Using HPCTOOLKIT with MPI Programs

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Abstract

HPCTOOLKIT is an integrated suite of tools that supports measurement, analysis, attribution and presentation of application performance for sequential and parallel programs. This paper describes how to use HPCTOOLKIT with MPI programs.

1 Introduction

HPCTOOLKIT's measurement tools collect data on each process and thread of an MPI program. HPCTOOLKIT can be used with pure MPI programs as well as hybrid programs that use OpenMP or pthreads for multi-threaded parallelism.

HPCTOOLKIT supports C, C++ and Fortran MPI programs. It has been successfully tested with MPICH, MVAPICH and OpenMPI and should work with almost all MPI implementations.

2 Running and Analyzing MPI Programs

Q: How do I launch an MPI program with hpcrun?

A: For dynamically-linked binaries, use a command line similar to the following example.

```
mpirun -np num hpcrun -e EVENT:count ... program arg ...
```

Note: The MPI launch command (mpirun, mpiexec, etc.) goes on the outside with its options first, then hpcrun and its options on the inside, and finally the application program and its command-line arguments last.

Q: How do I compile and run a statically-linked MPI program?

A: On systems such as Compute-Node Linux and BG/P that run only statically-linked binaries on the compute nodes, use hpclink to build a statically-linked version of your application with the HPCTOOLKIT library linked in. For example,

```
hpclink mpicc -o myprog file.o ... -l<lib> ...
```

Then, set the HPCRUN_EVENT_LIST environment variable in the launch script before running the application.

```
export HPCRUN_EVENT_LIST="PAPI_TOT_CYC@4000000" mpiexec -n 64 myprog arg ...
```

See the *Using HPCToolkit with Statically-Linked Programs* guide for more information.

Q: What files does hpcrun produce for an MPI program?

A: In this example, s3d_f90.x is the Fortran S3D program compiled with OpenMPI and run with the command line "mpiexec -n 4 hpcrun -e PAPI_TOT_CYC:2500000 ./s3d_f90.x". This produced 12 files in the following abbreviated 1s listing.

```
krentel 1889240 Feb 18
                       s3d_f90.x-000000-000-72815673-21063.hpcrun
krentel
           9848 Feb 18
                        s3d_f90.x-000000-001-72815673-21063.hpcrun
krentel 1914680 Feb 18
                        s3d_f90.x-000001-000-72815673-21064.hpcrun
           9848 Feb 18
                        s3d_f90.x-000001-001-72815673-21064.hpcrun
krentel
krentel 1908030 Feb 18
                        s3d_f90.x-000002-000-72815673-21065.hpcrun
krentel
           7974 Feb 18
                       s3d_f90.x-000002-001-72815673-21065.hpcrun
krentel 1912220 Feb 18
                        s3d_f90.x-000003-000-72815673-21066.hpcrun
krentel
           9848 Feb 18
                        s3d_f90.x-000003-001-72815673-21066.hpcrun
krentel 147635 Feb 18
                        s3d_f90.x-72815673-21063.log
krentel 142777 Feb 18
                        s3d_f90.x-72815673-21064.log
krentel 161266 Feb 18
                        s3d_f90.x-72815673-21065.log
krentel 143335 Feb 18
                        s3d_f90.x-72815673-21066.log
```

Here, there are four processes and two threads per process. Looking at the file names, s3d_f90.x is the name of the program binary, 000000-000 through 000003-001 are the MPI rank and thread numbers, and 21063 through 21066 are the process IDs.

We see from the file sizes that OpenMPI is spawning one helper thread per process. Technically, the smaller .hpcrun files imply only a smaller calling-context tree (CCT), not necessarily fewer samples. But in this case, the helper threads are not doing much work.

Q: Do I need to include anything special in the source code?

A: Just one thing. Early in the program, preferably right after MPI_Init(), the program should call MPI_Comm_rank() with communicator MPI_COMM_WORLD. Nearly all MPI programs already do this, so this is rarely a problem. For example, in C, the program might begin with:

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

```
{
   int size, rank;

MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &size);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
...
}
```

Note: The first call to MPI_Comm_rank() should use MPI_COMM_WORLD. This sets the process's MPI rank in the eyes of hpcrun. Other communicators are allowed, but the first call should use MPI_COMM_WORLD.

Also, the call to MPI_Comm_rank() should be unconditional, that is all processes should make this call. Actually, the call to MPI_Comm_size() is not necessary (for hpcrun), although most MPI programs normally call both MPI_Comm_size() and MPI_Comm_rank().

Q: What MPI implementations are supported?

A: Although the matrix of all possible MPI variants, versions, compilers, architectures and systems is very large, HPCTOOLKIT has been tested successfully with MPICH, MVAPICH and OpenMPI and should work with most MPI implementations.

Q: What languages are supported?

A: C, C++ and Fortran are supported.

3 Building and Installing HPCToolkit

Q: Do I need to compile HPCTOOLKIT with any special options for MPI support?

A: No, HPCTOOLKIT is designed to work with multiple MPI implementations at the same time. That is, you don't need to provide an mpi.h include path, and you don't need to compile multiple versions of HPCTOOLKIT, one for each MPI implementation.

The technically-minded reader will note that each MPI implementation uses a different value for MPI_COMM_WORLD and may wonder how this is possible. hpcrun (actually libmonitor) waits for the application to call MPI_Comm_rank() and uses the same communicator value that the application uses. This is why we need the application to call MPI_Comm_rank() with communicator MPI_COMM_WORLD.