Assignment 1

Quantum Information and Computing

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di Padova

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 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 test performance
- Matrices multiplied using three `for` loops, resulting in $O(n^3)$ time complexity

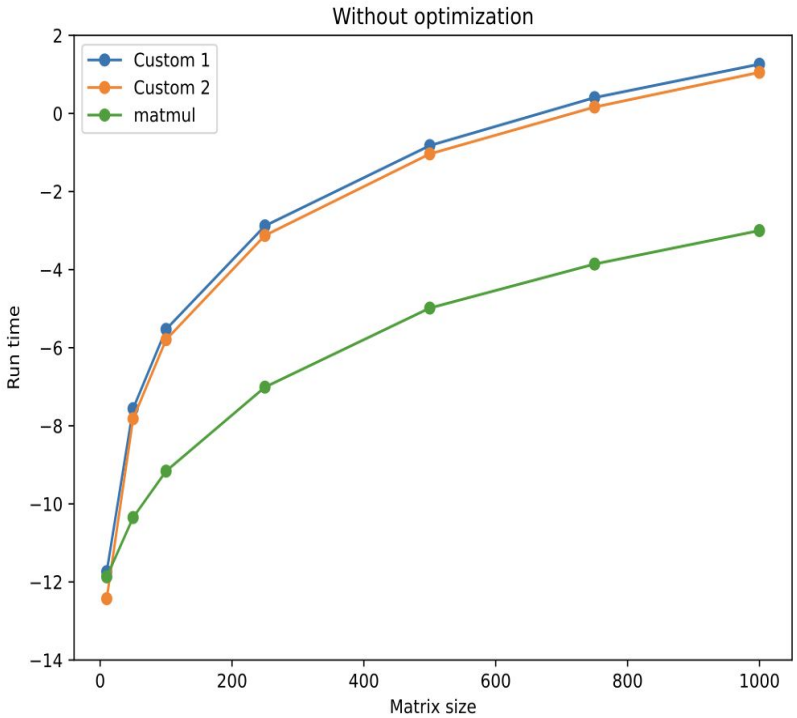
```
do i = 1, n_1
    do j = 1, n_4
        do k = 1, n_2
            matrix3(i, j) = matrix3(i, j) + matrix1(i, k) * matrix2(k, j)
        end do
    end do
end do
```

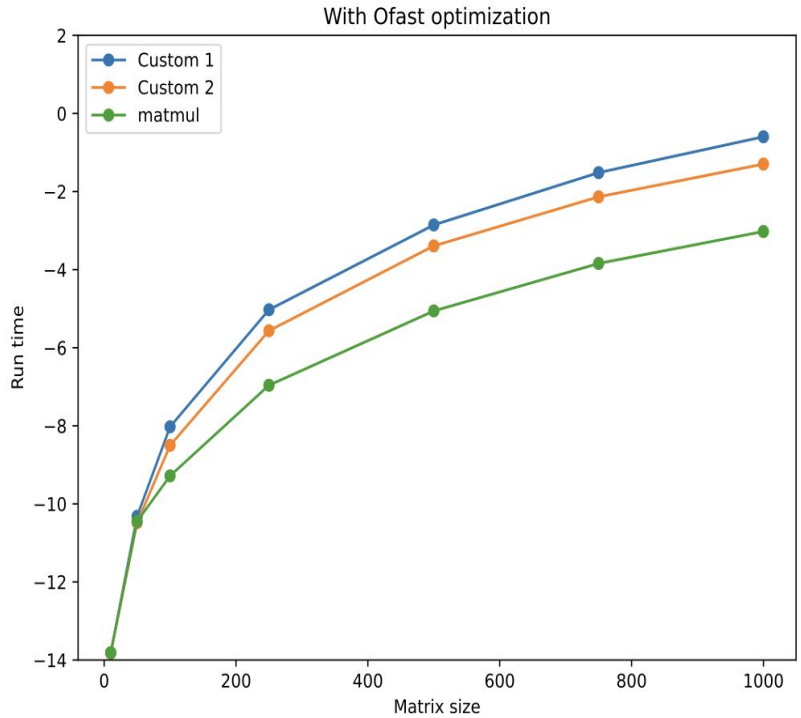
- Two different loop orders used, *ijk* and *kji*
- Methods timed against builtin `matmul` method, for example

```
Elapsed time for custom method 1 = 0.000020000
Elapsed time for custom method 2 = 0.000011000
Elapsed time for intrinsic method = 0.000026000
```

Exercise 3: Performance testing (cont'd)

- Different optimizations were used: `O1`–`O3`, `Os`, and `Ofast`
- `Ofast` reduced the performance gap between `matmul` and custom methods the most

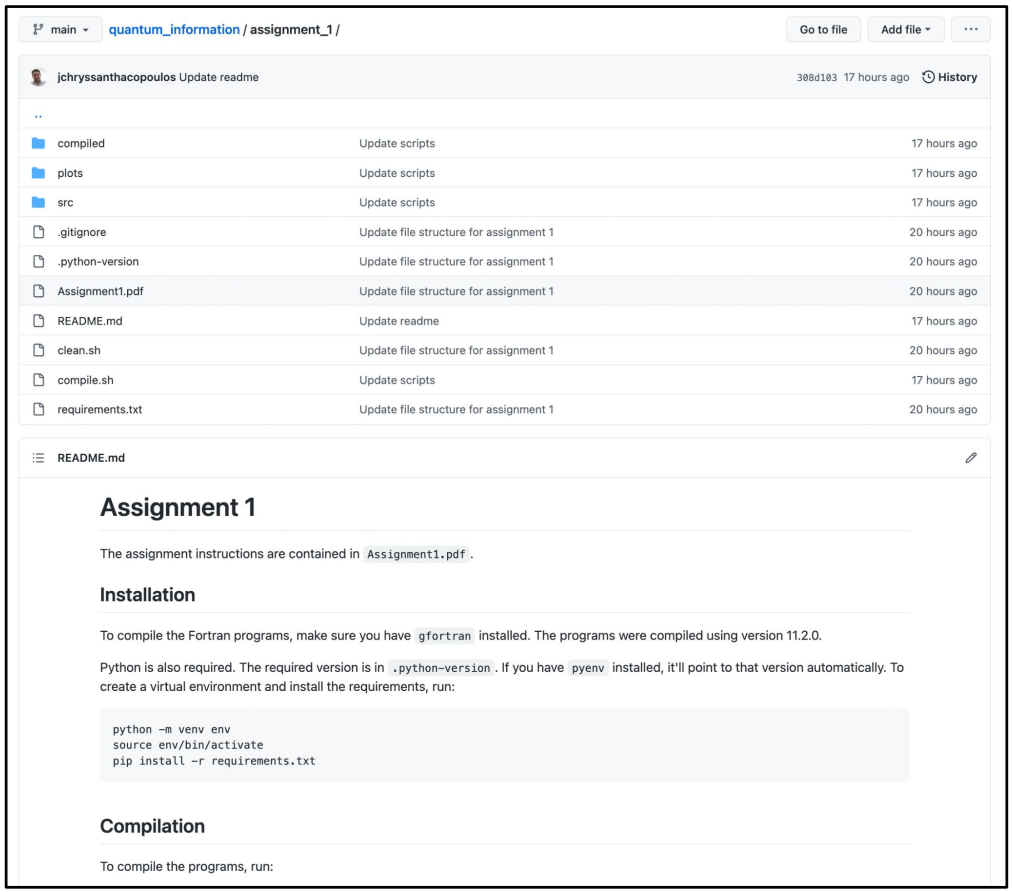




Code

Code on GitHub with instructions to install, compile, and run

`https://github.com/jchryssanthacopoulos/quantum_information`



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README.md

Assignment 1

The assignment instructions are contained in `Assignment1.pdf`.

Installation

To compile the Fortran programs, make sure you have `gfortran` installed. The programs were compiled using version 11.2.0.

Python is also required. The required version is in `.python-version`. If you have `pyenv` installed, it'll point to that version automatically. To create a virtual environment and install the requirements, run:

```
python -m venv env
source env/bin/activate
pip install -r requirements.txt
```

Compilation

To compile the programs, run: