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An introduction to numerical methods with BLAS

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Outline

- Setting up a system to compile a BLAS library and link it with executables
- Data representation for vector and matrices
- The interface of BLAS
- Effects of caches and cache aware programming
- Resources for testing and benchmarking

Not all evaluations perform the same!

Consider a simple matrix-vector multiplication:

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

The evaluation can be reduced with either 2 dot product or 2 scalar-matrix product operations:

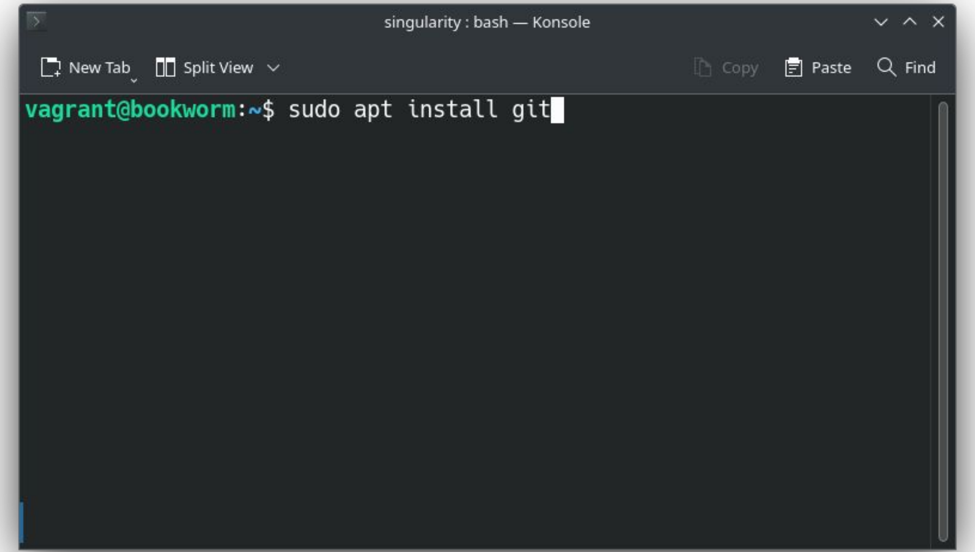
$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \end{pmatrix} \end{pmatrix}, \qquad \begin{pmatrix}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

Are there differences in the efficiency of the 2 evaluation methods?

Setting up your system to compile a BLAS library and link it with executables

Preparing your system to compile BLAS

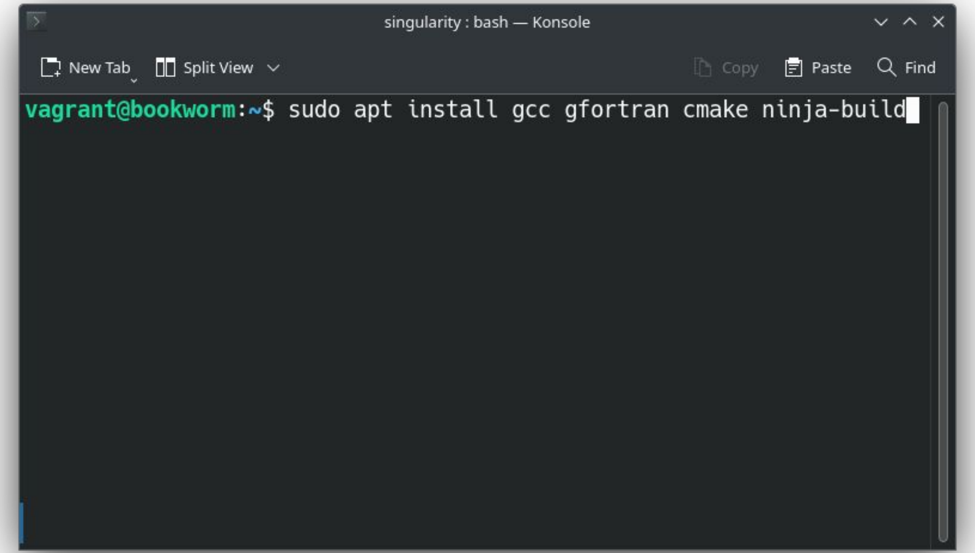
1. Install git



```
vagrant@bookworm:~$ sudo apt install git
```

Preparing your system to compile BLAS

1. Install git
2. Install build tools:
    - gcc
    - gfortran
    - CMake
    - Ninja (optional)



```
vagrant@bookworm:~$ sudo apt install gcc gfortran cmake ninja-build
```

Compiling Netlib BLAS

Fetching the code

- Clone the git repository from the UL HPC GitLab server.

```
$ git clone ssh://git@gitlab.uni.lu:8022/hlst/seminars/blas/lapack.git ~/Documents/blas/lapack
```

- Checkout the branch with the setup for the tutorial

```
$ cd ~/Documents/blas/lapack
$ git checkout blas-devel
```

Compiling Netlib BLAS

Build the BLAS components of Netlib LAPACK

- Configure the build system with the preset options

```
$ cmake --preset default-config
```

- The command will create a directory ‘build’ with the instructions to build the software

```
$ cmake --build build/Release --target all -- -j
$ cmake --build build/Release --target install
```

- The commands will:
  - build BLAS and CBLAS components
  - install the libraries in ‘~/.local/netlib’
- See the ‘CMakePresets.json’ for more information

Compiling the Matrix Market parser library

Build the Matrix Market Exchange Format parser

- Configure the build system with the preset options

```
$ cmake --preset default-config
```

- The command will create a directory ‘build’ with the instructions to build the software

```
$ cmake --build build/Release --target all -- -j
$ cmake --build build/Release --target install
```

- The commands will:
    - build ‘matrixmarket’ library
    - install the library and its headers in ‘~/.local/matrix-market’
- See the ‘CMakePresets.json’ for more information

Linking with Netlib BLAS

Fetch the example code

```
$ git clone ssh://git@gitlab.uni.lu:8022/hlst/seminars/blas/blas-tutorial.git ~/Documents/blas/blas-tutorial
```

- Configure the examples

```
$ cd ~/Documents/blas/blas-tutorial
$ cmake --preset default-config
```

Linking with Netlib BLAS

Build the example code

```
$ cmake --build build/Release --target 00_example_ddot --verbose
```

- The output is extensive, but we can reproduce the result with the following commands:

```
$ mkdir lib bin
$ gcc -I./include -isystem ${HOME}/.local/netlib/include -O3 -DNDEBUG -o src/00_example_ddot.c.o -c
src/00_example_ddot.c
$ gcc -O3 -DNDEBUG -o src/utils.c.o -c src/utils.c
$ ar qc lib/libutils.a  src/utils.c.o && ranlib lib/libutils.a
$ gcc -O3 -DNDEBUG -Wl,--no-as-needed src/00_example_ddot.c.o -o bin/00_example_ddot
-Wl,-rpath,${HOME}/.local/netlib/lib  lib/libutils.a ${HOME}/.local/netlib/lib/libcblas.so
${HOME}/.local/netlib/lib/libblas.so -lm
```

Linking with Netlib BLAS

Let’s break down the compilation commands

```
$ gcc -I./include -isystem ${HOME}/.local/netlib/include -O3 -DNDEBUG -o src/00_example_ddot.c.o -c
src/00_example_ddot.c
```

- Create an object file from ‘src/00_example_ddot.c’
- The file ‘src/00_example_ddot.c’ calls function from:
  - ‘utils/h’: add the location of the header file in the search path with ‘-I’
  - ‘cbals.h’: add the location of the header file in the system search path with ‘-isystem’
- Directories included with ‘-I’ are searched before directories included with ‘-isystem’
- Headers in directories included with ‘-isystem’ must use ‘<...>’ notation

Linking with Netlib BLAS

Let’s break down the compilation commands

```
$ gcc -O3 -DNDEBUG -o src/utils.c.o -c src/utils.c
```

- Creates an object file for the utility library from ‘src/utils.c’

```
$ ar qc lib/libutils.a  src/utils.c.o && ranlib lib/libutils.a
```

- Composes the object file into a static library
  - Effectively an object file with a lookup table to easily locate functions within the library

Linking with Netlib BLAS

Let’s break down the compilation commands

```
$ gcc -O3 -DNDEBUG -Wl,--no-as-needed src/00_example_ddot.c.o -o bin/00_example_ddot
-Wl,-rpath,${HOME}/.local/netlib/lib  lib/libutils.a ${HOME}/.local/netlib/lib/libcblas.so
${HOME}/.local/netlib/lib/libblas.so -lm
```

- The command links the executable ‘bin/00_example_ddot’
  - **-Wl,-rpath:** Adds the location of the BLAS and CBLAS library in the executable RUNPATH
  - **-Wl,--no-as-needed:** ensures that all dependencies are loaded from the correct location
  - **-lm:** links with a mathematical library (libm) used in ‘utilities.c’
- Dynamic libraries ‘libblas.so’ for BLAS and ‘libcblas.so’ and CBLAS will be required in runtime
- Static library ‘libutils.a’ is linked statically and will not be required in runtime

Linking with Netlib BLAS

Run the executable

- Compile the executable with the cmake build scripts:

```
$ cmake --build build/Release --target 00_example_ddot --verbose
```

- After the compilation you will be able to run the resulting executable with:

```
$ ./build/Release/bin/00_example_ddot # print help
$ ./build/Release/bin/00_example_ddot 100 2 # An example run
```

Linking with Netlib BLAS

Practical session

- Try compiling the CBLAS library
- Try compiling the executable ‘00_example_ddot’

Software libraries

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

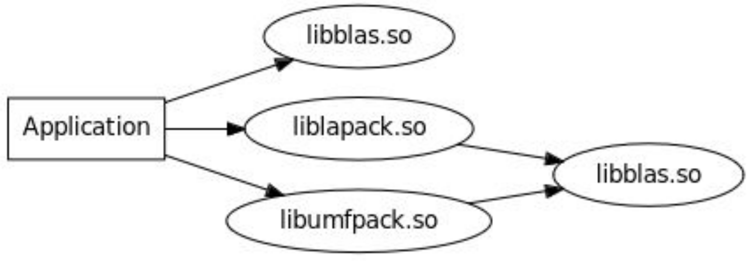
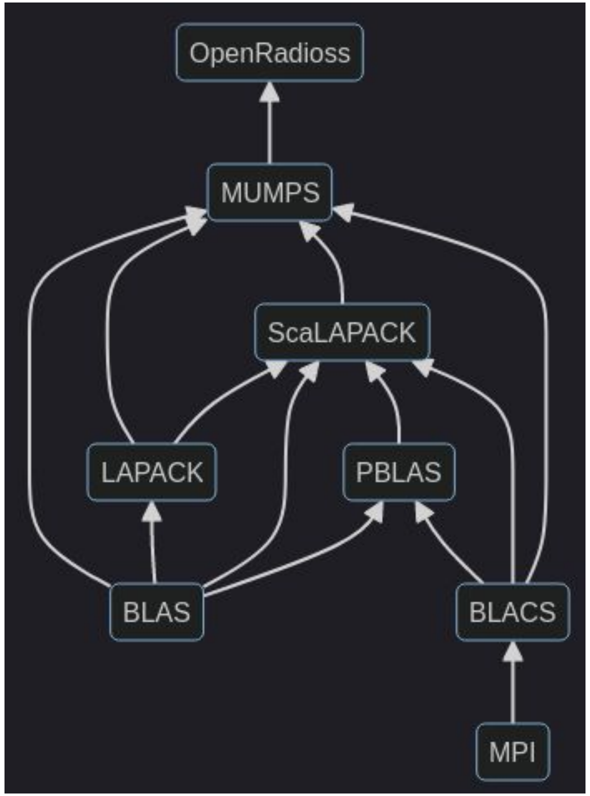
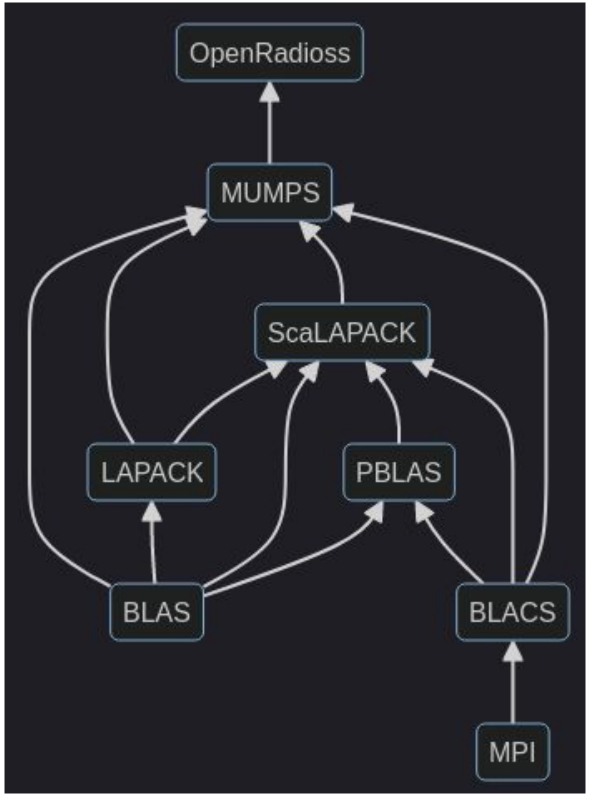
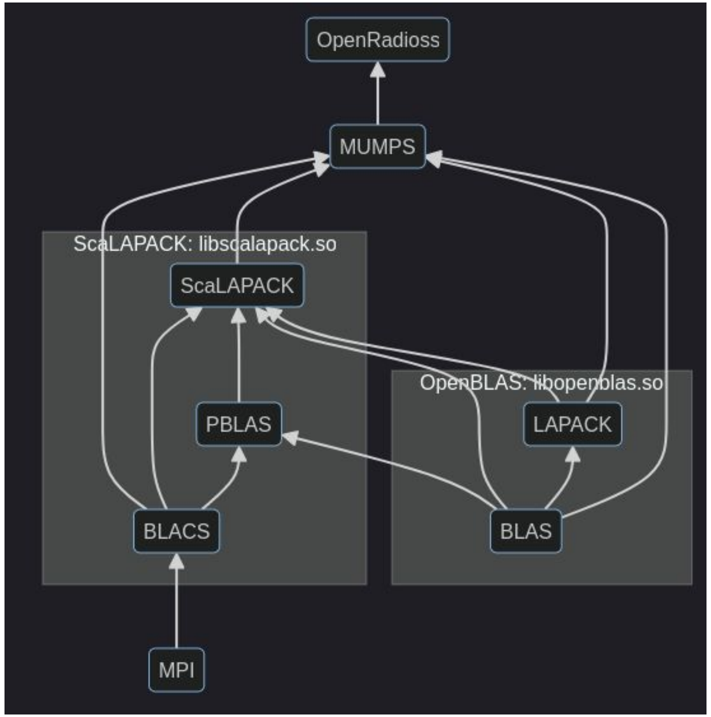


Figure 1: Shared library dependencies of an example application.



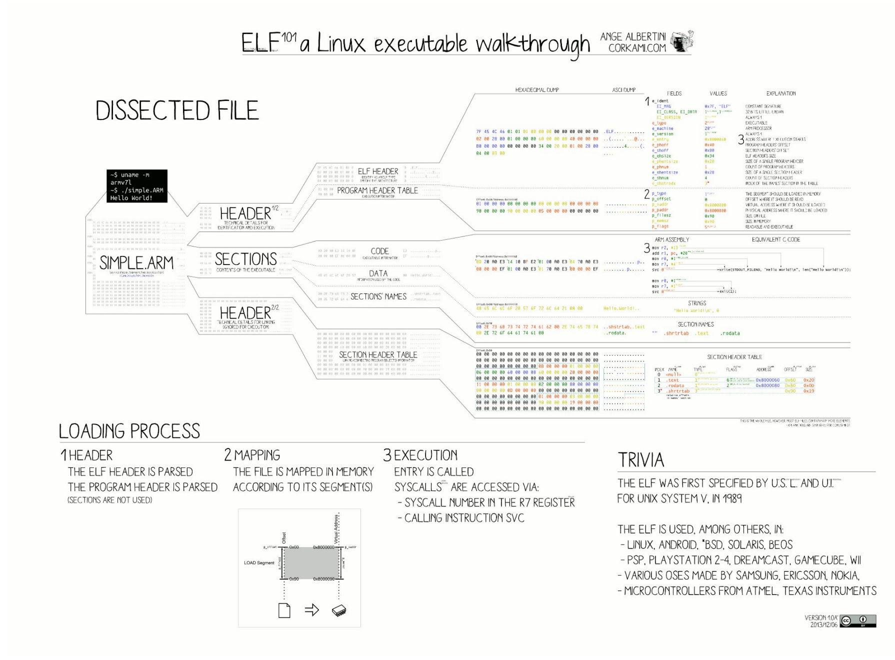
Software libraries





Tools for inspecting libraries and executables

- Does a particular ‘libopenblas.so’ instance implement the CBLAS interface?



```
~$ uname -m
armv7l
~$ ./simple.ARM
Hello World!
```

LOADING PROCESS

1 HEADER
THE ELF HEADER IS PARSED
THE PROGRAM HEADER IS PARSED
(SECTIONS ARE NOT USED)

2 MAPPING
THE FILE IS MAPPED IN MEMORY
ACCORDING TO ITS SEGMENT(S)

3 EXECUTION
ENTRY IS CALLED
SYSCALLS ARE ACCESSED VIA:
- SYSCALL NUMBER IN THE R7 REGISTER
- CALLING INSTRUCTION SVC

TRIVIA

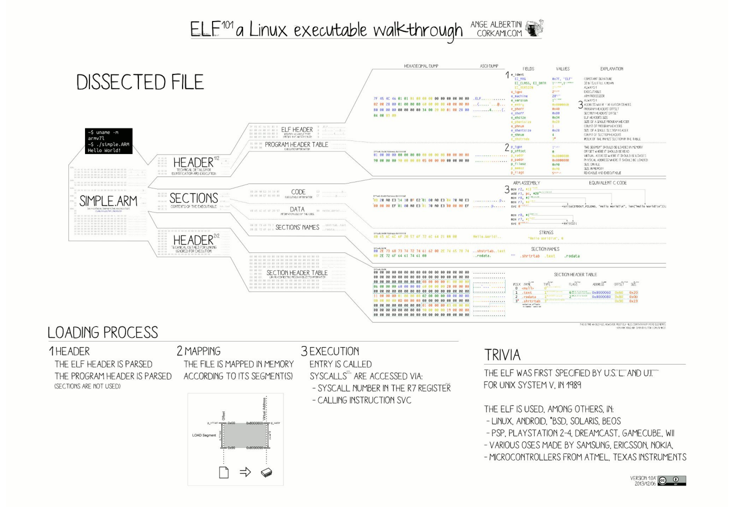
THE ELF WAS FIRST SPECIFIED BY U.S. L. AND U.I. FOR UNIX SYSTEM V, IN 1989

THE ELF IS USED, AMONG OTHERS, IN:
- LINUX, ANDROID, *BSD, SOLARIS, BEOS
- PSP, PLAYSTATION 2-4, DREAMCAST, GAMECUBE, WII
- VARIOUS OSES MADE BY SAMSUNG, ERICSSON, NOKIA,
- MICROCONTROLLERS FROM ATMEL, TEXAS INSTRUMENTS

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)


ELF101 a Linux executable walkthrough
ANGE ALBERTINI
CORKAMI.COM
DISSECTED FILE
SIMPLE.ARM
HEADER
SECTIONS
HEADER
ELF HEADER
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CODE
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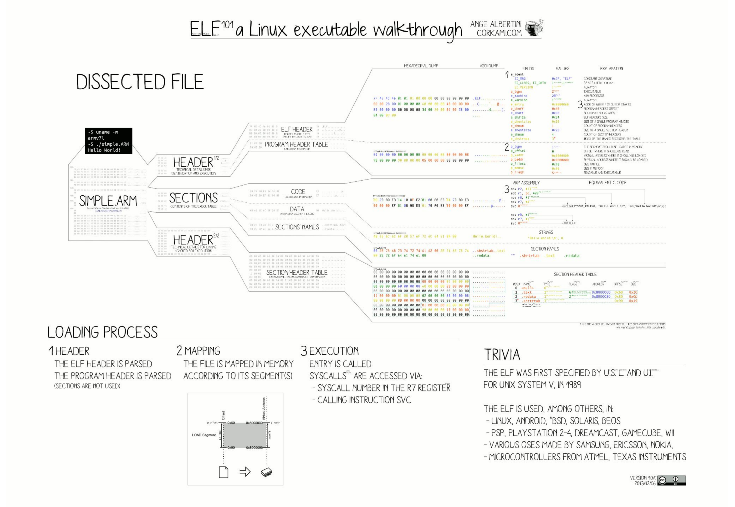
Tools for inspecting libraries and executables

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`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Tools for inspecting libraries and executables

Practical session

- Can you break the linking? Try removing the linker option: `--no-as-needed`

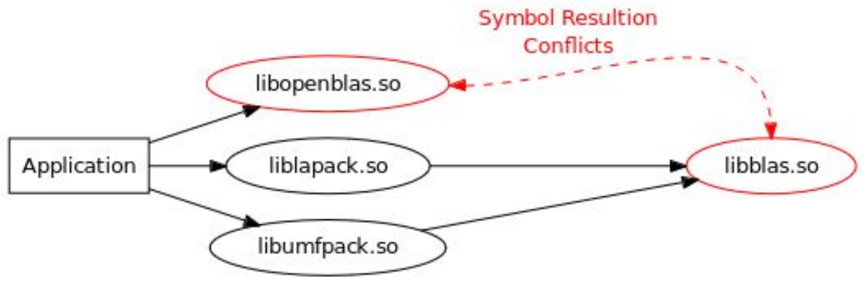


Figure 2: Wrong symbol resolution after relinking the example application.

Data representation for vector and matrices

Data representation

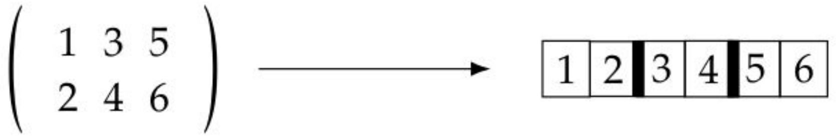
Matrices

- Computer memory is linear
- Matrices must be linearized:

$$\begin{pmatrix}1 & 3 & 5\\ 2 & 4 & 6\end{pmatrix} \longrightarrow \begin{array}{|c|c||c|c||c|c|}\hline 1 & 2 & 3 & 4 & 5 & 6\\ \hline\end{array}$$

Data representation

```
structure matrix(T)
    data : T*
    m : integer
    n : integer
end structure
```



- How useful is this representation?

Data representation

Example: Gaussian elimination algorithm

$$A^{(0)} = \begin{pmatrix} \begin{array}{|ccc} \hline 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 3 \end{array} \end{pmatrix} \sim A^{(1)} = \begin{pmatrix} 1 & 1 & 1 \\ \cline{2-3} 0 & \multicolumn{1}{|c}{1} & 1 \\ 0 & \multicolumn{1}{|c}{1} & 2 \end{pmatrix}$$

$$A^{(0)} \equiv \left(\begin{array}{ccc|ccc|ccc} 1 & 1 & 1 & 1 & 2 & 2 & 1 & 2 & 3 \end{array} \right)$$

$$A^{(1)} \equiv \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 2 \end{array} \right)$$

Data representation

Example: Gaussian elimination algorithm

```
structure matrix(T)
    data : T*
    ld : integer
    m : integer
    n : integer
end structure
```

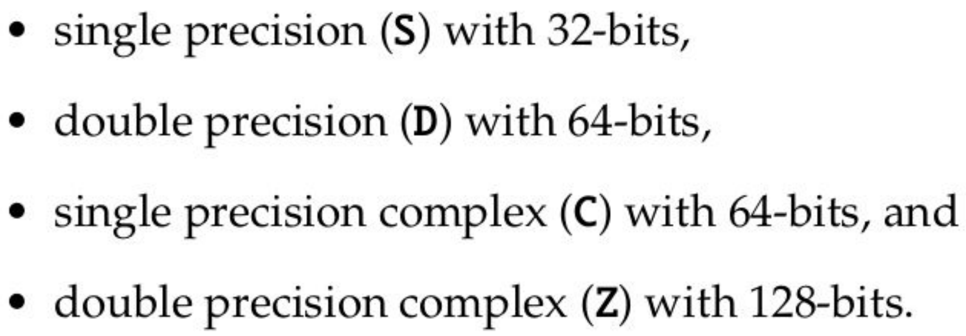
$$A^{(1)} \equiv \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 2 \end{array} \right)$$

$$A^{(1)} = \left(\begin{array}{c|cc} 1 & 1 & 1 \\ \cline{2-3} 0 & 1 & 1 \\ 0 & 1 & 2 \end{array} \right)$$

The interface of BLAS

The BLAS interface

- 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.

The BLAS interface

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

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

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

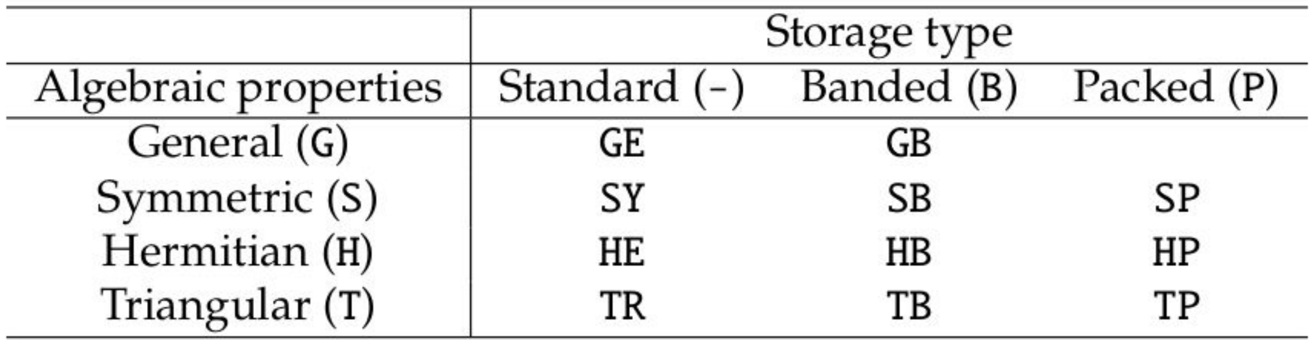
$$\textbf{TR:}\quad \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \longrightarrow \begin{array}{|c|c|c|c|c|c|c|c|c|}\hline a_{11} & a_{21} & a_{31} & a_{12} & a_{22} & * & a_{13} & * & * \\ \hline\end{array}$$

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

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

The BLAS interface

- The type of the matrix representation used forms the 2nd 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

The BLAS interface

- 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   ax+y

Data representation & BLAS interface

Practical session

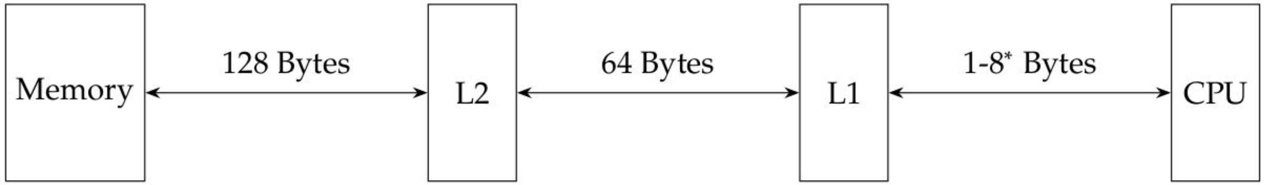
- Try exercises 01-03.
- You will need to find and call the appropriate BLAS functions.

Effects of caches and cache aware programming

Effects of caching

- Direct linearization of matrices can degrade performance!
- Caches affect the speed of memory access

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

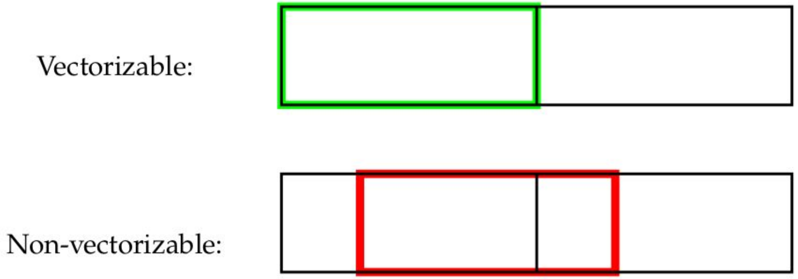


*up to 64 for some special SIMD instructions sets such as AVX-512

Effects of caching

- Direct linearization of matrices can degrade performance!
- Caches affect the speed of memory access

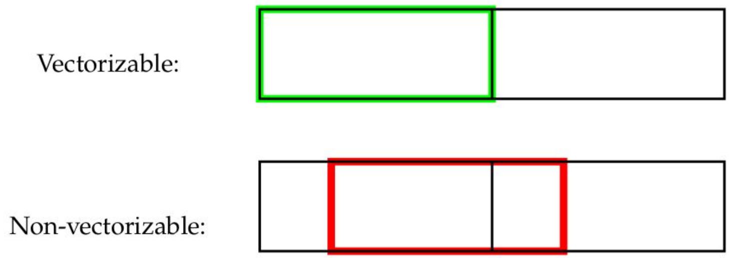
```
for ( int i = 0; i < n; ++i ) {

  a[i] = 0;
}
```



Effects of caching

- Direct linearization of matrices can degrade performance!
- Caches affect the speed of memory access

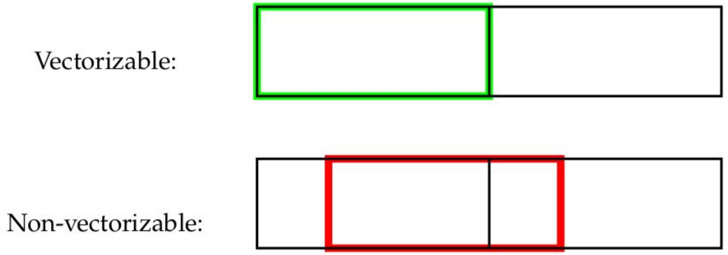
```
#pragma omp simd aligned(a:32)
for ( int i = 0; i < 4*n; i+=1 ) {
  a[i] = 0;
}
```



Effects of caching

- Direct linearization of matrices can degrade 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;
}
```



Effects of caching

Practical session

- Try exercises 04-05
- Demonstration of the use of ‘aligned_alloc’ in ‘src/read_and_execute.c’
- Hint: *for exercise 05 use the function ‘get_ld’ of the utilities library to get the leading dimension of arrays*

Resources for testing and benchmarking

Resources for testing and benchmarking

Resources for BLAS

- 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

Matrix benchmarks

- Matrix market: https://math.nist.gov/MatrixMarket/
- Matrix market exchange format reader: https://gitlab.uni.lu/hlst/seminars/blas/matrix-market-exchange-formats

Thank you!

Any questions?