Assignment 1

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

Quantum Information and Computing
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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
- Random `real*8` matrices multiplied using three `for` loops, resulting in $\mathcal{O}(n^3)$ time complexity

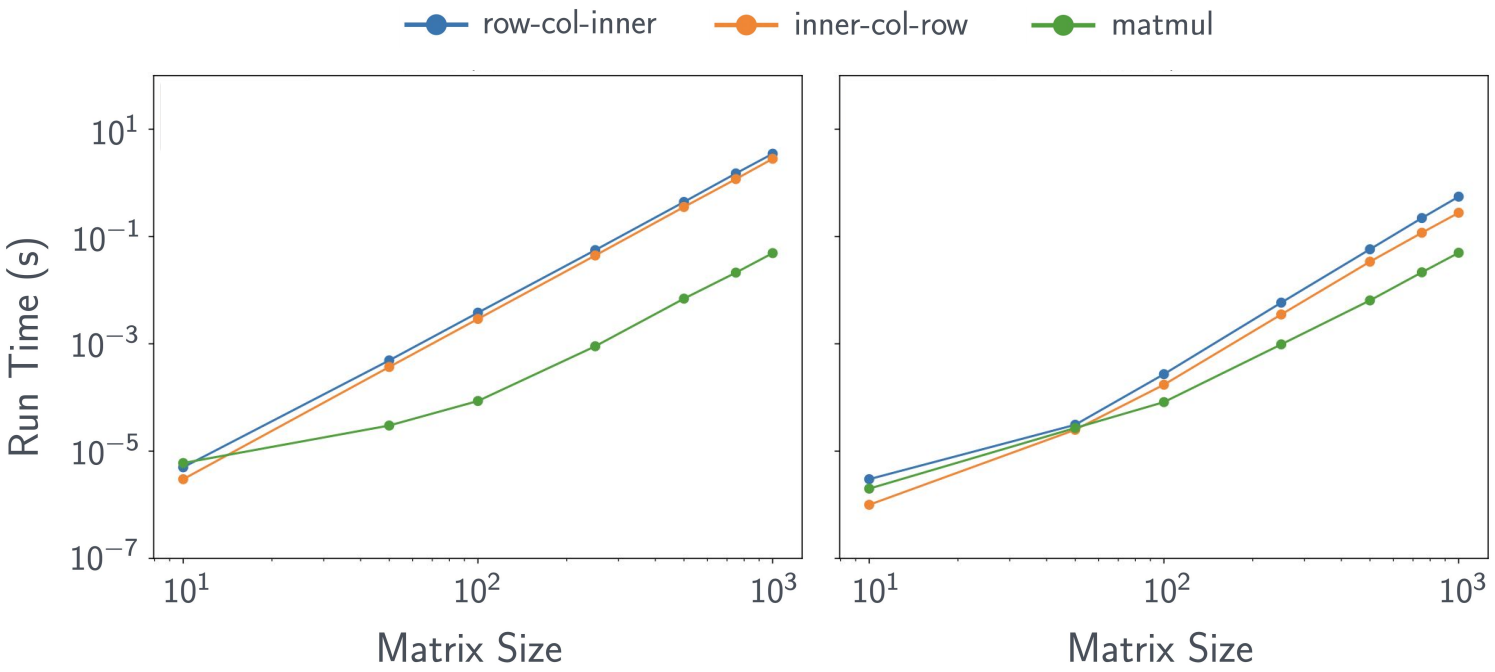
```
do i = 1, n_1
    do j = 1, n_2
        do k = 1, n_3
            matrix3(i, j) = matrix3(i, j) + matrix1(i, k) * matrix2(k, j)
        end do
    end do
end do
```

- 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 = 8.0370000000E-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)

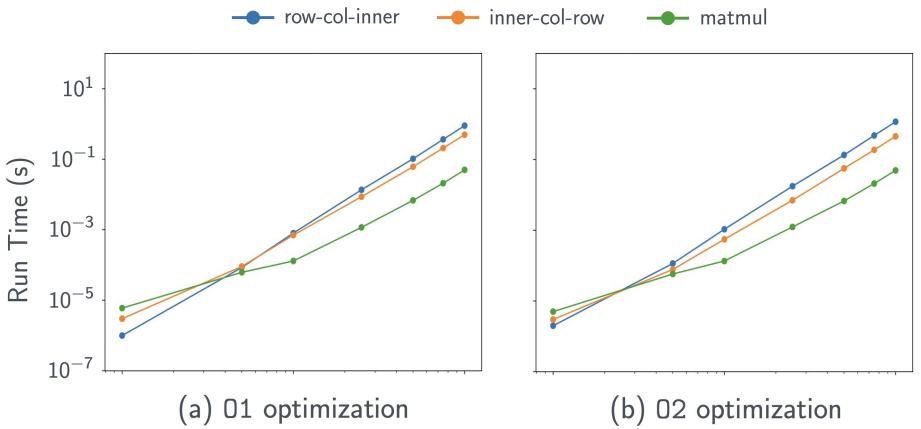
- Different optimizations were used: `O1`–`O3`, `Os`, and `Ofast`
- `Ofast` reduced performance gap between `matmul` and custom methods the most, $\sim \mathcal{O}(n^{2.8})_{\text{custom}}$ to $\sim \mathcal{O}(n^{2.2})_{\text{matmul}}$



(a) No optimization (b) `Ofast` optimization

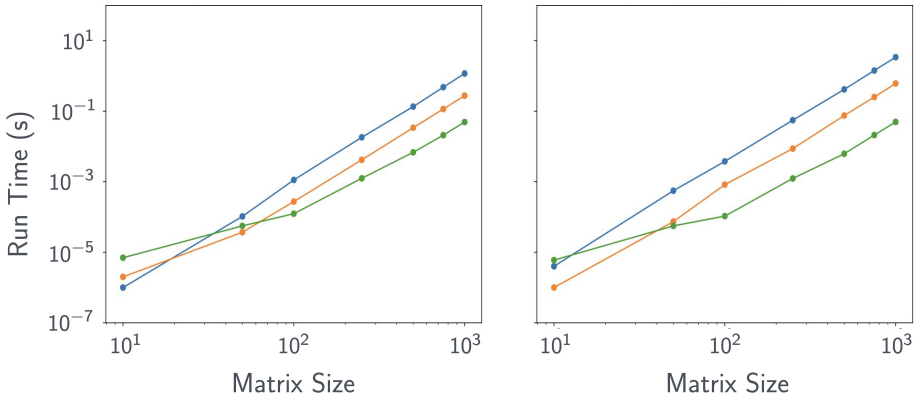
Exercise 3: Performance testing (3)

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



(a) O1 optimization

(b) O2 optimization



(c) O3 optimization

(d) Os optimization