ASYNCHRONOUS DATA TRANSFERS ON LARGE SCALE HPC SYSTEMS WITH EXPERIMENTS ON THE CRAY XT3/XT4

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ABSTRACT OF THE THESIS

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A key challenge faced by the emerging large scale scientific and engineering simulations is effectively and efficiently managing the large volumes of heterogeneous data generated. This includes offloading this data from the compute nodes at runtime, and transferring it over to service nodes or remote clusters for online monitoring, analysis, or archiving. To be effective, these I/O operations should not impose additional synchronization penalties on the simulation, should have minimal impact on the computational performance, maintain overall Quality of Service, and ensure that no data is lost.

This thesis describes the design, implementation, and operation of DART (Decoupled Asynchronous Remote Transfers). DART is a thin software layer built on RDMA (Remote Direct Memory Access) communication technology, and specifically the Portals RDMA library to allow fast, low-overhead access to data from simulations running on compute elements, and to support high-throughput low latency asynchronous I/O transfer of this data.

DART is part of the infrastructure for an integrated simulation of fusion plasma in a Tokamak being developed at the Center for Plasma Edge Simulation (CPES), a DoE Office of Fusion Energy Science (OFES) Fusion Simulation Projects (FSP). A performance evaluation on the Cray XT3/XT4 system at Oak Ridge National Laboratory demonstrates that DART can be used to offload expensive I/O operations to dedicated service nodes allowing more efficient utilization of the compute elements.

Acknowledgements

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Dedication

To my parents, Georgeta and Tudorel, whose permanent encouragements and unabated trust have helped me through every challenge I have faced. .

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Chapter 1

Introduction

The current advances in processor speed and architectures (e.g., from single to dual or quad core processors, and most recently the cell processors), enable scientists and engineers from different domains to cooperate and simulate complex phenomena with fine grain details and high accuracy. However, as the computing systems grow in computational capability and scale, efficiently utilizing these machines at full capacity and with the desired performance becomes increasingly challenging. Furthermore, complex scientific and engineering applications are based on live interactions and couplings across multiple and potentially distributed computational, data, and information services. For example, current fusion simulation efforts are exploring coupled models and codes that simultaneously simulate separate application processes and run on different resources at supercomputing centers. These codes will need to interact, at runtime, with each other, and with additional services (e.g., online data monitoring and analysis, data archiving, etc.).

These scientific simulations generate large amounts of data and thus require a robust substrate for data management and streaming between interacting components. In case of fusion simulations, for instance, large volumes and heterogeneous types of data generated have to be continuously streamed from dedicated compute nodes to specialized I/O nodes, and from there to local data analysis or storage machines or to remote clusters running coupled simulation components. A key challenge that such a substrate must address is transferring the large amounts of data generated by these simulations from the compute nodes to the service node (i.e., the I/O nodes) at runtime, and over to remote clusters for code coupling, online monitoring and analysis, and data archiving. To be viable and useful, the substrate has to comply with the simulation constraints for data transfers, i.e., (1) it should have minimum impact on the execution of the simulation in terms of performance and synchronization requirements, (2) it should satisfy stringent application/user space, memory, time and quality of service requirements, and (3) it should ensure that no data is lost. On most large scale parallel machines, a small number of service nodes usually service a much larger number of compute nodes, and offload their costly I/O operations. To meet the simulation requirements, the I/O substrate should be able to asynchronously transfer data from compute nodes to service node with minimal delay and overheads on the simulation. Technologies such as RDMA and the Portals library allow fast memory access into the address space of an application without interrupting the computational process, and provide a mechanism that can support these I/O requirements.

This work describes the DART (Decoupled Asynchronous Remote Transfers) system that aims to address these challenge and constraints. The objective of DART is to build a thin communication layer on top of Portals library that allows fast, low-overhead access to data at the compute elements and supports high-throughput low latency asynchronous I/O transfers. DART also provides a simple API that corresponds to traditional file I/O operations used in the simulation codes. This work also describes the design, implementation and operation of DART, and presents a performance evaluation on the Cray XT3/XT4 system at Oak Ridge National Laboratory. The evaluations demonstrate how DART can be used to offload expensive I/O operations to dedicated service nodes allowing more efficient utilization of compute elements. The performance evaluation also presents the results of using DART with two particle-in-cell FSP simulation codes GTC and XGC-1.

The rest of the thesis is organized as follows. Chapter 2 presents the background on existing I/O models, describes our testbed, and presents the generic RDMA communication technology and the Portals implementation of RDMA. Chapter 3 presents an overview of the related work. Chapter 4 presents the architecture of DART and describes its components. Chapter 5 discusses the implementation and operation of DART on a CRAY XT3/XT4 machine. Chapter 6 describes our experimental evaluation of DART and discusses the results, and chapter 7 concludes the thesis and presents directions for future work.

Chapter 2

Background

This chapter starts by categorizing and describing the existing I/O programming paradigmes, and emphasizes on the model that we used in this thesis. Next, it describes our testbed and its I/O communication features, i.e., support for RDMA data transfers. Following, we describe the Portals library that is an implementation for the RDMA communication framework.

2.1 I/O Models

We can categorize existing I/O programming practices or I/O models based on synchronous/asynchronous and blocking/non-blocking characteristics [13] into *synchronous blocking*, *synchronous non-blocking*, *asynchronous blocking* and *asynchronous non-blocking.* Each model has its own advantages and is suited for applications with a specific I/O pattern.

Synchronous blocking. Applications that implement this model have to synchronize send requests with receive requests. Thus, a receiver blocks until data from a send request becomes available or a sender blocks until data is consumed by a receive request.

To measure the I/O time for this model, let us consider the following piece of code:

```
1:  timer_start();
2:  write( fd, buffer, size );
3:  timer_stop();
4:  /* take the time difference */
```

When the application process makes the write call on line 2, the system call traps in kernel mode; the kernel copies data from application address space (or user space) to kernel space, and then tries to service the request. If, at the time of the call, a receiving process cannot transfer the available data entirely, the kernel blocks the application process on the completion of the I/O transfer, suspends and moves the process to a waiting queue, and schedules another process on the CPU. The application process remains suspended during the data transfer, and upon completion of the transfer, the kernel moves the application process from the waiting queue to the running queue and the process becomes eligible to be scheduled again on the CPU. Depending on the number of processes on the system, the application process can sit for a while in the running queue, until it is selected to run. When the process gets control back on the CPU, it continues execution with `timer_stop()` on line 3.

As we measure the total I/O time, we also account for some extra times that were not spent on actual I/O, e.g., time for the context switch (from user mode to kernel mode), time to copy data from user to kernel space, time to schedule another process to run, the running time of the other processes, and the time for a context switch back to our application process. In this case, the measured total I/O time is larger than the actual transfer time.

This I/O model is suited for applications where the sender and the receiver have to synchronize, since neither of them can proceed until the data exchange is completed. The negative side of this model is that it wastes valuable CPU cycles of the sender. While the sender blocks and waits for the I/O operation to complete, it could complete additional useful application computations. Due to the extra times required by this model, it is not well suited for applications that require a high throughput.

The **Synchronous Non-blocking** model is similar to the previous synchronous blocking one in that the sender and the receiver still have to synchronize, and the sender has to wait for the receiver to consume the data. Unlike the above model, in this case the sender does not block in the send call, which means that a send call will return immediately, regardless to whether the transfer is complete or not. This model requires the programmer to ensure the correctness of the transfer (e.g., ensure that a transfer completes). The user can determine the completeness of a transfer by checking on the return code of the send call; an error value of `EAGAIN` indicates the transfer is still in progress.

To measure the I/O time of this model, let us consider the following piece of code:

```
1:  timer_start();
2:  do {
```

```
3:  rc = write( fd, buffer, size );
4:  if( rc > 0 ) {
5:  size -= rc;
6:  buffer += rc;
7:  }
8:  else if( rc < 0 && errno != EAGAIN )
9:  break;
10:  } while( size > 0 );
11:  timer_stop();
12:  /* take the time difference */
```

When the application process makes the first write call (line 3), it traps into the kernel mode; the kernel copies the data from user space to kernel space and tries to service the request. Assuming the file descriptor `fd` supports non blocking calls, the write system call returns immediately and does not block the process. If a receiving process is not able to get the incoming data, the system call returns an error value of `EAGAIN` and the transfer is restarted. Moreover, if a receiving process cannot transfer all of the data at once, the system call returns with the partial value of the data transferred, and the transfer is restarted with the remaining data.

This I/O model, also accounts for some extra times when measuring the I/O time, e.g., time for a context switch from user to kernel mode, time to copy data from user to kernel space, time to restart the transfers, and so the I/O time is larger then the actual transfer time. In the worst case, the measured I/O time can equal the I/O time of a synchronous blocking I/O model. The improvement of the non-blocking model relative to the blocking I/O model is because the system call returns immediately and thus it does not block the application process. On a return from the system call, with a non-completion or partial completion code, the user may decide to do some more computation in the application and try the I/O operation later on.

This I/O model is suited for applications where the application process is required not to block (e.g., a server which handles multiple client connections simultaneous). The advantage of the non-blocking feature can be better exploited by the application programmer, but it introduces additional complexity to the code. Restarting the I/O operation adds penalties to the I/O performance and thus it degrades the overall throughput. This model is still inefficient for applications that require a high throughput.

Asynchronous blocking. Applications that implement this I/O model do not have to block in the I/O send call, but they can block in the data availability notification call `select()`. This model allows applications to exchange data in a decoupled way: the sender and the receiver are no longer required to be tightly synchronized. A sender application can check the communication channel using the `select()` system call, and it can send data only when the channel is available. In this way the send call does not block the application.

Let us consider the following example to analyze the I/O time of this model.

```
1:  rc = select( nfd, NULL, wfds, NULL, &timeout );
2:  if( rc > 0 ) {
3:  timer_start();
4:  write( fd, buffer, size );
5:  timer_stop();
6:  /* take the time difference */
7:  }
```

The `select()` system call traps in the kernel mode and blocks the application for a maximum specified value of `timeout` seconds (or milliseconds). The `select()` system call can monitor multiple file descriptors for I/O activity for both sending and receiving operations. When the kernel detects an event on any of the file descriptors monitored through the `select()` call, it takes the application process out of the waiting queue and adds it to the running queue, and selects it later on for the CPU control. When the process resumes, it continues with the `write` call on line 4, and at this moment the process knows that the communication channel is available for sending data and that the I/O call will not block. For this I/O model, the measurement of the I/O time is more accurate than for previous models, because the I/O call does not block.

The asynchronous blocking model is the most flexible model so far, because the `select()` call can monitor multiple descriptors and can control the total time to block through the `timeout` parameter. A user can transform this model into a non-blocking one by setting the `timeout` parameter to a small value. This way, the model becomes a polling mechanism and allows the user to schedule other application computations before retrying the I/O call, and to use its CPU more effectively. This flexibility has the cost of additional code complexity and the overhead of retrying the I/O operation. The negative side of this model is that it is not very efficient and it is not suited for high performance applications.

Asynchronous Non-blocking. This I/O model allows two applications to exchange data in a decoupled way (e.g., sender and receiver don't have to be synchronized), and allows an application to make the I/O calls without blocking the application process. When an application process makes an asynchronous I/O call, the asynchronous layer copies informations about the transfer (e.g., a reference to the memory region and the size of the region), then the call returns, and the application can continue its other computations. The data transfer should not impact the application run, and should proceed in parallel with the application. Depending on the implementation of the asynchronous layer, the system usually requires that the application does not modify the content of the data transfer buffer until the completion of the operation. The advantage of this model is that it tries to overlap data transfers with application computations for a better utilization of the CPU and a better transfer throughput. Moreover, the performance of this model could be even more significant if the system has hardware support so that the network interface card (NIC) can directly access an application memory address space without involving the CPU in the process (e.g., direct memory access).

2.2 Testbed System Description

The DART system described in this work was developed and tested on the Jaguar and Ewok machines at Oak Ridge National Labs (ORNL). Jaguar [18] is a CRAY XT3/XT4 parallel machine with more than 11,000 physical nodes. The nodes are logically divided into two partitions (Figure 2.1): a *compute partition* and a *service partition.* The compute partition has 11,500 nodes (*compute nodes*). Each compute node is a dual-core AMD Opteron 2.6GHz with 4GB memory, and runs the UNICOS/lc Operating System (OS) with the catamount micro-kernel [11]. The service partition has $\sim$ 200 nodes (*service nodes*). Each service node is a single-core AMD Opteron 2.4GHz with 4GB memory, and runs the GNU/Linux OS with a Linux kernel.

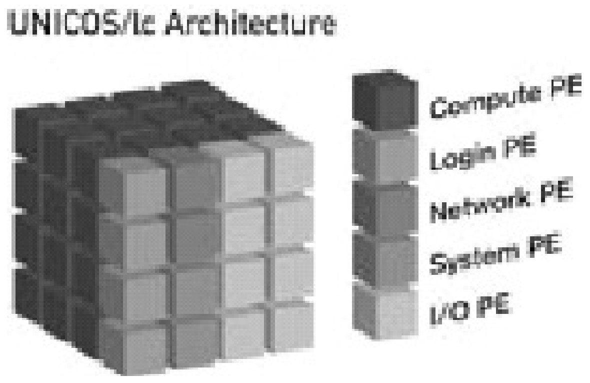


Figure 2.1: Jaguar architecture of a Cray XT3/XT4 machine [10]

The compute and service nodes are located on the same physical machine and the interconnect has a 3-D Torus topology using the *Cray Seastar* router and a very fast proprietary interconnection bus called the *HyperTransport* path (Figure 2.2). HyperTransport is a dedicated interconnection bus that is able to deliver 6.4GB/s transfer bandwidth. The compute nodes are dedicated nodes (i.e., non-shared) that run user batch jobs, whereas the service nodes are shared nodes that run system services (e.g., ssh, apache, etc.).

Service nodes on Jaguar machine connect to the Ewok cluster through a 5GB/s aggregated link. Ewok is a cluster with 128 nodes, where each node is a 2 Intel Xeon 3.4GHz CPU with 4GB memory. The nodes are interconnected by an Infiniband switch through 1GB/s links. Ewok is used to run analysis codes and serves as a sink for data generated by applications running on Jaguar.

On the Jaguar machine, the nodes in the system communicate through the *HyperTransport* path using the RDMA communication model.

2.3 RDMA and Portals Library

Remote Direct Memory Access. RDMA is a communication paradigm that enables a process to directly access another process's memory address space, independent of the location of the other process (e.g., the other process can be on the same node, or can be on a node on a remote cluster).

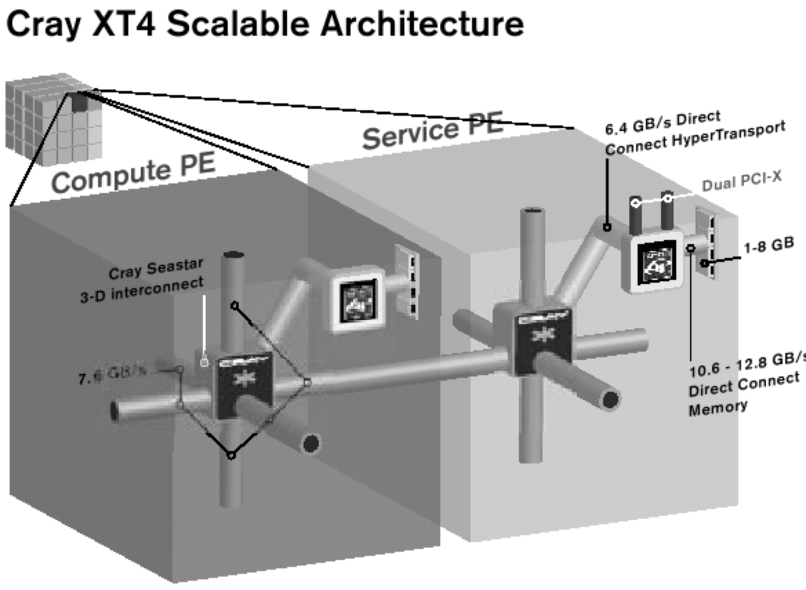

Cray XT4 Scalable Architecture
Compute PE
Service PE
6.4 GB/s Direct Connect HyperTransport
Dual PCI-X
1-8 GB
Cray Seastar 3-D interconnect
7.6 GB/s
10.6 - 12.8 GB/s Direct Connect Memory

Figure 2.2: Node interconnect on the Cray machine [10]

RDMA supports process to process communication models with zero-copy, and OS and application bypass. The zero-copy feature ensures that two nodes can exchange blocks of data in an I/O operation directly from the user memory address space, as opposed to first copying the data to the OS (kernel) memory space, and then exchange it. With the zero-copy feature, an application can avoid the overhead of making an extra copy of the data it sends. The OS and application bypass features ensure that an RDMA data transfer does not involve or interrupt the OS or the application in any phase of the transfer. However, this communication model does not directly provide a communication protocol, and the user has to provide, for example, other mechanisms to check for the completion of an I/O operation. The RDMA communication model restricts the application from accessing and modifying the memory region involved in the transfer until the completion of the transfer.

A machine provides the RDMA features/enhancements through a dedicated Network Interface Card (NIC) that can directly access the address space of a process without help from the operating system. The Jaguar machine exposes RDMA features to the user space through the Portals library.

Portals Library. The Portals library [3, 23] implements the RDMA communication model and provides a set of primitives that defines a communication protocol for RDMA data transfers. The provided primitives are one-side transfer operations. In the Portals

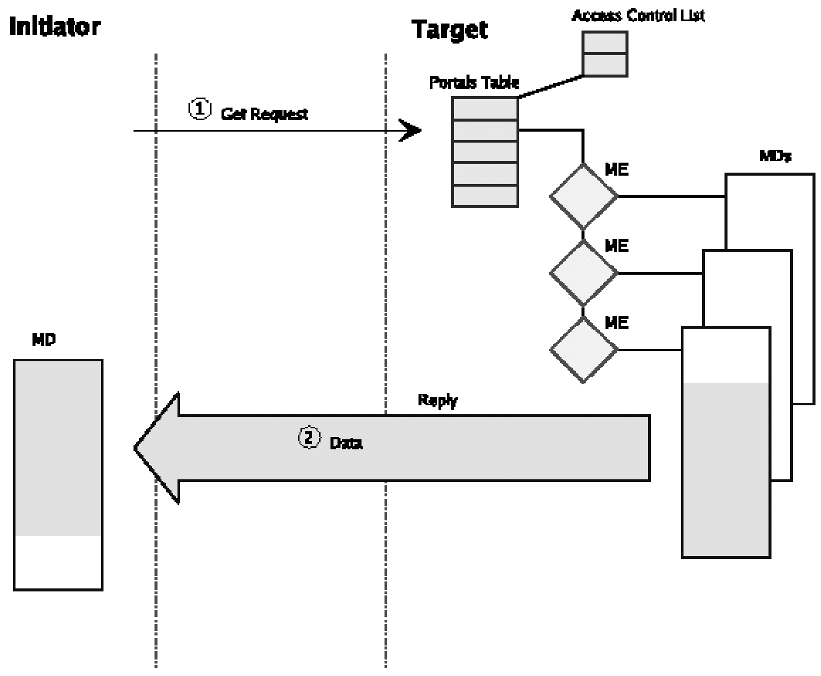


Figure 2.3: Portals *"get"* operation [23].

library, the two processes involved in a data transfer, i.e., the sender and the receiver are identified as the *source* and the *target*. Here, the source is the only active end envolved in a data transfer operation.

The Portals library supports two types of transfer operations, *get* shown in (Figure 2.3) and *put* shown in (Figure 2.4). The *get* operation extracts a block of data from a remote process memory, and the *put* operation injects a block of data into a remote process memory. In the *get* operation, the source initializes the data transfer, but it acts as a receiver for the transfer, while in the *put* operation, the source initializes the data transfer, but it acts as a sender for the transfer.

To support memory to memory data transfers between remote processes, the Portals library has to expose blocks of memory (memory buffers) from the address space of a process to the NIC, on the source as well as on the target. It exposes these blocks of memory through Memory Descriptors (MDs). These are Portals data types that contain internal bookkeeping information such as buffer start memory address and length, current transfer offsets, etc.

Portals also provide Access Control List (ACL) see (Figure 2.5) support for the MDs it

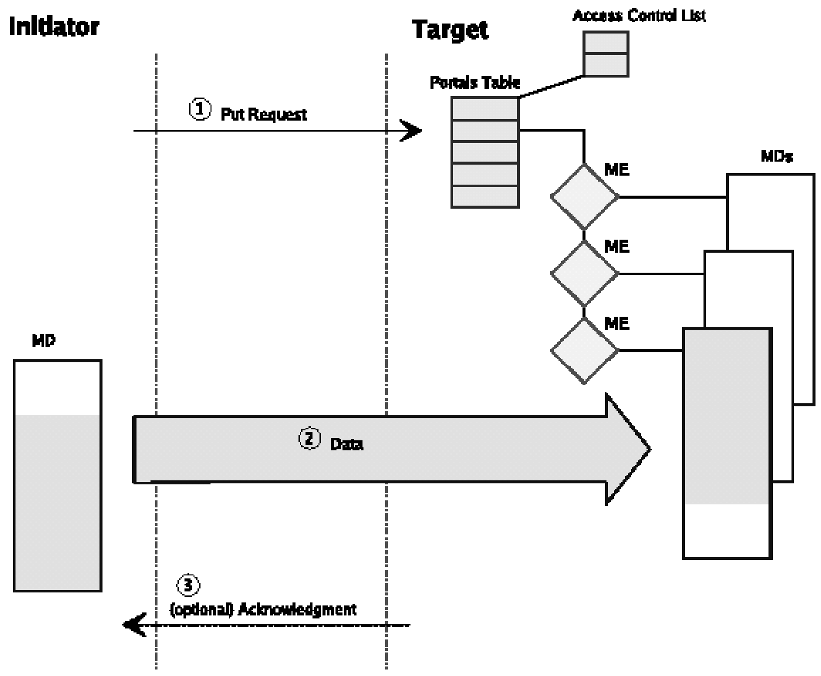


Figure 2.4: Portals *"put"* operation [23].

exposes. This way an application can control which processes and nodes have access to its memory address space. Each MD has to be attached to a Match Entry (ME) in a match list and each match list has to be associated with an entry in the Portals table. An entry in the Portals table can have associated multiple match lists linked together, and Portals checks each list sequentially to find a match for an ACL rule. Multiple applications can use the same Portals table entry and the same match list as long as they have distinct ACL matching rules.

Two remote processes can communicate through RDMA protocol provided that they know each other's "Portals addresses" and that the target has an ACL rule that matches the credential of the source. The access for a data transfer is checked only at the target side. The target and the source can use multiple MDs for communication, but each MD needs an unique ACL rule access key, so that Portals can identify the exact MD for a data transfer.

Portals also provides primitives to check the beginning or the completion of a data transfer operation, which are called events. An event in Portals is a data structure that defines a small log of an RDMA data transfer (e.g., source and target Portals addresses,

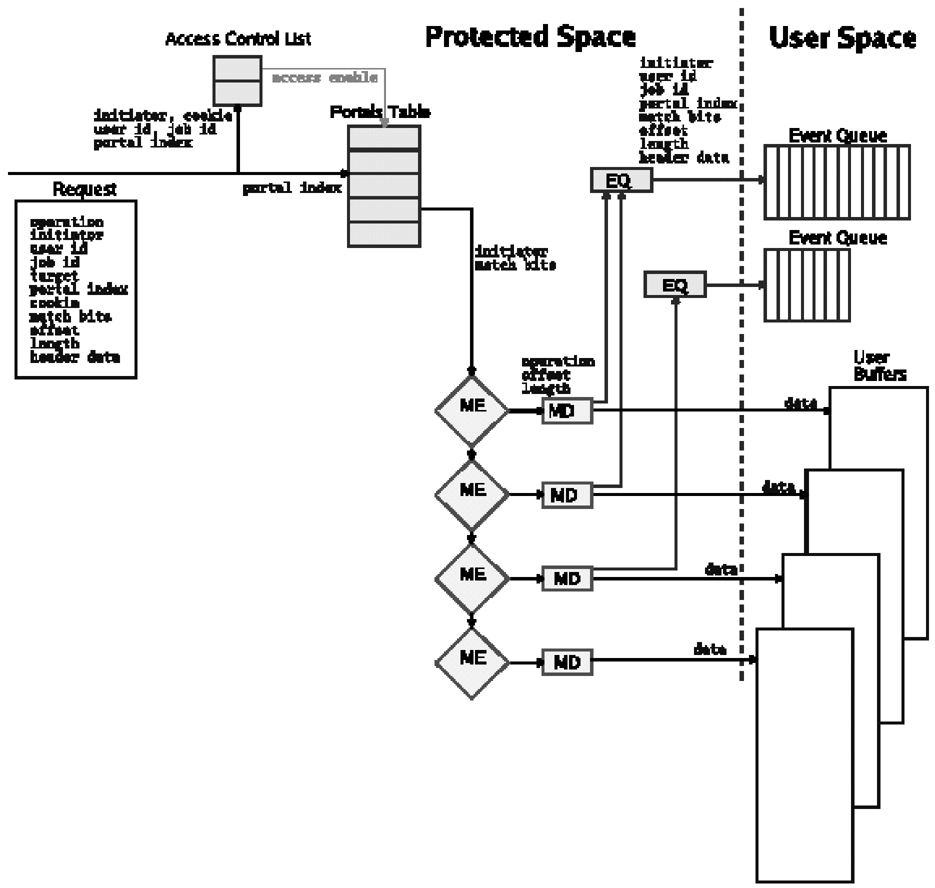


Figure 2.5: Portals *"acl"* rules [23].

number of bytes transfered, source or target offset of the transfer, etc.).

For each MD involved in a transfer, Portals generates events on both the source and the target. A MD has an Event Queue (EQ) associated with it, and each event generated for the MD is linked to the EQ.

With the availability of events, the Portals library is well suited to build an implementation of *asynchronous non-blocking* API semantics, that allows an application to send a block of data to a remote process without blocking or interrupting the application during the transfer.

Chapter 3

Prior Work

Many research efforts address the problem of enhancing the I/O performance for a class of applications in different ways. We can classify these approaches in two categories (1) system level approaches, and (2) application level approaches. The system level approach extends the services of the operating system, customizes them for the I/O needs of a specific class of applications, and preserves the I/O abstractions provided. For example, parallel and distributed network file systems extend the virtual file system (VFS) layer of the operating system, and provide the same file abstraction to an application. This approach has the great advantage of preserving binary compatibility for older applications. The application level approach consists in various transfer buffering and scheduling techniques, as well as collective collaboration between nodes of a parallel application. This approach is fine tuned for specific applications. For example, a database management system allocates and manages the storage system by itself for best performance, and bypasses the operating system interface.

Projects such as Lustre [9], GPFS [12], or PVFS [8] implement parallel filesystems. A parallel file system has a metadata server that keeps management information about a file, i.e., the file name, path, size, attributes or owner, and multiple backend storage servers that store the content of the file. This file system enhances the I/O performance of an applications at two levels. First, it separates management information from file content, and thus reduces the concurrency for file content access. Second, it stripes a file content across multiple storage servers and allows parallel accesses to the file content (e.g., both reads and writes). Accesses to a file are mediated by the metadata server, but an application transfers the content of a file directly and to and from a storage server, independent of the metadata server.

The MPI-IO and ROMIO [26] projects implement an application level solution, and they mainly target parallel applications. These systems provide a customized I/O interface that allows the processes of an application to collectively collaborate and write a file in parallel. The parallel file I/O interface allows an application to define relations such as 1-to-1, or 1-to-many, between compute nodes and the associated files produced, i.e., each compute node can write its own output file, or multiple compute node can cumulatively write to a single output file. This approach leverages the I/O performance of an application because it reduces the concurrency at the metadata server on a parallel file system.

The IO-Lite [22] and Client-Side File Caching [15] (CSFS) projects implement application level solution based on customized buffering techniques for specific applications. Thus, IO-Lite unifies the system caching and buffering mechanism by providing a single physical copy of the data which is shared between different system components, e.g., file system, networking system, interprocess communication system, etc. IO-Light improves an application I/O performance by avoiding multiple data copies. The CSFS project is specially tuned for applications that use the MPI-IO communication substrate. CSFS buffers and schedules the I/O operations at client side and bypasses the more general file system cache. The Direct Access File System [19] (DAFS) project also implements a caching technique in user space and bypasses the file system cache. It it optimized for zero-copy data transfers and is implemented on systems with RDMA support.

The LIVE Data Workspace project [1] at Georgia Tech and the underlying PBIO layer, has simular overall goals and approach as DART. However, there are several differences in the design, and the two systems make different tradeoffs. The focus of PBIO is on reconfigurability and ad hoc connections of components without a priori knowledge of data requirements. PBIO also supports multiple transports including Portals and Inifinband, while DART currently is only implemented over Portals. DART, in contrast, is more lightweight and is specifically tuned for streaming and was thus shown to be faster in the tests conducted at the Oak Ridge National Laboratory.

PDIO [24] is a related effort, and is specially designed to support runtime visualization of data from parallel simulations. It tries to virtually extend the file-system of Portals-enabled compute nodes to arbitrary destination locations. The design of PDIO is tightly coupled to the requirements of its target applications.

Asynchronous I/O API [25] is a recent effort that aims to provide a simple I/O interface capable of integrating with a variety of data transport layers, both synchronous and asynchronous. The goal of the AIO API is to provide an interface that is nearly as simple as standard Fortran I/O statements, while giving access to the power and flexibility of mature systems like MPI-IO, HDF-5 [7], parallel netCDF [20], and standard POSIX calls as well as more experimental systems like DART and the Georgia Tech LIVE system. Additionally, the data is encoded in a tagged, binary format with data and grouping attributes for easier data use without the overhead of parsing a plain text data format. The system consists of three parts: (1) the API that was designed primarily for Fortan use, but also tested with C, (2) an XML configuration file describing the data types, attributes, data transports, and buffer specifications selected, and (3) the data transport layer, for example, DART.

Chapter 4

DART Design and Architecture

The goal of the DART system is to efficiently manage and transfer large amounts of data from applications running on the compute nodes of a parallel system or cluster to the service nodes or remote locations, and support remote application monitoring, data analysis, coupling, or archiving. Figure 4.1 presents an overview of the DART system.

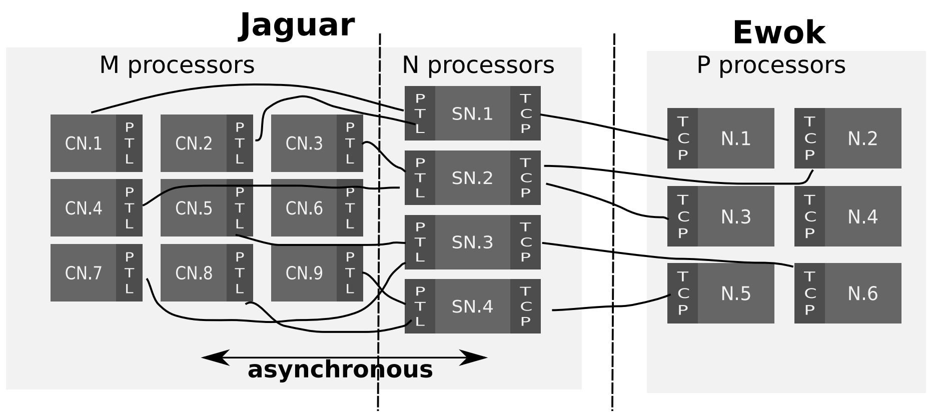


Figure 4.1: Architectural overview of DART.

The key objectives that DART tries to achieve include minimization of data transfer overhead on the application, high throughput, low latency data transfers, and prevention of data losses. To meet these requirements, DART asynchronously offloads the costly data I/O and streaming operations from the compute nodes to service nodes; on the service nodes, DART either saves data to local storage, or transfers it to remote locations.

DART system contains three components: a client library (*DARTClient*), a streaming server (*DARTSServer*) and a receiving server (*DARTReceiver*). *DARTClient* is a thin software layer on the application stack, built on the Portals library, that provides asynchronous API semantics. It runs on the compute nodes along with the application code and provides I/O services to the application. *DARTSServer* is the main component that schedules and initiates the I/O operations from DARTClients. It runs independently on a service node, extracts data from a running simulation on the compute nodes, and streams the data to a downstream *DARTReceiver*. Finally, *DARTReceiver* runs on nodes of a remote system (e.g., monitoring/analysis nodes, archiving nodes, nodes running a coupled simulation) and "consumes" the data streamed by *DARTSServer*.

4.1 The DART Client Layer

DARTClient is a "light" layer on the application software stack that is implemented directly on top of the Portals library that provides communication primitives to the above application layers such as the asynchronous I/O management layer (AIO) or directly to the simulation layer (e.g., GTC or XGC). It is implemented as a static library that is linked with the application at compile time.

DARTClient performs two main functions, (1) message signaling and coordination, and (2) data transfers. The message signaling function serves to notify the streaming server when the application has data available to send out, and to wait for an acknowledgment from the streaming server when it completes a data transfer operation or processes a notification message. For signaling and coordination, *DARTClient* registers a compute node with an instance of a streaming server and announces application requests for transfer events at runtime. During the registration phase, the *DARTClient* layer at the compute node and the streaming server at a service node exchange identification and communication parameters such as unique numerical process identifiers, Portals addresses, communication offsets, and memory descriptors identifiers (i.e., unique keys for Portals ACL rules). For data transfers, when the application at the compute nodes executes an I/O operation, *DARTClient* notifies the streaming server that it has data ready to be sent, and sets up the parameters and priorities for the transfer. Afterwards, it is the role of the streaming server to actually schedule and transfer the data.

DARTClient exposes two classes of memory descriptors to the streaming server, to support asynchronous and process to process direct memory communication. The first class is the application level memory descriptor. *DARTClient* creates these descriptors during the registration phase and communicates their ACL keys to the streaming server. They persist throughout the lifetime of the application. *DARTClient* defines two types of application level memory descriptors – one is used to notify the streaming server of a request for transfer, and the other is used to retrieve acknowledgments from the streaming server upon completion of a data transfer or processing of a notification message.

The second class of memory descriptors is the stream level memory descriptors, which *DARTClient* creates for each data stream opened by the application. Here the "data stream" equals the notion of a file. There are two types of stream level memory descriptors – one is used for transfer control messaging to store communication and signaling parameters for a stream, and the other is used to expose to the streaming server the memory area that maps the actual data written by the application. *DARTClient* creates these memory descriptors on-the-fly when a data stream is opened by the application, and announces their ACL key to the streaming server in a request for transfer message. These memory descriptors persist only during the lifetime of a data stream; they are destroyed afterwards.

DARTClient layer provides asynchronous API semantics to the above application layers, and thus enables the application to make asynchronous and non-blocking "write" calls, and to continue its computation without blocking and waiting for the data transfer to complete. *DARTClient* is built on the Portals library described previously, which is OS and application-bypass enabled, and allows the data transfers from compute nodes to overlap with application computations.

DARTClient uses multiple buffers to allow multiple data stream write operations to proceed in parallel. An application running on a compute node can open multiple data streams of different sizes sequentially (e.g., a diagnosis stream and a checkpoint stream). The data transfer operation is asynchronous, and transfers from streams of different sizes can overlap in time. A priority mechanism schedules smaller transfers with a higher priority to allow them to complete in parallel with larger transfers, but without being blocked by the larger ones, and thus multiple data streams are serviced in parallel.

4.2 The DART Streaming Server and Receiver

DARTSServer is the DART streaming server component that runs as a standalone application on the service nodes. It is responsible for scheduling and asynchronously extracting data from applications that run on the compute nodes, and streaming it to remote nodes or to local storage. Multiple instances of the *DARTSServer* can run on different service nodes and they serve data transfer requests from the large number of compute nodes in a cooperative manner.

The key functions of *DARTSServer* include registering communication parameters from a compute node, waiting for compute node notifications about data availability, scheduling and managing data transfers from the compute nodes, and streaming the data out to remote nodes or local storage as requested by the compute nodes. Data transfers have priorities based on the size of the data blocks and the frequency at which the application generates them. *DARTSServer* assigns a higher priority to smaller and more frequent data blocks, and assigns a lower priority to the less frequent and larger data blocks. This priority mechanism prevents transfers of smaller blocks from being blocked by the transfer of larger blocks, and enables them to proceed in parallel with the larger block transfers.

Two key performance goals underlying the *DARTSServer* are minimization of the transfer latencies and maximization of the transfer throughput. To achieve these goals, the streaming server pre-allocates resources (i.e., communication buffers associated with the memory descriptors for remote data transfers) during the server initialization phase at startup. The specific number of memory descriptors and the size of each buffer allocated is influenced by multiple factors such as (1) the limit on the number of file descriptors that can be used by a process (a memory descriptor counts as an open file), (2) the physical memory available on the service node, and (3) the size of the working set (to avoid trashing behaviors). On a Linux system, each process has a default maximum limit of 1024 file descriptors that it can use at any instant of time. In the current implementation, *DARTSServer* allocates 512 memory descriptors and a buffer of 4MB for each descriptor to accommodate the physical memory constraints of the server machine and to keep the communication buffers as part of the working set and avoid swapping penalties. *DARTSServer* adapts the data transfer scheduling algorithm to scale beyond 512 compute nodes, and up to 4096 compute nodes.

In addition to the memory descriptors used for the data transfers, the streaming server also allocates memory descriptors for node registration and message signaling. *DARTSServer* allocates two types of memory descriptors for node registration – one descriptor is used for compute node registration requests, and the other for service nodes registration requests. The latter is used when multiple server instances operate in a cooperative mode. When the *DARTSServer* runs in cooperative mode (i.e., there are multiple instances in the system), the first instance of the streaming server, also called the *master instance*, load balances the compute node registration across all instances of the streaming servers. The master instance uses the service node registration memory descriptor to also forward compute node registration requests to other *DARTSServer* instances to preserve the balance.

For message signaling, *DARTSServer* also uses two types of descriptors – one descriptor holds notifications from the compute nodes about data availability, and the other notifies a compute node when an asynchronous transfer completes. In case of the former, the access control policy [4] is set to allow the remote node (i.e., the compute node) to manage the offset for a write (*"push"*) operation. However, the streaming server establishes the write offset parameters for each individual node during the registration phase. This descriptor is large enough to hold requests from all the compute nodes associated with the streaming server, and is configured (via access control rules) to guarantee that the server does not miss any request.

The *DARTSServer* implementation is multi-threaded and consists of three threads including the main application process, viz., the *"Main"* thread t_1, the *"Portals"* thread t_2, and the *"Streaming"* thread t_3. The three threads are associated with three distinct queues as follows (1) $t_1 \rightleftharpoons ebq$, (2) $t_2 \rightleftharpoons pbq$, and (3) $t_3 \rightleftharpoons fbq$. Furthermore, the pre-allocated memory descriptors and the buffer are cycled between these threads by assigning them to the queues according to their status, i.e., available descriptors are assigned to *ebq*, in-progress descriptors are assigned to *pbq*, and used descriptors are assigned to *fbq*.

The overall data flow associated with the operation of the *DARTSServer* is illustrated in Figure 4.2. A data transfer starts when the application running on a compute node

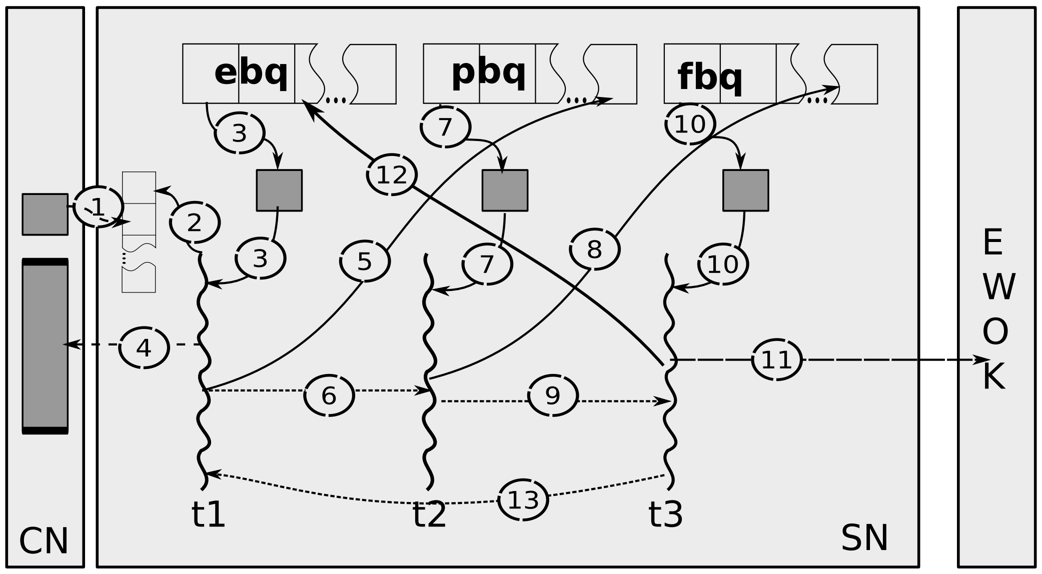


Figure 4.2: Data flow for DART operation.

generates a request for transfer message and posts a notification message on the notification memory descriptor at the streaming server (e.g., message sequence 1 in the figure). Thread t_1 continuously polls this memory descriptor for new incoming notification messages.

When a new notification arrives, t_1 extracts it (2), requests an empty buffer (3) for the transfer from the *ebq* queue, and starts the data transfer from the corresponding compute node (4). After t_1 thread initiates the asynchronous data transfer, it adds the buffer and the memory descriptor to the *pbq* queue (5), and signals thread t_2 (6). Thread t_2 blocks and waits for transfer completions, and when a transfer completes (7), it adds the corresponding buffer and memory descriptor to the fbq queue (8) and signals thread t_3 (9). The primary task of thread t_3 is to stream the data from a buffer (10) either to a remote location (11) or to local storage. Once it finishes streaming the data, it adds the buffer and memory descriptor back to the *ebq* queue (12) and signals thread t_1 (13).

4.3 DART API and Usage

The DART client layer (*DARTClient*) provides I/O primitives that are very similar to standard Fortran file operations, i.e., *dart_open(), dart_write()*, and *dart_close()*. The similarity in naming and signatures of these primitives with the file operations was chosen to make the library easy to use by scientists and to easily incorporate it into existing application codes.

Additionally DART provides function to initialize and finalize the library, i.e., *dart_init()*, and *dart_finalize()*.

DART I/O primitives are asynchronous. A typical usage of the API consists of a *dart_open()* operation that returns a handle that identifies a data stream, one or more non-blocking *dart_write()* operations on the handle of the data stream, and a *dart_close()* operation on the stream. Following the *close* operation, the stream is closed and the handle reference is no longer valid to the application (e.g., the application can no longer write to this stream), but the data transfer for this stream may not be completed yet. *DARTClient* releases the resources associated with a data stream only after the streaming server acknowledges the transfer completion. The application has to open another data stream if it needs to write more data.

Throughout the runtime of the application, an I/O operation may be in one of three states, *"not started"*, *"in progress"* or *"finished"*. In case of the first two states, *DARTClient* maintains status information for the data streams, and when the application calls *dart_finalize()*, it ensures that all of the in-progress operations are complete. As a result, a call to *dart_finalize()* can block and it should always be called at the end of the application so that it does not impact the simulation.

In the current implementation, DART assumes the application does not generate any sort of concurrency for the file streams (e.g., it does not open the same file from multiple nodes).

Chapter 5

DART Implementation and Operation on the Cray XT3/XT4

5.1 Compute Node Bootstrap Mechanisms

Compute nodes and service nodes on the Cray XT3/XT4 machine communicate using RDMA calls via the Portals protocol. Portals identifies each process in the system by a Portals address that is a tuple composed of unique numerical identifiers for the node (compute or service) and the process, i.e., *"nid"* and *"pid"*. Two processes in the system can communicate if they know each others Portals addresses.

When a user runs a simulation on the system (e.g., through the batch queuing system), he/she requests a certain number of compute nodes. However, the specific nodes that are assigned to the simulation, and consequently their Portals addresses, are only known at run-time. As a result, to enable the compute nodes to communicate with the streaming server, DART defines a customized bootstrap mechanism that is independent of the underlying execution mechanism (e.g., MPI or the batch queuing system). The bootstrap mechanism requires that the streaming server starts and runs before the application starts.

In the current implementation, DART supports two versions of the bootstrap mechanism. The first version relies on the environment variables to communicate the Portals address (i.e., the tuple {*"nid", "pid"*}) of the server to the compute nodes. *DARTSServer* sets the values of these variables, the job launching script picks the variables and passes them to the queuing system, and the queuing system replicates them on each compute node when it allocates and starts the application on the requested number of compute nodes.

While this approach is simple and elegant, it is not reliable. A job may wait in the batch queue for an undefined amount of time before its requested number of compute

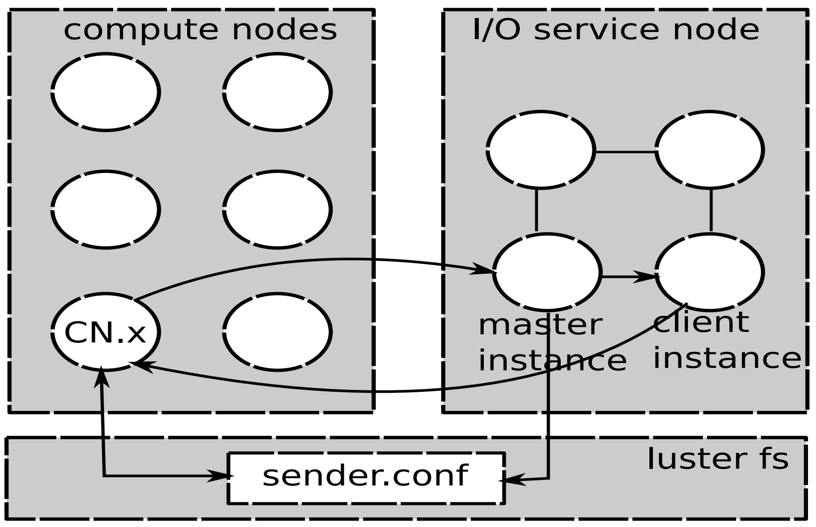


Figure 5.1: DART compute node bootstrap mechanism.

nodes becomes available. During the waiting time in the queue, the system may go down for maintenance. The queuing system automatically saves and restores the jobs waiting queue across system reboots, while the user has to manually restart the streaming server application (i.e., *DARTSServer*). On a manual restart, the streaming server process gets a new Portals address (the *"nid"* value may be the same if the server runs on the same service node, but it gets a different *"pid"* value), and this invalidates the address already announced to the compute nodes.

The second version, shown in Figure 5.1, relies on the file-system that is shared between the compute and service nodes. The server node writes its Portals address (i.e., the tuple *"nid"*, *"pid"*) to a persistent configuration file. When the application initializes, *DART-Client* parses this file and reads the Portals address of the streaming server. As part of the registration phase, it sends to the streaming server its own Portals address. This bootstrapping approach allows the streaming server to restart, get a different address, and modify the configuration file multiple times before the application starts on the compute nodes (which happens after the application is launched through the batch queuing system).

If the *DARTSServer* runs in cooperative mode, and multiple instances run on different service nodes, then the first server with the lowest "nid" value acts as a master and writes the configuration file, and the other servers follow the same bootstrap process as the compute nodes. During the application initialization phase, the master server maps each compute node to an instance of a streaming server via the bootstrap process, and later each compute node forwards all the requests to that server instance. At this phase, the master server uniformly distributes the compute nodes across the streaming servers, so that each server serves approximately the same number of compute nodes.

In the current implementation of DART, the initial mapping of compute nodes to streaming servers is preserved for the runtime of the applications. This is because the load on the servers is naturally balanced due to the SPMD (single program multiple data) nature of the applications. Cooperative load balancing between streaming servers is used in cases where this is not true (e.g., if local adaptivity is used at the application running on the compute nodes).

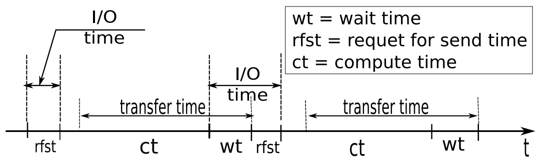
5.2 Data Transfer Protocol

The *DARTClient* is purposefully lightweight and implements the minimum required functionality so that it does not impact the application layers above. Consequently, *DARTSServer* implements all the logic necessary for scheduling, data extraction and data transport.

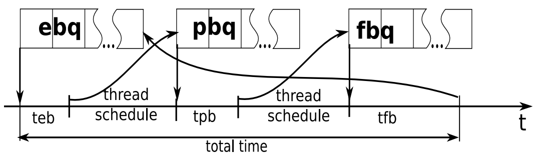
As described in Section 5.1, DART associates or maps each compute node of an application to an instance of *DARTSServer* during the registration phase through the bootstrap process. After the registration phase is completed a compute node sends all the I/O requests to the same server instance, and that instance services all the requests coming from the compute node.

When coupled with the asynchronous management layer *AIO layer* [25] or directly with the application, *DARTClient* caches all I/O operations corresponding to an application data stream to a communication buffer, until the application closes the stream. A compute node does not have to wait for a transfer operation corresponding to a data stream to complete, as *DARTClient* associates a distinct communication buffer to each stream of data. The *DARTClient* releases the resources associated with a data stream either on subsequent I/O operations, or upon the call to *dart_finalize()*.

The data transfer protocol has two stages. First, a compute node sends a small “request for send” notification message to its associated streaming server instance. Second, the



(a) DART client layer



(b) DART server

Figure 5.2: Timing diagrams for the operation of *DARTClient* and *DARTSServer*.

streaming server schedules the request, extracts the data from the memory of the compute node, and transfers it to the destination specified in the *"request for send"* notification (i.e., remote node or local storage). The streaming server, processes and services multiple data notification requests (from the same compute node or from different compute nodes) in a round robin fashion according to the priorities of the requests.

Figure 5.2 illustrates the operation of the transfer protocol using timing diagrams. Figure 5.2(a) presents the timing diagram at a compute node while running an application coupled with the *DARTClient* layer. An usual run of an application consists of sequences of computations (identified by c_t in the figure), followed by data transfer requests (identified by w_t and rfs_t in the figure). The data transfer protocol is asynchronous, and after a compute node posts a *"request for send"* notification message (e.g., this corresponds to rfs_t) on the streaming server, it can continue its computations without waiting for the actual transfer to complete. Due to this asynchronous nature, a data transfer can proceed in parallel with the application and can overlap computations, although it may not start immediately. A compute node may block before sending a notification (i.e., w_t), if the streaming server is busy and has not yet processed a previous notification message from the same compute node. The effective I/O time at the application level is the sum of w_t and rfs_t times. The value for rfs_t represents the time to post a notification message on the server, as well as the time to encode and cache the application data into the communication buffer.

Similarly, Figure 5.2(b) presents the timing diagram for the transfer of a block of data from a compute node to a remote node. In the figure, *"teb"* is the time the server takes for processing a notification message from a compute node and for scheduling the corresponding data extraction, *"tpb"* is the time the server takes for extracting the data from the compute node using the Portals interface, and *"tfb"* is the time the server takes to transfer the data to a remote node using the TCP interface. The value of these parameters corresponds to the processing times of threads t_1, t_2, and t_3 processing time as described in Section 4. The value for the total I/O time equals the sum of these three values plus some OS thread scheduling overheads.

Chapter 6
Experimental Evaluation

DART performance evaluation includes two sets of experiments. The first set evaluates the base performance of DART using synthetic testing simulations. The synthetic testing simulations clone the real simulation behavior by following the same computational pattern, i.e., a set of one or more computational stages followed by one I/O stage. The experiments evaluate the main parameters that influence data transfer rates from compute to service nodes, the amount of overlap between computations and data transfers, and the overhead of data transfers on the application. This includes (1) the size of data unit transfered, i.e., the block size, (2) the number of memory descriptors allocated at the service node, (3) the frequency of data transfers, and (4) the time required to stream the data, i.e., the time to store the message at the destination node.

The second set of experiments evaluates the performance of DART when it is integrated with real simulation codes, i.e., the GTC and XGC-1 fusion simulations. The key metrics used in these experiments are (1) the effective data transfer rate from the compute nodes and to the destination nodes, and (2) the overhead of using DART on the performance of the simulation.

6.1 Data Transfer Rate

This benchmark experiment evaluated the maximum application-level transfer rate that DART can achieve between compute and service nodes, using RDMA data transfers.

In the set up of this experiment, DART used two compute nodes and one service node, i.e., one streaming server transfered data from a simulation running on two compute nodes and measured the transfer rates. In this test, DART serviced a synthetic simulation code with a compute stage of 1 *msec*. This parameter however, did not influence the transfer

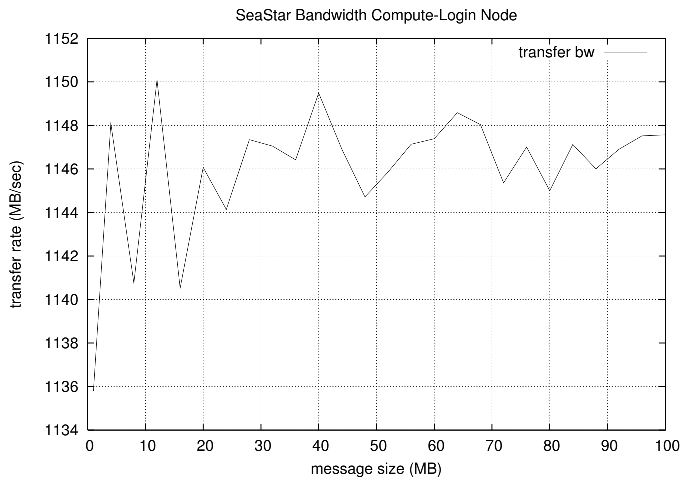


Figure 6.1: Data transfer rate between compute and service nodes.

rates since DART measured the transfer times and sizes at the streaming server.

During the test, the simulation varied the size of the data unit (i.e., the block size) from 1 to 100MB in increments of 4MB, and DART measured the achieved transfer rate for each value. The synthetic testing simulation ran for 100 iterations, and performed 100 data transfers for each distinct value of the block size.

The average transfer rate (over the 100 iterations) for each block size is plotted in Figure 6.1. The plot shows that DART can saturate the network link between compute and service nodes using a minimum block size of 4MB.

It should be noted that the streaming server used the `gettimeofday()` system call to measure the transfer times, and as a result, the measured values also include system operations such as OS process scheduling, etc., which explains the variability in the rate measurements.

6.2 Overhead on the Simulation

This experiment analyzed the additional overhead that DART transfer operations impose on a simulation running on the compute nodes, and expressed the value of the overhead as a percentage of the time the simulation spent in its compute stages.

In the setup of this experiment, DART used 128 compute nodes that ran the synthetic simulation and streamed the data to one streaming server. At the streaming server, DART used 128 memory descriptors to ensure that it can fetch data blocks from all the compute nodes in parallel. The testing simulation generated data in blocks of 4MB, and consequently, for this test, the streaming server allocated 4MB of memory to each memory descriptor to match the size of the data blocks from the application. Further, the streaming server transfered the data to a node on a remote cluster.

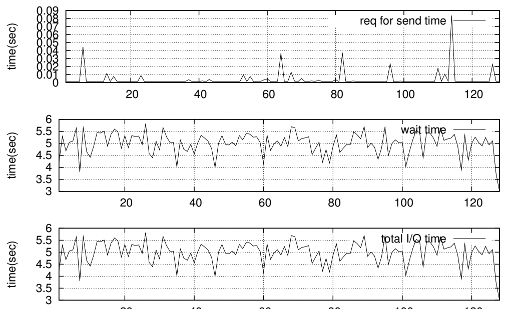
In order to analyse the influence of the I/O operation frequency on the data transfers overhead at the application level, the synthetic application simulated different durations for the compute stage in two different tests. The results of the two tests from this experiment are presented below. The values for the duration of the compute stages are selected to demonstrate the effect of I/O frequency on the overhead, and on the ability to overlap I/O with computations.

It should be noted that the synthetic simulation posted the "request for send" notifications from all the compute nodes at the same time, while the streaming server processed these notifications sequentially in round robin fashion. Consequently, the streaming server could service the $i+1^{st}$ notification request from a compute node only after it had serviced all i^{th} requests from all the other compute nodes. At the streaming server, the most time consuming operation while servicing a transfer request was streaming the data to the remote location.

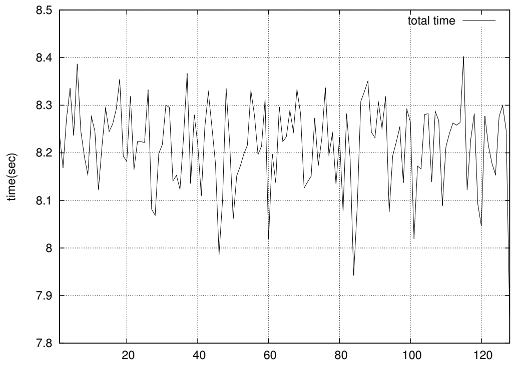
Furthermore, the upper bound for the time the server needed to service two consecutive requests for the same compute node was $t_{fb} * N + t_{pb}$, where t_{fb} was the time required to transfer one block of data to a node in the remote cluster (i.e., Ewok), N was the number of compute nodes, and t_{pb} was additional time to process and transfer the data from the compute nodes. The value of t_{pb} is typically negligible as compared to $t_{fb} * N$. Subsequently, the goal was to find a good balance between the duration of a compute stage and the data size streamed, in order to obtain a better overlap between computations and data transfers.

In each test, DART measured the *I/O time*, the *wait time*, the *"request to send" time* at the compute nodes, and the total *I/O time* for an operation (from the "request to send" notification to the end of streaming) at the streaming server.

In the first test, the testing application simulated a compute stage of 2 *sec*. This value was chosen based on previous experiments to demonstrate the effects of poor overlap. The results of this test are plotted in Figure 6.2(a) (for compute node) and Figure 6.2(b) (for the streaming server). In these plots, the x axis is the numerical identifier of each compute node and the y axis is the cumulative I/O time for 100 simulation iterations. The I/O time on the compute nodes equals the sum of *"request to send"* and *wait times*.



(a) Cumulative I/O time at the compute nodes.

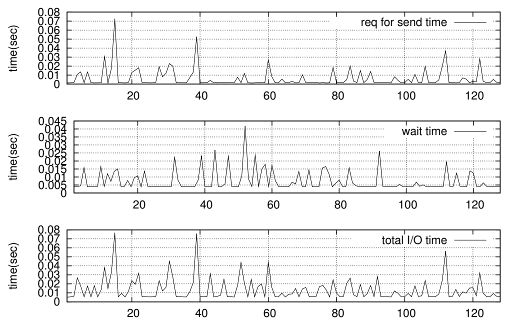


(b) Cumulative I/O time at the streaming server.

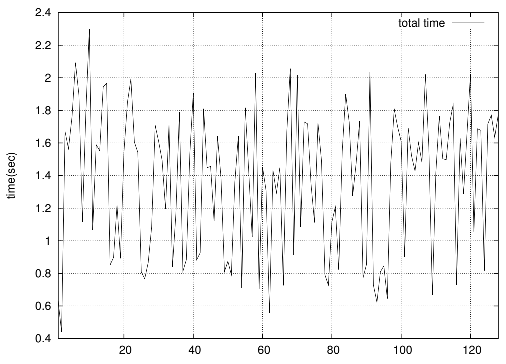
Figure 6.2: Overhead of DART on the application for a compute phase of 2 *sec*.

The values for *wait time* and *I/O time* in Figure 6.2(a) are almost identical, and this indicates that the I/O time is dominated by the wait time. A large value for the *wait time* indicates that a data notification operation blocks, and waits for a previous operation to finish. In this test, the duration for the compute stage is small, and the frequency of I/O stages is higher than the streaming server's ability to transfer the fetched data to the remote location (i.e., a node on the Ewok cluster). As a result, the streaming server delays the processing of "request for send" notifications from compute nodes and this causes the large *I/O time* in Figure 6.2(b). The results of this test show that the overlap between computations and the overhead of data extraction is not optimal, as the *wait time* is very high on compute nodes. The average time difference between the *I/O time* measured on the streaming server and the *I/O time* measured on the compute nodes is 34 *msec* per iteration, and represents the time required by the streaming server to transfer the data from a compute note to the remote node.

In the second test, the synthetic application established the value for the duration of the compute stage based on the results from the previous test and the discussion above to be 4.38 *sec*, so as to maximize the overlap. The rest of the setup and parameters remained the same. The results of the test are presented in Figure 6.3(a) for the compute node and



(a) Cumulative I/O time at the compute nodes.



(b) Cumulative I/O time at the streaming server.

Figure 6.3: Overhead of DART on the application for a compute phase of 4.38 *sec*.

in Figure 6.3(b) for the streaming server. Again, in these plots the x axis is the numerical identifier of each compute node and the y axis is the cumulative *I/O time* for 100 simulation iterations. The value for the *wait time* in this case is very small (5 *msec*), indicating that the $i + 1^{st}$ fetch operation from a compute node can proceed almost immediately, without having to wait for the i^{th} transfer to finish. These results demonstrate an efficient overlap of simulation computations with data extractions, resulting in very low I/O overhead on the simulation.

These experiments demonstrate that the data transfer latency and the simulation overhead depend very strongly on the duration of the computation stage (i.e., the frequency of I/O operations) and the size of the data blocks. At same time the overhead of transferring data from an application using RDMA calls can be very small if the application overlaps computations with data transfers.

6.3 Integration with Simulation Codes

In the second set of experiments, real scientific application codes replaced the synthetic simulations and DART performance was analyzed using multiple criteria. The first criteria was the throughput of the streaming server on both the Portals (compute nodes to streaming server) and TCP (streaming server to remote node) interfaces. The second criteria was the DART I/O overhead on the simulation, and the third criteria was DART scalability with the number of compute nodes.

6.3.1 Integration with GTC

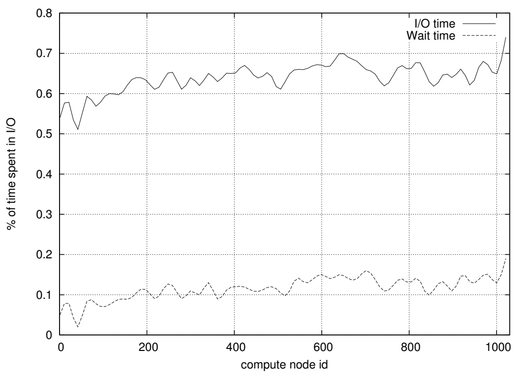
The first application used in this experiment was the Gyrokinetic Toroidal Code [17] (GTC) simulation. GTC is a highly accurate fusion modeling code that performs a highly complex analysis of non linear dynamics of plasma turbulence by using numerical simulations, thus requiring very large-scale computation capabilities.

The GTC code used the DART system as a transfer library and set the simulation parameters in the runs as described below. The key GTC parameters that influenced the size of the generated data and the frequency of I/O are *micell, mecell*, which determine the size of the domain, *npartdom*, which determines the number of particles in the domain, and *msnap*, which determines the frequency of I/O (e.g., frequency at which checkpoint files are generated).

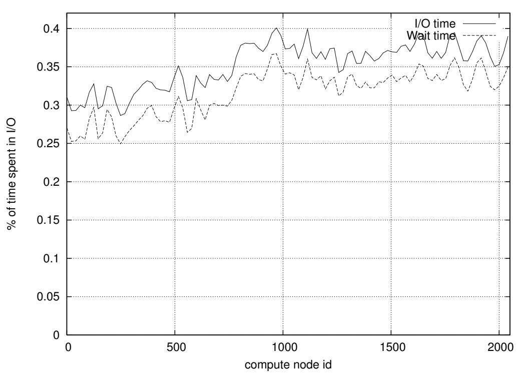
To test the scalability of DART, the GTC simulation ran initially on 1024 and later on 2048 compute nodes. For the test with 1024 compute nodes, the GTC simulation used the following values for the input parameters 160 for *micell* and *mecell* parameters, 16 for *npartdom*, and 13 for *msnap*. Corresponding to these parameter values, the GTC code generated a checkpoint file of 40MB for every 13 simulation iterations. Each simulation iteration took 8 *sec*, and the simulation ran for 200 iterations.

Proportionately, for the test on 2048 compute nodes, the GTC code used the following values: 160 for *micell* and *mecell* input parameters, 32 for *npartdom*, and 26 for *msnap*, and ran the computations for 400 iterations. Corresponding to these parameter values, the GTC code generated a checkpoint of 40MB every 26 simulation iterations, and each iteration took 8 *sec*.

In these experiments, the DART streaming server ran on a dedicated service node (i.e., no other users or I/O services were running on the same node). For performance analysis, DART measured the *wait* and *I/O times* at the simulation level for each of the compute nodes, and the throughput obtained on both Portals and TCP interfaces at the streaming server. During these experiments, the remote receiver received the data from the streaming server, but did not perform any processing on the data.



(a) I/O overhead on the GTC code on 1024 nodes.



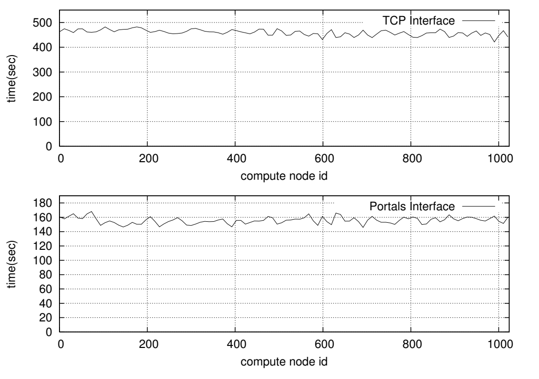
(b) I/O overhead on the GTC code on 2048 nodes.

Figure 6.4: Percentage of I/O and wait time overhead on the GTC simulation measured at the compute nodes.

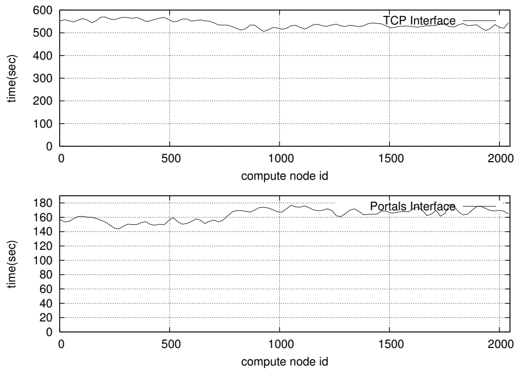
The I/O overhead on the GTC application caused by DART data extraction and streaming is plotted in Figure 6.4 as a percentage of the time taken by the compute stages. The x axis in these plots is a numerical identifier for each compute node, and the y axis is the overhead measured at each compute node of the simulation.

In Figure 6.4(a), the average value of the percentage *wait time* across the 1024 nodes is less than 0.15%, which indicates that DART was able to efficiently overlap computations with data extraction and transport. In addition, the average value of the I/O time is less than 0.65%, which indicates that the overhead on the simulation is very small. In Figure 6.4(b) the average value for the *I/O time* for 2048 nodes is still small at less than 0.4%. However, the difference between the *I/O* and *wait time* percentages is much smaller than in the 1024 case, indicating that the streaming server is aproaching the limit for the maximum number of compute nodes it can service simultaneously. The average value for the percentage overhead in the test with 2048 nodes was smaller than that for the test with 1024 nodes because the GTC code was generating the same amount of data for its checkpoint files, but the length of computing stage was doubled.

Figure 6.5 plots the cumulative *I/O times* at the streaming server for (1) extracting the checkpoint from the simulation using the Portals interface, and (2) transporting the data to a remote node using the TCP interface, for each compute node over the runtime of the simulation. In these plots, the x axis is a numerical identifier for each compute node and the y axis is the cumulative *I/O time*. As expected, the transfer times for the Portals interface



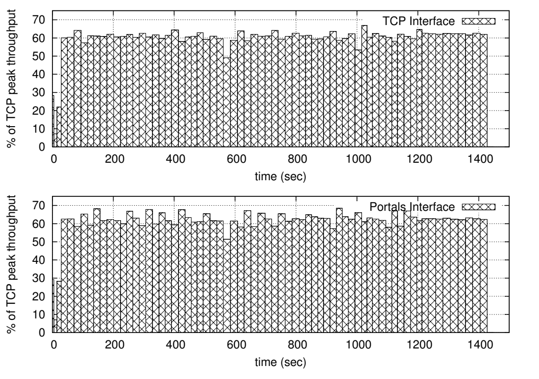
(a) Cumulative I/O time at the streaming server servicing 1024 compute nodes.



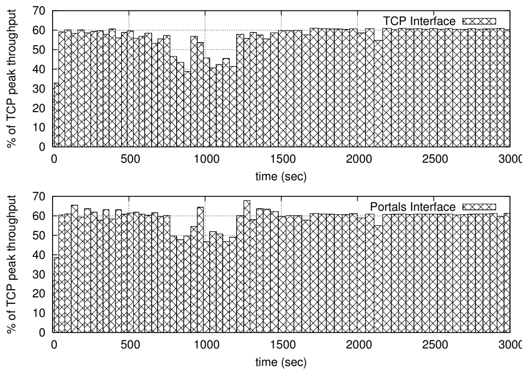
(b) Cumulative I/O time at the streaming server servicing 2048 compute nodes.

Figure 6.5: Cumulative I/O time times for the GTC simulation measured at the DART streaming server.

were smaller. The corresponding values for the transfer time on both Portals and TCP were comparable in the two cases (1024 and 2048 compute nodes), because the buffers that the streaming server allocated for communication were filled to capacity throughout the tests.



(a) DART streaming server servicing 1024 compute nodes.



(b) DART streaming server servicing 2048 compute nodes.

Figure 6.6: Throughput at the DART server using Portals (compute nodes to service node) and TCP (service node to remote node).

A benchmark test using the IPerf tool [14] for the maximum link throughput between the streaming server and the remote node using the TCP transport protocol, performed ahead of running these tests, showed a peak measured value of 5.01 *Gbps*. Figure 6.6 plots the throughput achieved using DART at the streaming server on both the Portals and TCP interfaces. In this plot, the x axis represents the runtime of the simulation, and the y axis represents the throughput as a percentage of the link peak value throughput. In both of the tests with 1024 and 2048 compute nodes, on the TCP interface, DART achieved an average sustained throughput of 60% of the peak TCP throughput. The streaming server spent the rest of the time to transfer the data on the Portals interface and to schedule the transfer operations. The average transfer throughput obtained on the Portals interface was comparable to the value of the TCP interface, i.e., 60%, which was expected since the communication buffer at the streaming server was fully utilized and became the bottleneck. Comparing the values of *I/O time* on Portals and TCP interfaces in the images of Figure 6.5(a), TCP transport is slower than Portals, but as the two transports share the same communication buffer at the streaming server, the Portals throughput adapts to the slower link.

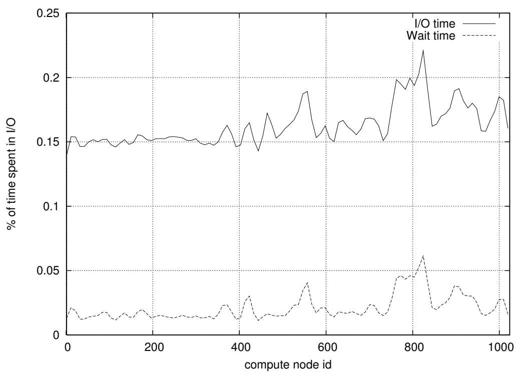
To summarize, in the experiment with 1024 compute nodes, the simulation ran for 1500 sec and each node generated 550MB of data, resulting in a total of 555GB across the system. The overhead on the simulation was less then 0.7%. In the experiment with 2048 compute nodes, the simulation ran for 3000 sec, and each node generated 550MB of data for a total of 1.2TB across the system and the overhead on the simulation of 0.4%.

6.3.2 Integration with XGC-1

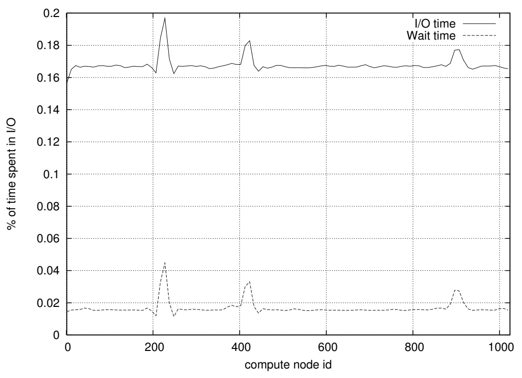
The second application used in the experiment was the Edge Gyrokinetic Code version 1 (XGC-1) [6] simulation code. XGC-1 is an edge turbulence particle-in-cell code, that uses numerical models to simulate a 2D dimensional density, the temperature, the bootstrap current and the viscosity profiles in accordance with neoclassical turbulent transport.

In the experiments with XGC-1, DART ran on 1024 compute nodes and one instance of the streaming server. The DART streaming server allocated the same set of resources as for the GTC experiment, i.e., 512 memory descriptors, and 4MB for each descriptor.

The numerical model that XGC-1 code is simulating can crash during the simulation execution, and XGC-1 protects against such crashes by repeatedly generating and saving *checkpoint files*. A checkpoint file is a snapshot of the state of the simulation computations at a given moment of time, and in case of a crash, the simulation can restart the computations from the latest file before the crash. The main XGC-1 input parameters



(a) *I/O* remote node streaming overhead on XGC



(b) *I/O* local storage saving overhead on XGC

Figure 6.7: Percentage of *I/O* and *wait time* overhead on the XGC-1 simulation measured at the compute nodes

that influence the size of a generated checkpoint file and the frequency of the I/O operations are *"ptl_num"*, which defines the number of particles to be used in the simulation, *"sml_mstep"*, which defines the number of iterations (computation cycles) the simulation performs, and *"sml_restart_write_period"*, defining the frequency at which the simulation generates checkpoint files.

XGC-1 used the DART system as a transfer library in two distinct experiments to (1) stream the checkpoint files to a remote destination and (2) to save the checkpoint files to a local storage system.

In the first experiment, DART transfered the data generated by the simulation to a remote node. In this experiment, the XGC-1 code used the following values for the input parameters 100 for *"sml_mstep"* parameter, 20 for the *"sml_restart_write_period"*, and 10^6 for the *"ptl_num"*. Corresponding to these values, XGC-1 generated a checkpoint file of 73MB every 20 iterations, and each iteration took 30 *sec*. The DART data transfer overhead on the simulation is plotted in Figure 6.7(a) as percentage of the compute stage duration (time). The value of the *wait time* is very small, which indicates that the data transfer overlapped computations and had a small overhead on the simulation less than 0.2%.

In the second experiment, DART saved the checkpoint files generated by the simulation to a local storage such as the Lustre [9] parallel file system. The values for the input parameters were similar, except for *"sml_mstep"*, which was set to 120, and *"sml_restart_write_period"*, which was set to 24. Corresponding to these values, XGC-1 generated a checkpoint file of 73MB every 24 iterations, and each iteration took 30 *sec*. The overhead on the simulation is also expressed as a percentage of the compute stage and results are plotted in Figure 6.7(b). Again, the value of the *wait time* is very small and the impact of data transfers on the simulation is less than 0.2%.

The difference between the two graphs in Figure 6.7 shows the data transfer to a local storage is more uniform across the nodes than in the streaming case. This behavior was expected, because Luster is a parallel file system, and the files were striped across multiple back-end storage servers, while for the streaming test DART used a single remote receiver.

To summarize, the behavior and performance of DART observed in these experiments were similar to that described above for GTC. The XGC-1 simulation ran for 3020 *sec*, and each node generated 760MB of data, resulting in a total of 380GB of data across the system. The overheads on the simulation due to DART operations was less than 0.2% of the simulation compute time. The difference in the values for the overhead on the simulation in the two case (e.g., GTC and XGC-1) is explained by the different values for the compute stages of the two simulations.

Chapter 7

Conclusions

This work presented the design, implementation, operation, and the evaluation of the DART system. DART is a library for fast, low latency and high throughput data transfers that uses the RDMA communication paradigm to provide an asynchronous API to the application layers of a scientific application.

DART system has three key components *DARTClient*, which is a thin transport layer on the application stack that runs in line with the application and provides the asynchronous API to the application, *DARTSServer*, which is a streaming server that runs as stand-alone application and transfers data from the application and *DARTReceiver*, which is an application that transports data from the streaming server to remote locations.

DART system was built and evaluated on top of Portals framework at Oak Ridge National Labs on a Cray XT3/XT4 machine. The evaluation presented three sets of experiments. The first set was a benchmark that measured the maximum data transfer rate that DART could achieve and sustain between a compute and a service node on the Jaguar machine. The second set of experiments used a synthetic test application (1) to analyse the main parameters that influence the performance of a data transfer (e.g., number of nodes an application runs on, the size of a transfer, the frequency of the transfers), and (2) to analyse the overhead of a data transfer using DART at the application level. The third set of experiments used DART as a transfer library for two real scientific applications GTC and XGC-1 fusion simulation codes.

The experimental results demonstrated that DART can saturate the interconnection link between a compute and a service nodes and that the performance of data transfers is strongly dependent on the computational pattern of the application (e.g., the duration of a compute stage), yet with a proper balance between computations and I/O stages, DART asynchronous transfer mechanism can overlap application computations with data transfers with a very small overhead on the application itself. Further, the results with real scientific simulation (i.e., GTC and XGC-1) showed that the DART library is scalable and can transfer large amounts of data with low overhead on the application, low latency and high throughput.

DART is currently built on the Cray system using the Portals library, and it is part of future work to extend and port DART to other platforms that supports RDMA communications such as BlueGene/P and Infiniband. The main features of DART demonstrated in this work include data transfers to either local or remote storage, yet DART can build other communication abstractions on top of it such as an end-to-end code-coupling layer.

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