Numascale
Best Practice Guide

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Revision History

Rev	Date	Author	Changes
0.1	2014-03-03	Atle Vesterkjær	First version
1.0	2014-03-05	Atle Vesterkjær	Added link to wiki. Updated with better fonts.
1.1	2014-03-16	Atle Vesterkjær	Installation hints
1.2	2014-08-28	Atle Vesterkjær	Added information about how to run hybrid applications (MPI+OpenMP)
1.3	2014-08-28	Atle Vesterkjær	Added information about how to run linear algebra code using thread safe scalapack
1.4	2015-05-22	Atle Vesterkjær	Fixed the MPI and Hybrid rankfiles to fit the interpretation of socket in newer kernels, tested on 3.19.5-numascale45+

1 INTRODUCTION

1.1 Abstract

This is a summary of best practices for achieving optimal results using Numascale Shared Memory Systems with emphasis on running and optimizing applications. Keywords are:

- OpenMP, affinity, different compilers
- MPI, linpack, NPB, rankfiles
- Vmstat, htop, top, numastat, *"cat /proc/cpuinfo"* etc.
- Numa-aware optimizations of code

1.2 Abbreviations

Throughout this document, we use the following terms:

Numascale AS	The name of the company that develops and owns NumaChip and NumaConnect.
NumaServer	A server equipped with a NumaConnect card.
NumaMaster	A NumaServer with an instance of the operating system installed.

1.3 Background

This document is an addendum to documents at http://www.numascale.com/numa_support.html that cover all aspects of setup, cabling and installation of a Numascale Shared Memory system:

- Numascale hardware installation guides
  - https://resources.numascale.com/Numascale-Hardware-Installation-IBM-System-x3755-M3.pdf
  - https://resources.numascale.com/Numascale-Hardware-Installation-H8QGL-iF+.pdf
- NumaManager Quick Start Guide, https://resources.numascale.com/nma-quickstart.pdf
  - a one page Quick Start Guide for deployment of NumaConnect
- NumaConnect Deployment with NumaManager, https://resources.numascale.com/nc-deployment-nma.pdf
  - a complete guide to get a NumaConnect system up and running. Using the NumaManager in this process is strongly recommended and the NumaManager is included in the NumaConnect delivery
- NumaConnect Deployment, https://resources.numascale.com/nc-deployment.pdf
  - a complete guide to get a NumaConnect system up and running when no NumaManager is available. It is recommended to use the NumaManager in this process

Any **multithreaded** application can run on Numascale Shared Memory System. The basic criteria's for being interested in a Numascale Shared Memory System are typically:

- You have a multithreaded application that can benefit from a larger number of cores then a single server can provide.
- You have an application that requires more memory than a single server can provide
- You have an application that requires both more cores and more memory than a single server can provide

2 MULTITHREADED APPLICATION THAT CAN BENEFIT FROM A LARGER NUMBER OF CORES THEN A SINGLE SERVER CAN PROVIDE

If you have a multithreaded application that can benefit from a larger number of cores than a single server can provide it is a good candidate for a Numascale Shared Memory System. Compared to other High-End ccNuma solutions and software only ccNuma solutions cores comes at a very low price in a NumaConnect Shared Memory System.

If your application scales well when you use more of the cores in your server, then there is a good chance that it will succeed running on a Numascale Shared Memory System with a larger number of cores than you have in your single server.

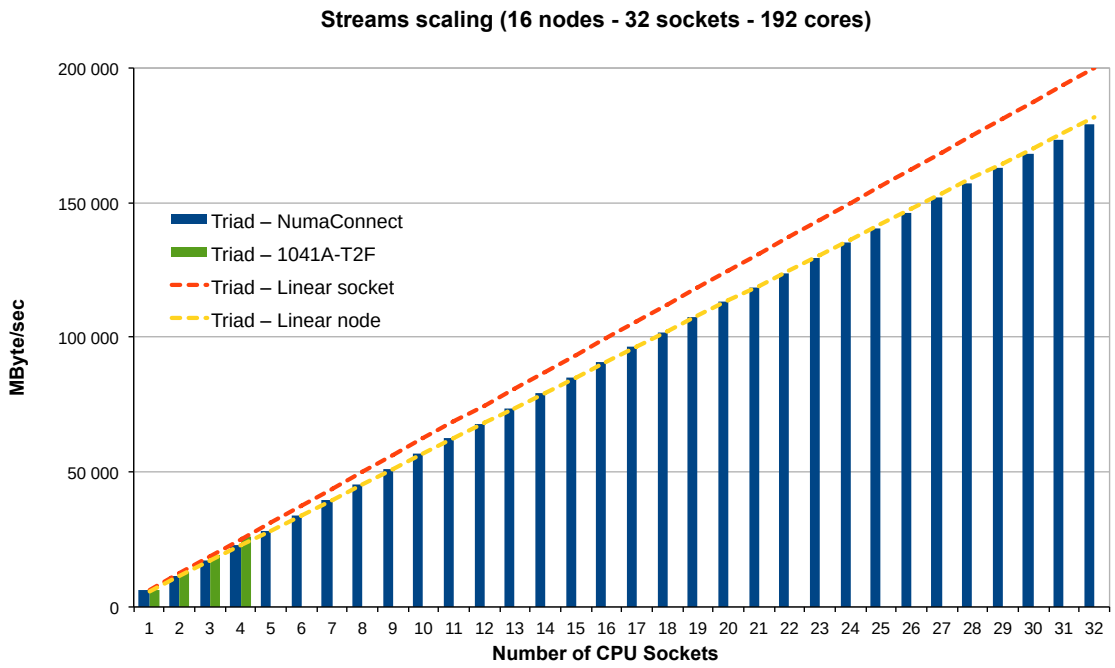


Figure 1: On a Numascale Shared Memory System the Streams benchmark can run in parallel on a larger number of cores than you have in your single server

The Stream benchmark is used as an example of such an application. Looking at the green bars in Figure 1 you see that the speedup increases when using more sockets inside the one server. This makes the application a good candidate for ccNuma systems.

In chapter 3 we will look into how a multithreaded application accesses memory in a ccNuma system. This is very relevant to how well it will scale in a large shared memory system when all CPUs and memory no longer are on the same physical server.

2.1 Tuning your application for a Numascale system

2.1.1 OpenMP

An OpenMP application has very nice runtime characteristics. It is the de-facto state of the art way of doing multithreaded programs. OpenMP pragmas allows you to parallelize code. OpenMP has a very nice way of parallelizing code as it gives the compiler a hint on where to place the parallel threads. Use environment variables in order to control the runtime of applications using OpenMP.

- GNU: `OMP_NUM_THREADS=64 GOMP_CPU_AFFINITY="0-255:4" bin/ep.C.x`
- GNU: `OMP_NUM_THREADS=128 GOMP_CPU_AFFINITY="0-127" bin/ep.C.x`
- GNU: `OMP_NUM_THREADS=128 GOMP_CPU_AFFINITY="0-255:2" bin/ep.C.x`
- PGI: `OMP_THREAD_LIMIT=128 OMP_PROCS_BIND=true OMP_NUM_THREADS=128 MP_BIND=yes MP_BLIST=$(seq -s, 0 2 255) bin_pgfortran/ep.C.x`

The AMD Opteron™ 6300 series processor is organized as a Multi-Chip Module (two CPU dies in the package), interconnected using a Hyper Transport link. Each die has its own memory controller interface to allow external connection of up to two memory channels per die. This memory interface is shared among all the CPU core pairs on each die. Each core pair appears to the operating system as two completely independent CPU cores. Thus, to the OS, the device shown in Figure 2 appears as 16 CPUs.

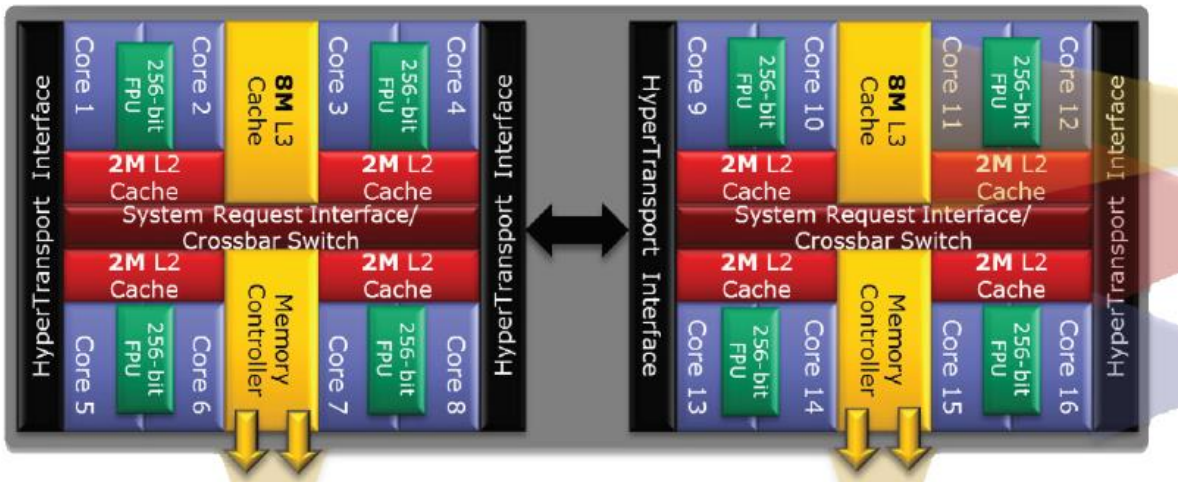


Figure 2: The AMD Opteron™ 6300 series processor is organized as a Multi-Chip Module

In Numascale Shared Memory System with AMD 6380 CPUs the most efficient way to run an FPU intensive OpenMP application with 128 threads in a 256 cores system is:

```
[atle@numademo NPB3.3-OMP]$ OMP_NUM_THREADS=128 GOMP_CPU_AFFINITY="0-255:2" bin/sp.D.x
```

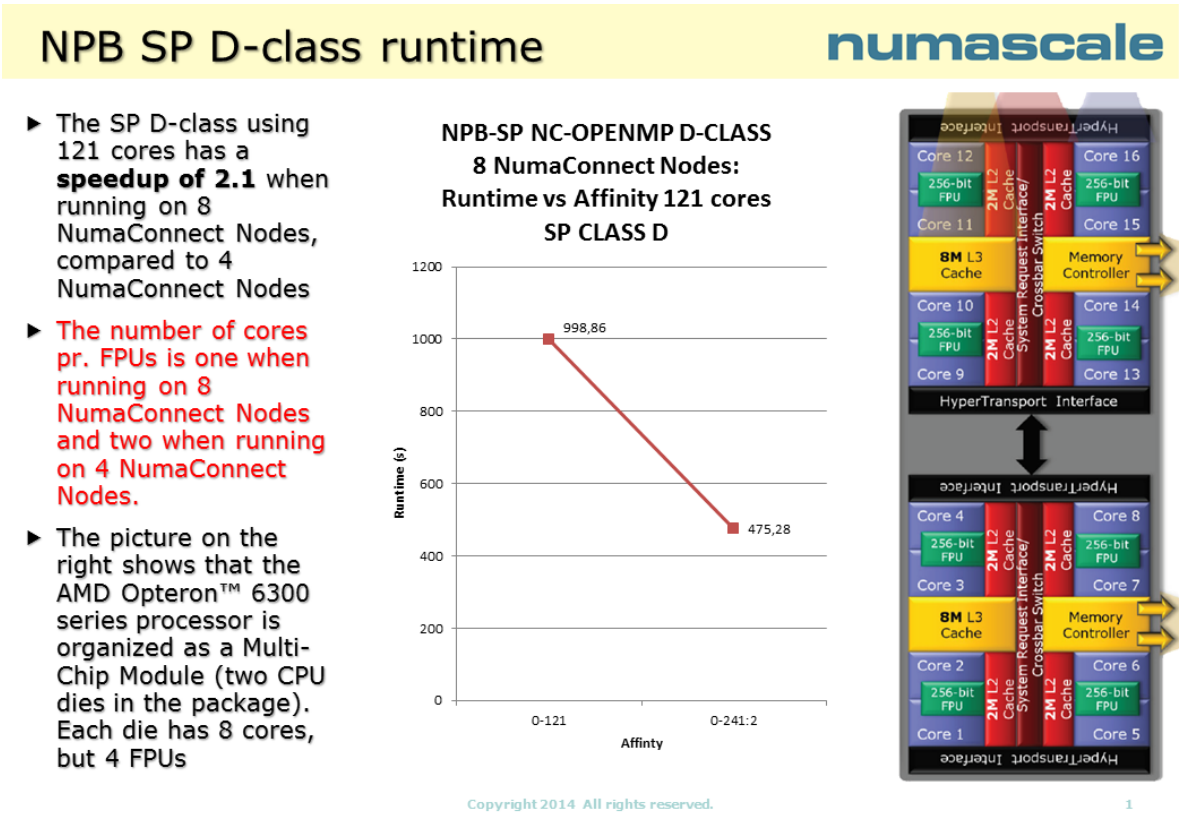


Figure 3: Speedup of Numascale OpenMP application when using more FPUs

If an OpenMP application uses 64 threads, the most efficient way to distribute the threads in the system is to get lower load on the memory interface and L3 cache shared among all the CPU core pairs on each die is using every fourth core in your system:

```
[atle@numademo NPB3.3-OMP]$ OMP_NUM_THREADS=64 GOMP_CPU_AFFINITY="0-255:4" bin/sp.D.x
```

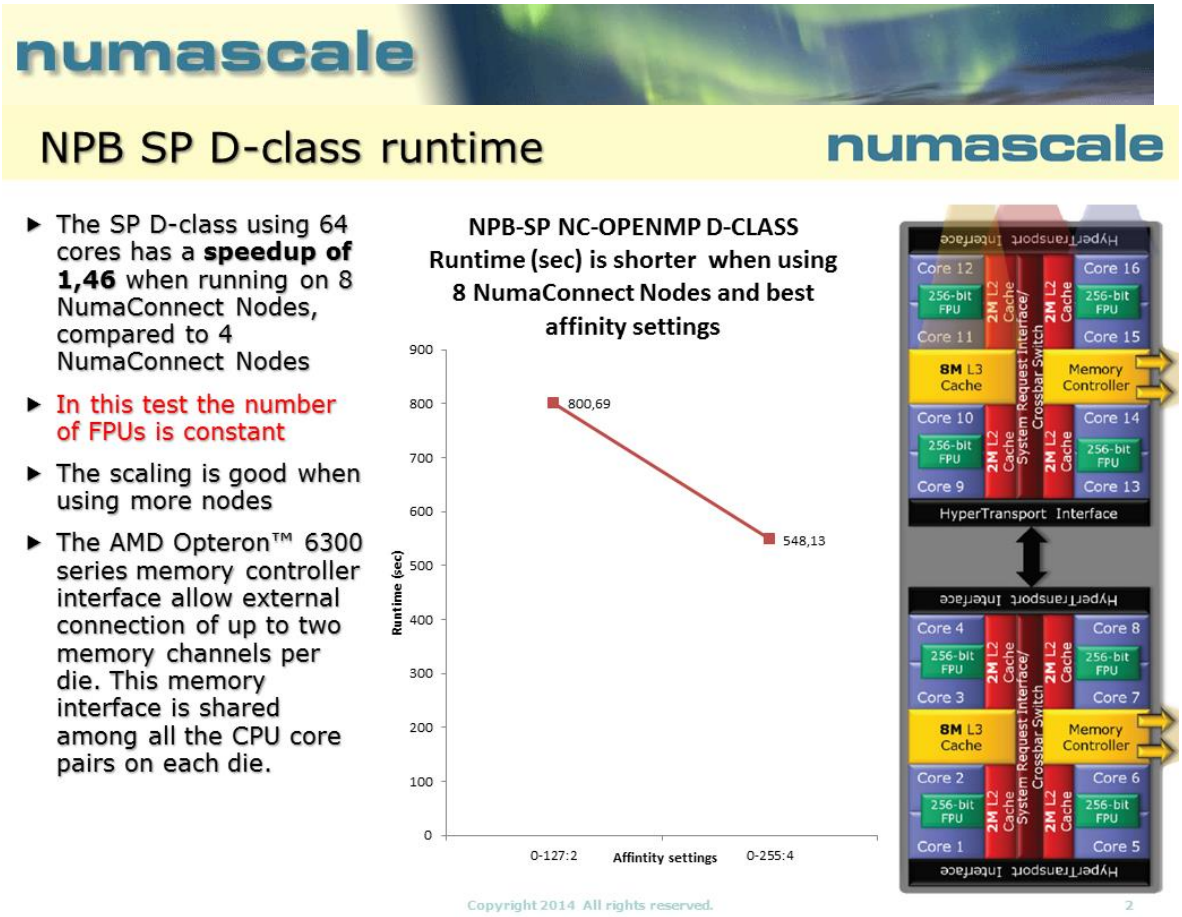


Figure 4: Speedup of Numascale OpenMP application when balancing the load to get a FAT link to memory and L3 cache

2.1.2 MPI

Numascale has developed a byte transfer layer (BTL) for OpenMPI that fully utilizes the NumaConnect. The Numascale OpenMPI implementation is very efficient compared to a standard shared memory BTL. Standard tests show a speedup of 4.5 – 19.9 on typical systems.

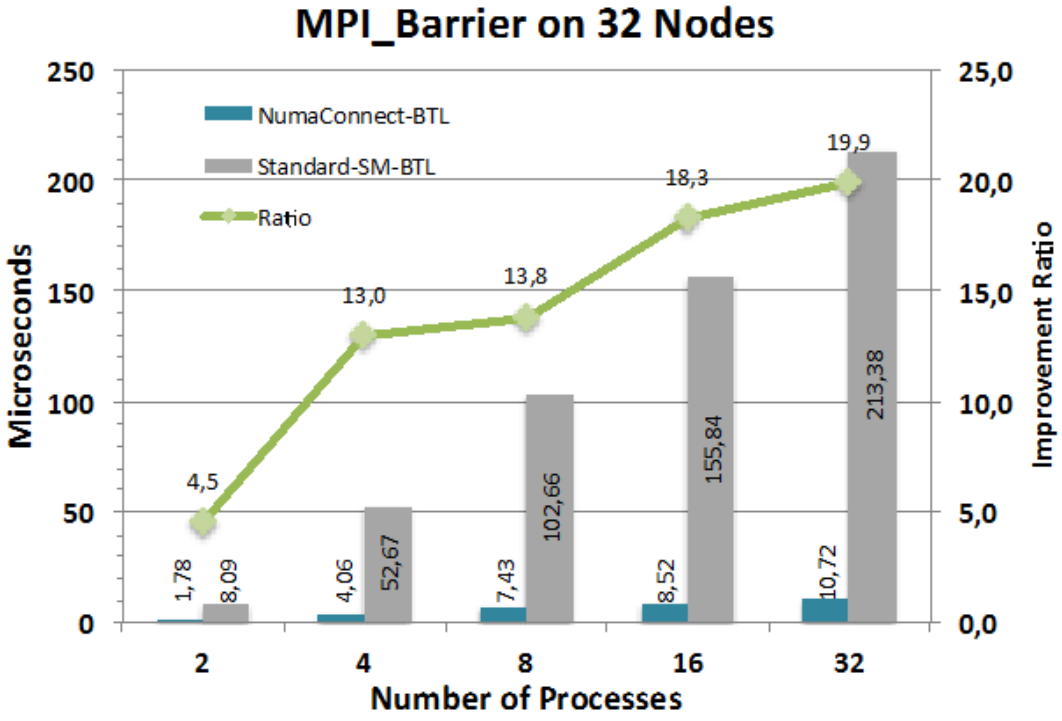


Figure 5: Numascale NumaConnect-BTL boosts your MPI performance

In order to use the NumaConnect-BTL make sure that it is included in the path:

```
[atle@numademo NPB3.3-MPI]$ export LD_LIBRARY_PATH=/opt/openmpi-1.7.2-numaconnect/lib:$LD_LIBRARY_PATH
[atle@numademo NPB3.3-MPI]$ export PATH=/opt/openmpi-1.7.2-numaconnect/bin:$PATH
[atle@numademo NPB3.3-MPI]$ which mpiexec
/opt/openmpi-1.7.2-numaconnect/bin/mpiexec
[atle@numademo NPB3.3-MPI]$
```

There are different ways of optimizing an MPI application. In order to avoid using slow disk IO we use tmpfs (dev/shm) as location for temporary OpenMPI files set by the flag `OMPI_PREFIX_ENV`.

Use the *–bind-to-core* option for jobs running on all the cores in the system:

```
[atle@numademo ~]$ OMPI_PREFIX_ENV=/dev/shm mpiexec -n 256 --bind-to-core -mca btl self,nc bin/lu.D.256
```

Use rankfiles when not running on all cores in the system.

An MPI application that utilizes less than all cores in a Numascale Shared Memory is optimized using rank files. In a 256 core system using AMD 6380 CPUs you can instruct your application to use one FPU per core by selecting every second core in a rankfile:

```
[atle@numademo NPB3.3-MPI]$ cat rank128_lu
rank  0=numademo slot=0:0
rank  1=numademo slot=0:2
```

```
rank  2=numademo slot=0:4
rank  3=numademo slot=0:6
….. until
rank 120=numademo slot=15:0
rank 121=numademo slot=15:2
rank 122=numademo slot=15:4
rank 123=numademo slot=15:6
rank 124=numademo slot=15:8
rank 125=numademo slot=15:10
rank 126=numademo slot=15:12
rank 127=numademo slot=15:14
atle@numademo NPB3.3-MPI]$
```

By using every fourth core in the system, it is possible to distribute the processes even more utilize all memory controllers and L3 caches in the system:

```
[atle@numademo NPB3.3-MPI]$ cat rank64
rank  0=numademo slot=0:0
rank  1=numademo slot=0:4
rank  2=numademo slot=0:8
rank  3=numademo slot=0:12
…..etc until
rank 60=numademo slot=15:0
rank 61=numademo slot=15:4
rank 62=numademo slot=15:8
rank 63=numademo slot=15:12
```

Start the application with these options set:

```
[atle@numademo NPB3.3-MPI]$ OMPI_PREFIX_ENV=/dev/shm mpiexec
-n 64 -rf rank64 -mca btl self,nc bin/lu.D.64
```

2.1.3 Hybrid (MPI+OpenMP)

Applications suites that comes with a hybrid version are able to run “out of the box” on a Numascale Shared Memory System.

Here is one example using the NAS Parallel Benchmarks, NPB-MZ-MPI applications suite that comes with a hybrid version. In this example each of the 16 MPI processes spawns two (2) threads using OpenMP, utilizing 32 cores.

[atle@numademo NPB3.3-MZ-MPI]$

export LD_PRELOAD=/opt/HOARD/libhoard.so

[atle@numademo NPB3.3-MZ-MPI]$

export OMP_NUM_THREADS=2;/opt/openmpi-1.6.0-numaconnect/bin/mpirun -n

16 --mca btl nc,self -rf rank16_colon2 bin_gnu/lu-mz.C.16

Here is the hybrid rank file used for the test:

```
[atle@numademo NPB3.3-MZ-MPI]$ cat rank16_2
rank  0=localhost slot=0:0,0:2
rank  1=localhost slot=0:4,0:6
rank  2=localhost slot=0:8,0:10
rank  3=localhost slot=0:12,0:14
…
rank  15=localhost slot=3:8,3:10
```

If you want to run a test on 16 MPI processes each spawning 8 OpenMP threads, in total 128 cores you can use this rank-file:

```
[atle@numademo NPB3.3-MZ-MPI]$ cat rank16_8
rank  0=h8qgl slot=0:0,0:2,0:4,0:6,0:8,0:10,0:12,0:14
rank  1=h8qgl slot=1:0,1:2,1:4,1:6,1:8,1:10,1:12,1:14
rank  2=h8qgl slot=2:0,2:2,2:4,2:6,2:8,2:10,2:12,2:14
rank  3=h8qgl slot=3:0,3:2,3:4,3:6,3:8,3:10,3:12,3:14
rank  4=h8qgl slot=4:0,4:2,4:4,4:6,4:8,4:10,4:12,4:14
rank  5=h8qgl slot=5:0,5:2,5:4,5:6,5:8,5:10,5:12,5:14
rank  6=h8qgl slot=6:0,6:2,6:4,6:6,6:8,6:10,6:12,6:14
rank  7=h8qgl slot=7:0,7:2,7:4,7:6,7:8,7:10,7:12,7:14
rank  8=h8qgl slot=8:0,8:2,8:4,8:6,8:8,8:10,8:12,8:14
rank  9=h8qgl slot=9:0,9:2,9:4,9:6,9:8,9:10,9:12,9:14
rank  10=h8qgl slot=10:0,10:2,10:4,10:6,10:8,10:10,10:12,10:14
rank  11=h8qgl slot=11:0,11:2,11:4,11:6,11:8,11:10,11:12,11:14
rank  12=h8qgl slot=12:0,12:2,12:4,12:6,12:8,12:10,12:12,12:14
rank  13=h8qgl slot=13:0,13:2,13:4,13:6,13:8,13:10,13:12,13:14
rank  14=h8qgl slot=14:0,14:2,14:4,14:6,14:8,14:10,14:12,14:14
rank  15=h8qgl slot=15:0,15:2,15:4,15:6,15:8,15:10,15:12,15:14
```

and run:

```
[atle@numademo NPB3.3-MZ-MPI]$ export
OMP_NUM_THREADS=8;/opt/openmpi-1.6.0-numaconnect/bin/mpirun -n 16
--mca btl nc,self -rf rank16_8 bin_gnu/lu-mz.C.16
```

2.1.4 Pthreads, or other multithreaded applications

taskset or numactl apply a mask for the creation of threads in a multithreaded program. Applications written with pthreads can use this to choose cores and memory segments for execution. In tests at Numascale, taskset and numactl perform equally well, but other online resources recommend using numactl for guaranteed memory binding.

```
[root@x3755 02_BWA_MEM]# taskset
taskset (util-linux-ng 2.17.2)
usage: taskset [options] [mask | cpu-list] [pid | cmd [args...]]
set or get the affinity of a process

p, --pid                  operate on existing given pid
c, --cpu-list             display and specify cpus in list format
h, --help                 display this help
V, --version              output version information

The default behavior is to run a new command:
taskset 03 sshd -b 1024
You can retrieve the mask of an existing task:
taskset -p 700
Or set it:
taskset -p 03 700
List format uses a comma-separated list instead of a mask:
taskset -pc 0,3,7-11 700
Ranges in list format can take a stride argument:
e.g. 0-31:2 is equivalent to mask 0x55555555
[root@x3755 02_BWA_MEM]# numactl
usage: numactl [--interleave=nodes] [--preferred=node]
[--physcpubind=cpus] [--cpunodebind=nodes]
[--membind=nodes] [--localalloc] command args ...
numactl [--show]
numactl [--hardware]
numactl [--length length] [--offset offset] [--shmmode shmmode]
[--strict]
[--shmid id] --shm shmkeyfile | --file tmpfsfile
[--huge] [--touch]
memory policy | --dump | --dump-nodes
memory policy is—interleave, --preferred, --membind, --localalloc
nodes is a comma delimited list of node numbers or A-B ranges or all.
cpus is a comma delimited list of cpu numbers or A-B ranges or all
all ranges can be inverted with !
all numbers and ranges can be made cpuset-relative with +
the old—cpubind argument is deprecated.
use—cpunodebind or—physcpubind instead
length can have g (GB), m (MB) or k (KB) suffixes
[root@x3755 02_BWA_MEM]#
```

"numactl –hardware" gives a good view of the hardware setup. Here a Numascale Shared Memory System with two NumaServers, 8 sockets and 64 cores is used:

```
[root@x3755 02_BWA_MEM]# numactl—hardware
available: 8 nodes (0-7)
node 0 cpus: 0 1 2 3 4 5 6 7
node 0 size: 65491 MB
```

```
node 0 free: 24474 MB
node 1 cpus: 8 9 10 11 12 13 14 15
node 1 size: 65536 MB
node 1 free: 56116 MB
node 2 cpus: 16 17 18 19 20 21 22 23
node 2 size: 65536 MB
node 2 free: 64338 MB
node 3 cpus: 24 25 26 27 28 29 30 31
node 3 size: 47104 MB
node 3 free: 46263 MB
node 4 cpus: 32 33 34 35 36 37 38 39
node 4 size: 65536 MB
node 4 free: 64358 MB
node 5 cpus: 40 41 42 43 44 45 46 47
node 5 size: 65536 MB
node 5 free: 62861 MB
node 6 cpus: 48 49 50 51 52 53 54 55
node 6 size: 65536 MB
node 6 free: 63288 MB
node 7 cpus: 56 57 58 59 60 61 62 63
node 7 size: 49152 MB
node 7 free: 46946 MB
node distances:
node   0   1   2   3   4   5   6   7
0:  10  16  16  22  100  100  100  100
1:  16  10  16  22  100  100  100  100
2:  16  16  10  16  100  100  100  100
3:  22  22  16  10  100  100  100  100
4:  100  100  100  100  10  16  16  22
5:  100  100  100  100  16  10  16  22
6:  100  100  100  100  16  16  10  16
7:  100  100  100  100  22  22  16  10
```

Here are some advices on how to tune a multithreaded application by selecting a runtime mask:

- Running only on the first socket

```
taskset -c 0-7 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -t ${REF} ${INP} ${INP2}
```

```
numactl—cpunodebind 0,1,2,3  --membind 0,1,2,3 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -t ${REF} ${INP} ${INP2}
```

- Running on all cores in the first NumaServer

```
taskset -c 0-31 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -M ${REF} ${INP} ${INP2}
```

```
numactl—cpunodebind 0,1,2,3,4,5,6,7  --membind 0,1,2,3,4,5,6,7 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -t ${REF} ${INP} ${INP2}
```

```
numactl—physcpubind 0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27
```

```
,28,29,30,31  --membind 0,1,2,3,4,5,6,7
/scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -t ${REF}
${INP} ${INP2}
```

- Running on all FPUs in the first NumaServer

```
taskset -c 0-31:2 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t
$procs -M ${REF} ${INP} ${INP2}
```

```
numactl—physcpubind 0,2,4,6,8,10,12,14,16,18,20,22,24,26,28,30  --membind
0,1,2,3,4,5,6,7 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t
$procs -t ${REF} ${INP} ${INP2}
```

- Running on all FPUs in the system

```
taskset -c 0-63:2 /scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t
$procs -M ${REF} ${INP} ${INP2}
```

```
numactl—physcpubind 0,2,4,6,8,10,12,14,16,18,20,22,24,26,28,30  --membind
0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15
/scratch/demouser04/04_Software/bwa-0.7.4/bwa mem -t $procs -t ${REF}
${INP} ${INP2}
```

Monitor the system usage with vmstat, htop, top and numastat to see if it behaves as intended with these runtime parameters. Please note that htop and top requires some system resources and might influence the performance. We recommend restarting the benchmark with the more lightweight vmstat for the final benchmark test when the runtime parameters have been qualified.

2.2 Running linear algebra libraries

ScaLAPACK is a scalable subset of the LAPACK (Linear Algebra Package) routines. It is open source and can be found at www.netlib.org. All commonly used linear algebra libraries like IBM ESSL, Intel MKL, AMD ADSL, IMSL, NAG use LAPACK and BLAS. The vensors supply a highly optimized version of the Netlib code. Numerical applications like Matlab or Fluent use these optimized libraries.

ScaLapack is based on MPI communication in Blacs and is not thread-save.

Our hardware supports solvers running threads distributed. We can provide a thread-save ScaLapack and OpenMP, shared memory based Blacs library.
This way the solvers run in a single process using OpenMP distributed on several machines.

Please check out https://wiki.numascale.com/tips/building-openmp-based-scalapack for more information.

3 MEMORY LAYOUT OF APPLICATIONS IN A NUMASCALE SHARED MEMORY SYSTEM

In order to illustrate the basic difference between a Numascale Shared Memory System and a cluster we consider a large job that can be solved in parallel by a large number of resources. In the clustering world, a large data set will be split into smaller fragment that will be distributed to individual nodes that are loosely coupled using the MPI protocol.

Imagine that such a job represents a large image like in Figure 6.

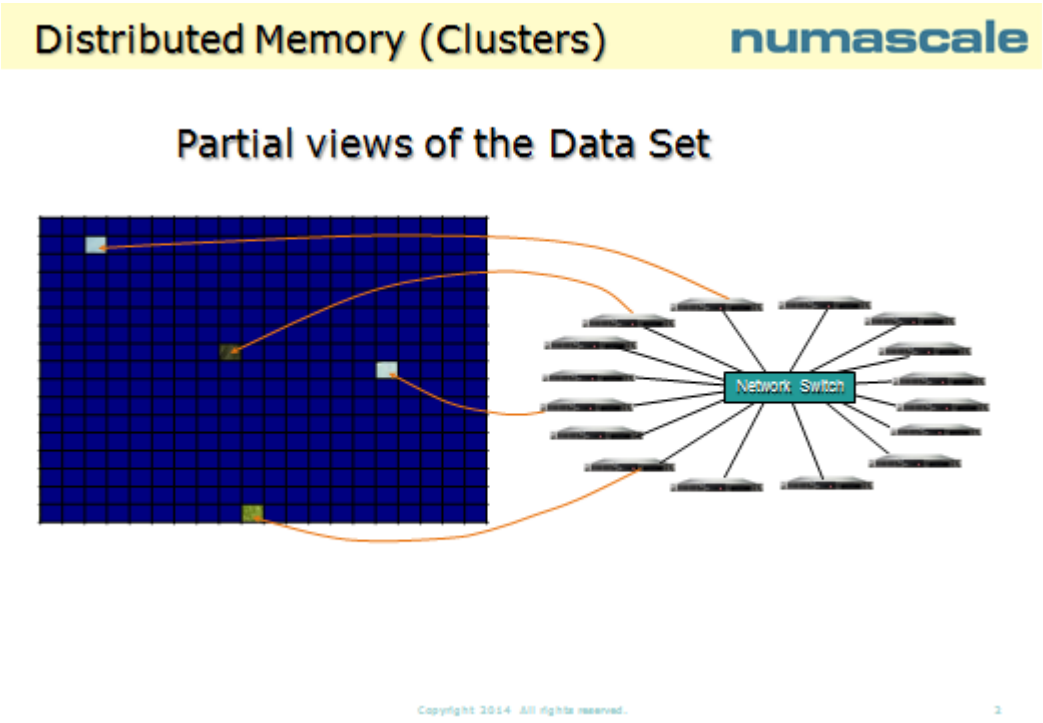


Figure 6: Distributed Memory (Clusters)

Consider the same job in the Numascale context. A shared view of the whole dataset is just as simple as on a standalone server.

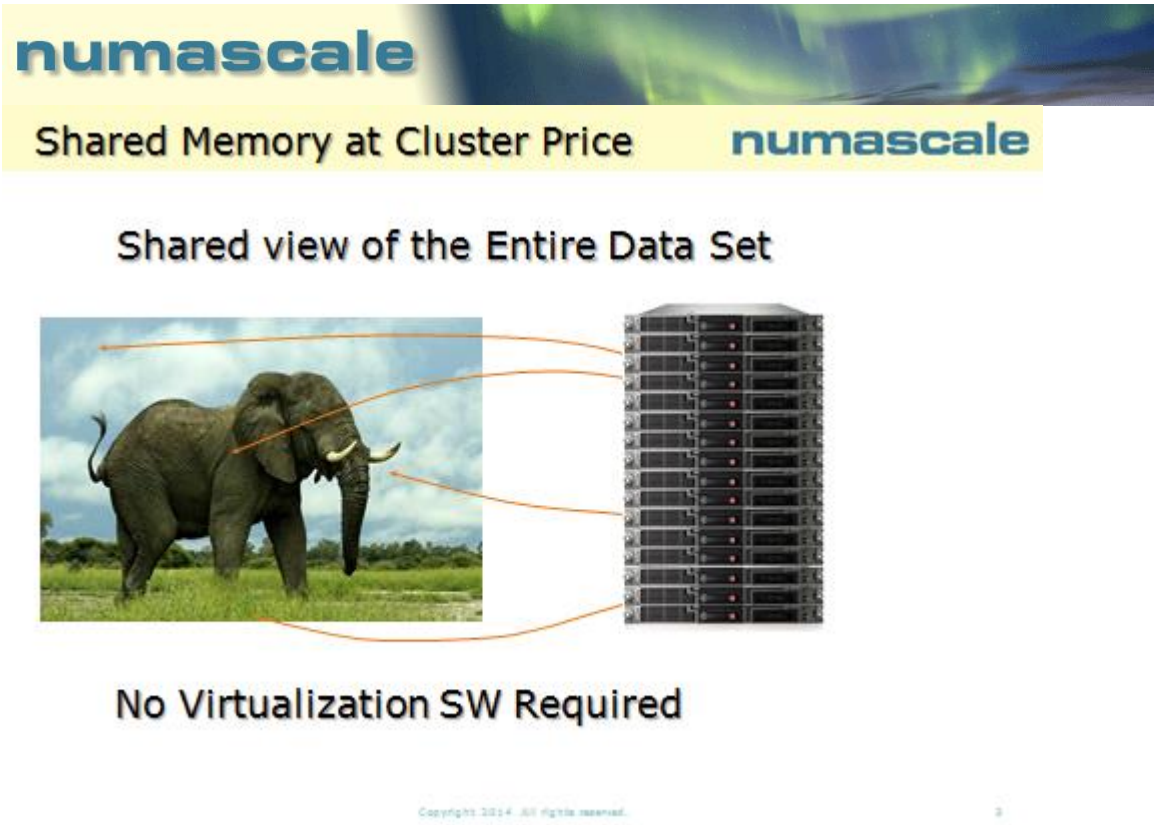


Figure 7: Shared Memory

Program a Numascale Shared Memory System just as a standalone server. The full memory range is available to all applications. You can run ”top” on a 1.5 TB system.

```
top - 09:29:57 up 20 days, 20:07,  6 users,  load average: 8.32, 8.31, 8.32
Tasks: 3068 total,   3 running, 3065 sleeping,   0 stopped,   0 zombie
Cpu(s):  1.4%us,  0.1%sy,  0.0%ni, 98.5%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  1583148160k total, 1185082348k used, 398065812k free,        4k buffers
Swap: 33046524k total,        0k used, 33046524k free,  4039576k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
202867 root      20   0 1119g 1.1t  524 R  815 74.1   3758:34 x.mod2as
197024 root      20   0 13180 3580 1204 R   37  0.0 403:40.55 htop
206397 root      20   0 13512 3704  924 R   14  0.0   0:04.48 top
197023 root      20   0 13512 3700  924 S   13  0.0 177:20.24 top
  1399 root      20   0     0    0    0 S    3  0.0   1:03.79 ksoftirqd/348
  2187 root      20   0     0    0    0 S    3  0.0   0:50.98 ksoftirqd/545
    10 root      20   0     0    0    0 S    2  0.0 290:26.05 rcu_sched
 11190 root      20   0     0    0    0 S    1  0.0  68:02.65 kworker/40:1
 11177 root      20   0     0    0    0 S    1  0.0 173:47.85 kworker/24:1
 11241 root      20   0     0    0    0 S    1  0.0  86:23.99 kworker/44:1
 11668 root      20   0     0    0    0 S    1  0.0  53:37.71 kworker/348:1
 11688 root      20   0     0    0    0 S    1  0.0  59:31.14 kworker/336:1
 12035 root      20   0     0    0    0 S    1  0.0  20:37.15 kworker/545:1
 11197 root      20   0     0    0    0 S    0  0.0  96:09.80 kworker/36:1
 11203 root      20   0     0    0    0 S    0  0.0 148:15.71 kworker/32:1
 11209 root      20   0     0    0    0 S    0  0.0 166:31.05 kworker/28:1
 11233 root      20   0     0    0    0 S    0  0.0  82:54.52 kworker/48:1
 11626 root      20   0     0    0    0 S    0  0.0  32:13.59 kworker/308:1
 11710 root      20   0     0    0    0 S    0  0.0  26:04.65 kworker/357:1
 11714 root      20   0     0    0    0 S    0  0.0  31:09.39 kworker/354:1
 47717 root      20   0  7764  576  484 S    0  0.0  22:06.24 tail
 47736 root      20   0  7764  576  484 S    0  0.0  22:13.57 tail
```

Figure 8: top on 1.5 TB system

3.1 All threads are available, e.g. through htop

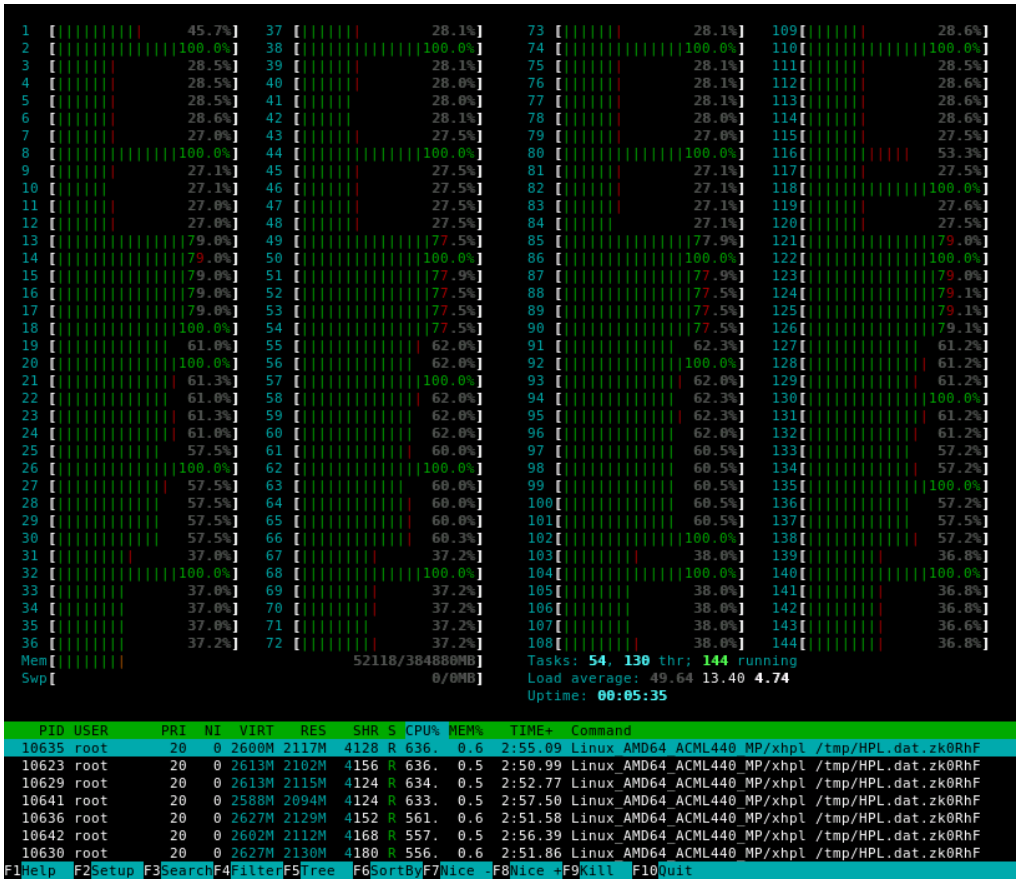


Figure 9: htop on 144 cores

The major difference from a single CPU server and a Numascale Shared Memory System is that there are differences in the memory latency. In a ccNuma system, the memory latency differs depending on where the actual memory is located.

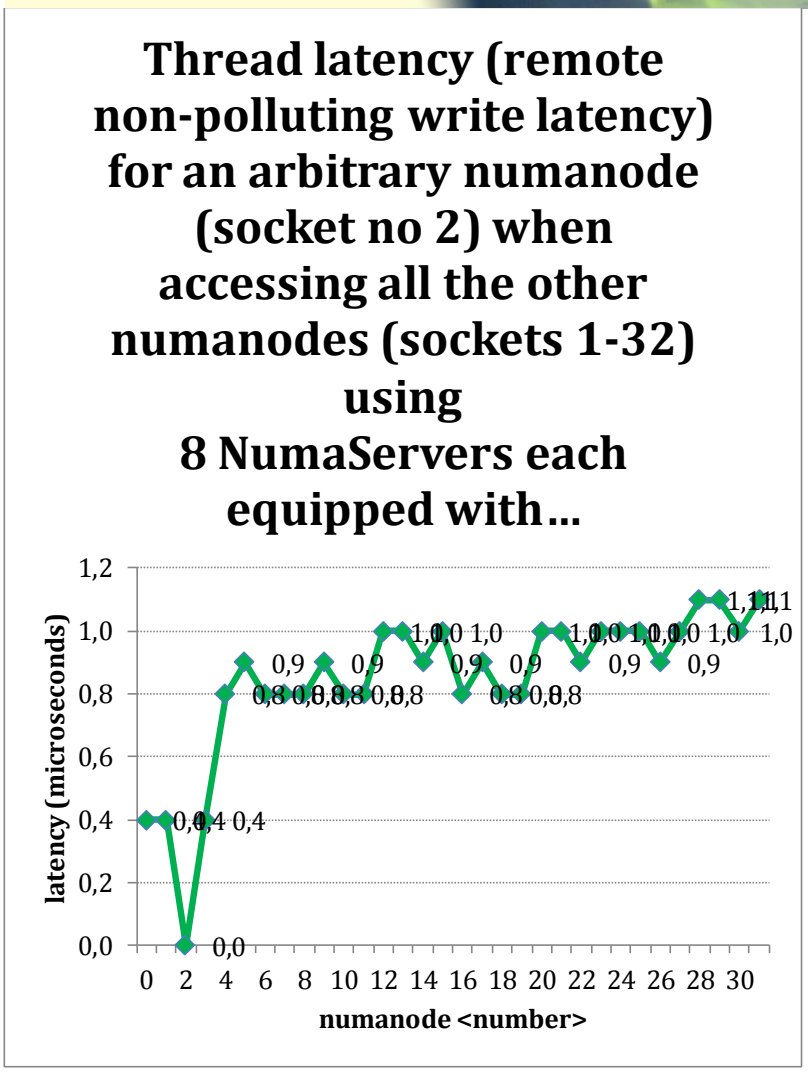


Figure 10: Memory latencies in a Numascale system

Although a ccNuma system is logically similar to a traditional SMP, it is physically different. The runtime of an application is very dependent on where the data is located relative to the running thread.

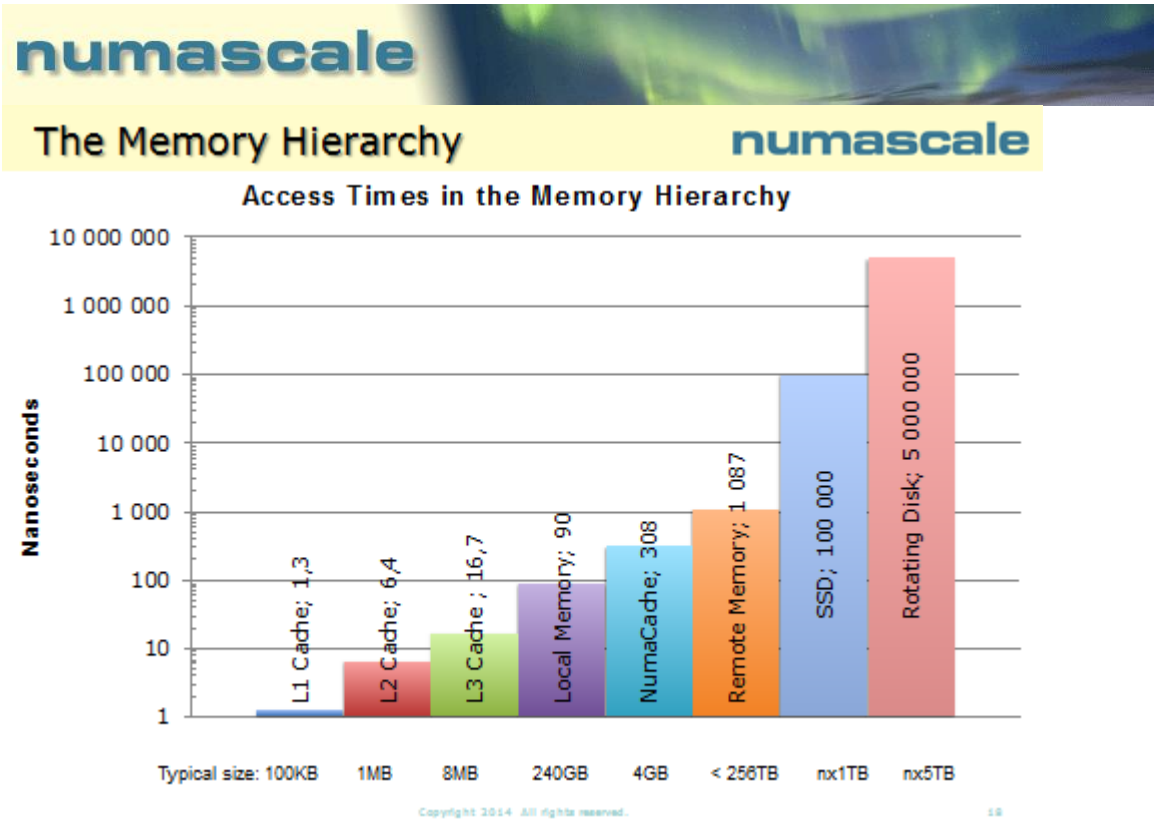


Figure 11: Memory hierarchy in a Numascale system

"numastat" monitor the memory access pattern in a system and can be used to verify the runtime the runtime parameters.

```
[atle@x3755 ~]$ numastat
                           node0           node1           node2           node3
numa_hit                116198855        22674225         1601598          326121
numa_miss                     0          390637               0               0
numa_foreign             390637               0               0               0
interleave_hit            26017           26221           26298           26107
local_node              116197682        22647868         1576067          299901
other_node                 1173          416994           25531           26220

                           node4           node5           node6           node7
numa_hit                2484895         4957523         4425252        25191604
numa_miss                     0               0               0               0
numa_foreign                  0               0               0               0
interleave_hit            26026           26209           26289           26088
local_node              2458717         4931194         4398832        25165424
other_node                26178           26329           26420           26180
[atle@x3755 ~]$
```

"numastat" can also be used to monitor the memory access pattern for a running process.

```
[atle@x3755 ~]$ ps -elf | grep bwa
4 S root     25459 25458 99  80   0 - 1274150 futex_ 10:29 pts/3  00:36:30
/home/demouser04/04_Software/bwa-0.7.4/bwa mem -t 128 -M
../../../00_RAW_DATA/EC_K12
../../../00_RAW_DATA/QBICECKH100001W4_GCCAAT_L001_R2_001.fastq
[root@x3755 atle]# numastat -p 25459
Per-node process memory usage (in MBs) for PID 25459 (bwa)
Node 0          Node 1          Node 2
```

```
                ---------------  ---------------  ---------------
Huge                       0.00             0.00             0.00
Heap                       0.00             0.00             0.00
Stack                      0.18             0.09             0.19
Private                   63.66            38.99            43.42
----------------  ---------------  ---------------  ---------------
Total                     63.85            39.07            43.61

                           Node 3           Node 4           Node 5
                ---------------  ---------------  ---------------
Huge                       0.00             0.00             0.00
Heap                       0.00             0.00             0.00
Stack                      0.18             2.52             0.38
Private                   31.44            82.00            66.58
----------------  ---------------  ---------------  ---------------
Total                     31.62            84.51            66.96

                           Node 6           Node 7            Total
                ---------------  ---------------  ---------------
Huge                       0.00             0.00             0.00
Heap                       0.00             0.00             0.00
Stack                     11.33             0.46            15.32
Private                 3434.12            64.36          3824.57
----------------  ---------------  ---------------  ---------------
Total                   3445.45            64.82          3839.89
[root@x3755 atle]#
```

Applications that take the different memory latencies in a ccNuma system into account scales well on a Numascale Shared Memory System. The RWTH TrajSearch code has the **most speedup on NumaConnect**, even if it was originally adapted to Scale MP.

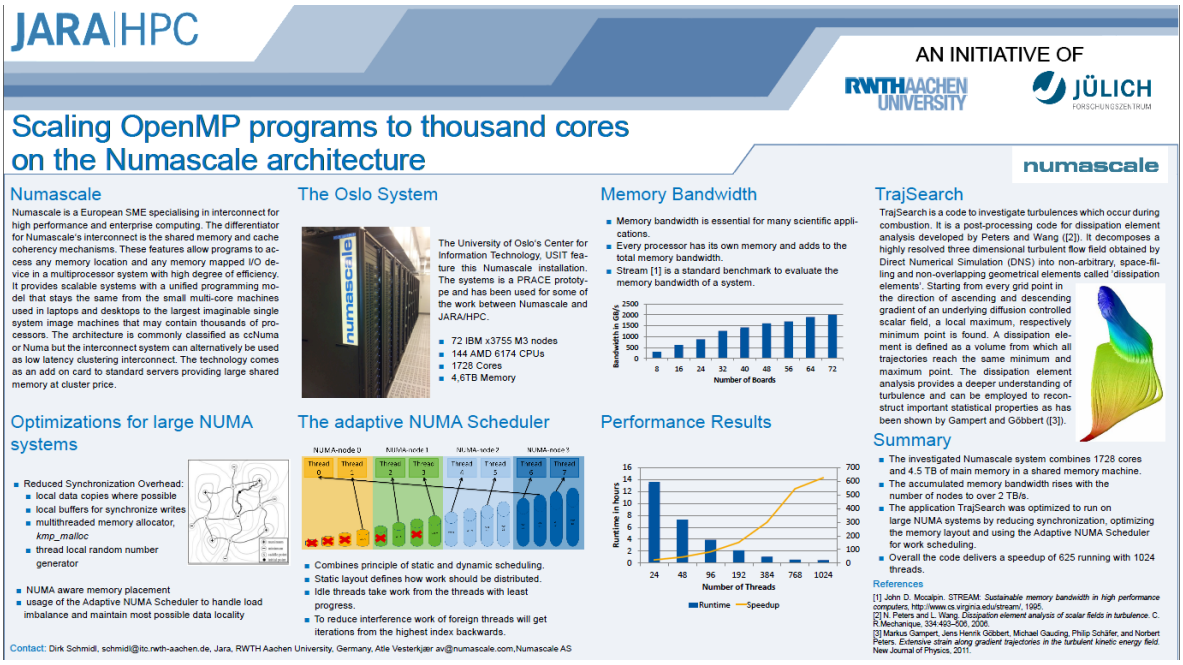


Figure 12: RWTH TrajSearch code

3.2 Keep Thread Local Storage (TLS) local

Numascale has patched the gcc and open64 OpenMP implementation to make sure that the stack and Thread Local Storage (TLS) is local to the running threads. This favors these compilers for OpenMP code. For more information about this feature, see https://wiki.numascale.com/tips/placing-stack-and-tls-memory .

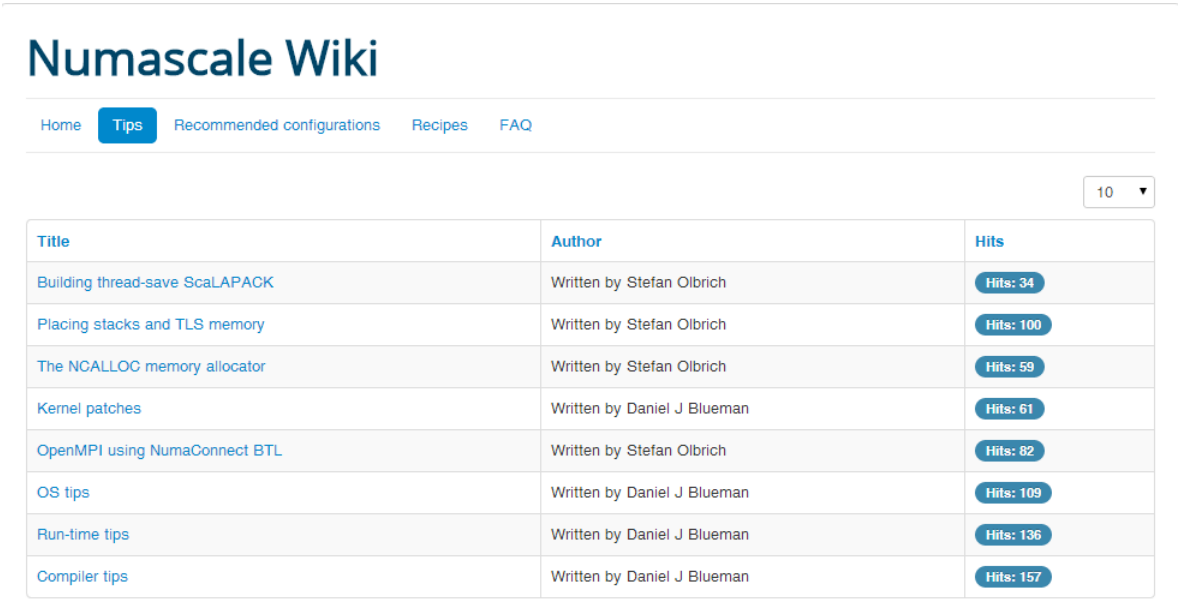


Figure 13: https://wiki.numascale.com/tips show best practice hints

3.1 Use a Numa-aware Memory allocator

3.1.1 The HOARD memory allocator

Numascale is experimenting with other memory allocators than libc in order to speed up the allocation process by not shifting around blocks between threads.

http://www.hoard.org/ reduces lock contention by using multiple heaps and avoids false sharing in its allocations.

```
export LD_PRELOAD=/opt/HOARD/libhoard.so
```

3.1.1 The NCALLOC memory allocator

Numascale has written its own memory allocator to ensure that the HEAP of a running thread is local to the core it is running on. You can experiment with both the NCALLOC and HOARD memory allocators. You can find more information about the NCALLOC memory allocator in https://wiki.numascale.com/tips/the-ncalloc-memory-allocator.

```
export LD_PRELOAD=/opt/HOARD/libncalloc.so
```

3.2 Arrange your data in a Numa-aware

The least efficient memory model for an application that you would like to scale well on ccNuma system is to have one big array of data on one node that all threads has to access. Try to distribute the data as much as possible in order to be able for threads to use memory local to the core they are running on.

4 COMPILERS

Check out https://wiki.numascale.com/tips for public tips from Numascale.

AMD has a good guide at http://amd-dev.wpengine.netdna-cdn.com/wordpress/media/2012/10/CompilerOptQuickRef-63004300.pdf for general compiler optimization flags for the AMD Opteron 6300 series.

AMD has done some work in optimizing compiler flags well-known applications:

- http://www.amd.com/us/products/server/benchmarks/Pages/gromacs-cluster-perf-d-dppc-two-socket-servers.aspx
- http://www.amd.com/us/products/server/benchmarks/Pages/high-performance-linpack-cluster-perf.aspx
- http://www.amd.com/us/products/server/benchmarks/Pages/molecular-dynamics-namd-cluster-performance-two-socket-servers.aspx

More can be found at http://www.amd.com/us/products/server/benchmarks/

The most common compilers used with the Numascale architecture are:

- GCC 4.8.1
- PGI compiler 13.3
- Open64 compiler (x86_open64-4.5.2.1)
- Intel compiler (yes this works for AMD systems as well)

Numascale has patched the gcc and open64 OpenMP implementation to make sure that the stack and Thread Local Storage (TLS) is local to the running threads. This favors these compilers for OpenMP code.

Please check out:
http://developer.amd.com/wordpress/media/2012/10/51803A_OpteronLinuxTuningGuide_SCREEN.pdf

5 INSTALLING NUMASCALE BTL

Download the source at:
https://resources.numascale.com/software/openmpi-1.7.2.tar.gz

It might be helpful to download:
https://resources.numascale.com/software/openmpi-tools.tar.gz

Remember to install numactl and numactl-devel using yum first.
Here are the installation steps on my system:

```
tar -zxvf ../openmpi-1.7.2.tar.gz
cd openmpi-tools/
cd automake-1.12.2/
./configure ; make; sudo make install
cd ..
cd autoconf-2.69/
./configure ; make; sudo make install
cd ../
cd flex-2.5.35/
sudo yum install help2ma
./configure ; make; sudo make install
cd ..
cd libtool-2.4.2/
./configure ; make; sudo make install
cd ../m4-1.4.16/
./configure ; make; sudo make install
cd ../../openmpi-1.7.2/
./autogen.sh
export CC=gcc F77=gfortran FC=gfortran LDFLAGS=-lnuma CFLAGS="-g -O3 -march=amdfam15"
./configure --disable-vt --prefix=/opt/openmpi-1.7.2-numaconnect
make
sudo make install
```

Start application like this:

```
mpirun -n 32 -rf rank32 -mca btl self,nc bin/lu.C.32
```

6 IPMI

6.1 Power control

To control the power of a IPMI based node, use the following command(s) :

```
% ipmitool -I lanplus -H <hostname>-ipmi -U <username> -P <password>
power on
% ipmitool -I lanplus -H <hostname>-ipmi -U <username> -P <password>
power off
% ipmitool -I lanplus -H <hostname>-ipmi -U <username> -P <password>
power reset
```

6.2 Console access

To open a serial console session towards an IPMI based node, use the following command :

```
% ipmitool -I lanplus -H <hostname>-ipmi -U <username> -P <password> sol
activate
```

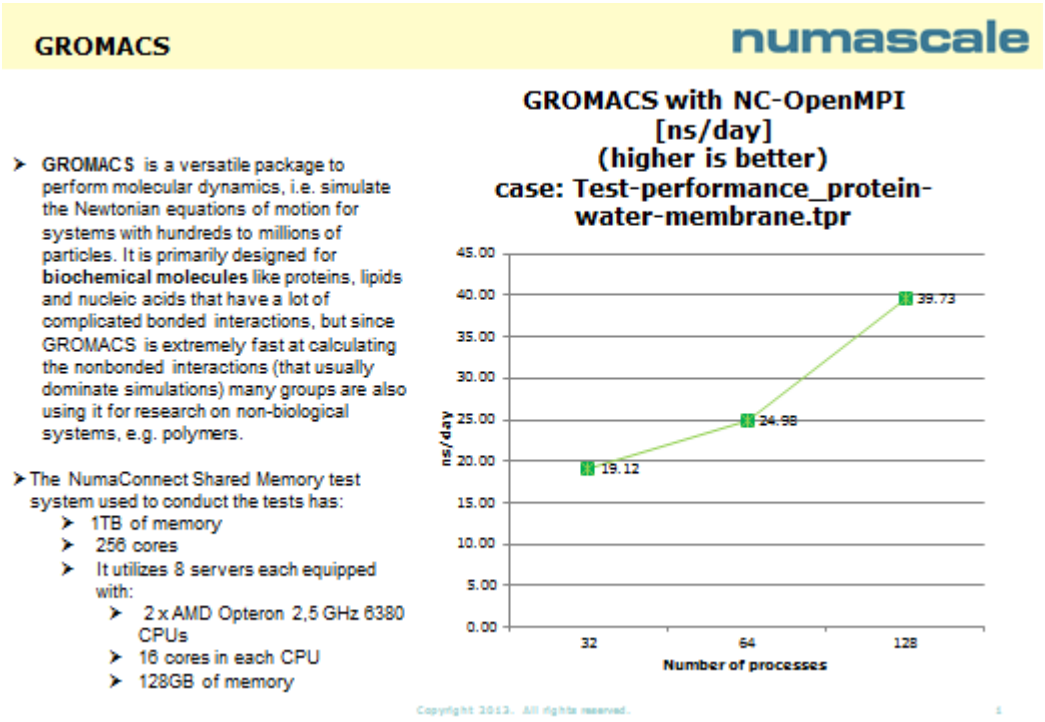
<username> and <password> may be different from device to device.

You can also pipe the console log to a file this way:

% ipmitool -I lanplus -H <hostname>-ipmi -U <username> -P <password> sol activate 2>&1 | tee <filename> &

7 INSTALLING APPLICATIONS

7.1 Gromacs



Gromacs scales positively when using our optimized NumaConnect BTL with OpenMPI:

Core	t (s)	Wall t (s)	%	ns/day	Hour/ns
32	2894.03	90.38	3201.90	19.12	1.26
64	4431.17	69.19	6404.20	24.98	0.96
128	5569.21	43.50	12803.70	39.73	0.60

Make sure you have a suitable FFTW version installed (i.e. single-precision and AMD-optimised). Find some info in
http://www.gromacs.org/Documentation/Installation_Instructions_for_5.0
http://www.gromacs.org/Documentation/Installation_Instructions_for_5.0#3.4._Fast_Fourier_Transform_library
http://www.gromacs.org/Documentation/Installation_Instructions_for_5.0#3.2.1._Running_in_parallel
Verify the installation by running "make check".

You can easily check your (acceleration) setup with "mdrun -version"

Relevant mdrun options include "-pin on", "-dlb yes", '-tunepme", "-nt [n]" where n is the number of threads. Should be equal to number of cores. If you specify 0, mdrun will guess but it might not guess correctly.

Here are the steps used on the Numascale system:

Compile FFTW:

CC=/opt/gcc-4.8.2/bin/gcc CFLAGS="-lnuma" CXX=g++ FC=/opt/gcc-4.8.2/bin/gfortran F77=/opt/gcc-4.8.2/bin/gfortran FFLAGS="-lnuma" ./configure --enable-float --enable-threads --enable-sse2 --prefix=/home/atle/GROMACS/fftw_lnuma

Gromacs:

CMAKE_PREFIX_PATH=/home/atle/GROMACS/fftw_lnuma cmake .. -DGMX_MPI=ON -DCMAKE_CXX_COMPILER=/opt/openmpi-1.7.2-numaconnect/bin/mpicxx -DCMAKE_C_COMPILER=/opt/openmpi-1.7.2-numaconnect/bin/mpicc -DCMAKE_C_FLAGS="-lnuma" -DCMAKE_CXX_FLAGS="-lnuma" -DCMAKE_BUILD_TYPE=Release -DCMAKE_INSTALL_PREFIX=/home/atle/GROMACS/MPI -DLIBXML2_LIBRARIES=/usr/lib64 -DGMX_PREFER_STATIC_LIBS=ON -DCMAKE_BUILD_TYPE=Release -DLIBXML2_INCLUDE_DIR=/usr/include/libxml2

Currently the MPI version works best on NumaConnect:

[atle@numademo mpi_numademo_128]$ mpirun -n 128 -rf rank128_lu -mca btl self,nc /home/atle/GROMACS/MPI_NUMADEMO/bin/mdrun_mpi -s Test-performance_protein-water-membrane.tpr