Re-designing Communication and Work Distribution in Scientific Applications for Extreme-scale Heterogeneous Systems

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Drivers of Modern HPC System Architectures

- Multi-core processors are ubiquitous
- Modern interconnects have high performance features such as RDMA and support for collectives
- Accelerators/Coprocessors becoming common in high-end systems
- Pushing the envelope for Exascale computing

Multi-core Processors | High Performance Interconnects | Accelerators / Coprocessors

- High compute density, high performance/watt >1 TFlop DP on a chip

Tianhe – 2 (1) | Titan (2) | Stampede (6) | Blue Waters
Challenges for Communication Runtimes

• Complex Architecture
  – Within a node
    • Accelerators connected via PCIe,
    • NUMA shared memory
  – Interconnect feature and topology consideration

• Scaling
  – Current algorithms developed and tested with 100s to 1000s of processes
  – few systems on which to run with 10,000s to 100,000s
Parallel Programming Models Overview

- Programming models provide abstract machine models
- Models can be mapped on different types of systems
  - e.g. Distributed Shared Memory (DSM), MPI within a node, etc.
- Many Core models
  - OpenMP, OpenACC, CUDA
Key Questions

• How do MPI collectives perform at extreme scales?
• How well do the CraySHMEM and UPC PGAS collective communications scale?
• Can both the CPU and GPU resources be leveraged effectively in a hybrid node system?
MPI on Blue Waters

- Domain applications such as weather forecasting, earthquake simulations, and many more have a real requirement for large throughput capability.
- MPI is the most dominant programming model for distributed memory systems.
- MPI jobs in order of 1K processes becoming common.
- MPI jobs in order of 1M processes is the maximum.
- Blue Waters is one of the first instances that can be used to test performance of MPI jobs at a really large scale.
Blue Waters MPI Collective Performance

• Point-to-point operations and Collective operations determine the performance of MPI programs
• Performance of point-to-point operations involve
  – Efficient utilization of underlying interconnection hardware
  – Design of high performance protocols
• Performance of collectives additionally involves
  – Design of efficient algorithms
• We evaluate performance of common collectives such as:
  – MPI_Bcast
  – MPI_Reduce
  – MPI_Allgather
Performance of MPI_Bcast (64 – 512 Processes)

- Latency is flat in the 1 byte – 32 byte range and then starts climbing – regardless of process count
- Latency of broadcast more than doubles in the short message range going from 128 processes to 256 processes which is undesirable
Performance of MPI_Bcast (1K – 8K Processes)

- For a process count over 1K, there is a spike in latency at the 256 byte range where bandwidth available starts getting stressed.
Performance of MPI_Bcast (16K – 128K Processes)

- Unlike the 64 – 8K process count there is variability – possible traffic effect
- The spike at 8K message range is indicative of algorithm selection problem
Performance of MPI_Reduce (64 – 512 Processes)

- Reduce latency is hardware accelerated and regardless of process count the latency is similar.
- There does seem to be a limitation with hardware acceleration at 128K byte range.
Performance of MPI_Reduce (1K – 8K Processes)

- Trends similar to smaller process count
Performance of MPI_Reduce (16K – 128K Processes)

- Notable increase in latency for 128K processes in the short message range
Scalability of MPI_Bcast and MPI_Reduce

- Scalability normalized to 64 process job case
- MPI_Reduce is highly scalable
- MPI_Bcast is not as scalable
Performance of MPI_Allgather (128K Processes)

• Allgather is equivalent to all processes performing broadcasts
• Bandwidth of the interconnection is tested
• Traditionally order of log (N) algorithms applicable to short message allgathers
• The above graph raises an alarm of latency growth for large scale dense collectives
Observations on MPI Collective Performance

• Performance of latency sensitive operations such as Reduce is competitive in the operational range with increasing scale

• Congestion effects, cross job traffic likely to play a role in performance of collectives as job sizes get larger (as seen in the 128K jobs)

• Performance of dense collectives like Allgather suffer from bandwidth limitations =>
  – Applications should perform such collectives in smaller communicators or using non-blocking variant of the collectives
  – Better algorithms need to be devised to overcome bandwidth limitations
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Partitioned Global Address Space (PGAS) programming models getting more traction

- Shared memory abstraction over distributed nodes
- Global view of data and one-sided communication calls
- Provides improved productivity
- Can express irregular communication patterns easily

Unified Parallel C (UPC) – a language based PGAS model

SHMEM – a library based model

Blue Waters provides a good platform to evaluate performance of UPC/SHMEM jobs at scale
Blue Waters UPC Performance Evaluations

- Point-to-point operations and Collective operations determine the performance of UPC programs
- Used Cray UPC and OSU UPC Microbenchmarks for evaluations
- Performance of point-to-point operations involve
  - upc_memput
  - upc_memget
- Performance of collectives additionally involves
  - upc_barrier
  - upc_broadcast
  - upc_reduce
Latency is flat in the 1 byte – 512 byte range and then starts climbing

- Latency for UPC Put (intra/inter) for 4 byte message: 0.13/2.34 us
- Latency for UPC Get (intra/inter) for 4 byte message: 0.07/1.17 us

Higher costs for Put operation might be because of the extra synchronization operation (upc_fence) for ensuring completion
UPC Barrier Performance

- Barrier Operation Latency at 32,768 process – **186us**
- Scalability graph shows the latency normalized to that at 1,024 processes
- Linear scalability observed for smaller system sizes
UPC Broadcast Performance

- Broadcast Latency for a 4byte message at 32,768 processes – **13us**
- Variation in latencies observed after 8192 processes, and the variation increases with scale
- Broadcast latency does not scale linearly with increase in system size
UPC Reduce Performance

- Reduce Latency for 4 byte message at 32,768 processes – **5.4us**
- Linear scalability observed for small message range
- Variation in operation latency observed as the system size increases
Blue Waters CraySHMEM Performance Evaluations

• Point-to-point operations and Collective operations determine the performance of SHMEM programs
• Used CraySHMEM library and OSU OpenSHMEM Microbenchmarks for evaluations
• Performance of point-to-point operations involve
  – shmem_put
  – shmem_get
• Performance of collectives additionally involves
  – shmem_barrier
  – shmem_broadcast
  – shmem_reduce
  – shmem_collect
CraySHMEM Put/Get Performance

- Latency is flat in the 1 byte – 512 byte range and then starts climbing after 1K bytes
  - Latency for 4byte Put operation (intra/inter) – 0.12/1.04 us
  - Latency for 4byte Get operation (intra/inter) – 0.05/1.41 us
- Significantly higher latency observed for get operation, with increase in message size
  - Get Latency for 512K message – 763 us
CraySHMEM Barrier Performance

- Barrier Latency at 16,384 processes – **138.64 us**
- Similar latencies as that of UPC barrier
- Shows good scalability trends with increase in system size
CraySHMEM Broadcast Performance

- Latency is flat in the 1 byte – 512 byte range and then starts climbing – regardless of process count
- Broadcast Latency for 4-byte message at 16,384 processes – 72.3us
- Variation in latencies observed with increase in system size
CraySHMEM Reduce Performance

- Latency for 4-byte message at 16K processes – **210 us**
- Scalability analysis shows good scalability trends with even higher system sizes as well
- Latencies smaller compared to UPC reduce operation – extra synchronization operations in UPC collective operations
CraySHMEM Collect Performance

- Latency for 4byte collect (all-gather) operation at 16K processes – 319.3 ms
- Scalability analysis shows collect operation scales well
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Current Execution of HPL on Heterogeneous GPU Clusters

- HPL (High Performance Linpack)
  Benchmark for ranking supercomputers in the top500 list

- Current HPL support for GPU Clusters
  - Heterogeneity inside a node CPU+GPU
  - Homogeneity across nodes

- Current HPL execution on heterogeneous GPU Clusters
  - Only CPU nodes (using all the CPU cores)
  - Only GPU nodes (using CPU+GPU on only GPU nodes)
  - As the ratio CPU/GPU is higher => report the “Only CPU” runs

- Hybrid HPL support for heterogeneous systems
  - Heterogeneity inside a node (CPU+GPU)
  - Heterogeneity across nodes (nodes w/o GPUs)

R. Shi, S. Potluri, K. Hamidouche, X. Lu, K. Tomko and D. K. Panda, A Scalable and Portable Approach to Accelerate Hybrid HPL on Heterogeneous CPU-GPU Clusters, IEEE Cluster (Cluster '13), Best Student Paper Award
Two Level Workload Partitioning: Inter-node

- **Inter-node Static Partitioning**
  
  Original design: uniform distribution, bottleneck on CPU nodes
  
  New design: identical block size, schedules more MPI processes on GPU nodes
  
  \[
  \text{MPI}_{\text{GPU}} = \frac{\text{ACTUAL\_PEAK\_GPU}}{\text{ACTUAL\_PEAK\_CPU}} + \beta
  \]
  
  \((\text{NUM\_CPU\_CORES} \mod \text{MPI}_{\text{GPU}} = 0)\)

  Evenly split the cores
Two Level Workload Partitioning: Intra-node

- **Intra-node Dynamic Partitioning**
  - MPI-to-Device Mapping
    - Original design: 1:1
    - New design: M: N (M > N), N= number of GPUs/Node, M= number of MPI processes
  - Initial Split Ratio Tuning: alpha = \( \frac{\text{GPU}_\text{LEN}}{\text{GPU}_\text{LEN} + \text{CPU}_\text{LEN}} \)
    - Fewer CPU cores per MPI processes
    - Overhead caused by scheduling multiple MPI processes on GPU nodes
Performance Tuning of Single CPU Node and GPU Node

Netlib-CPU: Standard HPL version from Netlib (UTK)
Hybrid-CPU: Hybrid HPL version with OpenMP support
NVIDIA-GPU: NVIDIA’s HPL version
* OpenBLAS Math Library is used

Peak Performance Scaling on Single CPU/GPU Node

- Netlib-CPU
- Hybrid-CPU
- NVIDIA-GPU

Performance (Gflops) vs. Problem Size N
Peak Performance Scaling of Pure CPU/GPU Nodes

Measure the peak performance of either pure CPU Nodes or pure GPU Nodes (1, 2, 4, 8, 16)
Strong and Weak Scalability of Hybrid CPU+GPU Nodes

Using Hybrid-HPL to measure the scalability with 4 GPU Nodes + (4, 8, 12, 16) CPU Nodes
Launch 1 MPI process / CPU node; 1, 2 or 4 MPI processes / GPU node
Strong Scalability: fixed problem size N for each combination of CPUs+GPUs (e.g. N=100,000 for 4 GPUs + 4 CPUs)
Weak Scalability: fixed memory usage (~40%) on GPU nodes for all cases

Strong Scalability

Weak Scalability
Peak Performance of Hybrid CPU Nodes + GPU Nodes

Measure the peak performance of 64 CPU Nodes and 16 GPU Nodes
Launch 1 MPI process / CPU node, and 4 MPI processes / GPU node

<table>
<thead>
<tr>
<th>Node Configuration</th>
<th>Peak Performance (Gflops)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 GPUs</td>
<td>6,480</td>
</tr>
<tr>
<td>64 CPUs</td>
<td>13,210</td>
</tr>
<tr>
<td>16 GPUs + 64 CPUs</td>
<td>14,520</td>
</tr>
</tbody>
</table>

Peak Performance Efficiency (Hybrid-HPL)
Peak Perf. of hybrid Nodes / (Peak Perf. of CPUs + Peak Perf. of GPUs)
(e.g. 14,520 / (6,480 + 13,210) = 73.7 %)
Conclusion

- The Blue Waters system provides unique opportunities
  - Communications at large scale
  - Hybrid system with XE6 and XK7 nodes

- MPI collectives study on up to 128K processes
  - Latency sensitive collectives such as reduce perform well
  - Bandwidth limitations impact dense collectives such as Allgather

- UPC and SHMEM communications study up 32K and 16K cores respectively
  - UPC and SHMEM point-to-point performance is good
  - Some collectives (UPC Scatter, SHMEM Broadcast) scale well, for others (SHMEM collect) we observed high latencies
Conclusions (continued)

- Hybrid HPL
  - Peak single CPU node performance 202 Gflops/sec
  - Peak GPU node performance 670 Gflops/sec
  - Performance efficiency of hybrid HPL compared to the sum of pure CPU and GPU nodes, above 70% efficiency with 16 GPU nodes and 64 CPU nodes.

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