the used programming languages. Works on Git version control.
covr	test coverage reports for R

Code styling

An important feature of a computer code is that it is understandable to other people reading it. To ensure this is the case, a clean and coherent style of coding should be used in a project. Some languages have a preferred coding style, and in some GUIs (graphical user interfaces) those styling rules can be set to be required. One can also use ones own coding style, but it should be one easily readable by others, and it should be the same style throughout the whole project.

Links

Link	Description
styleguide	Google guide for coding styles of the major programming languages
awesome guidelines	A guide to coding styles covering also documentations, tools and development environments
Pythonic rules	Intoduction to coding style in python.
R style	A post on R coding style

Containerized applications

In this section the benefits of project and package managers, that are a way of organizing packages in separated environments, will be outlined. However, a higher degree of isolation can be achieved by containerization than using environments. By containerizing, a user can virtualize the entire operating system, and make it ready to be deployed on any other machine. One can for example deploy a container without the need of installing anything on the hosting machine! Note that containers are a different concept from Virtual Machines, where it is the hardware being virtualized instead.

Links

Link	Description
Docker	An open source widespread container that is popular both in research and industry
Docker course	A course on the use of Docker freely hosted on youtube
Docker curriculum	Beginner's introduction to docker
Docker basics	Intoduction tutorials to Docker from the official documentation page
Singularity	Singularity is another containerization tool. It allows you to decide at which degree a container interacts with the hosting system
Singularity tutorial	A well done Singularity tutorial for HPC users
Singularity video tutorial	A video tutorial on Singularity
Reproducibility by containerization	A video on reproducibility with Singularity containers

Documentation

When creating a piece of software, it is always a good idea to create a documentation explaining the usage of each element of the code. For packages, there are software that automatically create a documentation by using the declarations of functions and eventually some text included into them as a string.

Links

Link	Description
MkDocs	A generator for static webpages, with design and themes targeted to documentation pages, but also other type of websites. This website is itself made with MkDocs.
mkdocstrings	Python handler to automatically generate documentation with MkDocs

Link	Description
pdoc3	A package that automatically creates the documentation for your coding projects. It is semi-automatic (infers your dependencies, classes, etc. but adds a description based on your docstrings)
pdoc3 101	How to run pdoc to create an HTML documentation
Roxygen2	A package to generate `R` documentation — it can be used also with `Rcpp`
Sphinx	Another tool to write documentation — it produces also printable outputs. `Sphinx` was first created to write the `python` language documentation. Even though it is a tool especially thought for `python` code, it can be used to generate static webpages for other projects.

Documents with live code

Programming languages like `python` and `R` allows users to write documents that contain text, images and equations together with executable code and its output. Text is usually written using the very immediate markdown `language`. Markdown files for `R` can be created in the GUI `Rstudio`, while `python` uses `jupyter notebooks`.

Links

Link	Description
Introduction to Markdown	Markdown for `R` in `Rstudio`
Jupyter notebooks	create interactive code with `python`. You can write `R` code in a jupyter notebook by using the `python` package rpy2

Package/Environment management systems

When coding, it is essential that all the projects are developed under specific software conditions, i.e. the packages and libraries used during development (dependencies) should not change along the project's lifetime, so that variations in things such as output formats and new algorithmic implementations will not create conflicts difficult to trace back under development. An environment and package manager makes the user able to create separated frameworks (environments) where to install specific packages that will not influence other software outside the environment in use. A higher degree of isolation can be achieved through containers (see the related part of this page).

Links

Link	Description
Conda	an easy to use and very popular environment manager
Getting started with conda	Introduction to `conda` setup and usage from the official documentation
Conda cheat sheet	Quick reference for `conda` usage
YARN	An alternative to `conda`

Many short jobs running

Every time a job is submitted to the job manager (e.g. Slurm) of a computing cluster, there is an overhead time necessary to elaborate resource provision, preparation for output, and queue organization. Therefore it is wise to create, when possible, longer jobs. One needs to find the correct balance for how to organizing jobs: if these are too long and fail because of some issue, than a lot of time and resources have been wasted, but such problems can be overcome by tracking the outputs of each step to avoid rerunning all computations. For example, at each step of a job outputting something relevant, there can be a condition checking if the specific output is already present.

Massive standard outputs

Try to avoid printing many outputs on the standard output (`stdout`), in other words a large amount of printed outputs directly to the terminal screen. This can be problematic when a lot of parallel jobs are running, letting `stdout` filling all the home directory up, and causing errors and eventual data loss. Instead use an output in software-specific data structures (such as `.RData` files for the `R` language) or at least simple text files.

Packaging a coding project

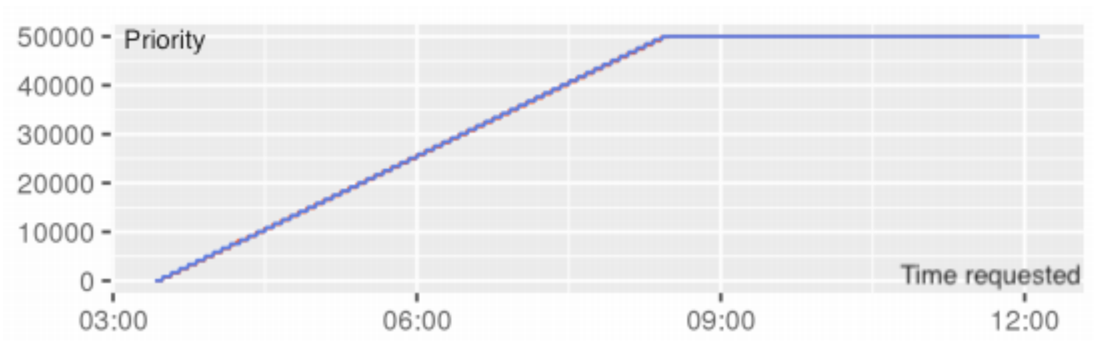
When coding a piece of software in which there are multiple newly implemented functions, it can be smart to organize all those functions as a package, that can be reused and eventually shared with ease. Such a practice is especially easy and can be mastered very quickly for coding projects in `python` and `R`.

Links

Link	Description
pyPA	`python` packaging user guide
R package development	Develop an `R` package using `Rstudio`

Pipe-lining and submitting jobs in Slurm

Slurm is a job scheduler. It allows a user to specify a series of commands and resources requirements to run such commands. Slurm does consider the job submission on an HPC system together with all the other jobs, and prioritize them among other things according to the resources requirement and the available computational power.



In figure above, the priority assigned to a Slurm job when the requested time increases, by keeping the memory and CPUs fixed. Decreased priority has higher values. Adapted from *A Slurm Simulator: Implementation and Parametric Analysis. Simakov et al 2017.*

The Danish national HPCs, and most of the other EuroHPC supercomputers, use Slurm as job manager.

Links

Link	Description
SLURM example 1 and SLURM example 2	Some examples of how to make a Slurm script to submit a job from the danish HPC GenomeDK and from Princeton Research Computing.
Gwf, a simple python tool to create interdependent job submissions	Gwf, developed at the University of Aarhus, makes it easy to create Slurm jobs and organize them as a pipeline with dependencies, using the python language (you need python 3.5+). You get to simply create the shell scripts and the dependencies, without the complicating syntax of Slurm. The page contains also a useful guide.

Version control

Version control is the tracking of your development history for a project. This allows multiple people working on the same material to keep changes in sync without stepping over each other's contributions. Version control tools allow to commit changes with a description, set up and assign project objectives, open software issues from users and contributors, test automatically the code to find bugs before users step into them. Version control is useful for both teams and single users, and it is a good practice to have version control as a standard for any project.

Links

Link	Description
GitHub	the most used tool for version control
Github 101	quick introduction to get started on Github
GitLab and BitBucket	Two other popular alternatives to `Github`

HPC programming

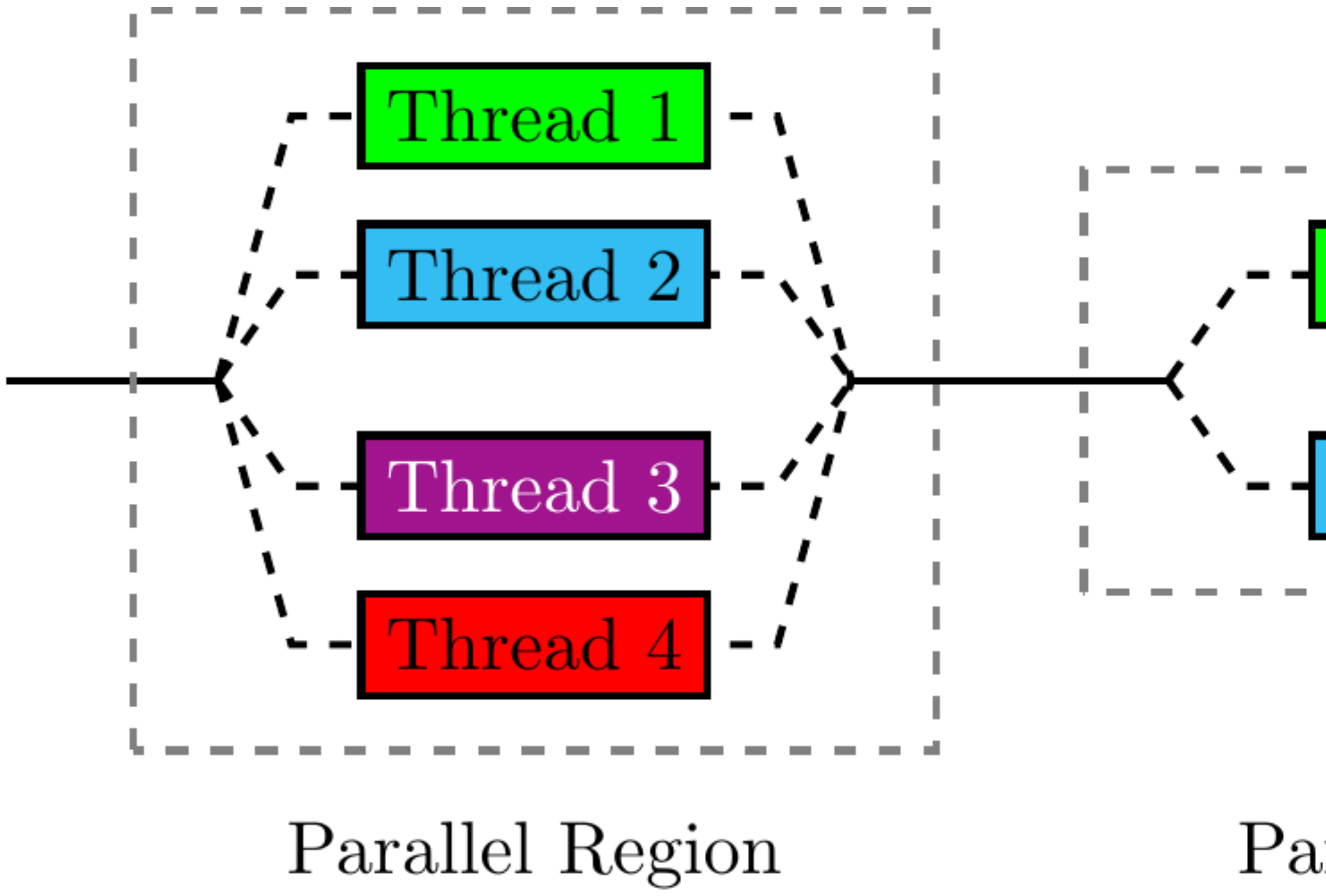
As with any other computer, an HPC system can be used with sequential programming. This is the practice of writing computer programs executing one instruction after the other, but not instructions simultaneously in parallel, i.e. parallel programming.

Parallel programming

There are different ways of writing parallelized code, while in general there is only one way to write sequential code, generally as a logic sequence of steps.

OpenMP (multithreading)

A popular way of parallel programming is through writing sequential code and pointing at specific pieces of code that can be parallelized into threads (fork-join mechanism, see figure below from ADMIN magazine). A thread is an independent execution of code with its own allocated memory.



If threads vary in execution time, when they have to be joined together to collect data, some threads might have to wait for others, leading to loss of execution time. It is up to the programmer to best balance the distribution of threads to optimize execution times when possible.

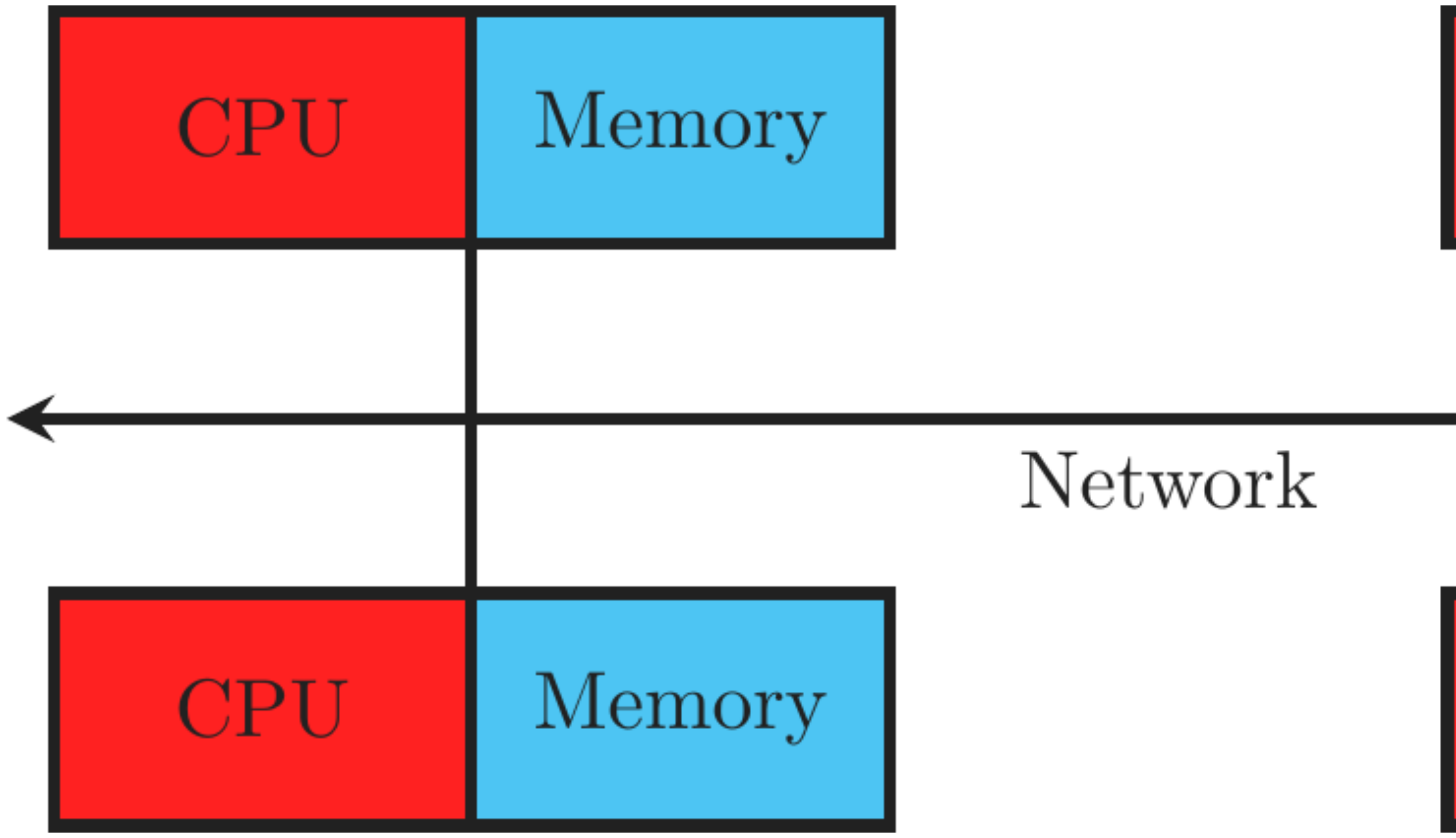
Modern CPUs support openMP in a natural way, since they are usually multicore CPUs and each core can execute threads independently. OpenMP is available as an extension to the programming languages C and Fortran and is mostly used to parallelize for loops that constitute a time bottleneck for the software execution.

Link	**Description**
Video course	a video course (here the link to the first lesson, you will be able to find all the other lessons associated to that) held by ARCHER UK.
OpenMP Starter	A starting guide for OpenMP
WikiToLearn course	An OpenMP course from WikiToLearn

Link	Description
MIT course	A course from MIT including also MPI usage (next section for more info about MP)

MPI (message passing interface)

MPI is used to distribute data to different processes, that otherwise could not access to such data (figure below inspired by LLNL).



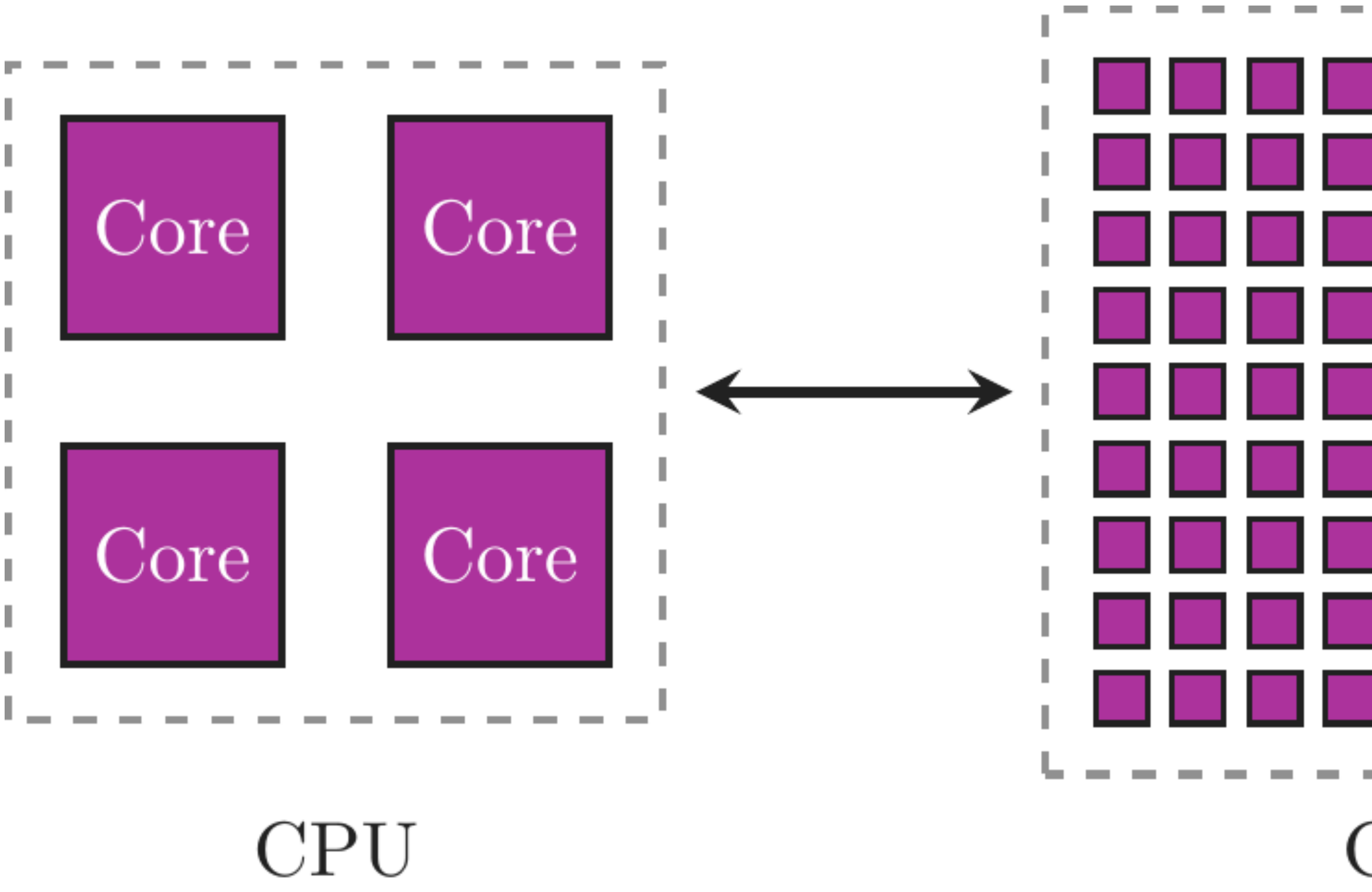
MPI is considered a very hard language to learn, but this reputation is mostly due to the fact that the message passing is programmed explicitly.

Link	Description
Video course	a video course (here the link to the first lesson, you will be able to find all the other lessons associated to that) held by ARCHER UK.
MPI Starter	A starting guide for OpenMP

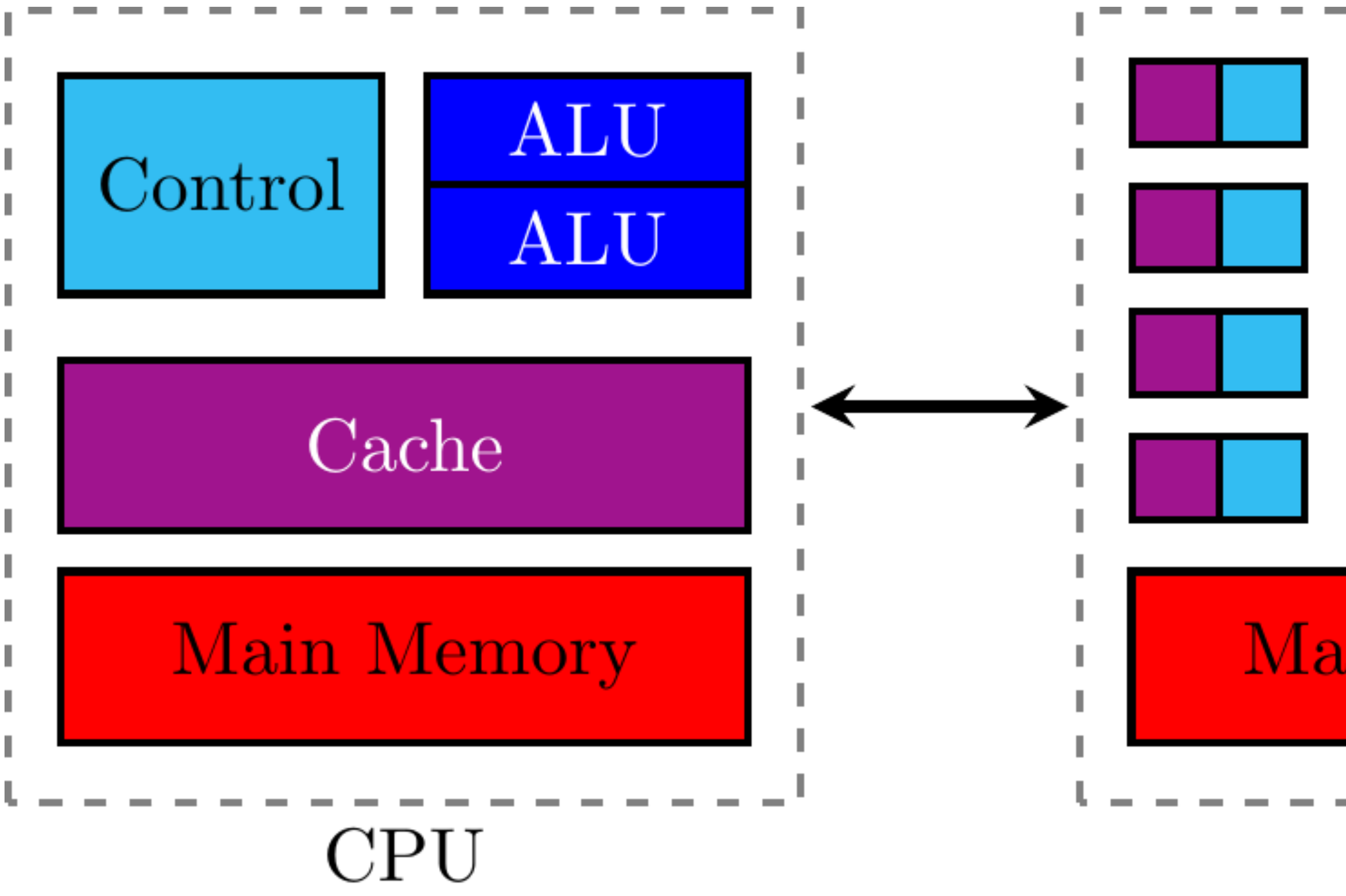
Link	Description
PRACE course	A PRACE course on the MOOC platform FutureLearn

GPU programming

GPUs (graphical processing units) are computing accelerators that are used to boosts heavy linear algebra applications, such as deep learning. A GPU usually features a large number of special processing units that enable massively parallel execute of code (figure below inspired by Astronomy Computing Today).



When utilized properly GPUs can enable performance of certain programs that is unachievable using only CPUs. To achieve this performance GPUs employ an architecture that is vastly different from that of a CPU which is illustrated below (figure inspired by omisci), where ALU is an acronym for arithmetic logic unit.



For the sake of clarity text is omitted in parts of the figure with the different parts indicated by their colour code.

When writing programs that utilize GPUs the different architecture of a GPU poses a different set of challenges compared to those of writing parallel programs for CPUs. Specifically as memory on GPUs is limited compared to CPUs a different approach to memory management is required.

AMD and Nvidia are the two main producers of GPUs, where the latter has dominated the market for a long time. The Danish HPCs Type 1 and 2 feature various models of Nvidia graphic cards, while Type 5 (LUMI) has the latest AMD Instinct.

The distinction between AMD and Nvidia is mainly due to the fact that they are programmed with two different dialects, and software with dedicated multithreading on GPUs need to be coded specifically for the two brands of GPUs.

Nvidia CUDA

CUDA is a C++ dialect that has also various library for the most popular languages and packages (e.g. python, PyTorch, MATLAB, ...).

Link	Description
Nvidia developer training	Nvidia developer trainings for CUDA programming
Book archive	An archive of books for CUDA programming
Advanced books	Some advanced books for coding with CUDA
PyCUDA	Code in CUDA with python

AMD HIP

HIP is a dialect for AMD GPUs of recent introduction. It has the advantage of being able to be compiled for both AMD and Nvidia hardware. CUDA code can be converted to HIP code almost automatically with some extra adjustments by the programmer.

The LUMI HPC consortia has already organized a course for HIP coding and CUDA-to-HIP conversion. Check out their page for new courses.

Link	Description
Video introduction 1	Video introduction to HIP
Video introduction 2	Video introduction to HIP
AMD programming guide	Programming guide to HIP from the producer AMD

Choose your HPC

Here you can quickly fill in an assessment form to understand which HPC is best suited to your application. Some Answers are not mandatory in case you are uncertain of some specific choice.

HPC types

DeiC Interactive HPC

DeiC Interactive HPC targets users who desire an interactive approach to HPC which ensures that the user's experience is as close to that of a laptop or desktop computer as possible. The computer is accessed through a browser from where a large range of applications can be used. Programs are run through a job which is scheduled through an interactive menu. Once the job is active the user can run the application, for which the job was created, either through the interactive editor, just like on an ordinary laptop or desktop computer, or through the terminal. The simplicity of use makes it ideal for new users, including students, and the large number of available applications provide experienced users with a vast array of tools for their projects. It is therefore well suited for both new and experienced HPC users. With DeiC Interactive HPC users have access to both ordinary CPU, large memory CPU and GPU nodes. More information on DeiC Interactive HPC is available at interactivehpc.dk.

DeiC Throughput HPC

DeiC Throughput HPC is the traditional HPC setup in which the user accesses a Linux server through an SSH connection. On the server everything is run through the terminal. Specifically the user accesses a front end node from where jobs can be submitted to a queue of jobs managed by a scheduling system, usually Slurm, which controls resource allocations and starts jobs in due time. Once a job is finished the output is returned to the user. Each job runs autonomously and the user can submit a detailed resource request tailored to each job. Users have access to both ordinary CPU, large memory CPU and GPU nodes. Throughput HPC can handle large amounts of data stored with high levels of security if necessary and is ideal for throughput intensive tasks that can be distributed among multiple cores and/or nodes. The fact that everything is handled through a Linux server using a scheduling system does however imply a steeper learning curve for new users relative to DeiC Interactive HPC.

DeiC Large Memory HPC

Like DeiC Throughput HPC, DeiC Large Memory HPC is configured as a Linux server with the Slurm scheduler accessed by the user through an SSH connection. DeiC Large Memory HPC however distinguishes itself from DeiC Throughput HPC in the hardware employed by offering a comparatively small number of nodes and CPU cores that have access to large amounts of fast memory. This setup tailors to tasks that cannot efficiently be distributed among cores and nodes or whose memory requirements exceed that offered by DeiC Throughput HPC. The documentation for the computer is available at docs.hpc-type3.sdu.dk.

DeiC Accelerated HPC

Like the use of GPUs have massively increased the possibilities for massively parallel tasks, extensive research is currently devoted to other types of hardware that can accelerate specific operations. DeiC Accelerated HPC is a testing ground to explore hardware accelerated solutions targetted at future HPC use. A leading hardware component for this type of research is the *Field-Programmable Gate Array* (FPGA). Where GPUs can accelerate massively parallel tasks as it is hardware designed specifically for such tasks, the goal is for FPGAs is to be hardware configurable to a specific task. In this way one can tackle a prohibiting bottleneck by optimization at the hardware level. Another approach to acceleration is *in-memory* computing which aims to tackle the following problem: Contemporary big data sets are becoming ever larger and currently exceed even that largest RAM units. This implies that data transfer between hard-drives or flash-drives and memory create a significant bottleneck for contemporary big data programs. In-memory computing aims to solve this problem by distributing the data amongst multiple RAM units each with its own CPU operating in parallel. This requires the use of software to communicate between CPUs in an efficient manner.

Capability HPC (LUMI pre-exascale)

Capability HPC provides a similar setup to DeiC Throughput HPC but with increased possibilities by virtue of state-of-the-art hardware. Specifically the interconnections between compute nodes is designed to minimize latency thereby addressing the issue of communication induced latency in distributed-memory programs running on separate nodes. Additionally the user can obtain access to large amounts of disk space also with low-latency interconnects. In this way Capability HPC enables computations that are prohibitive with DeiC Throughput HPC due to communication latency.

Currently Capability HPC consists of the LUMI pre-exascale computer and once they are operational also Leonardo and MareNostrum5. These machines are a part of the EuroHPC project where the international collaboration allows the purchase of otherwise inaccessible hardware. In particular LUMI will provide an extensive GPU partition designed to suit machine learning and artificial intelligence applications.