The Abdus Salam International Centre for Theoretical Physics

2494-21

Workshop on High Performance Computing (HPC) Architecture and Applications in the ICTP

14 - 25 October 2013

Introduction to Parallel Programming, Benchmarking & Profiling

Ivan Girotto
ICTP, Trieste

The Abdus Salam International Centre for Theoretical Physics

Introduction to Parallel Programming, Benchmarking & Profiling

Ivan Girotto – igirotto@ictp.it

Information & Communication Technology Section (ICTS)

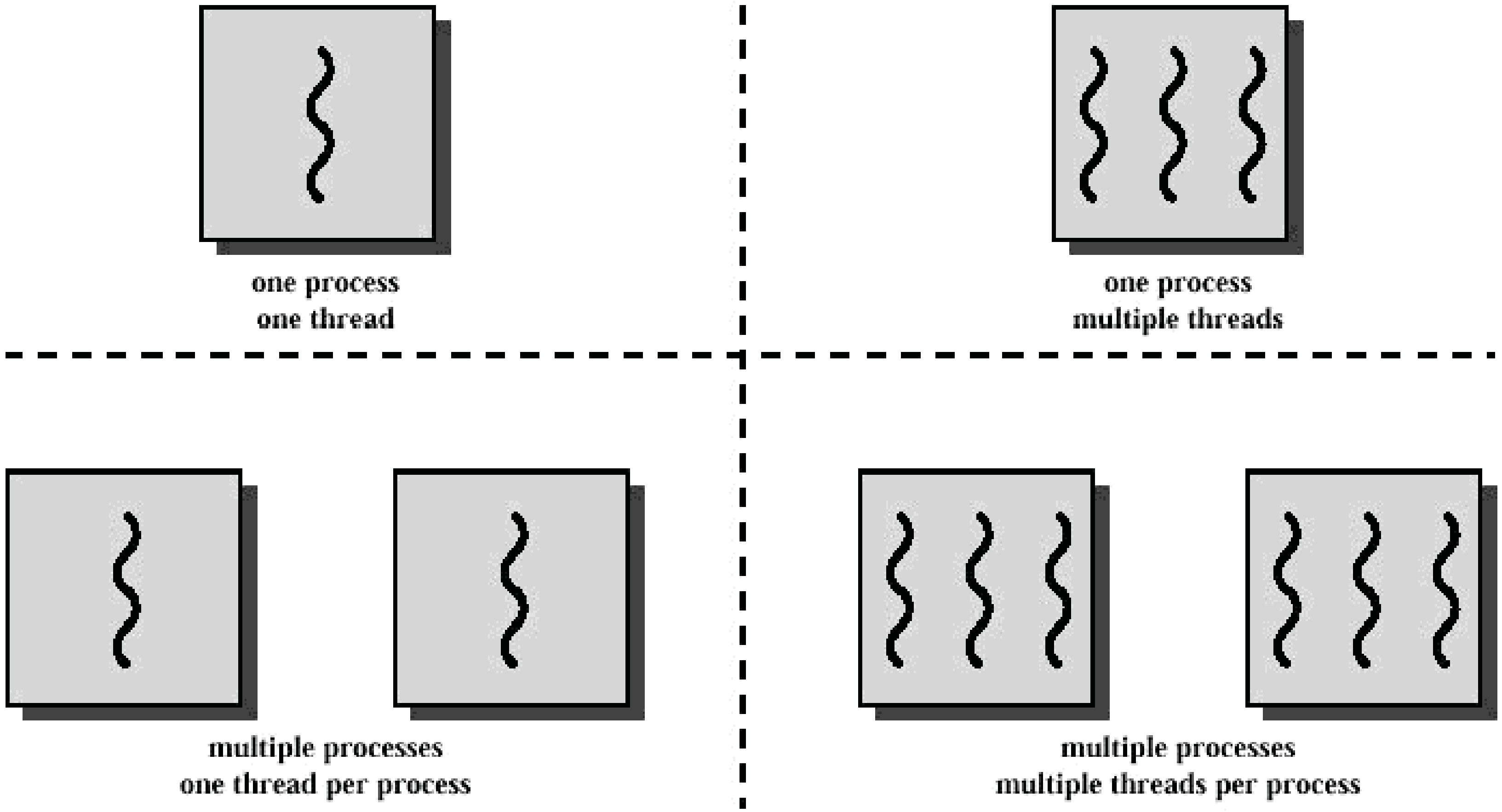
International Centre for Theoretical Physics (ICTP)

Outline

- Introduction to // Programming
- Compiling and Running // Programs
- Benchmarking
- Profiling
- Hands-on

Glossary

- Process: sequence of instructions execute by a given processing unit (core)
  - Unique memory address space
- Thread: sub-entity of a process. Portion of the content of a given process information. Each process can be seen as a single thread.
- Multiple process threads can be replicated to execute single/different instructions on the same/different data. Threads work on SPMD model.


one process
one thread
one process
multiple threads
multiple processes
one thread per process
multiple processes
multiple threads per process

Parallel Programming Models /1

- Shared memory
  - Process threads work together
  - Data are shared among the same address space
  - Communication is performed writing and reading data on a shared portion of the main memory
- Message passing (distribute memory model)
  - Compute processes work together
  - Data are distributed among different address spaces
  - Communication is performed among the exchange of distributed data with operations of send & recv
- On both models the compute units are uniquely identified (ID)

```
#include <stdlib.h>
#include <stdio.h>
#include <omp.h>

int main (int argc, char * argv[]){

 int myId, size, buffer = 0;

#pragma omp parallel private( myId, size )
 {
   myId = omp_get_thread_num();
   size = omp_get_num_threads();

   fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);

   if( myId == 0 ) buffer = 1;

#pragma omp barrier

   fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);
}

  return 0;
}
```

- Example of an OpenMP program for data exchange

```c
#include <stdlib.h>
#include <stdio.h>
#include <omp.h>

int main (int argc, char * argv[]){

  int myId, size, buffer = 0;

#pragma omp parallel private( myId, size )
  {
    myId = omp_get_thread_num();
    size = omp_get_num_threads();

    fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);

    if( myId == 0 ) buffer = 1;

#pragma omp barrier

    fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);
}

  return 0;
}
```

- Example of an OpenMP program for data exchange

```c
#include <stdlib.h>
#include <stdio.h>
#include <mpi.h>

int main (int argc, char * argv[]){

  int myId, size, buffer = 0;
  MPI_STATUS_SIZE status;

  MPI_Init( &argc, &argv );
  MPI_Comm_rank( MPI_COMM_WORLD, &myId );
  MPI_Comm_size( MPI_COMM_WORLD, &size );

  fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);

  if( myId == 0 ){
    buffer = 1;
    MPI_Send( &buffer, 1, MPI_INT, 1, 100, MPI_COMM_WORLD );
  }
  else MPI_Recv( &buffer, 1, MPI_INT, 0, 100, MPI_COMM_WORLD, &status )

  fprintf( stdout, "\nThread %d of %d. Buffer = %d.", myId, size, buffer);

  MPI_Finalize();

  return 0;
}
```

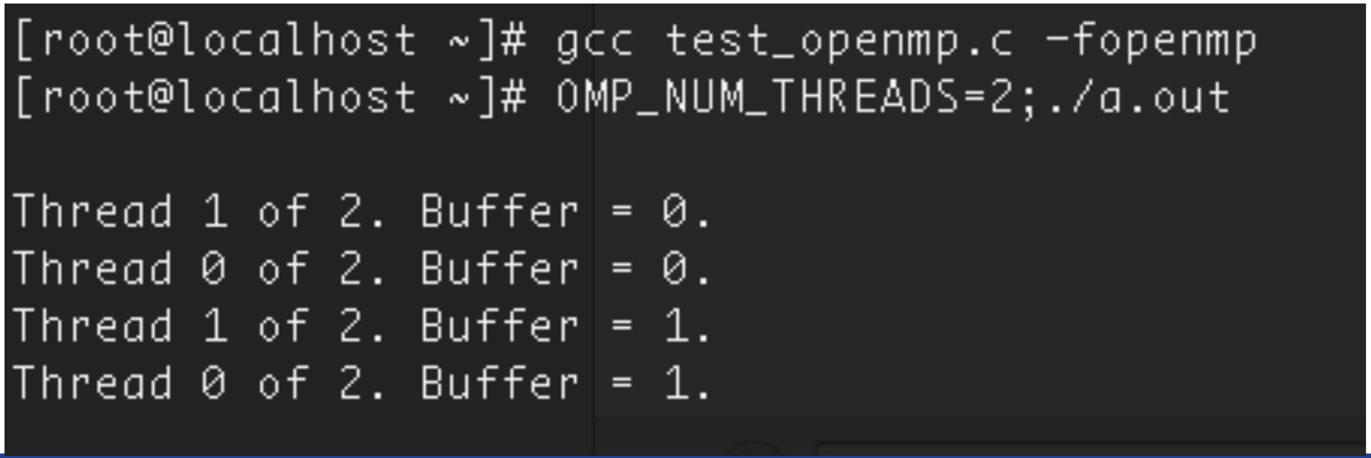
- Example of a MPI program for data exchange

Compile and Run an OpenMP program

gcc -O3 -o my_program.x my_program.c -fopenmp

or

icc -O3 -o my_program.x my_program.c -openmp



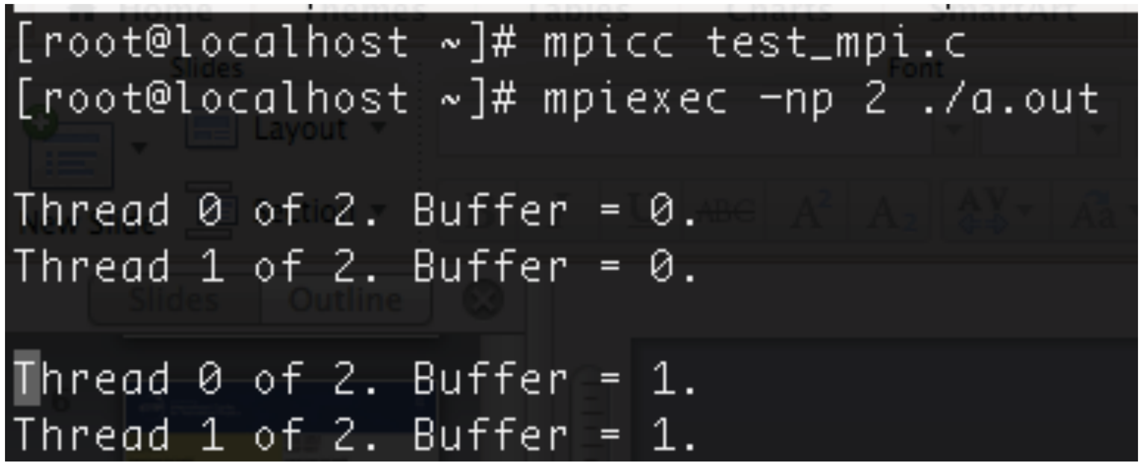
```
[root@localhost ~]# gcc test_openmp.c -fopenmp
[root@localhost ~]# OMP_NUM_THREADS=2;./a.out

Thread 1 of 2. Buffer = 0.
Thread 0 of 2. Buffer = 0.
Thread 1 of 2. Buffer = 1.
Thread 0 of 2. Buffer = 1.
```

Compile and Run an MPI program

mpicc -O3 -o my_program.x my_program.c

or

mpicc -O3 -o my_program.x my_program.c



```
[root@localhost ~]# mpicc test_mpi.c
[root@localhost ~]# mpiexec -np 2 ./a.out

Thread 0 of 2. Buffer = 0.
Thread 1 of 2. Buffer = 0.

Thread 0 of 2. Buffer = 1.
Thread 1 of 2. Buffer = 1.
```

Compile and Run an Hybrid program

mpicc -O3 -o my_program.x my_program.c -fopenmp

or

mpicc -O3 -o my_program.x my_program.c -openmp

```
[root@localhost ~]# mpicc -o test_hybrid.x test_hybrid.c -openmp
[root@localhost ~]# export OMP_NUM_THREADS=2
[root@localhost ~]# mpiexec -np 2 ./test_hybrid.x
```

CPU Architecture Benchmark /1

- Measure of Performance
- Architecture Assessment
- Basic key-points for obtaining useful outcomes:
  - Define what are the measures of interest
  - Define what are the tools
  - Define what is the SW environment
  - Define reasonable workloads
  - Data mining is essential (sooner or later)
- Synthetic Benchmark Vs. Application Benchmark

CPU Architecture Benchmark /2

- DGEMM - double precision Matrix-Matrix Multiplication to measure FLOP/s
  - C := alpha*op(A)*op(B) + beta*C
- DAXPY - adds a scalar multiple of a double precision vector to another double precision vector to measure memory bandwidth
  - y <-- alpha*x + y

Benchmark	DATA	FLOP
DAXPY	O(DIM)	O(DIM)
DGEMM	O(DIM^2)	O(DIM^3)

```
PROGRAM bench_dgemm
  IMPLICIT NONE
  INTEGER, PARAMETER :: dim = 8192
  REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
  ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
  y = 1.0d0 / ( DBLE( dim ) )
  z = 1.0d0 / ( DBLE( dim ) )
  x = 0.0d0
  t1 = cclock()
  call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
  t2 = cclock()
  [...]
  DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
PROGRAM bench_dgemm
  IMPLICIT NONE
  INTEGER, PARAMETER :: dim = 8192
  REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
  ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
  y = 1.0d0 / ( DBLE( dim ) )
  z = 1.0d0 / ( DBLE( dim ) )
  x = 0.0d0
  t1 = cclock()
  call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
  t2 = cclock()
  [...]
  DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
gcc -03 [...] ../LIBS/BLAS/blas_LINUX.a
```

```
PROGRAM bench_dgemm
  IMPLICIT NONE
  INTEGER, PARAMETER :: dim = 8192
  REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
  ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
  y = 1.0d0 / ( DBLE( dim ) )
  z = 1.0d0 / ( DBLE( dim ) )
  x = 0.0d0
  t1 = cclock()
  call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
  t2 = cclock()
  [...]
  DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
gcc -03 [...] -L/opt/intel/mkl/lib/intel64/ -lmkl_gf_lp64  -lmkl_gnu_thread -lmkl_core
```

```
PROGRAM bench_dgemm
 IMPLICIT NONE
 INTEGER, PARAMETER :: dim = 8192
 REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
 ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
 y = 1.0d0 / ( DBLE( dim ) )
 z = 1.0d0 / ( DBLE( dim ) )
 x = 0.0d0
 t1 = cclock()
 call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
 t2 = cclock()
 [...]
 DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
ifort -03 [...] -L/opt/intel/mkl/lib/intel64/ -lmkl_intel_lp64  -lmkl_intel_thread -lmkl_core
```

```
PROGRAM bench_dgemm
 IMPLICIT NONE
 INTEGER, PARAMETER :: dim = 8192
 REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
 ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
 y = 1.0d0 / ( DBLE( dim ) )
 z = 1.0d0 / ( DBLE( dim ) )
 x = 0.0d0
 t1 = cclock()
 call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
 t2 = cclock()
 [...]
 DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
ifort -03 [...] -L/opt/intel/mkl/lib/intel64/ -lmkl_intel_lp64  -lmkl_intel_thread -lmkl_core
gfortran -03 [...] -L${ACML_ROOT}/gfortran64/lib -lacml_mp
```

```
PROGRAM bench_dgemm
 IMPLICIT NONE
 INTEGER, PARAMETER :: dim = 8192
 REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
 ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
 y = 1.0d0 / ( DBLE( dim ) )
 z = 1.0d0 / ( DBLE( dim ) )
 x = 0.0d0
 t1 = cclock()
 call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
 t2 = cclock()
 [...]
 DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
ifort -03 -mmic [...] -L/opt/intel/mkl/lib/mic/ -lmkl_intel_lp64  -lmkl_intel_thread -lmkl_core
```

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```
PROGRAM bench_dgemm
  IMPLICIT NONE
  INTEGER, PARAMETER :: dim = 8192
  REAL*8, ALLOCATABLE :: x(:,:), y(:,:), z(:,:)
  ALLOCATE( x( dim, dim ), y( dim, dim ), z( dim, dim ) )
  y = 1.0d0 / ( DBLE( dim ) )
  z = 1.0d0 / ( DBLE( dim ) )
  x = 0.0d0
  t1 = cclock()
  call dgemm('N', 'N', dim, dim, dim, 1.0d0, y, dim, z, dim,  0.0d0, x, dim)
  t2 = cclock()
  [...]
  DEALLOCATE( x, y, z )
END PROGRAM bench_dgemm
```

```
nvcc -03  [...] -L${CUDA_HOME}/lib64/ -lcublas
```

CPU Architecture Benchmark /2

High Performance Linpack

HPC Challenge

Profiling

- Profiling usually means:
  - Instrumentation of code (e.g. during compilation)
  - Automated collection of timing data during execution
  - Analysis of collected data, breakdown by function
- Example:
  - `$gcc -o some_exe.x -pg some_code.c`
  - `$./some_exe.x`
  - `gprof some_exe.x gmon.out`
- Profiling is often incompatible with code optimization or can be misleading (inlining). But profiling DOES require to be performed with the production setting

PERF – Hardware Assisted Profiling

- Modern x86 CPUs contain performance monitor tools included in their hardware
- Linux kernel versions support this feature which allows for very low overhead profiling without instrumentation of binaries
- The perf command:
  - perf stat ./a.out -> profile summary
  - **perf record ./a.out; perf report**
  - **perf -h; perf [command] -h**

```
# gfortran -pg prog1.f ; ./a.out ; gprof --flat-profile ./a.out gmon.out

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
100.69      4.30     4.30    10000     0.00     0.00  xaver_
  0.00      4.30     0.00        1     0.00     4.30  MAIN__

# make CFLAGS=-pg mountain ; ./mountain ; gprof -p mountain gmon.out

  %   cumulative   self              self     total
 time   seconds   seconds    calls  ms/call  ms/call  name
 98.30      5.80     5.80     3206     1.81     1.81  test
  1.87      5.91     0.11        1   110.19   110.19  init_data
  0.00      5.91     0.00     2920     0.00     0.00  access_counter
  0.00      5.91     0.00     1460     0.00     0.00  get_counter
  0.00      5.91     0.00     1460     0.00     0.00  start_counter
  0.00      5.91     0.00     1459     0.00     0.00  add_sample
  0.00      5.91     0.00     1459     0.00     0.00  has_converged
  0.00      5.91     0.00      288     0.00    18.33  fcyc2
  0.00      5.91     0.00      288     0.00    18.33  fcyc2_full
[...]
```

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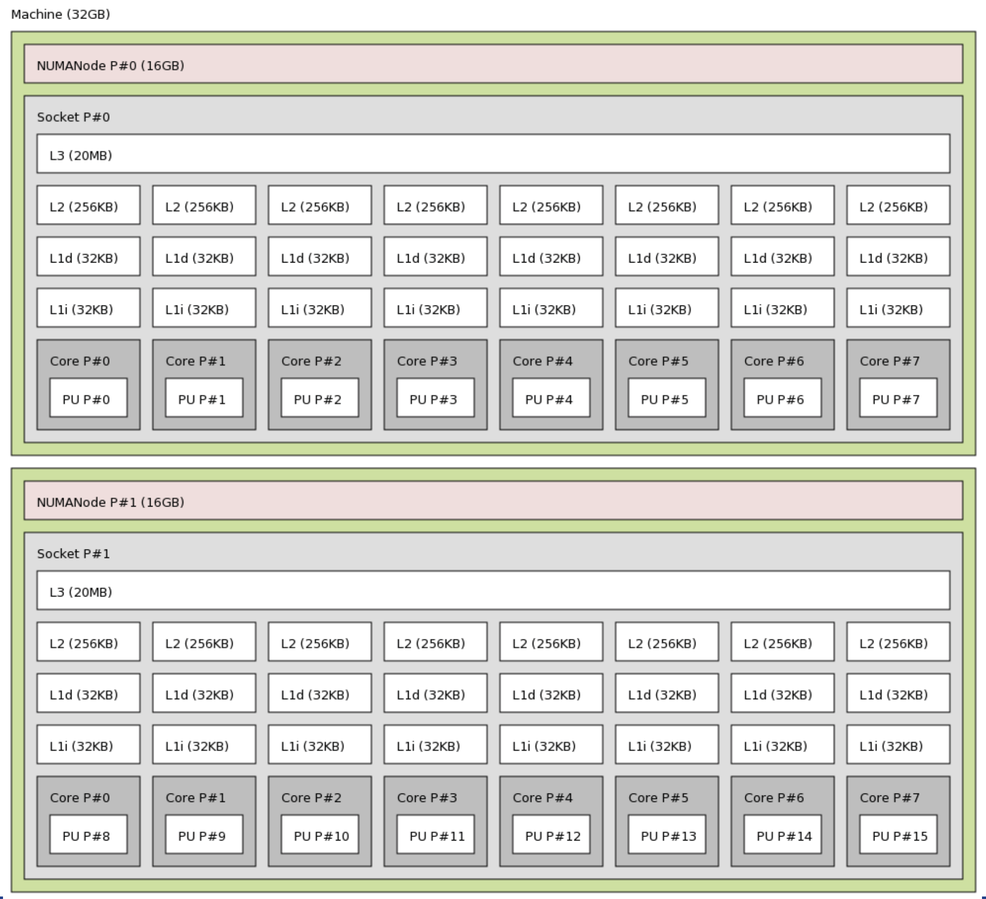
Hands-on

LAB-SESSION

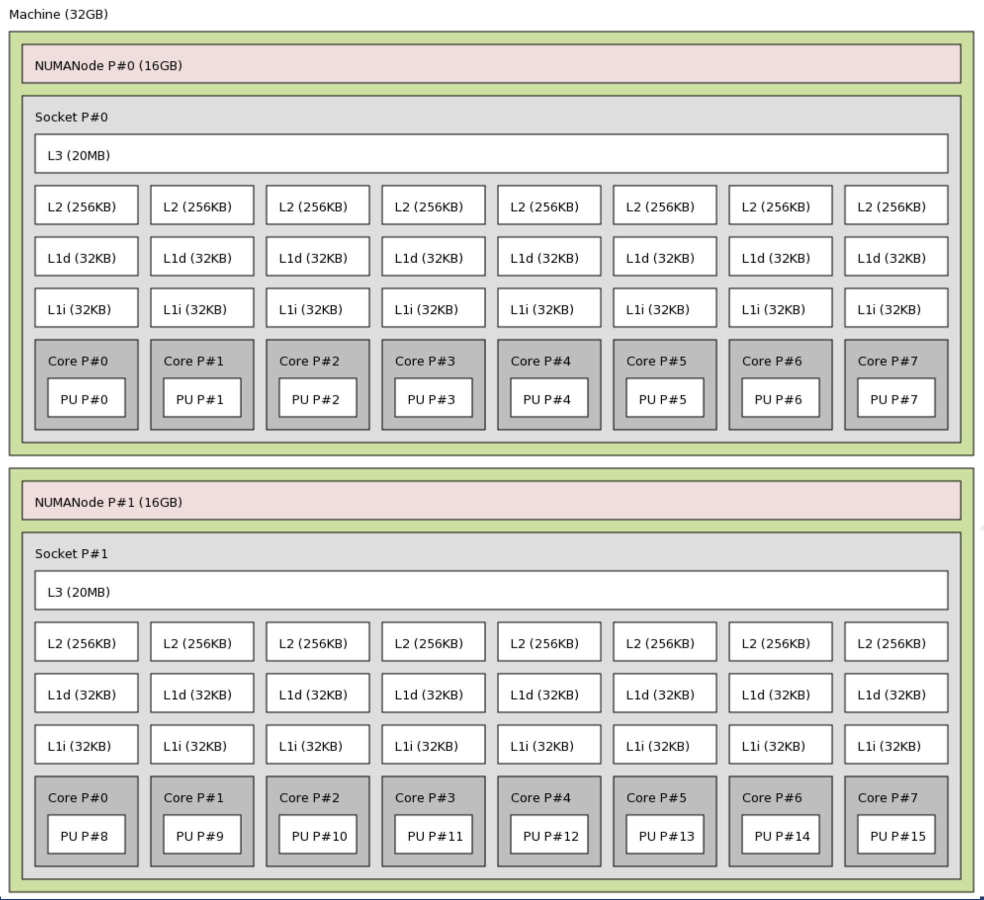
The Intel Xeon E5-2665 Sandy Bridge-EP 2.4GHz



cpu-only

The Intel Xeon E5-2665 Sandy Bridge-EP 2.4GHz

gpu


Machine (32GB)
NUMANode P#0 (16GB)
Socket P#0
L3 (20MB)
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Core P#0 PU P#0
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Core P#5 PU P#5
Core P#6 PU P#6
Core P#7 PU P#7
NUMANode P#1 (16GB)
Socket P#1
L3 (20MB)
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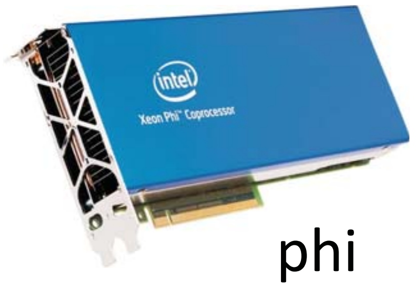
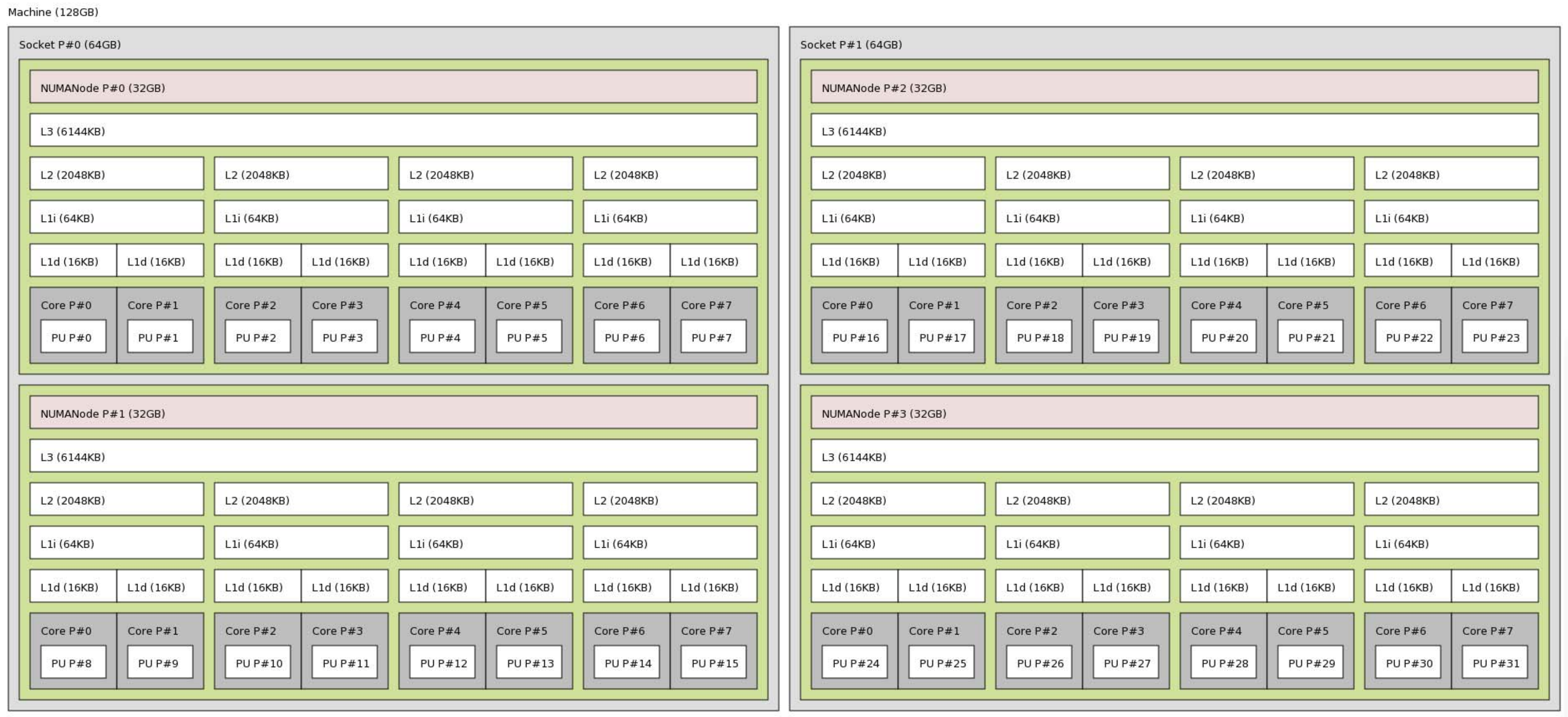
Core P#4 PU P#12
Core P#5 PU P#13
Core P#6 PU P#14
Core P#7 PU P#15



phi

The AMD Opteron 6380 Abu Dhabi 2.5GHz


Machine (128GB)
Socket P#0 (64GB)
NUMANode P#0 (32GB)
L3 (6144KB)
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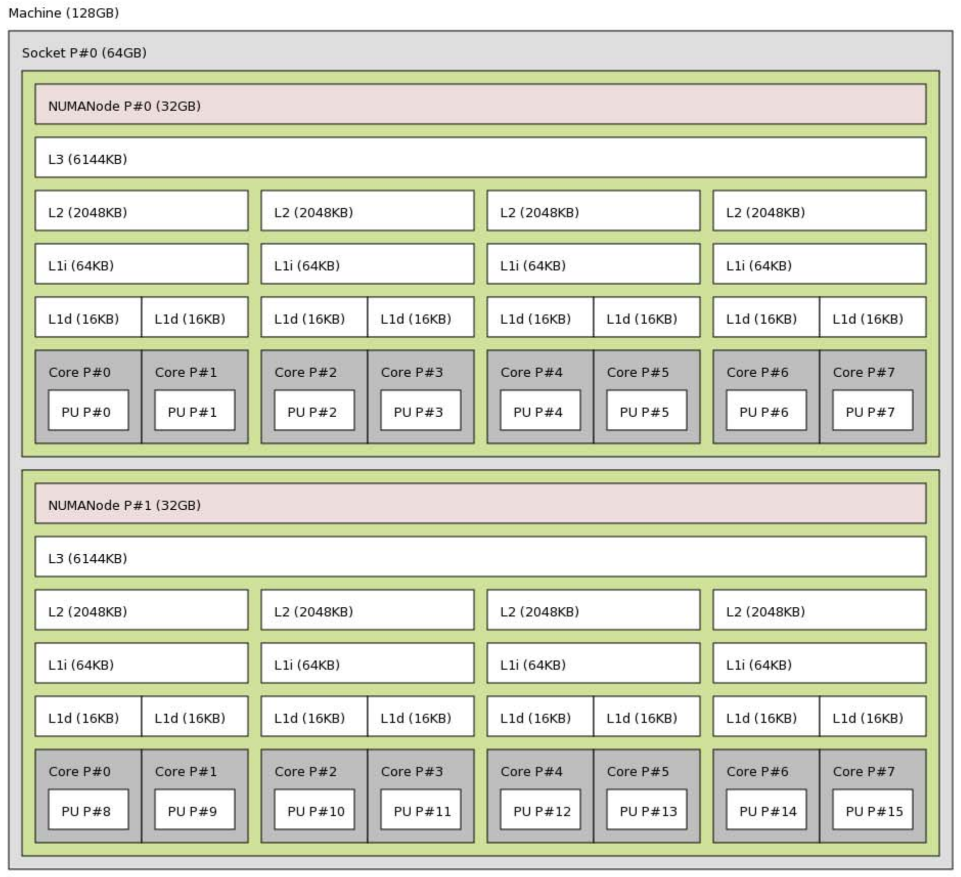
Core P#2 PU P#26
Core P#3 PU P#27
Core P#4 PU P#28
Core P#5 PU P#29
Core P#6 PU P#30
Core P#7 PU P#31

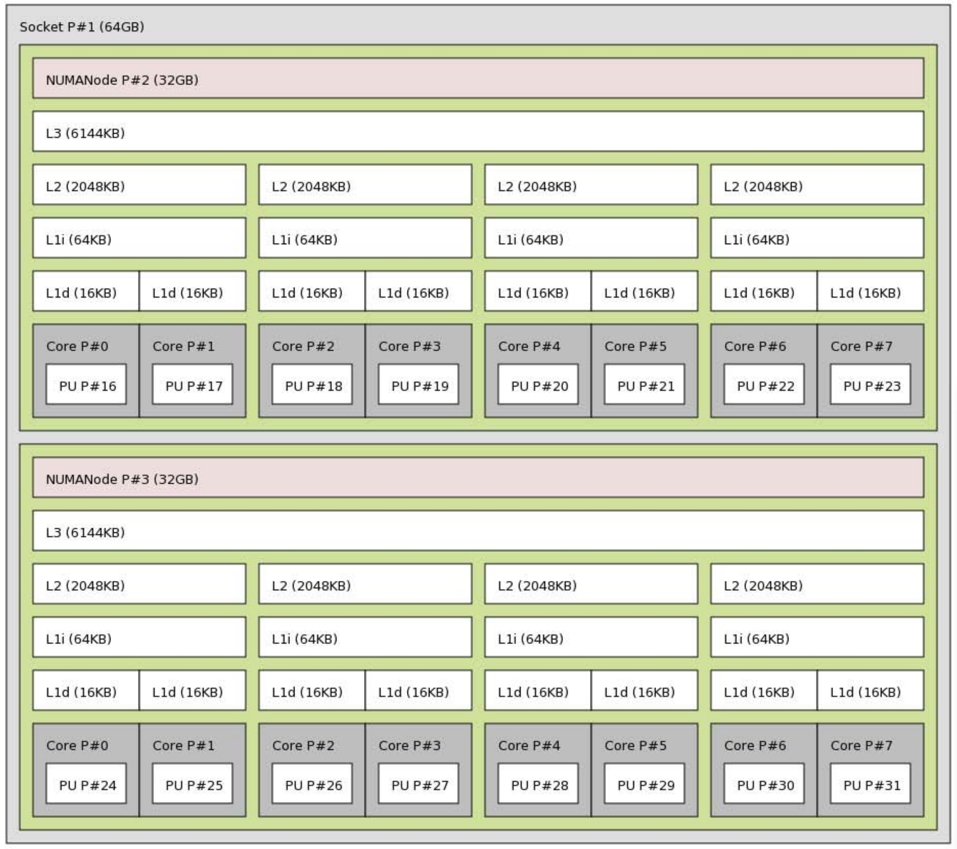
The AMD Opteron 6380 Abu Dhabi 2.5GHz



Socket #0 is used as Login Node

The AMD Opteron 6380 Abu Dhabi 2.5GHz

Socket #1 is used as Compute Node



ssh details

- AMD
  - ssh user[N]@94.82.133.184 -p 55566
- GPU-server
  - ssh user[N]@gpu-server
- password user[N] ... with N ∈ [1,24]

Exercises

1. Make a performance analysis using simple synthetic benchmarks (DGEMM, DAXPY) among the available architecture
2. Plot a scaling curve of the results obtained using DGEMM benchmark on multiple threads among the two computer architectures

Exercises Advanced /1

- Benchmark aggregate memory bandwidth using bench_mpi_daxpy.f90 measuring the scaling of the aggregate bandwidth at the increasing of the number of processes (use -D__MPI preprocessor macro)
- Perform a performance analysis using the pw.x binary of the Quantum-ESPRESSO package - application benchmark. Input provided in ex-lab/QE-Input on the gpu-server
  - mpiexec -np [N] ./pw.x -input input.it | tee output.out

Exercises Advanced /3

- Make a profiling analysis of either the provided synthetic benchmarks or an application benchmark at your choice.
- Use numactl or hwloc to map concurrent execution of processes among different cores. Analyze the increasing of cache-misses (perf command) while increasing the processes/ threads density

Exercises Advanced /4

- Run the benchmark on the INTEL PHI co-processors (no instructions template). See the list of links below:
  - Link1 (.pdf at the bottom of the page)
  - Native Compilation, Automatic Offload, Compiler Assisted Offload

Script Examples

- Interactive session:
  - qsub -I -q [queu] -l walltime=00:10:00 -l nodes=1:ppn=[cores_number_request]

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Best Results Obtained in Class

Benchmark	NVIDIA TITAN GPU	INTEL Xeon PHI	Xeon E5-2665 (2 - sockets)	Opteron 6380 (1 - socket)
DGEMM (GFlop/s)	1.1	766	164 (8 cores)	126 (8 cores)
			320 (16 cores)	104 (16 cores)
DAXPY (GByte/s)			12.8	7
MPI_DAXPY (GByte/s)			41	34

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Thanks for your attention!!