PARTEC CLUSTER COMPETENCE CENTER

MANAGED HPC

JURECA – Tuning for the platform

Usage of ParaStation MPI

2017-11-23

Outline

- ParaStation MPI
- Compiling your program
- Running your program
- Tuning parameters
- Resources

ParaStation MPI

- Based on MPICH (3.2)
  - *supports all MPICH tools (tracing, debugging, …)*
- Proven to scale up to 3,000 nodes and 85,000 procs per job
  - *JuRoPA running ParaStation MPI: **0.274** PFLOPS (2009)*
  - *JURECA running ParaStation MPI: **1.42** PFLOPS (2015)*
  - *JURECA & Booster ParaStation MPI: **3.78** PFLOPS (2017)*
- Supports a wide range of interconnects, even in parallel
  - *pscom library hides details*
  - *e.g. InfiniBand EDR on JURECA cluster in Jülich*
  - *Extoll on DEEP-ER*
- Tight integration with Cluster Management (healthcheck)

ParaStation MPI

- MPI libraries for several compilers
  - *especially for GCC and Intel*
- Recently added features include:
  - *Improved Omni-Path performance*
  - *Improved scalability*
  - *Improved InfiniBand bandwidth performance*
  - *Improved (dynamic) process management*

ParaStation History

- 1995: University project (→ University of Karlsruhe)
- 2004: Open source (→ ParaStation Consortium)
- 2004: Cooperation with JSC
  - *various precursor clusters*
  - *JUDGE*
  - *DEEP Cluster/Booster, DEEP-ER*
  - *JuRoPA2 (J2)*
  - *JuRoPA3 (J3)*
  - *JUAMS*
  - *JURECA*
  - *JURECA-Booster*

Recent Versions

- **JURECA**
  - *ParaStation MPI* → *psmpi-5.2.0-1 (MPI-3.1)*
  - *Intel Compilers* → *v 18.0.0 20170811*
  - *Gnu gcc* → *v 7.2.0*

Compiling on JURECA

- Currently MPI-3.1 version (5.2.0-1) available
- single thread tasks
  - `module load Intel ParaStationMPI`
  - `module load GCC ParaStationMPI`
- multi-thread tasks (mt)
  - `module load Intel ParaStationMPI/5.2.0-1-mt`
  - *no multi-thread GCC version available*
- ChangeLog available with
  - `less $(dirname $(which mpicc))/../ChangeLog`
- Gnu and Intel compilers available
  - *gcc-7.2.0 (`GCC`)*
  - *intel-2018.0.0 (`Intel`)*
- see also the previous talk JURECA - An overview

Wrapper vs. Manual Compilation

- Wrappers
  - *`mpicc`* *(C)*
  - *`mpicxx`* *(C++)*
  - *`mpif90`* *(Fortran 90)*
  - *`mpif77`* *(Fortran 77)*
- `mpi<LANG> -show`
  - *shows what would happen*
  - *useful for legacy Makefiles*
  - *allows to tweak compiler*
- When using the "mt" version (and using OpenMP), add
  - *`-fopenmp`* *(gcc)*
  - *`-qopenmp`* *(intel)*

Wrapper vs. Manual Compilation

- Intel C-Compiler + ParaStation MPI
  - *module load Intel ParaStationMPI*
  - *mpicc -show*

```
icc -Wl,-rpath-
link=/usr/local/software/jureca/Stages/2017b/software
/pscom/Default/lib -I/usr/local/software/jureca
/Stages/2017b/software/psmpi/5.2.0-1-iccifort-
2018.0.128-GCC-5.4.0/include -L/usr/local/software
/jureca/Stages/2017b/software/psmpi/5.2.0-1-iccifort-
2018.0.128-GCC-5.4.0/lib -Wl,-rpath -Wl,/usr/local
/software/jureca/Stages/2017b/software/psmpi/5.2.0-1-
iccifort-2018.0.128-GCC-5.4.0/lib -Wl,--enable-new-
dtags -lmpi
```

Did the wrapper link correctly?

- Libraries are linked at runtime according to **`LD_LIBRARY_PATH`**
- **`ldd`** shows the libarries attached to your binary
- Look for ParaStation libararies

```
ldd hello_mpi:
...
libmpi.so.12 => /usr/local/software/jureca/Stages/2017b/software
/psmpi/5.2.0-1-iccifort-2018.0.128-GCC-5.4.0/lib/libmpi.so.12
(0x00002ac9fca60000)
...
```

vs.

```
libmpi.so.12 => /usr/local/software/jureca/Stages/2017b/software
/psmpi/5.2.0-1-iccifort-2018.0.128-GCC-5.4.0-mt/lib/libmpi.so.12
(0x00002aaebb344000)
```

JURECA: start via srun

- Use **`srun`** to start MPI processes
- **`srun -N <nodes> -n <tasks>`** spawns task
  - *directly*
  - *interactively via salloc*
  - *from batch script via sbatch*
- Exports full environment
- Stop interactive run with (consecutive) **`^C`**
  - *passed to all tasks*
- No manual clean-up needed
- You can log into nodes which have an allocation/running job step
  - ***`squeue -u <user>`***
  - ***`sgoto <jobid> <nodenumber>`***
  - ***`e.g. sgoto 2691804 0`***
- Do not use mpiexec

hello_mpi.c

```c
/* C Example */
#include <stdio.h>
#include <mpi.h>

int main (int argc, char **argv) {

  int numprocs, rank, namelen;

  char processor_name[MPI_MAX_PROCESSOR_NAME];

  MPI_Init (&argc, &argv);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  MPI_Comm_size (MPI_COMM_WORLD, &numprocs);
  MPI_Get_processor_name (processor_name, &namelen);
  printf ("Hello world from process %d of %d on %s\n",
          rank, numprocs, processor_name);
  MPI_Finalize ();
  return 0;
}
```

Running on JURECA (Intel chain)

- `module load Intel`
- `module load ParaStationMPI`
- `mpicc -O3 -o hello_mpi  hello_mpi.c`
- **Interactive:**
- `salloc -N 2 # get an allocation`
- `srun -n 2 ./hello_mpi`
  - *`Hello world from process 0 of 2 on jrc0491`*
  - *`Hello world from process 1 of 2 on jrc0492`*
- **Batch:**
- `sbatch ./hello_mpi.sh`
- Increase verbosity:
  - *`PSP_DEBUG=[1,2,3,...] srun -n 2 ./hello_mpi`*

Process Placement

- ParaStation process pinning:
  - *Avoid task switching*
  - *Make better use of CPU cache*
- JURECA is pinning by default:
  - So *`--cpu_bind=rank`* may be omitted
- Manipulate pinning:
  - *e.g. for "large memory / few task" applications*
- Manipulate via `--cpu_bin=mask_cpu:<mask1>,<mask2>,…`
  - *CPU masks are always interpreted as hexadecimal values*
- For example on JURECA:

```
srun --cpu_bind=[verbose,]mask_cpu:0x1,0x1000
     -n 2 ./testcore
```

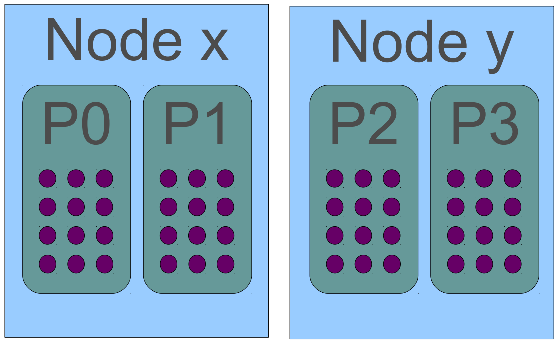
  - *`rank 0 running on core 0`*
  - *`rank 1 running on core 12`*

...	1000	...	80	40	20	10	8	4	2	1
...	12	...	7	6	5	4	3	2	1	0

Hybrid MPI/OpenMP

```
#include <stdio.h>
#include <mpi.h>
#include <omp.h>

int main(int argc, char *argv[]) {
  int numprocs, rank, namelen;
  char processor_name[MPI_MAX_PROCESSOR_NAME];
  int iam = 0, np = 1;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Get_processor_name(processor_name, &namelen);

#pragma omp parallel default(shared) private(iam, np)
  {
    np = omp_get_num_threads();
    iam = omp_get_thread_num();
    printf("Hello from thread %02d out of %d from process %d out of %d on %s\n",
           iam, np, rank, numprocs, processor_name);
  }

  MPI_Finalize();
}
```

Example:
2 Nodes, 2x2 Procs,
2x2x12 Threads



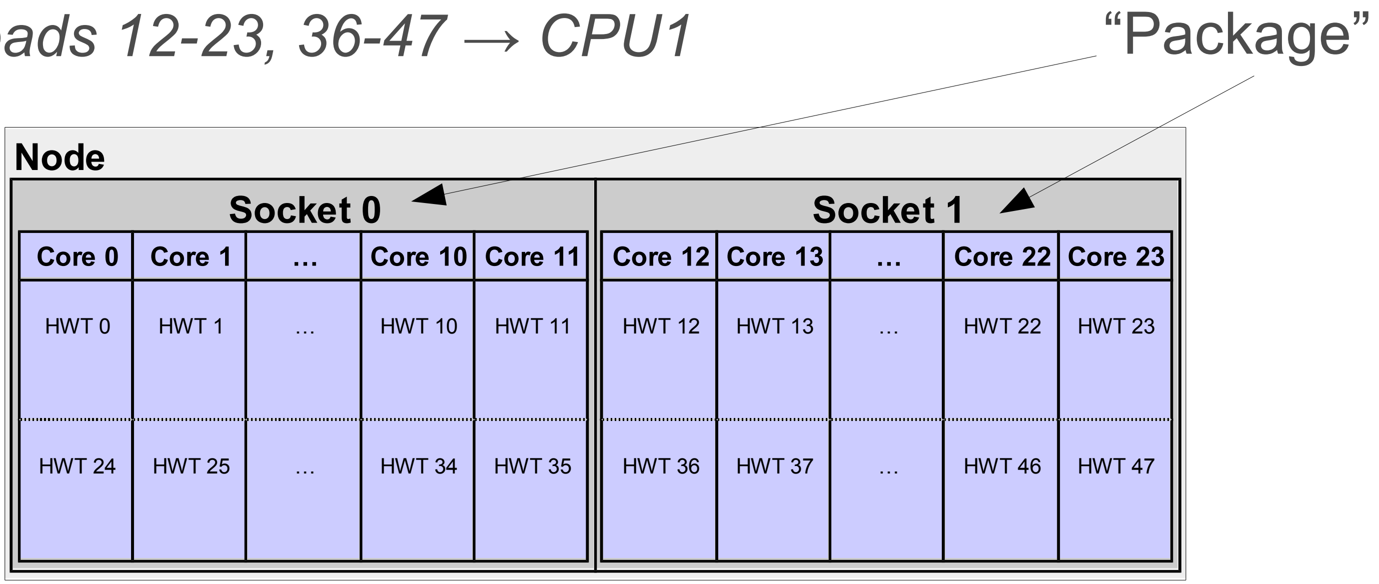
On JURECA

- `module load Intel ParaStationMPI/5.1.9-1-mt`
- `mpicc -O3 -qopenmp -o hello_hybrid hello_hybrid.c`
- `salloc -N 2 --cpus-per-task=12`
- `export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}`
- `srun -n 4  ./hello_hybrid`

```
Hello from thread 00 out of 12 from process 0 out of 4 on jrc0491
Hello from thread 01 out of 12 from process 0 out of 4 on jrc0491
Hello from thread 02 out of 12 from process 0 out of 4 on jrc0491
Hello from thread 03 out of 12 from process 0 out of 4 on jrc0491
                              .
                              .
                              .
Hello from thread 09 out of 12 from process 3 out of 4 on jrc0492
Hello from thread 10 out of 12 from process 3 out of 4 on jrc0492
Hello from thread 11 out of 12 from process 3 out of 4 on jrc0492
```

Pinning: Which core for a thread?

- JURECA:
  - *2 Sockets, 12 Cores per Socket*
  - *2 HW-Threads per Core*
  - *→ 48 Threads possible*
- Normally (SMT):
  - *Threads 0-11, 24-35 → CPU0*
  - *Threads 12-23, 36-47 → CPU1*



Pinning: Which core for a thread?

- No thread pinning by default on JURECA
- Allow the Intel OpenMP library thread placing
  - *`export KMP_AFFINITY=[verbose,modifier,]...`*

    `compact`: *place threads as close as possible*

    `scatter`: *as evenly as possible*
  - *`KMP_AFFINITY=granularity=fine,verbose,scatter srun ...`*

    ```
    OMP: Info #171: KMP_AFFINITY: OS proc 0 maps to
    package 0 core 0
    OMP: Info #242: KMP_AFFINITY: pid 4940 thread 1
    bound to OS proc set {1}
    ```
- Full environment is exported via `srun` on JURECA
- For GCC: set GOMP_CPU_AFFINITY (see manual)

Large Job Considerations

- Every MPI process talks to all others:
  - *(N-1) x 0.55 MB communication buffer space per process!*

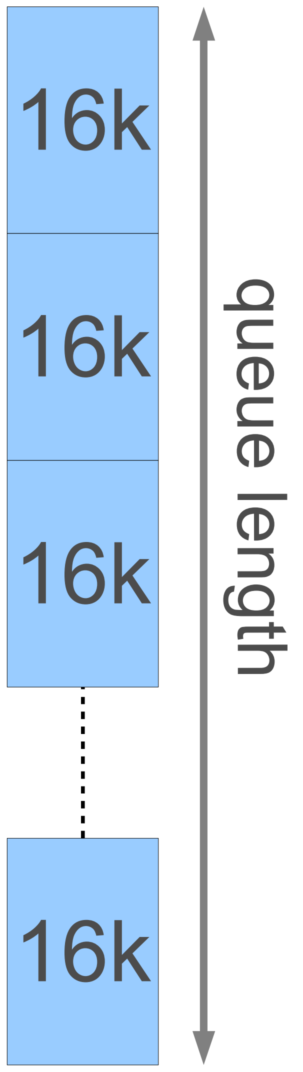
- Example 1 on JURECA:
  - *max job size 256 × 48 = 12,288 processes*
  - *12,288 × 0.55 MB → ~ 6758 MB / process*
  - *× 48 process / node → ~ 317 GB communication buffer space*
  - *But there are only 128 GB main memory per node*

- Example 2 on JURECA:
  - *job with 128 nodes and only one process per core*
  - *(128 × 24 - 1) × 0.55 MB × 24 → ~ 40 GB / node*
  - *Main memory – OS – GPFS – 40 GB → ~ 60 GB*
  - *60 GB / 24 procs → 2.5 GB left for each process*

On Demand / Buffer Size

Two possible solutions:

- 1. Create buffers on demand only:
  - *`export PSP_ONDEMAND=1`*
- 2. Reduce the buffer queue length:
  - *(Default queue length is 16)*
  - *`export PSP_OPENIB_SENDQ_SIZE=3`*
  - *`export PSP_OPENIB_RECVQ_SIZE=3`*
  - *Do not go below 3, deadlocks might occur!*
  - *Trade-off: Performance penalty (sending many small messages)*



On-Demand / Queue Size Guidelines

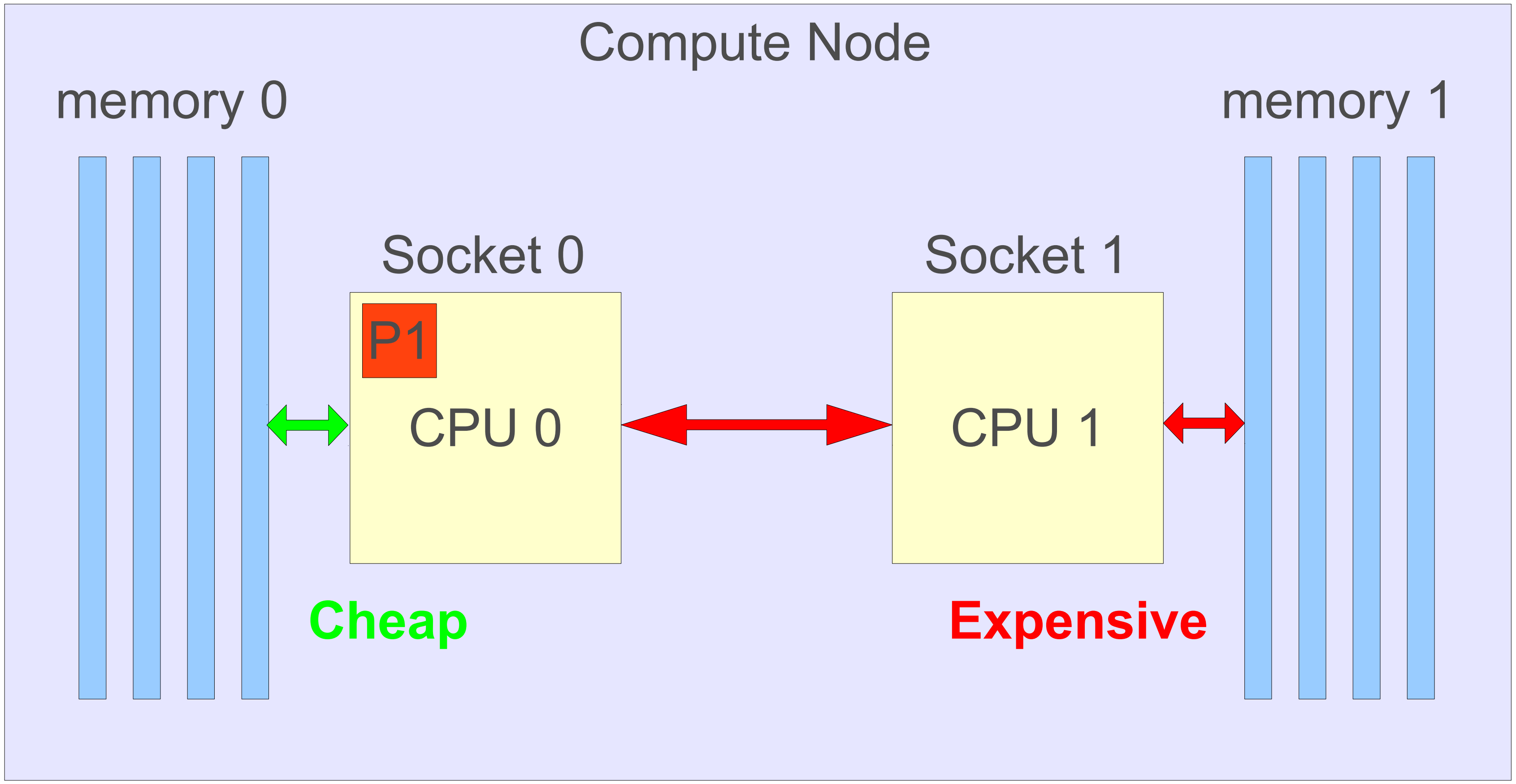
- On-Demand works best with nearest neighbor communications
  - *(Halo) Exchange*
  - *Scatter/Gather*
  - *All-reduce*
  - *...*
- But for *All-to-all* communication:
  - *queue size modification only viable option...*
- Example

```
    rank 0: for ( ; ; ) MPI_Send ()
    rank 1: for ( ; ; ) MPI_Recv ()
```

  - *`PSP_OPENIB_SENDQ/RECVQ_SIZE=4:` 1.8 seconds*
  - *`PSP_OPENIB_SENDQ/RECVQ_SIZE=16:` 0.6 seconds*
  - *`PSP_OPENIB_SENDQ/RECVQ_SIZE=64:` 0.5 seconds*

NUMA Considerations

- Non Uniform Memory Access (NUMA)



NUMA Policies

- If memory is bound to processes, only local memory is accessible → and can get exhausted (at about 55 GB):

  -
    ```
    srun -n 1 --mem_bind=rank|local ./blockmem_mpi
    srun: error: jrc0075: task 0: Killed
    srun: Force Terminated job step 1505858.15
    ```
- If memory is not bound to processes, all memory is accessible:

  -
    ```
    srun -n 1 --mem_bind=none ./blockmem_mpi
    ```
- On JURECA is `--mem_bind=none` used by default so it can be omitted
- But: membind off → data is crossing CPUs (NUMA)
  → ~15–20% performance drop!
- First-Touch Policy: Memory is allocated locally

Resources

- www.parastation.com
- www.fz-juelich.de/ias/jsc/jureca
- /opt/parastation/doc/pdf
- by mail: support@par-tec.com
- by mail: sc@fz-juelich.de
- Download ParaStation MPI at github:
  - *https://github.com/ParaStation/psmgmt*
  - *https://github.com/ParaStation/pscom*
  - *https://github.com/ParaStation/psmpi2*
  - *git clone https://github.com/ParaStation/psmpi2.git*

Summary

- You now should be able to
  - *compile*
  - *run your application*
  - *tune some runtime parameters*
  - *diagnose and fix specific errors*
  - *know where to turn to in case of problems*

Thank you!