

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN



https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose\_23/nqp/

## Sheet 1: Linear Algebra

Released: 04/21/23; Submit until: 05/05/23 (20 Points)

This sheet is about a very small introduction into elementary concepts of C++ and how to use them to implement fast linear algebra operations using Intel's <u>Math Kernel Library (MKL)</u>. In order to work through the problems, checkout the git repository nqp-exercises provided on the lecture's homepage and work with the code templates. While the header file la\_wrapper.h, which contains an interface to some linear algebra methods of the MKL, is complete, in each code template there are files which are erroneous and need to be corrected. In a Jupyter-Hub session, use the provided *Makefile* as well as a proper make.inc to compile the corrected code templates.

**Problem 1** Implementing a matrix class (5 Points)

Checkout the code template blas\_wrapper, which contains an elementary implementation of a wrapper of the widely used linear algebra MKL.

- (1.a) (3P) Correct the code template blas\_wrapper such that you can compile it using make build. As a consistency check, you can use the default implementation of the main-routine and check the output when executing the compiled binary.
- (1.b) (2P) You now have a rudimentary matrix class that implements fast linear algebra operations using Intel's MKL. Use this class and write a main-routine which performs a scaling analysis of the runtime needed to copy matrices with dimension  $m \times m$  for  $m \in \mathbb{N}$  and plot the runtime as a function of m. Extract the exponent  $\alpha$  determining the dominating scaling of the runtime  $t \sim m^{\alpha}$ .

**Problem 2** Implementing fast matrix contractions (10 Points)

For this exercise, checkout the code template gemm\_wrapper, which provides an elementary implementation of the fast xgemm operations. Here, the x denotes the fundamental data type, i.e., single, double, complex single, or complex double. The acronym gemm abbreviates <u>GE</u>neral <u>Matrix-Matrix multiplications</u> and this convention carries over for other provided operations, for instance, <u>GE</u>neral <u>Matrix-V</u>ector multiplications (checkout Intel's developer guide for a rather complete documentation about the blas/lapack interface).

(2.a) (5P) Proceed as in problem (1) and correct the code template. Note how la\_operations.h now also contains a multiplication operations, which is compiled into an object file la\_objects.o that now implements a general matrix-matrix multiplication. Write a test case, which tests the implemented xgemm-functionality and returns success (return code 0) or failure (return code 1) on exit, depending on whether a successful matrix-matrix multiplication has been performed. Why is such a test case useful?

(2.b) **(5P)** Write a trivial version of a matrix-matrix multiplication by implementing the calculations of the elements

$$C_{ij} = \sum_{k} A_{ik} B_{kj} \tag{1}$$

of the result of a matrix-matrix product  $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$ , explicitly. Here, we consider  $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathbb{V}_{\mathbb{R}}^{m \times m}$  for some  $m \in \mathbb{N}$ . Perform a runtime analysis comparing your naive implementation with xgemm calls, investigate the dependency of the runtime on the matrix dimension m and extract the exponent  $\beta$  determining the dominating scaling of the runtime  $t \sim m^{\beta}$ . Interpret you result.

## **Problem 3** Syntactic sugar for matrix contractions (5 Points)

For this exercise, checkout the code template  $expr\_templates$ , which provides an elementary implementation of expression templates to overload the multiplication operator. In problem (2) we introduced an operator overload to the multiplication operator \*, allowing for expression such as C=A\*B in C++. However, that implementation also required an intermediate copy operation, which is necessary because \* is a binary operator and the result of the matrix-matrix multiplication has to get through a temporary return value. This unfortunate fact can be avoided by delayed evaluation, which in C++ can be implemented using *expression templates*.

- (3.a) (3P) Proceed as in problem (1) and (2) and correct the code template. In particular note how the binary matrix-matrix multiplication operator \* is mapped to the unary assignment operator =, which assigns the result of the operation to an instance of LAMatrix without additional copy-operations.
- (3.b) (2P) Perform a runtime analysis and extract the speed-up as a function of the matrixdimension m obtained, using the xgemm-impementations of the \*-operator from problem (2) and (3).