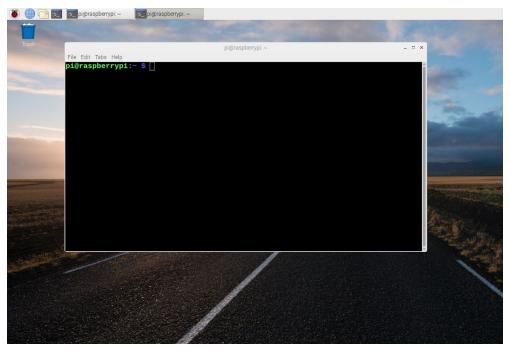
Parallel Programming Basics: Drug Design and DNA in Parallel:

Executed by Shilp Patel

Compilation:

Start terminal:



Here I opened terminal window by choosing its icon in the menu bar at the top So in this project, the most difficult part was compiling dd_omp and dd_threads. To do that I download TBB library, PIP and OpenCV.

I used this following steps provided by this sites to install TBB:

First I installed PIP for easier approach towards installing OpenCV using steps provided by https://www.pyimagesearch.com/2018/09/19/pip-install-opencv/

Second I installed OpenCV using steps provided by

 $\underline{https://circuit digest.com/microcontroller-projects/how-to-install-python-opencv-on-raspberry-\underline{pi}}$

Third I installed TBB Library using steps and packages provided by

https://packages.debian.org/experimental/libtbb-dev

https://github.com/abhiTronix/TBB Raspberry pi

https://www.theimpossiblecode.com/blog/intel-tbb-on-raspberry-pi/

The following screenshots are taken after I had finally installed and tried out the library correctly. It took me about 15 hrs to figure it out but in the end it was worth it.

Sequential (also called Serial) solution:
I made directory named sequential.
Downloads and copied the dd_serial and
Makefile provided by the professor, in to the
directory. And to compile I used make
command.

```
pi@raspberrypi:- $ mkdir sequential
mkdir: cannot create directory 'sequential': File exists
pi@raspberrypi:- $ cd sequential
pi@raspberrypi:-/sequential $ ls
dd serial dd_serial.cpp Makefile
pi@raspberrypi:-/sequential $ make
make: 'dd_serial' is up to date.
pi@raspberrypi:-/sequential $ []
```

OpenMP solution:

I made directory named openmp1.

Downloaded and copied the dd_omp and Makefile provided by the professor, in to the directory. And to compile I used make command.

```
pi@raspberrypi:- $ mkdir openmp1
mkdir: cannot create directory 'openmp1': File exists
pi@raspberrypi:- $ cd openmp1
pi@raspberrypi:-/openmp1 $ ls
dd_omp dd_omp.cpp Makefile
pi@raspberrypi:-/openmp1 $ make
make: 'dd_omp' is up to date.
pi@raspberrypi:-/openmp1 $ |
```

C++11 standard threads solution:

I made directory named cplusthreads, while figuring out how to compile I had it named threads for easier approach. Downloaded and copied the dd_threads and Makefile provided by the professor, in to the directory. And to compile I used make command.

```
pi@raspberrypi:- $ mkdir cplusthreads1
mkdir: cannot create directory 'cplusthreads1': File exists
pi@raspberrypi:- $ cd cplusthreads1
pi@raspberrypi:-/cplusthreads1 $ ls
dd threads dd threads.cpp Makefile
pi@raspberrypi:-/cplusthreads1 $ make
make: 'dd threads' is up to date.
pi@raspberrypi:-/cplusthreads1 $ |
```

Measure Run-Time:

Part A

```
pi@raspberrypi:-/sequential $ time ./dd_serial 7 120
maximal score is 5, achieved by ligands
acehch ieehkc

real 2m6.312s
user 2m5.822s
sys 0m0.360s
pi@raspberrypi:-/sequential $ cd
pi@raspberrypi:-/sequential $ cd
pi@raspberrypi:-/openmp1 $ time ./dd_omp 7 120 1
max_ligand=7 nligands=120 nthreads=1
0MP defined
maximal score is 5, achieved by ligands
acehch ieehkc

real 2m21.793s
user 2m21.206s
sys 0m0.110s
pi@raspberrypi:-/openmp1 $ time ./dd_omp 7 120 2
max_ligand=7 nligands=120 nthreads=2
0MP defined
^Z
[2]+ Stopped ./dd_omp 7 120 2

real 0m3.547s
user 0m0.000s
sys 0m0.001s
pi@raspberrypi:-/s cd threads/
pi@raspberrypi:-/s cd threads/
pi@raspberrypi:-/threads $ time ./dd_threads 7 120 1
max_ligand=7 nligands=120 nthreads=1
maximal score is 5, achieved by ligands
acehch ieehkc

real 2m15.081s
user 2m15.004s
sys 0m0.010s
```

Here I measured the running time of each implementation, using the time command and observing the real time for each solution. In the command I also included thread to be 1 and the default arguments for each value.

Results:

| Implementation | Time(s) |
|----------------|---------|
| dd_serial | 126.312 |
| dd_openmp | 141.793 |
| dd_threads | 135.081 |

Part B:

2 Threads:

Here I measured the running time of dd_omp and dd_threads implementation, using the time command and observing the real time for each solution. In the command I also included thread to be 2 and the default arguments for each value.

```
i@raspberrypi:~/threads $ cd
pi@raspberrypi:~ $ cd sequential/]
bash: cd: sequential/]: No such file or directory
pi@raspberrypi:~ $ cd sequential
pi@raspberrypi:~/sequential $ cd
pi@raspberrypi:~ $ cd openmp1/
pi@raspberrypi:~/openmp1 $ time ./dd_omp 7 120 2
max_ligand=7 nligands=120 nthreads=2
OMP defined
 maximal score is 5, achieved by ligands
ieehkc acehch
 real
           1m53.969s
           2m20.863s
user
           0m0.030s
pi@raspberrypi:~/openmp1 $ cd ~/threads/
pi@raspberrypi:~/threads $ time ./dd_threads 7 120 2
max_ligand=7 nligands=120 nthreads=2
maximal score is 5, achieved by ligands
ieehkc acehch
 real
           1m19.603s
user
           2m23.661s
           0m0.000s
```

3 Threads:

Here I measured the running time of dd_omp and dd_threads implementation, using the time command and observing the real time for each solution. In the command I also included thread to be 3 and the default arguments for each value.

```
real
          1m19.603s
user
          2m23.661s
          0m0.000s
pi@raspberrypi:~/threads $ cd ~/openmp1/
pi@raspberrypi:~/openmp1 $ time ./dd_omp 7 120 3
max_ligand=7 nligands=120 nthreads=3
OMP defined
maximal score is 5, achieved by ligands
ieehkc acehch
real
          1m39.225s
          2m23.822s
          0m0.050s
pi@raspberrypi:~/openmp1 $ cd ~/threads/
pi@raspberrypi:~/threads $ time ./dd_threads 7 120 3
max_ligand=7 nligands=120 nthreads=3
maximal score is 5, achieved by ligands
ieehkc acehch
          0m55.104s
          2m23.565s
```

4 Threads:

Here I measured the running time of dd_omp and dd_threads implementation, using the time command and observing the real time for each solution. In the command I also included thread to be 4 and the default arguments for each value.

```
0m55.104s
real
user
                2m23.565s
sys 0m0.020s
pi@raspberrypi:~/threads $ cd ~/openmp1/
pi@raspberrypi:-/threads 3 cd -/openmpl/
pi@raspberrypi:-/openmpl $ time ./dd_omp 7 120 4
max_ligand=7 nligands=120 nthreads=4
OMP defined
maximal score is 5, achieved by ligands
ieehkc acehch
real
                2m24.144s
sys 0m0.030s
pi@raspberrypi:~/openmp1 $ cd ~/threads/
pi@raspberrypi:~/threads $ time ./dd_threads 7 120 4
max_ligand=7 nligands=120 nthreads=4
maximal score is 5, achieved by ligands
 ieehkc acehch
 real
                0m42.148s
                2m23.918s
                0m0.020s
pi@raspberrypi:~/threads $ 🗍
```

Results:

| Implementation | Time(s) 2 Threads | Time(s) 3 Threads | Time(s) 4 Threads |
|----------------|-------------------|-------------------|-------------------|
| dd_omp | 113.969 | 99.225 | 80.768 |
| dd_threads | 79.603 | 55.104 | 42.148 |

Questions:

1. Which approach is fastest?

In part A dd_serial has the fastest approach; And in part B dd_thread with 4 threads has the fastest approach. The time depends on the numbers of threads that is used to run the program.

2. Determine the number of lines in each file (use wc -l). How does the C++11 implementation compare to the OpenMP implementations?

```
pi@raspberrypi:~/threads $ wc -1 dd_threads.cpp
205 dd_threads.cpp
pi@raspberrypi:~/threads $ cd ~/openmp1/
pi@raspberrypi:~/openmp1 $ wc -1 dd_omp.cpp
193 dd omp.cpp
```

- As shown above in the screenshot provided, The word count of dd_omp is 193 and word count of dd_threads is 205. The difference between C++11 implementation and the OpenMP implementations is 12 word count difference and as a result dd_threads has faster approach than dd omp.
 - 3. Increase the number of threads to 5 threads. What is the runtime for each?

| Implementation | Time(s) 5 Threads |
|----------------|-------------------|
| dd_omp | 75.339 |
| dd_threads | 44.445 |

```
pi@raspberrypi:~/threads $ wc -1 dd_threads.cpp
205 dd_threads.cpp
pi@raspberrypi:~/threads $ cd ~/openmp1/
pi@raspberrypi:~/openmp1 $ wc -1 dd_omp.cpp
193 dd_omp.cpp
pi@raspberrypi:~/openmp1 $ time ./dd_omp 7 120 5
max_ligand=7 nligands=120 nthreads=5
OMP defined
maximal score is 5, achieved by ligands ieehkc acehch
            1m15.339s
 real
            2m23.841s
            0m0.152s
pi@raspberrypi:~/openmp1 $ cd ~/threads/
pi@raspberrypi:~/threads $ time ./dd_threads 7 120 5
max_ligand=7 nligands=120 nthreads=5
 maximal score is 5, achieved by ligands
 acehch ieehkc
            0m44.445s
user
            2m23.887s
sys 0m0.122s
pi@raspberrypi:~/threads $
            0m0.122s
```

- Here I measured the running time of dd_omp and dd_threads implementation, using the time command and observing the real run time for each solution. In the command I used 5 thread and the default arguments for each value.
 - 4. Increase the maximum ligand length to 7, and rerun each program. What is the run time for each?

Run time for max_ligand = 7:

| Implementation | Time(s) |
|----------------|---------|
| dd_serial | 126.312 |
| dd_openmp | 141.793 |
| dd_thread | 135.081 |