## Assignment 1

# Quantum Information and Computing AA 2022–23

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1 November 2022



## Exercise 1: Setup



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

```
module first_module
    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: Cloud Veneto



- 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 (see Slide 7)
- 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



- 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_4
        do k = 1, n_2
            matrix3(i, j) = matrix3(i, j) + matrix1(i, k) * matrix2(k, j)
        end do
    end do
end do
```

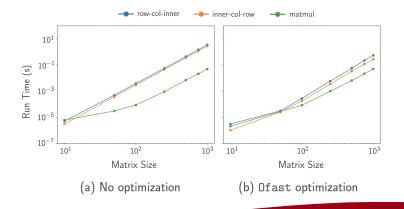
- Two different loop orders used, row-col-inner and inner-col-row
- Methods timed against builtin matmul method, for example

```
Elapsed time for row-col-inner = 1.800000000E-05
Elapsed time for inner-col-row = 1.00000000E-05
Elapsed time for matmul = 3.52000000E-04
```

### Exercise 3: Performance testing (cont'd)



- 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  $\sim \mathcal{O}(n^{2.2})_{\text{matmul}}$



#### Code



Code on GitHub with instructions to install, compile, and run https://github.com/jchryssanthacopoulos/quantum\_information

| P  | main -   | quantum_information / assignment_1 /   |  | Go to file Add f      | lie *        |
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|  |  | Assignment 1   |  |                       |              |
|  | The assignment instructions are contained in .Assignment1.pdf .  |  |  |                       |              |
|  |  | Installation   |  |                       |              |
|  | To compile the Fortran programs, make sure you have afortran installed. The programs were compiled using version 11.2.0. |  |  | 11.2.0.               |              |
| Python is also required. The required version is inpython-version . If you have pyenv installed, it'll point to to create a virtual environment and install the requirements, run: |  |  |  | ion automatically. To |              |
|  |  | gython -m vemv env<br>source env/bin/activate<br>pip install -r requirements.txt |  |                       |              |
|  |  | Compilation  |  |                       |              |
|  |  | To compile the programs, run:  |  |                       |              |