Expanse:SLURM Runtime Configurations and Tuning
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EXPANSE
COMPUTING WITHOUT BOUNDARIES

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NSF Award 1928224

Outline

- AMD EPYC Processor Architecture
  - Hardware details
  - NUMA options
  - Applications
- Expanse task layout and affinity scripts
  - ibrun
  - affinity
  - slurm-aff-prod (for MPI/pthreads)
- Summary

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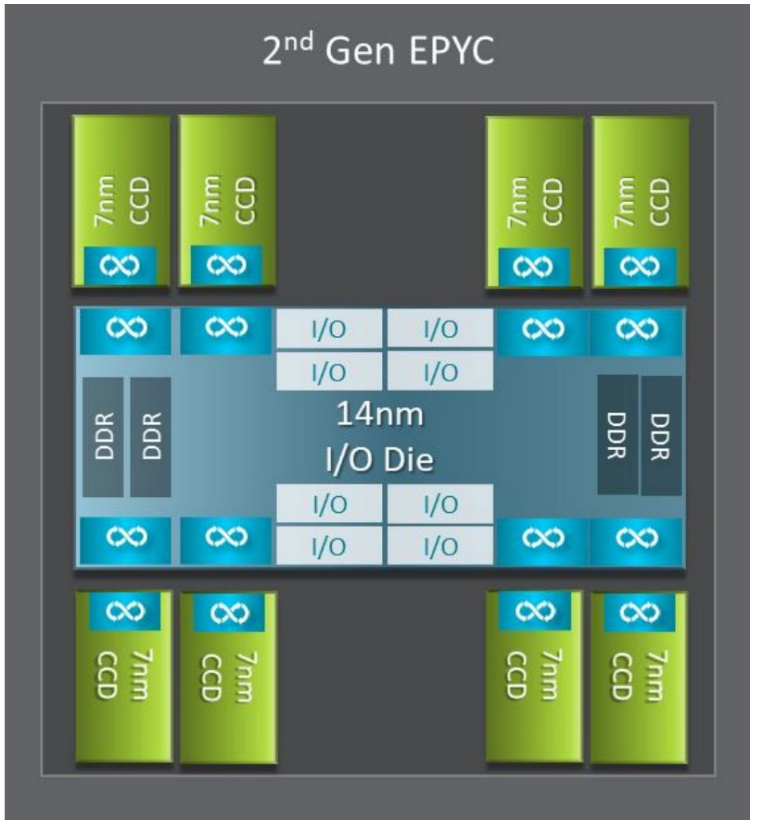
AMD EPYC 7742 Processor Architecture

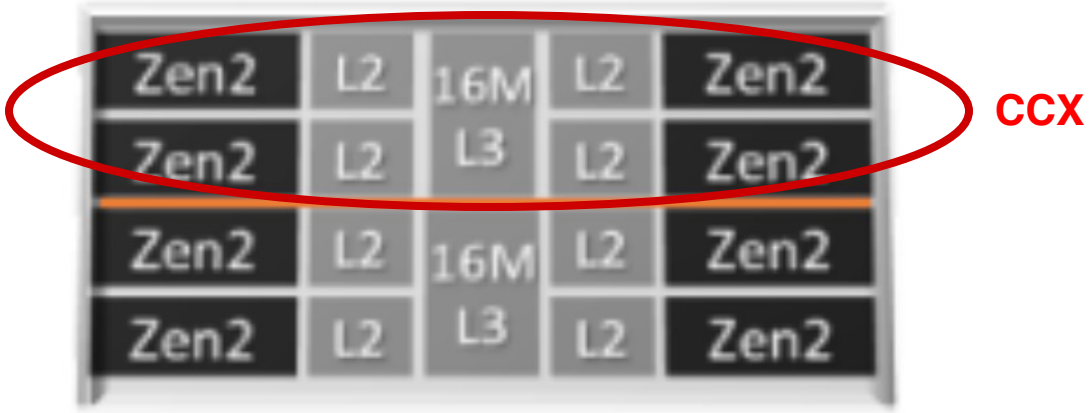
- 8 Core Complex Dies (CCDs).
- CCDs connect to memory, I/O, and each other through the I/O Die.
- 8 memory channels per socket.
- DDR4 memory at 3200MHz.
- PCI Gen4, up to 128 lanes of high speed I/O.
- Memory and I/O can be abstracted into separate quadrants each with 2 DIMM channels and 32 I/O lanes.



Reference: https://developer.amd.com/wp-content/resources/56827-1-0.pdf

AMD EPYC 7742 Processor: Core Complex Die (CCD)

- 2 Core Complexes (CCXs) per CCD
- 4 Zen2 cores in each CCX shared a 16M L3 cache. Total of 16 x 16 = 256MB L3 cache.
- Each core includes a private 512KB L2 cache.



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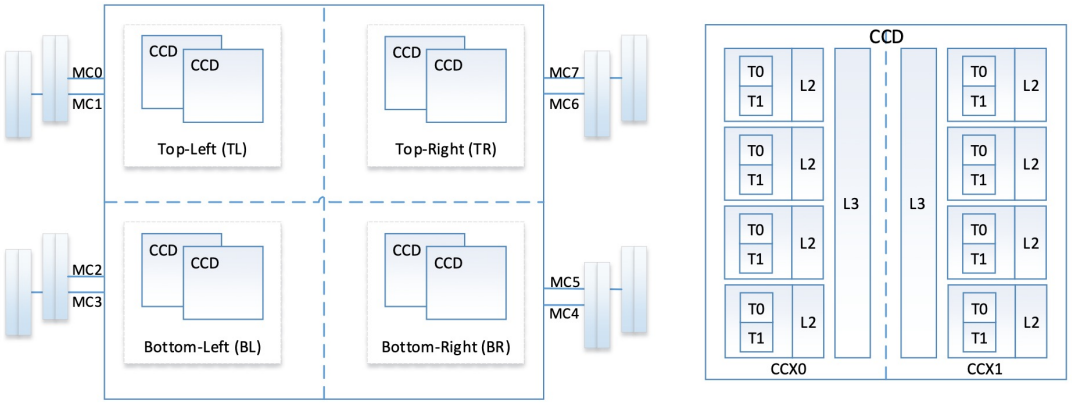
AMD EPYC 7742 Processor : NUMA Nodes Per Socket

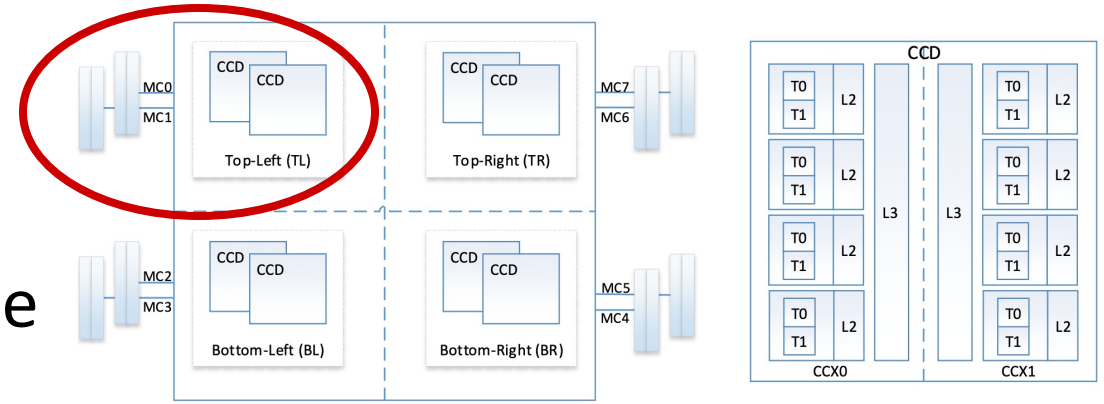
- The four logical quadrants allow the processor to be partitioned into different NUMA domains. Options set in BIOS.
- Domains are designated as NUMA per socket (NPS).
- **NPS4:** Four NUMA domains per socket is the typical HPC configuration.



https://developer.amd.com/wp-content/resources/56338_1.00_pub.pdf

NPS4 Configuration

- The processor is partitioned into four NUMA domains.
- Each logical quadrant is a NUMA domain.
- Memory is interleaved across the two memory channels
- PCIe devices will be local to one of four NUMA domains (the IO die that has the PCIe root for the device)
- ***This is the typical HPC configuration*** as workload is NUMA aware, ranks and memory can be pinned to cores and NUMA nodes.



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Using MPI options

- All MPI implementations have affinity options.
- Example OpenMPI run command:

  mpirun -np 32 --mca pml ucx --mca osc ucx --map-by l3cache xhpl

- Example Intel MPI setup:

  export OMP_NUM_THREADS=16

  mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./hello_hybrid

- Can also combine with application pinning options. For example for NAMD:

  mpirun -np 8 --map-by ppr:4:node namd2 +setcpuaffinity +ppn 31 +commap 0,32,64,96 +pemap 1-31,33-63,65-95,97-127 stmv.namd

ibrun and affinity options

- Basic usage
  - ibrun ./executable <executable_opions>
- With affinity
  - ibrun affinity <hints> ./executable <executable_opions>
- Affinity options
  - **scatter**: scatters the ranks across all numa domains in a cyclic manner
  - **scatter-ccd**: scatters the ranks across all AMD CCD domains in a cyclic manner
  - **scatter-ccx**: scatters the ranks across all AMD CCX domains in a cyclic manner
  - **scatter blk <blk_size>**: scatters the ranks across all numa domains in a cyclic manner, but with 'blk_size' (1-16) consecutive ranks packed into a single numa domain
  - **scatter-ccd blk <blk_size>**: scatters the ranks across AMD CCD domains in a cyclic manner, but with 'blk_size' (1-8) consecutive ranks packed into a single CCD domain
  - **scatter-ccx blk <blk_size>**: scatters the ranks across AMD CCX domains in a cyclic manner, but with 'blk_size' (1-4) consecutive ranks packed into a single CCX domain

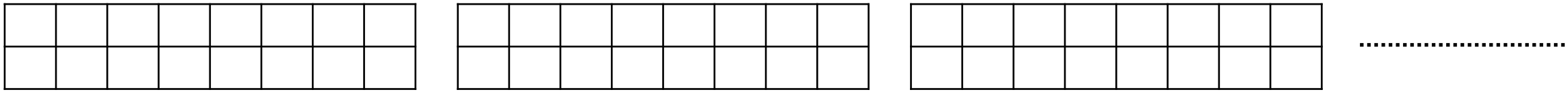
NOTE: valid blk_sizes depend on the **cpus-per-task a**nd the **domain type** (numa, CCD, CCX). 'blk' is optional and is set to '1' by default

Guide for Layout Diagrams (for upcoming slides)

NUMA Domain 1

NUMA Domain 2

NUMA Domain 3



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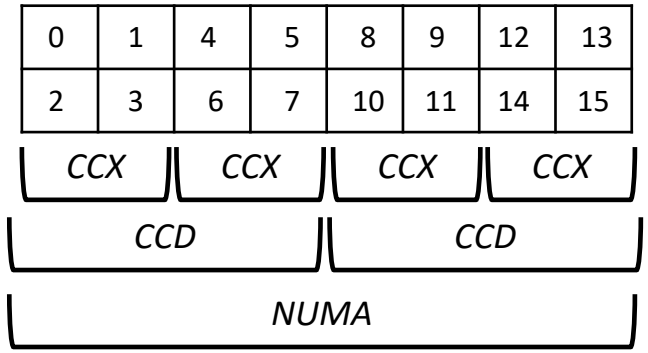


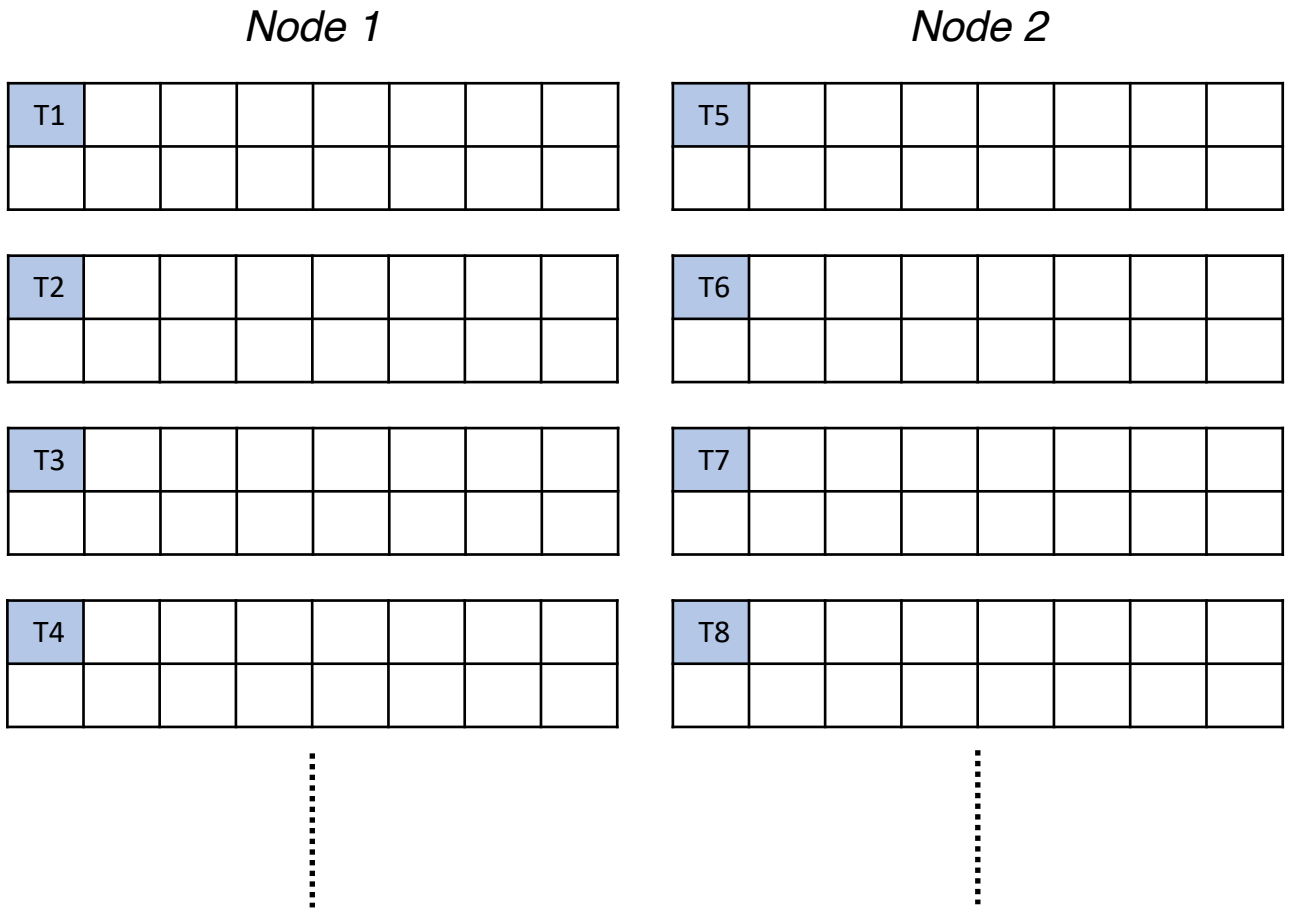
Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=4
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4

ibrun ./hy-gcc-openmpi.exe

(same as srun –n 8 ./hy-gcc-openmpi.exe)
```



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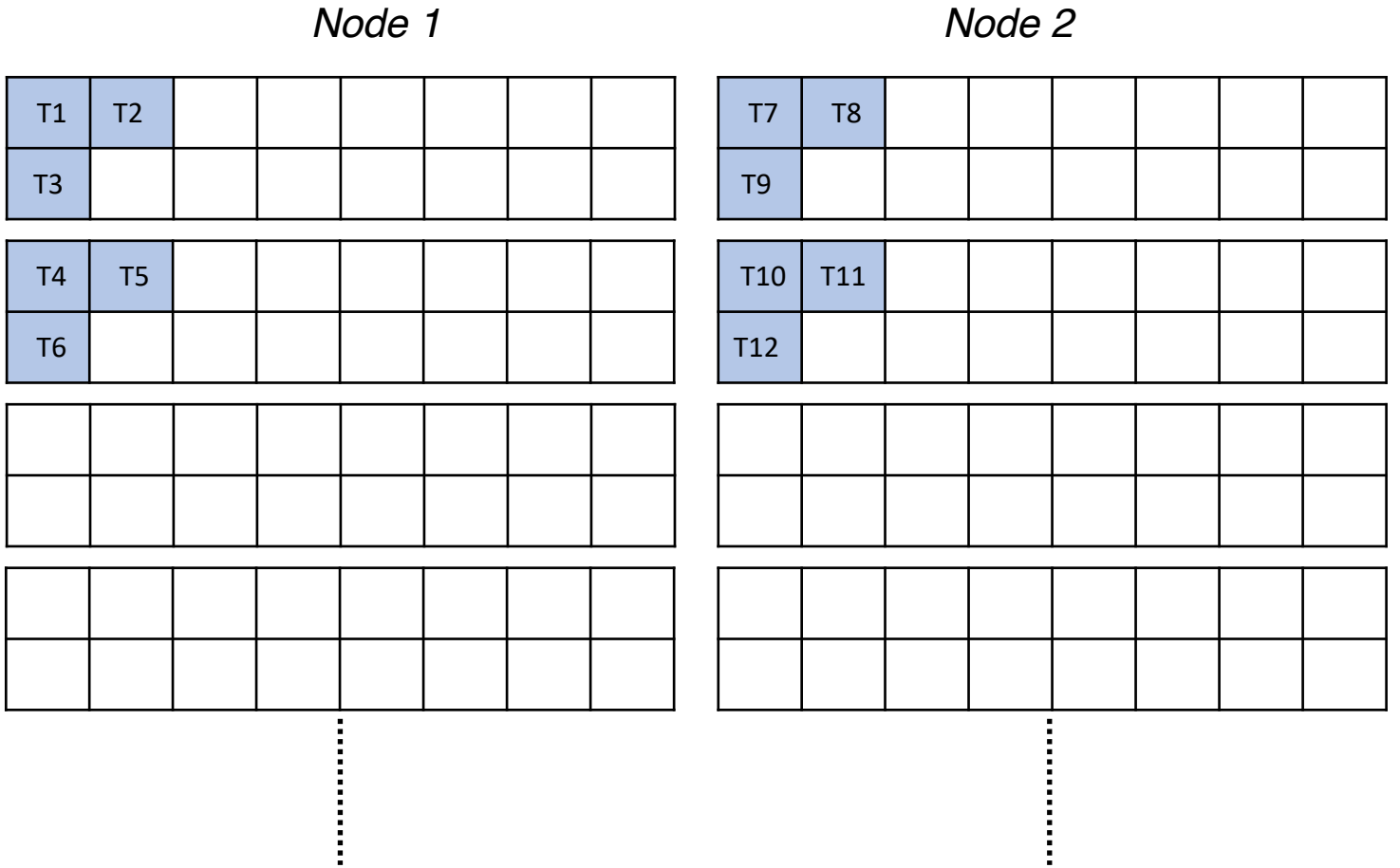
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
```

ibrun affinity scatter blk 3 ./hy-gcc-openmpi.exe



Example ibrun options and layouts

```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=2
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

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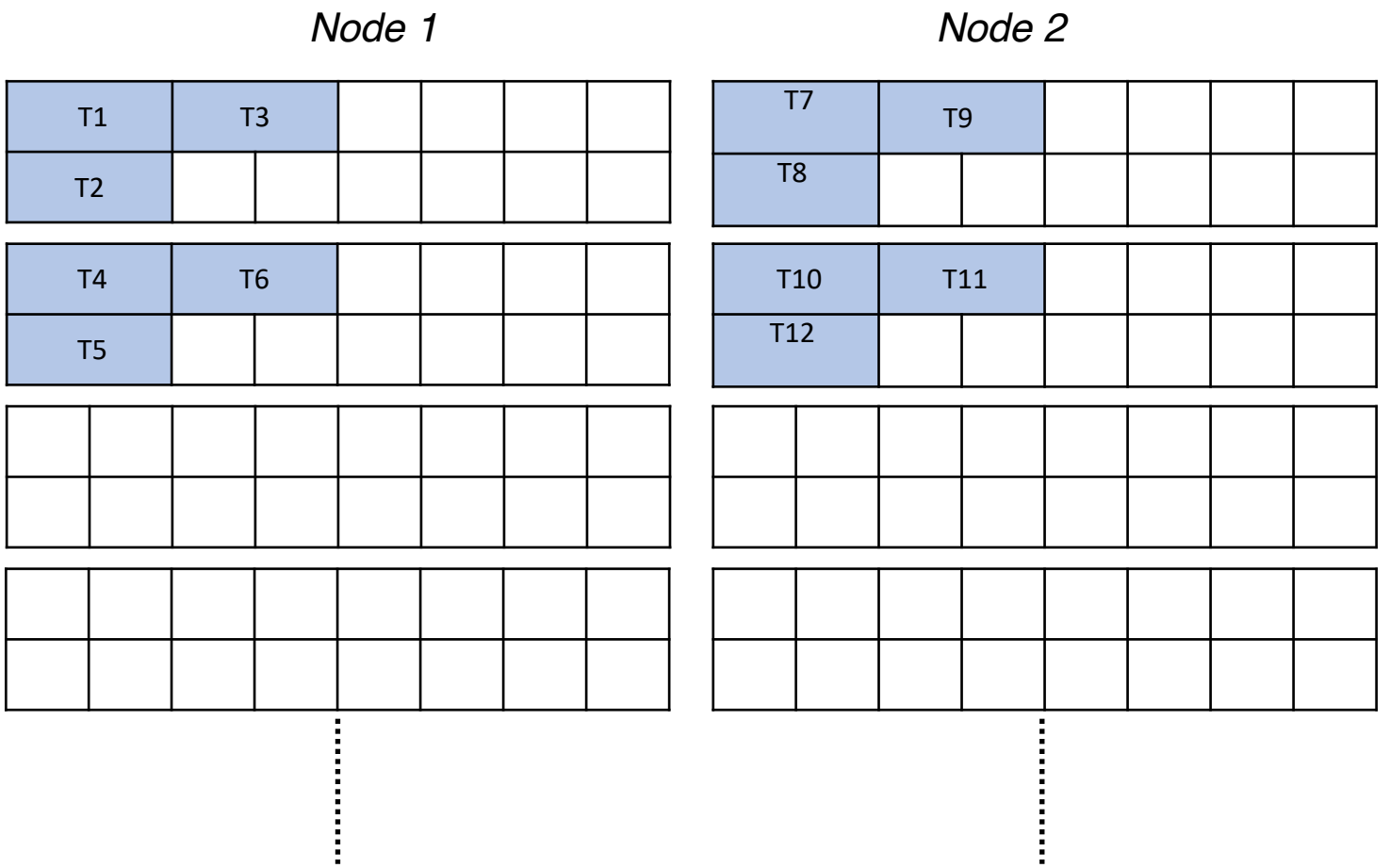

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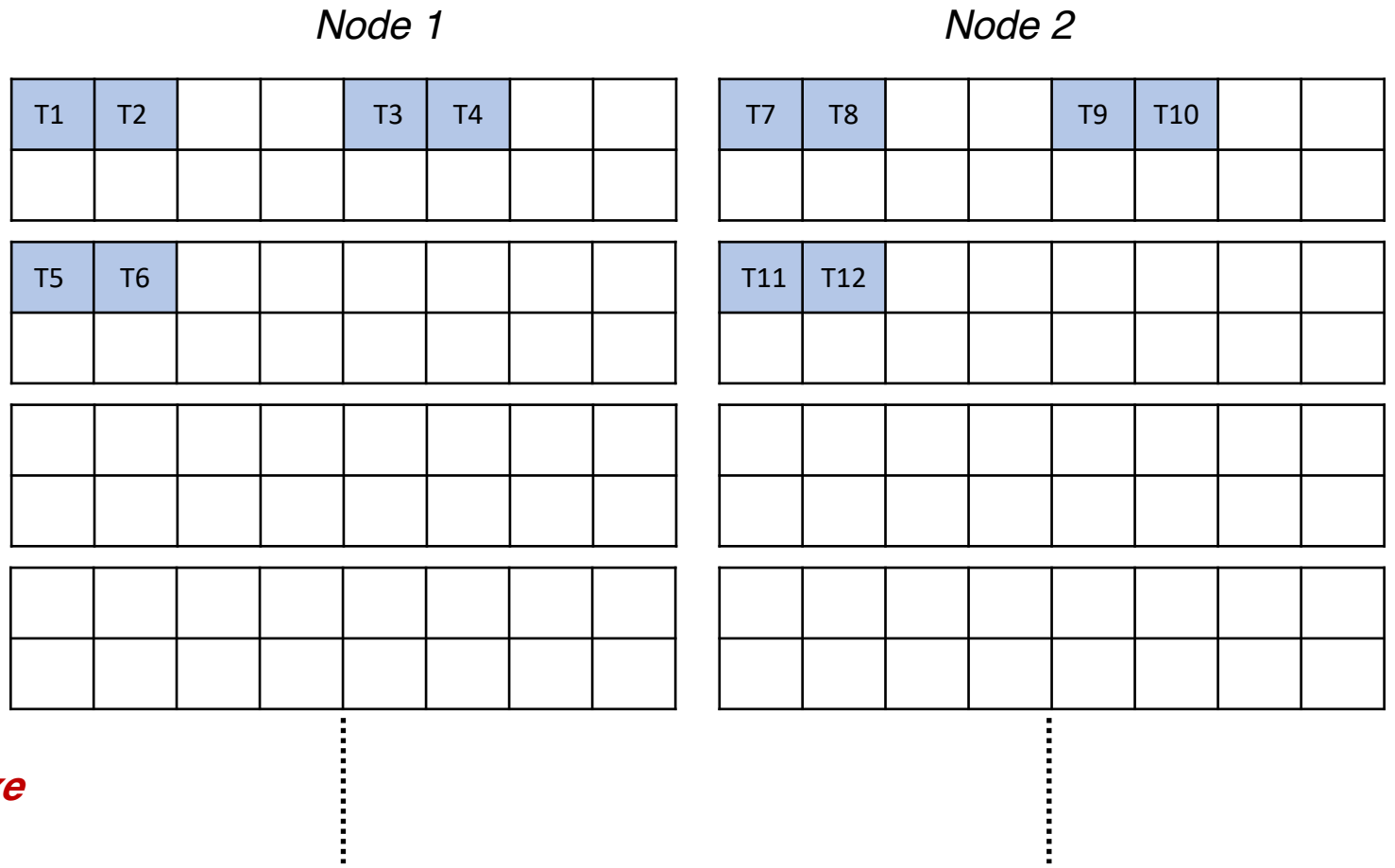
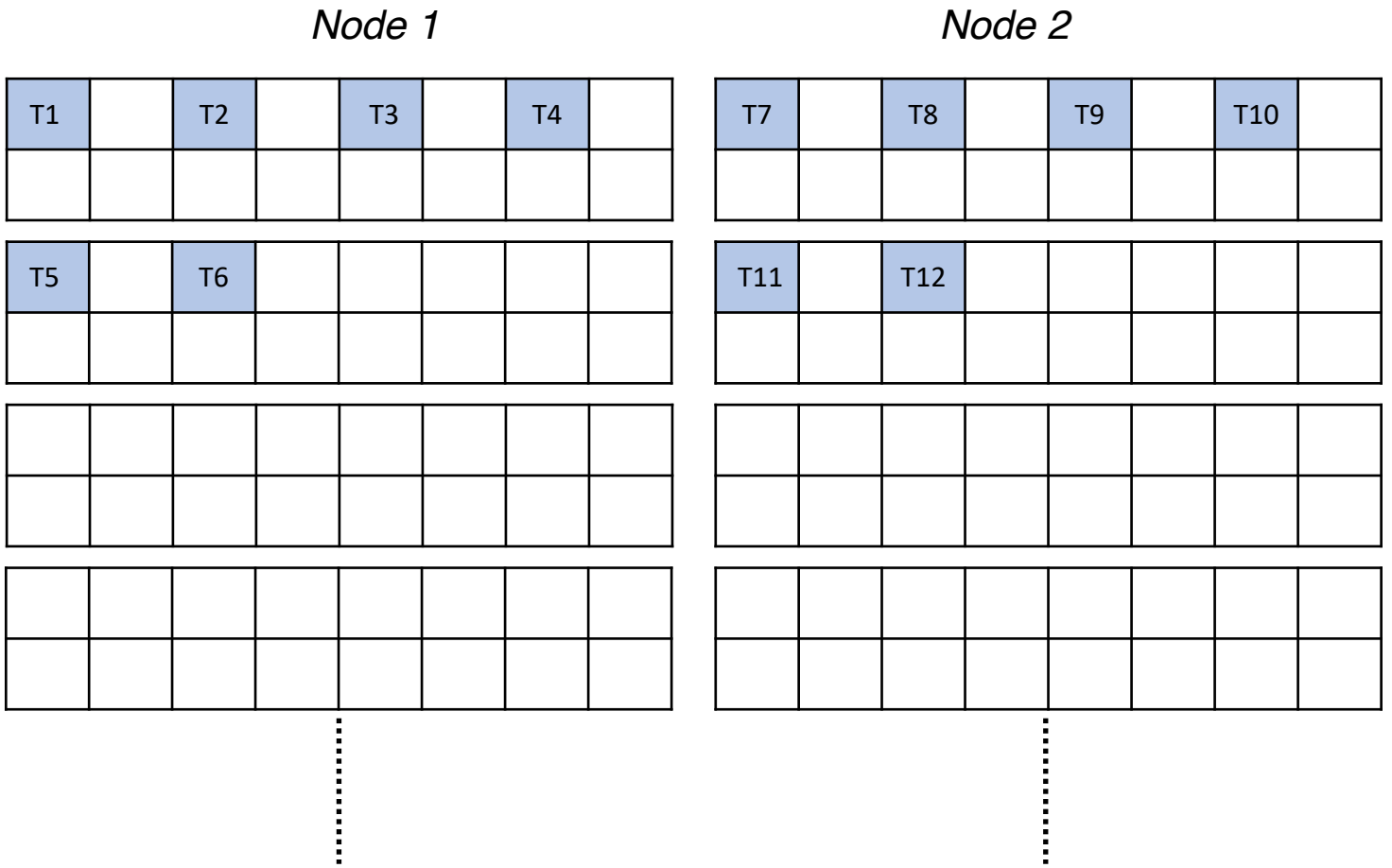


ibrun affinity scatter-ccd blk 2 ./hy-gcc-openmpi.exe

Example ibrun options and layouts

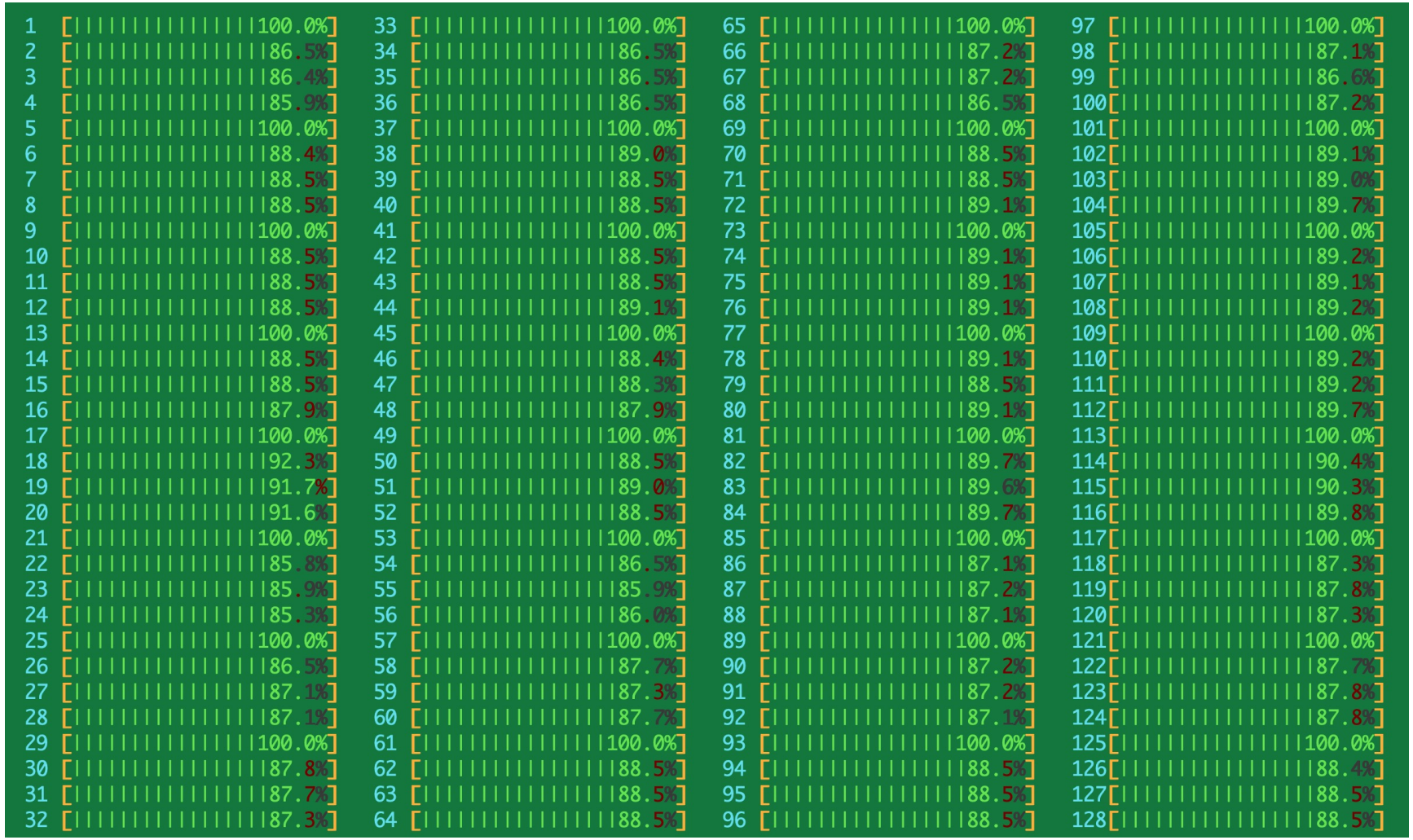
```
#!/bin/bash
#SBATCH -p compute
#SBATCH -N 2
#SBATCH -A <ACCT>
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=6
#SBATCH -t 00:20:00

### Expanse modules
module reset
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4

ibrun affinity scatter-ccx ./hy-gcc-openmpi.exe
```



Snapshot of task layout with scatter-ccx option

#SBATCH --nodes=1
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=4

ibrun affinity scatter-ccx $XHPL



Snapshot of task layout with scatter-ccx option

#SBATCH --nodes=1
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=4

ibrun affinity scatter-ccx $XHPL

```
82667 xhpl            mahidhar    2526976 R 98.4 00:02:10   0
82667 xhpl            mahidhar    2526976 S  0.0 00:00:00   0
82667 xhpl            mahidhar    2526976 S  0.8 00:00:01   0
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   1
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   2
82667 xhpl            mahidhar    2526976 R 87.9 00:01:49   3
82668 xhpl            mahidhar    2527544 R 98.4 00:02:09  40
82668 xhpl            mahidhar    2527544 S  0.0 00:00:00  40
82668 xhpl            mahidhar    2527544 S  0.9 00:00:01  40
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  41
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  42
82668 xhpl            mahidhar    2527544 R 88.3 00:01:49  43
82669 xhpl            mahidhar    2527532 R 98.3 00:02:09   4
82669 xhpl            mahidhar    2527532 S  0.0 00:00:00   4
82669 xhpl            mahidhar    2527532 S  0.7 00:00:00   4
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   5
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   6
82669 xhpl            mahidhar    2527532 R 87.7 00:01:48   7
```

slurm-aff-prod script for MPI/Pthreads codes

- The **slurm-aff-prod** script is used to bind Pthreads after MPI job launch. Can be used by wrapping binary based on name.

```
#!/bin/bash
#SBATCH -p shared
#SBATCH -N 1
#SBATCH --ntasks-per-node=10
#SBATCH --cpus-per-task=4
#SBATCH --mem=77G
#SBATCH -t 00:10:00
#SBATCH -J A76BE.GTRGAMMA.mpi10pt4NautoMRExfa
#SBATCH -o A76BE.GTRGAMMA.mpi10pt4NautoMRExfa.%j.%N.out
#SBATCH -e A76BE.GTRGAMMA.mpi10pt4NautoMRExfa.%j.%N.err
#SBATCH -A use300

export NP=$SLURM_TASKS_PER_NODE
export THREADS=$SLURM_CPUS_PER_TASK

rm RAx*

export AFFINITY_INFO=0
export AFFINITY_DEBUG=0

srun --mpi=pmi2 -n $NP ./raxmlHPC-HYBRID_8.2.12_expanse -s ./A76BE.txt -n A76BE.GTRGAMMA.mpi10pt4NautoMRExfa -m GTRGAMMA -N a
utoMRE -p 12345 -x 12345 -f a
```

```
#!/bin/sh

# This is for running on EXPANSE

#source $HOME/.bashrc

module reset
module load sdsc
module load gcc/10.2.0
module load openmpi/4.0.4
module load raxml/8.2.12
module load slurm

EXE='raxmlHPC-HYBRID-AVX'
slurm-aff-prod-test $EXE &

echo "running:"
echo " $EXE -T ${THREADS} $*"

$EXE -T ${THREADS} $*
```

Summary

- AMD Processor on Expanse has 4 NUMA domains with 16 cores each.
- 8 Core Complex Dies (CCDs) per processor, with 2 Core Complexes (CCXs) per CCD. Four cores in a CCX share L3 cache.
- For hybrid MPI/OpenMP and MPI/Pthreads codes it is important to lay out tasks correctly and binding is important for performance.
- **ibrun, affinity, and slurm-aff-prod** scripts available to make it easier to lay out and bind tasks.
- Follow all things Expanse at https://www.sdsc.edu/support/user_guides/expanse.html
- Tools are being updated so feedback is encouraged!

Thank you to our collaborators, partners, users, and the SDSC team!

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