Introduction to High Performance Computing

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SDS406 – Fall semester, 2024 - 2025

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L04: OpenMP and Optimization, 21st October 2024

Outline for today

OpenMP

- Review of OpenMP examples; `axpy` and `xdoty`

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Performance analysis and optimization

- Understanding of program performance
- Understanding of hardware characteristics in terms of performance
- Understanding of *potential* performance of a program given the hardware characteristics
- Optimization steps to approach potential performance

OpenMP Examples

Linear algebra

Operation:

$$z_i = a x_i + y_i$$

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Number of *floating point operations*

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  - One multiplication (ax_i)

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  - One addition ($+y_i$)

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```
double p = 2.0*n/t1/1e9;
printf(" nth = %2d, t0 = %lf sec, t1 = %lf sec, diff z norm = %e, perf = %lf Gflop/s\n", nth, t0, t1, norm, p);
```

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- For `n` iterations, `2*n/t1/1e9` in Gflops/s

OpenMP for linear algebra

```
[ikoutsou@front02 ex03]$ for ((n=1; n<=16; n++))
> do OMP_NUM_THREADS=${n} srun -N 1 -p p100 -n 1 --cpus-per-task=64 ./axpy $((32*1024*1024))
> done
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n_{OMP}	`axpy` [Gflop/s]	`xdoty` [Gflop/s]
1	0.509	0.791
2	0.999	1.564
3	1.443	2.226
4	1.890	2.907
5	2.294	3.594
6	2.705	4.268
7	3.000	4.922
8	3.102	5.465
9	3.247	5.651
10	3.179	6.183
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12	3.404	7.039
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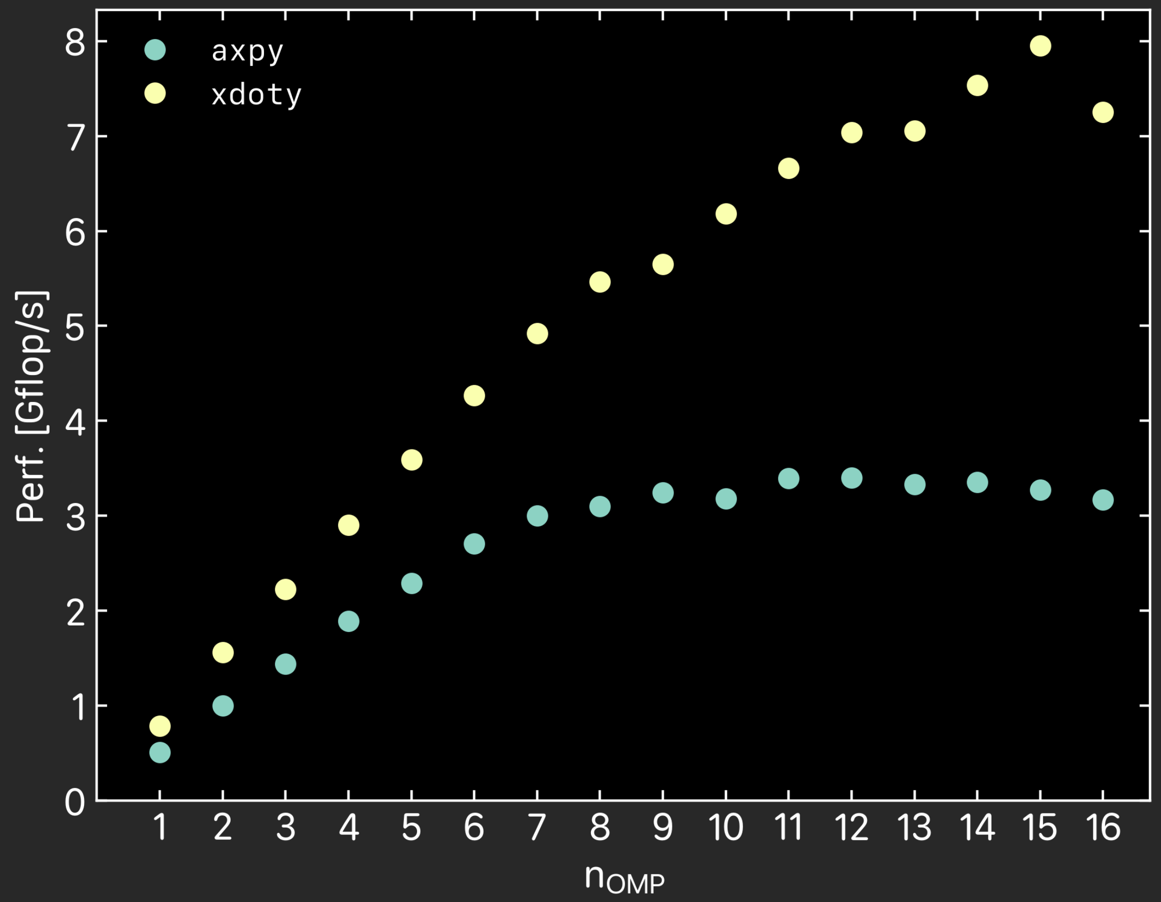

Performance Analysis

Performance analysis

Understand performance and hardware to evaluate the potential performance of your code

- Performance analysis: analysis of the performance of a code; comparison to what is expected
- Identification of bottlenecks
- Identification of improvements that can be made

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Hardware characteristics

Peak floating point rate

- The theoretical, highest number of floating point operations that can be carried out by a computational unit
- Depends on: clock rate, vector length, FPUs per core, cores per socket

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Peak bandwidth

- The theoretical, highest number of bytes that can be read/written from/to some level of memory (L1,2,3 cache, RAM, etc.)
- For RAM: data rate, channels, ranks, banks

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When optimizing, it is important to have these numbers in mind for the machine you're running on

`P100` GPU nodes

On Linux, you can obtain processor details via `cat /proc/cpuinfo`:

```
processor       : 0
vendor_id       : GenuineIntel
cpu family      : 6
model           : 85
model name      : Intel(R) Xeon(R) Gold 6130 CPU @ 2.10GHz
 ...
cpu MHz         : 2100.000
cache size      : 22528 KB
physical id     : 0
siblings        : 32
core id         : 0
cpu cores       : 16
 ...
flags           : fpu vme de pse tsc msr pae mce cx8 apic  ...
```

Look up the processor on https://ark.intel.com

Peak performance

- Peak Floating Point rate
    - 16-cores per socket, 2 sockets per node, clock: 2.1 GHz
    - Best case: two 512-bit multiply-and-add per cycle (AVX-512 FMA)
    - In double precision: $2 \times$ (8 `mul` + 8 `add`) per cycle = 32 flop/cycle
    - Therefore: $2.1\text{x}10^9$ cycles/s $\times$ 32 flop/cycle = 67.2 Gflop/s per core
    - 1,075.2 Gflop/s per socket
- Peak BW
    - Up to 6 channels per socket $\Rightarrow$ 128 GB/s to RAM per socket
    - Assuming all channels filled, two sockets $\Rightarrow$ 256 GB/s
      $\longrightarrow$ `p100` nodes: 4 channels per socket filled
        - Theoretical peak **80 GBytes/s** per socket
- Some (semi-)standard tools
    - On Linux, you can obtain processor details via `cat /proc/cpuinfo`.
    - You can obtain topology and memory info e.g. `hwloc`, `dmidecode` (latter requires access to `/dev/mem`)

Computational kernels

Sustained performance

- Sustained FP-rate: the measured, average number of floating point operations carried out by the kernel per unit time
    - `add`, `sub`, and `mul` count as 1 flop
    - `dev`, `sqrt`, `sin`, etc. count $\geqslant 2$ flops. Depends on architecture
    - Count number of flops in kernel and divide by runtime
    - Alternatively, or for more complex codes, use performance counters

In our examples we will see cases of kernels where the flops are countable

- Sustained BW: the measured, average bytes read/written from main memory per unit time
    - As in the case of FP-rate, count bytes needed to be read and bytes needed to be written to and from RAM and divide by run time
    - *Maximum data reuse* assumption: "local" data, once read from RAM, never needs to be re-read

Maximum data reuse

- A (hopefully) familiar example:

$$y_i = a \cdot x_i + y_i, i = 0, \ldots, L-1$$

- It's implementation in C:

```c
double y[L]; /* Or malloc() */
double x[L]; /* Or malloc() */
double a;

/*  ...  Some initialization of a, x, and y
 *  omitted here ...
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for(int i=0; i<L; i++) {
  y[i] = a*x[i] + y[i];
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- Number of flops
  - $N_{fp} = L \cdot 2$
- Number of bytes of I/O
  - $N_{IO} = w \cdot (3 \cdot L)$
    - Read each element of y once
    - Read each element of x once
    - Write an element of y once
  - w: word-length in bytes, e.g.
    - $w = 4$ bytes for single precision,
    - $w = 8$ bytes for double, etc.

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How about the memory accesses of a?

- Maximum data reuse assumption: a is read only in the first iteration and remains in *cache* for all following iterations

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- Another example:

$$y_i = \sigma \cdot (x_i - x_{i-1}), \quad i = 1, \ldots, L-1$$

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  - For practical purposes, when $L \gg$, this is $N_{fp} \simeq L \cdot 2$
- Number of bytes of I/O
  - In each iteration, read two elements of x and write one of y
  - **But**, one element of x has been read during previous iteration $\Rightarrow N_{IO} = w \cdot (2 \cdot (L-1) + 1) \simeq w \cdot 2 \cdot L$

Maximum data reuse

For counting N_{IO}, looking at the iteration unrolled may help to reveal data reuse

```
y[  1] = sigma*(x[  1] - x[  0]);
y[  2] = sigma*(x[  2] - x[  1]);
y[  3] = sigma*(x[  3] - x[  2]);
 ...
y[L-1] = sigma*(x[L-1] - x[L-2]);
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`sigma` and elements of `x[]` are required multiple times. However we assume they only need to be read once.

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- Given some measurement of the run-time $\bar{T}$
  - FP-rate: $\beta_{fp} = \frac{N_{fp}}{\bar{T}}$
  - IO-rate: $\beta_{IO} = \frac{N_{IO}}{\bar{T}}$

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- Given some measurement of the run-time $\bar{T}$
  - FP-rate: $\beta_{fp} = \frac{N_{fp}}{\bar{T}}$
  - IO-rate: $\beta_{IO} = \frac{N_{IO}}{\bar{T}}$
- This motivates defining their ratio, which is referred to as *intensity*

$$I = \frac{N_{fp}}{N_{IO}}$$

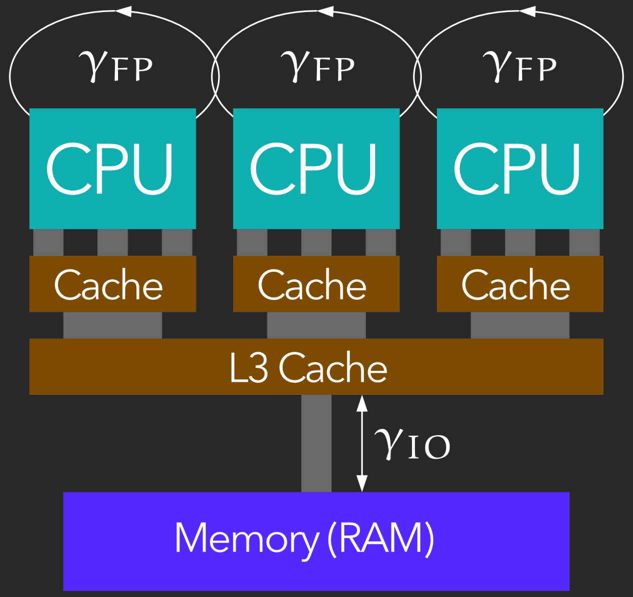
Intensities

Computational kernel intensity

- Ratio of kernel floating point operations to bytes of I/O
- For our previous example:
  - $\mathrm{I_k} = \frac{\mathrm{N_{fp}}}{\mathrm{N_{IO}}} = \frac{2\mathrm{L}}{2w\mathrm{L}} = 1/w$
  - Note how the problem size L drops out $\Rightarrow$ constant $\mathrm{I_k}$ irrespective of problem size
  - E.g. for double precision ($w = 8$), $\mathrm{I_k}$=0.125 flops/byte

Machine flop/byte ratio

- Similarly to $\mathrm{I_k}$, we can define the *machine flop/byte ratio* ($\mathrm{I_m}$)
- $\mathrm{I_m} = \frac{\gamma_{\mathrm{fp}}}{\gamma_{\mathrm{IO}}}$
- E.g. for the nodes of the `p100` partition: $\mathrm{I_m} = 8.4 \frac{\mathrm{flop}}{\mathrm{byte}}$



Intensities

Balance between kernel / hardware intensities

- $I_k \gg I_m$: Kernel is "compute-bound" on this architecture. Higher γ_{fp} would lead to higher performance, but higher γ_{IO} would not necessarily.
- $I_k \ll I_m$: Kernel is "bandwidth-" or "memory-bound" on this architecture. Higher γ_{IO} would lead to higher performance, but higher γ_{fp} would not necessarily.
- $I_k \simeq I_m$: Kernel is balanced on this architecture. Ideal situation.

For the example we have been studying

- $I_k \ll I_m \Rightarrow$ the kernel is memory-bound

Note the assumptions that enter I_k and I_m

- γ_{fp} considers all operations can be a sequence of multiply-and-add
- β_{IO} assumes maximum data reuse
- I_k constant if problem size L drops out

Kernel computational intensity

Another example: matrix-matrix multiplication

- Consider a matrix-matrix multiplication: $C_{M \times K} = A_{M \times N} \cdot B_{N \times K}$

```
double C[M][K];
double A[M][N];
double B[N][K];

for(int m=0; m<M; m++) {
  for(int k=0; k<K; k++) {
    C[m][k] = 0;
    for(int n=0; n<N; n++) {
      C[m][k] += A[m][n]*B[n][k];
    }
  }
}
```

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- $N_{fp} = 2 \cdot M \cdot K \cdot N$
- $N_{IO} = w \cdot (M \cdot K + M \cdot N + N \cdot K)$
- $I_k = \frac{2}{w} \frac{1}{\frac{1}{M} + \frac{1}{N} + \frac{1}{K}}$
- E.g. for a square problem $M = N = K, \Rightarrow I_k = \frac{2}{3}\frac{N}{w}$

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- E.g. for a square problem $M = N = K, \Rightarrow I_k = \frac{2}{3} \frac{N}{w}$

- This is an example of a kernel where I_k depends on the problem size.
- On a given architecture with I_m, the kernel transitions from bandwidth-bound to compute-bound as N increases.
- For double precision (w = 8 bytes), the kernel is balanced when $N \simeq 100$.

Optimization

Given a code you wish to optimize, for an architecture with I_m

- What is N_{fp} and N_{IO} and what is the resulting I_k?
- Is the kernel memory or compute bound on this architecture?
- What do you obtain for β_{fp} and β_{IO}
  - For this one requires measuring the performance on the targeted architecture
- What are the ratios $\frac{\beta_{fp}}{\gamma_{fp}}$ and $\frac{\beta_{IO}}{\gamma_{IO}}$?

These are questions you need to answer before considering optimization

- After answering the above, we can start considering targeted optimizations for our kernel on the given machine
  - If your kernel is memory-bound, we should be trying to optimize for memory I/O. Ideally we try to achieve a $\frac{\beta_{IO}}{\gamma_{IO}} \longrightarrow 1$.
  - If your kernel is compute-bound, we should be trying to optimize for a higher FP-rate. Ideally we try to achieve a $\frac{\beta_{fp}}{\gamma_{fp}} \longrightarrow 1$.

Performance analysis

Back to our linear algebra kernels

`axpy`:

$$y_i \leftarrow a \cdot x_i + y_i$$

`xdoty`:

$$r = \sum_i x_i \cdot y_i$$

Performance analysis

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- Run again for 1 to 16 OpenMP threads

Performance analysis

Back to our linear algebra kernels

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$$r = \sum_i x_i \cdot y_i$$

- Run again for 1 to 16 OpenMP threads
- But now, we care about understanding performance; first of all, enable additional compiler optimizations with `-O3`:

```
[ikoutsou@front02 l04]$ cc -O3 -fopenmp -o axpy axpy.c
```

Performance analysis

Back to our linear algebra kernels

`axpy`:

$$y_i \leftarrow a \cdot x_i + y_i$$

`xdoty`:

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- Run again for 1 to 16 OpenMP threads
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```
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```

- We would also like to ensure we're running each OpenMP thread on a *physical core*

Performance analysis

Back to our linear algebra kernels

`axpy`:

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- Run again for 1 to 16 OpenMP threads
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  ```
  [ikoutsou@front02 l04]$ cc -O3 -fopenmp -o axpy axpy.c
  ```

- We would also like to ensure we're running each OpenMP thread on a *physical core*

This needs to be ensured at two levels:

- Slurm's `salloc` or `srun`
- With the OpenMP runtime

Performance analysis

Back to our linear algebra kernels

`axpy`:

$$y_i \leftarrow a \cdot x_i + y_i$$

`xdoty`:

$$r = \sum_i x_i \cdot y_i$$

- Run again for 1 to 16 OpenMP threads
- But now, we care about understanding performance; first of all, enable additional compiler optimizations with `-O3`:

```
[ikoutsou@front02 l04]$ cc -O3 -fopenmp -o axpy axpy.c
```

- We would also like to ensure we're running each OpenMP thread on a *physical core*

This needs to be ensured at two levels:

- Slurm's `salloc` or `srun`
- With the OpenMP runtime

This thread placement is also referred to as the *OpenMP thread affinity*

Thread/process affinity

Affinity at the Slurm level

- Slurm sets defaults, but these are usually configured by the system administrators and can therefore be different on each system or even every Slurm partition
  - For example, `-n 16`, depending on this setup, may provide us with 16 cores (one CPU) or with 8 cores and two processes per core
  - Asking for 64 tasks (32 cores, 2 threads per core), ensures we have allocated all CPU resources of a node
  - But, running with `OMP_NUM_THREADS=16` may do one of several things, e.g.:
    - Place 8 OpenMP threads on 8 cores of the first CPU and 8 threads on the 8 cores of the second CPU
    - Place 16 OpenMP threads on the 8 cores of one of the two CPUs, thus "oversubscribing" each core by $\times 2$
    - Place 16 OpenMP threads on the 16 cores of one of the two CPUs

Thread/process affinity

Affinity at the Slurm level

- Slurm sets defaults, but these are usually configured by the system administrators and can therefore be different on each system or even every Slurm partition
    - For example, `-n 16`, depending on this setup, may provide us with 16 cores (one CPU) or with 8 cores and two processes per core
    - Asking for 64 tasks (32 cores, 2 threads per core), ensures we have allocated all CPU resources of a node
    - But, running with `OMP_NUM_THREADS=16` may do one of several things, e.g.:
        - Place 8 OpenMP threads on 8 cores of the first CPU and 8 threads on the 8 cores of the second CPU
        - Place 16 OpenMP threads on the 8 cores of one of the two CPUs, thus "oversubscribing" each core by $\times 2$
        - Place 16 OpenMP threads on the 16 cores of one of the two CPUs
    - You should be in position to:
        - Specify the desired placement of OpenMP threads to cores
        - Verify that the actual placement is indeed the desired placement

Thread/process affinity

Getting CPU info

- You can check which cores have been allocated and their placement with the `hwloc` tool

```
[ikoutsou@front02 ~]$ salloc -N 1 -n 1 --cpus-per-task=6 -p p100
[ikoutsou@cyc01 ~]$ module load gompi
[ikoutsou@cyc01 ~]$ hwloc-ls|more
[ikoutsou@cyc01 ex04]$ hwloc-ls|more
Machine (123GB total)
  Package L#0
    NUMANode L#0 (P#0 63GB)
    L3 L#0 (22MB)
      L2 L#0 (1024KB) + L1d L#0 (32KB) + L1i L#0 (32KB) + Core L#0
        PU L#0 (P#0)
        PU L#1 (P#32)
      L2 L#1 (1024KB) + L1d L#1 (32KB) + L1i L#1 (32KB) + Core L#1
        PU L#2 (P#1)
        PU L#3 (P#33)
      L2 L#2 (1024KB) + L1d L#2 (32KB) + L1i L#2 (32KB) + Core L#2
        PU L#4 (P#2)
        PU L#5 (P#34)
    HostBridge
     ...
```

- A `NUMANode` is one CPU socket. Each `L#` is a core.
- Slurm gave us 3 cores on the same CPU

Thread/process affinity

Getting CPU info

- We will reserve all cores on the node with `--cpus-per-task=64` and determine the placement via OpenMP

Thread/process affinity

Getting CPU info

- We will reserve all cores on the node with `--cpus-per-task=64` and determine the placement via OpenMP

```
[ikoutsou@front02 ~]$ salloc -N 1 -n 1 --cpus-per-task=64 -p p100
[ikoutsou@cyc01 ex04]$ hwloc-ls|more
Machine (123GB total)
  Package L#0
    NUMANode L#0 (P#0 63GB)
    L3 L#0 (22MB)
      L2 L#0 (1024KB) + L1d L#0 (32KB) + L1i L#0 (32KB) + Core L#0
        PU L#0 (P#0)
        PU L#1 (P#32)
      L2 L#1 (1024KB) + L1d L#1 (32KB) + L1i L#1 (32KB) + Core L#1
        PU L#2 (P#1)
        PU L#3 (P#33)
  ...
  Package L#1
    NUMANode L#1 (P#1 60GB)
    L3 L#1 (22MB)
      L2 L#16 (1024KB) + L1d L#16 (32KB) + L1i L#16 (32KB) + Core L#16
        PU L#32 (P#16)
        PU L#33 (P#48)
      L2 L#17 (1024KB) + L1d L#17 (32KB) + L1i L#17 (32KB) + Core L#17
        PU L#34 (P#17)
        PU L#35 (P#49)
```

- You should see two `NUMANode`, 16 cores for each, and each core has two `PU`s

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
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    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
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- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example A:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f96eefc77c0 affinity 0-63
level 1 thread 0x7f96ae60d700 affinity 0-63
level 1 thread 0x7f96ade0c700 affinity 0-63
level 1 thread 0x7f96ad60b700 affinity 0-63
nth =  4   t0 = 0.129383 sec, t1 = 0.035683 sec, diff z norm = 0.000000e+00, perf = 1.880688 Gflop/s
```

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
    - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
        - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
    - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
        - `spread`: Spread out consecutive OpenMP threads over `PLACES`
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- An additional environment variables allows us to check where the OpenMP threads are placed:
    - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example A:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f96eefc77c0 affinity 0-63
level 1 thread 0x7f96ae60d700 affinity 0-63
level 1 thread 0x7f96ade0c700 affinity 0-63
level 1 thread 0x7f96ad60b700 affinity 0-63
nth =  4   t0 = 0.129383 sec, t1 = 0.035683 sec, diff z norm = 0.000000e+00, perf = 1.880688 Gflop/s
```

- No affinity specified, so all threads can take all slots — from 0 to 63

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example B:

```
[ikoutsou@front02 l04]$ export OMP_PROC_BIND=true; export OMP_NUM_THREADS=4; export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f8a6703a7c0 affinity 0
level 1 thread 0x7f8a26680700 affinity 32
level 1 thread 0x7f8a25e7f700 affinity 1
level 1 thread 0x7f8a2567e700 affinity 33
 nth =   4   t0 = 0.130506 sec, t1 = 0.061074 sec, diff z norm = 0.000000e+00, perf = 1.098812 Gflop/s
```

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
    - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
        - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
    - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
        - `spread`: Spread out consecutive OpenMP threads over `PLACES`
        - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
    - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example B:

```
[ikoutsou@front02 l04]$ export OMP_PROC_BIND=true; export OMP_NUM_THREADS=4; export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f8a6703a7c0 affinity 0
level 1 thread 0x7f8a26680700 affinity 32
level 1 thread 0x7f8a25e7f700 affinity 1
level 1 thread 0x7f8a2567e700 affinity 33
 nth =  4   t0 = 0.130506 sec, t1 = 0.061074 sec, diff z norm = 0.000000e+00, perf = 1.098812 Gflop/s
```

- OpenMP threads bound to specific hardware thread

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example B:

```
[ikoutsou@front02 l04]$ export OMP_PROC_BIND=true; export OMP_NUM_THREADS=4; export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f8a6703a7c0 affinity 0
level 1 thread 0x7f8a26680700 affinity 32
level 1 thread 0x7f8a25e7f700 affinity 1
level 1 thread 0x7f8a2567e700 affinity 33
 nth =  4   t0 = 0.130506 sec, t1 = 0.061074 sec, diff z norm = 0.000000e+00, perf = 1.098812 Gflop/s
```

- OpenMP threads bound to specific hardware thread
- The numbering follows `hwloc-ls`, the `P#` entry $\Rightarrow$ `0` and `32` are two hardware threads of the same core. Same for `1` and `33`

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example C:

```
[ikoutsou@front02 l04]$ export OMP_PROC_BIND=true; export OMP_NUM_THREADS=4; export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ export OMP_PLACES=cores
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7fbb918d87c0 affinity 0,32
level 1 thread 0x7fbb50f1e700 affinity 1,33
level 1 thread 0x7fbb5071d700 affinity 2,34
level 1 thread 0x7fbb4ff1c700 affinity 3,35
nth =  4   t0 = 0.129853 sec, t1 = 0.035487 sec, diff z norm = 0.000000e+00, perf = 1.891086 Gflop/s
```

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example C:

```
[ikoutsou@front02 l04]$ export OMP_PROC_BIND=true; export OMP_NUM_THREADS=4; export OMP_DISPLAY_AFFINITY=true
[ikoutsou@front02 l04]$ export OMP_PLACES=cores
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7fbb918d87c0 affinity 0,32
level 1 thread 0x7fbb50f1e700 affinity 1,33
level 1 thread 0x7fbb5071d700 affinity 2,34
level 1 thread 0x7fbb4ff1c700 affinity 3,35
nth =  4   t0 = 0.129853 sec, t1 = 0.035487 sec, diff z norm = 0.000000e+00, perf = 1.891086 Gflop/s
```

- OpenMP threads are bound to cores, but can "float" between hardware threads of the same core

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example D:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true; export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ export OMP_PLACES="{0}:4:1"
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f70941da7c0 affinity 0
level 1 thread 0x7f7053820700 affinity 1
level 1 thread 0x7f705301f700 affinity 2
level 1 thread 0x7f705281e700 affinity 3
nth =  4   t0 = 0.130987 sec, t1 = 0.036052 sec, diff z norm = 0.000000e+00, perf = 1.861447 Gflop/s
```

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example D:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true; export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ export OMP_PLACES="{0}:4:1"
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7f70941da7c0 affinity 0
level 1 thread 0x7f7053820700 affinity 1
level 1 thread 0x7f705301f700 affinity 2
level 1 thread 0x7f705281e700 affinity 3
nth =  4   t0 = 0.130987 sec, t1 = 0.036052 sec, diff z norm = 0.000000e+00, perf = 1.861447 Gflop/s
```

- Explicitly specify the placement of OpenMP threads (therefore `OMP_PROC_BIND` is unnecessary)

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example E:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true; export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ export OMP_PLACES="{0}:4:8"
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7fe4deb797c0 affinity 0
level 1 thread 0x7fe49e1bf700 affinity 8
level 1 thread 0x7fe49d9be700 affinity 16
level 1 thread 0x7fe49d1bd700 affinity 24
nth =  4   t0 = 0.131311 sec, t1 = 0.035607 sec, diff z norm = 0.000000e+00, perf = 1.884705 Gflop/s
```

Thread/process affinity

Affinity at the OpenMP level

- Two environment variables:
  - `OMP_PLACES`: Specify what a "slot" is for OpenMP. Options are `sockets`, `cores`, `threads`
    - You can also specify *which* slots to use for OpenMP. I.e., which cores, which threads, which sockets
  - `OMP_PROC_BIND`: Specify whether OpenMP threads are allowed to move between `PLACES`. `OMP_PROC_BIND=false` means **don't bind**, i.e. allow OpenMP threads to move. In addition to `true`, you can specify:
    - `spread`: Spread out consecutive OpenMP threads over `PLACES`
    - `close`: Keep consecutive OpenMP threads over `PLACES` close
- An additional environment variables allows us to check where the OpenMP threads are placed:
  - `OMP_DISPLAY_AFFINITY`: prints out numbers indicating the hardware threads

Example E:

```
[ikoutsou@front02 l04]$ export OMP_DISPLAY_AFFINITY=true; export OMP_NUM_THREADS=4
[ikoutsou@front02 l04]$ export OMP_PLACES="{0}:4:8"
[ikoutsou@front02 l04]$ srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
level 1 thread 0x7fe4deb797c0 affinity 0
level 1 thread 0x7fe49e1bf700 affinity 8
level 1 thread 0x7fe49d9be700 affinity 16
level 1 thread 0x7fe49d1bd700 affinity 24
nth =  4   t0 = 0.131311 sec, t1 = 0.035607 sec, diff z norm = 0.000000e+00, perf = 1.884705 Gflop/s
```

- Two OpenMP threads on one CPU socket and two on the other

Performance analysis

- Rerun `xdoty.c` and `axpy.c`
- You can use your own from last lesson or take them from `/onyx/data/sds406f24/l04/ex01/`

Performance analysis

- Rerun `xdoty.c` and `axpy.c`
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```
[ikoutsou@front02 l04]$ for((n=1; n<=16; n++))
> do
> export OMP_PLACES="{0}:$n:1"
> export OMP_NUM_THREADS=$n
> srun -N 1 -n 1 --cpus-per-task=64 -p p100 ./axpy $((32*1024*1024))
> done
nth =  1   t0 = 0.033659 sec, t1 = 0.036666 sec, diff z norm = 0.000000e+00, perf = 1.830279 Gflop/s
nth =  2   t0 = 0.033601 sec, t1 = 0.019508 sec, diff z norm = 0.000000e+00, perf = 3.440089 Gflop/s
nth =  3   t0 = 0.033593 sec, t1 = 0.015206 sec, diff z norm = 0.000000e+00, perf = 4.413355 Gflop/s
nth =  4   t0 = 0.033526 sec, t1 = 0.014653 sec, diff z norm = 0.000000e+00, perf = 4.579882 Gflop/s
nth =  5   t0 = 0.033566 sec, t1 = 0.013098 sec, diff z norm = 0.000000e+00, perf = 5.123596 Gflop/s
nth =  6   t0 = 0.033436 sec, t1 = 0.012727 sec, diff z norm = 0.000000e+00, perf = 5.272943 Gflop/s
nth =  7   t0 = 0.033536 sec, t1 = 0.012487 sec, diff z norm = 0.000000e+00, perf = 5.374327 Gflop/s
nth =  8   t0 = 0.033525 sec, t1 = 0.013092 sec, diff z norm = 0.000000e+00, perf = 5.125928 Gflop/s
nth =  9   t0 = 0.033648 sec, t1 = 0.012486 sec, diff z norm = 0.000000e+00, perf = 5.374737 Gflop/s
nth = 10   t0 = 0.033825 sec, t1 = 0.012753 sec, diff z norm = 0.000000e+00, perf = 5.262198 Gflop/s
nth = 11   t0 = 0.033825 sec, t1 = 0.012249 sec, diff z norm = 0.000000e+00, perf = 5.478725 Gflop/s
nth = 12   t0 = 0.033886 sec, t1 = 0.012366 sec, diff z norm = 0.000000e+00, perf = 5.426861 Gflop/s
nth = 13   t0 = 0.033876 sec, t1 = 0.012259 sec, diff z norm = 0.000000e+00, perf = 5.474250 Gflop/s
nth = 14   t0 = 0.033799 sec, t1 = 0.012575 sec, diff z norm = 0.000000e+00, perf = 5.336727 Gflop/s
nth = 15   t0 = 0.034108 sec, t1 = 0.012522 sec, diff z norm = 0.000000e+00, perf = 5.359182 Gflop/s
nth = 16   t0 = 0.034084 sec, t1 = 0.014791 sec, diff z norm = 0.000000e+00, perf = 4.537138 Gflop/s
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OpenMP and controlling for affinity

n_{OMP}	`axpy` [Gflop/s]	`xdoty` [Gflop/s]
1	1.830	1.541
2	3.440	2.985
3	4.413	4.312
4	4.580	5.479
5	5.124	6.652
6	5.273	7.724
7	5.374	8.553
8	5.126	8.609
9	5.375	8.990
10	5.262	8.974
11	5.479	8.914
12	5.427	8.819
13	5.474	8.756
14	5.337	8.765
15	5.359	8.638
16	4.537	8.298

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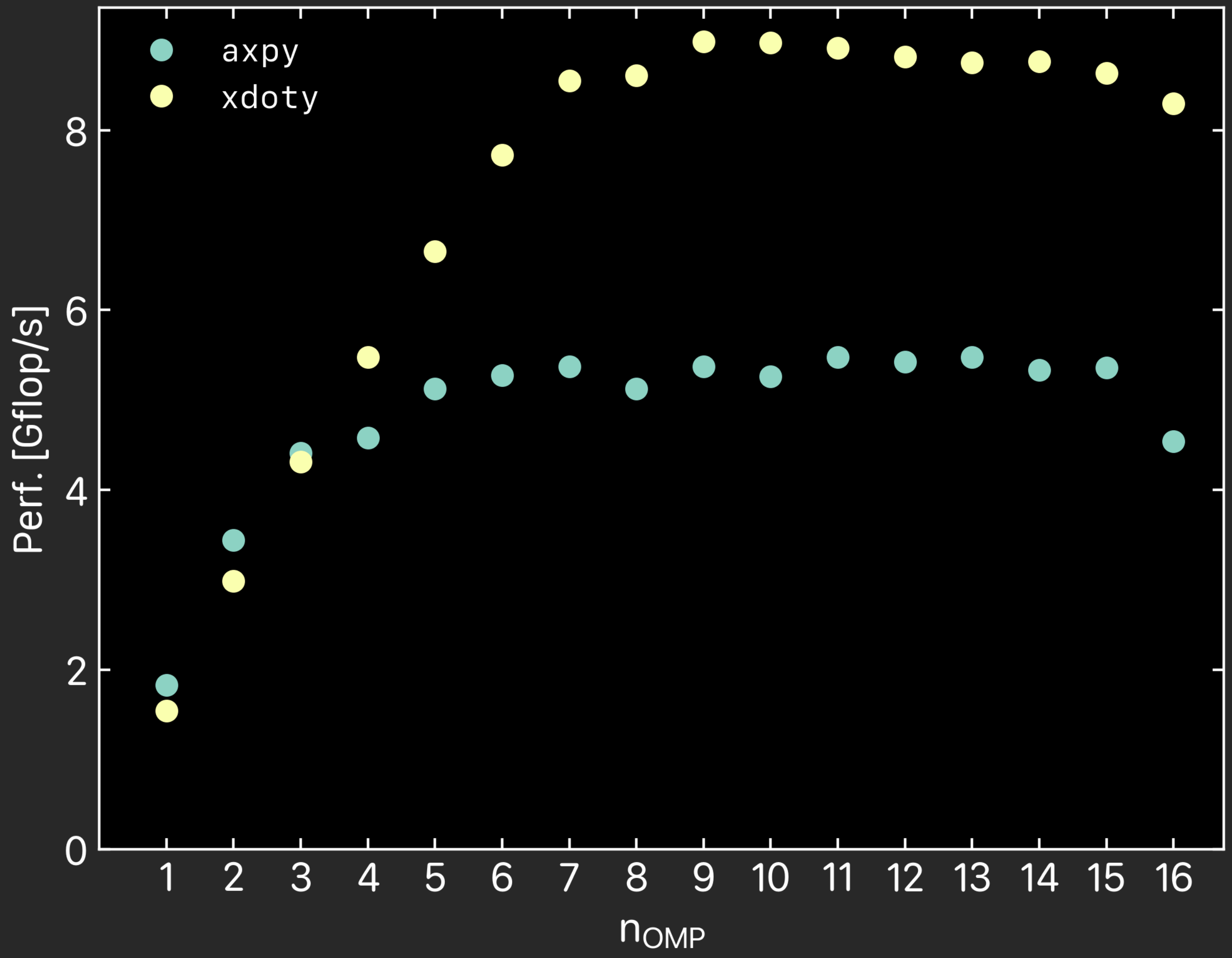

Performance analysis

Back to our linear algebra kernels

`axpy`:

$$y_i \leftarrow a \cdot x_i + y_i$$

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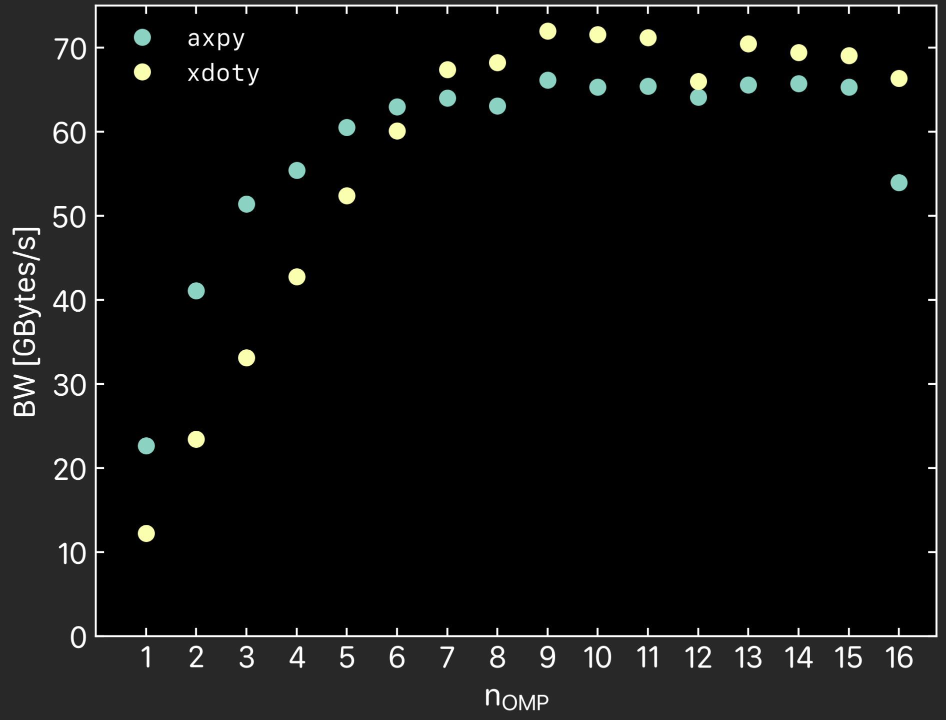

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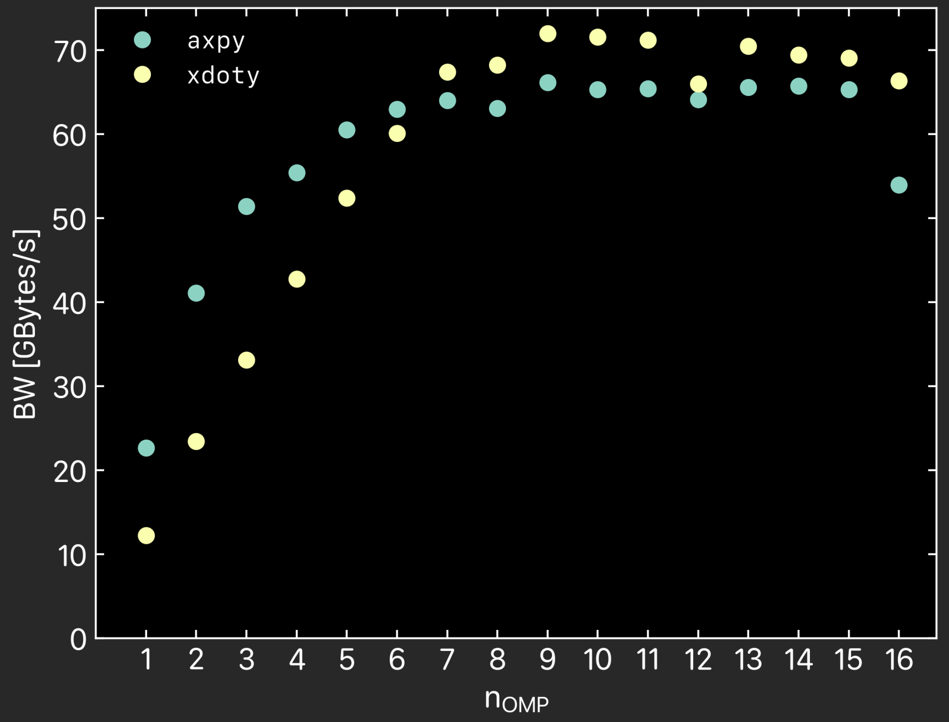

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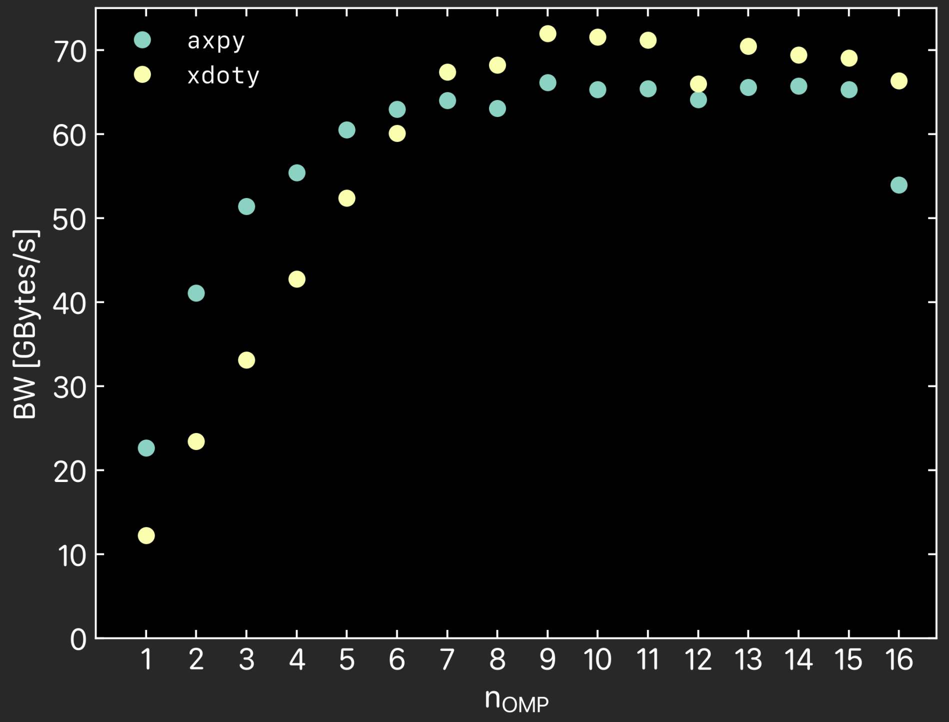
- Compare with *per socket theoretical peak* of $\sim$80 GBytes/s



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double t0 = stop_watch(0);
int niter = 0;
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$\longrightarrow$ *Warm-up*: Compile and run once using $n = 1024^2$ and 2 OpenMP thread

Performance analysis

Another example using `axpy()`:

$$y_i \leftarrow a \cdot x_i + y_i \quad i = 0, \ldots, L-1$$

```
[ikoutsou@front02 ex02]$ sbatch run.sh
Submitted batch job 181364
[ikoutsou@front02 ex02]$ cat axpy.txt
 nth =  2   t0 = 3.678e-04 sec   L =    1048576   niter =     8158   beta_fp = 5.702e+00 Gflop/s   beta_io = 6.843e+01 GBytes/s
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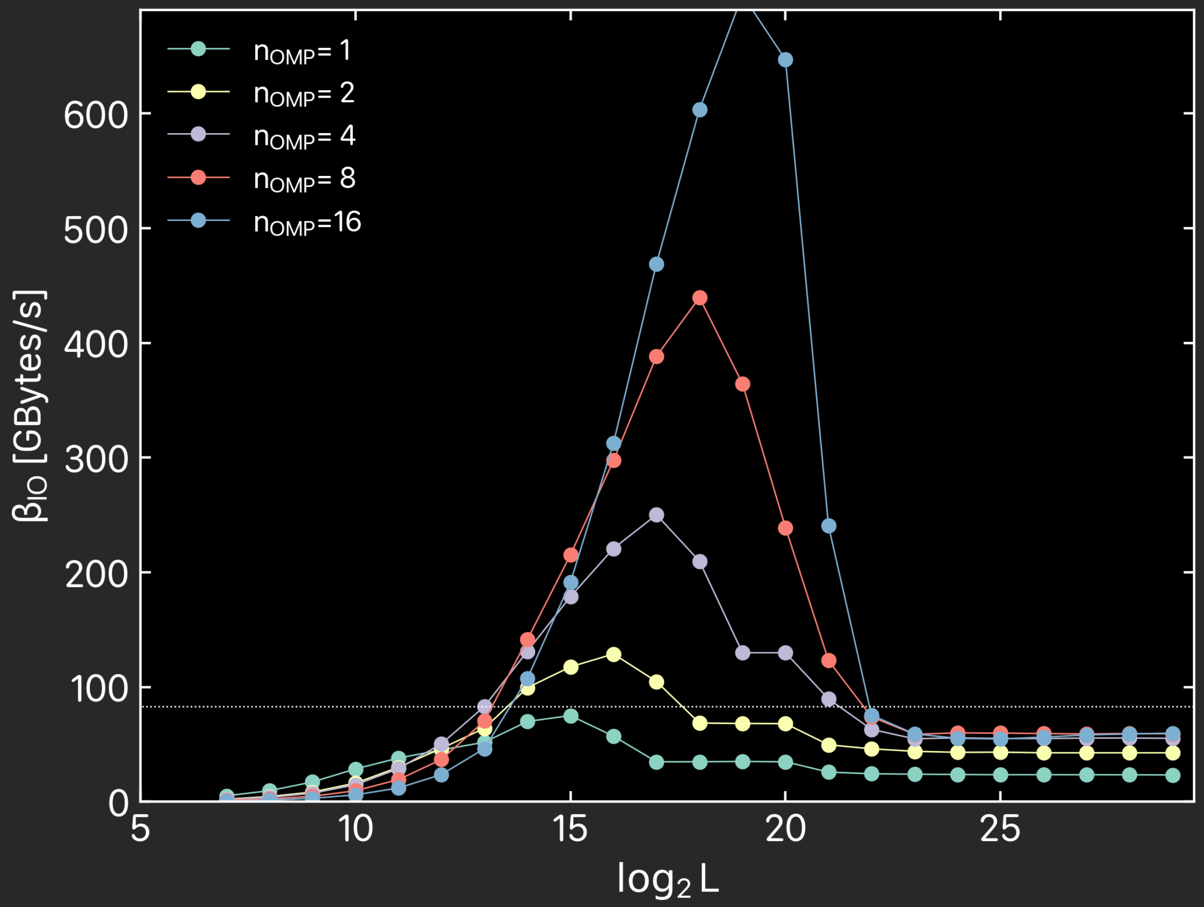
  $\longrightarrow$ best use log-scale on the x-axis

Performance analysis



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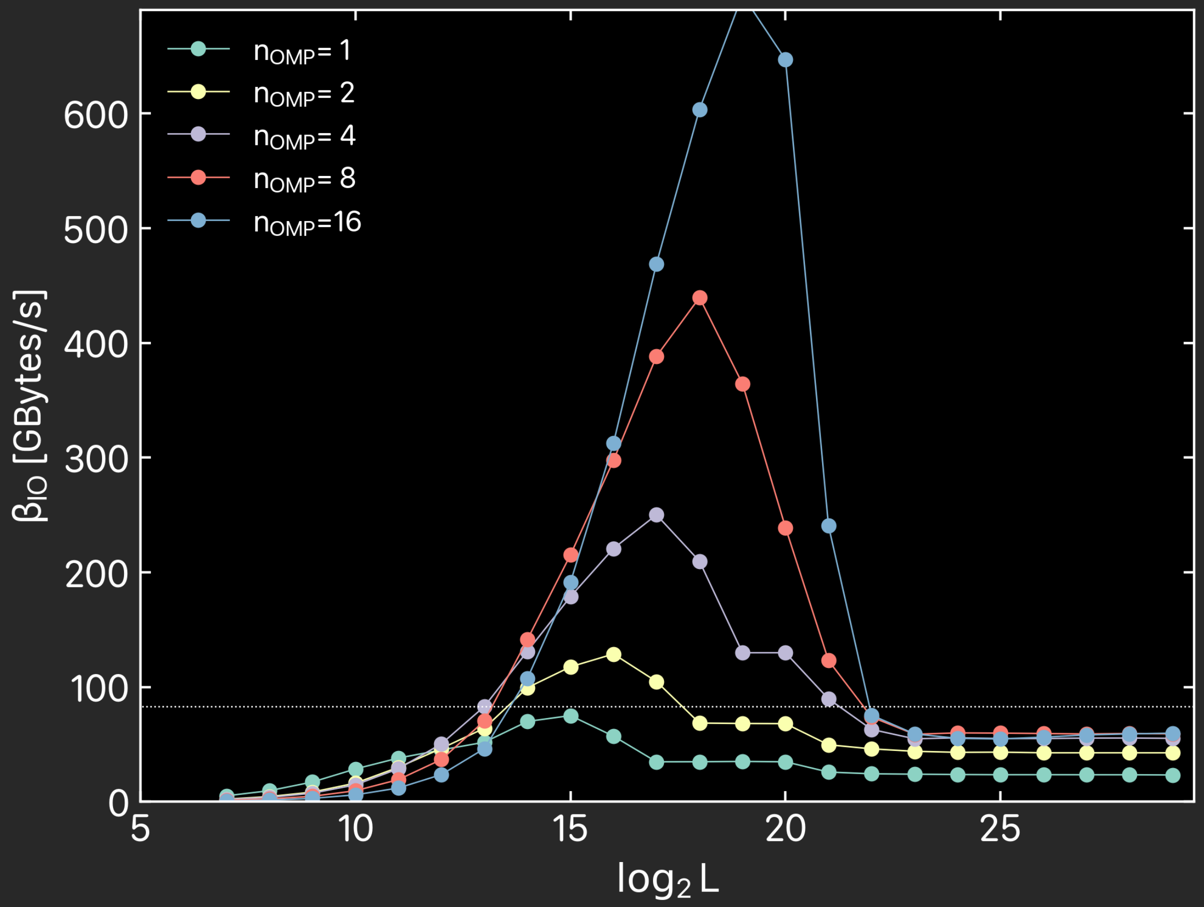

- Dashed horizontal line is theoretical peak bandwidth (single socket) of 83 GBytes/s

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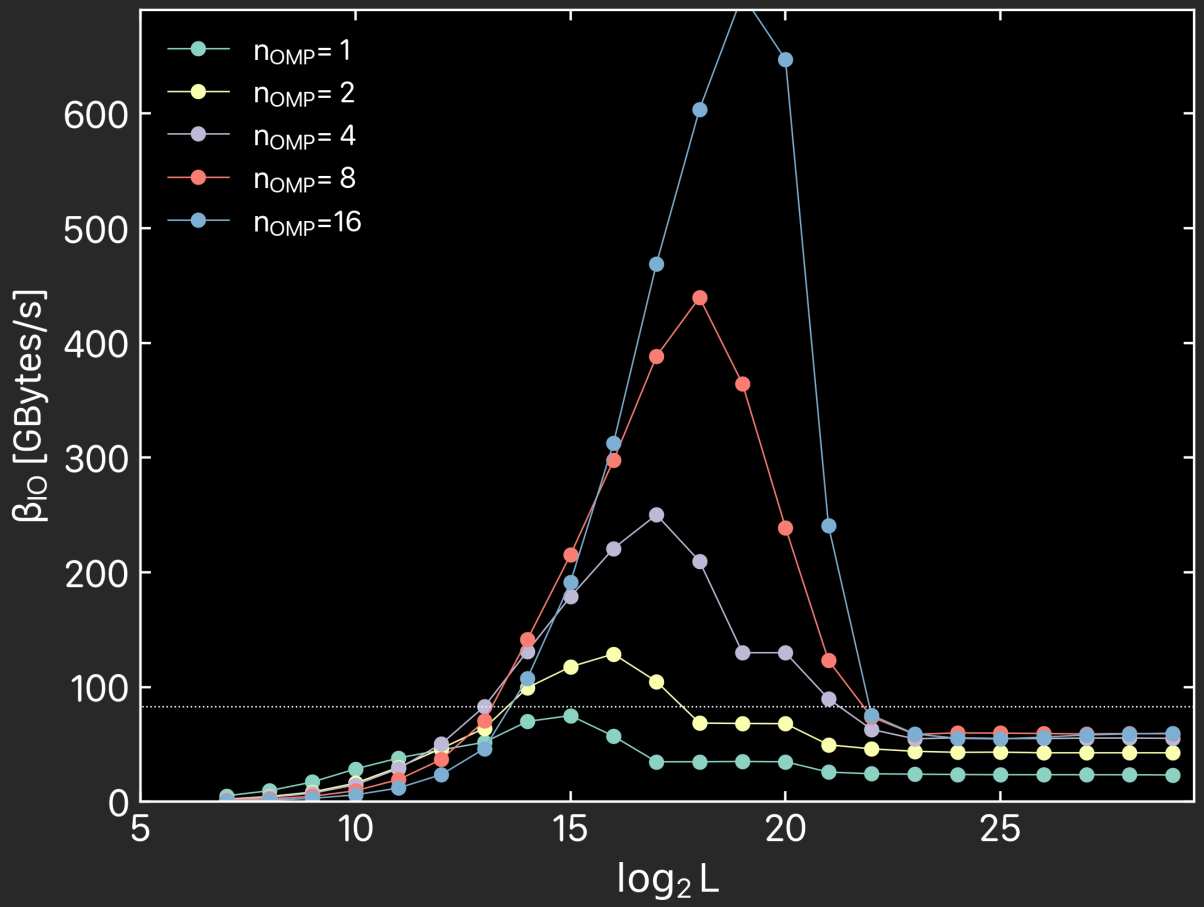

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- What is happening between $L = 2^{15}$ and 2^{20}?

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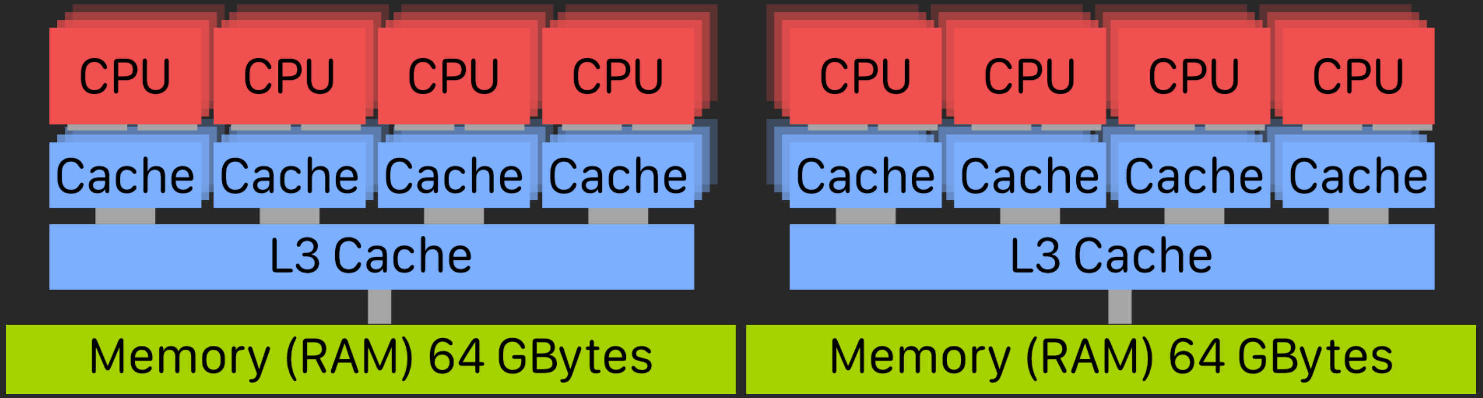

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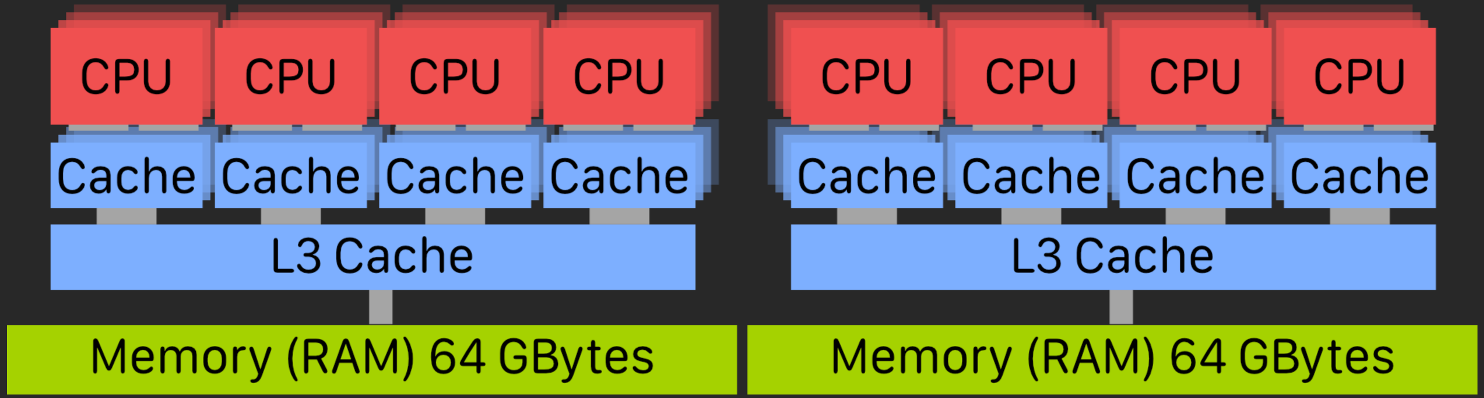

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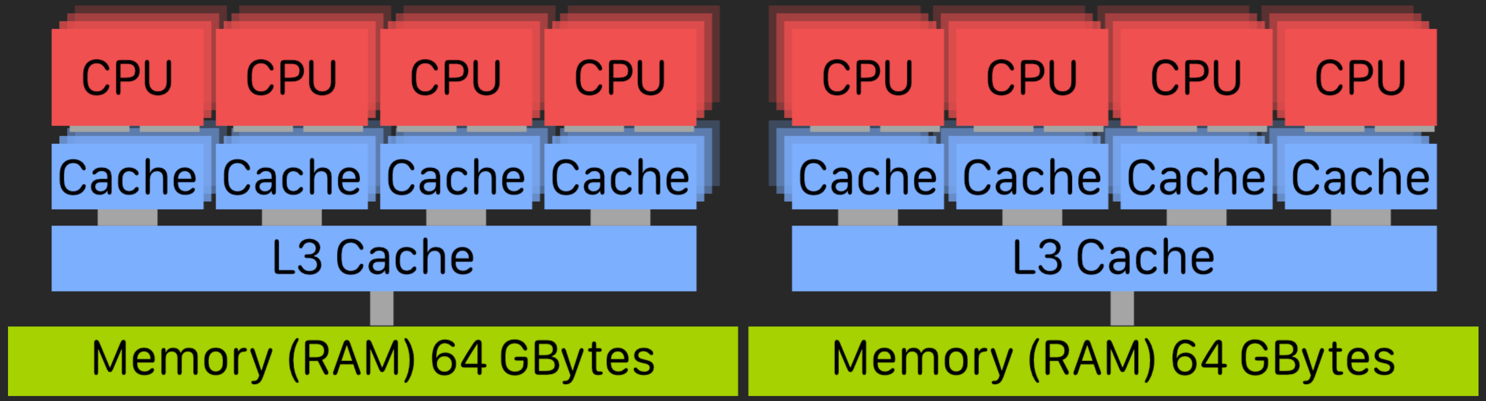

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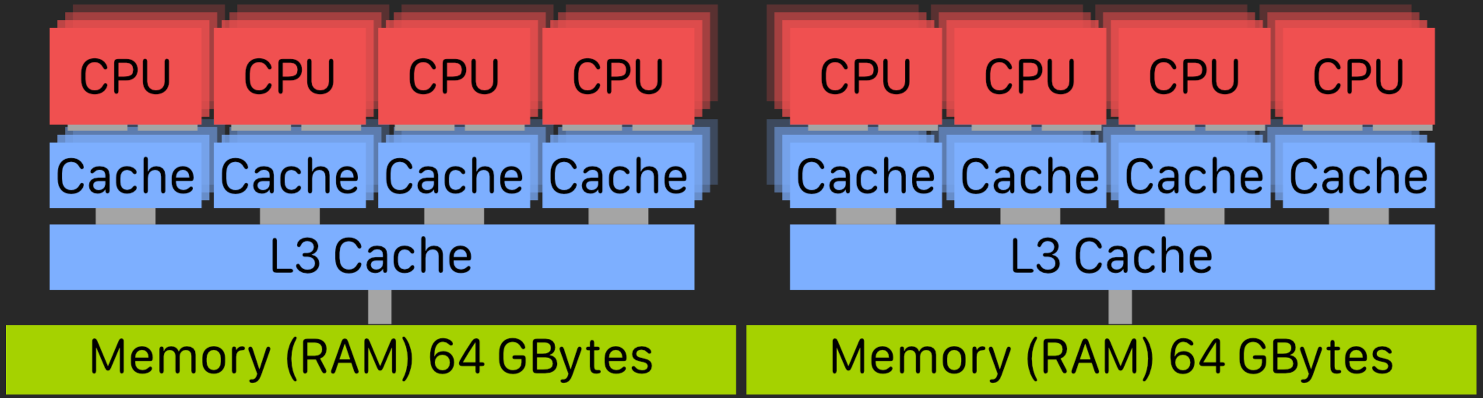

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- Increasing the number of cores used increases the bandwidth that can be sustained
- For L that fits in a single NUMA-node RAM (i.e. $<$ 64 GBytes) $\Rightarrow$ peak bandwidth is 83 GBytes/s

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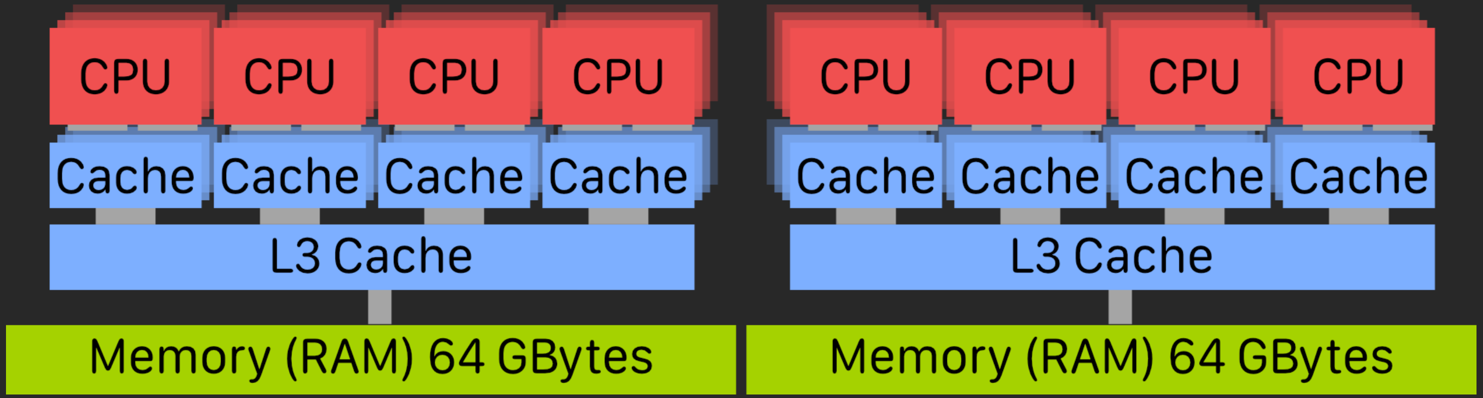

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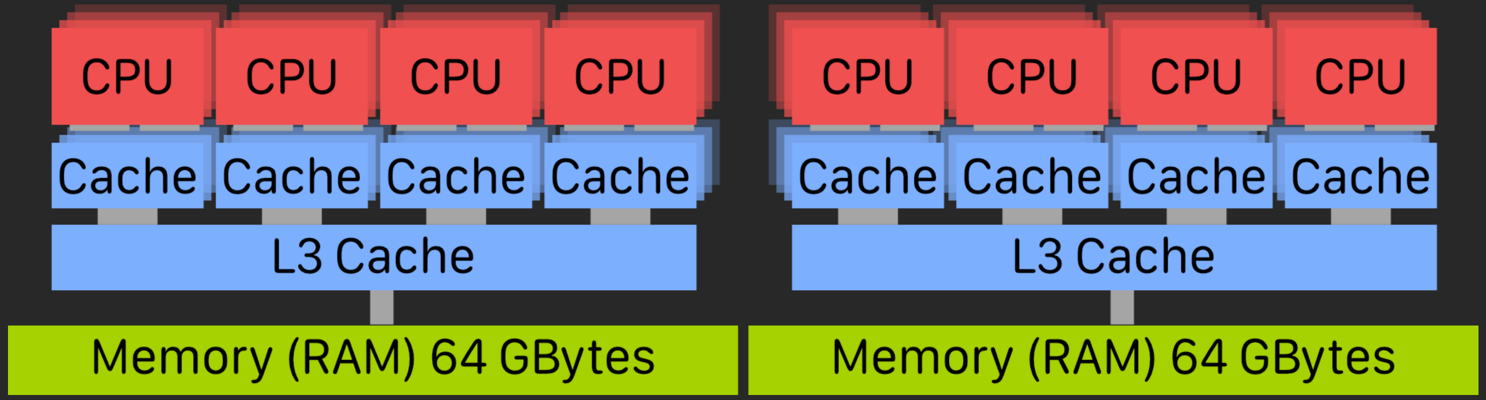

- What is the cache size?
  - 22 MBytes (for each socket)
  - See e.g. `/proc/cpuinfo` or `hwloc-ls`

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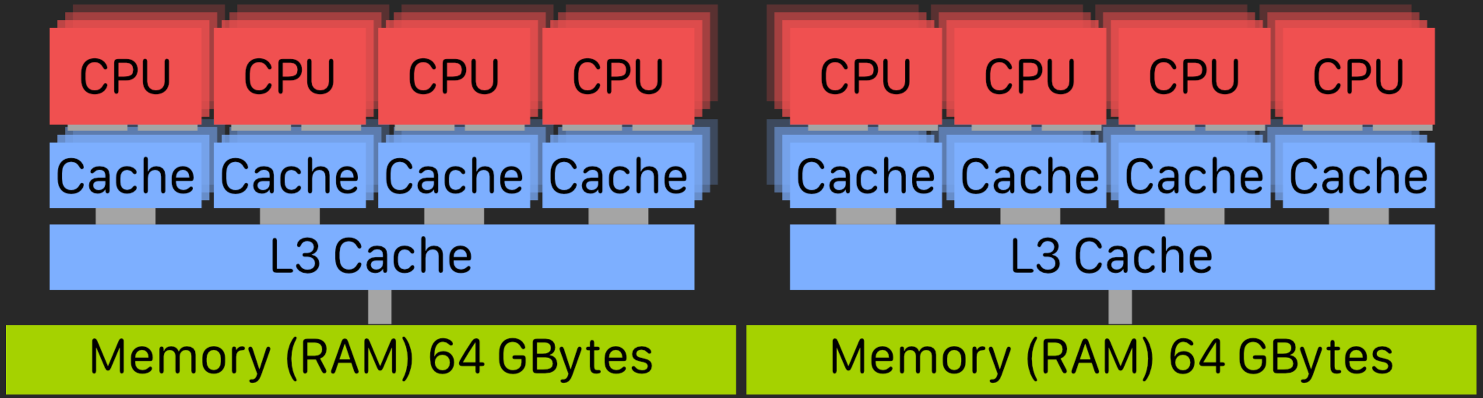

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    - 22 MBytes (for each socket)
    - See e.g. `/proc/cpuinfo` or `hwloc-ls`
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Performance analysis

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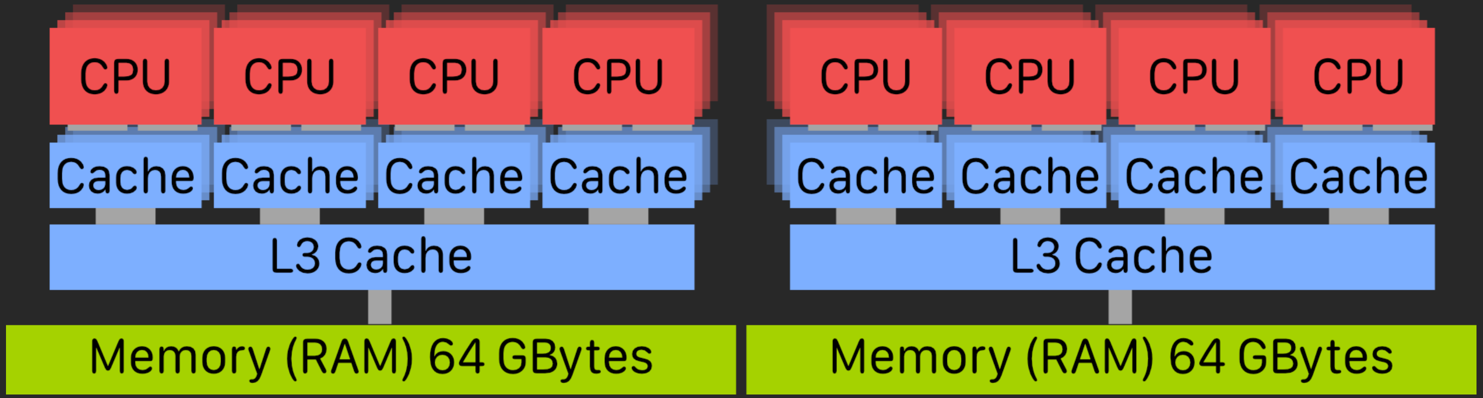

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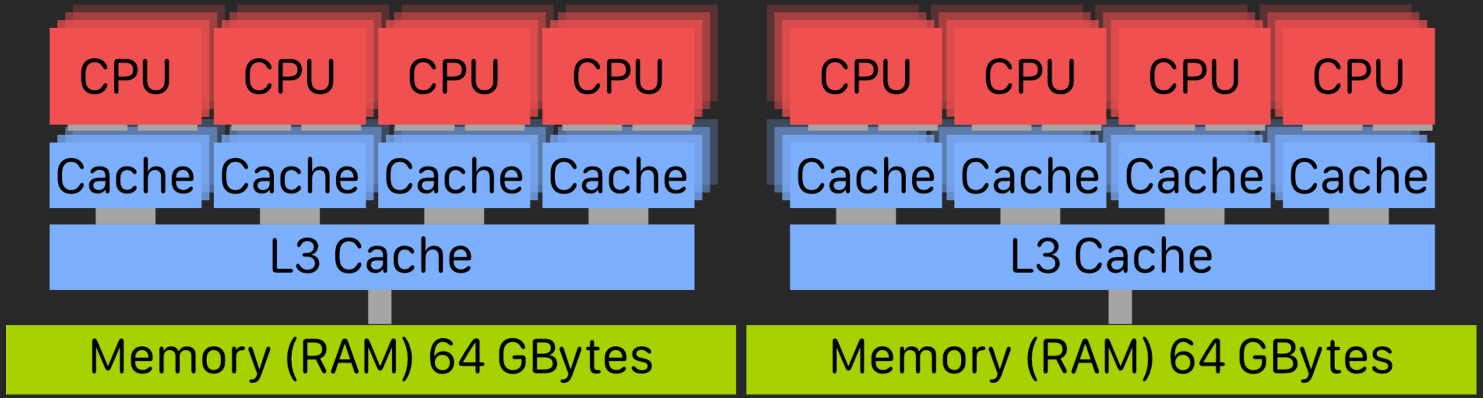

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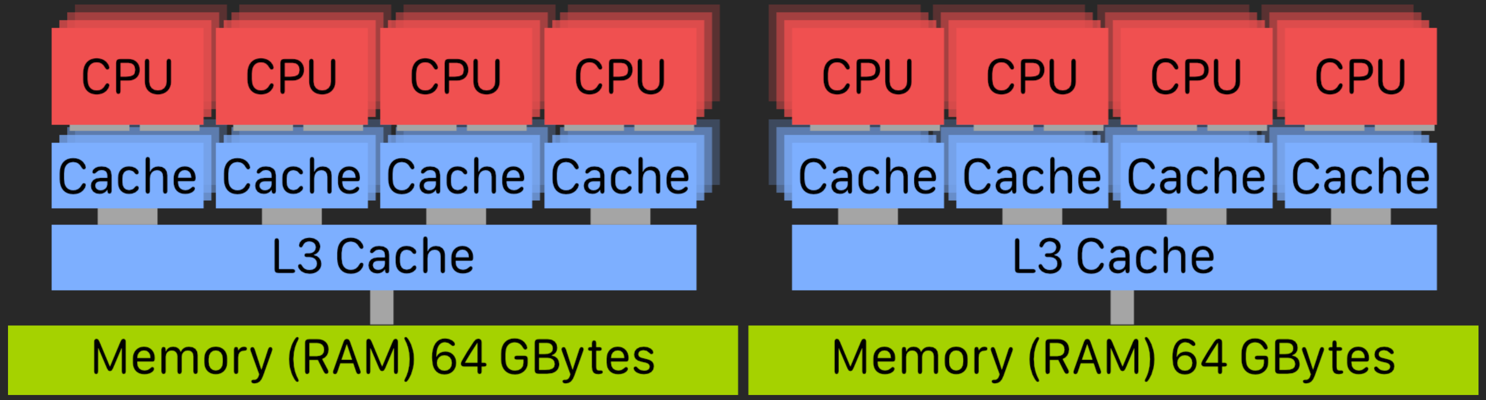

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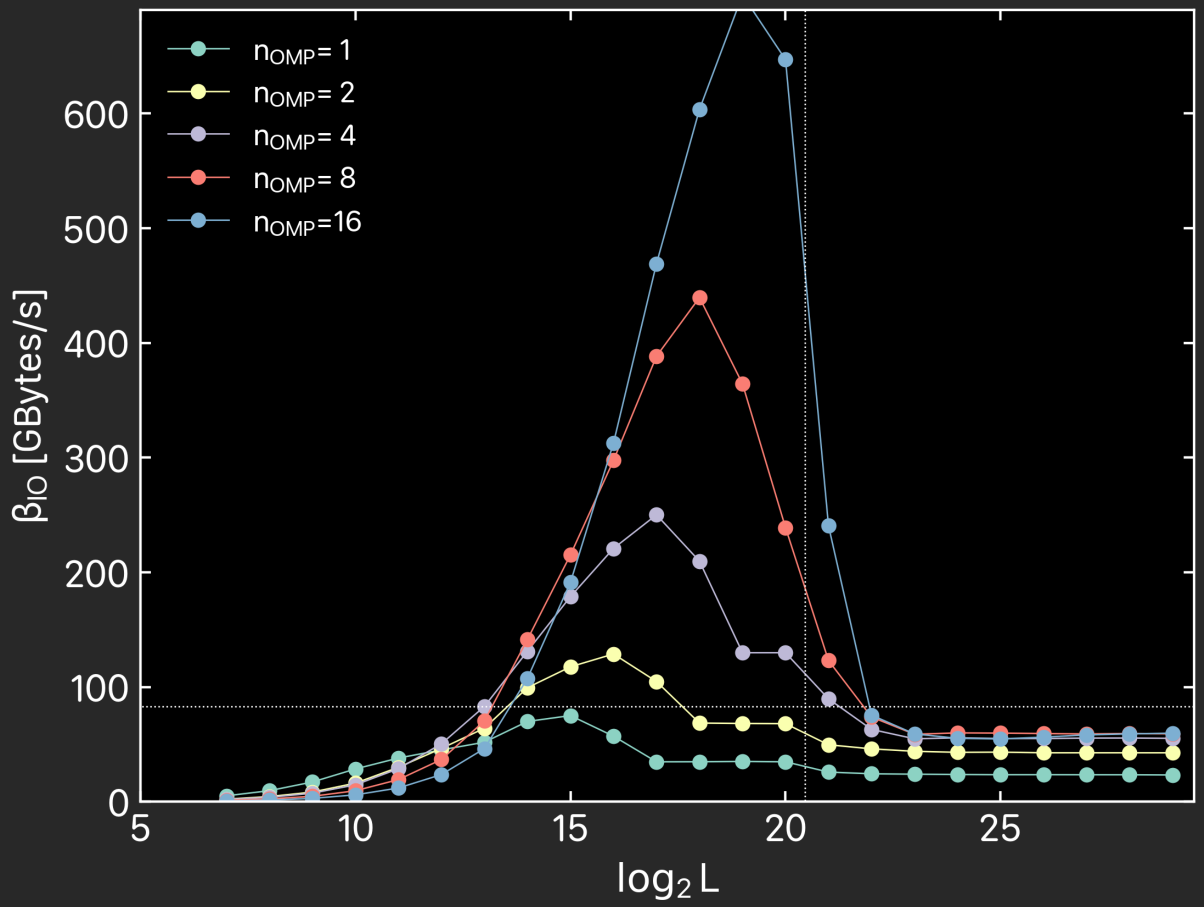
  - $\Rightarrow L_c$ =22 MBytes / (8 Bytes$\times 2$) $\simeq 2^{20}$

Performance analysis



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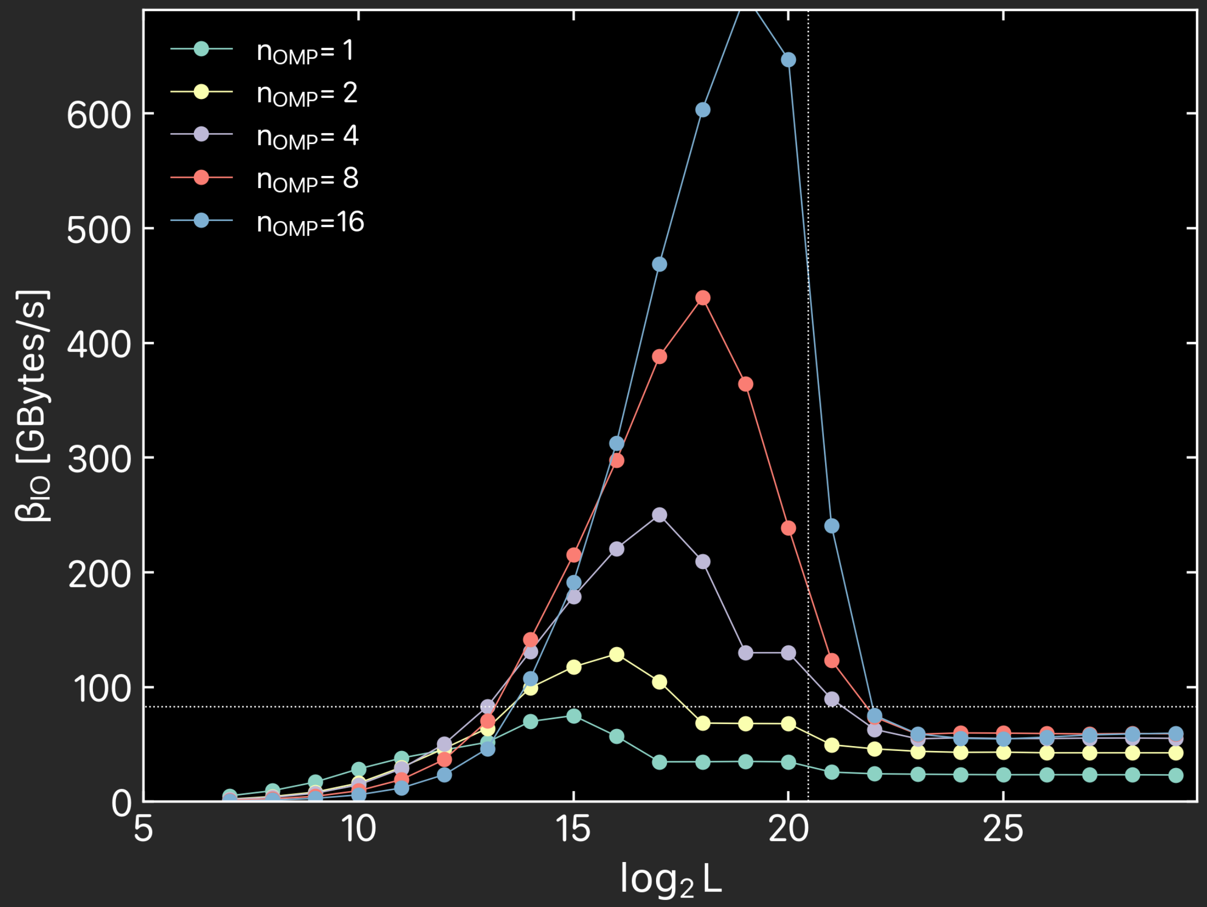

- Dashed vertical line indicates L_c, i.e. the largest value of L for which arrays `x[]` and `y[]` still fit in the L3 cache of 22 MBytes

Optimization

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- One good example though that can help demonstrate this effect it the matrix-matrix multiplication