Adding MPI to OpenMP

Hybrid programming: MPI + X

MPI vs. OpenMP

- Pure MPI Pro:
  - Portable to distributed and shared memory machines
  - Scales beyond one node
  - No data placement problem
  - Explicit communication
- Pure MPI Con:
  - Difficult to develop and debug
  - High latency, low bandwidth (max PCI-x bus)
  - Large granularity
  - Difficult load balancing

- Pure OpenMP Pro:
  - Easy to implement parallelism
  - Low latency, high bandwidth (max memory bus)
  - Implicit Communication
  - Coarse and fine granularity
  - Dynamic load balancing
- Pure OpenMP Con:
  - Difficult to develop and debug
  - Only on shared memory machines
  - Scale within one node
  - Possible data placement problem (on NUMA architectures)
  - No specific thread order

Why hybrid programming ?

- Hybrid MPI+X paradigm is the software trend for dealing with complexities of hybrid hierarchical architectures (such as heterogeneous multi-core architectures prevalent nowadays).
- Elegant in concept and architecture: using MPI across nodes and OpenMP within nodes. Good usage of shared memory system resource (memory, latency, and bandwidth).
- Avoids the extra communication overhead with MPI within node. Reduce memory footprint.
- OpenMP adds fine granularity (larger message sizes) and allows increased and/or dynamic load balancing.
- Some problems have two-level parallelism naturally.
- Some problems could only use restricted number of MPI tasks.
- Possible better scalability than both pure MPI and pure OpenMP.

Example 1

```
int main(int argc, char* argv[]) {
  MPI_Init(NULL, NULL);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  #pragma omp parallel private(omp_rank)
  {
    omp_rank = omp_get_thread_num();
    printf(”Rank %d thread %d\n”, rank, omp_rank);
  }
  MPI_Finalize();
}
```

- What is the expected outcome ?

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Initializing MPI with thread support

- MPI_INIT_THREAD (required, &provided, ierr)
  - IN: required, desired level of thread support (integer).
  - OUT: provided, provided level of thread support (integer).
  - Beware: Returned provided maybe less than required.
- Thread support levels:
  - MPI_THREAD_SINGLE: Only one thread will execute.
  - MPI_THREAD_FUNNELED: Process may be multi-threaded, but only master thread will make MPI calls (all MPI calls are ’’funneled'' to master thread)
  - MPI_THREAD_SERIALIZED: Process may be multi-threaded, multiple threads may make MPI calls, but only one at a time: MPI calls are not made concurrently from two distinct threads (all MPI calls are ’’serialized'').
  - MPI_THREAD_MULTIPLE: Multiple threads may call MPI, with no restrictions.

MPI_THREAD_SINGLE < MPI_THREAD_FUNNELED < MPI_THREAD_SERIALIZED < MPI_THREAD_MULTIPLE

OMP MASTER calls MPI

- The OMP master thread is the thread that entered main
  - In some OSes it might have specific properties and behaviors (signals, pid, …)
- MPI_THREAD_FUNNELED is required
- Inside a parallel region there are no implicit synchronizations

```
#pragma omp parallel
for(i = 0; i < BIG_NUMBER; i++)
  buf[i] = I;

#pragma omp master
  MPI_Send(buf, …);
```

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- MPI_THREAD_FUNNELED is required
- Inside a parallel region there are no implicit synchronizations
  - An explicit barrier before the MPI call is needed to ensure correctness of the input data
  - An explicit barrier after the MPI call is needed to ensure correctness of the output data
  - It also implies that all the other threads are wasting time

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```

OMP SINGLE calls MPI

- The OMP single directive ensure the only one thread executes the corresponding block
- MPI_THREAD_SERIALIZED is required
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```
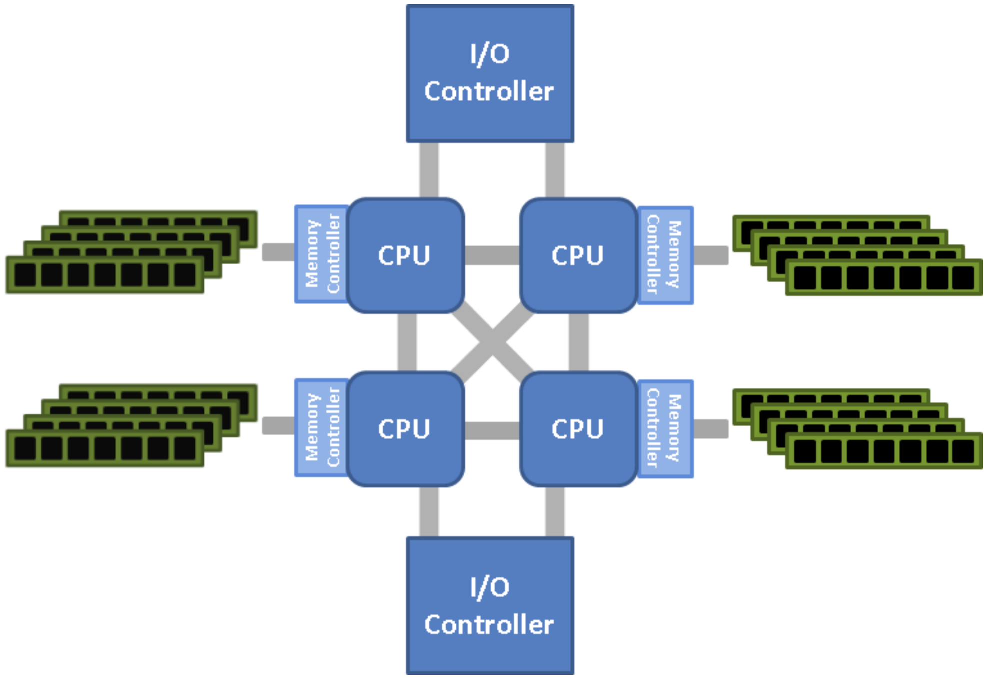

No pain, no gain

- Enforcing barriers limit the performance
- Removing the barriers depends on the algorithm and on the other implicit synchronizations between parts of the algorithm
  - When was the data updated ? Outside the parallel section ?
  - When will be the data used ? Outside this parallel section ?
- Without the barrier automatic overlap between computations and communications become automatic

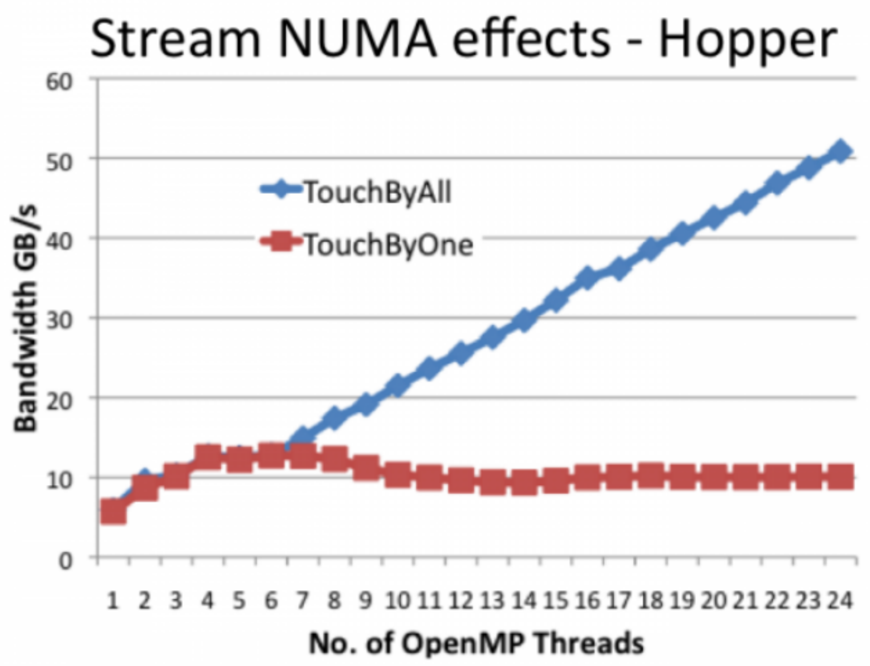
A word (or two) about affinity

- Single threaded MPI applications rarely raise affinity issues
- Unleashing multiple threads in the context of the same application is a different topic:
  - Thread affinity: floating vs. bound
    - Memory issues
  - Memory affinity: allocate memory as close as possible to the core that will use it most
    - Affinity is not decided during the allocation
    - The default policy is ”first touch”
- Each MPI library has it’s own affinity settings (read the man/documentation…)



More words about affinity

- Performance with and without correct data initialization
- HWLOC is the tool to use !



Courtesy Hongzhang Shan

```
#pragma omp parallel for
for( i = 0; i < MANY; i++) {
  a[i] = 1.0; b[i] = 2.0; c[i] = 0 }

#pragma omp parallel for
For( i = 0; i < MANY; i++ ) {
  c[i] = a[i] * b[i];
}
```

Hybrid Parallelization steps

- From sequential code, decompose with MPI first, then add OpenMP
- From OpenMP code, treat as serial code.
- From MPI code, add OpenMP.
- Simplest and least error-prone way is to use MPI outside parallel region, and allow only master thread to communicate between MPI tasks. MPI_THREAD_FUNNELED is usually the best choice.
  - Keep in mind the cost and implications of serializations
- Could use MPI inside parallel region with thread-safe MPI.
- MPI_THREAD_MULTIPLE comes with a performance cost. Inside the MPI library, thread synchronizations might be necessary, and this might show on the overheads of the MPI calls.