An introduction to numerical methods using BLAS

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Overview

- What are numerical libraries and how to use them?
- Functionality and uses of BLAS
- How computer architecture (caches) affect implementation of computations

Not all evaluations are the same!

Consider a simple matrix multiplication

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix}. \tag{1}$$

Can be evaluated in 2 ways, with a dot product or a scalar-matrix product:

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \end{pmatrix}, \qquad \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 1 \begin{pmatrix} 1 \\ 3 \end{pmatrix} + 2 \begin{pmatrix} 2 \\ 4 \end{pmatrix}.$$

Software libraries

- BLAS is a typical software library
- Libraries can be used in 2 forms:
    - Static
    - Dynamic

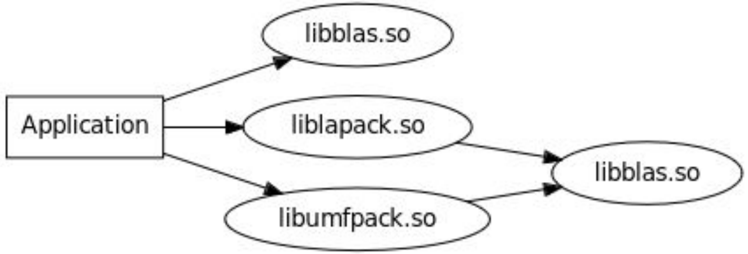
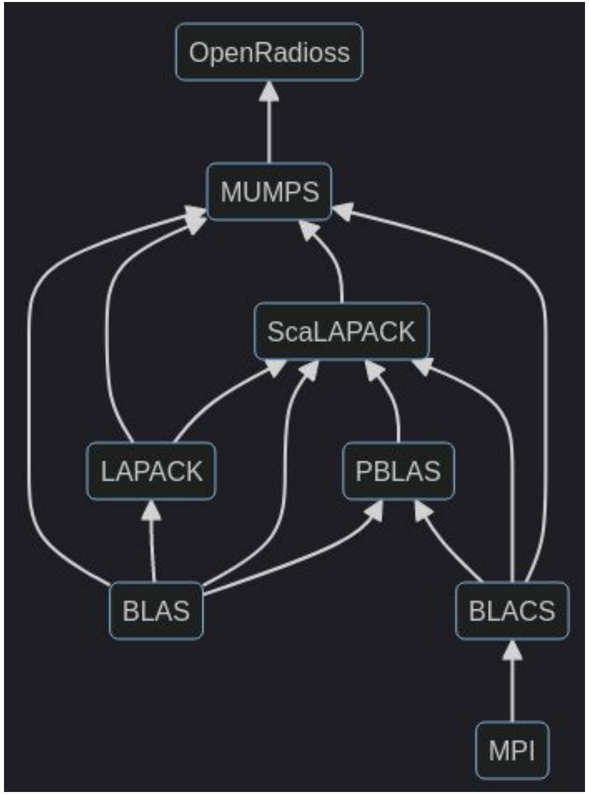
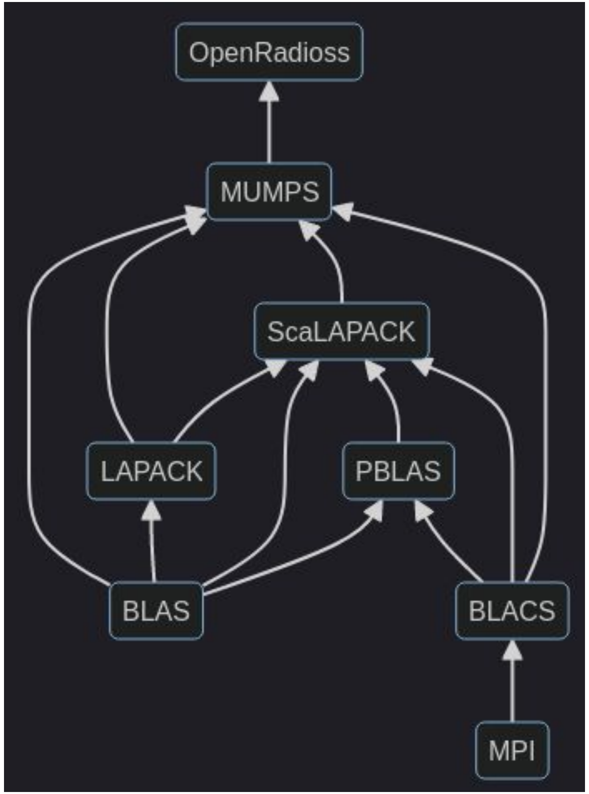
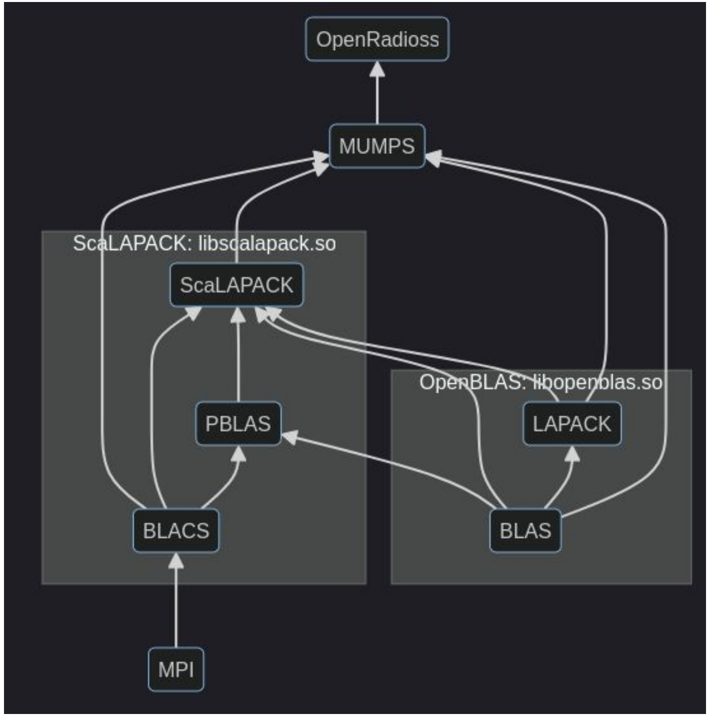


Figure 1: Shared library dependencies of an example application.



Software libraries





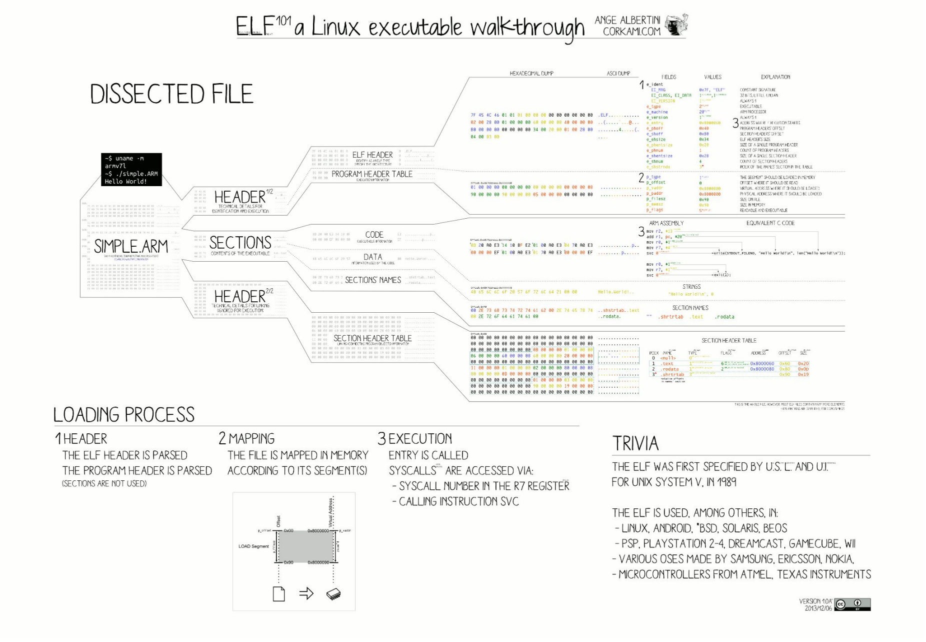
Practical session

Compile and install:

- BLAS: https://gitlab.com/greeklug/lapack/-/tree/greeklug-presentation
- Matrix-Market I/O library: https://gitlab.com/greeklug/matrix_market_exchange_formats

Tools for inspecting libraries and executables

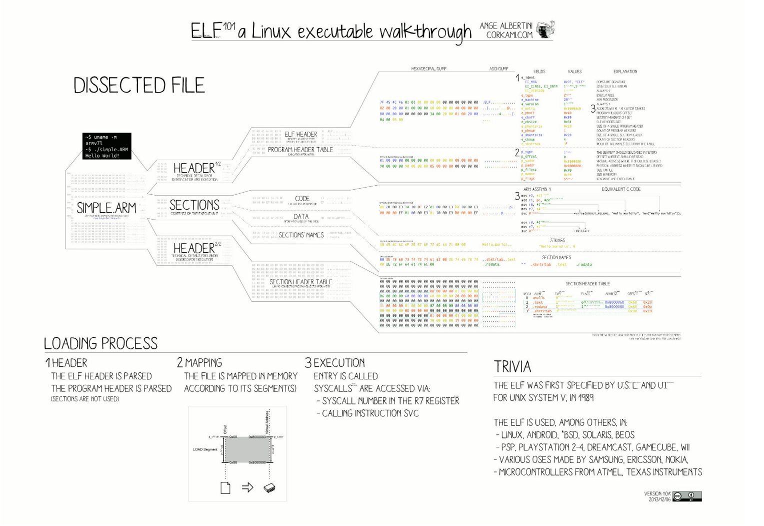
- Does this `libopeblas.so` instance implement the CBLAS interface?



Tools for inspecting libraries and executables

To investigate the shared object:

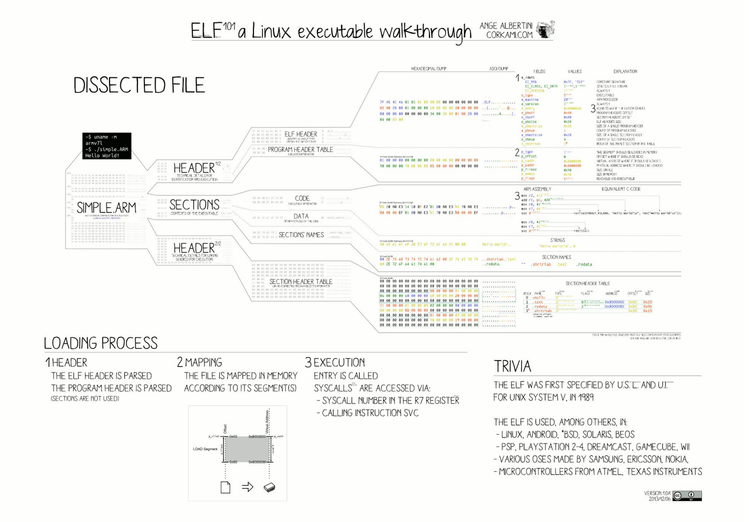
- `readelf`: display information about ELF files
  - `--all`: all sections
  - `--file-header`: information about interoperability
  - `--dynamic`: dynamically linked libraries and other information
- `objdump`: display information about objects
  - `--syms`: information for symbols (functions and variables)
  - `--demangle`: restore human readable names for objects generated from C++
- `nm`: list symbols
  - `--dynamic`: list only export symbols (only for dynamic libraries)



Tools for inspecting libraries and executables

Even extract information about function signatures (needs debug info, `-g`):

- Read debug info with `readelf`
  - `--debug-dump=info`
- Partially disassemble with `objdump`
  - `--disassemble`
  - `--disassemble-all`



Practical session

- Compile the tutorial example code: https://gitlab.com/greeklug/blas-tutorial
- Call some function Matrix Market I/O
- Can you break the linking? Try removing the linker option: `--no-as-needed`

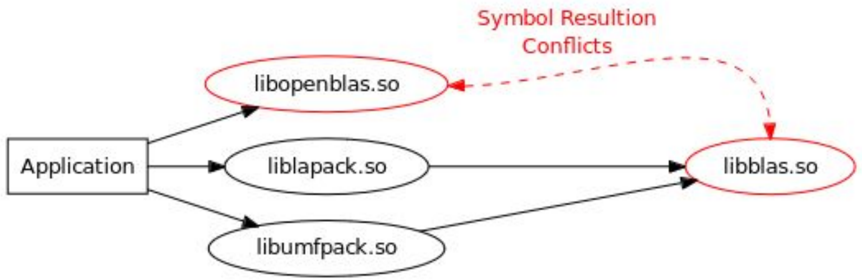


Figure 2: Wrong symbol resolution after relinking the example application.

Data representation

- Computer memory is linear
- Matrices are linearized:

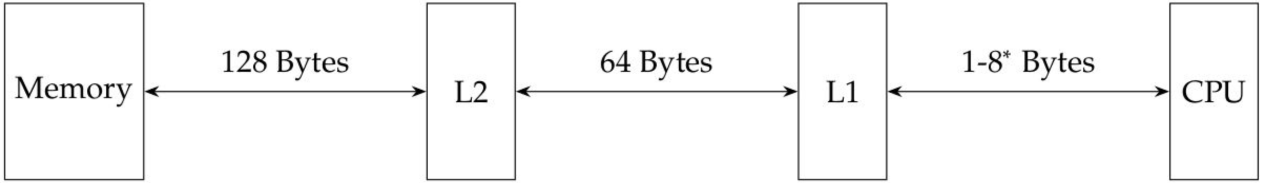
$$\begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix} \longrightarrow \boxed{1}\boxed{2}\boxed{3}\boxed{4}\boxed{5}\boxed{6}$$

```c
typedef struct _dense_matrix {
  /* Data structure storing matrix A */
  double* a; // Pointer to the C array with the entries of A
  int m;     // Number of rows in A
  int n;     // Number of columns in A
} dense_matrix;
```

Caching

- Direct linearization is not sufficient for good performance!
- Caches affect the speed of memory access

```
for ( int i = 0; i < n; ++i ) {

  a[i] = 0;
}
```

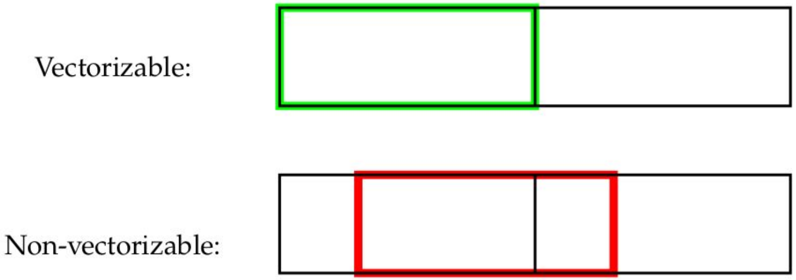


*up to 64 for some special SIMD instructions sets such as AVX-512

Caching

- Direct linearization is not sufficient for good performance!
- Caches affect the speed of memory access

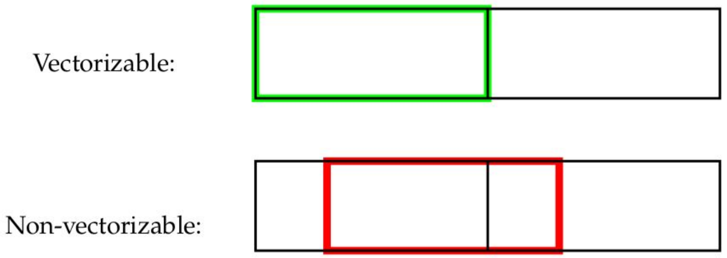
```
for ( int i = 0; i < n; ++i )
{
  a[i] = 0;
}
```



Caching

- Direct linearization is not sufficient for good performance!
- Caches affect the speed of memory access

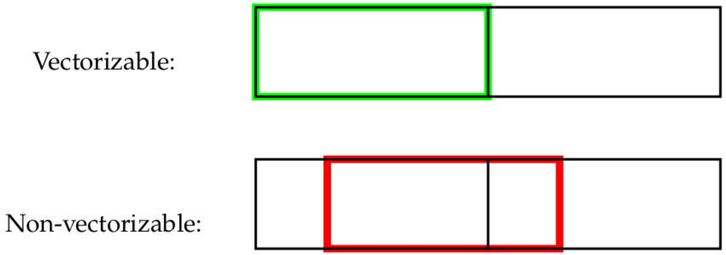
```
#pragma omp simd aligned(a:32)
for ( int i = 0; i < 4*n; i+=1 ) {

  a[i] = 0;
}
```



Caching

- Direct linearization is not sufficient for good performance!
- Caches affect the speed of memory access

```
for ( int i = 0; i < n; i+=1 ) {
  a[4*i] = 0;
  a[4*i+1] = 0;
  a[4*i+2] = 0;
  a[4*i+3] = 0;
}
```



Not all evaluations are the same!

Revisiting the simple matrix-vector product:

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix}. \tag{1}$$

The dot product evaluation jumps across cache lines!

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \end{pmatrix},$$

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 1 \begin{pmatrix} 1 \\ 3 \end{pmatrix} + 2 \begin{pmatrix} 2 \\ 4 \end{pmatrix}.$$

Caching

- Direct linearization is not sufficient for good performance!
- Caches affect the speed of memory access

```c
typedef struct _dense_matrix {
  /* Data structure storing matrix A */
  double* a; // Pointer to the C array with the entries of A
  int m;     // Number of rows in A
  int n;     // Number of columns in A
  int nzmax; // Maximum number of entries that can be stored in array a
  int lda;   // Leading dimension of the array A
} dense_matrix;
```

Practical session

- Call some function (DGEMV) of BLAS
- Try the code with aligned memory allocation!

BLAS naming conventions

- Operations organized by computational complexity
  - Level 1: O(n)
  - Level 2: O(n^2)
  - Level 3: O(n^3)
- BLAS supports various number types and numerical precision (first part of function names):

  - single precision (**S**) with 32-bits,
  - double precision (**D**) with 64-bits,
  - single precision complex (**C**) with 64-bits, and
  - double precision complex (**Z**) with 128-bits.

BLAS naming conventions

- Matrix properties are exploited to save space and reduce memory accesses:

GE:
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & a_{32} & a_{13} & a_{23} & a_{33} \\ \hline \end{array}$$

SY:
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & * & a_{13} & * & * \\ \hline \end{array}$$

TR:
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & * & a_{13} & * & * \\ \hline \end{array}$$

SP:
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & a_{13} \\ \hline \end{array}$$

TP:
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & a_{13} \\ \hline \end{array}$$

BLAS naming conventions

- Matrix properties are exploited to save space and reduce memory accesses.
- This forms the second part of the name:

	Storage type		
Algebraic properties	Standard (-)	Banded (B)	Packed (P)
General (G)	GE	GB	
Symmetric (S)	SY	SB	SP
Hermitian (H)	HE	HB	HP
Triangular (T)	TR	TB	TP

BLAS naming conventions

- Last part is the type of the operants:
  - V: vector
  - M: matrix
- For instance:

DGEMV:

- D: double precision
- GE: general matrix
- MV: matrix-vector multiplication

DGEMM:

- D: double precision
- GE: general matrix
- MM: matrix-matrix multiplication

- The convention does not work always, especially for Level 1 operations
  - DAXPY: $y \leftarrow ax+y$

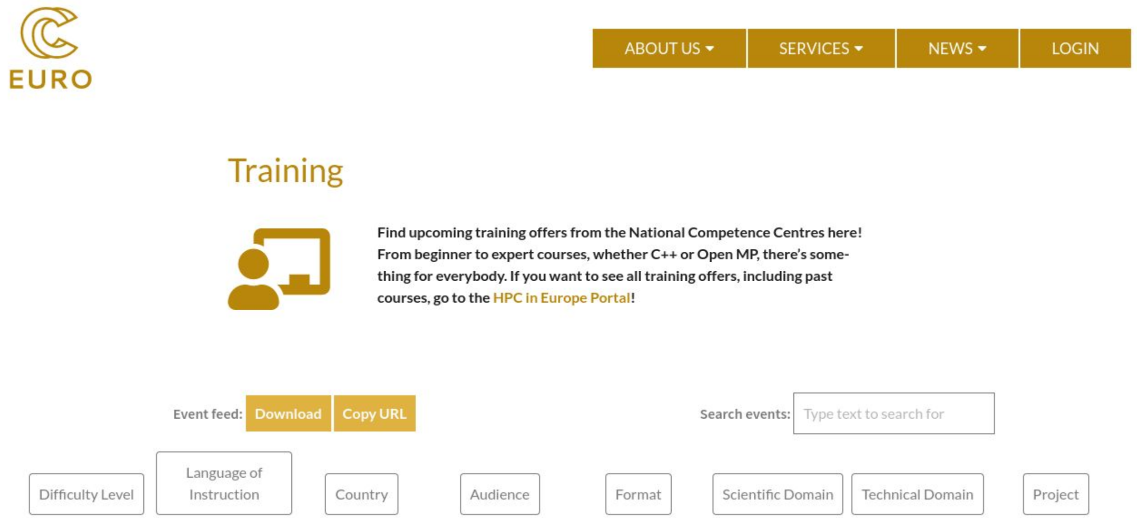
Course notes and resources

Will appear in the tutorial directory: https://gitlab.com/greeklug/blas-tutorial

Official BLAS webpage: https://www.netlib.org/blas/

- Quick reference (function list): https://www.netlib.org/blas/
- Reference BLAS implementation: https://www.netlib.org/lapack/explore-html/d1/df9/group__blas.html

Seminar on numerical methods coming soon in EurroCC:
https://www.eurocc-access.eu/services/training/

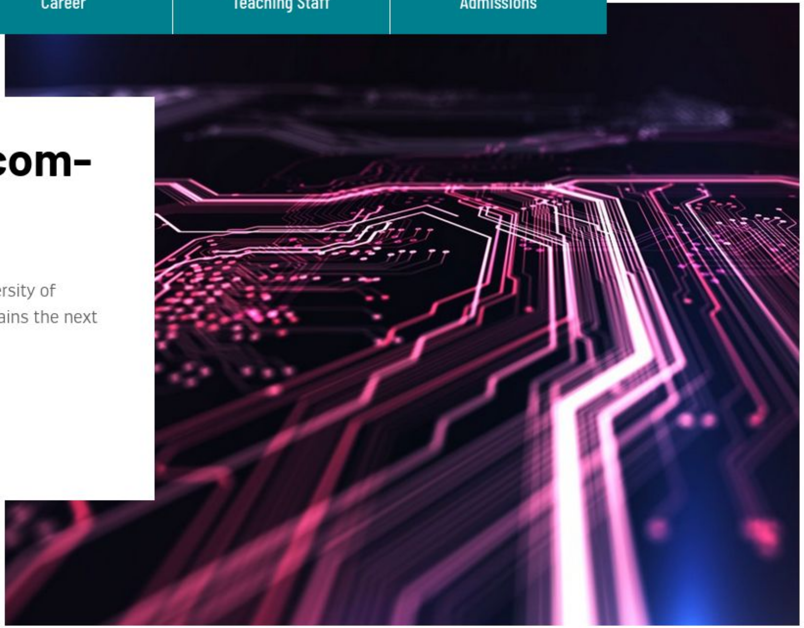


Thank you!

Study Programme

Master in High Performance Computing

Overview | Programme | Career | Teaching Staff | Admissions



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Language: EN

Admissions
EU: 1 Feb-28 Aug 2024
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Fees: €200/sem

Format: Full time

Campus: Belval

Available places: 40

Study Programme

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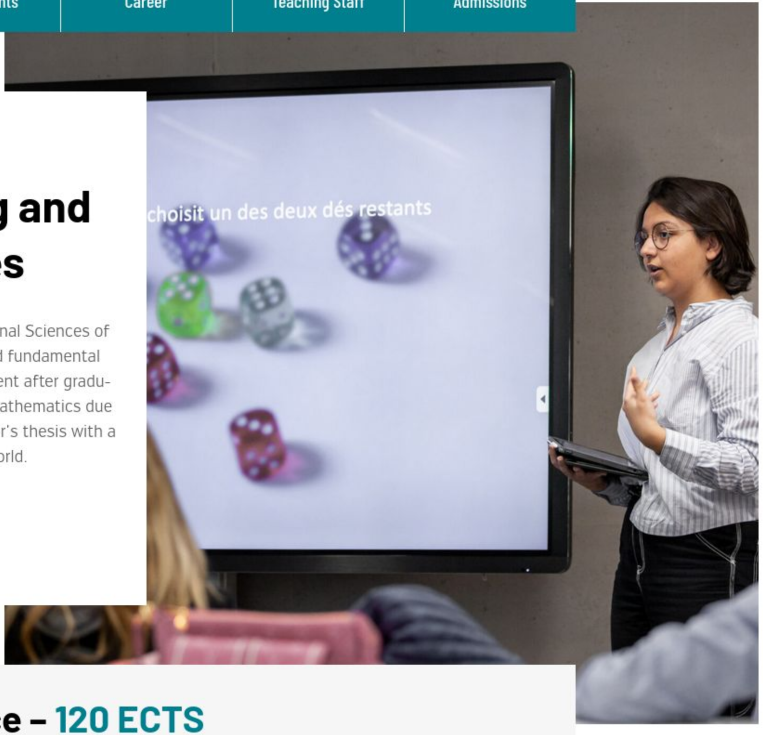
Learn more

Teachers



The Programme at a glance – 120 ECTS

Duration:
2 years / 4 sem

Teaching Languages:
EN

Admissions:
EU: 1 Feb 2023 – 31 Aug 2023
Non-EU: 1 Feb 2023 – 30 Apr 2023

Fees:
200€/ sem. (semester 1)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- European Master For High Performance Computing: https://eumaster4hpc.uni.lu/