Assignment 1

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/assignment_1

Quantum Information and Computing AA 2022–23

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Exercise 1: Setup (1)



- First program to test basic features
- Contains module and function to compute square root

```
module first_module
   implicit none

  real*8 var1, var2

  contains
     function mysqrt(x) result(sx)
        real*8 x
        real*8 sx
        sx = sqrt(x)
        end function

end module first_module
```

■ Program output

The square root of 5.0 is 2.2361

Exercise 1: CloudVeneto (2)



- Key-pair and virtual machine created on CloudVeneto
- Private key copied onto gateway machine

 scp /path/to/private/key [username]@gate.cloudveneto.it:~
- SSHed into gateway machine, then VM
 ssh [username]@gate.cloudveneto.it
 ssh -i /path/to/private/key ubuntu@[VM_IP_address]
- Installed gfortran
- git cloned my repository
- All code compiled and executed

Exercise 2: Number precision



- Program to test limits of integers and real numbers
- Part (a)
 - Add 2.000.000 and 1 using INTEGER*2 and INTEGER*4
 - Since INTEGER*2 only has range of $\approx 10^4$, storing 2.000.000 causes overflow

```
The sum of -31616 and 1 using INTEGER*2 is -31615 The sum of 2000000 and 1 using INTEGER*4 is 2000001
```

■ Part (b)

- Sum $\pi \cdot 10^{32}$ and $\sqrt{2} \cdot 10^{21}$ with single and double precision
- Since single has 8 digits of precision, summing has no effect

The sum of 3.14159278E+32 and 1.41421360E+21 using REAL*4 is 3.14159278E+32
The sum of 3.1415926535897933E+32 and 1.4142135623730950E+21 using REAL*8 is 3.1415926536039354E+32

Exercise 3: Performance testing (1)



- Program to implement matrix multiplication and time it
- Matrices multiplied using three for loops, resulting in $\mathcal{O}(n^3)$ time complexity

```
do i = 1, n_1

do j = 1, n_2

do k = 1, n_3

matrix3(i, j) = matrix3(i, j) + matrix1(i, k) * matrix2(k, j)

end do

end do

end do
```

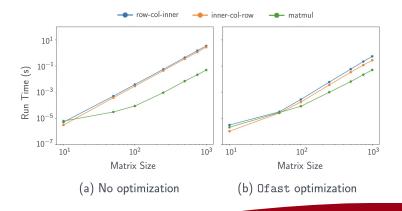
- Two different loop orders used, row-col-inner and inner-col-row
- Methods timed against builtin matmul method, for example

```
Elapsed time for matmul = 2.1500000000E-04
Max abs error for row-col-inner = 3.1974423109E-14
Elapsed time for row-col-inner = 8.037000000E-03
Max abs error for inner-col-row = 3.1974423109E-14
Elapsed time for inner-col-row = 6.2030000000E-03
```

Exercise 3: Performance testing (2)



- Different optimizations were used: 01-03, 0s, and 0fast
- Ofast reduced performance gap between matmul and custom methods the most, $\sim \mathcal{O}(n^{2.8})_{\text{custom}}$ to $\sim \mathcal{O}(n^{2.2})_{\text{matmul}}$



Exercise 3: Performance testing (3)



Performance of other optimization methods (run on 10-core M1 Pro 32 GB)

