A preliminary evaluation of the hardware acceleration of the Cray Gemini Interconnect for PGAS languages and comparison with MPI

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ABSTRACT

The Gemini interconnect on the Cray XE6 platform provides for lightweight remote direct memory access (RDMA) between nodes, which is useful for implementing partitioned global address space languages like UPC and Co-Array Fortran. In this paper, we perform a study of Gemini performance using a set of communication microbenchmarks and compare the performance of one-sided communication in PGAS languages with two-sided MPI. Our results demonstrate the performance benefits of the PGAS model on Gemini hardware, showing in what circumstances and by how much one-sided communication outperforms two-sided in terms of messaging rate, aggregate bandwidth, and computation and communication overlap capability. For example, for 8-byte and 2KB messages the one-sided messaging rate is 5 and 10 times greater respectively than the two-sided one. The study also reveals important information about how to optimize one-sided Gemini communication.

Keywords

PGAS, CAF, UPC, MPI, Gemini, Hardware Acceleration, Performance, Message Rate, Overlap

1. INTRODUCTION

The classic parallel programming model, MPI, faces several new challenges on petaflop computing platforms, which are dominated by multicore-node architectures [9, 21]. To address these challenges, researchers are starting to investigate other programming models to understand whether they could replace or used in combination with MPI. Among these studied programming models, the Partitioned Global Address Space (PGAS) family of languages, represented by Co-Array Fortran (CAF) [16] and Unified Parallel C (UPC) [5], show great promise as the near-term alternative to MPI. Compared with MPI, a big difference is that PGAS provides a global shared address space while controlling locality. This is designed to simplify programming as with this global shared space abstraction PGAS languages allow the ability to directly build distributed data structures that can be accessed throughout the machine. By integrating communication and synchronization into the language itself, PGAS languages allow the compiler or runtime system to distribute and schedule remote memory accesses in an optimal manner

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without the need for maintaining a global, uniform access view of memory on a distributed memory system [1].

Both CAF and UPC have been around for a decade or so. However these two languages still have not been widely adopted by user community; partly because of the lack of a developer environment, and partly because not enough convincing performance results have been presented to demonstrate they are superior and viable alternatives to the MPI programming model.

Hopper is a 1.28 PF peak Cray XE6 computing platform recently installed at NERSC. The defining feature of this platform is the custom interconnect, called Gemini, which provides a hardware accelerated global address space and allows remote direct memory access (RDMA) from any node to any other in the system. In this work, we will investigate what the effect of this special Gemini hardware support for global address space and one-sided messaging is upon the performance of the PGAS languages. We compare whether PGAS languages can outperform MPI, with an aim to determining if PGAS is a superior and viable alternative to MPI and under which circumstances.

The principle contributions of this paper are

- We translated several popular MPI benchmarks into PGAS languages to measure network bandwidth and messaging rate and facilitate comparisons. Our results show that in the bandwidth limit, with large messages, MPI and PGAS performance is identical. For mediumsized and small messages, the lower overhead of the single-sided PGAS messages allows greater effective bandwidths to be achieved.
- We developed an independent micro-benchmark to measure the capability to overlap computation and communication for PGAS languages and MPI. Our results show that with large messages almost complete overlap of computation and communication is possible with PGAS languages using Gemini whereas with MPI this is currently not possible.
- We translated the NAS FT benchmark into Co-Array Fortran and achieved up to $2.8 \times$ the performance of the original MPI version on 16K cores.

The paper is organized as follows. Related work is discussed in Section 2. Section 3 describes the experimental platforms. The messaging rate is examined in Section 4. As the number of cores on the future supercomputing platforms increases rapidly, the average message size will become smaller, therefore overall performance will become more sensitive to the performance of fine-grain communication thus the throughput of small messages is carefully studied in this section. Section 5 examines the capability of PGAS and MPI to overlap computation and communication. In Section 6, we compare the performance differences of an MPI and a CAF version of the NAS FT benchmark. Finally, we summarize our conclusions and future work in Section 7.

2. RELATED WORK

The related work can be divided into two categories based on the programming models used: CAF and UPC. For CAF, Mellor-Crummey et al. have proposed Co-array Fortran 2.0 [11]. The applications they studied include MG, CG, BT, and SP from the NAS parallel benchmark suite and the Sweep3D neutron transport benchmark. The codes have been tested on several small clusters which consist of different processors and networks. The CAF programs show nearly equal or slightly better performance than their MPI counterparts [6, 7]. Barrett [3] studied different Co-array Fortran implementations of Finite Differencing Methods on Cray X1 and found that CAF exhibits better performance for smaller grid sizes and similar results for larger ones. Bala [2] demonstrated performance improvements over et al. MPI in a molecular dynamics application on a legacy HPC platform (Cray T3E). In addition, parallel linear algebra kernels for tensors [15] and matrices [18] benefit from a Coarray based one-sided communication model due to a raised level of abstraction with little or no loss of performance over MPL.

Comparing the performance of UPC and MPI have been the subject of many papers [8, 4, 10, 19, 13]. El-Ghazawi and Cantonnet [8] discussed UPC performance and potential advantage using NPB applications. With proper hand tuning and optimized collective libraries, UPC delivered comparable performance to MPI. Shan [19] and Jin [10] also compared the performance of NPB on several different platforms and similar conclusions were drawn. Nishtala and other researchers [13, 4] discussed the scaling behavior and better performance of NAS FT for UPC on several different platforms using the Berkeley UPC compiler with GASNET communication system.

The principle difference of our study is that it is performed on a platform with the Cray Gemini interconnect which provides hardware acceleration for one-sided communication, which is advantageous for the performance of PGAS languages. In this study, we examine how this special hardware support affects the performance of PGAS languages as compared to MPI.

3. EXPERIMENTAL PLATFORM

3.1 Hopper

A majority of our work has been performed on a Cray XE6 platform, called Hopper, which is located at NERSC and consists of 6,384 dual-socket nodes each with 32GB of memory. Each socket within a node contains an AMD "Magny-Cours" processor at 2.1 GHz with 12 cores. Each Magny-Cours package is itself a MCM (Multi-Chip Module) containing two hex-core dies connected via hyper-transport.

Each die has its own memory controller that is connected to two 4-GB DIMMS. This means each node can effectively be viewed as having four chips and there are large potential performance penalties for crossing the NUMA domains. Every pair of nodes is connected via hypertransport to a Cray Gemini network chip, which collectively form a 17x8x24 3-D torus. In this work we used the Cray compiler version 7.4.0 which provides support for Co-Array Fortran (CAF) and Unified Parallel C (UPC).

3.1.1 Gemini

The defining feature of the Cray XE6 architecture is the Gemini interconnect, which provides a global address space. There are two mechanisms to transfer the internode messages using one-sided communication with Gemini. The first uses Fast Memory Access (FMA) and the second uses the Block Transfer Engine (BTE). The FMA transport mechanism involves the CPU, has low latency and more than one transfer can be active at the same time. Transfers using the BTE are performed by the Gemini network chip, asynchronously with CPU so that the communication and computation can overlap. In general, FMA is used to transfer short messages and BTE for long messages. The point at which this transition occurs is controlled by the environment variable MPICH_GNI_RDMA_THRESHOLD for MPI and by PGAS_OFFLOAD_THRESHOLD for PGAS languages. All the results shown here using two nodes are for two nodes connected to different Gemini's, unless otherwise mentioned.

3.2 Franklin

For comparison purposes, we also performed some of the tests on a Cray XT4 platform, called Franklin, which is also located at NERSC. Each node consists of a quad-core AMD Budapest 2.3GHz processor and 8 GB DDR3 800 MHz memory. The nodes are connected through a proprietary SeaStar2 interconnect which is designed to optimize MPI performance by handling the handshaking protocol needed by MPI. As with Hopper the interconnect is a 3D-torus but in this case each node represents a distinct point on the torus.

4. MESSAGING RATE

Messaging rate is an important performance metric for measuring the viability of the interconnects on HPC platforms, especially for PGAS programming languages [20]. Also, as we look towards exascale architectures, where because of memory constraints problems are likely to be strongscaled, messaging rate is likely to become a more and more important performance metric.

4.1 Implementation

The MPI version is obtained from OSU Micro benchmark suite [12] and slightly changed to use a different buffer for each iteration. In the MPI version, a process sends a series of same size messages to its partner using nonblocking MPI_Isend. The number of messages in is determined by a variable called "window size" and our experiments show that setting the window size to 64 is large enough to achieve converged performance. After the partner has received all the messages, it will send an acknowledgement back to the sender. In the CAF implementation, the nonblocking MPI_Isend is substituted by a loop with direct load/store assignment (corresponding to one-sided put operation). However for each loop iteration the starting address is incremented by one so that the data sent is not contiguous between loop iterations. This prevents the compiler collapsing the loop into one put. In order to ensure that non-blocking communication was used the delayed synchronization compiler directive pgas defer_sync was used. Then, at the end, a synchronization is called to ensure all data have been received.

4.2 Performance

The codes are executed using two sets of processes, one on each node. The messaging rate between two nodes using 1, 6, and 24 communicating pairs per node for CAF and MPI are shown in Fig. 1 and 2 respectively. (The two nodes have a 1-hop network distance.) For small messages, MPI achieves the best performance when 6 pairs are used, a rate of 9 million messages per second. Using 24 pairs, the message rate drops slightly. ¹ On the contrary, the message rates of CAF for small messages increase steadily with the number of communicating pairs used. The best performance is obtained when 24 pairs are used, which is about 4.7 times better than the best MPI message rate. CAF clearly shows much better scalability for small messages.

We also measured the messaging rate using get instead of put for CAF. In the bandwidth limit, as one might expect, the get and put performance is identical. However, for small messages put performs significantly better than get. The messaging rates with 8-byte messages are 1.46, 1.64, and $3.46 \times$ greater than get using one, six, and 24 pairs respectively.



Figure 1: The messaging rate for MPI using 1, 6, and 24 pairs per node.

The corresponding bandwidths for the message rates shown in Fig. 1 and 2 are shown in Fig. 3. The CAF performance increases much faster with increasing message size. The main performance difference between CAF and MPI occurs for message sizes in the middle of the range where the benefits of single-sided messaging are mostly strongly felt. For a 512 byte message, using 24 pairs, the CAF performance has reached 4.75 GB/s, which is much higher than the corresponding MPI bandwidth of 2.4 GB/s. This result indicates that for PGAS languages, by using more frequent medium-sized messages instead of the large bulk transfers favored by explicit message passing, better performance can



Figure 2: The messaging rate for CAF using 1, 6, and 24 pairs per node.



Figure 3: The corresponding bandwidth of MPI and CAF for message rates in Fig. 1 and 2.

be achieved due to increased messaging rate and less network contention. This is in agreement with a recent study of the GTS fusion application on a Cray XE6 [17].

For very small messages aggregation is still necessary. As shown in Fig. 2, the messaging rate for 8-byte and 16-byte messages is very close, thus using 16-byte messages will achieve almost double the bandwidth of 8-byte messages. Even so, because of the increased messaging rate, in the latency limit the PGAS effective bandwidth for 8-bytes messages is about $4.5 \times$ the MPI one.

As the message size increases there is a performance drop for MPI when the message size reaches 1KB. This is the threshold value for switching from using FMA to using the BTE for transferring internode MPI message data. The startup cost for the BTE is the reason for the sudden performance drop, which cannot be amortized well for such small message sizes.

There is also a performance drop for CAF when the message size reaches 4096 bytes, which is the threshold in CAF to switch from the FMA mechanism to using the BTE. We also note that as more communicating pairs are used, the phenomenon becomes more explicit, which is simply because the BTE processes requests through the kernel and therefore sequentially which means the startup cost will be accumulated as more communicating pairs are used.

Using one pair the highest bandwidth for CAF is around 6GB/s, which is close to the peak injection bandwidth to the Gemini interconnect from a node. Using 24 pairs this is reduced to around 5 GB/s, presumably because of contention for resources. The highest bandwidth for MPI is achieved using 1 pair and is a little lower than the CAF result, around 5.5GB/s.

¹Note that in order to achieve this result with 24 pairs the environment variable MPICH_GNI_MBOX_PLACEMENT was changed to "nic". With it set to the default value the performance for 24 pairs is approximately equal to that for one pair.

4.3 Performance on Cray XT4 with SeaStar Interconnect

In order to better understand the performance benefits of the Gemini interconnect for PGAS languages, we examined the message rates on Franklin, a Cray XT4 platform, with a custom SeaStar interconnect. The SeaStar interconnect does not support a global shared address space. Instead it was designed to optimize the MPI performance, managing the handshaking protocol.



Figure 4: The message rates for MPI and CAF on XT4 for 1 and 4 pairs communicating per node.



Figure 5: The bandwidth corresponding to the Message Rate Measurements for MPI and CAF on XT4 for one and four communicating pairs per node.

The XT4 messaging rates for MPI and CAF for one and four pairs over two nodes are shown in Fig. 4 and the corresponding aggregate bandwidths are displayed in Fig. 5. For large messages, both MPI and CAF deliver very similar performance and the network can be saturated easily by using 1 pair only. For the smallest messages, especially 8 and 16 bytes, contrary to the Hopper results, MPI performs much better than CAF. Across all the rest of the message size range the differences in performance between MPI and CAF are less significant, and the noticeable differences that were present for Gemini are not longer present, due to the absence of hardware acceleration for one-sided messaging.

The absolute message rate of CAF and MPI for 8 bytes and 2M bytes messages on SeaStar and Gemini Interconnects are shown in Table 1. They are measured using 1 communication pair. For 8-byte messages, on SeaStar, it's the MPI that achieves the best performance while on Gemini, it's CAF. From SeaStar to Gemini, the MPI perfor-



Figure 6: Ratio of the CAF performance to the MPI for the Gemini (XE6) and SeaStar (XT4) based machines.



Figure 7: Ratio of the Gemini (XE6) to SeaStar (XT4) performance for CAF and MPI.

mance has been improved about 6 times while the CAF performance have been increased over 40 times. The results clearly demonstrated the critical importance of the hardware support to programming models and languages. For 2MB messages, the performance will be bound by the network bandwidth. On SeaStar, both MPI and CAF deliver similar performance while on Gemini, CAF performs slightly better. As one might expect in the bandwidth limit the importance of the hardware support is diminished.

The performance differences between the XE6 and XT4 are shown in figures 6 and 7. Fig. 6 shows the ratio of the CAF to MPI performance for the two systems as a function of message size and illustrates the benefits of the hardware acceleration for PGAS. In the best case, for 1024 byte messages, CAF is almost 10 times faster than MPI on the XE6, whereas on the XT4 CAF is never faster. Fig.7 shows the Gemini/Seastar (XE6/XT4)performance ratio for CAF and MPI. Apart from the fluctuations in the performance caused by the change in protocol the MPI performance ratio is always significantly less than the CAF one. For both machines, the performance differences between MPI and CAF are not present in the bandwidth limit.

5. COMPUTATION AND COMMUNICATION OVERLAP

One important technique to tolerate the cost of communication is to overlap it with local computation. To measure the overlap capability of different programming models using Gemini, a synthetic micro-benchmark has been developed.

Table 1: The message rate for 8B and 2MB messages using 1 pair on SeaStar and Gemini Interconnects

			SeaSta	r		Gemini	Gemini/SeaStar		
		CAF	MPI	CAF/MPI	CAF	MPI	CAF/MPI	CAF	MPI
Γ	8B	86,347	325,053	0.27	3,625,000	1,903,663	1.90	41.98	5.86
L	2MB	846	847	1.00	3,074	2,812	1.09	3.63	3.32

5.1 Implementation

The micro benchmark has two input parameters, one is the communication message size (S), another is the time ratio of computation to communication (R). The communication time is first measured based on the input message size and is used to determine the loop length of the computational kernel

for (i = 0; i < Length; i++) {
temp += buf1[i] * buf2[i] }</pre>

so that Computation Time = Ratio * Communication Time.

The arrays used for the communication kernel and the arrays used for the computation kernel are independent. Therefore, ideally, the computation and communication can be completely overlapped. The MPI version uses the nonblocking MPI_Isend, MPI_Irecv, and MPI_Wait functions. In UPC, the nonblocking call upc_memput_nb is used. In CAF, get statements are used with the compiler directive, pgas_defer_sync, as above in the STREAM example. In principle, such statements can also be used in UPC, however, we found that this approach does not work for UPC using the Cray compiler currently.

5.2 Performance

A metric called overlapped_fraction is computed using following formula:

$$overlapped_fraction =$$

$$1 - \left(\frac{T_{TotalRunningTime} - max(T_{Comp}, T_{Comm})}{min(T_{Comp}, T_{Comm})}\right)$$

where T_{comp} is the computation time and T_{comm} is the communication time. In the case that the runtime is equal to the maximum of the separate measurements of computation and communication the overlap is perfect. This fraction represents the amount of work that it was not possible to overlap.



Figure 8: The overlap capability of MPI, UPC, and CAF.

Fig. 8 shows the results for MPI, UPC, and CAF using two cores, one on each node. The computation time to com-

munication time ratio is set as 1. Several message sizes are tested, ranging from 8 to 512 KB bytes. For MPI, we observe around 20% overlap fraction for messages up to 2 KB. Beyond that point, the overlapped fraction goes down dramatically and the overlap almost completely disappears when the message size reaches 512 KB. UPC and CAF show the opposite overlap capability to MPI as a function of message size. For small messages, the overlap fraction is only around 5%. However, for large messages, such as 512KB, the overlap fraction can reach above 80%. CAF performs even better than UPC, for message size 512KB, over 90% of the communication time is overlapped with computation time. Presumably the difference between the CAF and UPC results is due to the slightly different mechanisms used in each case, as described above.

The higher overlap capability of UPC and CAF for large messages is related to the BTE message transfer mechanism. The BTE is part of the Gemini, and works asynchronously with respect to the CPU.

The poor overlap capability of MPI is related with the handshaking protocol needed between the sender and the receiver in MPI programming model, which may consume a lot of CPU cycles. The Gemini has no special hardware support for this, unlike SeaStar interconnect, and therefore it is much more difficult for MPI to overlap the communication and computation. (We note that a software based mechanism for this is in development at Cray currently.)

For smaller messages using PGAS, FMA is used to transfer the message data. FMA needs CPU involvement to initiate the transfer activity leading to lower overlap capability. Setting the input parameter R higher (i.e. more local computation time), could improve the overlapped fraction.

The above computational kernel involves a lot of data access to memory; it is a STREAM-like loop. We also developed a computation intensive kernel with reduced memory activity that worked only on data in cache and obtained similar results, which indicates we are not subject to contention for memory bandwidth between the CPU and the BTE, at least for these experiments.

6. NAS FT

In this section, we examine the performance differences between a MPI and a CAF version of a popular benchmark application, NAS FT. The NAS FT benchmark solves partial differential equations using Fast Fourier Transform (FFT) method. The MPI version is obtained directly from NPB3.3 benchmark suite [14]. The CAF version is converted from the MPI version by replacing the dominant MPI call, an MPI_Alltoall, with a CAF implementation. We also added some necessary synchronizations, and changed the corresponding data array to a co-array. The implementation of the CAF alltoall communication uses a round-robin communication pattern.

The performance in terms of Mflops for the Class B prob-

Table 2: The message sizes for NAS FT Class B (BYTE)

	64	128	256	512	1024	2048	4096	8192	16384	32768	65536
transpose 1	131072	32768	8192	4096	2048	1024	512	256	128	64	32
transpose 2				524288	131072	32768	8192	2048	512	128	32

lem size is shown in Fig. 9 for up to 64K cores. The 3D grid size is $512 \times 256 \times 256$ in X, Y, and Z direction individually. When the total number of processes (nprocs) is less or equal to grid size in Z direction (256 for Class B), a 1-D partitioning scheme is used and the grid will be partitioned among the cores along the Z direction. When the total number of processes becomes greater than the grid size in the Z direction, 2-D partitioning will be used and in addition to partitioning the grid along Z direction, the grid will also be partitioned in Y direction. The corresponding process grid is 256*(nprocs/256) and two new sub-communicators will be created. Therefore, there will be two transposes under 2-D partition, one for each new communicator. Table 2 shows the alltoall message size for different number of processes.

The overall performance comparison between MPI and CAF in terms of mflops is shown in Fig. 9 and the corresponding communication times are shown in Fig. 10.



Figure 9: The performance of NAS FT for Class B for the CAF and MPI versions.



Figure 10: The global communication time of NAS FT for Class B in CAF and MPI .

Up to 256 tasks, MPI and CAF deliver similar performance. This is for two reasons. Firstly, for these three cases, 1-D partitioning is used, and the message size is large, in the regime where CAF and MPI performance is almost the same. This is clearly shown in Fig. 10 which compares the alltoall communication times in CAF to those of the MPI version. Secondly, local computation and local transpose time dominate the runtime at these core counts and affect the overall performance much more than global communication time. For 512 processes, we notice that the communication time for CAF has a sudden jump. This is because the message size for the first global alltoall communication is 4 KB bytes, which is the switch threshold from using FMA to the BTE. We have seen this phenomena in our earlier micro benchmarks. If we change the PGAS_OFFLOAD_THRESHOLD to 1MB, the performance of CAF is significantly improved at 512 cores and the performance is no longer anomalous. For MPI a similar effect occurs at 2048 cores, as shown in Fig. 10, where we can see that MPI has the highest global communication time at this core count.

For all other core counts, CAF performs significantly better than MPI as the message sizes become smaller. The best performance is obtained by using 16K cores, at which CAF is about 2.8 times faster than MPI. However, the performance gap shrinks when 64K cores are used. As shown in Fig. 10, from 16K to 64K cores, the global communication time for CAF is relatively stable while for MPI, it continues to drop but maintains higher than corresponding CAF time. Again this is due to a change in communication protocol, for messages smaller than 128 bytes, MPI uses a store and forward protocol instead of the default, as it has better performance. At 65536 cores both transposes involve messages below this limit, and hence the improved algorithm is used. Experiments increasing the threshold of the cutoff for the change in algorithm to 1 KB bytes at 16384 and 32768 cores show performance improvements of almost 50% for the MPI version.

7. SUMMARY AND CONCLUSIONS

Compared with the popular MPI programming model, PGAS languages provide substantial ease of programming, and the ability to construct globally accessible data structures. However, they still have not been widely adopted by user community today. This is mainly due to lack of the direct hardware support, a mature developer environment and lack of convincing performance results that they are superior to MPI.

In this work we evaluated the performance of PGAS languages on a Cray XE6 high-performance computing platform for which the Gemini interconnect provides direct support for a globally addressable memory and hardware-accelerated one-sided messaging. We examined the performance in terms of bandwidth, message rate, and capability to overlap computation with communication. The results demonstrated that with this special hardware acceleration, PGAS languages can outperform MPI, especially for messages a few KB in size, and therefore provide a viable alternative. However, they also show that simply swapping MPI calls for equivalent PGAS constructs may not necessarily be the optimal path forward for achieving good performance with PGAS, as the performance in the bandwidth limit is identical to that of MPI. Codes may need to be modified to send smaller messages more frequently than one would with MPI in order to achieve the greatest benefit from using PGAS languages, Our future work will focus on converting existent scientific applications into PGAS codes and study their performance on Hopper.

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