Computational Quantum Physics

Week 1

Due on Week 3

DELIVER THE CODE AND SOME PLOTS (PLOTS NOT NECESSARY)

Exercise 1: **Setup**

(a) Create a working directory.

(b) Open emacs and write your first program in FORTRAN puoi scegliere quello che vuoi

(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.

where to get pi from? up to me non-trivial (different ways)

Exercise 3: **Test performance**

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

(a) Write explicitely the matrix-matrix multiplication loop in two different orders. e.g. between rows and cols

(b) Use the Fortran intrinsic function. matmul

(c) Increase the matrix size and use the Fortran Function CPUTIME to monitor the code performance.

you can start from square matrices and then play

(d) Use the compiler different optimization flags and monitor the performances

gfortran at first
then optimization flags