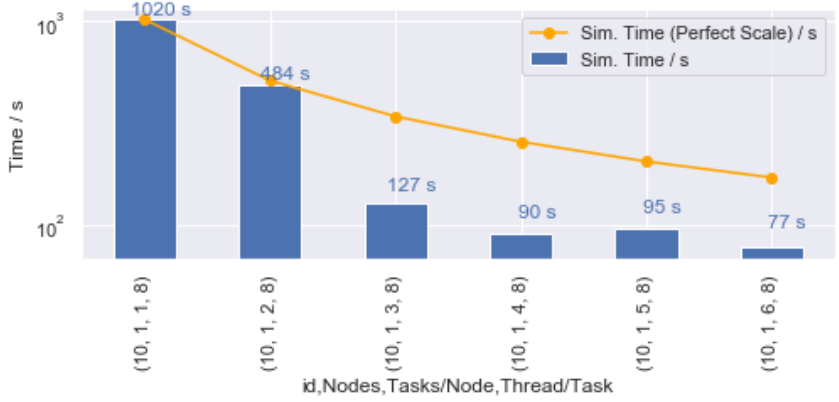
P^6

PROPER PINNING PREVENTS PRETTY POOR PERFORMANCE

Nov'24 | T. Hater | JSC

Superlinear Speed-Up?



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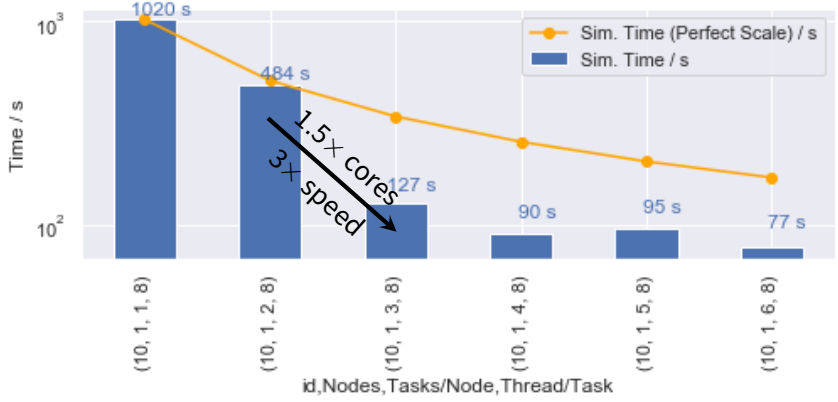

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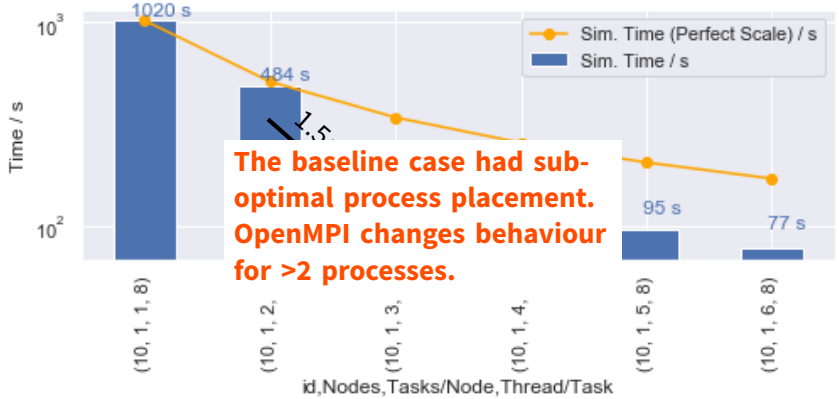

The baseline case had sub-optimal process placement. OpenMPI changes behaviour for >2 processes.

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What is Pinning?

Also: Binding, Affinity, …

- Force a process or thread to execute only on a given set of cores.

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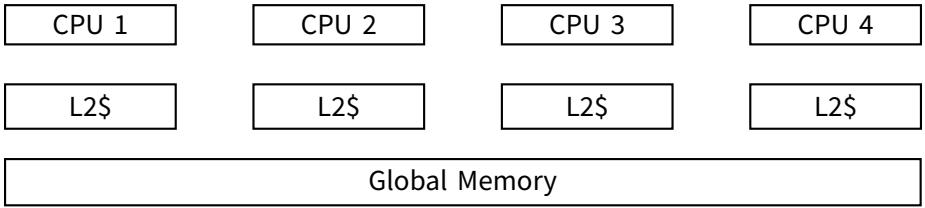
- But you can (should?) take control.
- We have seen as much as a gain (loss?) of $2\times$ in bandwidth

Why Pinning?

A Cartoon CPU



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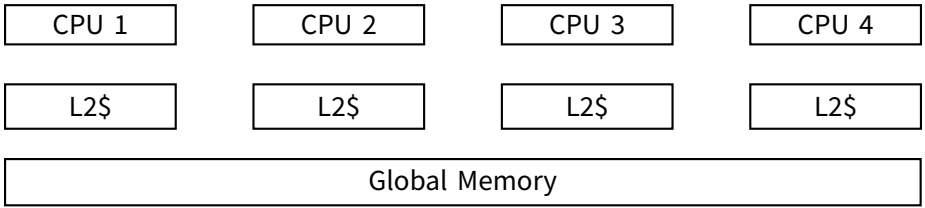

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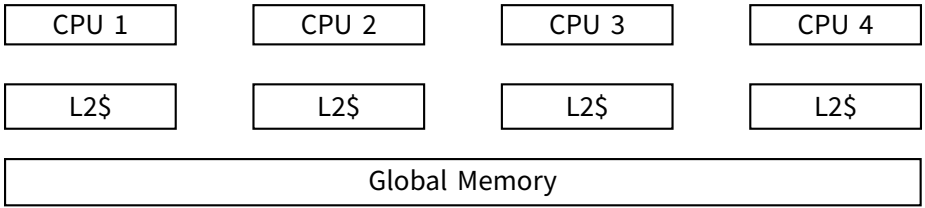

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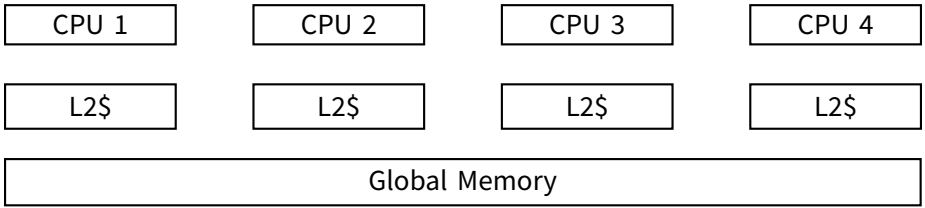

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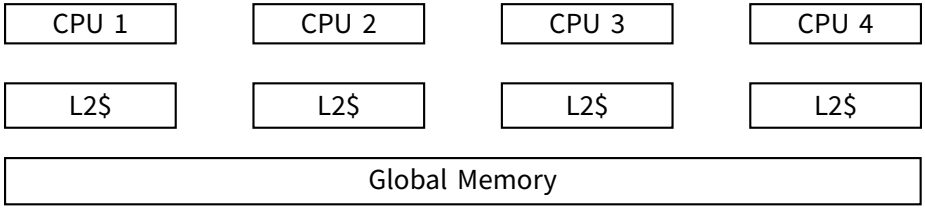

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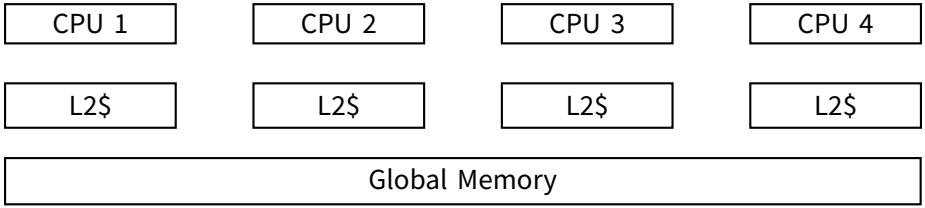
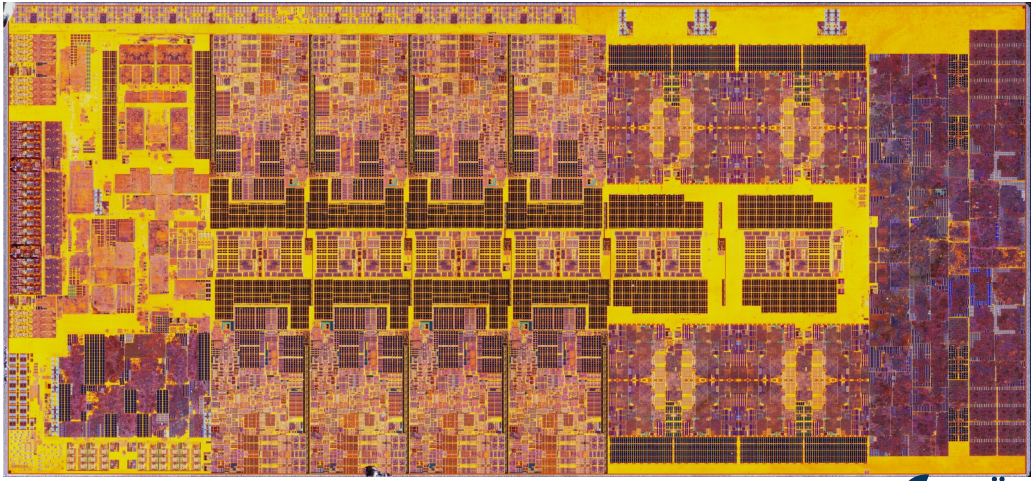


- Many cores, each with its own memory hierarchy.
- Shared global memory, but…
- …*affinity* to memory partitions.

- OS manages allocation,…
- …task placement, and…
- …swaps tasks in and out.

Reality is more Complex

Intel 13 gen: Raptor Lake



(Image: Fritzchens Fritz)

Why Pinning?

Scenario 1: Task Migration

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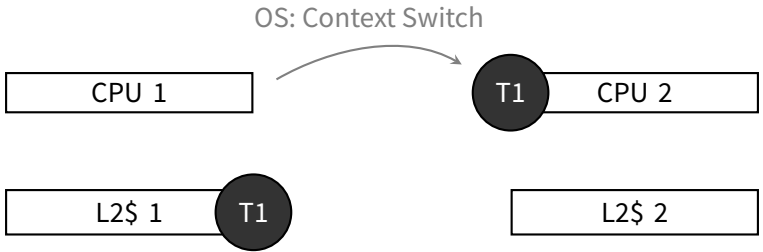

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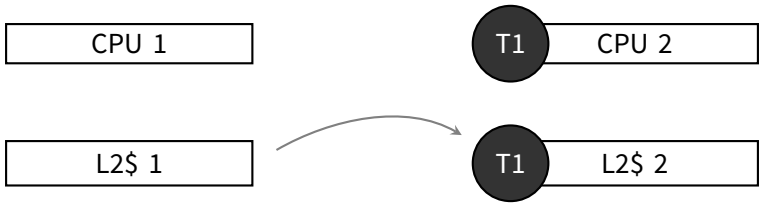

Why Pinning?

Scenario 1: Task Migration

Important

Swapping tasks in and out is basically free, but task *migration* leads to data migration. Granularity is a *cache line* (often 128 *B*); be aware of *false sharing*.

Why Pinning?

Scenario 2: NUMA

NUMA: Non-Uniform Memory Access, ie memory performance depends on relative location.

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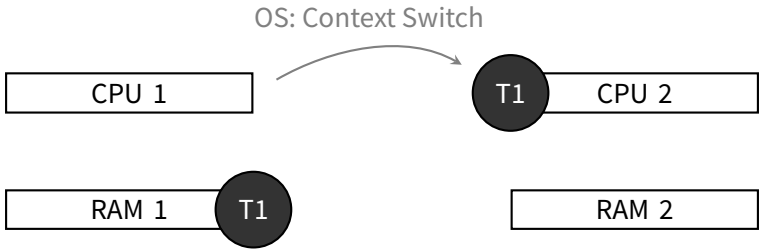

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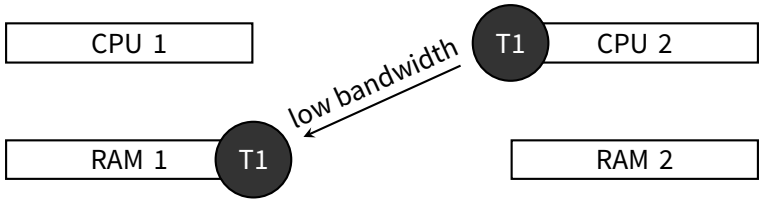

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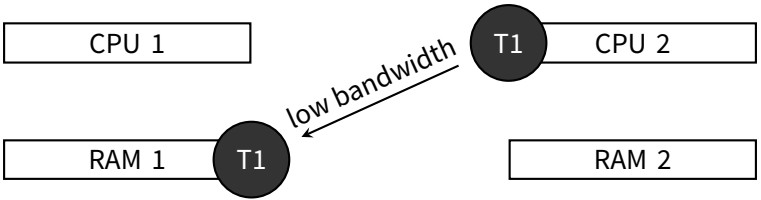


Important

All modern CPUs are NUMA architectures; might even have more than one NUMA domain!
Memory is actually allocated on initialisation, use same parallel configuration as consumer.
There will be no automatic migration.

Why Pinning?

Scenario 3: Sharing Resources

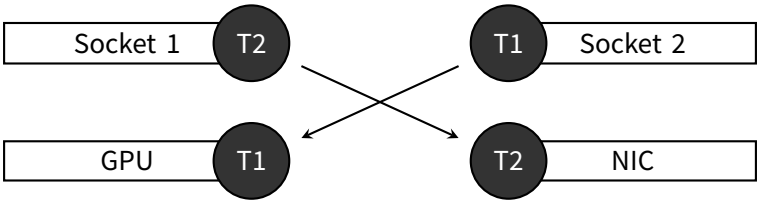
In some instances resources might be shared

- Hardware Threads (HWT) on a core might share computational units.
- Cores on a socket might share memory bandwidth, caches, …

This can lead to sub-optimal performance by leaving some parts idle and others saturated. The inverse *might also be true*, eg it might be beneficial to share caches for read-only data.

Why Pinning?

Scenario 4: Specialisation



- Accelerators/network interfaces might be attached to a specific socket.
- If tasks/threads have specialised jobs, like MPI communication, …
- …scheduling them close to the relevant hardware can improve performance.
- Again: Beware the context switch.

This Talk

- ✓ Motivation: Suboptimial and/or unpredictable performance
- ✓ Definition: What is pinning?
- ✓ Mechanism: Why does it improve performance?
- ☐ Learn to know your hardware.
- ☐ How to pin your processes.
- ☐ How to bind your threads.

Exploring a Node

```
> ml hwloc
> hwloc-ls # IMPORTANT: Run this on the *compute node*, eg via srun!
Machine (754GB total)
  Package L#0
    NUMANode L#0 (P#0 376GB)
    L3 L#0 (28MB)
      L2 L#0 (1024KB) + L1d L#0 (32KB) + L1i L#0 (32KB) + Core L#0
        PU L#0 (P#0)
        PU L#1 (P#40)
      L2 L#1 (1024KB) + L1d L#1 (32KB) + L1i L#1 (32KB) + Core L#1
        PU L#2 (P#1)
        PU L#3 (P#41)
[...]
    HostBridge
      PCIBridge
        PCI 3b:00.0 (InfiniBand)
          Net "ib0"
          OpenFabrics "mlx5_0"
  Package L#1
    NUMANode L#1 (P#1 378GB)
    L3 L#1 (28MB)
[...]
```

hwloc documentation

Exploring a Node

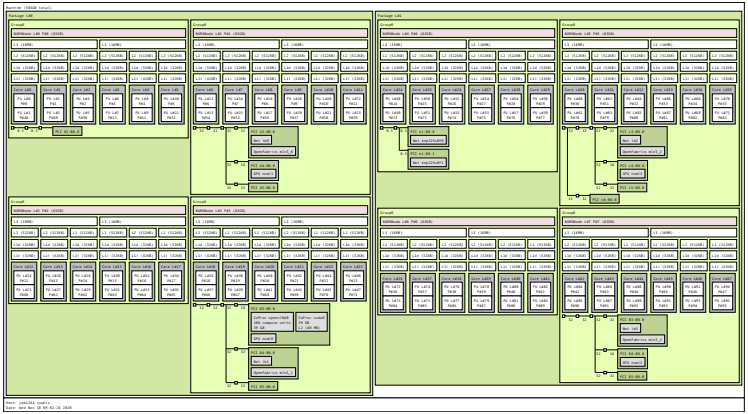
ASCII Art Edition

```
> hwloc-ls --output-format ascii # IMPORTANT: Run this on the *compute node*, eg via srun!
+-------------------------------------------------------------------------------------------------------------------+
| Machine (504GB total)                                                                                             |
| +---------------------------------------------------------------------------------------------------------------+ |
| | Package L#0                                                                                                   | |
| | +-----------------------------------------------------------------------------------------------------------+ | |
| | | NUMANode L#0 P#0 (252GB)                                                                                  | | |
| | | +-------------------------------------------+     +-------------------------------------------+ | | |
| | | | L3 (16MB)                                 | ... | L3 (16MB)                                 | | | |
| | | | +-------------+  +-------------+  +-------------+     +-------------+  +-------------+  +-------------+ | | |
| | | | | L2 (512KB)  |  | L2 (512KB)  |  | L2 (512KB)  |     | L2 (512KB)  |  | L2 (512KB)  |  | L2 (512KB)  | | | |
| | | | | L1d (32KB)  |  | L1d (32KB)  |  | L1d (32KB)  |     | L1d (32KB)  |  | L1d (32KB)  |  | L1d (32KB)  | | | |
| | | | +-------------+  +-------------+  +-------------+     +-------------+  +-------------+  +-------------+ | | |
| | | | +-------------+  +-------------+  +-------------+     +-------------+  +-------------+  +-------------+ | | |
| | | | | Core L#0    |  | Core L#1    |  | Core L#2    |     | Core L#21   |  | Core L#22   |  | Core L#23   | | | |
| | | | | +---------+ |  | +---------+ |  | +---------+ |     | +---------+ |  | +---------+ |  | +---------+ | | | |
| | | | | | PU L#0  | |  | | PU L#2  | |  | | PU L#4  | |     | | PU L#42 | |  | | PU L#44 | |  | | PU L#46 | | | | |
| | | | | | PU L#1  | |  | | PU L#3  | |  | | PU L#5  | |     | | PU L#43 | |  | | PU L#45 | |  | | PU L#47 | | | | |
| | | | | +---------+ |  | +---------+ |  | +---------+ |     | +---------+ |  | +---------+ |  | +---------+ | | | |
| | | | +-------------+  +-------------+  +-------------+     +-------------+  +-------------+  +-------------+ | | |
| | | +-------------------------------------------+     +-------------------------------------------+ | | |
| | +-----------------------------------------------------------------------------------------------------------+ | |
| +---------------------------------------------------------------------------------------------------------------+ |
+-------------------------------------------------------------------------------------------------------------------+
```

Exploring a Node

Accelerators and Network Devices

```
hwloc-ls --output-format=pdf > node.pdf
```



Exploring a Node

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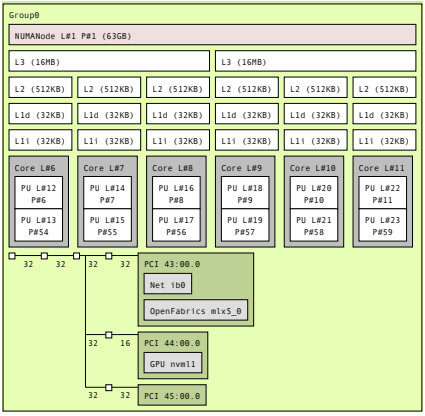

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Options for Binding

Usually, a hybrid model is used: MPI tasks $\times$ threads (OpenMP/pthreads/…)

Processes

- Resource Managers: SLURM, …
- MPI implementations: OpenMPI, PSMPI, …
- Linux: taskset, numactl, …
- HWLoc CLI tools

Threads

- OpenMP Environment variables (if used)
- Linux Kernel API
- OpenMP API (if used)
- HWLoc API

Processes: SLURM

Bind

`--cpu-bind=[options]` Enable binding

`verbose`	Print binding masks.
`cores|threads`	Use preset masks.
`rank`	Bind tasks to CPU IDs matching to task rank.
`rank_ldom`	Like rank, but distribute across NUMA domains.
`mask_cpu=0x..`	List of bit masks, can be generated by `hwloc` tools.

Note: binding a process with threads still allows migration between the available HWT.

Good News!

The PinningWebtool is a great help, if not yet fully updated to recent SLURM changes. Some options shown here are missing.

Processes: SLURM

Distribution

`-N n -n t -c k`	Request n nodes for t tasks × k CPUs per task
`--distribution=L:M:N`	Distribute tasks across
`L=block|cyclic`	Nodes
`M=block|cyclic|fcyclic`	Sockets
`N=block|cyclic|fcyclic`	HWT

The matter of `--exact`

When srun is invoked with `--exact`, SLURM will allocate *as few HWT as possible* to satisfy the requested allocation. Example: `srun -n 6 --exact` will use 6 HWT while `srun -n 6` *may* use 6 *cores*, thus allocating 6 × *#HWT*. NB. That might actually be useful, sometimes.
The crux is in recent versions of SLURM `-c|--cpus-per-task` implies `--exact`. You may use `--oversubscribe` to counteract this automatism.

Processes: SLURM

Distribution II

`-N n -n t -c k`	Request n nodes for t tasks × k CPUs per task
`--distribution=L:M:N`	Distribute tasks across
`L=block|cyclic`	Nodes
`M=block|cyclic|fcyclic`	Sockets
`N=block|cyclic|fcyclic`	HWT

slurm documentation

Processes: SLURM

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slurm documentation

Nodes, `default=block`

`block`	Close; consecutive task use one node, until full, then the next.
`cyclic`	Round-robin; one task per node until all nodes, then start again.

Processes: SLURM

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slurm documentation

Sockets, `default=cyclic`

`block`	Fill one sockect, then use the next.
`cyclic`	Round-robin across sockets.
`fcyclic`	Tasks round-robin **and** round-robin cores of each task.

Processes: SLURM

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`N=block|cyclic|fcyclic`	HWT

slurm documentation

Cores, `default=$socket-level`

`block`	keep tasks as close together as possible
`cyclic`	Round-robin across CPUs.
`fcyclic`	Tasks round-robin **and** round-robin cores of each task.

Processes: SLURM

Recommended Usage

```
srun --nodes=<nodes>
     --tasks-per-node=<tasks/node>
     --cpus-per-task=<threads/task>
     --distribution=block:cyclic:cyclic -- ./your_exe <args>
```

Processes: SLURM

Recommended Usage

```
srun --nodes=<nodes>
     --tasks-per-node=<tasks/node>
     --cpus-per-task=<threads/task>
     --distribution=block:cyclic:cyclic -- ./your_exe <args>
```

Note

`--cpus-per-task` is required here if you want to set the thread count. Setting `SLURM_CPUS_PER_TASK` or `--cpus-per-task` in your sbatch script is no longer supported. Also, remember that `--cpus-per-task` implies `--exact`!.

Processes: SLURM

Examples: Advanced Usage

System JUWELS Booster: NIC/GPUs attached to NUMA domains 1, 3, 5, 7

Goal 4 dedicated tasks for driving accelerators and communication each.

Processes: SLURM

Examples: Advanced Usage

System JUWELS Booster: NIC/GPUs attached to NUMA domains 1, 3, 5, 7

Goal 4 dedicated tasks for driving accelerators and communication each.

```
> # Compute masks for all HWT in the relevant NUMA domains
> numa=`hwloc-calc numa:1 numa:3 numa:5 numa:7`
> # Generate masks for the distribution of 8 tasks across these
> mask=`hwloc-distrib 8 --single --taskset --restrict $numa | xargs | tr ' ' ','`
> # Run application
> srun --cpu_bind=verbose,cpu_mask=$mask -N 1 -n 8 -c 1 -- app.exe
```

Processes: SLURM

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> srun --cpu_bind=verbose,cpu_mask=$mask -N 1 -n 8 -c 1 -- app.exe
```

Warning

This example is purely educational, GPU affinity is handled by default.
Masks can be computed by hand, but keeping track of the numbering and bitsets is tedious and errorprone. The numbering scheme may change by: vendor, CPU generation, OS, …

Processes: SLURM

JUWELS Booster Default

Just use the default if your application does not have special requirements.

```
srun -N 1 -n 4 --gpus=4 --cpus-per-task=12 --cpu-bind=socket -- app.exe
```

This does the right thing and **also** restricts the tasks' visible GPUs to the closest one.

Threads

- When using threads within tasks, these can use affinity as well.
- Without, threads will be mobile within the task-level masks.
- Consequently, we need to add another level of bindings…
- …and take care not to conflict with task-level masks.

Threads: OpenMP Environment Variables

`OMP_PROC_BIND=[...]` Inhibit migration, bind threads to

- `true` First location it runs on.
- `spread` Spread over allowable set.
- `close` Block threads together.

`OMP_PLACES=[...]` Bind threads to a set of places

- `threads` Individual hardware threads
- `cores` All HWT of a core
- `sockets` All cores of a socket
- `{1, …}` List of HWT ids

Migration is still allowed within a `place` when binding is not enabled.
Using `threads`|`cores`|`sockets` with task binding is safe.

OpenMP specification

Summary

- Be aware of your application, we cannot provide a general solution.
- Binding for more performance and more predictability.
- Tools like hwloc allow mapping node topologies.
- High-level settings for performance and portability.
  Example: SLURM and OpenMP.
- Low-level tools, eg hwloc-API, for ultimate control.

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