

<https://github.com/UCR-HPC/cs211-hw2-solving-large-linear-system-private-MoonlyTower>

vate-MoonlyTower

Rui Liu

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## Q1

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 13 & 18 \\ 7 & 54 & 78 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 40 & 57 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

M is the lower triangular,

$$M = \begin{pmatrix} 0 & 0 & 0 \\ 4 & 0 & 0 \\ 7 & 8 & 0 \end{pmatrix} \quad L = M + I = \begin{pmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 7 & 8 & 1 \end{pmatrix}$$

U is the upper triangular,

$$U = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 5 & 6 \\ 0 & 0 & 9 \end{pmatrix}$$

so that,  $A = LU$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 7 & 8 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 5 & 6 \\ 0 & 0 & 9 \end{pmatrix}$$

## Q2

### step1:log into the hpc-001

```
scp -r /Users/ruiliu/Downloads/lapack-3.12.0 ssh -J rui001@bolt.cs.ucr.edu  
rui001@hpc-001  
scp -r /Users/ruiliu/Downloads/lapack-3.12.0 rui001@hpc-001.cs.ucr.edu  
/home/rui001/CS211-hw/l_BaseKit_p_2024.2.1.100.sh  
ssh -J rui001@bolt.cs.ucr.edu rui001@hpc-001
```

### step2:download the MKL library form the Intel on hpc-001

The following tools have been installed successfully:

Intel® oneAPI Math Kernel Library

Installation location: /home/rui001/intel/oneapi

Intel® oneAPI Math Kernel Library | 2024.2.2

```
[rui001@cluster-001-login-node ~]$ source /home/rui001/intel/oneapi/setvars.sh
```

```
:: initializing oneAPI environment ...
-bash: BASH_VERSION = 4.4.20(1)-release
args: Using "$@" for setvars.sh arguments:
:: compiler -- latest
:: mkl -- latest
:: tbb -- latest
:: oneAPI environment initialized ::
```

### step3:code /compiler and test on file main2.

I give the detailed comments process when using file main2 to debugging and verify the correctness of the code.

资源管理器

问题 输出 调试控制台 端口 终端

RUI001 [SSH: HPC-001.CS...

> .vscode-server

✓ CS211-hw

> hw1

> hw2

> extern

◆ .gitignore

≡ .nfs00000000... U

≡ func\_call.c

≡ include.h

≡ lapack.c

≡ main

≡ main.c

≡ main2 U

≡ main2.c U

≡ makefile

≡ my\_block.c

≡ my.c M

≡ mylu U

≡ pad.txt

≡ starter.py

> lapack-3.12.0

\$ l\_BaseKit\_p\_2024.2....

\$ l\_onemkl\_p\_2024.2....

> lapack-3.12.0.tar

≡ test\_mkl

≡ test\_mkl.c

大纲

时间线

Matrix A after LU factorization:

-0.865367 0.324562 -0.571642 -0.402492 0.546081 -0.143504 0.536445 0.567530 0.988226 -0.115777

-0.522515 1.071072 0.034204 -1.042182 -0.692322 -0.592811 -0.407617 0.442498 1.298387 -0.600616

-0.777394 -0.478120 -1.070278 -1.644396 0.366007 -0.703901 -0.255174 0.936692 1.094184 -0.275433

-0.040643 -0.030346 0.793164 2.070068 -0.181983 0.376359 -0.212329 -1.629902 -1.104095 0.368456

-0.853179 0.875634 0.371728 0.133576 1.788122 0.000349 0.724988 -0.683310 0.123207 0.972633

-0.168867 0.637587 0.068753 -0.042380 -0.012966 1.218015 0.072017 -0.919788 -1.632044 -0.048442

-0.156482 0.620882 -0.733388 -0.151293 0.662255 -0.091264 -1.205219 -0.373143 -0.167320 -0.605230

-0.129645 -0.798361 0.377964 -0.058655 -0.804866 -0.665317 0.554355 -2.110945 -0.884717 0.688650

0.895295 0.513499 -0.196381 -0.148092 0.034006 -0.415157 0.185580 0.370581 -2.675141 -0.580604

-0.204266 -0.661267 0.589822 -0.280163 -0.662701 0.031582 0.472380 0.339359 -0.361098 -0.495711

Pivot indices:

7 9 5 0 8 1 3 2 6 4

tempB[0] after pivoting: -0.949390

tempB[1] after pivoting: -0.378045

tempB[2] after pivoting: 0.330522

tempB[3] after pivoting: 0.348874

tempB[4] after pivoting: -0.101949

tempB[5] after pivoting: 0.916656

tempB[6] after pivoting: 0.777232

tempB[7] after pivoting: 0.784441

tempB[8] after pivoting: -0.366271

tempB[9] after pivoting: -0.485835

B[0] before forward substitution (after pivoting): -0.949390

B[1] before forward substitution (after pivoting): -0.378045

B[2] before forward substitution (after pivoting): 0.330522

B[3] before forward substitution (after pivoting): 0.348874

B[4] before forward substitution (after pivoting): -0.101949

B[5] before forward substitution (after pivoting): 0.916656

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B[0] after forward substitution: -0.949390

<div> <div>RUI001 [SSH: HPC-001.CS...</div> <div> <div> <div>&gt; .vscode-server</div> <div> <div>CS211-hw</div> <div> <div>&gt; hw1</div> <div> <div>hw2</div> <div> <div>&gt; extern</div> <div> <div>.gitignore</div> <div> <div>≡ .nfs00000000... 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```
• [rui001@cluster-001-login-node hw2]$ gcc main2.c -o main2 -lm
• [rui001@cluster-001-login-node hw2]$ ./main2
```

```
Matrix A:
6.000000 3.000000 1.000000
1.000000 3.000000 4.000000
3.000000 7.000000 5.000000
Vector B:
2.000000 10.000000 5.000000
Initial Matrix A:
6.000000 3.000000 1.000000
1.000000 3.000000 4.000000
3.000000 7.000000 5.000000
Initial Vector B:
2.000000 10.000000 5.000000
```

```
Step 0: Current max = 6.000000 at row 0
Row 1 after division: 0.166667 3.000000 4.000000
Row 2 after division: 0.500000 7.000000 5.000000
Matrix A after step 0:
6.000000 3.000000 1.000000
0.166667 2.500000 3.833333
0.500000 5.500000 4.500000
```

```
Step 1: Current max = 2.500000 at row 1
Swapping rows 1 and 2
Row 2 after division: 0.166667 0.454545 3.833333
Matrix A after step 1:
6.000000 3.000000 1.000000
0.500000 5.500000 4.500000
0.166667 0.454545 1.787879
```

```
Matrix A after LU factorization:
6.000000 3.000000 1.000000
0.500000 5.500000 4.500000
0.166667 0.454545 1.787879
Pivot indices:
0 2 1
```

```
tempB[0] after pivoting: 2.000000
tempB[1] after pivoting: 5.000000
tempB[2] after pivoting: 10.000000
B[0] before forward substitution (after pivoting): 2.000000
B[1] before forward substitution (after pivoting): 5.000000
B[2] before forward substitution (after pivoting): 10.000000
B[0] after forward substitution: 2.000000
B[i]: 4.000000
A[i * n + j]: 0.500000
B[1] after forward substitution: 4.000000
B[i]: 9.666667
A[i * n + j]: 0.166667
B[i]: 7.848485
A[i * n + j]: 0.454545
B[2] after forward substitution: 7.848485
Vector B after forward substitution:
2.000000 4.000000 7.848485
```

```
B[i]: 7.848485
A[i * n + i]: 1.787879
#####B[2] after backward substitution: 4.389831
B[i]: 4.000000
A[i * n + i]: 5.500000
#####B[1] after backward substitution: -2.864407
B[i]: 2.000000
A[i * n + i]: 6.000000
#####B[0] after backward substitution: 1.033898
Vector B after backward substitution (Solution X):
1.033898 -2.864407 4.389831
```

```
Solution X:
1.033898 -2.864407 4.389831
```

#### step4:code /compiler and test on file main.

##### complier:

```
cd /path/to/your/project
```

```
CURDIR=$(pwd)
```

```
export CURDIR
```

```
LD_LIBRARY_PATH=$CURDIR/extern:/act/opt/intel/composer_xe_2013.3.1/mkl/lib/intel64:$LD_LIBRARY_PATH
```

```
export LD_LIBRARY_PATH
```

```
make
```

#### I have shown the final experiment outcome as above.

##### ./main function num

```
[rui001@cluster-001-login-node hw2]$ ./main my 1000
n=1000, pad=1
time=0.146002s
[rui001@cluster-001-login-node hw2]$ ./main my 2000
n=2000, pad=1
time=1.642781s
[rui001@cluster-001-login-node hw2]$ ./main my 3000
n=3000, pad=1
time=6.559644s
[rui001@cluster-001-login-node hw2]$ ./main my 4000
n=4000, pad=1
time=15.823135s
[rui001@cluster-001-login-node hw2]$ ./main my 5000
n=5000, pad=1
time=30.574100s

[rui001@cluster-001-login-node hw2]$ ./main lapack 100
n=100, pad=1
time=0.040017s
[rui001@cluster-001-login-node hw2]$ ./main lapack 1000
n=1000, pad=1
time=0.073281s
[rui001@cluster-001-login-node hw2]$ ./main lapack 1000
n=1000, pad=1
time=0.074497s
[rui001@cluster-001-login-node hw2]$ ./main lapack 2000
n=2000, pad=1
time=0.239922s
[rui001@cluster-001-login-node hw2]$ ./main lapack 3000
n=3000, pad=1
time=0.707063s
[rui001@cluster-001-login-node hw2]$ ./main lapack 4000
n=4000, pad=1
time=1.424908s
[rui001@cluster-001-login-node hw2]$ ./main lapack 5000
n=5000, pad=1
time=2.850201s
[rui001@cluster-001-login-node hw2]$ █
```

##### srtn main function num

- [rui001@cluster-001-login-node hw2]\$ export LD\_LIBRARY\_PATH=/home/act-software/opt/intel/cor  
b/intel64:/home/rui001/CS211-hw/hw2/extern:\$LD\_LIBRARY\_PATH
- [rui001@cluster-001-login-node hw2]\$ srun main my 1000  
n=1000, pad=1  
time=0.133002s
- [rui001@cluster-001-login-node hw2]\$ srun main my 2000  
n=2000, pad=1  
time=1.292453s
- [rui001@cluster-001-login-node hw2]\$ srun main my 3000  
n=3000, pad=1  
time=5.619809s
- [rui001@cluster-001-login-node hw2]\$ srun main my 4000  
n=4000, pad=1  
time=14.073875s
- [rui001@cluster-001-login-node hw2]\$ srun main my 5000  
n=5000, pad=1  
time=28.704089s
- [rui001@cluster-001-login-node hw2]\$ srun main lapack 1000  
n=1000, pad=1  
time=0.039766s
- [rui001@cluster-001-login-node hw2]\$ srun main lapack 2000  
n=2000, pad=1  
time=0.203340s
- [rui001@cluster-001-login-node hw2]\$ srun main lapack 3000  
n=3000, pad=1  
time=0.640516s
- [rui001@cluster-001-login-node hw2]\$ srun main lapack 4000  
n=4000, pad=1  
time=1.304958s
- [rui001@cluster-001-login-node hw2]\$ srun main lapack 5000  
n=5000, pad=1  
time=2.614344s

Compare the outcome of my function and the lapack:

We firstly calculate the Number of Floating-Point Operations (FLOPs).  
For an LU decomposition of an  $n \times n$  matrix, the number of operations can be approximated by  $\frac{n^3+6n^2-4n}{3}$ .

So Gflops=  $\frac{n^3+6n^2-4n}{3} / \text{time(seconds)} * 10^9$ .

### Matrix Size 1000

FLOPs=3.35332\*10<sup>8</sup>

my function:Time: 0.133002s

Gflops=3.35332\*10<sup>8</sup> / 0.133002×10<sup>9</sup>≈2.5212 Gflops

LAPACK:Time: 0.039766s

Gflops=3.35332\*10<sup>8</sup> / 0.039766×10<sup>9</sup>≈8.43051 Gflops

### Matrix Size 2000

FLOPs=2.674664\*10<sup>9</sup>

my function:Time: 1.242953s

Gflops=2.674664\*10<sup>9</sup> / 1.242953×10<sup>9</sup>≈2.151826 Gflops

LAPACK:Time: 0.203340s

Gflops=2.674664\*10<sup>9</sup> / 0.203340×10<sup>9</sup>=13.153654 Gflops

### Matrix Size 3000

FLOPs=9.017996\*10<sup>9</sup>

my function:Time: 5.619809s

Gflops= $9.017996 \times 10^9 / 5.619809 \times 10^{-9} \approx 1.60468$ Gflops

LAPACK:Time: 0.640516s

Gflops= $9.017996 \times 10^9 / 0.640516 \times 10^{-9} \approx 14.0793$  Gflops

### Matrix Size 4000

FLOPs= $2.1365328 \times 10^{10}$

my function:Time: 17.044483s

Gflops= $2.1365328 \times 10^{10} / 14.073875 \times 10^{-9} \approx 1.518$ Gflops

LAPACK:Time: 1.424908s

Gflops= $2.1365328 \times 10^{10} / 1.304958 \times 10^{-9} \approx 16.3724$ Gflops

### Matrix Size 5000

FLOPs= $4.171666 \times 10^{10}$

my function:Time: 33.782017s

Gflops= $4.171666 \times 10^{10} / 28.704089 \times 10^{-9} \approx 1.4534$ Gflops

LAPACK:Time: 2.850201s

Gflops= $4.171666 \times 10^{10} / 2.614344 \times 10^{-9} \approx 18.0412$  Gflops

### Q3

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 9 & 12 & 15 \\ 3 & 26 & 41 & 49 \\ 5 & 40 & 107 & 135 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 9 & 12 & 15 \\ 3 & 26 & 41 & 49 \\ 5 & 40 & 107 & 135 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 12 & 15 \\ 3 & 20 & 41 & 49 \\ 5 & 30 & 107 & 135 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 12 & 15 \\ 3 & 4 & 41 & 49 \\ 5 & 6 & 107 & 135 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 4 & 41 & 49 \\ 5 & 6 & 107 & 135 \end{pmatrix}$$

$$\text{we calculate } \begin{pmatrix} 3 & 4 \\ 5 & 6 \end{pmatrix} \begin{pmatrix} 3 & 4 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 33 & 44 \\ 51 & 62 \end{pmatrix}$$



$$\text{so } A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 4 & 8 & 9 \\ 5 & 6 & 56 & 73 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 4 & 8 & 9 \\ 5 & 6 & 7 & 10 \end{pmatrix}$$

$$L \text{ is the lower triangular, which is } \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 4 & 1 & 0 \\ 5 & 6 & 7 & 1 \end{pmatrix},$$

$$U \text{ is the upper triangular, which is } \begin{pmatrix} 1 & 2 & 3 & 4 \\ 0 & 5 & 6 & 7 \\ 0 & 0 & 8 & 9 \\ 0 & 0 & 0 & 10 \end{pmatrix}.$$

#### Q4

```
void mydgemm(int n, double *A, double *B, double *C) {
    #pragma omp parallel for collapse(2)
    for (int i = 0; i < n; i += BLOCK_SIZE) {
        for (int j = 0; j < n; j += BLOCK_SIZE) {
            for (int k = 0; k < n; k += BLOCK_SIZE) {
                for (int ii = i; ii < i + BLOCK_SIZE && ii < n; ++ii) {
                    for (int jj = j; jj < j + BLOCK_SIZE && jj < n; ++jj) {
                        double sum = 0.0;
                        for (int kk = k; kk < k + BLOCK_SIZE && kk < n; ++kk) {
                            sum += A[ii * n + kk] * B[kk * n + jj];
                        }
                        C[ii * n + jj] += sum;
                    }
                }
            }
        }
    }
}
```



```

void mydgetrf_block(int n, double *A) {
    for (int k = 0; k < n; k += BLOCK_SIZE) {
        int end = k + BLOCK_SIZE < n ? k + BLOCK_SIZE : n;

        // Factorize the diagonal block
        for (int i = k; i < end; ++i) {
            for (int j = k; j < i; ++j) {
                A[i * n + j] /= A[j * n + j];
                for (int l = j + 1; l < end; ++l) {
                    A[i * n + l] -= A[i * n + j] * A[j * n + l];
                }
            }
        }

        // Update the trailing submatrix
        #pragma omp parallel for collapse(2)
        for (int i = end; i < n; ++i) {
            for (int j = k; j < end; ++j) {
                A[i * n + j] /= A[j * n + j];
                for (int l = end; l < n; ++l) {
                    A[i * n + l] -= A[i * n + j] * A[j * n + l];
                }
            }
        }

        // Perform matrix multiplication for the trailing submatrix
        #pragma omp parallel for collapse(2)
        for (int i = end; i < n; i += BLOCK_SIZE) {
            for (int j = end; j < n; j += BLOCK_SIZE) {
                for (int ii = i; ii < i + BLOCK_SIZE && ii < n; ++ii) {
                    for (int jj = j; jj < j + BLOCK_SIZE && jj < n; ++jj) {
                        double sum = 0.0;
                        for (int kk = k; kk < end; ++kk) {
                            sum += A[ii * n + kk] * A[kk * n + jj];
                        }
                        A[ii * n + jj] -= sum;
                    }
                }
            }
        }
    }
}

```

test result:

on block size=32

n=1000, pad=1

Time taken: 0.068316 seconds

n=2000, pad=1

Time taken: 0.537873 seconds

n=3000, pad=1

Time taken: 1.862734 seconds

n=4000, pad=1

Time taken: 4.064807 seconds

n=5000, pad=1

Time taken: 8.126369 seconds

#### on block size=64:

```
n=1000, pad=1
Time taken: 0.074267 seconds

n=2000, pad=1
Time taken: 0.535702 seconds

n=3000, pad=1
Time taken: 1.738807 seconds

n=4000, pad=1
Time taken: 4.140256 seconds

n=5000, pad=1
Time taken: 8.497961 seconds
```

#### on block size=128

```
n=1000, pad=1
Time taken: 0.099635 seconds

n=2000, pad=1
Time taken: 0.577570 seconds

n=3000, pad=1
Time taken: 1.811601 seconds

n=4000, pad=1
Time taken: 4.347364 seconds

n=5000, pad=1
Time taken: 8.669026 seconds
```

We can see that compare to non-block algorithm is much quicker, especially as the n size increase, the block pattern get a better time cost than non-block one.

- [rui001@cluster-001-login-node hw2]\$ export LD\_LIBRARY\_PATH=/home/act-software/opt/intel/cor  
b/intel64:/home/rui001/CS211-hw/hw2/extern:\$LD\_LIBRARY\_PATH
- [rui001@cluster-001-login-node hw2]\$ srun main my 1000  
n=1000, pad=1  
time=0.133002s
- [rui001@cluster-001-login-node hw2]\$ srun main my 2000  
n=2000, pad=1  
time=1.292453s
- [rui001@cluster-001-login-node hw2]\$ srun main my 3000  
n=3000, pad=1  
time=5.619809s
- [rui001@cluster-001-login-node hw2]\$ srun main my 4000  
n=4000, pad=1  
time=14.073875s
- [rui001@cluster-001-login-node hw2]\$ srun main my 5000  
n=5000, pad=1  
time=28.704089s

We get the conclusion that maybe as the block size is too large, the performance is began to lose, so the appropriate size like 32 or 64 would be much better.