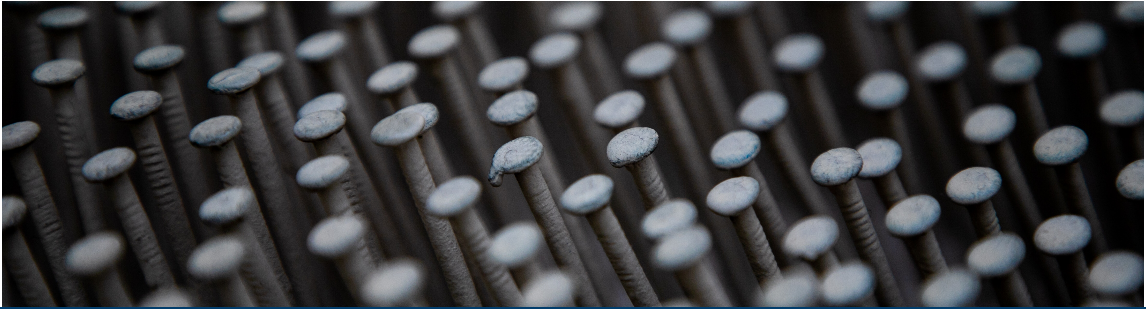

P^6

PROPER PINNING PREVENTS PRETTY POOR PERFORMANCE

November ’23 | T. Hater | JSC

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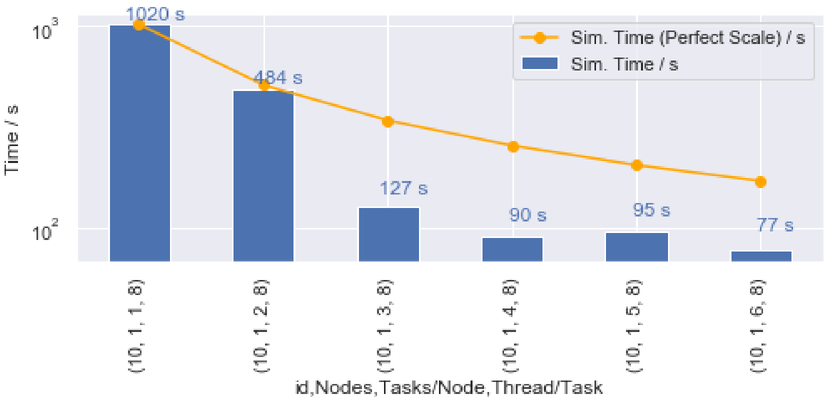
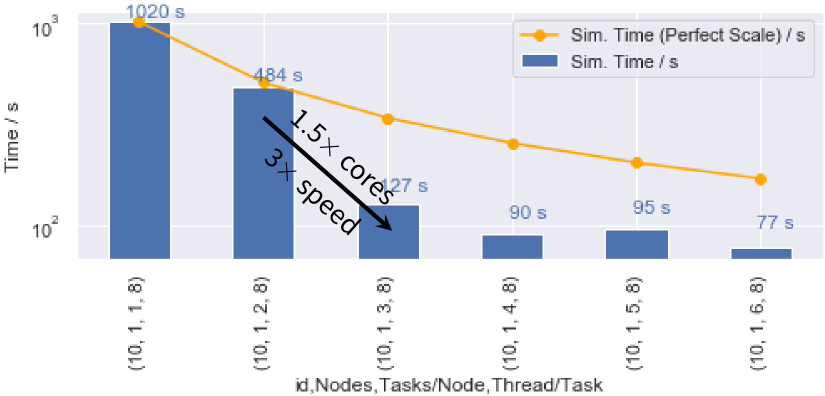
Superlinear Speed-Up?



Superlinear Speed-Up?



Superlinear Speed-Up?

No, just a bad baseline…

- Default process placement switched between two cases.

Superlinear Speed-Up?

No, just a bad baseline…

- Default process placement switched between two cases.
- Second configuration is better for this benchmark.

STREAM benchmark

Heavily Optimised for Target Architecture, …

- Target: 2 sockets $\times$ 10 cores $\times$ 8-way SMT
- 1GiB, only `triad` (3 `double` per element).
- De-activated bindings by MPI and OpenMP.
- 10 runs each averaged over 5 repetitions, pick top result.
- `-Ofast -march=native -mtune=native`
- `-std=c++17 -fno-builtin -fno-rtti -fno-exceptions -fopenmp`
- Cache line blocked and aligned, SIMD, single fork/join, first touch aware, RMW optimised.

STREAM benchmark

Heavily Optimised for Target Architecture

- Target: 2 sockets ×
- 1GiB, only triad (3
- De-activated bindi ?.
- 10 runs each avera pick
- -0fast -march=nat
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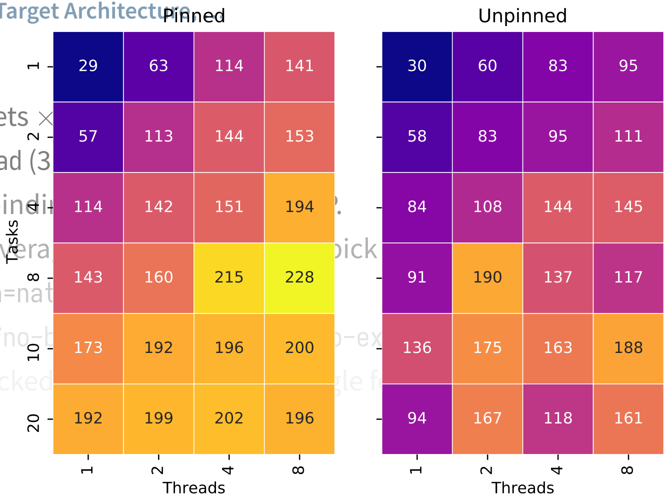

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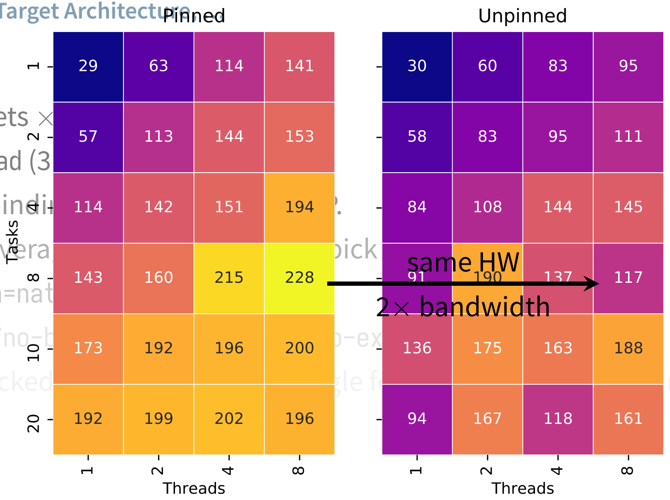

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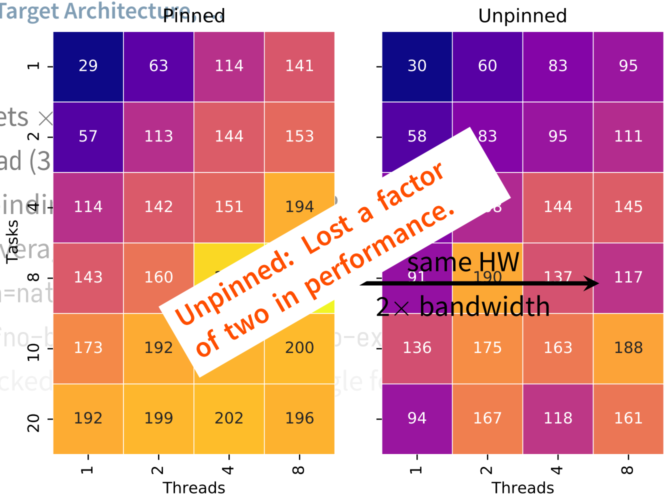

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What is Pinning?

Also: Binding, Affinity, …

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

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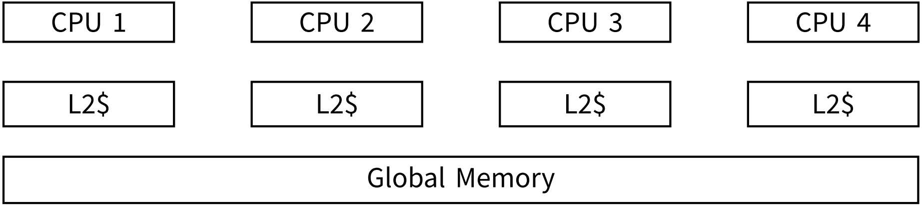
- Enforced by the OS, driven by user space tools.
- In HPC this is (partially!) handled by the scheduler (SLURM) or MPI.
- But you can (should?) take control.

Why Pinning?

A Cartoon CPU



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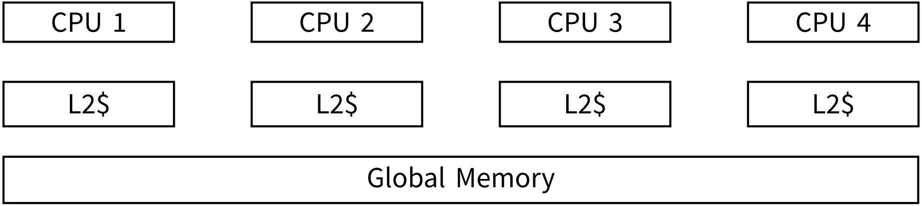

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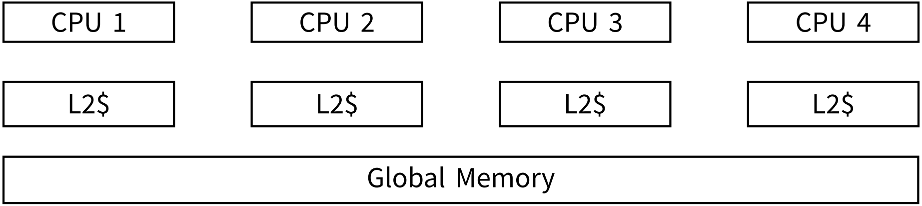

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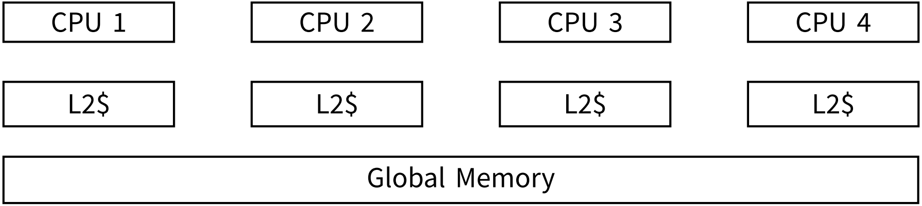

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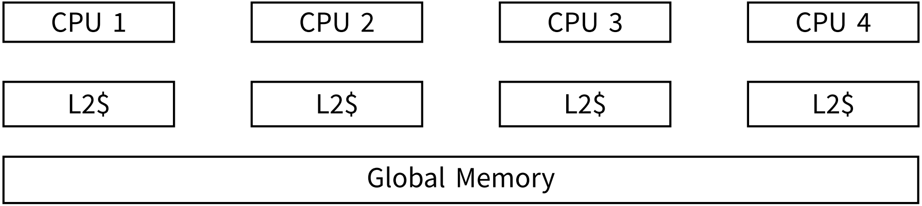

- Many cores, each with its own memory hierarchy.
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- …task placement, and…

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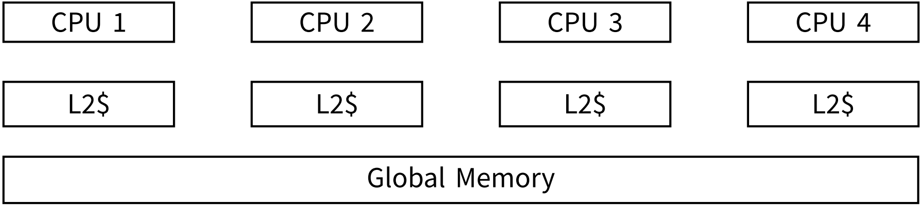


- Many cores, each with its own memory hierarchy.
- Shared global memory, but…
- …*affinity* to memory partitions.

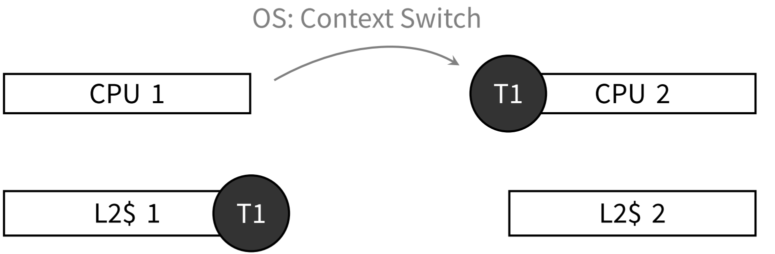
- OS manages allocation,…
- …task placement, and…
- …swaps tasks in and out.

Why Pinning?

Scenario 1: Task Migration

Why Pinning?

Scenario 1: Task Migration



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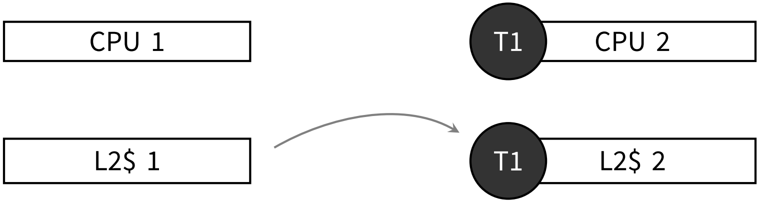
Why Pinning?

Scenario 1: Task Migration



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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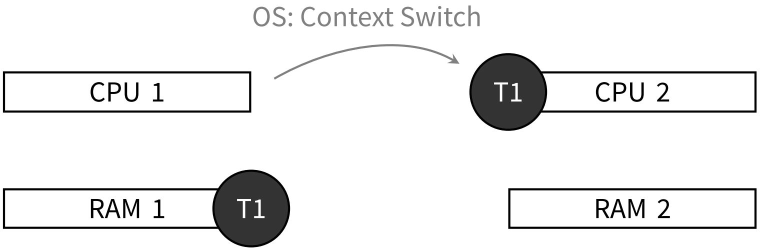

Why Pinning?

Scenario 2: NUMA

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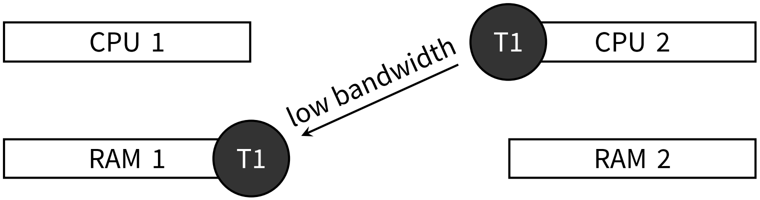

Why Pinning?

Scenario 2: NUMA

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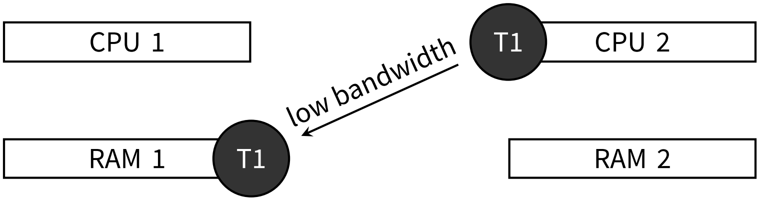


Important

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

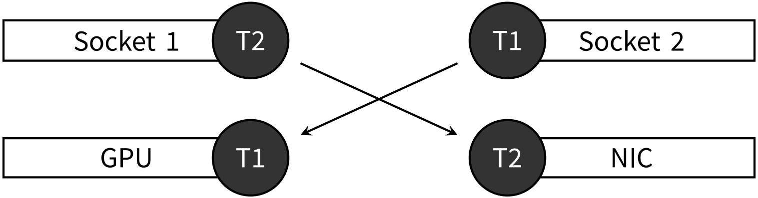
In some instances resources might be shared

- 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

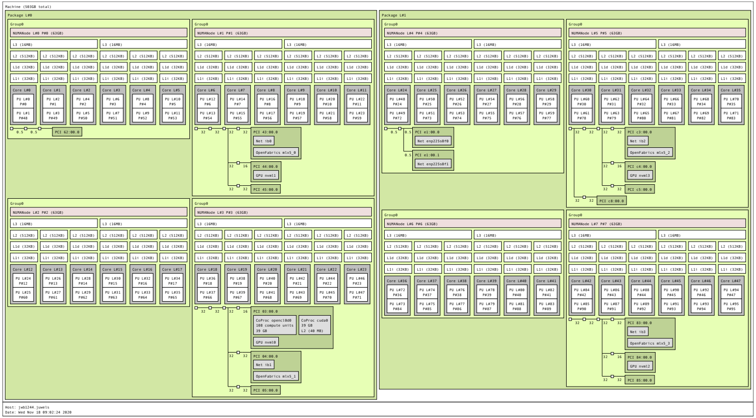
ASCII Art Edition

```
> 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
```



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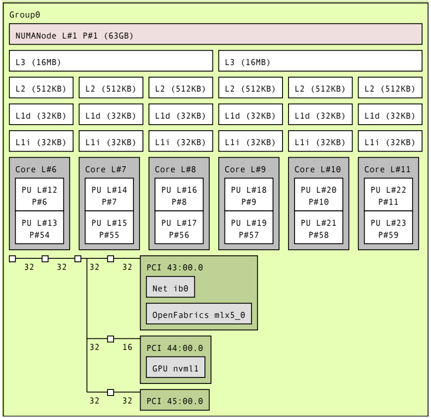
Exploring a Node

Accelerators and Network Devices



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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.

Warning

SLURM at JSC is currently (v22) in an inconsistent state and will change soon (v23). It is thus highly important to monitor the masks generated for your application and the resulting performance.

Worse, the PinningWebtool **is not yet updated** to recent SLURM changes.

Processes: SLURM

Distribution

`-N n -n t -c k`	Request n nodes for t tasks $\times$ 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 $\times$ #*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

Distribution II

`-N n -n t -c k`	Request n nodes for t tasks $\times$ 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

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

Distribution II

`-N n -n t -c k`	Request n nodes for t tasks $\times$ 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

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

Distribution II

`-N n -n t -c k`	Request n nodes for t tasks $\times$ 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

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

Maximising hardware use, assume no benefit from co-locating tasks.

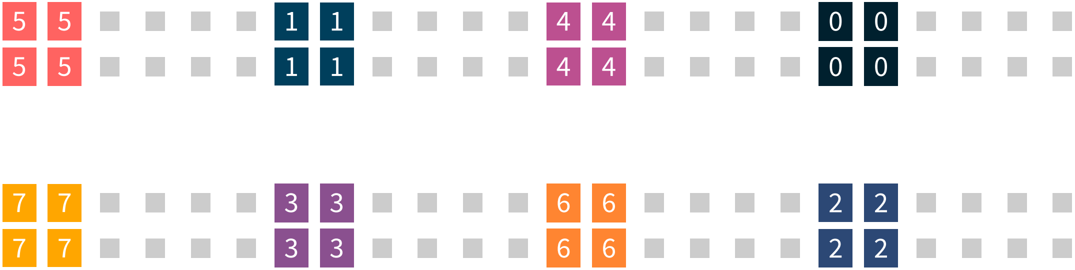
System	JUWELS Booster
Node	2 sockets $\times$ 20 cores $\times$ 2 HWT
Request	1 node with 8 tasks $\times$ 3 CPUs

Recipe

```
# Execute command <cmd> with some binding <bind> and print the masks
$> srun --cpu_bind=verbose,<bind> -n 8 -c 3 <cmd>
cpu_bind=DEFAULT - jwb0149, task  0  0 [12565]: mask 0xc0040 set
cpu_bind=DEFAULT - jwb0149, task  2  2 [12574]: mask 0xc0001000 set
cpu_bind=DEFAULT - jwb0149, task  4  4 [12577]: mask 0x3001000000 set
cpu_bind=DEFAULT - jwb0149, task  1  1 [12575]: mask 0xc000000080 set
cpu_bind=DEFAULT - jwb0149, task  3  3 [12576]: mask 0x2003 set
cpu_bind=DEFAULT - jwb0149, task  6  6 [12579]: mask 0x400000000c000000000000 set
cpu_bind=DEFAULT - jwb0149, task  7  7 [12578]: mask 0x800c0000000000000000000 set
cpu_bind=DEFAULT - jwb0149, task  5  5 [12580]: mask 0xc000000002000000 set
# Feed masks to hwloc, receive logical HWT ids.
$> hwloc-calc --pi 0x400000000c000000000000 --intersect PU
13,15,85
```

Example: Cores

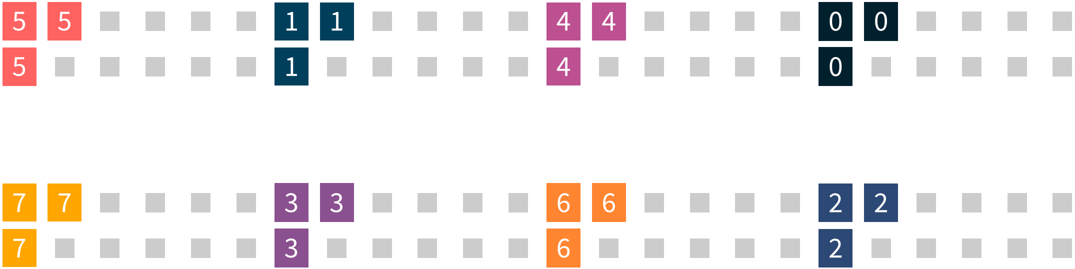
```
srun --cpu_bind=verbose,cores -n 8 -c 3 …
```



- The default!
- ✗ Using 16 cores, but we could employ 24, sans SMT
- ✗ We still use more than the minimum HWT

Example: Rank_LDom

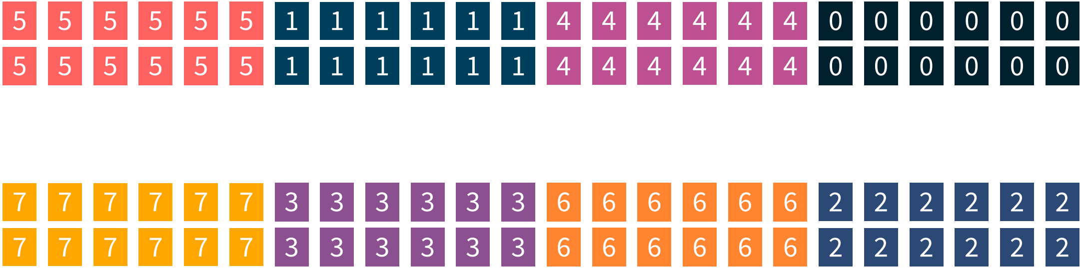
```
srun --cpu_bind=verbose,rank_ldom -n 8 -c 3 …
```



- ✗ Using 16 cores, but we could employ 24, sans SMT.

Example: LDom

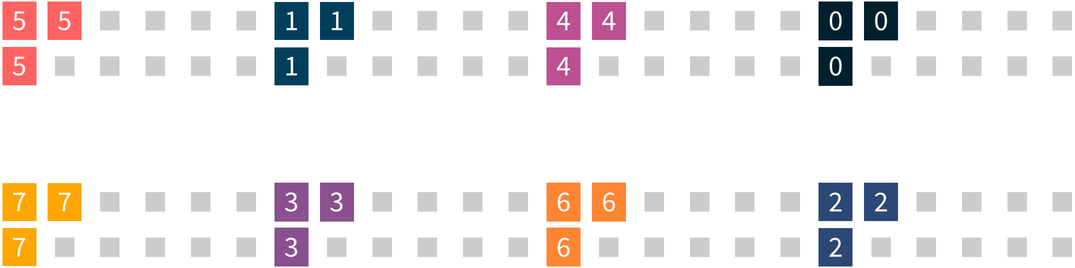
```
srun --cpu_bind=verbose,rank -n 8 -c 3 …
```



- ✓ Even distribution.
- ✓ All cores used.
- ✗ Masks are not minimal.

Example: Threads

```
srun --cpu_bind=verbose,threads -n 8 -c 3 …
```



- ✗ Using 16 cores, but we could employ 24, sans SMT.
- ✗ We still use more than the minimum HWT.
- Same as `rank_ldom`?
- This *used* to be the best option pre v22.05

Processes: SLURM

Conclusion

- Less pathological examples than pre v22.05
- But, the results require constant monitoring and are hard to interpret.
- Out of the options above, LDom seems best. Currently.
- We did not explore the effect of `--distribution`.
- Consider generating your own masks using `hwloc`.
- Expect more changes in the coming weeks.

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

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.

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> 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
```

Warning

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 --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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