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Center for High-Performance Computing

Hybrid MPI/OpenMP programming

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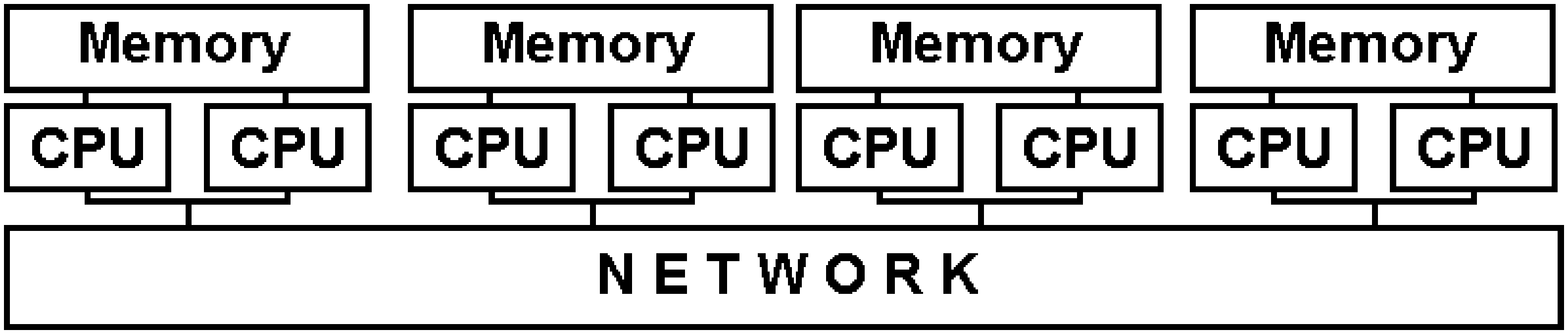
Overview

- Single and multilevel parallelism.
- Example of MPI-OpenMP buildup.
- Compilation and running.
- Performance suggestions.
- Code examples.

Single level parallelism

- Shared memory computers
  - N processors, single system image
  - thread-based parallelism - OpenMP, shmem
  - message-based parallelism - MPI
- Distributed memory computers
  - nodes with local memory, coupled via network
  - message-based parallelism – MPI
  - partitioned global space – UPC, Coarray Fortran

Shared-Distributed memory



- Each node has N processors that share memory
- Nodes loosely connected (network)
- CHPC:
  - 12, 16, 20, 24, 28, 32, 64 core cluster nodes

Multilevel parallelism

- Coarse and fine grain level
  - coarse – nodes, processors (sockets)
    fine – CPU cores
  - MPI - nodes, CPU sockets
    OpenMP, pthreads, shmem – CPU cores
  - OpenMP works best with processing intensive loops
- Multilevel advantages
  - memory limitations – extra memory for each copy of executable on the node
  - process vs. thread overhead
  - message overhead
  - portability, ease to maintain (can disable OpenMP)

MPI and OpenMP

- MPI (Message Passing Interface)
  - standardized library (not a language)
  - collection of processes communicating via messages
  - available for most architectures
  - http://www.mpi-forum.org/

- OpenMP
  - API for shared memory programming
  - available on most architectures as a compiler extension (C/C++, Fortran)
  - includes compiler directives, library routines and environment variables
  - www.openmp.org

Processes vs. threads

- Process
  - have own address space
  - can have multiple threads

- MPI
  - many processes
  - shared-nothing architecture
  - explicit messaging
  - implicit synchronization
  - all or nothing parallelization

- Thread
  - executes within process
  - same address space
  - share process's stack
  - thread specific data

- OpenMP
  - 1 process, many threads
  - shared-everything architecture
  - implicit messaging
  - explicit synchronization
  - incremental parallelism

Pi example

- Calculation of value of π using integral:

$$\int_0^1 \frac{dx}{x^2+1} = \frac{\pi}{4}$$

- trapezoidal rule
- simple loop easy to parallelize both with MPI and OpenMP

Serial code

```
#include <stdio.h>
#include <math.h>
#include "timer.h"
int main(int argc, char *argv[]){
const int N = 10000000000;
const double h = 1.0/N;
const double PI = 3.141592653589793238462643;
double x,sum,pi,error,time; int i;

time = ctimer();
sum = 0.0;
for (i=0;i<=N;i++){
  x = h * (double)i;
  sum += 4.0/(1.0+x*x);}

pi = h*sum;
time += ctimer();

error = pi - PI;
error = error<0 ? -error:error;
printf("pi = %18.16f +/- %18.16f\n",pi,error);
printf("time = %18.16f sec\n",time);
return 0;}
```

- **User-defined timer**
- **Calculation loop**
- **Print out result**

OpenMP code

```
#include <stdio.h>
#include <math.h>
#include "timer.h"
int main(int argc, char *argv[]){
const int N = 10000000000;
const double h = 1.0/N;
const double PI = 3.141592653589793238462643;
double x,sum,pi,error,time; int i;

time = -ctimer();
sum = 0.0;
#pragma omp parallel for shared(N,h),private(i,x),reduction(+:sum)
for (i=0;i<=N;i++){
  x = h * (double)i;
  sum += 4.0/(1.0+x*x);}

pi = h*sum;
time += ctimer();

.......

return 0;}
```

- **OpenMP directive**

MPI code

```
#include <stdio.h>
#include <math.h>
#include "timer.h"
int main(int argc, char *argv[]){
const int N = 10000000000;
const double h = 1.0/N;
const double PI = 3.141592653589793238462643;
double x,sum,pi,error,time,mypi; int i;
int myrank,nproc;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);
MPI_Comm_size(MPI_COMM_WORLD,&nproc);

time = -ctimer();
sum = 0.0;
for (i=myrank;i<=N;i=i+nproc){
  x = h * (double)i;
  sum += 4.0/(1.0+x*x);}
mypi = h*sum;
MPI_Reduce(&mypi,&pi,1,MPI_DOUBLE,MPI_SUM,0,MPI_COMM_WORLD);
time += ctimer();
......
return 0;}
```

- **MPI initialization**
- **Distributed loop**
  OK here, inefficient for vectors due to strided memory access
- **Global reduction**

MPI-OpenMP code

```
#include <stdio.h>
#include <math.h>
#include "timer.h"
int main(int argc, char *argv[]){
const int N = 10000000000;
const double h = 1.0/N;
const double PI = 3.141592653589793238462643;
double x,sum,pi,error,time,mypi; int i;
int myrank,nproc;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);
MPI_Comm_size(MPI_COMM_WORLD,&nproc);

time = -ctimer();
sum = 0.0;

#pragma omp parallel for shared(N,h,myrank,nproc),private(i,x),reduction(+:sum)
for (i=myrank;i<=N;i=i+nproc){
  x = h * (double)i;
  sum += 4.0/(1.0+x*x);}
mypi = h*sum;
MPI_Reduce(&mypi,&pi,1,MPI_DOUBLE,MPI_SUM,0,MPI_COMM_WORLD);
time += ctimer();
......
return 0;}
```

- **OpenMP directive to parallelize each MPI task loop using threads**
- **Sum MPI task local values of π**

Compilation

- GNU, PGI, Intel compilers, OpenMP with –fopenmp, -mp, -qopenmp switch
- MPICH, MVAPICH2, OpenMPI or Intel MPI

`module load mpich` **MPICH**

`module load mvapich2` **MVAPICH2**

`module load openmpi` **OpenMPI**

`module load impi` **Intel MPI**

```
mpicc -mp=numa source.c -o program.exe (PGI)
mpif90 -fopenmp source.f -o program.exe (Intel gfortran)
mpiifort -qopenmp source.f -o program.exe (Intel ifort)
mpif90 -fopenmp source.f -o program.exe (GNU)
```

Third party libraries

- BLASes and FFTW are threaded
- Intel compilers:

```
-I$FFTW_INCDIR -lfftw3 -lfftw3_omp -L$FFTW_LIBDIR
-Wl,-rpath=$MKLROOT/lib/intel64 -L$MKLROOT/lib/intel64
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread
```

- PGI compilers:

```
-I$FFTW_INCDIR -lfftw3 -lfftw3_omp -L$FFTW_LIBDIR -lacml_mp
```

- MKL ScaLAPACK w/ Intel

```
-Wl,-rpath=$MKLROOT/lib/intel64 -L$MKLROOT/lib/intel64
-lmkl_scalapack_ilp64 -lmkl_intel_ilp64 -lmkl_core
-lmkl_intel_thread -lmkl_blacs_intelmpi_ilp64 -liomp5 -lpthread -lm
```

https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

Running

- Ask for #MPI processes
- Use SLURM environment variables to get OpenMP thread count
- Interactive batch (asking for 2 nodes, 2 tasks/node)

```
salloc -n 4 -N 2 -t 1:00:00 -p kingspeak -A chpc   … wait
for prompt …

set TPN=`echo $SLURM_TASKS_PER_NODE | cut -f 1 -d \(`
set PPN=`echo $SLURM_JOB_CPUS_PER_NODE | cut -f 1 -d \(`
@ THREADS = ( $PPN / $TPN )
mpirun -genv OMP_NUM_THREADS=$THREADS -np $SLURM_NTASKS
./program.exe
```

- Non-interactive batch
  - same thing, except in a Slurm script

Running – process pinning

- Current NUMA architectures penalize memory access on neighboring CPU sockets
- Distribute and bind processes to CPU sockets
- Intel compilers can also pin threads to cores

```
module load intel mvapich2
mpirun -genv KMP_AFFINITY granularity=fine,compact,1,0 -genv
   MV2_BINDING_POLICY scatter -genv MV2_BINDING_LEVEL socket
   -genv OMP_NUM_THREADS 8 -np 4
```

- Intel MPI binds processes to sockets by default

```
module load intel impi
mpirun -x KMP_AFFINITY granularity=fine,compact,1,0
   -genv OMP_NUM_THREADS 8 -np 4
```

or use `I_MPI_PIN_DOMAIN=socket`

Running – process pinning cont'd

- Default pinning policies for compilers and MPI distributions vary
- See analysis of the situation at https://aci ref.org/how-to-gain-hybrid-mpi-openmp-code-performance-without-changing-a-line-of-code-a-k-a-dealing-with-task-affinity/
- Some applications can gain up to 30% performance with pinning processes AND threads
- Using pinthreads.sh script from the article with common compilers (Intel, PGI, GNU) and MPIs (MPICH, MVAPICH2, IMPI, OpenMPI) on a 24 core node, 8 MPI tasks 3 threads each:

```
mpirun -np 8 -genv OMP_NUM_THREADS 3 -bind-to socket -map-by socket ./pinthreads.sh ./myprogram
```

- Check the pinning by this bash one-liner:

```
for i in $(pgrep myprogram); do for tid in $(ps --no-headers -mo tid -p $i |grep -v -); do taskset -cp "${tid}"; done ;
```

General multilevel approach

- Parallelize main problem using MPI
  - task decomposition
    - frequencies in wave solvers
  - domain decomposition
    - distribute atoms in molecular dynamics
    - distribute mesh in ODE/PDE solvers
- Exploit internal parallelism with OpenMP
  - use profiler to find most computationally intense areas
    - internal frequency loop in wave solvers
    - local force loop in MD
    - local element update loop in ODE/PDE solvers
  - measure the efficiency to determine optimal number of threads to use
  - Intel Advisor can be helpful (`module load advisor`)

Things to be aware of

- Not every MPI program will benefit from adding threads
  - not worth with loosely parallel codes (too little communication)
    - overhead with thread creation about 10^4 flops
  - time with different node/thread count to get the best performing combination
- MPI communication within OpenMP
  - can be tricky if each thread communicates
  - be aware of thread safety in MPI when using MPI_THREAD_MULTIPLE

Thread safety

- Defines if it is safe to use program or library with parallel threads
- Most libraries these days are thread safe
  - But it's good to check, usually there is some note in the documentation or in the build scripts
  - Some libraries have threaded and non-threaded versions
- Most often thread safety relates to the concurrent access of shared data
- MPI defines several threading models, some allow communication from threads, some don't

Four MPI threading models

- MPI_THREAD_SINGLE
  - only non-threaded section communicates (default)
- MPI_THREAD_FUNNELLED
  - process may be multithreaded but only master thread communicates
- MPI_THREAD_SERIALIZED
  - multiple threads may communicate but only one at time
- MPI_THREAD_MULTIPLE
  - all threads communicate (fully thread safe)

Example of single thread communication.

- Complex norm routine

```
int main(int argc, char **argv){
.......
MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
MPI_Comm_rank(MPI_COMM_WORLD,&myid);
.......

double _Complex stabWmnorm(double *Wm, double _Complex *stab, int size)
{
  double _Complex norm, vec, norml;
  int i;

  norml = 0 + I*0;
  #pragma omp parallel for private(i,vec) reduction(+:norml)
  for (i=0;i<size;i++)
  {
     vec = stab[i]*Wm[i];
     norml = norml + vec*conj(vec);
  }
  MPI_Allreduce(&norml,&norm,1,MPI_DOUBLE_COMPLEX,MPI_SUM,MPI_COMM_WORLD);

  return sqrt(norm);
}

MPI_Finalize();
```

Parallel OpenMP for loop

MPI communication outside OpenMP

Multiple threads comm. - initialization

- Special MPI_Init
  - Returns variable thread_status which indicates what level of threading is supported

```
int thread_status;

MPI_Init_thread(&argc, &argv,MPI_THREAD_MULTIPLE,&thread_status);
if (thread_status!=MPI_THREAD_MULTIPLE)
{
 printf("Failed to initialize MPI_THREAD_MULTIPLE\n");
 exit(-1);
}

...

MPI_Finalize();
```

Multiple threads point-to-point communication

```
#pragma omp parallel private(iis,niip,iip,iisf)
{
 double _Complex *ne, *nh; int comlab, mythread, nthreads;
 MPI_Status statx[fwdd->Nz];
 MPI_Request reqx[fwdd->Nz];

#ifdef _OPENMP
 mythread = omp_get_thread_num(); nthreads = omp_get_num_threads();
#endif

 ne = (double _Complex *)malloc(sizeof(double _Complex)*3*Nxy);

 comlab=mythread*10000; // different tag for each proc/thread

 for (iis=mythread; iis < Ncp[0]; iis+=nthreads)
 {
   … calculate pieces of large distributed vector Ebb as a local vector ne
   if (cpuinfo[0] == iip)
   {
    MPI_Isend( &ne[0], Nxy, MPI_DOUBLE_COMPLEX, Dp[0], comlab, MPI_COMM_WORLD, reqx[Nreqi[0]]);
    Nreqi[0]++; comlab++;
   }
   else if (cpuinfo[0] == Dp[0])
   {
    MPI_Irecv(&Ebb[ie[0]*Nxy], Nxy, MPI_DOUBLE_COMPLEX, iip, comlab, MPI_COMM_WORLD, reqx[Nreqi[0]]);
    Nreqi[0]++; comlab++;
   }
   MPI_Waitall(Nreqi[0], &reqx[0], &statx[0]);
 }

 free(ne);
}
```

Start parallel OpenMP section

Data structures for non-blocking communication

Find thread # and # of threads

Allocate local thread arrays

Each thread does different iteration of this loop

Each communication pair has unique tag

Finalize non-blocking communication

Free local thread arrays
End OpenMP parallel section

-> use message tag to differentiate between threads

Multiple threads collective communication

```
MPI_Comm comm_thread[NOMPCPUS];

#pragma omp parallel private(iis,niip,iip,iisf)
{
 double _Complex *ne; int mythread, nthreads

#ifdef _OPENMP
 mythread = omp_get_thread_num(); nthreads = omp_get_num_threads();
#endif

 ne = (double _Complex *)malloc(sizeof(double _Complex)*3*Nxy);

 for(ithr=0;ithr<nthreads;ithr++)
 {
   #pragma omp barrier // synchronize so that each process gets the right thread
   if (ithr==mythread) MPI_Comm_dup(comm_domain,&comm_thread[mythread]);
 }
 for (iis=mythread; iis < Ncp[0]; iis+=nthreads)
 {
    … calculate ne …
    MPI_Gatherv( &ne[indgbp[iic]],Nxy_loc,MPI_DOUBLE_COMPLEX, &Gb[ie[ic]*Nxy2 + iit2], Nxy_rec,
    Nxy_disp, MPI_DOUBLE_COMPLEX, Dp[ic],comm_thread[mythread]);
 }

 for(ithr=0;ithr<nthreads;ithr++)
 {
   if (ithr==mythread) MPI_Comm_free(&comm_thread[mythread]);
 }

 free(ne);
}
```

Start parallel OpenMP section

Local thread variables

Find thread # and # of threads

Allocate local thread arrays

Per thread communicator

Each thread does different iteration of this loop

Thread communicator

Free thread communicators

Free local thread arrays

End OpenMP parallel section

-> use communicators to differentiate between threads

Future outlook

- Mixed MPI-OpenMP has become commonplace
  - reduces memory footprint per core
  - better locality of memory access per core
  - faster inter-node communication – larger messages, smaller overhead
  - One sided MPI communication further improves parallel efficiency

Summary

- Single and multilevel parallelism
- Simple MPI-OpenMP example
- Compilation, running
- A few advices

`http://www.chpc.utah.edu/short_courses/mpi_omp`

References

- MPI

  `http://www.mpi-forum.org/`
- OpenMP

  `http://www.openmp.org/`
- MPI+OpenMP

  Pacheco – Introduction to Parallel Programming
- XSEDE HPC Summer Boot Camp

  OpenMP, OpenACC, MPI

  https://www.youtube.com/XSEDETraining