Exercise C4a: Writing a simple library

In this task you are supposed to write a small tools file that contains useful functions. This file can be used through out this course, for your convenience. The input and output of the functions are both defined in the tools.c and tools.h. Complete the functions, then run the test to make sure that you have implemented the functions correctly. The makefiles and project structure is something that you can reuse throughout the course.

Functions that are to be written

- elementwise_addition
- addition_with_constant
- elementwise_multiplication
- multiplication_with_constant
- dot_product
- create_2D_array
- destroy_2D_array
- matrix_multiplcation
- vector_norm
- normalize_vector
- average
- standard_deviation
- distance_between_vectors
- cumulative_integration
- write_xyz
- fft_freq

look in the header file for descriptions of the functions. The fft_freq should have the same output as numpy.fft.fftfreq with 2π .

You can visualize the atoms written to atoms.extxyz with ase, ase gui atoms.extxyz (which might be useful for later). There is also more advanced programs, such as, ovito and vmd.