

# Computational Quantum Physics

## Week 1

### Due on Week 3

#### Exercise 1: **Setup**

- (a) Create a working directory.
- (b) Open emacs and write your first program in FORTRAN
- (c) Submit a test job.
- (d) *(Optional)* Connect to the cluster spiro.fisica.unpd.it via ssh and repeat the execution

#### Exercise 2: **Number precision**

Integer and real numbers have a finite precision. Explore the limits of INTEGER and REAL in Fortran.

- (a) Sum the numbers 2.000.000 and 1 with INTEGER\*2 and INTEGER\*4
- (b) Sum the numbers  $\pi \cdot 10^{32}$  and  $\sqrt{2} \cdot 10^{21}$  in single and double precision.

#### Exercise 3: **Test performance**

Matrix matrix multiplication is many times the bottleneck of linear algebra computations.

- (a) Write explicitly the matrix-matrix multiplication loop in two different orders.
- (b) Use the Fortran intrinsic function.
- (c) Increase the matrix size and use the Fortran Function CPUTIME to monitor the code performance.
- (d) Use the compiler different optimization flags and monitor the performances