Mathematical Software Programming (02635)

Lecture 8 — October 30, 2025

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Fall 2025

Announcement

Assignment

- Posted on DTU Learn
- Due on November 19, 2025 (submit report on DTU Learn and code on Autolab)
- Please post your questions on DTU Learn

Learning objectives

- call external (third party) programs and libraries
- design, implement, and document a program that solves a mathematical problem
- debug and **test** mathematical software

This week

Topics

- External libraries and basic linear algebra

Learning objectives

- Call external (third party) programs and libraries

Basic Linear Algebra Subroutines (BLAS)

- building blocks for linear algebra (*de facto* standard)
- started as a FORTRAN library (late 1970s)
- linear algebra *engine* in MATLAB, Python (Numpy, Scipy), R, Mathematica, ...
- high performance when optimized for a specific system
- many vendors: Intel MKL, AMD AOCL, Accelerate, OpenBLAS, ATLAS

BLAS

BLAS level 1 routines (1970s)

- vector operations, e.g.,

$$x^T y, \quad \|x\|_2, \quad x \leftarrow \alpha\, x, \quad y \leftarrow \alpha\, x + y$$

- use $O(n)$ operations for vectors of length n

BLAS level 2 routines (1980s)

- matrix-vector operations, e.g.,

$$y \leftarrow \alpha\, Ax + \beta\, y, \quad A \leftarrow \alpha\, xx^T + A, \quad x \leftarrow T^{-1}x,\ T \text{ triangular}$$

- use $O(mn)$ operations for matrices of size $m \times n$

BLAS

BLAS level 3 routines (1980s)

- matrix-matrix routines, e.g.,

$$C \leftarrow \alpha\, AB + \beta\, C, \quad X \leftarrow T^{-1}X,\ T \text{ triangular}$$

- use $O(n^3)$ operations for matrices of size $n \times n$

What's in a name?

BLAS naming scheme

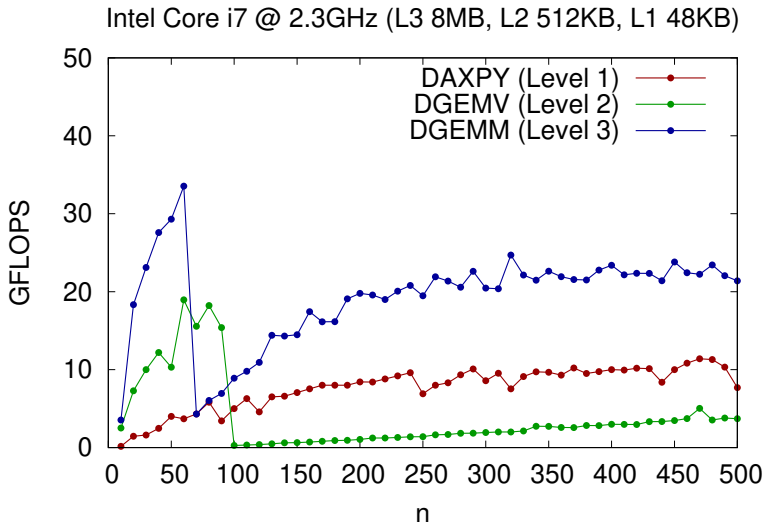
`XYYZZ`

- First character `X` indicates data type (`S`, `D`, `C`, `Z`)
- BLAS level 1: letters `YYZZ` indicate mathematical operation
- BLAS level 2+3: letters `YY` indicate matrix type
- BLAS level 2+3: letters `ZZ` indicate mathematical operation

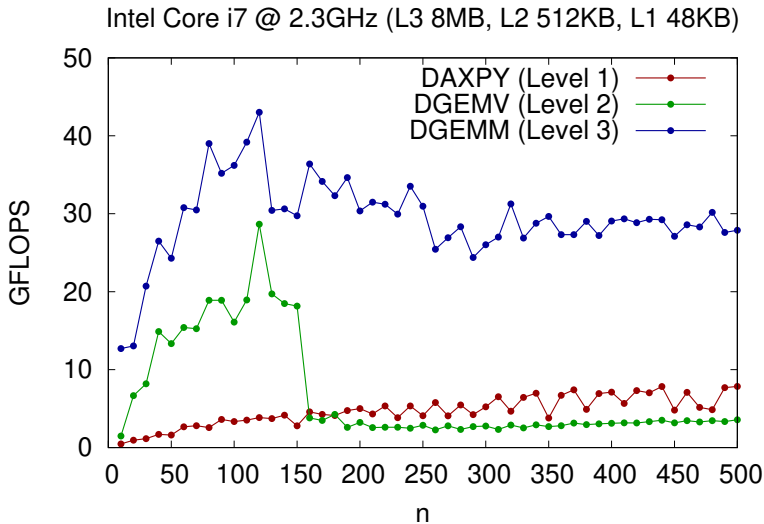
Examples

- `dscal` — *double scale* ($x \leftarrow \alpha x$)
- `saxpy` — *single a x plus y* ($y \leftarrow \alpha x + y$)
- `dgemv` — *double general matrix-vector* ($y \leftarrow \alpha A x + \beta y$)
- `dtrsv` — *double triangular solve vector* ($x \leftarrow T^{-1} x$)
- `ssymm` — *single symmetric matrix-matrix* ($C \leftarrow \alpha S B + \beta C$)

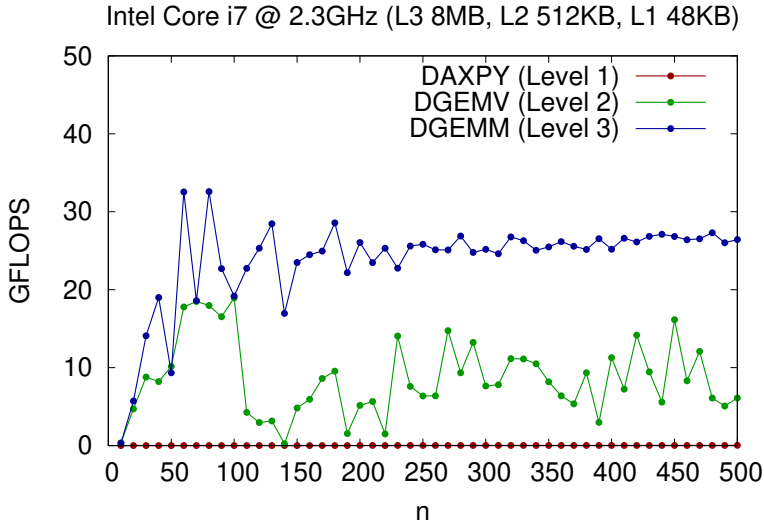
BLAS performance (OpenBLAS)



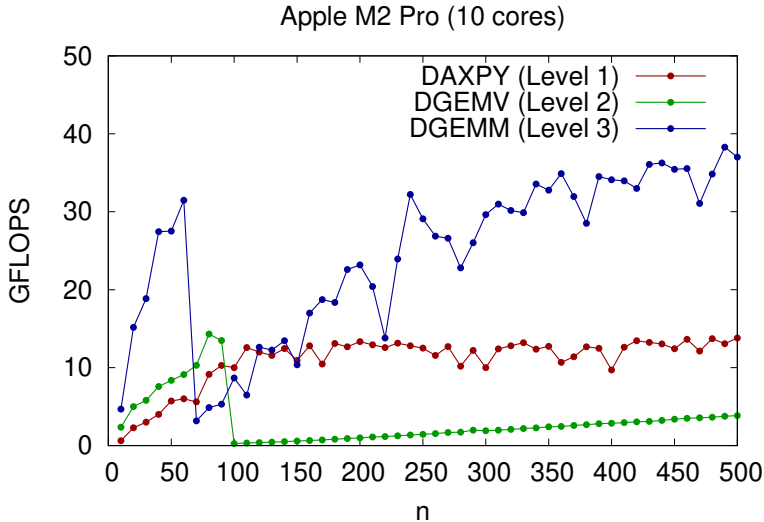
BLAS performance (Accelerate)



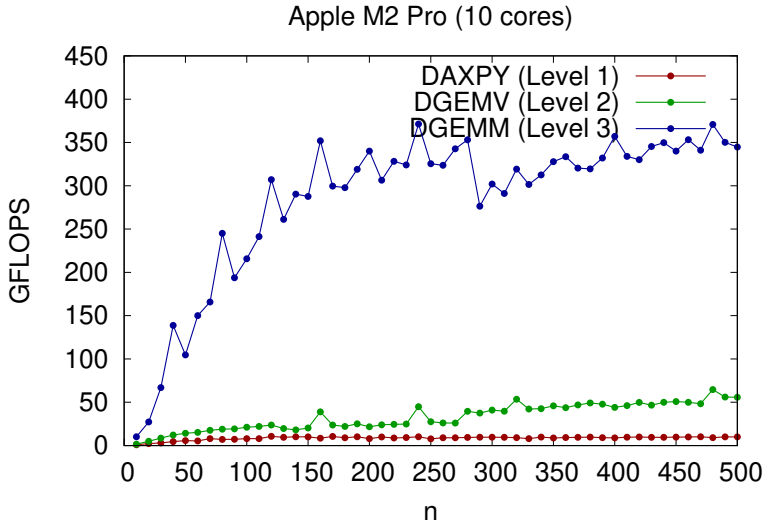
BLAS performance (MKL)



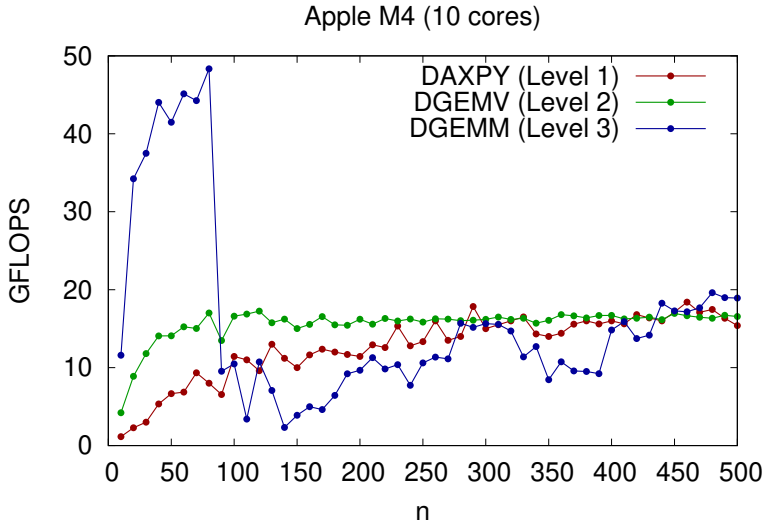
BLAS performance (OpenBLAS)



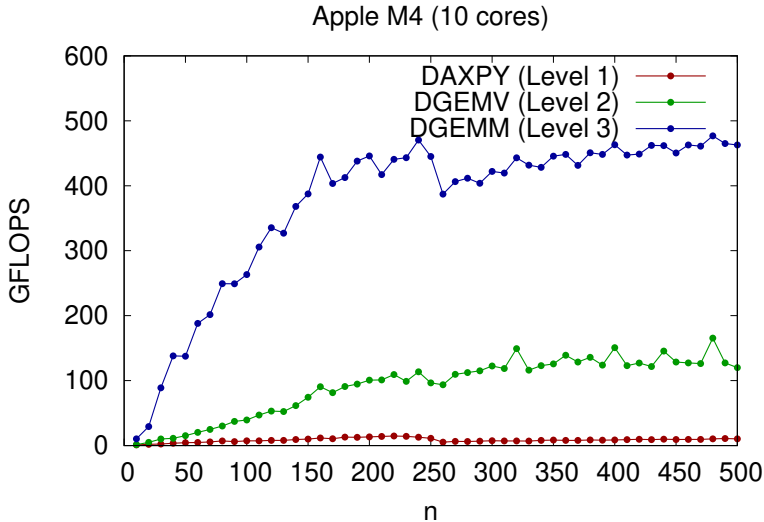
BLAS performance (Accelerate)



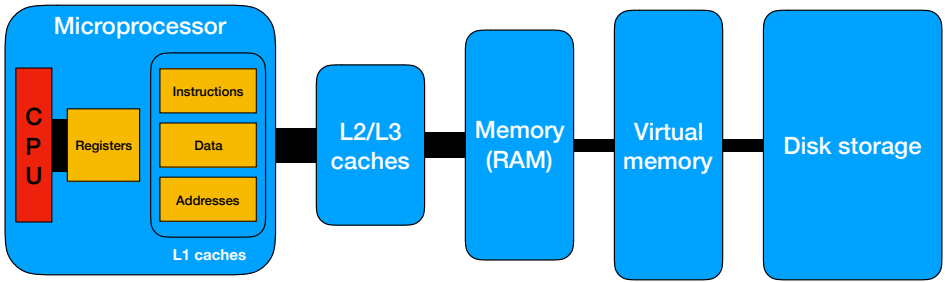
BLAS performance (OpenBLAS)



BLAS performance (Accelerate)



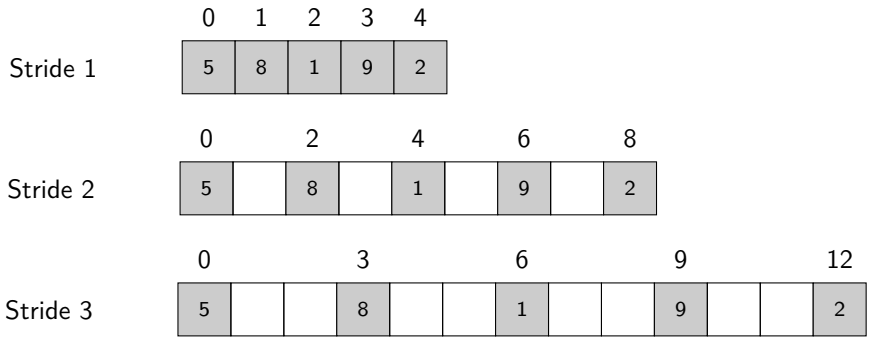
Memory hierarchy



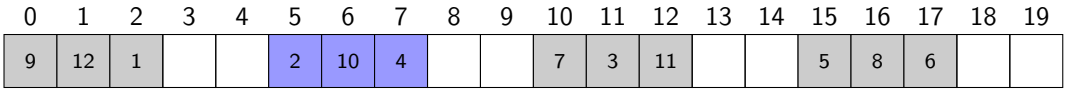
Possible bottlenecks

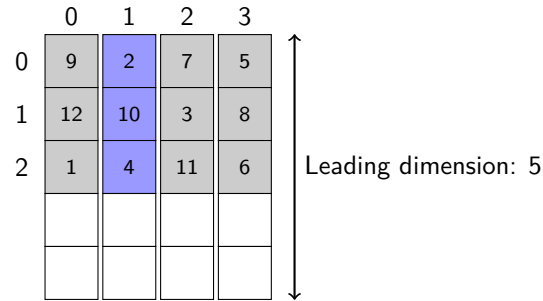
- CPU speed is a bottleneck — *CPU bound*
- cache size/speed is a bottleneck — *cache bound*
- memory size/speed is a bottleneck — *memory bound*
- disk or network speed is a bottleneck — *I/O bound*

BLAS vector storage



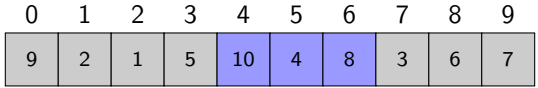
BLAS matrix storage: full

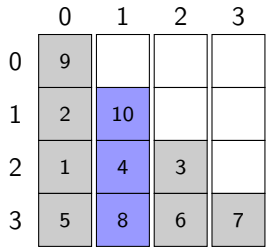




GE (general), SY (symmetric), HE (Hermitian), TR (triangular)

BLAS matrix storage: packed





TP (triangular packed), SP (symmetric packed), HP (Hermitian packed)

BLAS matrix storage: band

$$A = \begin{bmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{22} & a_{23} & & & \\ a_{31} & a_{32} & a_{33} & a_{34} & & \\ & a_{42} & a_{43} & a_{44} & a_{45} & \\ & & a_{53} & a_{54} & a_{55} & a_{56} \end{bmatrix}$$

5×6 matrix with $l = 2$ subdiagonals and $u = 1$ superdiagonal

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
	a_{11}	a_{21}	a_{31}	a_{12}	a_{22}	a_{32}	a_{42}	a_{23}	a_{33}	a_{43}	a_{53}	a_{34}	a_{44}	a_{54}		a_{45}	a_{55}			a_{56}			

	0	1	2	3	4	5
0		a_{12}	a_{23}	a_{34}	a_{45}	a_{56}
1	a_{11}	a_{22}	a_{33}	a_{44}	a_{55}	
2	a_{21}	a_{32}	a_{43}	a_{54}		
3	a_{31}	a_{42}	a_{53}			

BLAS memory model

- vectors and matrices are contiguous arrays
- matrices are stored in column-major ordering
- *stride* refers to distance between *consecutive* elements
- *leading dimension* (LDA) refers to distance between columns

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \end{bmatrix}, \qquad \begin{bmatrix} * & * & * & * & * \\ * & * & A_{23} & A_{24} & A_{25} \\ * & * & A_{33} & A_{34} & A_{35} \\ * & * & * & * & * \end{bmatrix}$$

- ith column of A is a vector of length 4 with stride 1
- ith row of A is a vector of length 5 with stride 4
- $(A_{11}, A_{22}, A_{33}, A_{44})$ is a vector of length 4 with stride 5
- A is a matrix with 4 rows, 5 columns, stride 1, LDA 4
- *slice* (submatrix to the right) has 2 rows, 3 columns, stride 1, LDA 4
- see Stride Visualizer

Example: BLAS level 1

```
void dscal_(                    /* Prototype for BLAS dscal */
   const int * n,               /* length of array      */
   const double * a,            /* scalar a             */
   double * x,                  /* array x              */
   const int * incx             /* array x, stride      */
);

int main(void) {
    int i,incx,n;
    double a, x[5] = {1.0,2.0,3.0,4.0,5.0};
    n = 5; a = 3.0; incx = 1;
    dscal_(&n, &a, x, &incx);   // Scale the vector x by 3.0
    return 0;
}
```

Makefile

Windows

```
LDLIBS=-lopenblas
```

macOS

```
LDLIBS=-lblas
```

DTU Unix system (Gbar)

```
LDFLAGS=-L/usr/lib64/atlas
LDLIBS=-lsatlas
```

```
# Requires: "module load openblas"
CPPFLAGS=-I$(MODULE_OPENBLAS_BASE_DIR)/include
LDFLAGS=-L$(MODULE_OPENBLAS_BASE_DIR)/lib
LDLIBS=-l$(MODULE_OPENBLAS_LIB)
```

Example: CBLAS

```c
#include <stdio.h>
#if defined(__MACH__) && defined(__APPLE__)
#include <Accelerate/Accelerate.h>
#else
#include <cblas.h>
#endif

int main(void) {
   int i,incx,n;
   double a, x[5] = {1.0,2.0,3.0,4.0,5.0};
   n = 5; a = 3.0; incx = 1;
   cblas_dscal(n, a, x, incx); // Scale the vector x by 3.0
   return 0;
}
```

Makefile

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macOS

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LDLIBS=-lcblas
```

DTU Unix system (Gbar)

```
LDFLAGS=-L/usr/lib64/atlas
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```

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LDFLAGS=-L$(MODULE_OPENBLAS_BASE_DIR)/lib
LDLIBS=-l$(MODULE_OPENBLAS_LIB)
```

Linear Algebra Package (LAPACK)

Library of routines for numerical linear algebra (1990s)

- matrix factorizations (LU, Cholesky, QR, SVD, Schur, ...)
- systems of linear equations
- least-squares problems
- eigenvalue and singular value problems
- uses BLAS routines as building blocks

Assignment

Self-contained program for solving a system of equations with LAPACK routine `DGESV`

$$Ax = b, \qquad A \in \mathbb{R}^{n \times n},\ b \in \mathbb{R}^n$$

Today's exercises

1. Run BLAS/CBLAS examples

   Linux and Windows WSL users: install OpenBLAS first

   ```
   $ sudo apt-get install libopenblas-dev
   ```

2. Autolab
   - BLAS level 1 (`dscal`, `daxpy`)
   - BLAS level 2 (`dtrsv`)

Remember: BLAS assumes column-major storage!