Optimizing Python codes

Google Colab

Mahendra Verma
IIT Kanpur

mkv@iitk.ac.in

Python codes

On MacPro (16”, 2019)   Big Sur

Google Colab
Intel(R) Xeon(R) CPU @ 2.20GHz
(!cat /proc/cpuinfo)

TIME in seconds

Fluctuations around 10% due to other jobs

HPC_python.ipynb

File Edit View Insert Runtime Tools Help All changes saved

Comment Share

Table of contents

+ Code + Text

RAM
Disk

```
!cat /proc/cpuinfo
```

Strong and Weak Scaling

[2]

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.colors as colors
from google.colab import files

def strong_scale(N):
  return 1/(1-f+f/N)

def Gustafson_scale(N):
  return 1-f+f*N

N = np.linspace(1,100,100)

fig, ax = plt.subplots(figsize = (3,2.5))

f = 0.5
```

Data size

$A = 10^8$

$A = [10^4, 10^4]$

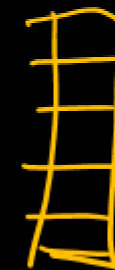
Vectorization

```python

from datetime import datetime
import numpy as np
a =  np.random.random(10**8)
b =  np.random.random(10**8)
c = np.empty(10**8)

# with loop
t1 = datetime.now()
for i in range(10**8):
    c[i] = a[i]*b[i]
t2 = datetime.now()
print ("for loop, time = ", t2-t1)


t1 = datetime.now()
c=(a*b)
t2 = datetime.now()
print ("for vectorised ops, time = ", t2-t1)
```



$c_i = a_i \quad b_i$

$2 \quad 3$

$\dot{v} = -v^2$

for i in range(100):
$v(t+\Delta t) = v(t) + \Delta t\, v(t)^2$

MAC	Colab
Loop: T = 39 sec	Loop: T = 48 sec
Vector: T = 0.11 sec	Vector: T = 0.36 sec

Storage of Arrays

Row colum

	0	1	2	3
0	0	1	2	3
1	4	5	6	7
2	8	9	10	11
3	12	13	14	15

0,0
0,1
0,2
0,3
1,0
1,1
⋮

0	1	2	3

for i = 0:3
for j = 0:3
c[i][j] = a[i][j] * b[i][j]

c(i,j)

(i j)

C: Column index varies faster than row index (i,j)

Row major
C, Python

Column major
Fortran

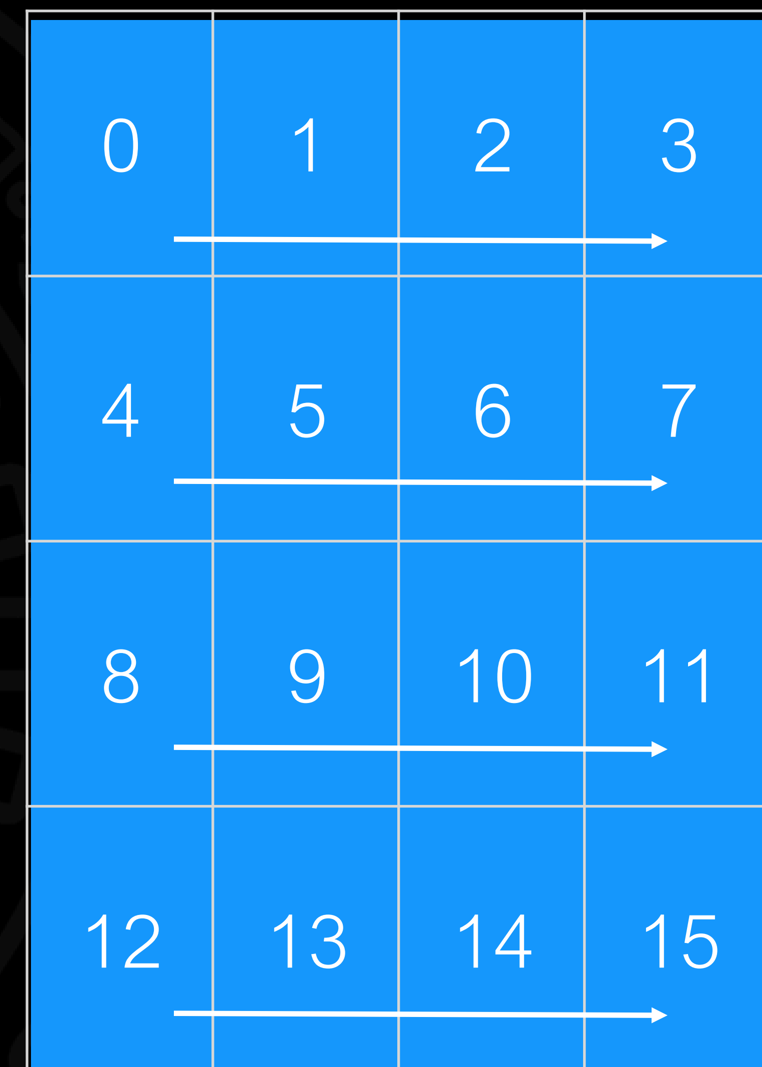
Loop

```
t1 = datetime.now()
for i in range(N):
    for j in range(N):
        c2[i,j] = a2[i,j]*b2[i,j]

t2 = datetime.now()
print ("for loop_i_j, time = ", t2-t1)
#for loop_i_j, time =  0:00:55.346258


t1 = datetime.now()
for j in range(N):
    for i in range(N):
        c2[i,j] = a2[i,j]*b2[i,j]

t2 = datetime.now()
print ("for loop_j_i, time = ", t2-t1)
#for loop_j_i, time =  0:01:06.284808
```



MAC

Loop i_j: T = 53 sec

Loop j_i: T = 1:12 sec

Colab

Loop i_j: T = 1:16 76

Loop j_i: T = 1:53 113

2D vectorized

```
a =  np.random.random((10**4,10**4))
b =  np.random.random((10**4,10**4))

t1 = datetime.now()

c = a*b

t2 = datetime.now()
print ("for 2D array, time = ", t2-t1)
```

MAC

T = 0.16 sec

Colab

T = 0.38 sec

Loop with if

```
t1 = datetime.now()
for i in range(N):
    for j in range(N):
        if (a2[i,j] > 0.5):
            c2[i,j] = a2[i,j]*b2[i,j]
        else:
            c2[i,j] = -a2[i,j]*b2[i,j]

t2 = datetime.now()
print ("for loop_i_j, time = ", t2-t1)
# for loop_i_j, time =  0:01:23.087140
```

MAC

Loop_i_j with if: T = 1:23 sec

Colab

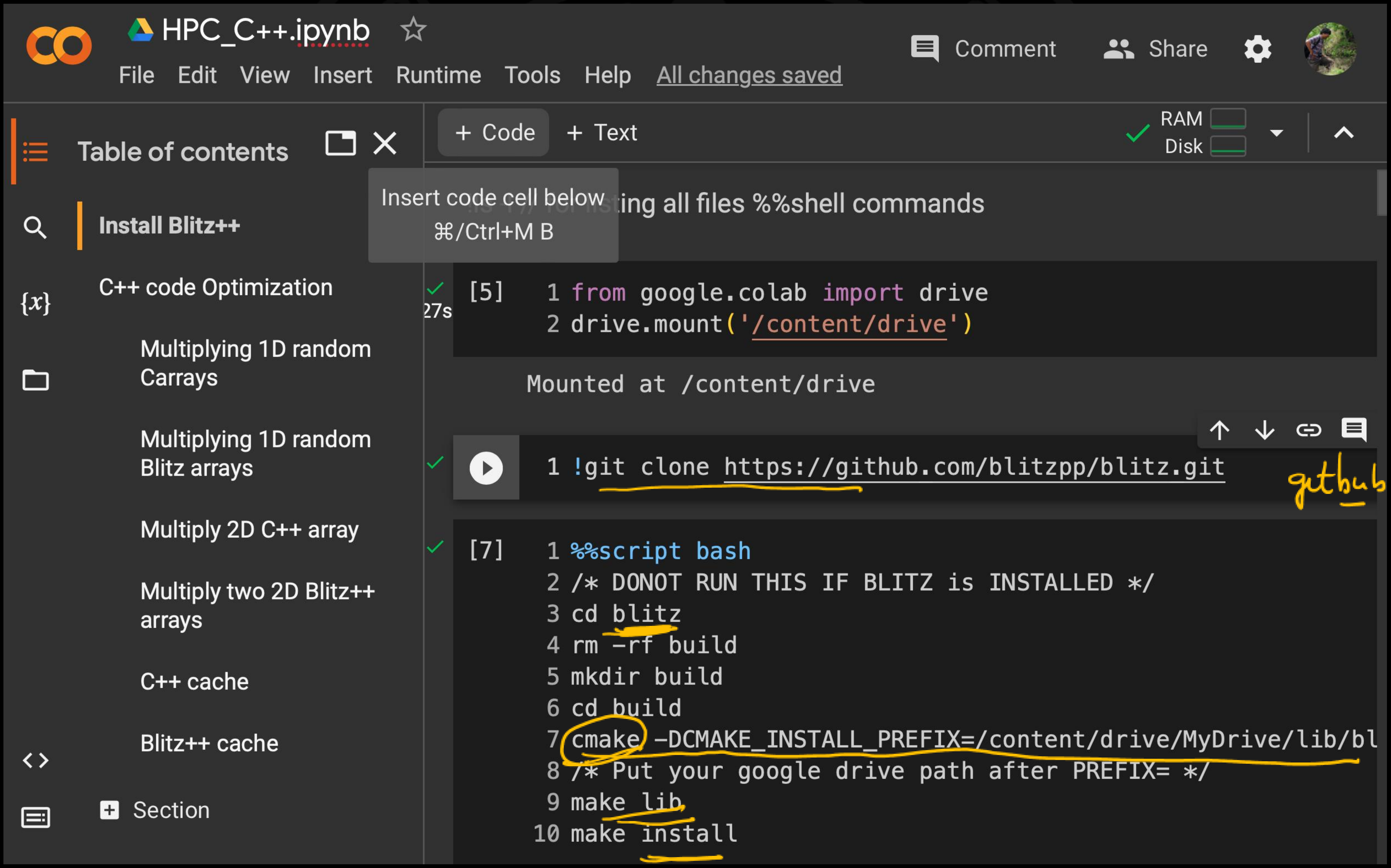
Loop_i_j with if: T = 1:44 sec

Optimizing C++ codes

Mahendra Verma
IIT Kanpur

mkv@iitk.ac.in

Using Google Colab



Using gcc

On Macbook Pro (16”, 2019)
Big Sur

Fluctuations around 10% due to other jobs

Install gcc in mac

$ brew install gcc

$gcc - -version

Install gcc in ubuntu

$ sudo apt update

$sudo apt install build-essential

$sudo apt install build-essential

$gcc - -version

Timing using

```
#include <chrono>
using namespace std::chrono;
```

```
auto start = high_resolution_clock::now();
auto stop = high_resolution_clock::now();
auto duration = duration_cast<microseconds>(stop - start)/1e6;
cout << duration.count() << endl;
```

1e3

TIME in seconds

Using compiler options

-O1 -O2 -O3

- Compilers have many optimisation options.
- It tries to generate faster codes for advanced options. Compiling takes longer for such options.
- Try -O3 or -Ofast, which could yield speedup of the order of 10.
- Study these options for other compilers.

Loop

#define N 100000000

```
for (int i=0; i<N; i++) {
    a[i] = rand();
    b[i] = rand();
}
```

```
for (int i=0; i<N; i++) {
    c[i] = a[i]*b[i];
}
```

Without any option: dt = 675 ms

Uncertainty 10%

With -O1: T = 79.7 ms

With -O2: T = 0

With -O3: T = 0

With -Ofast: T = 0

2D C++ array

#define N 10000

```
for (int i=0; i<N; i++)
  for (int j=0; j<N; j++) {
      c[i][j]  =  a[i][j] *b[i][j] ;
}
```

Without any option: T = 1.49 s

With -O3: T = 0

j-i loop: Without any option: T = 12.4 s

With -O3: T = 0

Using blitz++

Blitz++

Blitz++ utilizes advanced C++ template metaprogramming techniques, including expression templates,[1] to provide speed-optimized mathematical operations on sequences of data without sacrificing the natural syntax provided by other mathematical programming systems. Indeed, it has been recognized as a pioneer in the area of C++ template metaprogramming.[2]

Taken from Wikipedia

With blitz array

#define N 100000000

```
int main()
{
    Uniform<float> x;

    x.seed((unsigned int)time(0));

    Array<double,1> a(N), b(N), c(N);

    auto start = high_resolution_clock::now();
    for (int i=0; i<N; i++) {
        a(i) = x.random();
        b(i) = x.random();
        c(i) = a(i)*b(i);
    }
```

Without any option: T = 2.69

With -O3: T = 0.52

2

$\boxed{c=a*b}$

4

Without any option:
T = 5.39

With -O3: T = 0.24

Blitz++ 2D array

#define N 10000

```
for (int i=0; i<N; i++)
    for (int j=0; j<N; j++)  {
        a(i,j) = x.random();
        b(i,j) = x.random();
        c(i,j) = a(i,j)*b(i,j);
}
```

With -O3

T (ij) = 3.43   T (ij) = 0.21

T (ji) = 38.7   T (ji) = 10

c=a*b

T = 5.49

With -O3: dt = 0.22

Summary

$A = 10^8$

$A = [10^4, 10^4]$

Time in seconds

Structure	Python	C++	C++ (-O3 opt)	Blitz	Blitz (-O3)
1D loop	48	0.675	0	2.7	0.505
1D vector	0.35			5.39	0.239
2D loop (i,j)	1.16	1.48	0	3.43	0.213
2D loop (j, i)	1.53	12.37	0	38.8	10.096
2D vector	0.38			5.49	0.223

Optimizing Python codes

Mahendra Verma
IIT Kanpur

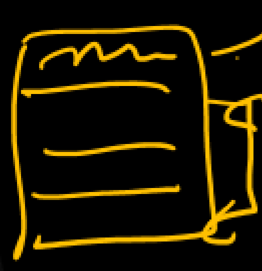
mkv@iitk.ac.in

Python codes

Google Colab

Intel(R) Xeon(R) CPU @ 2.20GHz

(!cat /proc/cpuinfo)



TIME in milliseconds (ms)

Fluctuations around 10% due to other jobs

HPC_python.ipynb

File Edit View Insert Runtime Tools Help All changes saved

Comment Share

+ Code + Text

RAM Disk


```
[ ] !cat /proc/cpuinfo
```

Strong and Weak Scaling

```
[2]
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.colors as colors
from google.colab import files

def strong_scale(N):
  return 1/(1-f+f/N)

def Gustafson_scale(N):
  return 1-f+f*N

N = np.linspace(1,100,100)

fig, ax = plt.subplots(figsize = (3,2.5))

f = 0.5
```

Data size

$A = 10^8$

$A = [10^4, 10^4]$

sum(a*b)

sum (sin (a))

1D array sum(a*b)

```python
# with loop
t1 = datetime.now()
tot = 0
for i in range(10**8):
    tot += a[i]*b[i]
t2 = datetime.now()
print ("for loop, time, tot = ", t2-t1, tot)
## 1D vectorized
t1 = datetime.now()
tot = np.sum(a*b)
t2 = datetime.now()
print ("for 1D vectorised a*b, time, tot = ", t2-t1, tot)
```

import numpy as np

01: 2: 3.001 GMT

loop

a**3

80 times faster !!

	None	-O1	-O2	-O3	-Ofast
C++	361	357	352	261	155
Loop	30910				
Vector	473				

Storage of Arrays

0 1 2 3 4 5 ----

a[i,j]

a(0,0)
a[0,1]
a[0,2]
⋮

A[0,0]
A[1,0]

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

for i=0 : N_x - 1
  for j=0 : N_y - 1
    A[i,j]

for j=0 ...
  for i= ...
    A[i,j]

C: Column index varies faster than row index (i,j)

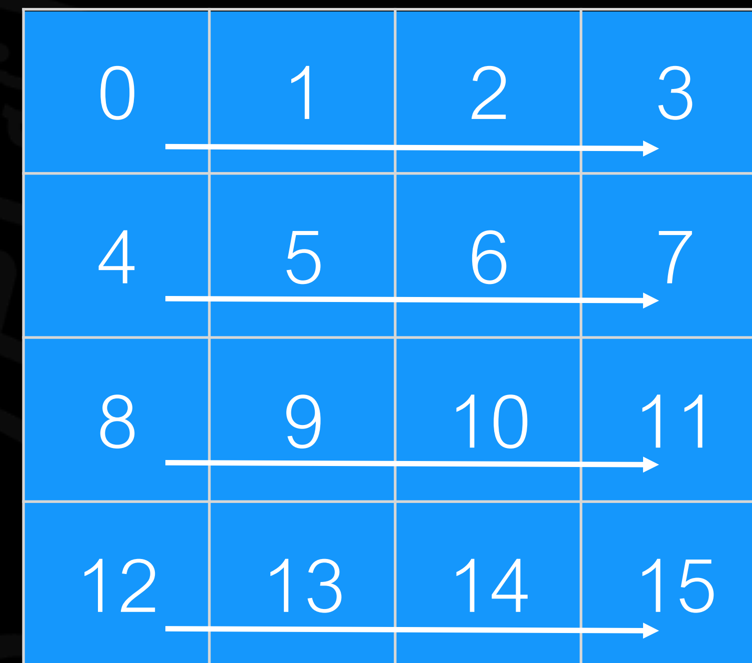
Row major
C, Python

Column major
Fortran

Loop

```
t1 = datetime.now()
tot = 0
for i in range(N):
  for j in range(N):
    tot += a2[i,j]*b2[i,j]
t2 = datetime.now()
print ("for loop_i_j, time, tot = ", t2-t1, tot)

t1 = datetime.now()
tot = 0
for j in range(N):
  for i in range(N):
    tot += a2[i,j]*b2[i,j]
t2 = datetime.now()
print ("for loop_j_i, time, tot = ", t2-t1, tot)
```



sum(a*b)

	None	-O1	-O2	-O3	-Ofast
C++ ij	359	350	421	289	133
C++ ji	5753	5826	6205	5910	143
Py ij	37920				
Py ji	45400				
Py Vector	746				

Loop with if

```
for i in range(N):
  for j in range(N):
    if (a2[i,j] > 0.5):
      c2[i,j] += a2[i,j]*b2[i,j]
    else:
      c2[i,j] += -1.098*a2[i,j]*b2[i,j]

t2 = datetime.now()
print ("for loop_i_j_with_if, time, tot = ", t2-t1, tot)
```

for tot

Loop_i_j with if: T = 62230 sec

sum(sin(a))

```
for i in range(10**8):
    tot += np.sin(a[i])
```

loop

```
tot = np.sum(np.sin(a))
```

Vector

	None	-O1	-O2	-O3	-Ofast
C++	1727	2293	1351	1353	653
Py Loop	92150				
Py Vector	1313				

2D sum(sin(a))

exp
log

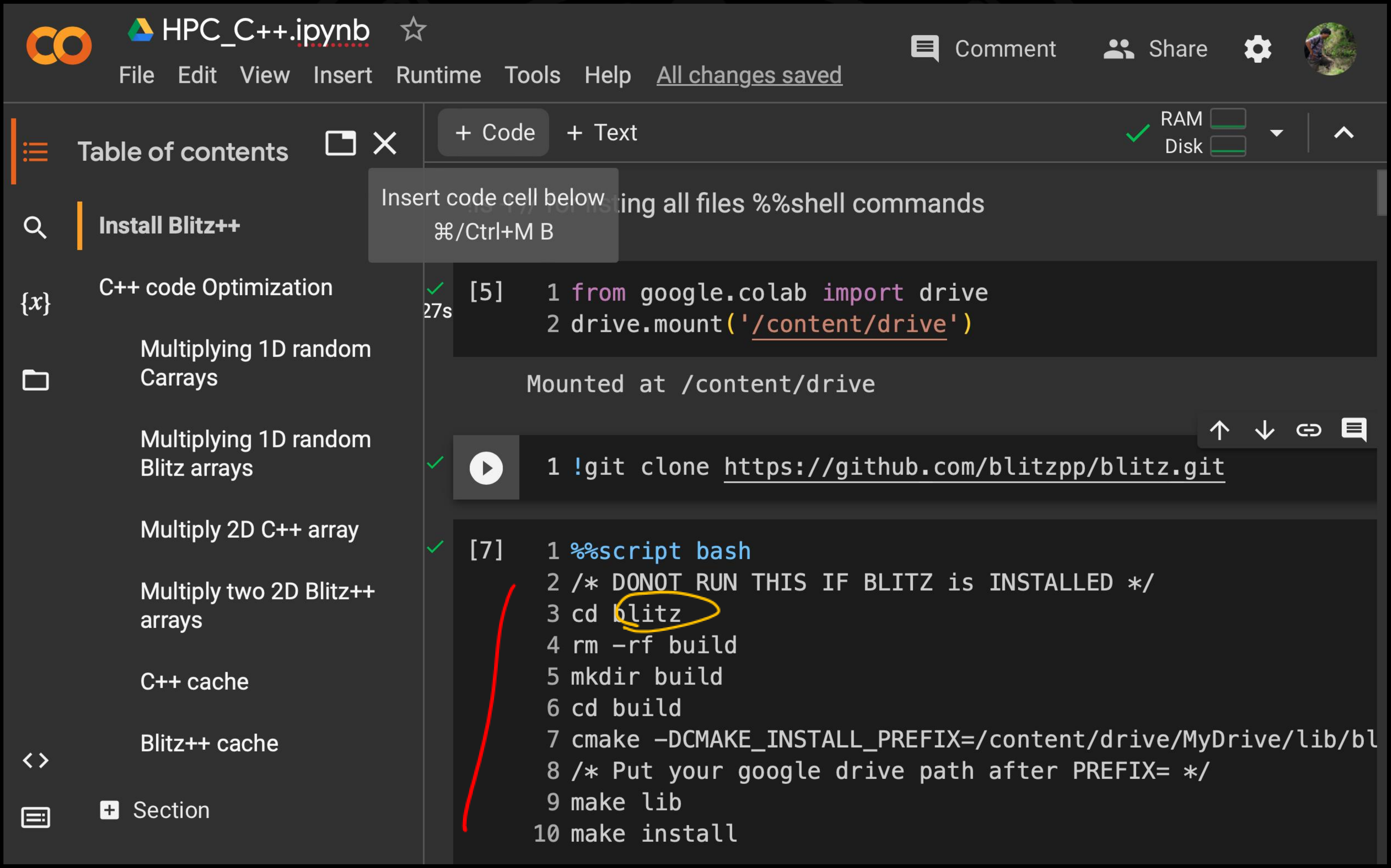
	None	-O1	-O2	-O3	-Ofast
C++ ij	1775	2149	2165	1794	836
C++ ji	9750	6624	6217	6272	652
Py ij	90390				
Py ji	102400				
Py Vector	1141				

Optimizing C++ codes

Mahendra Verma
IIT Kanpur

mkv@iitk.ac.in

Using Google Colab



Install gcc in mac

$ brew install gcc

$gcc - -version

Install gcc in ubuntu

$ sudo apt update

$sudo apt install build-essential

$sudo apt install build-essential

$gcc - -version

Timing using

```
#include <chrono>
using namespace std::chrono;
```

```
auto start = high_resolution_clock::now();
auto stop = high_resolution_clock::now();
auto duration = duration_cast<microseconds>(stop - start)/1e6;
cout << duration.count() << endl;
```

TIME in milliseconds (ms)

Using compiler options

- Compilers have many optimisation options.
- It tries to generate faster codes for advanced options. Compiling takes longer for such options.
- Options: ~~-O1, -O2, -O3, -Ofast~~
- -Ofast yields the most efficient code among the above.
- Study these options for other compilers.

O

-O1 -fopenmp

g++ fn.cc -o fn

./fn

a.out

sum(a*b)

#define N 100000000

```
for (int i=0; i<N; i++) {
  a[i] = (float)(rand()) / (float)(RAND_MAX);
  b[i] = (float)(rand()) / (float)(RAND_MAX);
}
```

```
for (int i=0; i<N; i++) {
    sum += a[i]*b[i];
}
```

None	-O1	-O2	-O3	-Ofast
361	357	352	261	155

Uncertainty 10%

2D C++ array sum(a*b)

#define N 10000

```
for (int j=0; j<N; j++)
  for (int i=0; i<N; i++) {
    sum += a[i][j] *b[i][j] ;
```

	None	-O1	-O2	-O3	-Ofast
ij	359	350	421	289	133
Ji	5753	5826	6205	5910	143
ij (with if)	4681	4147	4142	4256	4228

sum(sin(A))

#define N 100000000

```
for (int i=0; i<N; i++) {
    a[i] = rand();
    b[i] = rand();
}
```

```
for (int i=0; i<N; i++) {
    sum += a[i]*b[i];
}
```

sin(a[i])

None	-O1	-O2	-O3	-Ofast
1727	2293	1351	1353	653

2D C++ array sum(sin(a))

#define N 10000

```
for (int i=0; i<N; i++)
  for (int j=0; j<N; j++) {
      sum  +=  sin(a[i][j]) ;
}
```

	None	-O1	-O2	-O3	-Ofast
ij	1775	2149	2165	1794	836
Ji	9750	6624	6217	6272	652

Using blitz++

Blitz++

Blitz++ utilizes advanced C++ template metaprogramming techniques, including expression templates,[1] to provide speed-optimized mathematical operations on sequences of data without sacrificing the natural syntax provided by other mathematical programming systems. Indeed, it has been recognized as a pioneer in the area of C++ template metaprogramming.[2]

1997

Taken from Wikipedia

sum(a*b) for 1D blitz array

#define N 100000000

```
for (int i=0; i<N; i++) {
  a(i) = x.random();
  b(i) = x.random();
}
```

```
for (int i=0; i<N; i++)
  sum_arr += a(i)*b(i);
```

c =

sum(a*b)

sum(c)

	None	-O1	-O2	-O3	-Ofast
C++	1727	2293	1351	1353	155
Loop	2020	354	353	270	135
Vector	5778	669	790	537	454

blitz++

sum(a*b) for 2D blitz array

#define N 1000

	None	-O1	-O2	-O3	-Ofast
C++ ij	359	350	421	289	133
C++ ji	5753	5826	6205	5910	143
Blitz ij	2239	350	352	263	185
Blitz ji	10542	5203	5045	5010	5061
Vector	5051	317	327	258	273

sum(sin(a)) blitz array

#define N 100000000

```
for (int i=0; i<N; i++)
  sum_arr += sin(a(i));
```

c=sin(a)
sum(c)

	None	-O1	-O2	-O3	-Ofast
C++	1727	2293	1351	1353	653
Loop	3409	1790	1336	1352	677
Vector	5501	5779	2303	1818	1230

sum(sin(a)) for 2D Blitz array

#define N 100000000

	None	-O1	-O2	-O3	-Ofast
C++ ij	1775	2149	2165	1794	836
C++ ji	9750	6624	6217	6272	652
Blitz ij	2846	1386	1325	1315	667
Blitz ji	8690	6421	6534	6885	3464
Vector	5404	1439	1445	1497	777

Summary

$A = 10^8$

$A = [10^4, 10^4]$

sum(a*b): Time in mili sec

Structure	Python	C++ (-Ofast)	Blitz (-Ofast)
1D loop	30013	155	135
1D vector	473		454
2D loop (i,j)	37920	133	185
2D loop (j, i)	45400	143	5061
2D vector	746		273

sin(a): Time in mili sec

Structure	Python	C++ (-Ofast)	Blitz (-Ofast)
1D loop	92150	653	677
1D vector	1313		1230
2D loop (i,j)	90390	836	667
2D loop (j,i)	102400	652	3464
2D vector	1141		777

Optimizing C++ codes

Mahendra Verma
IIT Kanpur

mkv@iitk.ac.in

Cache locality

Timings with -O3 & -Ofast on Colab

cted.com/c-programming-hacks-4-matrix-multiplication-are-we-doi

$$C[i,j] = \sum_k A[i,k] * B[k,j]$$

C = A*B

N = 2048

```
for (int i=0; i<N; i++)
    for (int j=0; j<N; j++)
        for (int k=0; k<N; k++)
        {
            c[i][j]  += a[i][k] *b[k][j] ;
        }
```

-O3: 53.1812 s

-Ofast: 6.9823 s

```
for (int i=0; i<N; i++)
    for (int k=0; k<N; k++)
        for (int j=0; j<N; j++)
        {
            c[i][j]  += a[i][k] *b[k][j] ;
        }
```

-O3: 6.4822 s

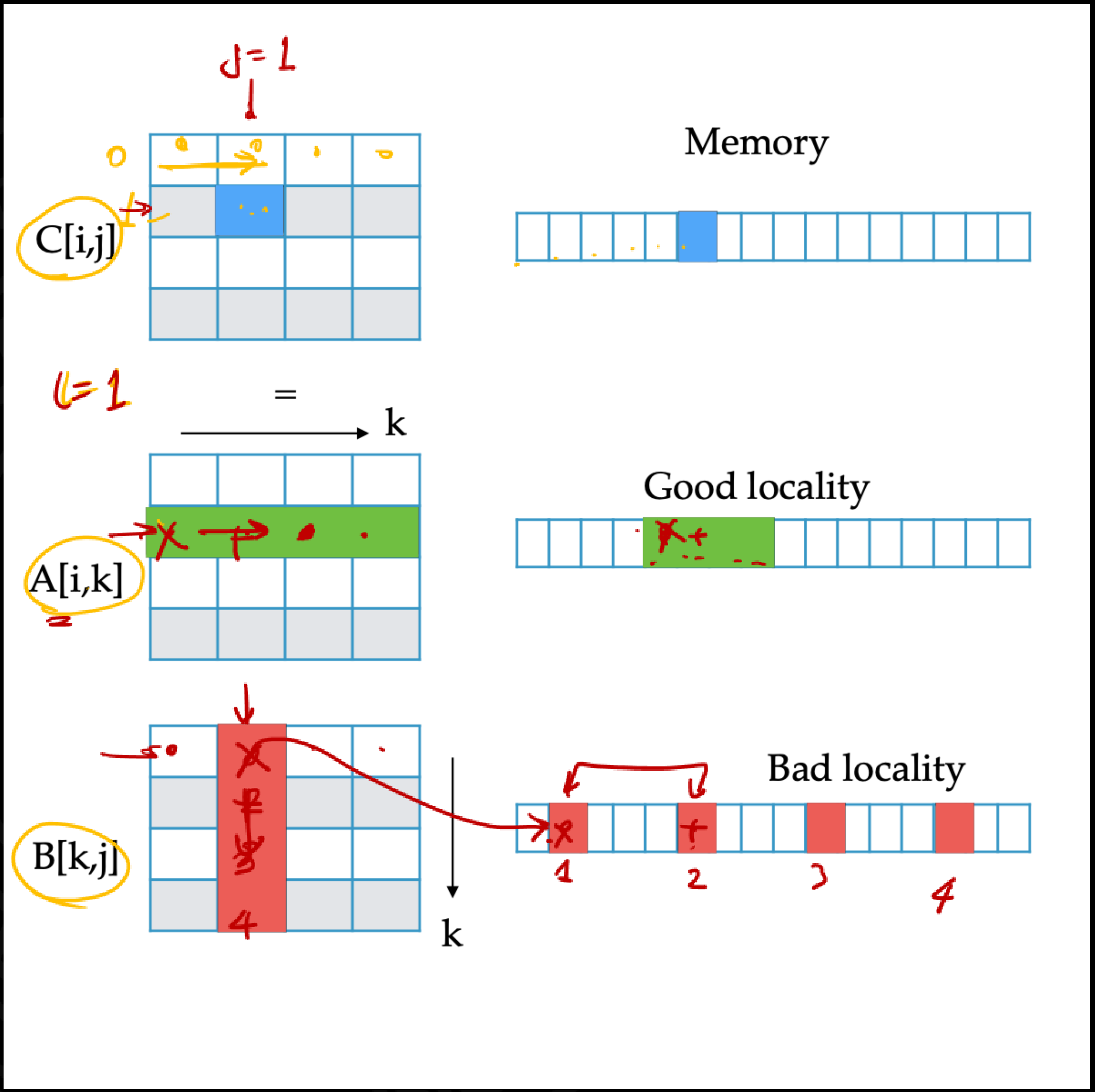
-Ofast: 6.5144 s

```
for (int k=0; k<N; k++)
    for (int i=0; i<N; i++)
        for (int j=0; j<N; j++)
        {
            c[i][j]  += a[i][k] *b[k][j] ;
        }
```

-O3: 6.9082 s

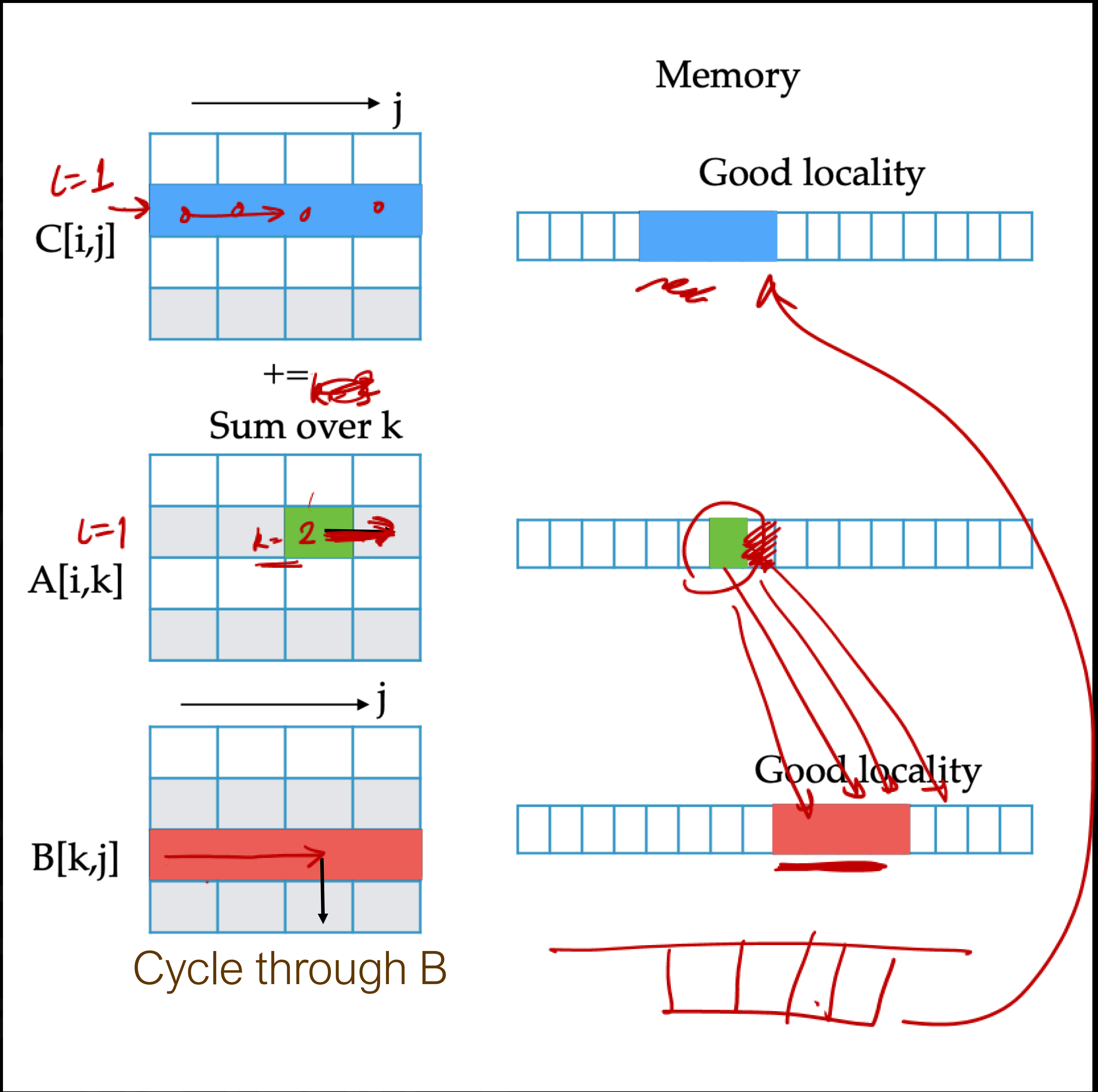
-Ofast: 6.8868 s

```
for (int i=0; i<N; i++)
    for (int j=0; j<N; j++)
        for (int k=0; k<N; k++)
        {
            C(i,j) += A(i,k)*B(k,j);
        }
```



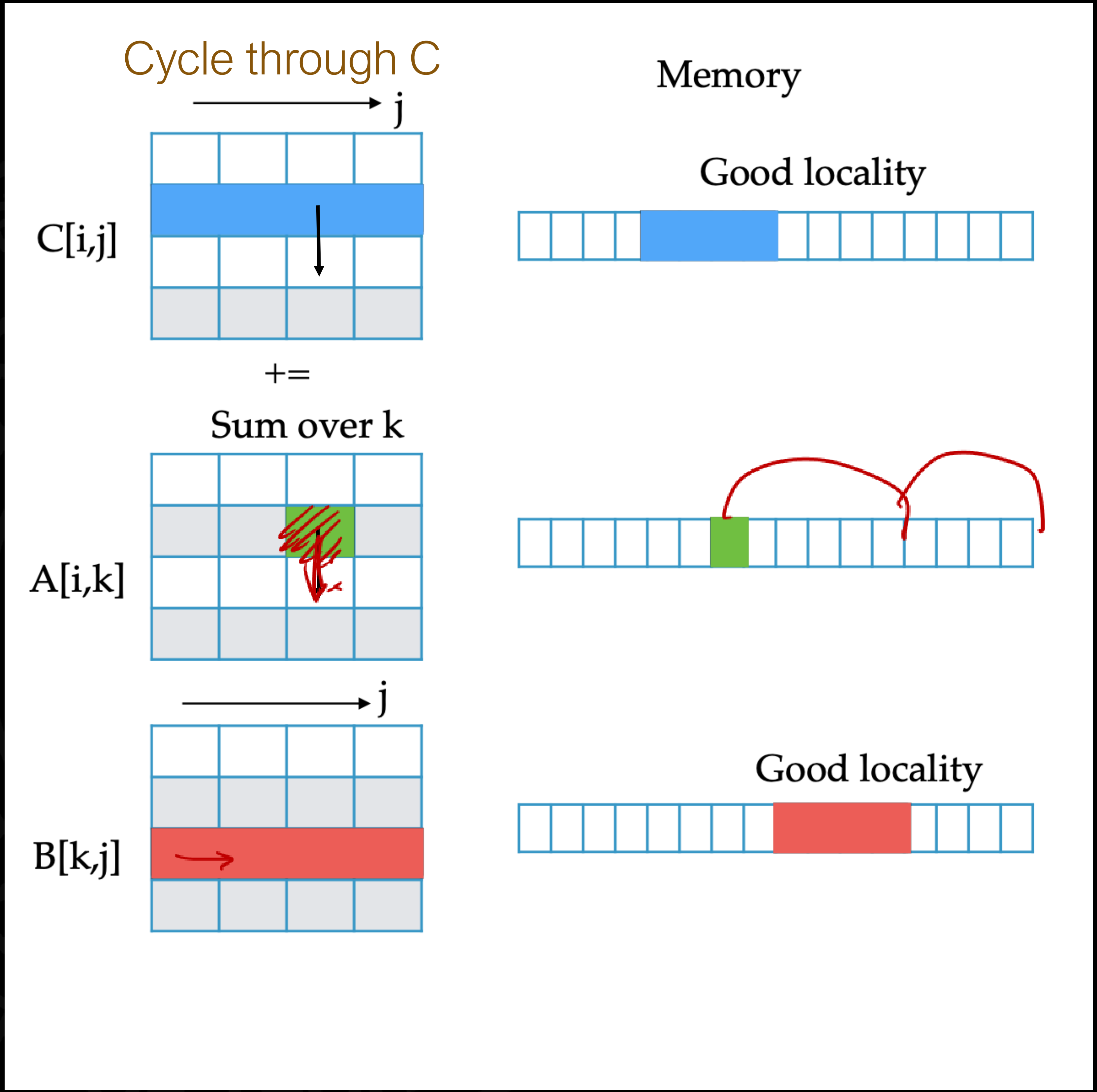
Bad locality of B leads to inefficiency

```
for (int i=0; i<N; i++)
    for (int k=0; k<N; k++)
        for (int j=0; j<N; j++)
        {
            C(i,j) += A(i,k)*B(k,j);
        }
```



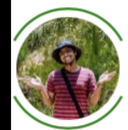
Good locality of B & C leads to efficient code

```
for (int k=0; k<N; k++)
    for (int i=0; i<N; i++)
        for (int j=0; j<N; j++)
        {
            C(i,j) += A(i,k)*B(k,j);
        }
```



Good locality of B & C leads to efficient code

The impact of cache locality on performance in C through matrix multiplication



Gunavaran Brihadiswaran Follow

Jul 29, 2020 · 5 min read ★

The Experiment

I changed the order of the nested loops and performed three iterations for each combination. The results are as follows.

	Elapsed Time (seconds)					
Iteration	i,j,k	i,k,j	j,i,k	j,k,i	k,i,j	k,j,i
1	195.92	34.78	183.97	274.35	35.53	286.1
2	198.37	34.86	189.94	278.82	35.29	278.64
3	196.41	34.71	183.9	280.99	35.18	274.59
Average	196.90	34.78	185.94	278.05	35.33	279.78

cted.com/c-programming-hacks-4-matrix-multiplication-are-we-doi

Speeding up using Numba

Mahendra Verma
IIT Kanpur

mkv@iitk.ac.in

Numba

- Numba translates Python functions to optimized machine code at runtime using LLVM lib.

- JIT: *Just in time* compiler

- Performance comparable to C or Fortran codes.

- Apply Numba decorators on python functions.

- https://numba.pydata.org/

```python
from numba import jit, njit, prange

@jit
def my_log_nocache(a):
    M, N = a.shape
    tot = 0
    for i in prange(M):
        for j in prange(N):
            tot += np.log(a[i,j])
    return tot
```

gcc x.cc — O   x.o

Cache option

- @njit(cache=True)
- This decorator (command) instructs Python to save the compiled code in a cache.

```
from numba import jit, njit, prange

@jit(cache = True)
def my_log_cache(a):
  M, N = a.shape
  tot = 0
  for i in prange(M):
    for j in prange(N):
      tot +=  np.log(a[i,j]) + np.sin(a[i,j])
  return tot
```

Timing in Python

```python
from numba import jit, njit, prange
@njit
def dummy():
    return None

@jit
def my_log_nocache(a):
    M, N = a.shape
    tot = 0
    for i in prange(M):
        for j in prange(N):
            tot +=  np.log(a[i,j]) + np.sin(a[i,j])
    return tot
```

(Cache

sum(log(a))

```
Dummy timing 0.036316633224487305
No cache 1st timing 2.4474663734436035 tot= -54026001.04944232
No cache 2nd timing 1.6440708637237549 tot= -54026087.339905575
Cache 1st timing 1.7453806400299072 tot= -54024569.87402726
Cache 2nd timing 1.6321403980255127 tot= -54034193.91120762
Cache 3rd timing 1.658315896987915 tot= -54028264.60840158
```

Timings in ms

C++ (-Ofast)	653
Py Loop	92150
Py Vector	1313
Numba	1171

nopython mode

- @jit(nopython=True)
- Or @njit
- This mode generates fast non-python code.

Parallel option

- @njit(parallel=True)
- This mode generates parallel code if possible
- Use *prange* instead of *range*

```
from numba import jit, njit, prange
n
@jit(parallel = True)
def my_log_nocache(a):
  M, N = a.shape
  tot = 0
  for i in prange(M):            2048      256 x8
    for j in prange(N):          2048      2048
      tot +=  np.log(a[i,j]) + np.sin(a[i,j])
  return tot
```

On MacBook Pro 16” (2019): 8 cores

Without parallel

```
(base) codes/codes23 $python numba_pll.py
Dummy timing 0.08803677558898926
No cache 1st timing 1.0817480087280273 tot= -54012060.12899187
No cache 2nd timing 1.0117287635803223 tot= -54026917.40798862
Cache 1st timing 1.1753530502319336 tot= -54015353.38920122
Cache 2nd timing 1.0465059280395508 tot= -54032690.54539104
Cache 3rd timing 1.076902151107788 tot= -54024366.320906855
```

With parallel

```
Dummy timing 0.16474199295043945
No cache 1st timing 0.607647180557251 tot= -54030760.91180665
No cache 2nd timing 0.1352088451385498 tot= -54042526.14654334
Cache 1st timing 0.6361870765686035 tot= -54047140.20137752
Cache 2nd timing 0.13567590713500977 tot= -54034882.26079227
Cache 3rd timing 0.13421010971069336 tot= -54036017.213262975
```

Advanced features

- nogil = True
- The @vectorize decorator
- The @guvectorize decorator

No speedup with Numba

@jit

```
start = time.time()
tot = np.sum(np.log(a))
end = time.time()
print(f'No Python sum timing {end - start}', f'tot= {tot}’)
```

```
start = time.time()
tot = my_sum(a)
end = time.time()
print(f'No Jit sum 1st timing {end - start}', f'tot= {tot}')
```

@jit
def mysum(c)
return np.sum(a)

np.sum(a) is already optimized.
Hence, Numba does not speedup the code.

Summary

- Numba yields C/Fortran like high performance in Python.
- Numba: Cheap way to speedup!
- No need to make changes in the code. We just need to put Numba decorators ahead of functions.