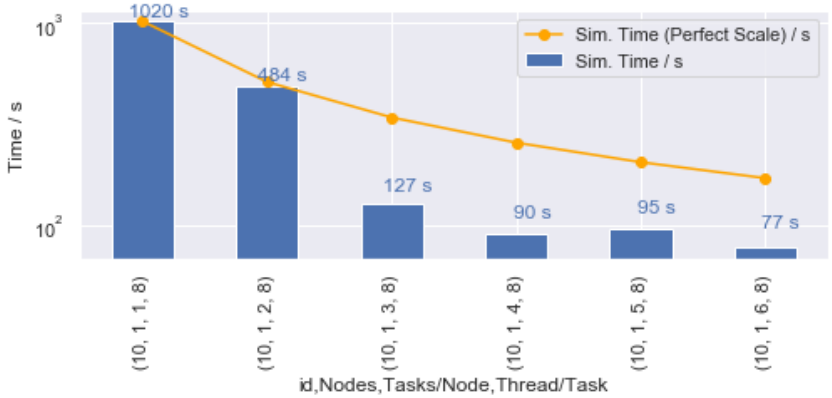
P^6

PROPER PINNING PREVENTS PRETTY POOR PERFORMANCE

Nov ’22 | T. Hater | JSC

JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

Superlinear Speed-Up?



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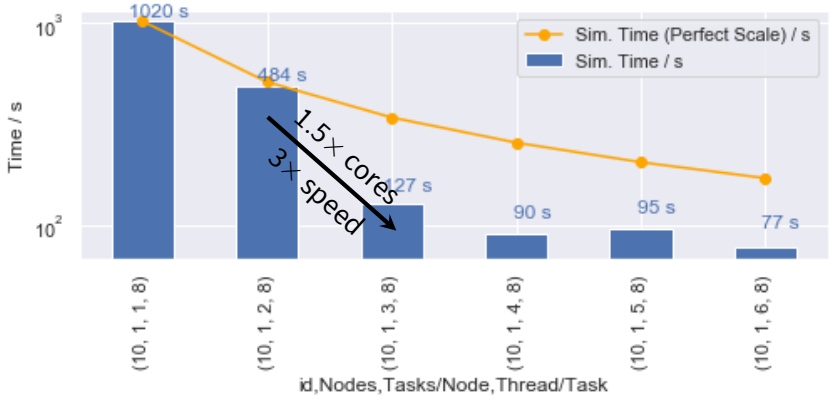

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No, just a bad baseline…

- 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 × 10 cores × 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.

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Heavily Optimised for Target Architecture

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- -Ofast -march=nat
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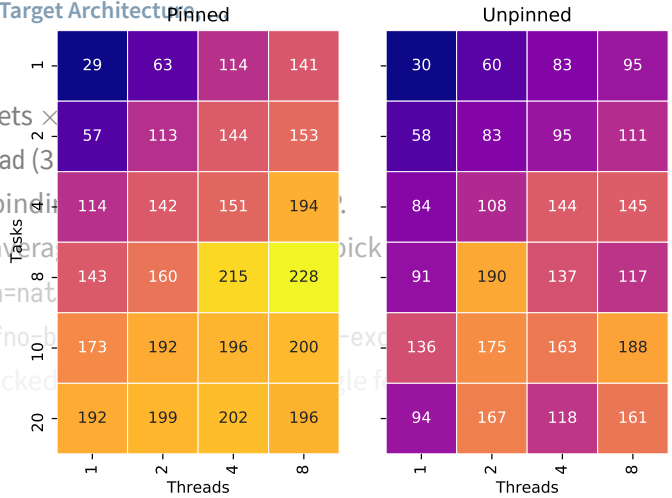

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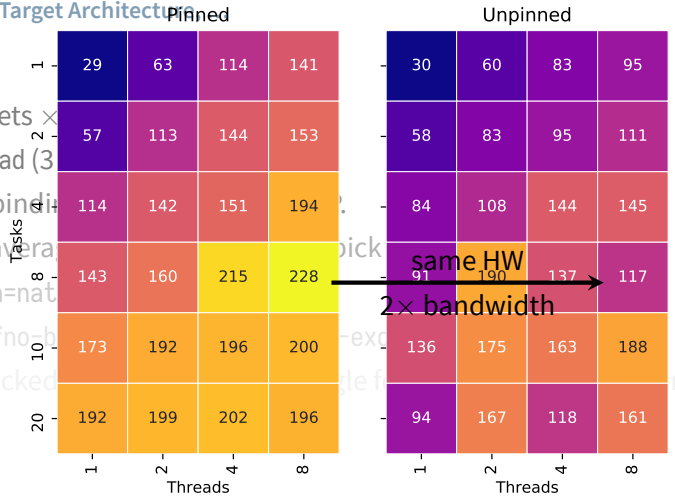

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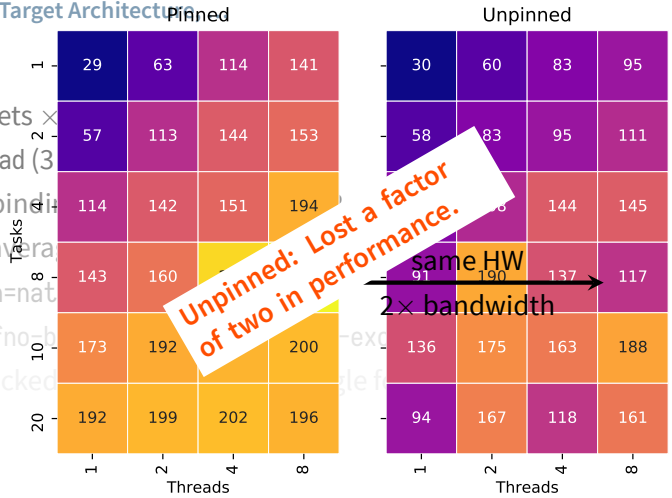

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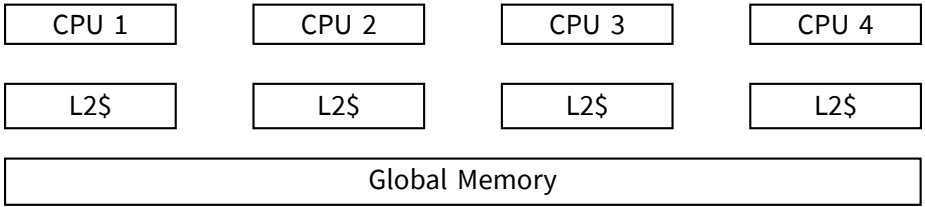
- But you can (should?) take control.

Why Pinning?

A Cartoon CPU



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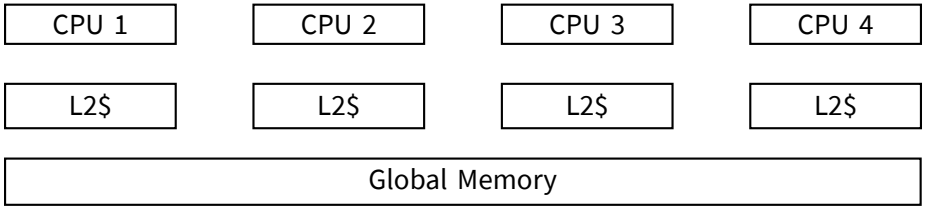

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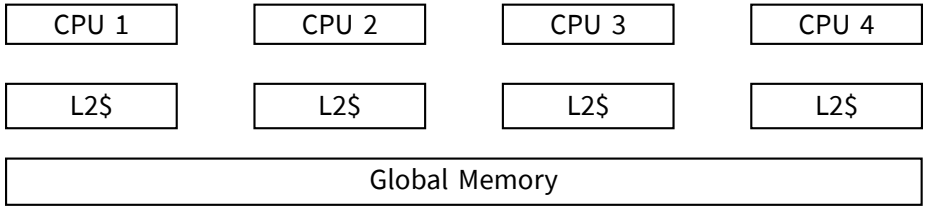

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- …*affinity* to memory partitions.

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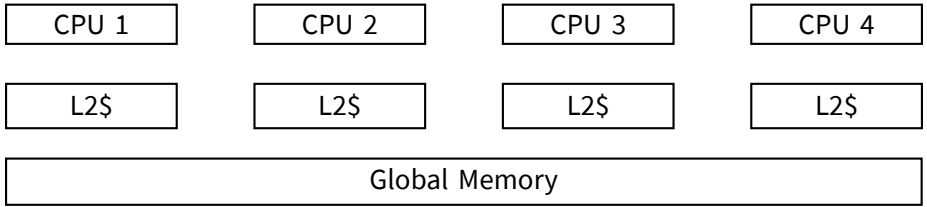

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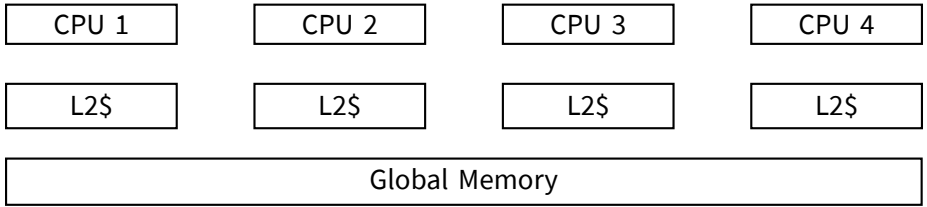

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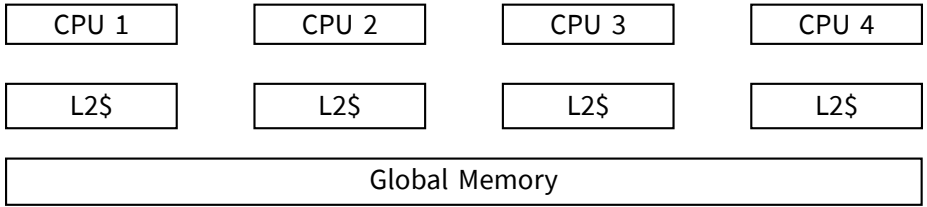

- Many cores, each with its own memory hierachy.
- Shared global memory, but…
- …*affinity* to memory partitions.

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

Why Pinning?

Scenario 1: Task Migration

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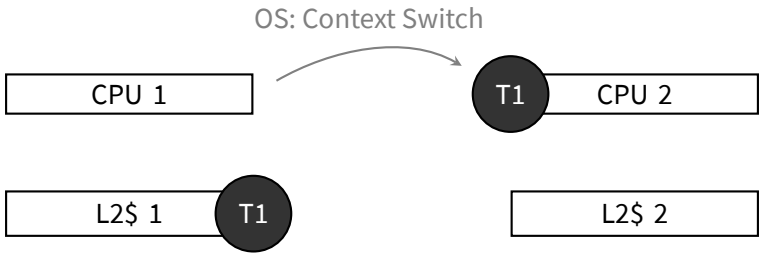

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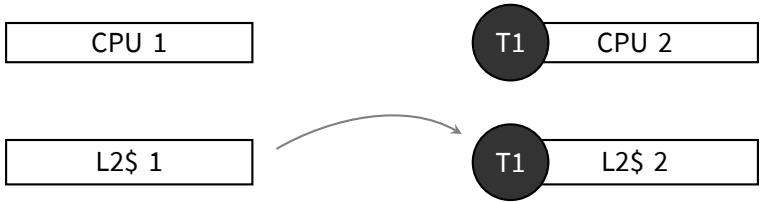

Why Pinning?

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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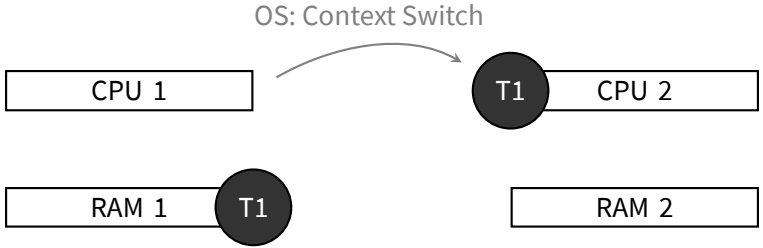

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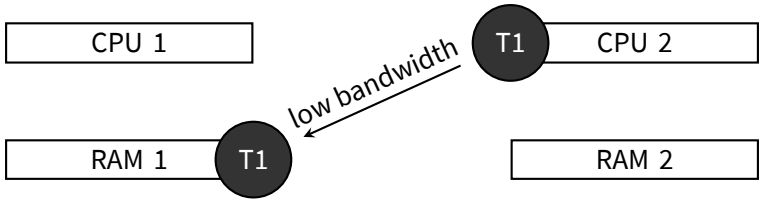

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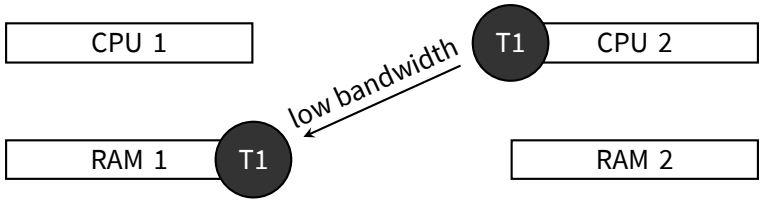


Important

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

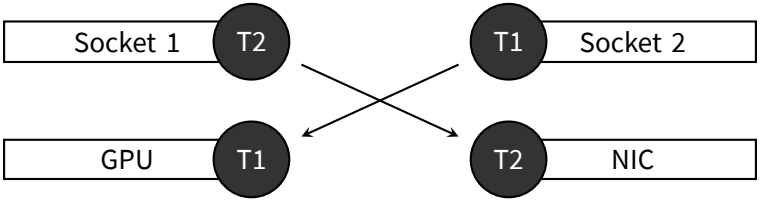
In some instances resources might be shared

- 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

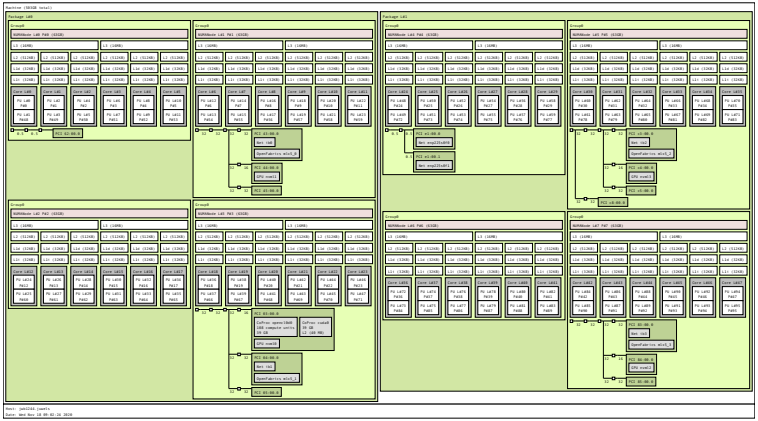
ASCII Art Edition

```
> 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
```



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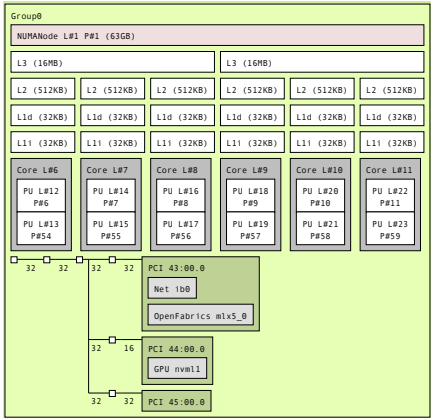


Options for Binding

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

`--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 might still generate **bad distributions**, see examples later on.

Processes: SLURM

Distribute

`-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

where

`block`	keep tasks as close together as possible
`fcyclic`	round-robin distribution, threads round-robin
`fcyclic`	round-robin distribution, threads close

When a task use more than one CPU, `cyclic` will allocate all as a group within the one socket if possible while `fcyclic` would distribute across sockets.

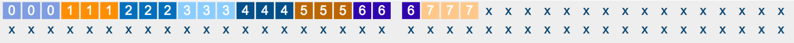
slurm documentation

Processes: SLURM

Examples: Single-node

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

Goal: Optimise for using as much of the hardware as possible, assuming the application does not benefit from co-locating tasks.



`bind=rank`

✗ Task 6 is split over two sockets.

✗ Uneven load across sockets.

Processes: SLURM

Examples: Single-node

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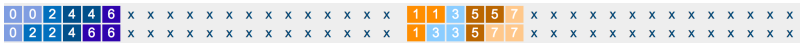

`bind=rank_ldom`

✗ Tasks share cores

✗ SMT used before filling HWT

Processes: SLURM

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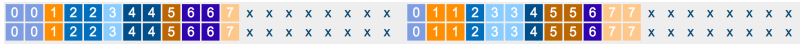

`bind=cores`

✗ Tasks split over sockets.

Each requested CPU acquires a full physical core.

Processes: SLURM

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Goal: Optimise for using as much of the hardware as possible, assuming the application does not benefit from co-locating tasks.

`bind=threads`

✓ Goal achieved

Processes: SLURM

Examples: Multi-node

System	JUWELS GPUs
Node	2 sockets × 20 cores × 2 HWT
Request	2 nodes with 20 tasks × 2 CPUs


```
bind=threads
distribution=block:cyclic:fcyclic
```

Processes: SLURM

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Images: PinningWebtool

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

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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

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Goal 4 dedicated tasks for driving accelerators and communication each.

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> # 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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