JURECA – Tuning for the platform

Usage of ParaStation MPI

2017-05-22
Outline

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

- Based on MPICH (3.1.4)
  - 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)
- 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 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 → psmipi-5.1.9-1 (MPI-3)
  - Intel Compilers → v 17.0.2 20170213
  - Gnu gcc → v 5.4.0
Compiling on JURECA

- Currently MPI-3 version (5.1.9-1) available
- single thread tasks
  - `module load Intel ParaStationMPI`
  - `module load GCC ParaStationMPI`
- multi-thread tasks (mt)
  - `module load Intel ParaStationMPI/5.1.9-1-mt`
  - no multi-thread GCC version available
- ChangeLog available with
  - `less $(dirname $(which mpicc))/../ChangeLog`
- Gnu and Intel compilers available
  - `gcc-5.4.0 (GCC)`
  - `intel-2017.0.2 (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`

```plaintext
icc -Wl,-rpath-
link=/usr/local/software/jureca/Stages/2017a/software/
pscom/Default/lib
-I/usr/local/software/jureca/Stages/2017a/software/ps
mpi/5.1.9-1-iccifort-2017.2.174-GCC-5.4.0/include
-L/usr/local/software/jureca/Stages/2017a/software/ps
mpi/5.1.9-1-iccifort-2017.2.174-GCC-5.4.0/lib -Wl,-
rpath
-Wl,/usr/local/software/jureca/Stages/2017a/software/
psmpi/5.1.9-1-iccifort-2017.2.174-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 libraries attached to your binary
- Look for ParaStation libraries

```bash
ldd hello_mpi:
...
libmpi.so.12 => /usr/local/software/jureca/Stages/2017a/software/psmpi/5.1.9-1-iccifort-2017.2.174-GCC-5.4.0/lib/libmpi.so.12 (0x00002b40213a4000)
...
```

vs.

```bash
libmpi.so.12 => /usr/local/software/jureca/Stages/2017a/software/psmpi/5.1.9-1-iccifort-2017.2.174-GCC-5.4.0-mp/lib/libmpi.so.12 (0x00002b05cc3e6000)
```
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
/* 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
```c
#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

Node x
(P0 P1)
(P2 P3)

Node y
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

<table>
<thead>
<tr>
<th>Node</th>
<th>Socket 0</th>
<th></th>
<th>Socket 1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Core 0</td>
<td>Core 1</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>HWT 0</td>
<td>HWT 1</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>HWT 24</td>
<td>HWT 25</td>
<td>...</td>
</tr>
</tbody>
</table>

"Package"
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:
  - \((N-1) \times 0.55 \text{ MB communication buffer space per process!}\)

- Example 1 on JURECA:
  - \(\text{max job size } 256 \times 48 = 12,288 \text{ processes}\)
  - \(12,288 \times 0.55 \text{ MB} \rightarrow \sim 6758 \text{ MB / process}\)
  - \(\times 48 \text{ process / node} \rightarrow \sim 317 \text{ GB communication buffer space}\)
  - But there are only 128 GB main memory per node

- Example 2 on JURECA:
  - \(\text{job with 128 nodes and only one process per core}\)
  - \((128 \times 24 - 1) \times 0.55 \text{ MB} \times 24 \rightarrow \sim 40 \text{ GB / node}\)
  - \(\text{Main memory – OS – GPFS – 40 GB} \rightarrow \sim 60 \text{ GB}\)
  - \(60 \text{ GB / 24 procs} \rightarrow 2.5 \text{ GB left for each process}\)
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!