Usage of TAMPI

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Quick Overview

The **Task-Aware MPI** or TAMPI library ensures a **deadlock-free** execution of hybrid applications by implementing a cooperation mechanism between the MPI library and the parallel task-based runtime system.

TAMPI extends the functionality of standard MPI libraries by providing new mechanisms for improving the interoperability between parallel task-based programming models, such as **OpenMP** or **OmpSs-2**, and both **blocking** and **non-blocking** MPI operations.

Presently OpenMP programs (based on a derivative version of the LLVM OpenMP, yet to be released) can only make use of the non-blocking mode of TAMPI, whereas OmpSs-2 programs can leverage both blocking and non-blocking modes.

TAMPI is compatible with mainstream MPI implementations that support the **MPI_THREAD_MULTIPLE** threading level, which is the minimum requirement to provide its task-aware features.

Additional information about the TAMPI can be found at:

• OmpSs-2 repository. ?https://github.com/bsc-pm/tampi

Quick Setup on DEEP System for a Hybrid Application

We highly recommend to interactively log in a cluster module (CM) node to begin using TAMPI.

Presently, it seems that system affinity is not correctly setup for hybrid applications using multi-threading, therefore multi-threading will be ignored from now on.

A truly hybrid application should simply execute two MPI ranks, one on each NUMA socket to mitigate suboptimal memory accesses. Such an application will then use all the cores/threads available on each NUMA socket to run a shared-memory parallel application.

The command below requests an entire CM node for an interactive session with 2 MPI ranks (one per NUMA socket) and each rank using the 12 **physical** cores available on each socket (multi-threading disabled):

```
srun -p dp-cn -N 1 -n 2 -c 12 --pty /bin/bash -i
```

Once you have entered a CM node you can check the system affinity via the NUMA command srun numactl --show:

```
policy: bind
preferred node: 1
physcpubind: 12 13 14 15 16 17 18 19 20 21 22 23
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 0
physcpubind: 0 1 2 3 4 5 6 7 8 9 10 11
cpubind: 0
nodebind: 0
membind: 0
```

It can be readily seen that the each MPI process is bind to a different socket with no interleaving of processes or memory thus yielding optimal performance.

TAMPI has already been installed on DEEP and can be used by simply executing the following commands:

```
modulepath="/usr/local/software/skylake/Stages/2018b/modules/all/Core:$modulepath"
modulepath="/usr/local/software/skylake/Stages/2018b/modules/all/Compiler/mpi/intel/2019.0.117-GCC-7.3.0:$modulepath"
modulepath="/usr/local/software/skylake/Stages/2018b/modules/all/MPI/intel/2019.0.117-GCC-7.3.0/psmpi/5.2.1-1-mt:$modulepath
export MODULEPATH="$modulepath:$MODULEPATH"
```

Note that loading the TAMPI module will automatically load the **OmpSs-2** and **Parastation MPI** modules (notice that this MPI library has been compiled with multi-threading support enabled).

You might want to request more MPI ranks per socket depending on your particular application. See the examples below and the system affinity report (note that all of them ignore multi-threading):

```
srun -p dp-cn -N 1 -n 4 -c 6 --pty /bin/bash -i
```

module load TAMPI

```
$ srun numactl --show
policy: bind
preferred node: 0
physcpubind: 6 7 8 9 10 11
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
physcpubind: 0 1 2 3 4 5
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 1
physcpubind: 18 19 20 21 22 23
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 12 13 14 15 16 17
cpubind: 1
nodebind: 1
membind: 1
```

```
srun -p dp-cn -N 1 -n 12 -c 2 --pty /bin/bash -i
```

```
$ srun numactl --show
policy: bind
preferred node: 0
physcpubind: 0 1
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
```

```
physcpubind: 4 5
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
physcpubind: 2 3
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
physcpubind: 8 9
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
physcpubind: 6 7
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 0
physcpubind: 10 11
cpubind: 0
nodebind: 0
membind: 0
policy: bind
preferred node: 1
physcpubind: 14 15
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 16 17
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 20 21
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 18 19
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 22 23
cpubind: 1
nodebind: 1
membind: 1
policy: bind
preferred node: 1
physcpubind: 12 13
```

cpubind: 1
nodebind: 1
membind: 1

Nbody Benchmark (MPI+OmpSs-2+TAMPI)

Users must clone/download this example's repository from https://pm.bsc.es/gitlab/ompss-2/examples/nbody and transfer it to a DEEP working directory.

Description

This benchmark represents an N-body simulation to numerically approximate the evolution of a system of bodies in which each body continuously interacts with every other body. A familiar example is an astrophysical simulation in which each body represents a galaxy or an individual star, and the bodies attract each other through the gravitational force.

There are **7 implementations** of this benchmark which are compiled in different binaries by executing the command make. These versions can be blocking, when the particle space is divided into smaller blocks, or non-blocking, when it is not.

The interoperability versions (MPI+OmpSs-2+TAMPI) are compiled only if the environment variable TAMPI_HOME is set to the Task-Aware MPI (TAMPI) library's installation directory.

Execution Instructions

The binaries accept several options. The most relevant options are the number of total particles (-p) and the number of timesteps (-t). More options can be seen with the -h option. An example of execution could be:

```
mpiexec -n 4 -bind-to hwthread:16 ./nbody -t 100 -p 8192
```

in which the application will perform 100 timesteps in 4 MPI processes with 16 hardware threads in each process (used by the OmpSs-2 runtime). The total number of particles will be 8192 so that each process will have 2048 particles (2 blocks per process).

References

- ?https://pm.bsc.es/gitlab/ompss-2/examples/nbody
- ?https://en.wikipedia.org/wiki/N-body_simulation

Heat Benchmark (MPI+OmpSs-2+TAMPI)

Users must clone/download this example's repository from https://pm.bsc.es/gitlab/ompss-2/examples/heat and transfer it to a DEEP working directory.

Description

This benchmark uses an iterative Gauss-Seidel method to solve the heat equation, which is a parabolic partial differential equation that describes the distribution of heat (or variation in temperature) in a given region over time. The heat equation is of fundamental importance in a wide range of science fields. In mathematics, it is the parabolic partial differential equation par excellence. In statistics, it is related to the study of the Brownian motion. Also, the diffusion equation is a generic version of the heat equation, and it is related to the study of chemical diffusion processes.

There are 9 implementations of this benchmark which are compiled in different binaries by executing the command make.

The interoperability versions (MPI+OmpSs-2+TAMPI) are compiled only if the environment variable TAMPI_HOME is set to the Task-Aware MPI (TAMPI) library's installation directory.

Execution Instructions

The binaries accept several options. The most relevant options are the size of the matrix in each dimension (-s) and the number of timesteps (-t). More options can be seen with the -h option. An example of execution could be:

```
mpiexec -n 4 -bind-to hwthread:16 ./heat -t 150 -s 8192
```

in which the application will perform 150 timesteps in 4 MPI processes with 16 hardware threads in each process (used by the OmpSs-2 runtime). The size of the matrix in each dimension will be 8192 (8192² elements in total), this means that each process will have 2048x8192 elements (16 blocks per process).

References

- ?https://pm.bsc.es/gitlab/ompss-2/examples/heat
- ?https://pm.bsc.es/ftp/ompss-2/doc/examples/local/sphinx/04-mpi+ompss-2.html
- ?https://en.wikipedia.org/wiki/Heat_equation

Krist Benchmark (OmpSs-2+CUDA)

Users must clone/download this example's repository from https://pm.bsc.es/gitlab/ompss-2/examples/krist and transfer it to a DEEP working directory.

Description

This benchmark represents the krist kernel, which is used in crystallography to find the exact shape of a molecule using Rntgen diffraction on single crystals or powders.

There are 2 implementations of this benchmark, krist and krist-unified using regular and unified CUDA memory, repectively.

Execution Instructions

./krist N_A N_R

where:

- N_A is the number of atoms (1000 by default).
- N_R is the umber of reflections (10000 by default).

References

• ?https://pm.bsc.es/gitlab/ompss-2/examples/krist