Globus Service Enhancements for Exascale Applications and Facilities

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Abstract

Many extreme-scale applications require the movement of large quantities of data to, from, and among leadership computing facilities, as well as other scientific facilities and the home institutions of facility users. These applications, particularly when leadership computing facilities are involved, can touch upon edge cases (e.g., terabyte files) that had not been a focus of previous Globus optimization work, which had emphasized rather the movement of many smaller (megabyte to gigabyte) files. We report here on how automated client-driven chunking can be used to accelerate both the movement of large files and the integrity checking operations that have proven to be essential for large data transfers. We present detailed performance studies that provide insights into the benefits of these modifications in a range of file transfer scenarios.

Introduction

Modern science applications often involve the processing of massive data from a wide spectrum of sources, encompassing both experimental and observational facilities, such as synchrotron light sources (Liu et al. 2021a) and telescopes, and supercomputers, as in climate science (Reichstein et al. 2019) and cosmology (Heitmann et al. 2019). Workflows underpinning these science applications must be able to deliver these data to processing resources that best suit each applications' scale, timeliness, and hardware requirements. When data producers are remote from consumers, as they often are, these workflows must be able to transfer large data across high-bandwidth networks. Reliable and rapid wide area data movement thus becomes a vital element of exascale computing systems (Alexander et al. 2020).

The sharing of even extremely large data among geographically distributed resources and researchers has become increasingly feasible thanks to the widespread availability of high-bandwidth networks, the deployment of specialized network architectures (Dart et al. 2013), and the development of specialized data transfer protocols and services, notably the GridFTP protocol (Allcock et al. 2005) and the Globus service (Chard et al. 2016) which is widely used to manage GridFTP-based file transfers. Thus it has become commonplace to transfer petabytes over networks such as Internet2 and the U.S. Department of Energy's ESnet (Kettimuthu et al. 2018; Lacinski et al. 2024). However, emerging applications pose new challenges relating to the transfer of small numbers of extremely large (e.g., multi-TB) files, a workload for which Globus has not been optimized. Here, we report on work that tackles these challenges by developing and evaluating enhancements to Globus for such transfers. These enhancements focus on enabling the partitioning of large files, during a transfer, into many chunks that can be transmitted concurrently. We show that this chunking can accelerate both data transfer and integrity checking operations performed as part of a transfer.

Background

Scientific Data Transfer Infrastructure

Modern scientific computing environments employ specialized data transfer infrastructure designed to maximize the speed achievable when moving data among geographically distributed storage systems. These infrastructures typically combine a high-speed network; high-speed parallel file systems; a network and data transfer node (DTN) architecture to remove barriers to the rapid transfer of data over the network to/from file systems; and the Globus service and agents to achieve high-speed data movement.

Contemporary science networks such as ESnet connect research institutions at 100 Gb/s or higher rates. These networks are optimized for high-speed, reliable packet transport. At the end of these networks are typically highperformance parallel file systems such as Lustre (of which more below) that incorporate large degrees of internal parallelism to achieve high I/O rates. The elements that sit in between the external network and the file system play a crucial role in enabling high-speed data transfers. Two essential elements (Dart et al. 2013) are a clean network path to the external networks (without, for example, firewalls) and one or more Data Transfer Nodes (DTNs) configured to drive transfers at high speeds. DTNs are specialized servers configured specifically for efficient, high-speed data transfers. Specifically, they are equipped with highperformance network interfaces, often 10 Gigabit Ethernet or higher; are configured to optimize the data path to minimize latency and maximize throughput; are typically connected directly to ESnet to take full advantage of its

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Figure 1. A modern data transfer infrastructure connects high-speed storage to wide area networks via a clean, high-bandwidth network path with one or more data transfer nodes (DTNs) hosting **Globus Connect agents**. The cloud-hosted **Globus service** acts as a client to the Globus Connect agents, instructing them to perform file transfers in response to user requests.

high-speed capabilities; are also connected directly to highspeed storage; and run Globus Connect servers to handle large datasets, support reliable multi-stream file transfers, and manage security, access control, and logging.

DTNs typically sit outside any corporate firewall(s) so that data can move between wide area network and HPC storage without interference. To ensure that this configuration does not create security exposures, DTNs are configured with security measures tailored to the protection of data during transfer. This is particularly important when handling sensitive or proprietary information.

GridFTP and Globus

GridFTP (Allcock 2003) is an extension of the standard File Transfer Protocol (FTP) designed specifically for high-performance, secure data transfer tasks. Its most widely employed implementation is that included in Globus (Allcock et al. 2001; Chard et al. 2016), and in this brief summary we focus our discussion on that instantiation (Allcock et al. 2005).

The GridFTP protocol and its Globus implementation incorporate a variety of features designed for high-speed, reliable, and secure file transfer. For performance, Globus GridFTP employs *parallelism*, whereby a single data mover employs multiple concurrent connections to transfer different parts of a single file, and *concurrency*, whereby multiple data movers communicate different files: see Figure 2. It also employs *pipelining*, in which multiple file transfer requests can be in flight without acknowledgments (see Figure 3), and can handle third-party transfers, whereby the data transfer operation is initiated by one machine but involves data moving directly between two other machines. The latter capability is fundamental to Globus, because it allows for transfers to be initiated, monitored, and managed by the cloud-hosted Globus service.

Globus GridFTP incorporates fault recovery mechanisms that enable the resumption of data transfers upon failure, rather than a total restart—a crucial capability when

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transferring large datasets, where a failure can occur due to various network or system issues. For security, Globus GridFTP supports strong authentication and data encryption to ensure that data transfers are secure and that only authorized users can access the service. It also implements integrity checking to detect data corruption at any point along the path between source storage and destination storage. (Data corruption while data at rest, while a concern (Bairavasundaram et al. 2008), is viewed as out of scope.) In addition, its modular architecture allows for integration with a wide variety of storage systems, from conventional POSIX to high-performance parallel file systems and a range of object stores (Liu et al. 2021b).

The GridFTP protocol supports what we refer to here as chunked data transfer by defining new commands such as SPAS (Striped Passive) and SPOR (Striped Port), and by adding stripe layout and block size options to the FTP RETR command (Allcock 2003). The original Globus implementation of GridFTP (Allcock et al. 2005) implemented these commands, which enabled it to achieve \sim 17 Gb/s of throughput between parallel file systems at NCSA and SDSC almost two decades ago. In this server-side chunking mechanism, the server determined how many GridFTP server processes to use for a chunked data transfer request. Though a powerful capability, a significant limitation is that the GridFTP control server must decide the number of nodes and processes to use for a chunked transfer, and in practice the GridFTP control server at one end had no knowledge about the configuration of the GridFTP server (e.g., number of DTNs) at the other end. This difficulty, plus some stability issues in the server-side chunking implementation, meant this mechanism was not widely used in practice.

From 2010 forward, Globus was re-architected as a hybrid architecture in which a cloud-hosted Globus service manages the activities of Globus Connect agents, for example by requesting pairs of such agents to perform file transfers in response to user requests (Foster 2011). Today, tens of thousands of such agents are deployed on storage systems at thousands of institutions worldwide. Globus service state is maintained in geographically replicated and thus highly reliable cloud storage, while file transfers proceed directly from one agent to another under the direction of the Globus service. As we describe in the following, the Globus service's knowledge of Globus Connect agent configurations allows for the implementation of *client-side chunking*, in which the Globus service, acting as a client to those agents, leverages partial file transfer mechanisms in the GridFTP protocol, in the form of ERET/ESTO (Extended Retrieve / Extended Store) commands (Allcock 2003), to drive chunked transfers.

Previous Performance Evaluations

Many studies of data transfer performance have been performed over the years, involving a wide variety of network environments, protocols, and workloads. Here we comment just on some recent studies of Globus performance, as they provide context for subsequent discussion.

Allcock et al. (2005) and Ito et al. (2005) studied the impact of concurrency and parallelism on achieved transfer performance. Yildirim et al. (2012) conduct a more detailed investigation of the impact of GridFTP pipelining, parallelism, and concurrency on performance, and provide guidelines for setting these parameters. Kettimuthu et al. (2015) showed that by ensuring a sufficient, but not excessive, allocation of concurrency to the right transfers, overall performance of the resources can be improved significantly. Arslan et al. (2018) present algorithms for dynamic adaptation of these parameters to improve performance.

Liu et al. (2017) applied machine learning methods to a large collection of Globus log data to estimate parameters for predictive models that yielded insights into factors determining end-to-end transfer performance. One observation was that "contention at endpoints can significantly reduce aggregate performance of even overprovisioned networks."

Liu et al. (2018a) analyzed 40 billion GridFTP command logs totaling 3.3 exabytes and 4.8 million transfer logs collected by the Globus transfer service from 2014/01/01 to 2018/01/01. Among many interesting observations, we note two: First, they saw one integrity check failure per 1.26 TB, although admitting that the integrity checking protocol could not distinguish between true data corruption and a file changed deliberately during a transfer. Second, they observed that most datasets transferred by Globus had only one file, and that 17.6% of those datasets (or 11% of the total) had a file size of \geq 100 MB—motivating the need for distributing single-file transfers over multiple servers.

Kettimuthu et al. (2018) undertook a study in which they sought to move 1 PiB (2^{50} B = 1.125 PB) in 24 hours over a 100 Gb/s network connecting Argonne National Laboratory and the National Center for Supercomputing Applications. They succeeded ultimately in moving 1 PiB in 24 h 3 min without integrity checking (an average rate of 92.4 Gb/s) and in 30 h 52 min (72 Gb/s) with integrity checking. They achieved this rate via careful optimization of transfer parameters, including organizing the data to be transferred into 4 GB files and setting concurrency to 128 and parallelism to 1 (i.e., transferring 128 files concurrently, with a total of 128 TCP streams).

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Liu et al. (2019) conducted a detailed study of per-file overheads in wide area Globus transfers. Their results are applicable mainly to smaller files.

The Petascale DTN project (Dart et al. 2021b) was motivated, in the first instance, by the observation that despite HPC facilities being connected by 100 Gb/s networks and equipped with dedicated DTNs, achieved end-to-end data transfer performance among HPC facilities was often disappointing, rarely exceeding 10 Gb/s. Thus in 2020 researchers at four such facilities (ALCF, NERSC, OLCF, and NCSA) undertook a systematic investigation of data transfer performance, with the goal of achieving routine transfer rates of 1 PB/week (a sustained 15 Gb/s) among the participating sites. They used for these studies a \sim 4.4 TB output dataset from a HACC simulation run (Dart et al. 2021a), comprising a total of 211 directories and 19260 files, ranging in size from zero bytes to 11.3 GB. As shown in Table 1, performance among the four sites improved substantially over the course of the studies. The authors acknowledge multiple reasons for these improvements, from network upgrades to improved DTN hardware and changes to both the Globus implementation (e.g., see Section IV.C in Liu et al. (2018b)) and policies, and emphasize the importance of sustained monitoring to guide optimizations.

Table 1. Pairwise average data transfer rates, in Gb/s, reported by the Petascale DTN project (Dart et al. 2021b) between pairs of sites before (upper sub-table) and after (lower sub-table) optimization of DTN configurations.

	Destination			
Source	ALCF	NCSA	NERSC	OLCF
Performance at start of project				
ALCF	-	13.4	10.0	10.5
NCSA	8.2	-	6.8	6.9
NERSC	7.3	7.6	-	6.0
OLCF	11.1	13.3	6.7	-
Performance at end of project				
ALCF	-	50.0	35.0	46.8
NCSA	56.7	-	22.6	34.7
NERSC	42.2	33.7	-	39.0
OLCF	47.5	43.4	33.1	-

Methodology

Our major focus in this work is to enable rapid transfer of large files. To this end, we focus our attention on two goals.

Our first goal is to extend the Globus transfer service to orchestrate the actions of multiple data movers when moving large files, with the goal of achieving improved performance for large file transfer on POSIX file systems. With this mechanism, large files are chunked, and transferred, in parallel across multiple DTNs, from their source to their destination. We investigate the optimal chunk size capable of keeping all concurrent transfer sessions used, and incorporate changes to the transfer service to implement client-side chunking. (We use the term chunking for this Globus capability here, rather than striping, so as to avoid confusion with striping as implemented in the Lustre file system, which we also discuss in the following.)



Figure 2. Concurrency (multiple data movers) and parallelism (multiple TCP connections) as implemented in Globus GridFTP.

The second related goal is to optimize the process used by Globus to verify the integrity of transferred data, as the associated checksum computations and additional read operation have been shown to introduce significant costs in high-bandwidth transfers (Kettimuthu et al. 2018).

Distribution of Transfers Over Multiple DTNs

As described above, Globus leverages concurrency to transmit multiple files at one time, with the degree of concurrency supported by a particular Globus endpoint determined by configuration parameters that may be adjusted by the endpoint administrator.

Concurrency is a powerful accelerator of data transfers when many files are to be transmitted at the same time. By allowing different data movers to proceed independently with reading and transmitting (or receiving and writing), aggregate achieved I/O rates to the storage system increase, as do aggregate achieved network bandwidth in many cases—for example, when individual DTN connections to a border router have lower capacity than that router's connection to the wide area network. Furthermore, as each data mover can operate on a separate file concurrently, no coordination costs are incurred. However, concurrency provides no benefits at all when transferring a single large file, as in that case just a single data mover will engage in data movement, leaving other data movers idle. Whether transfer speed is limited by data mover file read/write performance



Figure 3. Pipelining in Globus GridFTP. Delays due to waiting for acknowledgements (left) are reduced by sending multiple requests at once (right).

or network send/receive performance (Liu et al. 2018a), the single data mover imposes a bottleneck. Similar concerns arise, albeit at a reduced level, when the number of large files is less than the optimal concurrency level for an endpoint.

This analysis suggests that a superior approach to transferring a single large file (or a small number of large files) could instead be to partition the task of transferring the large file(s) among multiple data movers. To investigate the feasibility of this approach, we leveraged the partial file transfer capability of the Globus GridFTP server implementation to engage multiple data mover pairs at the source and destination to process disjoint file *chunks* independently, reading and transmitting them at the source, and receiving and writing them at the destination.

In more detail, the transfer of a file with chunking proceeds as follows. First, during the set up phase, we: determine chunk size, S, and concurrency, N, either via some heuristic or by reference to a configuration parameter; create N source-destination data mover pairs, and establish connections between the data movers in each pair; and allocate chunks among data movers. Then, each data mover pair proceeds to transmit chunks, using the extended retrieve (ERET) and extended store (ESTO) rather than the regular retrieve and store (RETR and STOR) commands, so as to allow for partial transfers. Pipelining is also used to ensure that individual data movers are not kept waiting for acknowledgements; as a consequence, chunks should not be too large. The implementation keeps track of which chunks have been transmitted successfully so as to enable efficient partial restarts upon failures.

Optimization of Integrity Checking Calculations

The Globus transfer service is configured by default to perform integrity checking on all files that it transfers, in order to detect data corruption due to such factors as faulty file system I/O or data transmission. Specifically, a Globus source node computes a 32-bit MD5 checksum for a file when reading it to transmit; the corresponding Globus destination node, upon receiving the file, first writes it to storage and then re-reads the file and computes a second checksum. If the two checksums differ, an error is recorded and the file transfer is repeated. Integrity checking errors are rare but do occur, often but not always in bursts due



Figure 4. A sketch of activity over time for a non-chunked (above) and chunked (below) transfers, both with integrity checking. With 'time' on the horizontal axis, the non-chunked transfer must wait until the entire file is transferred (blue) before performing its integrity check (orange), leading to longer end-to-end times. In the chunked file case, not only do multiple GridFTP processes transfer different portions of a file in parallel, but transfer and integrity checks execute concurrently. (For simplicity, we show the integrity check cost being incurred only after the transfer; in practice, some modest cost also is incurred when first reading the file.)

to faulty equipment, and thus this feature is an important element of the Globus service that, as far as we know, is rarely disabled. We note that Globus checksumming is in addition to and independent of checksumming performed by TCP, which only concerns data transmission, not file I/O, and furthermore uses an inadequate 16-bit checksum value (Stone and Partridge 2000).

While essential for most if not all science applications, the costs of both computing the checksums and re-reading the file at the destination can be considerable. Thus, we explored the feasibility of leveraging file chunking to enable concurrency and pipelining of checksum computations. Specifically, we extended the algorithm described above to compute and transmit a partial checksum with each ERET / ESTO pair, thus distributing the costs of checksumming and performing the additional file read operation over multiple data movers, as illustrated in Figure 4.

Experiments and Results

We conducted experiments between three HPC systems: the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory; the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory; and the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory. Our experiments engaged high-performance Lustre file systems (Schwan 2003) at each facility: at ALCF, the Eagle file system; at NERSC, the Perlmutter scratch file system; and at OLCF, the Orion file system. Each facility operates multiple DTNs that are connected at high speeds to their associated file system, and to the ESnet wide area network at 100 Gb/s. We performed five main sets of experiments, to measure:

- The impact of Lustre striping on transfer performance.
- The impact of Globus chunk size on transfer performance.
- The impact of integrity checking on transfer performance.
- The impact of varying the number of files being transferred on transfer performance.
- The impact of chunking on transfers involving varying numbers of files.

All experiments were run with concurrency = 64 and parallelism = 4, and all experiments that involved checksumming employed the default MD5SUM algorithm.

Striping in Lustre

The Lustre file system is employed widely in HPC systems, including at the three facilities considered in this work. We determined during our early investigations that a Lustre configuration parameter, specifically the number of Object Storage Targets (OSTs) over which a file was distributed, has a significant impact on the performance achieved when transferring one or a small number of large files. Here we report on experiments that quantify this impact and guide choices made in subsequent experiments.

Lustre allows administrators and users to specify striping of data across multiple OSTs, at the file system, directory, or individual file level. Striped files can then be accessed concurrently by multiple processes, boosting aggregate data throughput. Striping also enables the storage of files whose size exceeds the capacity of a single OST.



Figure 5. Impact of Lustre stripe count on Globus transfer performance for a 1×2.5 TB file transfer between ALCF (A) and NERSC (N), both with and without chunking. All transfers were conducted without integrity checking.

Striping also has drawbacks such as increased system overhead from heightened network activities and server competition, and can increase the numbers of files corrupted by a single hardware failure. Lustre allows users to manage tradeoffs among these different factors by finetuning striping parameters, including stripe size and count, to optimize performance and reliability for specific needs subject however to limits imposed by system administrators.

Unlike Globus chunking, which impacts both file I/O and network transfers, Lustre striping impacts file I/O alone. Thus, for example, if transferring a chunked file with concurrency level of 2, then at the source endpoint two data movers work concurrently to read independent chunks of the file; if Lustre striping is engaged with striping 3, each data mover read operation retrieves data from three OSTs, and thus overall we would see read operations from the two data movers engaging up to six OSTs. Thus, depending on configuration details, Globus chunking and Lustre striping can either complement each other or work at cross purposes. Care must be taken to configure these different parameters in order to optimize performance and storage scalability.

Here we report on experiments in which we study the impact on data transfer performance of varying the Lustre stripe count, with the goal of determining the Lustre configurations that yield the highest transfer speeds. We measure speeds achieved for a 1×2.5 TB transfer with Lustre stripe counts from 1 to 16, both with and without chunking, and without integrity checking. We perform transfer tests between ALCF and NERSC, in both directions—from ALCF to NERSC (A2N) and from NERSC to ALCF (N2A). The Lustre stripe size is set to 1 MB.

Our results, in Figure 5, show that in most test scenarios transfer speeds vary little (by less than 20%) with Lustre stripe count. However, for NERSC to ALCF transfers with chunking, increasing stripe count from 1 (the default on both systems) to 16 increased throughput by $8.1 \times$, from 3.92 Gb/s to 31.76 Gb/s. (It then declines for a stripe count of 64.) We did not explore this phenomenon further, but observe that it highlights the importance of Lustre configuration for Globus transfers, which in many cases are rate-limited as much by

file system I/O performance as by network bandwidth. In all subsequent experiments, we set the Lustre stripe count to 16.

Impact of Globus Chunk Size

Chunk size, the size of each data segment transferred when using chunking, is a critical parameter for Globus transfers. To determine the impact of chunk size on Globus transfer throughput, we conducted tests between ALCF (A) and NERSC (N) for a variety of chunk sizes. We performed experiments for three 500 GB transfer scenarios, involving 1×500 GB, 5×100 GB, and 20×25 GB files, respectively. We tested each configuration both from ALCF to NERSC (A2N) and NERSC to ALCF (N2A).

We present our results in Figure 6. (In these results and those that follow, we ran each experiment 3–4 times and show in the figure both the average and one standard deviation either side of that average.) In all three cases $(1 \times 500 \text{ GB}, 5 \times 100 \text{ GB}, 20 \times 25 \text{ GB})$, performance tends first to *increase* with chunk size over the range 50 MB to 500 MB and then to *decrease* as chunk size increases further to 5000 MB. We attribute the initial increasing trends to the larger chunk sizes allowing for more effective utilization of network bandwidth, and the subsequent decreases to decreased opportunities for parallelism for larger chunk sizes (e.g., with a chunk size of 5000 MB for a single 500 GB file, only 100 chunks are available, which is less than the product of the number of GridFTP control channel sessions and the number of separate TCP connections, which is $64 \times 4 = 256$.)

We note that the performance gains from increasing chunk size are significantly less (at most 15%) in the 1×500 GB case. We attribute this result to greater bottlenecks and increased competition for resources when handling a single file. This observation is underscored by the fact that the throughput improvement for the 20×25 GB case is significantly greater than that with 5×100 GB files.

Integrity checking Costs

We emphasize that in most cases, Globus integrity checking is crucial for ensuring correct data tranmission. Nevertheless, we want to understand the performance impact of integrity checking so as to guide optimizations. To that end, we conducted tests across ALCF, NERSC, and OLCF in which we measured data transfer performance for the same three tasks considered in the chunk size study (i.e., 1×500 GB, 5×100 GB, and 20×25 GB files), with and without integrity checking. For the chunking experiments, we experimented with different chunk sizes and selected the configuration that delivered the fastest throughput, which in all subsequent experiments was either 200 MB or 500 MB.

We show in Figure 7 throughput with and without integrity checking, both without (above) and with (below) chunking. We observe first (upper subfigures) that integrity checking impacts throughput significantly in the non-chunking cases. For example, transfer speed is roughly halved for both A2N and N2A, an effect that declines somewhat for some source-destination pairs with more files, but remains pronounced. With chunking (lower subfigures), the performance degradation persists but is much less pronounced, particularly when more files are involved.



Figure 6. Impact of Globus chunk sizes on performance achieved for 500 GB transfers between ALCF and NERSC, for different numbers of files. All transfers were conducted with integrity checking.



Figure 7. 500 GB transfers, in from 1 to 20 files, among three facilities, with and without integrity checking. Above: Without chunking. Below: With chunking.

To focus in on these differences, we show in Figure 8 a different view of the A2N and N2A data. Transfer and integrity checking ('checksum') times, averaged across the sets of 4 experiments for which results are provided in Figure 7, are presented in stacked bar chart form, both with and without chunking. We observe, looking left to right, that as the number of files increases from 1 to 20, transfer and integrity checking times both decrease substantially. For example, for transfer tasks without chunking from ALCF to NERSC, the average integrity checking time decreases significantly, from 773 s to 60.7 s, as the number of files increases from 1 to 20. With chunking, the decrease is from 53.7 s to 21.7 s. For the 1×500 GB task, integrity checking times without and with chunking are 773 s and 53.7 s, respectively, emphasizing the importance of chunking for single (or few) large file(s) transfers. Overall, we see that by allowing integrity checking operations to be performed in parallel, chunking enhances throughput significantly. These results underscore the benefits of parallelizing integrity checking for data transfer performance.

Single vs. Multiple File Transfers

Here we investigate how performance varies with the number of files in a task. In addition to the 1×500 GB, 5×100 GB, and 20×25 GB tasks considered in previous experiments, we also consider 100×5 GB and 500×1 GB. We measured throughput both with and without chunking, and with integrity checking. For the tests that employ chunking, we also assessed multiple chunk sizes to determine the configuration that yields optimal performance.

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Our results, in Figure 9, demonstrate that for this fixed total transfer size of 500 GB, it is always faster to transfer multiple smaller files than a single large file, due to the considerable opportunities for parallelism in the former case, although the magnitude of this difference is reduced when chunking is employed. For example, for ALCF to NERSC *without* chunking (the upper row in the figure), increasing the number of files from 1 to 500 boosted transfer speed from 1.98 Gb/s to 46.48 Gb/s: a 23-fold increase. Similarly, for NERSC to ALCF, increasing the file count to 500 results in more than a 28-fold speedup. However, when Globus chunking is enabled (the bottom row), the performance differential between single-file and many-file



Figure 8. Average transfer and integrity check times for three different 500 GB transfer tasks between ALCF and NERSC, with and without chunking. **Above**: Stacked transfer and integrity check times. **Below**: Integrity check times only.

transfers decreases significantly. For the ALCF to NERSC route, the speedup reduces from 23 to 1.9, and for NERSC to ALCF, from 28 to 3.

Transfers With and Without Chunking

Finally, we explore the impacts of chunking on transfer tasks involving 1×500 GB, 5×100 GB, and 20×25 GB files. Our results, in Figure 10, show that chunking has clear benefits when transferring a few files, but that these benefits largely disappear for many files. Specifically, we find that chunking yields peak speedups of up to $9.5 \times$ (for A2N) and $5 \times$ (for A2N) for the single-file and five-file transfer cases, respectively, but for the 20-file case, the maximum speedup diminishes to 1.6 (O2N), while there is even some slowdown in some cases (e.g., O2N). It may be significant that chunking performs better in the 20-file case for the larger round-triptime (RTT) ALCF-NERSC and NERSC-OLCF cases than for the lower RTT ALCF-OLCF case.

Related Work

We summarized above several studies that focused particularly on Globus GridFTP performance. Here we note other relevant work.

Tierney et al. (1994, 1999) conducted pioneering work on striping as a means of accelerating remote data access applications, and Kettimuthu et al. (2010) reviewed factors that can influence the speed of large transfers.

The performance achieved for a particular data transfer can depend significantly on numerous configuration choices, including the network protocol used: e.g., TCP or UDPbased alternatives (He et al. 2002; Gu and Grossman 2007); number of data movers (Kettimuthu et al. 2014); number of TCP streams (Sivakumar et al. 2000; Hacker et al. 2002; Lu et al. 2005); TCP window size (Floyd 2003); TCP variant (Bullot et al. 2003; Leith and Shorten 2004; Wei et al. 2006); degree of pipelining, file system striping; and use of redundant paths (Zhang et al. 2004). Researchers have investigated the impact of such parameters on the performance achieved for different transfer tasks and in different environments (Ito et al. 2005), and proposed methods for selecting such parameters automatically (Prasad et al. 2003; Yildirim et al. 2015; Arslan and Kosar 2018). They have also investigated the impact of transfer parameters on different performance metrics (e.g., latency vs. bandwidth) and on properties other than performance, such as energy consumption (Alan et al. 2015) and impact on competing flows (Hacker et al. 2002; Lu et al. 2005). These are factors that could be considered in Globus, which currently focuses on bandwidth.

In other related work, Liu et al. (2016) discuss blocklevel streaming computation of checksums to accelerate integrity checking, while Arslan and Alhussen (2018) discuss ways in which integrity checking costs can be reduced by careful organization of checksum computations and file I/O operations. Arifuzzaman and Arslan (2021) use online optimization to select transfer parameters. Charyyev and Arslan (2020) examine how detection of file corruption errors can be enhanced by ensuring that checksum calculations are performed on disk-resident rather than cached data. Various researchers have investigated compression of data to be communicated over networks (Cappello et al. 2019; Foster et al. 2017).

Conclusions

We have reported on our development and evaluation of a new capability in the Globus transfer service designed to accelerate movement of individual large files. The key development here is the addition of support for the (logical) chunking of large files into disjoint subsets that are then transmitted by distinct data movers, in ways that also allow for enhanced overlapping of checksum computations with data movement. We demonstrate by careful experimentation that these developments can deliver significant performance benefits. For example, we find that when transferring a single 500GB file from ALCF to NERSC, chunking increases performance by a factor of 9.5.

We can also point to other opportunities for further optimizations. In the current implementation, chunking is enabled manually, either on a per-user basis or by a user labeling a transfer. Large-scale deployment would likely require automation of decisions concerning which transfers to chunk and what chunk size to employ, with the latter potentially being set based on the file in hand. Our results also suggest that significant opportunities remain for further



Figure 9. 500 GB transfers, of from 1 to 500 files, among different pairs of three facilities. **Above**: Without chunking. **Below**: With chunking. Integrity checking is enabled for all tasks



Figure 10. Transfer speed for 500 GB data, in 1×500 GB, 5×100 GB, and 20×25 GB, among the three facilities, with and without chunking. Integrity checking is enabled for all tasks.

optimization of integrity checking, perhaps by application of methods proposed by Arslan et al. (2018).

This work also points to the importance of managing parallel file system striping parameters. We found that for transfers between Lustre file systems, tuning the Lustre stripe count can improve the transfer throughput by up to $8.1 \times$. Thus we may want Globus to allow the administrator of a Globus collection that contains a few large files to enable chunking for that dataset. The specified stripe width would then need to be communicated from the Globus service to the local Globus Connect Server agent, which in turn would set the stripe width using the API or CLI provided by the file system.

Our experiments also provide insights into the growing costs of integrity checking as increased network speeds reduce the time taken for data transmission. Such trends may motivate the use of alternative checksumming algorithms.

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References

- Ismail Alan, Engin Arslan, and Tevfik Kosar. Energy-aware data transfer algorithms. In *International Conference for High Performance Computing, Networking, Storage and Analysis*, pages 1–12. IEEE, New York, NY, USA, 2015.
- Francis Alexander, Ann Almgren, John Bell, Amitava Bhattacharjee, Jacqueline Chen, Phil Colella, David Daniel, Jack DeSlippe, Lori Diachin, Erik Draeger, Anshu Dubey, Thom Dunning, Thomas Evans, Ian Foster, Marianne Francois, Tim Germann, Mark Gordon, Salman Habib, Mahantesh Halappanavar, Steven Hamilton, William Hart, Zhenyu Huang, Aimee Hungerford, Daniel Kasen, Paul R. C. Kent, Tzanio Kolev, Douglas B. Kothe, Andreas Kronfeld, Ye Luo, Paul Mackenzie, David McCallen, Bronson Messer, Sue Mniszewski, Chris Oehmen, Amedeo Perazzo, Danny Perez, David Richards, William J. Rider, Rob Rieben, Kenneth Roche,

Andrew Siegel, Michael Sprague, Carl Steefel, Rick Stevens, Madhava Syamlal, Mark Taylor, John Turner, Jean-Luc Vay, Artur F. Voter, Theresa L. Windus, and Katherine Yelick. Exascale applications: Skin in the game. *Philosophical Transactions of the Royal Society A*, 378(2166):20190056, 2020.

- William Allcock. GridFTP: Protocol extensions to FTP for the grid. In *Global Grid Forum*, 2003, 2003. https://zenodo. org/records/6828.
- William Allcock, Ian Foster, Steven Tuecke, Ann Chervenak, and Carl Kesselman. Protocols and services for distributed dataintensive science. In *AIP Conference Proceedings*, volume 583, pages 161–163. American Institute of Physics, 2001.
- William Allcock, John Bresnahan, Rajkumar Kettimuthu, Michael Link, Catalin Dumitrescu, Ioan Raicu, and Ian Foster. The Globus striped GridFTP framework and server. In ACM/IEEE Conference on Supercomputing, page 54. IEEE Computer Society, 2005.
- Md Arifuzzaman and Engin Arslan. Online optimization of file transfers in high-speed networks. In *International Conference for High Performance Computing, Networking, Storage and Analysis*, pages 1–13, 2021.
- Engin Arslan and Ahmed Alhussen. A low-overhead integrity verification for big data transfers. In *International Conference* on *Big Data*, pages 4227–4236. IEEE, 2018.
- Engin Arslan and Tevfik Kosar. High-speed transfer optimization based on historical analysis and real-time tuning. *IEEE Transactions on Parallel and Distributed Systems*, 29(6):1303– 1316, 2018.
- Engin Arslan, Bahadir A Pehlivan, and Tevfik Kosar. Big data transfer optimization through adaptive parameter tuning. *Journal of Parallel and Distributed Computing*, 120:89–100, 2018.
- Lakshmi N Bairavasundaram, Andrea C Arpaci-Dusseau, Remzi H Arpaci-Dusseau, Garth R Goodson, and Bianca Schroeder. An analysis of data corruption in the storage stack. *ACM Transactions on Storage*, 4(3):1–28, 2008.
- Hadrien Bullot, Roger Les Cottrell, and Richard Hughes-Jones. Evaluation of advanced TCP stacks on fast long-distance production networks. *Journal of Grid Computing*, 1(4):345– 359, 2003.
- Franck Cappello, Sheng Di, Sihuan Li, Xin Liang, Ali Murat Gok, Dingwen Tao, Chun Hong Yoon, Xin-Chuan Wu, Yuri Alexeev, and Frederic T Chong. Use cases of lossy compression for floating-point data in scientific data sets. *The International Journal of High Performance Computing Applications*, 33(6): 1201–1220, 2019.
- Kyle Chard, Steven Tuecke, and Ian Foster. Globus: Recent enhancements and future plans. In *XSEDE16 Conference on Diversity, Big Data, and Science at Scale*, pages 1–8, 2016.
- Batyr Charyyev and Engin Arslan. RIVA: Robust integrity verification algorithm for high-speed file transfers. *IEEE Transactions on Parallel and Distributed Systems*, 31(6):1387–1399, 2020.
- Eli Dart, Lauren Rotman, Brian Tierney, Mary Hester, and Jason Zurawski. The Science DMZ: A network design pattern for data-intensive science. In *International Conference on High Performance Computing, Networking, Storage and Analysis*, pages 1–10, 2013.
- Eli Dart, William Allcock, Wahid Bhimji, Tim Boerner, Ravinderjeet Cheema, Andrew Cherry, Brent Draney, Salman Habib,

Damian Hazen, Jason Hill, Matt Kollross, Suzanne Parete-Koon, Daniel Pelfrey, Adrian Pope, Jeff Porter, and David Wheeler. Petascale DTN project host network configurations and test data set, 2021a. https://zenodo.org/ records/3880669.

- Eli Dart, William Allcock, Wahid Bhimji, Tim Boerner, Ravinderjeet Cheema, Andrew Cherry, Brent Draney, Salman Habib, Damian Hazen, Jason Hill, Matt Kollross, Suzanne Parete-Koon, Daniel Pelfrey, Adrian Pope, Jeff Porter, and David Wheeler. The Petascale DTN project: High performance data transfer for HPC facilities. arXiv preprint arXiv:2105.12880, 2021b.
- Sally Floyd. HighSpeed TCP for large congestion windows RFC 3649, Experimental, 2003. URL http://www.faqs.org/rfcs/rfc3649.html.
- Ian Foster. Globus Online: Accelerating and democratizing science through cloud-based services. *IEEE Internet Computing*, 15 (3):70–73, 2011.
- Ian Foster, Mark Ainsworth, Bryce Allen, Julie Bessac, Franck Cappello, Jong Youl Choi, Emil Constantinescu, Philip E Davis, Sheng Di, Wendy Di, Hanqi Guo, Scott Klasky, Kerstin Kleese Van Dam, Tahsin Kurc, Abid Malik, Kshitij Mehta, Klaus Mueller, Todd Munson, George Ostouchov, Manish Parashar, Tom Peterka, Line Pouchard, Dingwen Tao, Ozan Tugluk, Stefan Wild, Matthew Wolf, Justin Wozniak, Wei Xu, and Shinjae Yoo. Computing just what you need: Online data analysis and reduction at extreme scales. In 23rd International Conference on Parallel and Distributed Computing, pages 3– 19. Springer, 2017.
- Yunhong Gu and Robert L Grossman. UDT: UDP-based data transfer for high-speed wide area networks. *Computer Networks*, 51(7):1777–1799, 2007.
- Thomas J Hacker, Brian D Athey, and Brian Noble. The end-to-end performance effects of parallel TCP sockets on a lossy widearea network. In *16th International Parallel and Distributed Processing Symposium*, pages 10–pp, New York, NY, USA, 2002. IEEE.
- Eric He, Jason Leigh, Oliver Yu, and Thomas A DeFanti. Reliable blast UDP: Predictable high performance bulk data transfer. In *International Conference on Cluster Computing*, pages 317– 324, New York, NY, USA, 2002. IEEE.
- Katrin Heitmann, Thomas D. Uram, Hal Finkel, Nicholas Frontiere, Salman Habib, Adrian Pope, Esteban Rangel, Joseph Hollowed, Danila Korytov, Patricia Larsen, Benjamin S. Allen, Kyle Chard, and Ian Foster. HACC cosmological simulations: First data release. *The Astrophysical Journal Supplement Series*, 244(1):17, 2019.
- Takeshi Ito, Hiroyuki Ohsaki, and Makoto Imase. On parameter tuning of data transfer protocol GridFTP for wide-area grid computing. In 2nd International Conference on Broadband Networks, pages 1338–1344, New York, NY, USA, 2005. IEEE.
- Rajkumar Kettimuthu, Alex Sim, Dan Gunter, Bill Allcock, Peer-Timo Bremer, John Bresnahan, Andrew Cherry, Lisa Childers, Eli Dart, Ian Foster, Kevin Harms, Jason Hick, Jason Lee, Michael Link, Jeff Long, Keith Miller, Vijaya Natarajan, Valerio Pascucci, Ken Raffenetti, David Ressman, Dean Williams, Loren Wilson, and Linda Winkler. Lessons learned from moving Earth System Grid data sets over a 20 Gbps widearea network. In 19th ACM International Symposium on High

Performance Distributed Computing, pages 316–319, 2010.

- Rajkumar Kettimuthu, Gayane Vardoyan, Gagan Agrawal, and P. Sadayappan. Modeling and optimizing large-scale wide-area data transfers. In *14th IEEE/ACM International Symposium* on Cluster, Cloud, and Grid Computing, CCGRID '14, page 196–205. IEEE Press, 2014. ISBN 9781479927838.
- Rajkumar Kettimuthu, Gayane Vardoyan, Gagan Agrawal, P. Sadayappan, and Ian Foster. An elegant sufficiency: load-aware differentiated scheduling of data transfers. In International Conference for High Performance Computing, Networking, Storage and Analysis, SC '15, New York, NY, USA, 2015. Association for Computing Machinery.
- Rajkumar Kettimuthu, Zhengchun Liu, David Wheeler, Ian Foster, Katrin Heitmann, and Franck Cappello. Transferring a petabyte in a day. *Future Generation Computer Systems*, 88:191–198, 2018.
- Lukasz Lacinski, Lee Liming, Steven Turoscy, Cameron Harr, Kyle Chard, Eli Dart, Paul Durack, Sasha Ames, Forrest M. Hoffman, and Ian T. Foster. Automated, reliable, and efficient continental-scale replication of 7.3 PB climate simulation data: A case study, 2024. Arxiv 2404.19717.
- Douglas Leith and Robert Shorten. H-TCP: TCP for high-speed and long-distance networks. In 2nd International Workshop on Protocols for Fast Long-Distance Networks, 2004.
- Si Liu, Eun-Sung Jung, Rajkumar Kettimuthu, Xian-He Sun, and Michael Papka. Towards optimizing large-scale data transfers with end-to-end integrity verification. In *International Conference on Big Data*, pages 3002–3007. IEEE, 2016.
- Yuanlai Liu, Zhengchun Liu, Rajkumar Kettimuthu, Nageswara Rao, Zizhong Chen, and Ian Foster. Data transfer between scientific facilities–bottleneck analysis, insights and optimizations. In 19th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, pages 122–131. IEEE, 2019.
- Zhengchun Liu, Prasanna Balaprakash, Rajkumar Kettimuthu, and Ian Foster. Explaining wide area data transfer performance. In 26th International Symposium on High-Performance Parallel and Distributed Computing, pages 167–178, 2017.
- Zhengchun Liu, Rajkumar Kettimuthu, Ian Foster, and Nageswara SV Rao. Cross-geography scientific data transferring trends and behavior. In 27th International Symposium on High-Performance Parallel and Distributed Computing, pages 267–278. IEEE, 2018a.
- Zhengchun Liu, Rajkumar Kettimuthu, Ian T Foster, and Yuanlai Liu. A comprehensive study of wide area data movement at a scientific computing facility. In 38th International Conference on Distributed Computing Systems, pages 1604–1611, 2018b.
- Zhengchun Liu, Ahsan Ali, Peter Kenesei, Antonino Miceli, Hemant Sharma, Nicholas Schwarz, Dennis Trujillo, Hyunseung Yoo, Ryan Coffee, Naoufal Layad, Jana Thayer, Ryan Herbst, Chunhong Yoon, and Ian Foster. Bridging data center AI systems with edge computing for actionable information retrieval. In 3rd Annual Workshop on Extremescale Experiment-in-the-Loop Computing, pages 15–23. IEEE, 2021a.
- Zhengchun Liu, Rajkumar Kettimuthu, Joaquin Chung, Rachana Ananthakrishnan, Michael Link, and Ian Foster. Design and evaluation of a simple data interface for efficient data transfer across diverse storage. ACM Transactions on Modeling and Performance Evaluation of Computing Systems, 6(1), 2021b.

- Dong Lu, Yi Qiao, Peter A Dinda, and Fabián E Bustamante. Modeling and taming parallel TCP on the wide area network. In 19th IEEE International Parallel and Distributed Processing Symposium, pages 10–pp, New York, NY, USA, 2005. IEEE.
- Ravi S Prasad, Manish Jain, and Constantinos Dovrolis. Socket buffer auto-sizing for high-performance data transfers. *Journal* of Grid computing, 1(4):361–376, 2003.
- Markus Reichstein, Gustau Camps-Valls, Bjorn Stevens, Martin Jung, Joachim Denzler, Nuno Carvalhais, and Prabhat. Deep learning and process understanding for data-driven Earth system science. *Nature*, 566(7743):195–204, 2019.
- Philip Schwan. Lustre: Building a file system for 1000node clusters. In *Linux Symposium*, pages 380–386, 2003. https://www.kernel.org/doc/ols/2003/ ols2003-pages-380-386.pdf.
- Harimath Sivakumar, Stuart Bailey, and Robert L Grossman. PSockets: The case for application-level network striping for data intensive applications using high speed wide area networks. In ACM/IEEE Conference on Supercomputing, pages 38–38, New York, NY, USA, 2000. IEEE.
- Jonathan Stone and Craig Partridge. When the CRC and TCP checksum disagree. ACM SIGCOMM Computer Communication Review, 30(4):309–319, 2000.
- Brian Tierney, Jason Lee, Ling Tony Chen, Hanan Herzog, Gary Hoo, Guojun Jin, and William E Johnston. Distributed parallel data storage systems: A scalable approach to high speed image servers. In 2nd ACM International Conference on Multimedia, pages 399–405, 1994.
- Brian L Tierney, Jason Lee, Brian Crowley, Mason Holding, Jeremy Hylton, and Fred L Drake. A network-aware distributed storage cache for data intensive environments. In 8th International Symposium on High Performance Distributed Computing, pages 185–193. IEEE, 1999.
- David X Wei, Cheng Jin, Steven H Low, and Sanjay Hegde. FAST TCP: Motivation, architecture, algorithms, performance. *IEEE/ACM Transactions on Networking*, 14(6):1246–1259, 2006.
- Esma Yildirim, JangYoung Kim, and Tevfik Kosar. How GridFTP pipelining, parallelism and concurrency work: A guide for optimizing large dataset transfers. In 2012 SC Companion: High Performance Computing, Networking Storage and Analysis, pages 506–515. IEEE, 2012.
- Esma Yildirim, Engin Arslan, Jangyoung Kim, and Tevfik Kosar. Application-level optimization of big data transfers through pipelining, parallelism and concurrency. *IEEE Transactions on Cloud Computing*, 4(1):63–75, 2015.
- Ming Zhang, Junwen Lai, Arvind Krishnamurthy, Larry L Peterson, and Randolph Y Wang. A transport layer approach for improving end-to-end performance and robustness using redundant paths. In USENIX Annual Technical Conference, pages 99–112, New York, NY, USA, 2004. USENIX.

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