Computational Quantum Physics

Week 2

Due on Week 4

Exercise 1: **Checkpoints**

Write a subroutine to be used as a checkpoint for debugging.

(a) Include a control on a logical variable (DEBUG=.TRUE. or .FALSE.)

(b) Include an additional (optional) string to be printed

(c) Include additional (optional) variables to be printed

Exercise 2: **Documentation**

Rewrite Exercise 3 of Week 1 including:

(a) Documentation.

(b) Comments.

(c) Pre- and post- conditions.

(d) Error handling

(e) Checkpoints

Exercise 3: **Derived Types**

In Fortran90 write a MODULE which contains a double complex matrix derived TYPE that includes the components: Matrix elements, Matrix Dimensions, Matrix Trace, and Matrix Determinant.

(a) Define the correspondent TYPE.

(b) Define a function/subroutine that initializes this new TYPE

(c) Define the functions/subroutines TRACE and ADJOINT

(d) Define the correspondent INTERFACES of the previous points.

(e) Define a subroutine that writes on file the Matrix TYPE in a readable form.

(f) Include everything in a test program.