Lab: Hybrid Programming and NUMA Control

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Introduction to Parallel Computing
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Based on materials developed by Kent Milfeld at TACC

What You Will Learn

- How to use numactl in the execution of serial, threaded, and 4xN hybrid (i.e., 4 MPI tasks, each with N threads) codes
- How to structure communications in a 2x16 hybrid code that involves threaded MPI calls between 2 nodes
  - MPI calls from serial region
  - MPI calls from master thread in a parallel region
  - MPI calls from all threads in a parallel region
- How to measure the performance of the above codes
- The performance implications of using numactl and threaded MPI
  - Location of data is important in serial codes
  - Initialization of data is important in threaded codes
  - For less than 16-way, MPI executables need to be assigned to sockets
Getting Started

- Untar the file numahybrid.tar
  - cd ~ (start in your home directory)
  - tar xvf ~train100/labs/numahybrid.tar (extract files)
  - cd numahybrid

numactl_serial

- Run the memory intensive daxpy program on four different sockets using local, interleave and off-socket-memory policies.
  - Use the commands below to make the daxpy executable and run it with numa control commands.
  - See the job script and the table on the next page for the numa options.
  - Run the job and report the times and relative performance.

- Procedure:
  - cd numactl_serial (change directory to numactl_serial)
  - module unload mvapich; module swap pgi intel; module load mvapich
  - make
  - qsub job (submits job)
numactl_serial – Results

• From the job output fill in the table.

<table>
<thead>
<tr>
<th>Command</th>
<th>Time (secs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>numactl -l C 0</td>
<td></td>
</tr>
<tr>
<td>numactl -l C 1</td>
<td></td>
</tr>
<tr>
<td>numactl -l C 2</td>
<td></td>
</tr>
<tr>
<td>numactl -l C 3</td>
<td></td>
</tr>
<tr>
<td>numactl -i all -C 0</td>
<td></td>
</tr>
<tr>
<td>numactl -i all -C 1</td>
<td></td>
</tr>
<tr>
<td>numactl -i all -C 2</td>
<td></td>
</tr>
<tr>
<td>numactl -i all -C 3</td>
<td></td>
</tr>
<tr>
<td>numactl -m 3 -C 0</td>
<td></td>
</tr>
</tbody>
</table>

Rank the performance of local, interleave, and off-socket-memory policies, from best to poorest
1.)
2.)
3.)

numactl_alloc

• The daxpy algorithm is parallelized to run as 4 threads. It is run on 4 different sockets through the code statements:

```plaintext
ithread = OMP_GET_THREAD_NUM()*4
call f90_setaffinity(ithread)
```

– In master_alloc_daxpy, the a, b, and c matrices are allocated preferentially on the default socket for the master thread (0).
– In thread_alloc_daxpy, sections of a, b, and c are allocated where the threads are executing (cores 0,4,8,12 on sockets 0,1,2,3).

• Procedure:
  – cd numactl_alloc  (change directory to numactl_alloc)
  – if you have done this already, don’t do it again:
    module unload mvapich; module swap pgi intel; module load mvapich
  – make       (note, must link with -l numa to obtain set_mempolicy)
  – qsub job   (submits job)
numactl_alloc – Results

- From the job output fill in the table.

<table>
<thead>
<tr>
<th>Command</th>
<th>Time (secs)</th>
<th>Rank the performance of master-allocated memory vs. thread-allocated, from best to poorest</th>
</tr>
</thead>
<tbody>
<tr>
<td>master_alloc_daxpy</td>
<td></td>
<td>1.)</td>
</tr>
<tr>
<td>thread_alloc_daxpy</td>
<td></td>
<td>2.)</td>
</tr>
</tbody>
</table>

numactl_4x1, numactl_4x4

- Run the daxpy program as 4 tasks in a node (4x1) and 4 tasks with 4 threads in a node (4x4), following the instructions below.
  - Use the commands below to make the daxpy executable and run it with numa control commands.
  - See the job script and the table on the next page for the numa options.
  - Run the job and report the times and relative performance.

- Procedure:
  - cd numactl_4x1 or numactl_4x4 (change directory as needed)
  - if you have done this already, don’t do it again:
    module unload mvapich; module swap pgi intel; module load mvapich
  - make
  - qsub job (submits job)
numactl_4x1, numactl_4x4 – Results

- From the job output fill in the tables.

<table>
<thead>
<tr>
<th>Command (4x1)</th>
<th>Time (secs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;no numactl&gt;</td>
<td></td>
</tr>
<tr>
<td>numactl -l</td>
<td></td>
</tr>
<tr>
<td>numactl -i all</td>
<td></td>
</tr>
<tr>
<td>numactl tacc affinity</td>
<td></td>
</tr>
</tbody>
</table>

Rank 4x1 performance from best to poorest
1.)
2.)
3.)
4.)

<table>
<thead>
<tr>
<th>Command (4x4)</th>
<th>Time (secs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;no numactl&gt;</td>
<td></td>
</tr>
<tr>
<td>numactl -l</td>
<td></td>
</tr>
<tr>
<td>numactl -i all</td>
<td></td>
</tr>
<tr>
<td>numactl tacc affinity</td>
<td></td>
</tr>
</tbody>
</table>

Rank 4x4 performance
1.)
2.)
3.)
4.)

What’s the Explanation?

- This is a bandwidth-limited code, so the best results are achieved when executions are distributed across all sockets.
- For both 4x1 and 4x4 cases, the default kernel policy puts all tasks on socket 0; tweaking the memory allocation doesn’t help much 😞
- tacc_affinity spreads the tasks across sockets, which is 2-4x faster
  - 4x1 case is 2-3x faster
  - 4x4 case is 4x faster because the default affinity puts ALL threads on a single socket
What is tacc_affinity?

It's a script: /share/sge6.2/default/pe_scripts/tacc_affinity

```bash
#!/bin/bash
MODE=/share/sge6.2/default/pe_scripts/getmode.sh
# First determine "wayness" of PE
myway=echo $PE | sed s/way//'
# Determine local compute node rank number
if [ x"$MODE" == "xmvapich2_ssh" ]; then
  export MV2_USE_AFFINITY=0
  export MV2_ENABLE_AFFINITY=0
  my_rank=$PMI_ID
  elif [ x"$MODE" == "xmvapich1_ssh" ]; then
    export VIADEV_USE_AFFINITY=0
    export VIADEV_ENABLE_AFFINITY=0
    my_rank=$MPIRUN_RANK
    else
    echo "TACC: Could not determine MPI stack. Exiting!"
    exit 1
    fi
local_rank=$(( $my_rank % $myway ))

# Based on "wayness" determine socket layout on local node
# if less than 4-way, offset to skip socket 0
if [ $myway -eq 2 ]; then
  numnode="0,1,2,3"
# if 2-way, set 1st task on 0,1 and second on 2,3
elif [ $myway -eq 2 ]; then
  numnode="$(( 2 * $local_rank )),$(( 2 * $local_rank + 1 ))"
  elif [ $myway -lt 4 ]; then
    numnode=$( ( $local_rank + 1 ) / 4 )
else
  numnode=$( ( $local_rank + 1 ) / 4 )
fi
#exec /usr/bin/numactl -c $numnode -m $numnode $*
```
Communications in Hybrid Codes

- The tmpi (threaded mpi) code illustrates different ways of doing point-to-point and broadcast communications in a hybrid code. Using both mvapich and openmpi, we will:
  - check to make sure the code performs correctly
  - measure the cost for sending a single large message in the serial region
  - compare the cost for sending 16 small messages in the parallel region

- Procedure:
  - cd threaded_mpi
  - if you have done this already, don’t do it again:
    module unload mvapich; module swap pgi intel; module load mvapich
  - ./build.sh (this builds tmpi.mvapich1 and tmpi.openmp)

Hybrid Job Script

Script for 10 interactive minutes of 2 nodes (=32/16), 1 task per node (1way), 2 tasks total, in the development queue. 16 threads (OMP_NUM_THREADS 16) are launched on each node.

```bash
#!/bin/tcsh
#
#$ -V                      # inherit submission environment
#$ -cwd                    # use submission directory
#$ -N threadedmpi          # jobname (threadedmpi)
#$ -j y                    # stdout/err combined
#$ -o $JOB_NAME.o$JOB_ID   # output name jobname.ojobid
#$ -pe 1way 32             # 1 task/node, 32 cores total
#$ -q development          # queue name !! use normal
#$ -1 h_rt=00:10:00        # request 10 minutes
#$ -A TACCacct             # Accounting: training project
set echo
setenv MY_NSLOTS 2
setenv OMP_NUM_THREADS 16
ibrun ./tmpi < input
```

If # of tasks is not equal to wayness*total_cores/16, set value here.
Submit the Batch Job

% qsub job
...
------ Welcome to TACC's Ranger System, an NSF TeraGrid Resource -------
...
Your job 18073 ("threadedmpi") has been submitted

% qstat

job-ID prior name user state submit/start at queue slots
--- -------- ---- -------- ------ -------------------------- --------
18075 0.00001 threadedmp milfeld r 01/17/2008 22:48:54 normal@i104-408 32

% showq
...

Communication from Serial Region

include "mpif.h"

call MPI_Init_thread(MPI_THREAD_MULTIPLE, iprovided,ierr)
call MPI_Comm_size(MPI_COMM_WORLD,nranks, ierr)
call MPI_Comm_rank(MPI_COMM_WORLD,irank,ierr)

if(irank == 0) then
  call mpi_send(as,n,MPI_REAL8, 1,9,MPI_COMM_WORLD, ierr)
call mpi_recv(as,n,MPI_REAL8, 1,1,MPI_COMM_WORLD, istatus,ierr)
else if (irank == 1) then
  call mpi_recv(as,n,MPI_REAL8, 0,9,MPI_COMM_WORLD, istatus,ierr)
call mpi_send(as,n,MPI_REAL8, 0,1,MPI_COMM_WORLD, ierr)
endif

if(irank .eq. 0) read(*,'(i5)') iread1
call MPI_Bcast(iread1,1,MPI_INTEGER, 0,iwcomm, ierr)

(don't forget error argument in f90 codes)
Broadcast in Parallel Region

```fortran
!$OMP PARALLEL private(i,ithread,nthreads, icpl, icp2, icpd)

ithread = OMP_GET_THREAD_NUM()

if(ithread == 0) then
    if(irank .eq. 0) read(*,'(i5)') iread2
    call MPI_Bcast(iread2,1,MPI_INTEGER, 0,iwcomm, ierr)
end if

!$OMP PARALLEL private(i,ithread,nthreads, icpl, icp2, icpd)

... (don't forget error argument in f90 codes)
```

Point-to-point in Parallel Region

```fortran
!$OMP DO ordered
do i = 1,nthreads
!$OMP ordered
if(irank == 0) then
    call mpi_send(as,ns,MPI_REAL8, 1,ithread,MPI_COMM_WORLD, ierr)
    call mpi_recv(as,ns,MPI_REAL8, 1,ithread,MPI_COMM_WORLD, istatus,ierr)
else if (irank == 1) then
    call mpi_recv(as,ns,MPI_REAL8, 0,ithread,MPI_COMM_WORLD, istatus,ierr)
    call mpi_send(as,ns,MPI_REAL8, 0,ithread,MPI_COMM_WORLD,ierr)
end if
!$OMP end ordered
end do
if(irank == 0 .and. ithread == 0) then
    call mpi_send(as,n,MPI_REAL8, 1,ithread,MPI_COMM_WORLD, ierr)
    call mpi_recv(ar,n,MPI_REAL8, 1,ithread,MPI_COMM_WORLD, istatus,ierr)
else if (irank == 1 .and. ithread == 0) then
    call mpi_recv(ar,n,MPI_REAL8, 0,ithread,MPI_COMM_WORLD, istatus,ierr)
    call mpi_send(as,n,MPI_REAL8, 0,ithread,MPI_COMM_WORLD, ierr)
end if
!$OMP barrier
!$OMP END PARALLEL
```

Not needed with mvapich2

End of Parallel
End of MPI
Hybrid Communication Cost (Output from tmpi)

Mvapich
Serial Region Ping Pong (words:secs) 400000: 0.00509
Serial Region Broadcast (sec) 0.00002
Parallel Region Broadcast (sec) 0.00001
Parallel region messages:
One Large message size:secs 400000 tot time: 0.00561
16 Small messages size:secs 25000 tot time: 0.00534
individual times: 0.00034 0.00033 0.00034 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033 0.00033

OpenMPI
Serial Region Ping Pong (words:secs) 400000: 0.00501
Serial Region Broadcast (sec) 0.00005
Parallel Region Broadcast (sec) 0.00001
Parallel region messages:
One Large message size:secs 400000 tot time: 0.00550
16 Small messages size:secs 25000 tot time: 0.08949
individual times: 0.08383 0.00037 0.00037 0.00038 0.00037 0.00065 0.00035 0.00036 0.00034 0.00035 0.00034 0.00035 0.00035 0.00035 0.00036

Why the Difference in Results?

- Explanation: mvapich has a special queue service which allows multiple short messages (all having the same destination) to be sent as quickly as one long message!