Optimizing Noncontiguous Accesses in MPI-IO*

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Abstract

The I/O access patterns of many parallel applications consist of accesses to a large number of small, noncontiguous pieces of data. If an application's I/O needs are met by making many small, distinct I/O requests, however, the I/O performance degrades drastically. To avoid this problem, MPI-IO allows users to access noncontiguous data with a single I/O function call, unlike in Unix I/O. In this paper, we explain how critical this feature of MPI-IO is for high performance and how it enables implementations to perform optimizations. We first provide a classification of the different ways of expressing an application's I/O needs in MPI-IO—we classify them into four *levels*, called level 0 through level 3. We demonstrate that, for applications with noncontiguous access patterns, the I/O performance improves dramatically if users write their applications to make level-3 requests (noncontiguous, collective) rather than level-0 requests (Unix style). We then describe how our MPI-IO implementation, ROMIO, delivers high performance for noncontiguous requests. We explain in detail the two key optimizations ROMIO performs: data sieving for noncontiguous requests from one process and collective I/O for noncontiguous requests from multiple processes. We describe how we have implemented these optimizations portably on multiple machines and file systems, controlled their memory requirements, and also achieved high performance. We demonstrate the performance and portability with performance results for three applications—an astrophysics-application template (DIST3D), the NAS BTIO benchmark, and an unstructured code (UNSTRUC)—on five different parallel machines: HP Exemplar, IBM SP, Intel Paragon, NEC SX-4, and SGI Origin2000.

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1 Introduction

I/O is a major bottleneck in many parallel applications. Although the I/O subsystems of parallel machines may be designed for high performance, a large number of applications achieve only about a tenth or less of the peak I/O bandwidth. One of the main reasons for poor application-level I/O performance is that I/O systems are optimized for large accesses (on the order of megabytes), whereas many parallel applications make lots of small requests (on the order of kilobytes or even less). These small requests occur for the following reasons:

- In many parallel applications (for example, those that access distributed arrays from files) each process needs to access a large number of relatively small pieces of data that are not contiguously located in the file [1, 3, 11, 19, 18, 24].
- Most parallel file systems have a Unix-like API (application programming interface) that allows a user to access only a single, contiguous chunk of data at a time from a file.[1] Noncontiguous data sets must therefore be accessed by making separate function calls to access each individual contiguous piece.

With such an interface, the file system cannot easily detect the overall access pattern of one process individually or that of a group of processes collectively. Consequently, the file system is constrained in the optimizations it can perform. Many parallel file systems also provide their own extensions to or variations of the traditional Unix interface, and these variations make programs nonportable.

To overcome the performance and portability limitations of existing parallel I/O interfaces, the MPI Forum (made up of parallel-computer vendors, researchers, and applications scientists) defined a new interface for parallel I/O as part of the MPI-2 standard [9]. This interface is commonly referred to as MPI-IO. MPI-IO is a rich interface with many features designed specifically for performance and portability. Multiple implementations of MPI-IO, both portable and machine specific, are available [5, 7, 13, 15, 26]. To avoid the above-mentioned problem of many distinct, small I/O requests, MPI-IO allows users to specify the entire noncontiguous access pattern and read or write all the data with a single function call. MPI-IO also allows users to specify collectively the I/O requests of a group of processes, thereby providing the implementation with even greater access information and greater scope for optimization.

A simple way to port a Unix I/O program to MPI-IO is to replace all Unix I/O functions with their MPI-IO equivalents. For applications with noncontiguous access patterns, however, such a simple port is unlikely to improve performance. In this paper, we demonstrate that to get significant performance benefits with MPI-IO, users must use some of MPI-IO's advanced features, particularly noncontiguous accesses and collective I/O.

An application can be written in many different ways with MPI-IO. We provide a classification of the different ways of expressing an application's I/O access pattern in MPI-IO. We classify them into four *levels*, called level 0 through level 3. We explain why, for high performance, users should write their application programs to make level-3 MPI-IO requests (noncontiguous, collective) rather than level-0 requests (Unix style). Similarly, I/O libraries, such as HDF5 [27], that are written on top of MPI-IO should also strive to make level-3 requests.

We describe how our portable implementation of MPI-IO, called ROMIO, delivers high performance when the user makes noncontiguous, collective I/O requests. We explain in detail the two key optimizations ROMIO performs: data sieving for noncontiguous requests from one process and collective I/O for noncontiguous requests from multiple processes. We describe how we have implemented these optimizations portably on multiple machines and file systems, controlled their memory requirements, and also achieved high performance. We demonstrate the performance and portability with performance results for three applications on five different parallel machines: HP Exemplar, IBM SP, Intel Paragon, NEC SX-4, and SGI Origin2000. The applications we used are the following:

1. DIST3D, a template representing the I/O access pattern in an astrophysics application, ASTRO3D [24], from the University of Chicago. This application does a large amount of I/O and is representative of applications that access distributed arrays.

[1] Unix does have functions `readv` and `writev`, but they allow noncontiguity only in memory and not in the file. POSIX has a function `lio_listio` that allows the user to specify a list of requests at a time. However, the requests in the list can be a mixture of reads and writes, and the POSIX standard says that each of the requests will be submitted as a separate nonblocking request [6]. Therefore, POSIX implementations cannot optimize I/O for the entire list of requests, for example, by performing data sieving as described in Section 5. Furthermore, since the `lio_listio` interface is not collective, implementations cannot perform collective I/O.

2. The NAS BTIO benchmark [5], a well-known MPI-IO benchmark developed at NASA Ames Research Center.
3. An unstructured code (UNSTRUC) from Sandia National Laboratories that is representative of applications that have irregular access patterns.

The rest of this paper is organized as follows. In Section 2, we explain how MPI-IO supports noncontiguous file accesses. In Section 3, we present a classification of the different ways of expressing an application's I/O access pattern in MPI-IO. We describe our MPI-IO implementation, ROMIO, in Section 4. In Sections 5 and 6, we describe in detail how data sieving and collective I/O are implemented in ROMIO. Performance results are presented and analyzed in Section 7, followed by conclusions in Section 8.

2 Noncontiguous Accesses in MPI-IO

In MPI, the amount of data a function sends, receives, reads, or writes is specified in terms of instances of a *datatype* [10]. Datatypes in MPI are of two kinds: basic and derived. Basic datatypes correspond to the basic datatypes in the host programming language—integers, floating-point numbers, and so forth. In addition, MPI provides datatype-constructor functions to create derived datatypes consisting of multiple basic datatypes located either contiguously or noncontiguously. The different kinds of datatype constructors in MPI are as follows:

- **contiguous** Creates a new datatype consisting of contiguous copies of an existing datatype.
- **vector/hvector** Creates a new datatype consisting of equally spaced copies of existing datatype.
- **indexed/hindexed/indexed_block** Allows replication of a datatype into a sequence of blocks, each containing multiple copies of an existing datatype; the blocks may be unequally spaced.
- **struct** The most general datatype constructor, which allows each block to consist of replications of different datatypes.
- **subarray** Creates a datatype that corresponds to a subarray of a multidimensional array.
- **darray** Creates a datatype that describes a process's local array obtained from a regular distribution a multidimensional global array.

The datatype created by a datatype constructor can be used as an input datatype to another datatype constructor. Any noncontiguous data layout can therefore be represented in terms of a derived datatype.

MPI-IO uses MPI datatypes to describe the data layout in the user's buffer in memory and also to define the data layout in the file. The data layout in memory is specified by the `datatype` argument in each read/write function in MPI-IO. The data layout in the file is defined by the *file view*. When the file is first opened, the default file view is the entire file; that is, the entire file is visible to the process, and data will be read/written contiguously starting from the location specified by the read/write function. A process can change its file view at any time by using the function `MPI_File_set_view`, which takes as argument an MPI datatype called the *filetype*. From then on, data will be read from or written to only those parts of the file specified by the filetype; any "holes" will be skipped. The file view and the data layout in memory can be defined by using any MPI basic or derived datatype; therefore, any general noncontiguous access pattern can be compactly represented.

Several studies have shown that, in many parallel applications, each process needs to access a number of relatively small, noncontiguous portions of a file [1, 3, 11, 19, 24]. From a performance perspective, it is critical that the I/O interface can express such an access pattern, as it enables the implementation to optimize the I/O request. The optimizations typically allow the physical I/O to take place in large, contiguous chunks, even though the user's request may be noncontiguous. MPI-IO's file views, therefore, are critical for performance. Users must ensure that they describe noncontiguous access patterns in terms of a file view and then call a single I/O function; they must not try to access each contiguous portion separately as in Unix I/O.

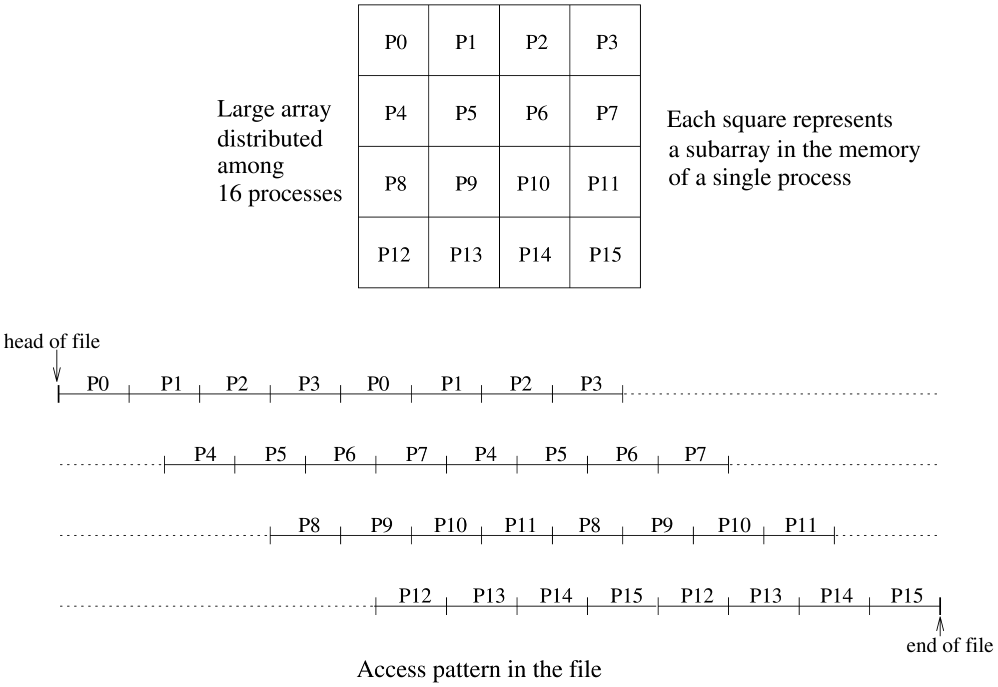


Figure 1: Distributed-array access

3 A Classification of I/O Request Structures

Any application has a particular "I/O access pattern" based on its I/O needs. The same I/O access pattern can be presented to the I/O system in different ways, however, depending on which I/O functions the application uses and how. We classify the different ways of expressing I/O access patterns in MPI-IO into four "levels," level 0 through level 3. We explain this classification with the help of an example, accessing a distributed array from a file, which is a common access pattern in parallel applications. (One of the benchmark applications we used for performance evaluation, DIST3D, has such an access pattern.)

Consider a two-dimensional array distributed among 16 processes in a (block, block) fashion as shown in Figure 1. The array is stored in a single file corresponding to the global array in row-major order, and each process needs to read its local array from the file. (Note that the file could be physically distributed among disks, but appears to the program as a single logical file.) The data distribution among processes and the array storage order in the file are such that the file contains the first row of the local array of process 0, followed by the first row of the local array of process 1, the first row of the local array of process 2, the first row of the local array of process 3, then the second row of the local array of process 0, the second row of the local array of process 1, and so on. In other words, the local array of each process is located noncontiguously in the file.

Figure 2 shows four ways in which a user can write a program in which each process reads its local array from this file using MPI-IO. In level 0, each process does Unix-style accesses—one independent read request for each row in the local array. Level 1 is similar to level 0 except that it uses collective I/O functions, which indicates to the implementation that all processes that together opened the file will call this function, each with its own access information. Independent I/O functions, on the other hand, convey no information about what other processes will do. In level 2, each process creates an MPI derived datatype to describe the noncontiguous access pattern, defines a file view, and calls independent I/O functions. Level 3 is similar to level 2 except that it uses collective I/O functions.

The four levels represent increasing amounts of data per request, as illustrated in Figure 3.[2] The more the amount

[2] In this figure, levels 1 and 2 represent the same amount of data per request, but, in general, when the number of noncontiguous accesses per process is greater than the number of processes, level 2 represents more data than level 1.

```
MPI_File_open(..., "filename", ..., &fh)
for (i=0; i<n_local_rows; i++) {
   MPI_File_seek(fh, ...)
   MPI_File_read(fh, row[i], ...)
}
MPI_File_close(&fh)
```

Level 0
(many independent, contiguous requests)

```
MPI_File_open(MPI_COMM_WORLD, "filename", ..., &fh)
for (i=0; i<n_local_rows; i++) {
   MPI_File_seek(fh, ...)
   MPI_File_read_all(fh, row[i], ...)
}
MPI_File_close(&fh)
```

Level 1
(many collective, contiguous requests)

```
MPI_Type_create_subarray(..., &subarray, ...)
MPI_Type_commit(&subarray)
MPI_File_open(..., "filename", ..., &fh)
MPI_File_set_view(fh, ..., subarray, ...)
MPI_File_read(fh, local_array, ...)
MPI_File_close(&fh)
```

Level 2
(single independent, noncontiguous request)

```
MPI_Type_create_subarray(.., &subarray, ...)
MPI_Type_commit(&subarray)
MPI_File_open(MPI_COMM_WORLD, "filename", ..., &fh)
MPI_File_set_view(fh, ..., subarray, ...)
MPI_File_read_all(fh, local_array, ...)
MPI_File_close(&fh)
```

Level 3
(single collective, noncontiguous request)

Figure 2: Pseudo-code that shows four ways of accessing the data in Figure 1 with MPI-IO

of data per request, the greater is the opportunity for the implementation to deliver higher performance. Users should therefore strive to express their I/O requests as level 3 rather than level 0. How good the performance is at each level depends, of course, on how well the implementation takes advantage of the extra access information at each level.

If an application needs to access only large, contiguous pieces of data, level 0 is equivalent to level 2, and level 1 is equivalent to level 3. Users need not create derived datatypes in such cases, as level-0 requests themselves will likely perform well. Most parallel applications, however, do not fall into this category. Several studies of I/O access patterns in parallel applications [1, 3, 11, 19, 18, 24] have shown that each process in a parallel program may need to access a number of relatively small, noncontiguous portions of a file. From a performance perspective, it is critical that the I/O interface can express such an access pattern, as it enables the implementation to optimize the I/O request. The optimizations typically allow the physical I/O to take place in large, contiguous chunks, even though the user's request may be noncontiguous. Users, therefore, should ensure that they describe noncontiguous access patterns in terms of a file view and then call a single I/O function; they should not try to access each contiguous portion separately as in Unix I/O. Figure 4 shows the detailed code for creating a derived datatype, defining a file view, and making a level-3 I/O request for the distributed-array example of Figure 1.

4 ROMIO Implementation of MPI-IO

We have developed a freely available, portable implementation of MPI-IO, called ROMIO [14, 25]. It runs on at least the following machines: IBM SP; Intel Paragon; Cray T3E; HP Exemplar; SGI Origin2000; NEC SX-4; other symmetric multiprocessors from HP, SGI, Sun, DEC, and IBM; and networks of workstations (Sun, SGI, HP, IBM, DEC, Linux, and FreeBSD). Supported file systems are IBM PIOFS, Intel PFS, HP HFS, SGI XFS, NEC SFS, NFS, PVFS, and any Unix file system (UFS).

A key component of ROMIO that enables such a portable MPI-IO implementation is an internal layer called ADIO [23]. ADIO, an abstract-device interface for I/O, is a mechanism for implementing parallel I/O APIs portably on multiple file systems. ADIO consists of a small set of basic functions for parallel I/O. We have implemented MPI-

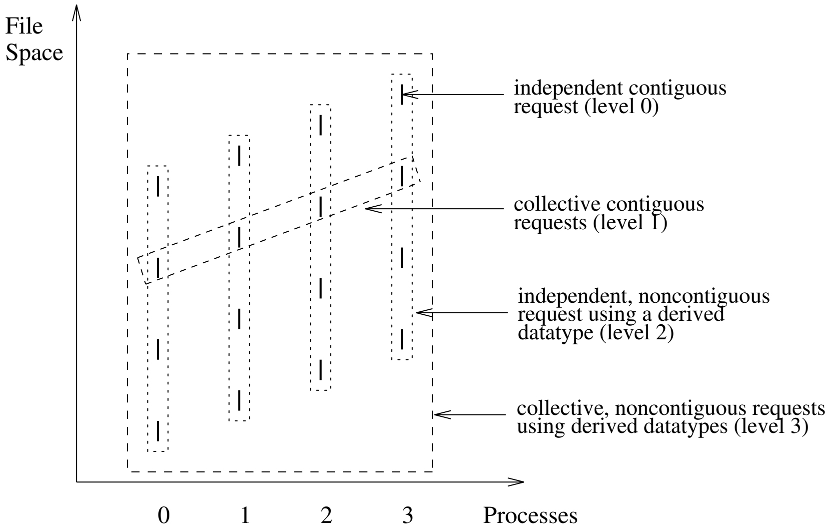


Figure 3: The four levels representing increasing amounts of data per request

```
array_of_gsizes[0] = num_global_rows;
array_of_gsizes[1] = num_global_cols;
array_of_distribs[0] = array_of_distribs[1] = MPI_DISTRIBUTE_BLOCK;
array_of_dargs[0] = array_of_dargs[1] = MPI_DISTRIBUTE_DFLT_DARG;
array_of_psizes[0] = array_of_psizes[1] = 4;
MPI_Comm_rank(MPI_COMM_WORLD, &mynode);
MPI_Type_create_darray(16, mynode, 2, array_of_gsizes, array_of_distribs,
                       array_of_dargs, array_of_psizes, MPI_ORDER_C,
                       MPI_FLOAT, &filetype);
MPI_Type_commit(&filetype);
local_array_size = num_local_rows * num_local_cols;
MPI_File_open(MPI_COMM_WORLD, "/pfs/test", MPI_MODE_CREATE | MPI_MODE_RDWR,
              MPI_INFO_NULL, &fh);
MPI_File_set_view(fh, 0, MPI_FLOAT, filetype, "native", MPI_INFO_NULL);
MPI_File_read_all(fh, local_array, local_array_size, MPI_FLOAT, &status);
MPI_File_close(&fh);
```

Figure 4: Detailed code for the distributed-array example of Figure 1 using a level-3 request

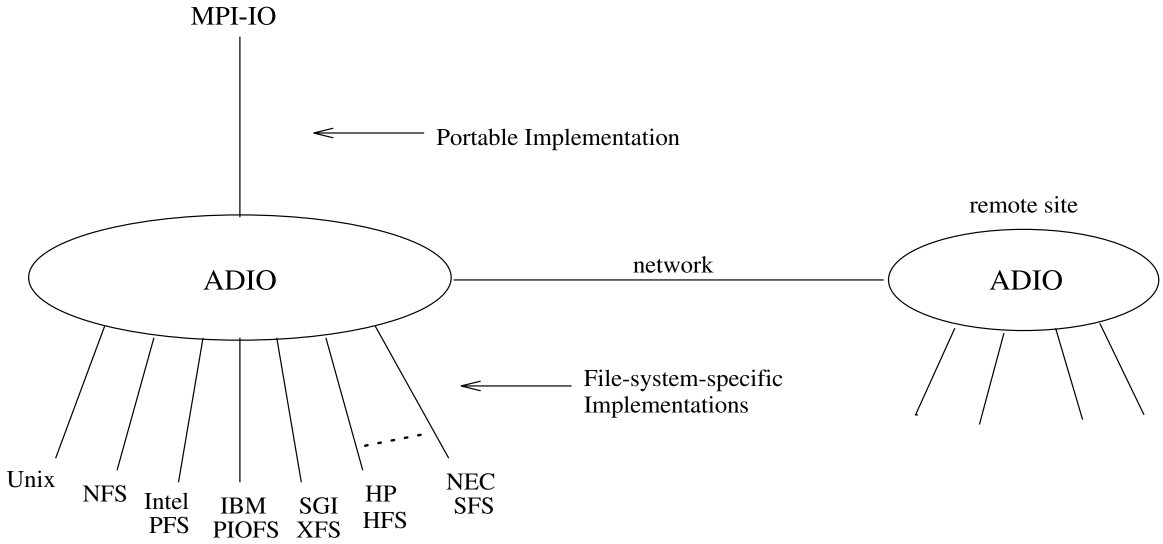


Figure 5: ROMIO Architecture: MPI-IO is implemented portably on top of an abstract-device interface called ADIO, and ADIO is optimized separately for different file systems.

IO portably on top of ADIO, and only ADIO is implemented separately on each different file system (see Figure 5). ADIO thus separates the machine-dependent and machine-independent aspects involved in implementing MPI-IO.

The following two sections describe the optimizations ROMIO performs for noncontiguous I/O requests, namely, data sieving for noncontiguous requests from one process and collective I/O for noncontiguous requests from multiple processes.

5 Data Sieving

To reduce the effect of high I/O latency, it is critical to make as few requests to the file system as possible. Data sieving is a technique that enables an implementation to make a few large, contiguous requests to the file system even if the user's request consists of several small, noncontiguous accesses. Data sieving was used in the PASSION I/O library [20, 22] to access sections of out-of-core arrays. We have extended it in ROMIO to handle *any* general noncontiguous access pattern (as can be described by an MPI datatype) and to use only a constant amount of extra memory regardless of the access pattern. The user can control the memory usage dynamically by setting a runtime parameter.

Figure 6 illustrates the basic idea of data sieving. Assume that the user has made a single read request for five non-contiguous pieces of data. Instead of reading each noncontiguous piece separately, ROMIO reads a single contiguous chunk of data starting from the first requested byte up to the last requested byte into a temporary buffer in memory. It then extracts the requested portions from the temporary buffer and places them in the user's buffer. The user's buffer happens to be contiguous in this example, but it could well be noncontiguous.

A potential problem with this simple algorithm is its memory requirement. The temporary buffer into which data is first read must be as large as the *extent* of the user's request, where extent is defined as the total number of bytes between the first and last byte requested (including holes). The extent can potentially be very large—much larger than the amount of memory available for the temporary buffer—because the holes (unwanted data) between the requested data segments could be very large. The basic algorithm, therefore, must be modified to make its memory requirement independent of the extent of the user's request.

ROMIO uses a user-controllable parameter that defines the maximum amount of contiguous data that a process can read at a time during data sieving. This value also represents the maximum size of the temporary buffer. The default value is 4 Mbytes (on each process), but the user can change it at run time via MPI-IO's hints mechanism. If the extent

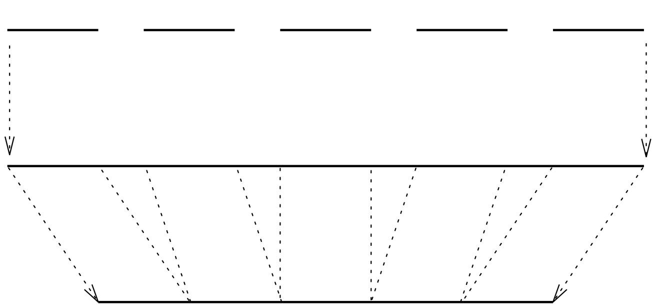


Figure 6: Data sieving

of the user's request is larger than the value of this parameter, ROMIO performs data sieving in parts, reading only as much data at a time as defined by the parameter.

The advantage of data sieving is that data is always accessed in large chunks, although at the cost of reading more data than needed. For many common access patterns, the holes between useful data are not unduly large, and the advantage of accessing large chunks far outweighs the cost of reading extra data. In some access patterns, however, the holes are so large that the cost of reading the extra data outweighs the cost of accessing large chunks. The BTIO benchmark (see Section 7), for example, has such an access pattern. An intelligent data-sieving algorithm can handle such cases as well. The algorithm can analyze the user's request and calculate the sizes of holes in it. Based on empirically determined prior knowledge of how large holes can get before data sieving is no longer beneficial, the algorithm can decide whether to perform data sieving or access each contiguous data segment separately.

Data sieving can similarly be used for writing data. A read-modify-write must be performed, however, to avoid destroying the data already present in the holes between contiguous data segments. For writing with data sieving, ROMIO first reads a contiguous chunk of data from the file into a temporary buffer in memory, copies data from the user's buffer into appropriate locations in the temporary buffer, and then writes the temporary buffer back to the file. The portion of the file being accessed must also be locked during the read-modify-write to prevent concurrent updates by other processes.

ROMIO also uses another user-controllable parameter that defines the maximum amount of contiguous data that a process can write at a time during data sieving. This parameter, by default, has a smaller value than the one used for reading, because writing involves locking the region of the file being accessed. If the region being locked is too large, many processes remain idle waiting for the lock to be released. Consequently, parallelism in I/O is lost, and performance decreases. On the other hand, if the region being locked is too small, there is greater parallelism, but the size of each I/O access also decreases, and performance is again adversely affected. In other words, a compromise is needed between allowing greater concurrency and having large access sizes. We determined experimentally that a write size of 512 Kbytes provides a good trade-off between the two conflicting goals and gives good performance. ROMIO therefore sets the default value of the maximum buffer size for writing to 512 Kbytes. The user can, of course, change this value at run time.

One could argue that most file systems perform data sieving anyway because they perform caching. That is, even if the user makes many small I/O requests, the file system always reads multiples of disk blocks and may also perform a read-ahead. The user's requests, therefore, may be satisfied out of the file-system cache. Our experience, however, has been that the cost of making many system calls, each for small amounts of data, is extremely high, despite the caching performed by the file system. In most cases, it is more efficient to make a few system calls for large amounts of data and extract the needed data. (See the performance results in Section 7.)

ROMIO performs data sieving when the user makes a level-2 (noncontiguous, noncollective) MPI-IO request. For level-3 requests (noncontiguous, collective), data sieving is used within the collective I/O implementation to perform the local I/O on each process, as explained in the next section.

6 Collective I/O

The preceding section explained how data sieving can be used to optimize I/O when the entire (noncontiguous) access information of a single process is known. Further optimization is possible if the implementation is given the entire access information of a group of processes. Such optimization is broadly referred to as collective I/O.

In many parallel applications, although each process may need to access several noncontiguous portions of a file, the requests of different processes are often interleaved and may together span large contiguous portions of the file. If the user provides the MPI-IO implementation with the entire access information of a group of processes, the implementation can improve I/O performance significantly by merging the requests of different processes and servicing the merged request, that is, by performing collective I/O.

Collective I/O can be performed in different ways and has been studied by many researchers in recent years. It can be done at the disk level (disk-directed I/O [8]), at the server level (server-directed I/O [17, 16]), or at the client level (two-phase I/O [4, 21] or collective buffering [12]). Each method has its advantages and disadvantages. Since ROMIO is a portable, user-level library with no separate I/O servers, it performs collective I/O at the client level by using a generalized version of two-phase I/O.

ROMIO performs collective I/O when the user makes level-3 MPI-IO requests. Most level-1 requests do not contain enough information for ROMIO to perform collective optimizations, and ROMIO therefore implements them internally as level-0 requests. Some level-1 requests, such as those that represent a read-broadcast type of access pattern, are optimized collectively, however.

6.1 Two-Phase I/O

Two-phase I/O was first proposed in [4] in the context of accessing distributed arrays from files. Consider the example of reading a two-dimensional array from a file into a (block,block) distribution in memory, as shown in Figure 7. Assume that the array is stored in the file in row-major order. As a result of the distribution in memory and the storage order in the file, the local array of each process is located noncontiguously in the file: each row of the local array of a process is separated by rows from the local arrays of other processes. If each process tries to read each row of its local array individually, the performance will be poor because of the large number of relatively small I/O requests. Note, however, that all processes together need to read the entire file, and two-phase I/O uses this fact to improve performance as explained below.

If the entire I/O access pattern of all processes is known to the implementation, the data can be accessed efficiently by splitting the access into two phases. In the first phase, processes access data assuming a distribution in memory that results in each process making a single, large, contiguous access. In this example, such a distribution is a row-block or (block,*) distribution. In the second phase, processes redistribute data among themselves to the desired distribution. The advantage of this method is that by making all file accesses large and contiguous, the I/O time is reduced significantly. The added cost of interprocess communication for redistribution is (almost always) small compared with the savings in I/O time.

The basic two-phase method was extended in [21] to access sections of out-of-core arrays. Since MPI-IO is a general parallel I/O interface, I/O requests in MPI-IO can represent *any* access pattern, not just sections of arrays. The two-phase method in [21] must therefore be generalized to handle any noncontiguous I/O request. We have implemented such a scheme in ROMIO.

Two-phase I/O does increase the memory requirements of a program. For reading a distributed array, for example, the amount of extra memory needed on each process (to store the data read in the first phase) is equal to the size of the local array itself. Since this amount of memory may not be available, the basic two-phase algorithm must be modified to read and communicate smaller parts of the array at a time. Similarly, on machines in which the I/O performance does not scale with the number of processes making simultaneous file accesses, it may be beneficial to have only a subset of processes perform I/O, with the remaining processes participating only in the redistribution phase. All these generalizations—any access pattern, fixed memory requirement, and variable number of processes performing I/O—are incorporated in ROMIO's collective I/O implementation.

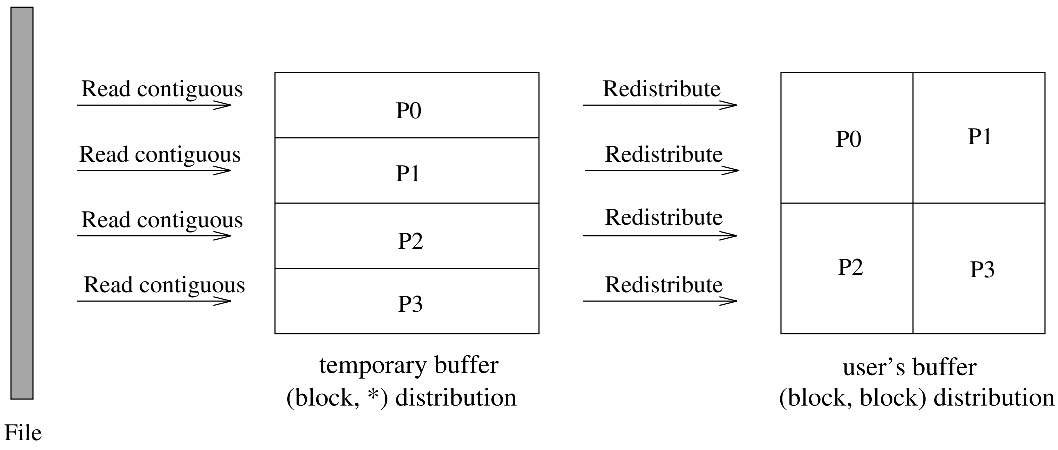


Figure 7: Reading a distributed array by using two-phase I/O

6.2 Generalized Two-Phase I/O in ROMIO

ROMIO uses two user-controllable parameters for collective I/O: the number of processes that should directly access the file and the maximum size on each process of the temporary buffer needed for two-phase I/O. By default, all processes perform I/O in the I/O phase, and the maximum buffer size is 4 Mbytes per process. The user can change these values at run time via MPI-IO's hints mechanism (see Figure 8).

We first explain the algorithm that ROMIO uses for collective reads and then describe how the algorithm differs for collective writes. Figure 9 shows a simple example that illustrates how ROMIO performs a collective read. In this example, all processes perform I/O, and each process is assumed to have as much memory as needed for the temporary buffer.

In MPI-IO, the collective I/O function called by a process specifies the access information of that process only. If an MPI-IO implementation needs the access information of all processes participating in a collective I/O operation, it must gather the information from those processes during the execution of the collective I/O function. Also, file accesses in collective I/O refer to accesses from multiple processes to a *common* file.

6.2.1 Collective Reads

In ROMIO's implementation of collective reads, each process first analyzes its own I/O request and creates a list of offsets and a list of lengths, where `length[i]` gives the number of bytes that the process needs from location `offset[i]` in the file. Each process also calculates the locations of the first byte (start offset) and the last byte (end offset) it needs from the file and then broadcasts these two offsets to other processes. As a result, each process has the start and end offsets of all processes.

In the next step, each process tries to determine whether this particular access pattern can benefit from collective I/O, that is, whether the accesses of any of the processes are interleaved in the file. Since an exhaustive check can be expensive, each process checks only whether, for any two processes with consecutive ranks (i and $i+1$), the following expression is true: (start-offset$_{i+1}$ $<$ end-offset$_i$). If the expression is not true, each process concludes that collective I/O will not improve performance for this particular access pattern, since the requests of different processes cannot be merged. In such cases, each process just calls the corresponding independent I/O function, which uses data sieving to optimize noncontiguous requests.

If the above expression is true, the processes perform collective I/O as follows. Portions of the file are "assigned" to each process such that, in the I/O phase of the two-phase operation, a process will access data only from the portion of the file assigned to it. This portion of the file assigned to a process is called the process's *file domain*. If a process needs data located in another process's file domain, it will receive the data from the other process during the communication phase of the two-phase operation. Similarly, if this process's file domain contains data needed by other processes, it

```
/* create new info object */
MPI_Info_create(&info);

/* specify buffer size for collective I/O */
MPI_Info_set(info, "cb_buffer_size", "8388608");

/* specify that only half the processes should perform I/O in collec-
tive I/O */
sprintf(value, "%d", nprocs/2);
MPI_Info_set(info, "cb_nodes", value);

/* specify buffer size for data sieving in independent reads */
MPI_Info_set(info, "ind_rd_buffer_size", "1048576");

/* specify buffer size for data sieving in independent writes */
MPI_Info_set(info, "ind_wr_buffer_size", "262144");

/* use this info object in the open function */
MPI_File_open(MPI_COMM_WORLD, "/pfs/test", MPI_MODE_CREATE | MPI_MODE_RDWR,
              info, &fh);
```

Figure 8: Example showing how to specify hints in MPI-IO. The two collective I/O hints, `cb_buffer_size` and `cb_nodes`, are predefined hints in MPI-IO; the two data-sieving hints, `ind_rd_buffer_size` and `ind_wr_buffer_size`, are additional hints that ROMIO supports.

must send this data to those processes during the communication phase.

File domains are assigned as follows. Each process calculates the minimum of the start offsets and the maximum of the end offsets of all processes. The difference between these two offsets gives the total extent of the combined request of all processes. The file domain of each process is obtained by dividing this extent equally among the processes. For example, if the combined request of all processes spans from offset 100 to offset 399 in the file, and there are three processes, the file domain of process 0 will be from offset 100 to 199; the file domain of process 1 will be from offset 200 to 299; and the file domain of process 2 will be from offset 300 to 399.

When file domains are selected in this manner, the file domain of a process may not contain data needed by any process (e.g., if the access pattern has large holes). In such a case, the process will not perform any I/O and will participate only in communication. (It is possible to design a more intelligent file-domain selection scheme that analyzes the access pattern and then assigns file domains in a manner that ensures an even balance of the I/O workload and/or reduces the communication needs.)

After the file domains are determined, each process calculates in which other process's file domain its own I/O request (or a portion of it) is located. For each such process, it creates a data structure containing a list of offsets and lengths that specify the data needed from the file domain of that process. It then sends this access information to the processes from which it expects to receive data. Similarly, other processes that need data from the file domain of this process send the corresponding access information to this process. After this exchange has taken place, each process knows what portions of its file domain are needed by other processes and by itself. It also knows which other processes are going to send the data that it needs.

The next step is to read and communicate the data. This step consumes the majority of the time because all the I/O and data communication takes place here. Note that the communication in earlier steps involved only access information. The access information is usually much smaller than actual data, unless the access pattern is so irregular that an index is needed to represent the location of every basic datatype needed from the file.

As mentioned above, ROMIO performs the read-and-communicate step in several parts to reduce its memory re-

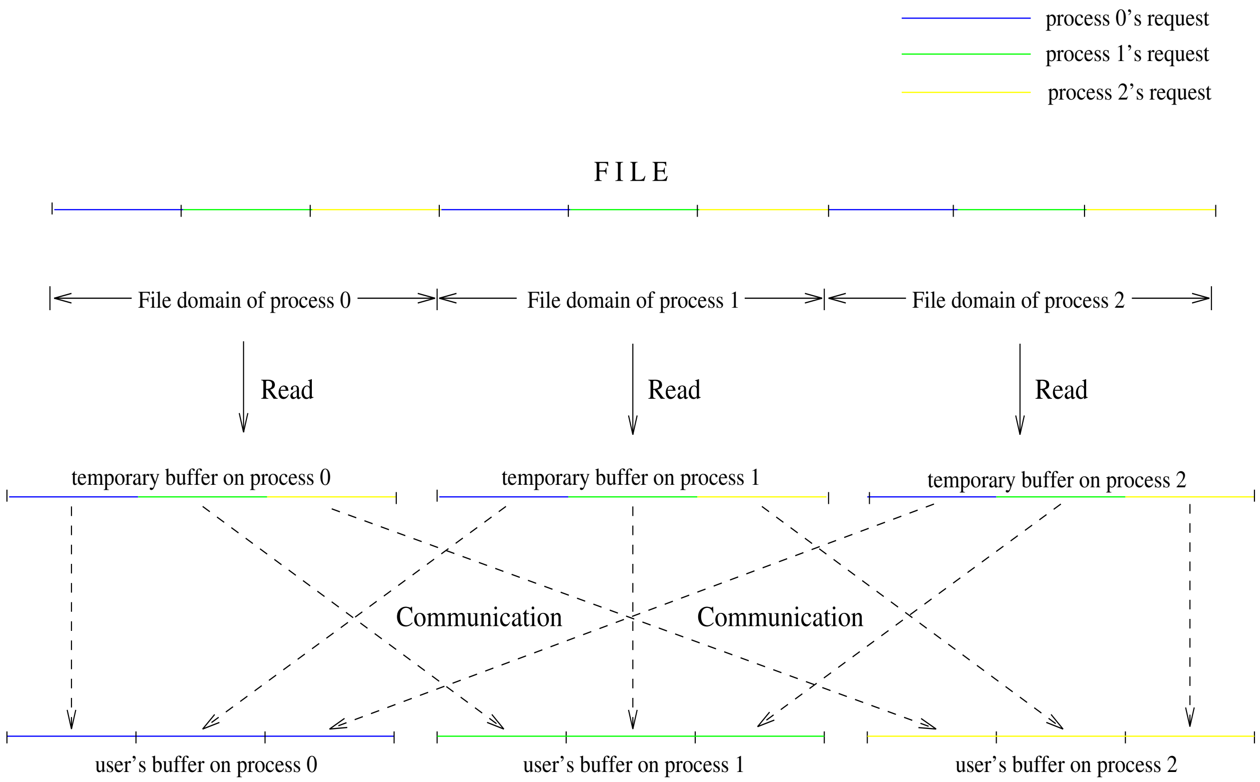


Figure 9: A simple example illustrating how ROMIO performs a collective read

quirement. Each process first calculates the offsets corresponding to the first and last bytes needed (by any process) from its file domain. It then divides the difference between these offsets by the maximum size allowed for the temporary buffer (4 Mbytes by default). The result is the number of times (`ntimes`) it needs to perform I/O. All processes then perform a global-maximum operation on `ntimes` to determine the maximum number of times (`max_ntimes`) any process needs to perform I/O. Even if a process has completed all the I/O needed from its own file domain, it may need to participate in communication operations thereafter to receive data from other processes. Each process must therefore be ready to participate in the communication phase `max_ntimes` number of times.

For each of the `ntimes` I/O operations, a process does the following operations. It checks whether the current portion of its file domain (no larger than the maximum buffer size) has data that any process needs, including itself. If it does not have such data, the process does not need to perform I/O in this step; it then checks whether it needs to receive data from other processes, as explained below. If it does have such data, it reads with a single I/O function call all the data from the first offset to the last offset needed from this portion of the file domain into a temporary buffer in memory. The process effectively performs data sieving, as the data read may include some unwanted data. Now the process must send portions of the data read to processes that need them.

Each process first informs other processes how much data it is going to send to each of them. The processes then exchange data by first posting all the receives as nonblocking operations, then posting all the nonblocking sends, and finally waiting for all the nonblocking communication to complete. MPI derived datatypes are used to send noncontiguous data directly from the temporary buffer to the destination process. On the receive side, if the user has asked for data to be placed contiguously in the user-supplied buffer, the data is received directly into the user's buffer. If data is to be placed noncontiguously, the process first receives data into a temporary buffer and then copies it into the user's buffer. (Since data is received in parts over multiple communication operations from different processes, we found this approach easier than creating derived datatypes on the receive side.)

Each process performs I/O and communication `ntimes` number of times and then participates only in the communication phase for the remaining `(max_ntimes - ntimes)` number of times. In some of these remaining communication steps, a process may not receive any data; nevertheless, the process must check whether it is going to receive data in a particular step.

6.2.2 Collective Writes

The algorithm for collective writes is similar to the one for collective reads except that the first phase of the two-phase operation is communication and the second phase is I/O. In the I/O phase, each process checks to see whether any holes (gaps) exist in the data it needs to write. If holes exist, it performs a read-modify-write; otherwise it performs only a write. During the read-modify-write, a process need not lock the region of the file being accessed (unlike in independent I/O), because the process is assured that no other process involved in the collective I/O operation will directly try to access the data located in this process's file domain. The process is also assured that concurrent writes from processes other than those involved in this collective I/O operation will not occur, because MPI-IO's consistency semantics [9] do not automatically guarantee consistency for such writes. (In such cases, users must use `MPI_File_sync` and ensure that the operations are not concurrent.)

6.2.3 Performance Issues

Even if I/O is performed in large contiguous chunks, the performance of the collective I/O implementation can be significantly affected by the amount of buffer copying and communication. We were able to improve ROMIO's collective I/O performance by as much as 50% on some machines by tuning the implementation to minimize buffer copying, minimize the number of communication calls, and use the right set of MPI communication primitives.

Initially, in each of the communication steps, we always received data into a temporary buffer and then copied it into the user's buffer. We realized later that this copy is needed only when the user's buffer is to be filled noncontiguously. In the contiguous case, data can be received directly into the appropriate location in the user's buffer. We similarly experimented with different ways of communicating data in MPI and measured the effect on overall collective I/O performance with different MPI implementations and on different machines. We selected nonblocking communication with the receives posted first and then the sends, a strategy that performs well on most systems. It may be possible, however, to tune the communication further on some machines by posting the sends before the receives or by using MPI's persistent requests.

6.2.4 Portability Issues

We were able to implement these optimizations portably, and without sacrificing performance, by using ADIO as a portability layer for I/O (see Section 4) and by using MPI for communication. Data sieving and collective I/O are implemented as ADIO functions [23]; data sieving is used in the ADIO functions that read/write noncontiguous data, and collective I/O is used in ADIO's collective I/O functions. Both these optimizations ultimately make contiguous I/O requests to the underlying file system, which are implemented by using ADIO's contiguous I/O functions. The contiguous I/O functions, in turn, are implemented by using the appropriate file-system call for each different file system.

7 Performance Evaluation

We describe the three applications used in the performance experiments, the machines on which we ran the applications, and the set of experiments performed. We then present and analyze the performance results.

7.1 Applications

The first application we used is DIST3D, a template representing the I/O access pattern in an astrophysics application, ASTRO3D [24], from the University of Chicago. It measures the performance of reading/writing a three-dimensional array distributed in a (block,block,block) fashion among processes from/to a file containing the global array in row-major order.

The second application is the BTIO benchmark [5] from NASA Ames Research Center, which simulates the I/O required by a time-stepping flow solver that periodically writes its solution matrix. The solution matrix is distributed among processes by using a multipartition distribution [2] in which each process is responsible for several disjoint subblocks of points (cells) of the grid. The cells are arranged such that, for each direction of the solve phase, the cells belonging to a certain process will be evenly distributed along the direction of solution. The solution matrix is stored on each process as C three-dimensional arrays, where C is the number of cells on each process. (The arrays are actually four dimensional, but the first dimension has only five elements and is not distributed.) Data is stored in the file in an order corresponding to a column-major ordering of the global solution matrix. Note that this distribution is different from the (block,block,block) distribution of DIST3D. The benchmark performs only writes, but we modified it to perform reads also, in order to measure the read bandwidths.

The third application we used is an unstructured code (which we call UNSTRUC) written by Larry Schoof and Wilbur Johnson of Sandia National Laboratories. It is a synthetic benchmark that emulates the I/O access pattern in unstructured-grid applications. It generates a random irregular mapping from the local one-dimensional array of a process to a global array in a common file shared by all processes. The mapping specifies where each element of the local array is located in the global array. The size of each element can also be varied in the program.

7.2 Machines

We ran the codes portably and measured the performance on five different parallel machines: the HP Exemplar and SGI Origin2000 at the National Center for Supercomputing Applications (NCSA), the IBM SP at Argonne National Laboratory, the Intel Paragon at the California Institute of Technology, and the NEC SX-4 at the National Aerospace Laboratory (NLR) in Holland. These machines cover almost the entire spectrum of high-performance systems, and they represent distributed-memory, shared-memory, and parallel vector architectures. They also represent a wide variation in I/O architecture, from the "traditional" parallel file systems on distributed-memory machines such as the SP and Paragon, to the so-called high-performance file systems on shared-memory machines such as the Origin2000, Exemplar, and SX-4.

We used the native file systems on each machine: HFS on the Exemplar, XFS on the Origin2000, PIOFS on the SP, PFS on the Paragon, and SFS on the SX-4. At the time we performed the experiments, these file systems were configured as follows: HFS on the Exemplar was configured on twelve disks; XFS on the Origin2000 had two RAID units with SCSI-2 interfaces; the SP had four servers for PIOFS, each server with four SSA disks attached to it in one SSA loop; the Paragon had 64 I/O nodes for PFS, each with an individual Seagate disk; and SFS on the NEC SX-4 was configured on a single RAID unit comprising sixteen SCSI-2 data disks.

7.3 Experiments

We modified the I/O portions of these applications to correspond to each of the four levels of requests (see Section 3) and ran the programs on all five machines. In all experiments, we used the default values of the sizes of the internal buffers ROMIO uses for data sieving and collective I/O (see Sections 5 and 6). We also used the default values of the file-striping parameters on all file systems. On PFS and PIOFS the default striping unit was 64 Kbytes.

On each machine, we used as many processors as we could reasonably access. We also tried to use the same number of processors on a given machine for each application but were at times constrained by the application's requirements: BTIO requires that the number of processors be a perfect square, whereas UNSTRUC requires that the number of processors be a power of two. On some machines, therefore, we could not use the same number of processors for both BTIO and UNSTRUC; for example, on the NEC SX-4 we had to run BTIO on 9 processors and UNSTRUC on 8 processors.

The access patterns in DIST3D and BTIO are such that level-1 requests cannot be optimized with collective I/O. In such cases, ROMIO internally translates level-1 requests into level-0 requests (with some overhead incurred in analyzing the level-1 request). In UNSTRUC, the I/O access pattern is irregular, and the granularity of each access is very small (64 bytes). Level-0/1 requests are not feasible for this kind of application because they take an excessive

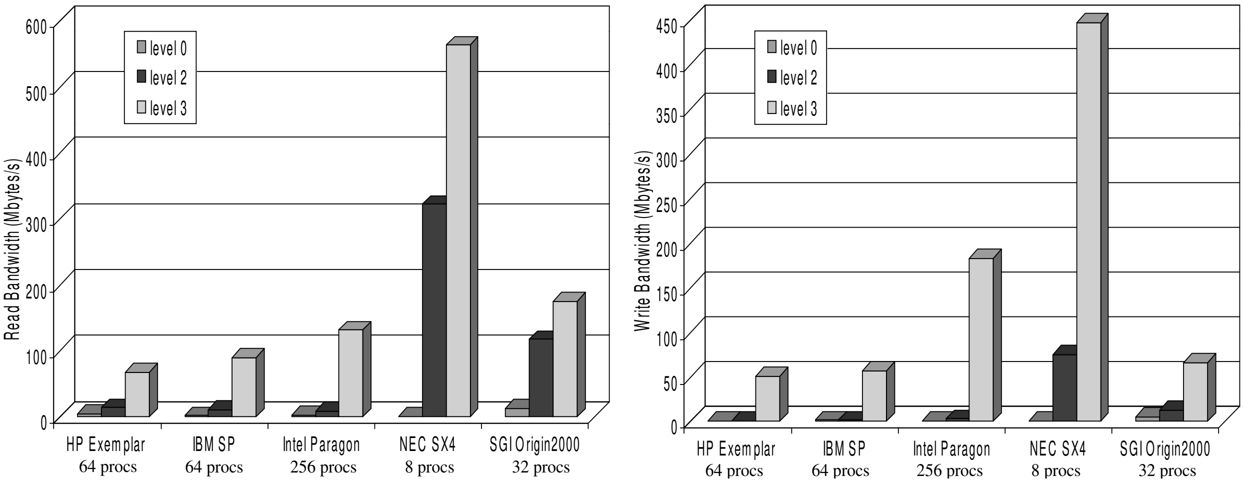


Figure 10: Performance of DIST3D (array size 512x512x512 integers = 512 Mbytes). Level-1 results are not shown because, for this access pattern, ROMIO simply translates level-1 requests internally into level-0 requests.

amount of time. Therefore, we present results with level-0, level-2, and level-3 requests for DIST3D and BTIO, and with level-2 and level-3 requests for UNSTRUC.

7.4 Results

Figure 10 shows the read and write bandwidths for DIST3D. We calculated the bandwidth as the total data transferred by all processes divided by the maximum of the time taken for I/O by any one process. The performance with level-0 requests was, in general, very poor because level-0 requests result in too many small read/write calls. For level-2 requests—for which ROMIO performs data sieving—the read bandwidth improved over level-0 requests by a factor ranging from 2.6 on the HP Exemplar to 453 on the NEC SX-4. Similarly, the write bandwidth improved by a factor ranging from 2.3 on the HP Exemplar to 121 on the NEC SX-4. On the IBM SP, however, level-2 write requests performed the same as level-0 requests. This is because ROMIO cannot perform data sieving for writing on the SP's PIOFS file system, since PIOFS does not support file locking. On PIOFS, ROMIO internally translates level-2 requests into level-0 requests.

The performance improved considerably with level-3 requests because ROMIO performs collective I/O in this case. The read bandwidth improved by a factor of as much as 793 over level-0 requests (NEC SX-4) and as much as 14 over level-2 requests (Intel Paragon). Similarly, with level-3 requests, the write performance improved by a factor of as much as 721 over level-0 requests (NEC SX-4) and as much as 40 over level-2 requests (HP Exemplar).

Figure 11 presents results for Class C of the BTIO benchmark. For BTIO, level-0 requests performed better than level-2 requests on three out of the five machines. The reason is that the holes between data segments needed by a process are large in BTIO—more than five times the size of the data segment. As a result, a lot of unwanted data was accessed during data sieving (level 2), resulting in lower performance than with Unix-style accesses (level 0). As mentioned in Section 5, an intelligent data-sieving algorithm could detect such large holes and internally perform Unix-style accesses. ROMIO's data-sieving algorithm does not currently do this, however.

Level-3 requests performed extremely well on BTIO because no unwanted data was accessed during collective I/O and all accesses were large. The performance improved by a factor of as much as 512 over level-0 requests for reading and 597 for writing, both on the NEC SX-4.

Figures 12 shows the read and write bandwidths for UNSTRUC. We ran a problem size of 8 million grid points on all machines except the Origin2000 where, because of memory limitations imposed by the scheduler, we had to run a smaller problem size of 4 million grid points. Level-3 requests again performed much better than level-2

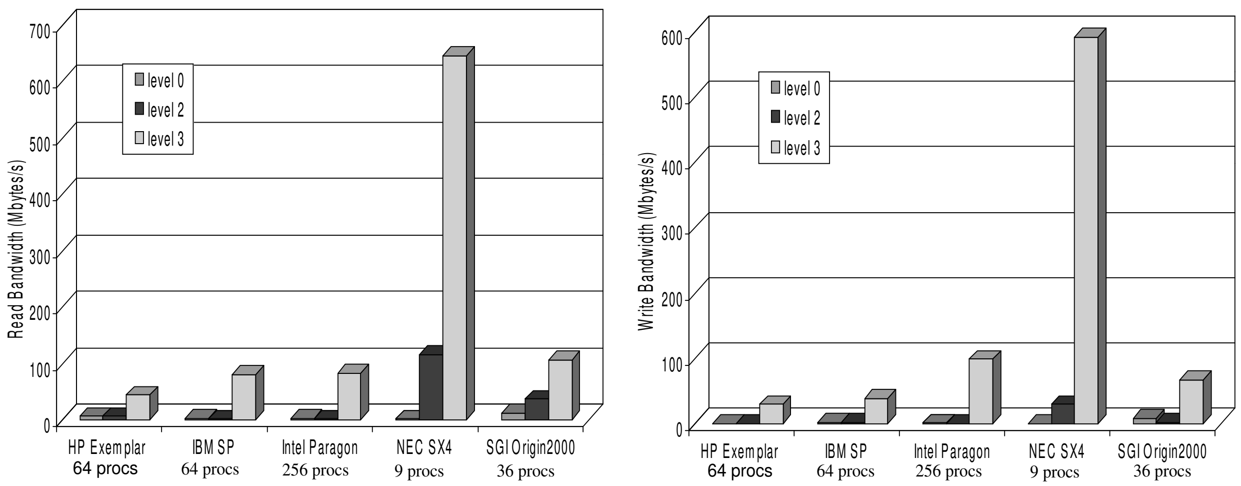


Figure 11: Performance of BTIO (Class C, problem size 5x162x162x162 double precision $\approx$ 162 Mbytes). Level-1 results are not shown because, for this access pattern, ROMIO simply translates level-1 requests internally into level-0 requests.

requests, the only exception being for reads on the NEC SX-4. In this case, because of the high read bandwidth of NEC's Supercomputing File System (SFS), data sieving by itself outperformed the extra communication required for collective I/O.

7.5 Impact of Architecture and System Configuration

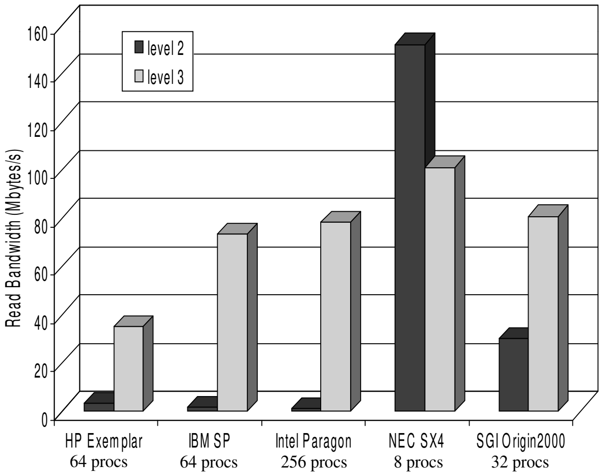
The above results show that although level 3 performed the best on each machine, there was a wide variation in the performance of the applications among the different machines. This variation is because the machines were configured with different amounts and types of I/O hardware (disks), different amounts of memory, and, of course, they had different I/O architectures and file systems. Our goal in this study was to compare the performance of the different levels of requests on a given machine, rather than comparing the performance of different machines. In general, the parallel I/O performance of a machine depends on the following factors:

- the I/O architecture;
- the speed and amount of I/O hardware (disks, etc.);
- how well the file system can handle concurrent reads and writes; and
- how well the file system's caching policies (read-ahead, write-behind) work for the given application.

The performance on the NEC SX-4 was the best among the five machines. We believe that is because the machine has high memory and I/O bandwidth and it was configured with sufficient I/O hardware for high performance. We believe the performance would have been similar even if the machine had more processors.

8 Conclusions

The results in the preceding section demonstrate that MPI-IO can deliver good I/O performance to applications. To achieve high performance with MPI-IO, however, users must use some of MPI-IO's advanced features, particularly noncontiguous accesses and collective I/O. By making level-3 MPI-IO requests (noncontiguous, collective),



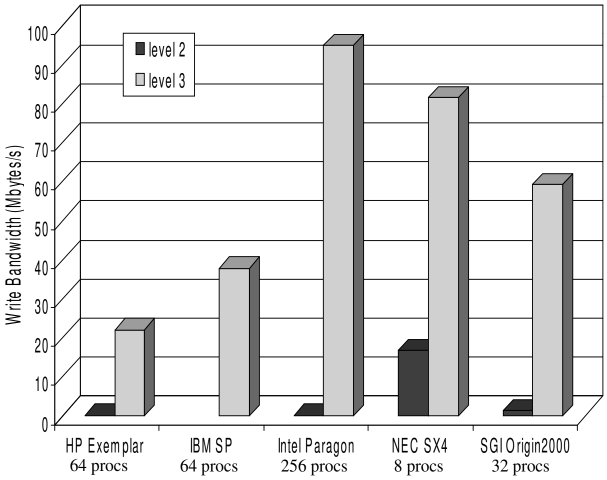


Figure 12: Performance of UNSTRUC. Level 0/1 results are not feasible for this application because they take an excessive amount of time because of the small granularity of each request. On the IBM SP, because of the absence of file locking in the PIOFS file system, ROMIO translates level-2 writes into level-0 writes, which are very slow in this case. Hence, results for level-2 writes on the SP are not shown.

we achieved I/O bandwidths on the order of hundreds of Mbytes/sec, whereas with level-0 requests (Unix style) we achieved less than 15 Mbytes/sec even when using high-performance file systems. With level-3 requests, the bandwidth achieved was limited only by the I/O capabilities of the machine and underlying file system. We believe that such performance improvements with level-3 requests can also be expected in applications other than those considered in this paper.

We have described in detail the optimizations ROMIO performs for noncontiguous requests: data sieving and collective I/O. We note that, to achieve high performance, these optimizations must be carefully implemented to minimize the overhead of buffer copying and interprocess communication. Otherwise, these overheads can impact performance significantly.

To carry out these optimizations, an MPI-IO implementation needs some amount of temporary buffer space, which reduces the total amount of memory available to the application. The optimizations, however, can be performed with a constant amount of buffer space that does not increase with the size of the user's request. Our results demonstrate that by allowing the MPI-IO implementation to use as little as 4 Mbytes of buffer space per process, which is a small amount on today's high-performance machines, users can gain orders of magnitude improvement in I/O performance.

We note that the MPI-IO standard does not *require* an implementation to perform any of these optimizations. Nevertheless, even if an implementation does not perform any optimization and instead translates level-3 requests into several level-0 requests to the file system, the performance would be no worse than if the user made level-0 requests. Therefore, there is no reason not to use level-3 requests (or level-2 requests where level-3 requests are not possible).

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