


AUTHOR QUERY FORM





 ELSEVIER	Journal: PARCO Article Number: 2016	Please e-mail or fax your responses and any corrections to: E-mail: corrections.esch@elsevier.sps.co.in Fax: +31 2048 52799
--	--	---

Dear Author,

Please check your proof carefully and mark all corrections at the appropriate place in the proof (e.g., by using on-screen annotation in the PDF file) or compile them in a separate list. To ensure fast publication of your paper please return your corrections within 48 hours.

For correction or revision of any artwork, please consult <http://www.elsevier.com/artworkinstructions>.

Any queries or remarks that have arisen during the processing of your manuscript are listed below and highlighted by flags in the proof. Click on the 'Q' link to go to the location in the proof.

Location in article	Query / Remark: click on the Q link to go Please insert your reply or correction at the corresponding line in the proof
Q1	The given (Written to) sentence s th to be incomplete. Please check for missing words/phrases and complete the sentence 
Q2	Please provide publisher details for Ref. [13] 
	Additional note 1 
	Additional note 2 

Thank you for your assistance.

Research highlights

► We show how MapReduce operations can be performed on top of the message-passing interface (MPI) in parallel and out-of-core, and describe our open-source implementation, called the MR-MPI library. ► We describe MapReduce algorithms for several graph computations: generation of random R-MAT graphs (or matrices), vertex ranking via PageRank, triangle and connected-component finding, maximal independent set identification, and single-source shortest-path. ► We give performance data for running these algorithms on graphs with up to billions of edges.



Contents lists available at ScienceDirect

Parallel Computing

journal homepage: www.elsevier.com/locate/parcoMapReduce in MPI for Large-scale **graph algorithms**

Steven J. Plimpton, Karen D. Devine*

Sandia National Laboratories, Albuquerque, NM, United States

ARTICLE INFO

Article history:
Available online xxxx

Keywords:
MapReduce
Message-passing
MPI
Graph algorithms
R-MAT matrices

ABSTRACT

We describe a parallel library written with message-passing (MPI) calls that allows algorithms to be expressed in the MapReduce paradigm. This means the calling program does not need to include explicit parallel code, but instead provides “map” and “reduce” functions that operate independently on elements of a data set distributed across processors. The library performs needed data movement between processors. We describe how typical MapReduce functionality can be implemented in an MPI context, and also in an out-of-core manner for data sets that do not fit within the aggregate memory of a parallel machine. Our motivation for creating this library was to enable graph algorithms to be written as MapReduce operations, allowing processing of terabyte-scale data sets on traditional MPI-based clusters. We outline MapReduce versions of several such algorithms: vertex ranking via PageRank, triangle finding, connected component identification, Luby’s algorithm for maximally independent sets, and single-source shortest-path calculation. To test the algorithms on arbitrarily large artificial graphs we generate randomized R-MAT matrices in parallel; a MapReduce version of this operation is also described. Performance and scalability results for the various algorithms are presented for varying size graphs on a distributed-memory cluster. For some cases, we compare the results with non-MapReduce algorithms, different machines, and different MapReduce software, namely Hadoop. Our open-source library is written in C++, is callable from C++, C, Fortran, or scripting languages such as Python, and can run on any parallel platform that supports MPI.

© 2011 Elsevier B.V. All rights reserved.

1. Introduction

MapReduce is the programming paradigm popularized by Google researchers Dean and Ghemawat [9]. Their motivation was to enable rapid development and deployment of analysis programs to operate on massive data sets residing on Google’s large distributed clusters. They introduced a novel way of thinking about certain kinds of large-scale computations as a “map” operation followed by a “reduce” operation. The power of the paradigm is that when cast in this way, a nominally serial algorithm now becomes two highly parallel operations working on data local to each processor, sandwiched around an intermediate data-shuffling operation that requires inter-processor communication. The user need only write serial code for the application-specific map and reduce functions; the parallel data shuffle can be encapsulated in a library since its operation is independent of the application.

The Google implementation of MapReduce is a C++ library with communication between networked machines via remote procedure calls. It allows for fault tolerance when large numbers of machines are used, and can use disks as out-of-core memory to process petabyte-scale data sets. Tens of thousands of MapReduce programs have since been written by Google researchers and are a significant part of the daily compute tasks run by the company [10].

* Corresponding author.

E-mail addresses: sjplimp@sandia.gov, kddevin@sandia.gov (K.D. Devine).

Similarly, the open-source Hadoop implementation of MapReduce [1], has become widely popular in the past few years for parallel analysis of large-scale data sets at Yahoo and other data-centric companies, as well as in university and laboratory research groups, due to its free availability. MapReduce programs in Hadoop are typically written in Java, although it also supports use of stand-alone map and reduce kernels, which can be written as shell scripts or in other languages.

More recently, MapReduce formulations of traditional number-crunching kinds of scientific computational tasks have been described, such as post-processing analysis of simulation data [22], graph algorithmics [8,16,18], and linear algebra operations [11]. The paper by Tu et al. [22] was particularly insightful to us, because it described how MapReduce could be implemented on top of the ubiquitous distributed-memory message-passing interface (MPI), and how the intermediate data-shuffle operation is conceptually identical to the familiar MPI_Alltoall operation. Their implementation of MapReduce was within a Python wrapper to simplify the writing of user programs. The paper motivated us to develop our own C++ library built on top of MPI for use in graph analytics, which we initially released as open-source software in mid-2009. We have since worked to optimize several of the library's underlying algorithms and to enable its operation in out-of-core mode for larger data sets. These algorithmic improvements are described in this paper and are part of the current downloadable version; see Section 7 for details.

The MapReduce-MPI (MR-MPI) library described in this paper is a simple, lightweight implementation of basic MapReduce functionality, with the following features and limitations:

- *C++ library using MPI for inter-processor communication:* The user writes a (typically) simple main program which runs on each processor of a parallel machine, making calls to the MR-MPI library. For map and reduce operations, the library calls back to user-provided `map()` and `reduce()` functions. The use of C++ allows precise control over the memory and format of data allocated by each processor during a MapReduce. Library calls for performing a map, reduce, or data shuffle, are synchronous, meaning all the processors participate and finish the operation before proceeding. Similarly, the use of MPI within the library is the traditional mode of MPI_Send and MPI_Recv calls between pairs of processors using large aggregated messages to improve bandwidth performance and reduce latency costs. A recent paper [15] also outlines the MapReduce formalism from an MPI perspective, although they advocate a more asynchronous approach, using one-way communication of small messages.
- *Small, portable:* The entire MR-MPI library is a few thousand lines of standard C++ code. For parallel operation, the program is linked with MPI, a standard message passing library available on all distributed-memory machines and many shared-memory parallel machines. For serial operation, a dummy MPI library (provided) can be substituted. As a library, MR-MPI can be embedded in other codes [2] to enable them to perform MapReduce operations.
- *In-core or out-of-core operation:* Each MapReduce object that a processor creates allocates “pages” of memory, where the page size is determined by the user. MapReduce operations can be performed using a few such pages (per processor). If the data set fits in a single page (per processor), the library performs its operations in-core. If the data set exceeds the page size, processors each write to temporary disk files (on local disks or a parallel file system) as needed and subsequently read from them. This out-of-core mode of operation allows processing of data sets larger than the aggregate memory of all the processors, i.e. up to the aggregate available disk space.
- *Flexible programmability:* An advantage of writing a MapReduce program on top of MPI, is that the user program can also invoke MPI calls directly, if desired. For example, one-line calls to MPI_Allreduce are often useful in determining the status of an iterative graph algorithm, as described in Section 4. The library interface also provides a user data pointer as an argument passed to all callback functions, so it is easy for the user program to store “state” on each processor, accessible during the map and reduce operations. For example, various flags can be stored that alter the operation of a map or reduce operation, as can richer data structures that accumulate results.
- *C++, C, and Python interfaces:* The C++ interface to the MR-MPI library allows user programs to instantiate and then invoke methods in one or more MapReduce objects. The C interface allows the same operations to be called from C or other high-level languages such as Fortran. The C interface also allows the library to be easily wrapped by Python via the Python “ctypes” module. The library can then be called from a Python script, allowing the user to write `map()` and `reduce()` callback functions in Python. If a machine supports running Python in parallel, a parallel MapReduce can also be run in this mode.
- *No fault tolerance or data redundancy:* Current MPI implementations do not enable easy detection of a dead processor or retrieval of the data it was working on. So like most MPI programs, a parallel program calling the MR-MPI library will hang or crash if a processor goes away. Unlike Hadoop, and its file system (HDFS) which provides data redundancy, the MR-MPI library reads and writes simple, flat files. It can use local per-processor disks, or a parallel file system, if available, but these typically do not provide data redundancy.

The remainder of the paper is organized as follows. Sections 2 and 3 describe how in-core and out-of-core MapReduce primitives are formulated as MPI-based operations in the MR-MPI library. Section 4 briefly describes the formulation of several common graph algorithms as MapReduce operations. Section 5 gives performance results for these algorithms running on a parallel cluster for graphs ranging in size from 8 million to 2 billion edges. We highlight the performance and complexity trade-offs of a MapReduce approach versus other more special-purpose algorithms. The latter generally perform better but are harder to implement efficiently on distributed memory machines, due to the required explicit management of par-

allelism, particularly for large out-of-core data sets. Section 6 summarizes some lessons learned from the implementation and use of our library.

2. MapReduce in MPI

The basic datums stored and operated on by any MapReduce framework are key/value (kv) pairs. In the MR-MPI library, individual keys or values can be of any data type or length, or combinations of multiple types (one integer, a string of characters, two integers and a double, etc.); they are simply treated as byte strings by the library. A kv pair always has a key; its value may be NULL. kv pairs are stored within a MapReduce (MR) object. A user program may create one or more MR objects to implement an algorithm. Various MapReduce operations (map, reduce, etc.) are invoked on an object and its kv pairs; kv pairs can also be passed between and combined across objects.

A related data type in the MR-MPI library is the key/multivalue (KMV) pair, where all values associated with the same key are collected and stored contiguously as a multivalue, which is just a longer byte string with an associated vector of lengths, one integer length per value. In this section, we assume the kv and KMV datums operated on by each processor fit in local memory.

A typical MR-MPI program makes at least three calls to the MR-MPI library, to perform map(), collate(), and reduce() operations on a MR object it creates. In a map(), zero or more key/value pairs are generated by each processor. Often this is done using data read from files, but a map() may generate data itself or process existing kv pairs to create new ones. The kv pairs produced are stored locally by each processor; a map() thus requires no inter-processor communication. Users call the library with a count of tasks to perform and a pointer to a user function; the MR-MPI map() operation invokes the user function multiple times as a callback. Depending on which variant of map() is called, the user function may be passed a file name, a chunk of bytes from a large file, a task ID, or a kv pair. Options for assigning map tasks to processors are specified by the user and include assigning consecutive chunks of tasks to processors, striding the tasks across processors, or using a master-slave model that is useful when tasks have widely varying workloads.

The collate() operation (or data shuffle in Hadoop) identifies unique keys and collects all the values associated with those keys to create KMV pairs. This is done in two stages, the first of which requires communication, since kv pairs with the same key may be owned by any processor. Each processor hashes each of its keys to determine which processor will “own” it. The k-byte length key is hashed into a 32-bit value whose remainder modulo P processors is the owning processor rank. Alternatively, the user can provide a hash function that converts the key into a processor rank. Each processor then sends each of its kv pairs to the owning processor.

After receiving new kv pairs, the second stage is an on-processor computation, requiring no further communication. Each processor reorganizes its kv pairs into KMV pairs, one for each unique key it owns. This is done using a hash table, rather than a sort. A sort scales as $N \log_2(N)$, i.e. it requires $\log_2(N)$ passes through the N kv pairs. With hashing, the list of KMV pairs can be created in two passes. The first pass populates the hash table with needed count and length information; the second pass copies the key and value datums into the appropriate location in a new KMV data structure. Since the cost to lookup a key in a well-formed hash table is a constant-time $O(1)$ operation, the cost of the data reorganization is also $O(N)$. This methodology has the added benefit that the number of values in each KMV pair is known and can be passed to the user function during a reduce. For some reduce operations, this count is all the information a reduce requires; the values need not be looped over. The count is not available in Hadoop-style data shuffles, which sort the values; counting the values associated with the same key requires iterating over the values.

Note that the first portion of the collate() operation involves all-to-all communication since each processor exchanges kv pairs with every other processor. The communication can either be done via a MPI_Alltoall() library call, or by a custom routine that aggregates datums into large messages and invokes point-to-point MPI_Send() and MPI_Recv() calls.

The reduce() operation processes KMV pairs and can produce new kv pairs for continued computation. Each processor operates only on the KMV pairs it owns; no communication is required. As with the map(), users call the library with a pointer to a user function. The MR-MPI reduce() operation invokes the user function, once for each KMV pair.

Several related MapReduce operations are provided by the library. For example, the collate() function described above calls two other functions: aggregate(), which performs the all-to-all communication, and convert(), which reorganizes a set of kv pairs into KMV pairs. Both functions can be called directly. The compress() function allows on-processor operations to be performed; it is equivalent to a convert() with on-processor KVs as input, followed by a reduce(). The clone() function turns a list of kv pairs into KMV pairs, with one value per key. The collapse() function turns N kv pairs into one KMV pair, with the keys and values of the kv pairs becoming 2N values of a single multivalue assigned to a new key. The gather() function collects kv pairs from all processors to a subset of processors; it is useful for doing output from one or a few processors. Library calls for sorting datums by key or value or for sorting the values within each multivalue are also provided. These routines invoke the C-library quicksort() function to compute the sorted ordering of the kv pairs (or values within a multivalue), using a user-provided comparison function. The kv pairs (or values in a multivalue) are then copied into a new data structure in sorted order.

The interface to various low-level operations is provided so that a user's program can string them together in various ways to construct useful MapReduce algorithms. For example, output from a reduce() can serve as input to a subsequent map() or collate(). Likewise, data can be partitioned across multiple MapReduce (MR) objects, each with its own set of

kV pairs. For example, as will be illustrated in Section 4, one MR object can store the edges of a graph, and another its vertices. **kV** pairs from multiple MR objects can be combined to perform new sequences of **map ()**, **collate ()**, and **reduce ()** operations.

The above discussion assumed that the **kV** or KMV pairs stored by a processor fit in its physical memory. In this case, the MR-MPI library performs only “in-core” processing and no disk files are written or read by any of the processors, aside from initial input data (if it exists) or final output data (if it is generated). Note that the aggregate physical memory of large parallel machines can be multiple terabytes, which allows for large data sets to be processed in-core, assuming the **kV** and KMV pairs remain evenly distributed across processors throughout the sequence of MapReduce operations. The use of hashing to assign keys to processors typically provides for such load-balancing. In the next section, we discuss what happens when data sets do not fit in available memory.

3. Out-of-core Issues

Since the MapReduce paradigm was designed to enable processing of extremely large data sets, the MR-MPI library also allows for “out-of-core” processing, which is triggered when the **kV** or KMV pairs owned by one or more processors do not fit in local memory. When this occurs, a processor writes one or more temporary files to disk, containing **kV** or KMV pairs, and reads them back in when required. Depending on the parallel machine’s hardware configuration, these files can reside on disks local to each processor, on the front end (typically a NFS-mounted file system for a parallel machine), or on a parallel file system and its associated disk array.

When a user program creates a MapReduce object, a “pagesize” can be specified, which defaults to 64 Mbytes. As described below, each MR-MPI operation is constrained to use no more than a handful of these pages. The *pagesize* setting can be as small as 1 Mbyte or as large as desired, though the user should ensure the allocated pages fit in physical memory; otherwise a processor may allocate slow virtual memory. The *pagesize* is also the typical size of individual reads and writes to the temporary disk files; hence a reasonable *pagesize* ensures good I/O performance.

We now explain how the MapReduce operations described in the previous section work in out-of-core mode. The **map ()** and **reduce ()** operations are relatively simple. As a **map ()** generates **kV** pairs via the user callback function, a page of memory fills up, one **kV** pair at a time. When the page is full, it is written to disk. If the source of data for the **map ()** operation is an existing set of **kV** pairs, those datums are read, one page at a time, and a pointer to each **kV** pair is given to the user function. Similarly, a **reduce ()** reads one page of KMV pairs from disk, and passes a pointer to each pair, one at a time, to the user callback function that typically generates new **kV** pairs. The generated pairs fill up a new page, which is written to disk when full, just as with the **map ()** operation. Thus for both a **map ()** and **reduce ()**, out-of-core disk files are read and written sequentially, one page at a time, which requires at most two pages of memory.

A special case is when a single KMV pair is larger than a single page. This can happen, for example, in a connected component finding algorithm if the graph collapses into one or a few giant components. In this case, the set of values (graph vertices and edges) associated with a unique key (the component ID), may not fit in one page of memory. The individual values in the multivalued are then spread across as many pages as needed. The user function that processes the KMV pair is passed a flag indicating it received only a portion of the values. Once it has processed them, it can request a new set of values from the MR-MPI library, which reads in a new page from disk.

Performing an out-of-core **collate ()** operation is more complex. Recall that the operation occurs in two stages. First, keys are hashed to “owning” processors and the **kV** pairs are communicated to new processors in an all-to-all fashion. In out-of-core mode, this operation is performed on one page of **kV** data (per processor) at a time. Each processor reads in a page of **kV** pairs, the communication pattern is determined (which processors receive which datums in that page), and all-to-all communication is performed. Each processor allocates a two-page chunk of memory to receive incoming **kV** pairs. On average each processor should receive one page of **kV** pairs; the two-page allocation allows for some load imbalance. If the **kV** pairs are distributed unevenly so that this limit is exceeded, the all-to-all communication is performed in multiple smaller passes until the full page contributed by every processor has been communicated. Performing an **MPI_Alltoall ()**, or using the custom all-to-all routines provided by the MR-MPI library, requires allocation of auxiliary arrays that store processor indices, datum pointers, and datum lengths. For the case of many tiny **kV** pairs, the total number of memory pages required to perform the all-to-all communication, including the source and target **kV** pages is at most seven.

When the communication stage of the **collate ()** operation is complete, each processor has a set of **kV** pages, stored in an out-of-core **kV** file, that need to be reorganized into a set of KMV pages, likewise stored in a new out-of-core KMV file. In principle, creating one page of KMV pairs would require all **kV** pages be scanned to find all the keys that contribute values to that page. Doing this for each output page of KMV pairs could be prohibitively expensive. A related issue is that, as described in the previous section, a hash table is needed to match new keys with previously encountered keys. But there is no guarantee that the hash table itself will not grow arbitrarily large for data sets with many unique keys. We need an algorithm for generating KMV pairs that operates within a small number of memory pages and performs a minimal number of passes through the **kV** disk file. An algorithm that meets these goals is diagrammed in Fig. 1; it reads the **kV** pages at most four times, and writes out new **kV** or KMV pages at most three times. It also uses a finite-size in-memory hash table, that stores unique keys as they are encountered while looping over the **kV** pages, as well as auxiliary information needed to construct the output pages of KMV pairs.

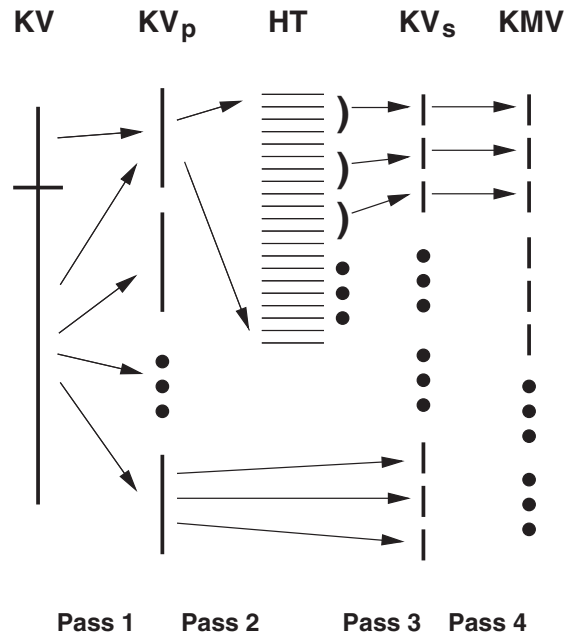


Fig. 1. Multi-pass algorithm for converting kV data to KMV data within a processor. The vertical lines represent out-of-core data sets. kV is key/value pairs; HT is an in-memory hash table; KMV is key/multivalue pairs.

- (Pass 1) The **kV** pairs are read, one page at a time, and split into “partition” files, represented by **KV_p** in the figure. Each partition file contains **kV** pairs whose unique keys (likely) fit in the hash table (HT). Initially, all **kV** pairs are assigned to the first partition file as the HT is populated. When the HT becomes full, e.g. at the point represented by the horizontal line shown on the leftmost vertical line as a downward scan is performed, the fraction of **kV** pairs read thus far is used to estimate the number of additional partition files needed. As subsequent **kV** pairs are read, they are assigned to the original partition file if the **kV** pair’s key is already in the current HT. If not, a subset of bits in the hash value of the key is used to assign the **kV** pair to one of the new partition files. The number of needed partition files is estimated conservatively, rounding up to the next power-of-two, so that extra passes through the **kV** pairs are almost never needed, and so that the bit masking can be done quickly. This first pass entails both a read and write of all the **kV** pairs.
- (Pass 2) The partition files are read, one at a time. The key for each **kV** pair is hashed into the HT, accumulating data about the number and size of values associated with each unique key. Before the next partition file is read, passes 3 and 4 are completed for the current partition. Eventually this pass entails a read of all **kV** pairs.
- (Pass 3) The unique keys in the HT for one partition are scanned to determine the total size of KMV for keys in the HT. The associated values create KMV pairs that span M memory pages. If $M > 1$, the associated partition file of **kV** pairs is read again, and each **kV** pair is assigned to one of M smaller “set” files, represented by **KV_s** in the figure. Each set file contains the **kV** pairs that contribute to the KMV pairs that populate one page of KMV output. If a single KMV pair spans multiple pages because it contains a very large number of values, the corresponding **kV** pairs are still written to a single set file. Eventually, this pass reads all partition files, entailing both a read and write of all **kV** pairs.
- (Pass 4) A set file is read and the key/value data for each of its **kV** pairs is copied into the appropriate location in the page of KMV pairs, using information stored in the HT. When complete, the KMV page is written to disk. This pass eventually reads all set files, entailing a final read of all **kV** pairs. It also writes all KMV pairs to disk. If each **kV** pair has a unique key, the volume of KMV output is roughly the same as that of the **kV** input.

In summary, this data reorganization for the **collate()** operation is somewhat complex, but requires only a small, constant number of passes through the data. The **kV** datums are read from disk at most four times, and written to disk three times. The first two write passes reorganize **kV** pairs into partition and set files; the final write pass creates the KMV data set. Depending on the size and characteristics of the **kV** datums (e.g., the number of unique keys), some of these passes may not be needed. By contrast, a full out-of-core sort of the **kV** pairs, performed via a merge sort as discussed below is still an $O(N \log_2 N)$ operation. The number of read/write passes through the **kV** data files depends on the amount of **kV** data that can be held in memory, but can be a large number for big data sets.

The memory page requirements for the out-of-core **collate()** operation are as follows. Two contiguous pages of memory are used for the hash table. Intermediate passes 2 and 3 can require numerous partition or set files to be opened simultaneously and written to. To avoid small writes of individual **kV** datums, a buffer of at least 16K bytes is allocated for each file.

The precise number of simultaneously open files is difficult to bound, but typically one or two additional pages of memory suffice for all needed buffers. Thus the total number of pages required for the data reorganization stage of the `collate()` operation is less than the seven used by the all-to-all communication stage.

Other MR-MPI library calls discussed in the previous section, such as `clone()`, `collapse()`, and `gather()`, can also operate in out-of-core mode, typically with one pass through the `kV` or KMV data and the use of one or two memory pages. Sorting `kV` pairs, by key or value, is an exception. An out-of-core merge sort is performed as follows. Two pages of `kV` datums are read from disk. Each is sorted in local memory using the C-library `quicksort()` function, as discussed in the previous section. The two pages are then scanned and merged into a new file which is written to disk as its associated memory page fills up. This process requires five memory pages, which includes vectors of `kV` datum pointers and lengths needed by the in-memory `quicksort()` operation. Once all pairs of pages have been merged, the sort continues in a recursive fashion, merging pairs of files into a new third file, without the need to perform additional in-memory sorts. Thus the overall memory requirement is five pages. The number of read/write passes through the `kV` data set for the merge sort is $O(\log_2 M)$, where M is the number of pages of `kV` pairs. The number of passes could be reduced at the cost of allocating more in-memory pages.

4. Graph algorithms in MapReduce

We begin with a MapReduce procedure for creating large, sparse, randomized graphs, since they are the input for the algorithms discussed below. R-MAT matrices [7] are recursively generated graphs with power-law degree distributions. They are commonly used to represent web and social networks. The user specifies six parameters that define the graph: the number of vertices N and edges M , and four parameters a, b, c, d that sum to 1.0 and are discussed below. The algorithm in Fig. 2 uses a single MapReduce object to generate M unique non-zero entries in a sparse $N \times N$ matrix G , where each entry G_{ij} represents an edge between graph vertices (V_i, V_j) , with V_i an integer from 1 to N .

In the `map()`, each of P processors generates a $1/P$ fraction of the desired edges. A single random edge (V_i, V_j) is computed recursively as follows. Pick a random quadrant of the G matrix with relative probabilities a, b, c , and d . Treat the chosen quadrant as a sub-matrix and select a random quadrant within it, in the same manner. Perform this process a total of n times where $N = 2^n$. At the end of the recursion, the final “quadrant” is a single non-zero matrix element G_{ij} .

Though G is very sparse, the `map()` typically generates some small number of duplicate edges. The `collate()` and `reduce()` remove the duplicates. The entire map-collate-reduce sequence is repeated until the number of resulting key/value (`kV`) pairs $N_{kv} = M$. For reasonably sparse graphs, only a few iterations are typically needed.

Note that the degree distribution of vertices in the graph depends on the choice of parameters a, b, c, d . If one of the four values is larger than the other three, a skewed distribution results. Variants of the algorithm can be used when N is not a power-of-two, to generate graphs with weighted edges (assign a numeric value to the edge), graphs without self edges (require $i \neq j$), or graphs with undirected edges (require $i < j$). Or the general R-MAT matrix can be further processed by MapReduce operations to meet these requirements. For some algorithms below (e.g., triangle finding and maximal independent set generation), we post-process R-MAT matrices to create upper-triangular R-MAT matrices representing undirected graphs. For each edge (V_i, V_j) with $i > j$, we add edge (V_j, V_i) , essentially symmetrizing the matrix; we then remove duplicate edges and self edges, leaving only edges with $i < j$.

By using an additional MapReduce object, we can improve the performance of the R-MAT generation algorithm, particularly when out-of-core operations are needed. In the enhanced algorithm (Fig. 3), we emit newly created edges into MapReduce object G_{new} and `aggregate()` the edges to processors. We then add those edges to the MapReduce object G , containing all previously generated unique edges; the edges of G are already aggregated to processors using the same mapping as G_{new} . We

```

Input:
  MapReduce object  $G$  = edges of graph, initially empty

 $M_{\text{remain}} = M$ 
while  $M_{\text{remain}} > 0$ :
  Map  $G$ :      Generate  $M_{\text{remain}}/P$  random edges  $(V_i, V_j)$  on each processor
               Output: Key =  $(V_i, V_j)$ , Value = NULL

  Collate  $G$ 
  Reduce  $G$ :   Remove duplicate edges
               Input: Key =  $(V_i, V_j)$ , MultiValue = one or more NULLs
               Output: Key =  $(V_i, V_j)$ , Value = NULL

   $M_{\text{remain}} = M - N_{kv}$ 

Output:
  MapReduce object  $G$  = edges of graph: Key =  $(V_i, V_j)$ , Value = NULL

```

Fig. 2. MapReduce algorithm for R-MAT graph generation on P processors, using a single MapReduce object G .


```

Input:
  MapReduce object  $G$  = edges of graph, initially empty
  MapReduce object  $G_{new}$  = new edges of graph, initially empty

 $M_{remain} = M$ 
while  $M_{remain} > 0$ :
  Map  $G_{new}$ :   Generate  $M_{remain}/P$  random edges  $(V_i, V_j)$  on each processor
               Output: Key =  $(V_i, V_j)$ , Value = NULL

  Aggregate  $G_{new}$ 
  Add  $G_{new}$  to  $G$ ,  $G_{new} = \text{empty}$ 
  Compress  $G$ : Remove duplicate edges
               Input: Key =  $(V_i, V_j)$ , MultiValue = one or more NULLs
               Output: Key =  $(V_i, V_j)$ , Value = NULL

   $M_{remain} = M - N_{kv}$ 

Output:
  MapReduce object  $G$  = edges of graph: Key =  $(V_i, V_j)$ , Value = NULL

```

Fig. 3. Enhanced MapReduce algorithm for R-MAT graph generation on P processors, using two MapReduce objects G and G_{new} .

can use a `compress()` to reduce duplicates locally on each processor. The enhanced algorithm runs faster due to the smaller number of `kV` pairs communicated in the `aggregate()`, compared to the `collate()` of the original algorithm, particularly in later iterations of the algorithm where few new edges are generated.

4.1. PageRank

The PageRank algorithm assigns a relative numeric rank to each vertex in a graph. In an Internet context, it models the web as a directed graph $G(V, E)$, with each vertex $V_i \in V$ representing a web page and each edge $(V_i, V_j) \in E$ representing a hyperlink from V_i to V_j . The probability of moving from V_i to another vertex V_j is $\alpha/d_{out}(V_i) + (1 - \alpha)/|V|$, where α is a user-defined parameter (usually 0.8–0.9), $d_{out}(V_i)$ is the outdegree of vertex V_i , and $|V|$ is the cardinality of V . The first term represents the probability of following a given link on page V_i ; the second represents the probability of moving to a random page. For pages with no outlinks, the first term is changed to $\alpha/|V|$, indicating equal likelihood to move to any other page. Equivalently, the graph can be represented by a matrix A [17], with matrix entries $A_{ij} = \alpha/d_{out}(V_i)$ if vertex V_i links to V_j . To keep A sparse, terms for random jumps and zero out-degree vertices are not explicitly stored as part of the matrix. Rather, they are computed separately as adjustments to the PageRank vector. The kernel of the PageRank algorithm is thus a power-method iteration consisting of `matrix-vector` multiplications $A^T x = y$, where x is the PageRank vector from the previous iteration. A few additional dot product and norm computations per iteration are also required.

The algorithm in Fig. 4 performs these iterations, using linear-algebra concepts implemented in a MapReduce framework. Related algorithms, each with their own optimizations, are discussed in [16,18]. In this version data is stored in four MapReduce objects: A , MT , x , and y . A stores the matrix; MT stores the row index of “empty” rows of A ; and x and y are vectors of length $|V|$. The nonzeros of matrix A are initialized as described above; the PageRank vector x is initialized uniformly. A MapReduce object MT contains the indices of all-zero rows of A , corresponding to vertices with no outlinks. The PageRank algorithm is made more efficient by invoking the `aggregate()` operation once on each of these MapReduce objects before the PageRank iterations begin. Since the objects are all keyed by vertex, pre-aggregating them moves all `kV` pairs with a given key to the same processor. Many of the subsequent PageRank operations then become local operations, replacing a `collate()` (which is equivalent to an `aggregate()` followed by `convert()`) with simply a `convert()`. In Fig. 4, steps where `convert()` is substituted for `collate()` are marked with an asterisk. This strategy of pre-aggregating to improve data locality is useful in many MapReduce algorithms; it assumes that identical keys in different MapReduce objects can be mapped to the same processor.

Step 1 of a PageRank iteration is, effectively, a dot-product of MT and x to compute an adjustment c_{dot} to the PageRank vector that represents random jumps and the uniform probability of going from a leaf page to any other page. MT is unchanged by the operation. In Step 2, the `matrix-vector` product $A^T x$ is computed and the result stored in y . This is the most expensive part of the computation, requiring two passes over the nonzero structure of A . In the first pass, a `convert()` gathers all local row entries A_{ij} with their associated x_i entry, and a `reduce()` computes $A_{ij} x_i$. In the second pass, a `collate()` gathers, for each j , all contributions to the column sum $\sum_i A_{ij} x_i$, which is computed by a second `reduce()`. Steps 3 and 4 adjust and scale the product vector; the work is proportional to $|V|$. Step 5 computes the residual as an infinity norm to determine whether the PageRank vector has converged; work is again proportional to $|V|$. Note that y and x are both keyed by vertex at this point, so they can be joined via an `add()` and `convert()` without need for the communication required by a full `collate()`. In Step 6,

```

Input:
  Pre-aggregated MapReduce object  $A = |V| \times |V|$  matrix: Key =  $i$ , Value =  $[j, A_{ij}]$ 
  Pre-aggregated MapReduce object  $MT$  = indices of all-zero rows of  $A$ : Key =  $i$ , Value = NULL
  Pre-aggregated MapReduce object  $x$  = initial PageRank vector: Key =  $i$ , Value =  $1/|V|$ 
  MapReduce object  $y$  = vector, initially empty; user-defined parameter  $\alpha$ 

while ( $residual > tolerance$ )
  1 Compute adjustment for random jumps and zero-outdegree vertices
    Add  $x$  to  $MT$ 
  *
    Convert  $MT$ : Key is vertex  $i$ 
    Reduce  $MT$ :
      Input: Key =  $i$ , MultiValue =  $(x_i, NULL)$  if  $i \in MT$ ; else MultiValue =  $x_i$ 
      If ( $nvalues = 2$ )  $c_{dot} = c_{dot} + x_i$ ; else  $c_{dot} = c_{dot} + \alpha$ 
      Output: Key =  $i$ , Value = NULL if  $nvalues = 2$ 
       $c_{dot} = \text{MPIAllreduce}(c_{dot}, \text{MPI\_SUM}) / |V|$ 
  2 Compute  $y = A^T x$ 
    Copy  $x$  to  $y$ 
    Add  $A$  to  $y$ 
  *
    Convert  $y$ : Key is row index of  $A$ 
    Reduce  $y$ :
      Input: Key =  $i$ , MultiValue =  $y_i, [j, A_{ij}]$  for nonzeros  $A_{ij}$  in  $A$ 
      Output: Key =  $j$ , Value =  $A_{ij}y_i$ 
    Collate  $y$ : Key is column index of  $A$ 
    Reduce  $y$ :
      Input: Key =  $j$ , MultiValue =  $A_{ij}y_i$  for nonzeros  $A_{ij}$  in column  $j$  of  $A$ 
      Output: Key =  $j$ , Value =  $\sum_i A_{ij}y_i$ 
  3 Add  $c_{dot}$  to  $y$ ; compute  $y_{max} = \max$  element in  $y$ 
    Map  $y$ :
      Input: Key =  $i$ , Value =  $y_i$ 
       $y_i = y_i + c_{dot}$ ;  $y_{max} = \max(y_i, y_{max})$ 
      Output: Key =  $i$ , Value =  $y_i$ 
       $y_{max} = \text{MPIAllreduce}(y_{max}, \text{MPI\_MAX})$ 
  4 Scale  $y$  by  $y_{max}$ 
    Map  $y$ :
      Input: Key =  $i$ , Value =  $y_i$ 
      Output: Key =  $i$ , Value =  $y_i/y_{max}$ 
  5 Compute residual
    Add  $y$  to  $x$ 
  *
    Convert  $x$ : Key is vertex  $i$ 
    Reduce  $x$ :
      Input: Key =  $i$ , MultiValue =  $x_i, y_i$ 
       $residual = \max(|x_i - y_i|, residual)$ 
       $residual = \text{MPIAllreduce}(residual, \text{MPI\_MAX})$ 
  6 Copy  $y$  to  $x$ 

Output:
  MapReduce object  $x$  = PageRank vector: Key =  $i$ , Value =  $x_i$  = numeric rank

```

Fig. 4. MapReduce algorithm for PageRank vertex ranking, using four MapReduce objects A , MT , x , and y . Pre-aggregating several of the MapReduce objects allows several communication intensive *collate()* operations to be replaced by local *convert()* operations (marked with asterisks).

the PageRank vector is overwritten prior to the next iteration. Throughout the algorithm, we exploit the ability to call `MPI_Allreduce` to compute global dot products and norms.

This linear-algebra approach is attractive because it allows construction of the MapReduce PageRank algorithm from simple kernels (matrix–vector multiplication, dot products) on commonly used data types (matrices, vectors). One can build a variety of algorithms based on these primitives; indeed, linear-algebra toolkits such as Trilinos [14] and PETSc [3] naturally exploit this idea. In parallel, each of these toolkits shares pre-computed data layouts and communication maps among its distributed objects to enable efficient operations on the objects. In a MapReduce context, however, separating the data into vectors and matrices results in additional overhead to gather kV pairs with the same key into a key-multivalue (KMV) pair.

This overhead could be reduced in the PageRank algorithm, for example, by storing the x and y vectors in a single MapReduce object, with key i and value (x_i, y_i) . Doing this would eliminate the `copy()` in Step 2 of Fig. 4, as well as the `add()` and `convert()` in Step 5. A further performance improvement would store an entire row of A along with x and y in a single MapReduce object, with key i and value $(x_i, y_i, d_{out}, [j_1, A_{ij_1}], [j_2, A_{ij_2}], \dots, [j_{d_{out}}, A_{ij_{d_{out}}}]$) (that is, storing together, for each vertex, its old and new PageRank value along with all out-going edges incident to the vertex). This data layout would eliminate an additional `convert()` at the cost of code reusability. This data layout would be efficient for PageRank, but is more complex and less likely to be useful for additional algorithms. In addition, since each k_v pair must fit within a single page of memory (in MR-MPI), storing entire matrix rows in a single k_v pair limits the size of matrices to which the algorithm can be applied. The more general approach used in Fig. 4 of storing non-zeros separately, enables arbitrarily large problems to be solved. The detailed timing break-downs in section 5.2 allow estimation of the benefit of these possible enhancements.

4.2. Triangle enumeration

A triangle in a graph is any triplet of vertices (V_i, V_j, V_k) where the edges (V_i, V_j) , (V_j, V_k) , (V_i, V_k) exist. Fig. 5 outlines a MapReduce algorithm that enumerates all triangles, assuming an input graph G of undirected edges (V_i, V_j) where $V_i < V_j$ for every edge, i.e., an upper-triangular R-MAT matrix. This exposition follows the triangle-finding algorithm presented in [8].

The initial step is to store a copy of the graph edges as k_v pairs in an auxiliary MapReduce object G_0 , for use later in the algorithm. The first `map()` on G converts edge keys to vertex keys with edge values. After a `collate()`, each vertex has the list of vertices it is connected to; the first `reduce()` can thus flag one vertex V_i in each edge with a degree count D_i . The second `collate()` and `reduce()` assign a degree count D_j to the other vertex in each edge. In the third `map()`, only the lower-degree vertex in each edge emits its edges as k_v pairs. The task of the third `reduce()` is to emit “angles” for each of these low-degree vertices. An “angle” is a root vertex V_i with two edges to vertices V_1 and V_2 , i.e. a triangle without the third edge (V_1, V_2) . The `reduce()` emits a list of all angles of vertex V_i by a double loop over the edges of V_i . Note that the aggregate number of k_v pairs emitted at this stage is minimized by having only the low-degree vertex in each edge generate angles.

In stage 4, k_v pairs from the original graph G_0 are added to the current working set of k_v pairs in MapReduce object G . The k_v pairs in G_0 contain edges that complete triangles for the angle k_v pairs just generated. After the fourth `collate()`, a pair of vertices (V_i, V_j) is the key, and the multivalued value is the list of all root vertices in angles that contain V_i and V_j . If the multivalued value also contains a NULL, contributed by G_0 , then there is a (V_i, V_j) edge in the graph. Thus all vertices in the multivalued value are roots of angles that are complete triangles and can be emitted as a triplet key.

4.3. Connected component labeling

A connected component (CC) of a graph is a set of vertices where all pairs of vertices in the set are connected by a path of edges. A sparse graph may contain many such components. Fig. 6 outlines a MapReduce algorithm that labels each vertex in a graph with a component ID. All vertices in the same component are labeled with the same ID, which is the ID of some vertex in the component. We assume an input graph E of undirected edges (V_i, V_j) . Kang et. al. [16] propose a MapReduce CC algorithm based on a `matrix-vector` multiplication kernel. This exposition follows the CC algorithm presented in [8], with the addition of logic that load-balances data across processors, which is important when one or a few giant components exist in the graph.

The algorithm begins (before the iteration loop) by assigning each vertex to its own component or “zone,” so that $Z_i = V_i$ and storing this assignment in MapReduce object V . Each iteration grows the zones, one layer of neighbors at a time. As zones collide due to shared edges, a winner is chosen (the smaller zone ID), and vertices in the losing zone are reassigned to the winning zone. When the iterations complete, each zone has become a fully connected component and the MR object V holds the zone assignment for every vertex. The algorithm thus finds all CCs in the graph simultaneously. The number of iterations required depends on the largest diameter of any component in the graph.

The first `map()` uses MapReduce object E as input to the empty MapReduce object W to emit the vertices in each edge as keys, with the edge as a value. The current zone assignment of each vertex in V is added to the set of k_v pairs in W . The first `collate()` collects all the edges of a vertex and its zone assignment together in one multivalued value. The first `reduce()` re-emits each edge, tagged by the zone assignment of one of its vertices.

Since each edge was emitted twice, the second `collate()` on W collects the zone assignments for its two vertices together. If the two zone IDs are different, the second `reduce()` chooses a winner (the smaller of the two IDs), and emits the loser ID as a key, with the winning ID as a value. If no zone ID changes are emitted, the algorithm is finished, and the iterations cease.

The third `map()` inverts the vertex/zone k_v pairs to become zone/vertex k_v pairs. The partitioning logic in Fig. 6 for this step (and subsequent ones) is described below. The fourth `map()` adds the changed zone assignments in W to the set of k_v pairs in V . The fourth `collate()` can now collect all the vertices in each zone along with any reassignments of that zone ID. Since a zone could collide with multiple other zones on the same iteration due to shared edges, the new zone ID for a zone becomes the minimum ID of any of its neighboring zones. If no zone reassignment values appear in the multivalued value resulting from the fourth `collate()`, the zone ID is unchanged. The final `reduce()` emits a k_v pair for each vertex in the zone, with the vertex as a key and the new zone ID as a value. This is an updated version of MapReduce object V , ready to be used as input for the next iteration.

```

Input:
  MapReduce object  $G$  = edges of graph: Key =  $(V_i, V_j)$  with  $V_i < V_j$ , Value = NULL
  MapReduce object  $G_0$  = edges of graph, initially empty

1 Copy  $G$  to  $G_0$ 
1 Map  $G$ :   Convert edges to vertices
           Input: Key =  $(V_i, V_j)$ , Value = NULL
           Output: Key =  $V_i$ , Value =  $V_j$ 
           Output: Key =  $V_j$ , Value =  $V_i$ 

1 Collate  $G$ 
1 Reduce  $G$ : Add first degree to one vertex in edge
           Input: Key =  $V_i$ , MultiValue =  $(V_j, V_k, \dots)$ 
           for each  $V$  in MultiValue:
             if  $V_i < V$ : Output: Key =  $(V_i, V)$ , Value =  $(D_i, 0)$ 
             else: Output: Key =  $(V, V_i)$ , Value =  $(0, D_i)$ 

2 Collate  $G$ 
2 Reduce  $G$ : Add second degree to other vertex in edge
           Input: Key =  $(V_i, V_j)$ , MultiValue =  $((D_i, 0), (0, D_j))$ 
           Output: Key =  $(V_i, V_j)$ , Value =  $(D_i, D_j)$  with  $V_i < V_j$ 

3 Map  $G$ :   Low degree vertex emits edges
           if  $D_i < D_j$ : Output: Key =  $V_i$ , Value =  $V_j$ 
           else if  $D_j < D_i$ : Output: Key =  $V_j$ , Value =  $V_i$ 
           else: Output: Key =  $V_i$ , Value =  $V_j$ 

3 Collate  $G$ 
3 Reduce  $G$ : Emit angles of each vertex
           Input: Key =  $V_i$ , MultiValue =  $(V_j, V_k, \dots)$ 
           for each  $V_1$  in MultiValue:
             for each  $V_2$  beyond  $V_1$  in MultiValue:
               if  $V_1 < V_2$ : Output: Key =  $(V_1, V_2)$ , Value =  $V_i$ 
               else: Output: Key =  $(V_2, V_1)$ , Value =  $V_i$ 

4 Add  $G_0$  to  $G$ 
4 Collate  $G$ 
4 Reduce  $G$ : Emit triangles
           Input: Key =  $(V_i, V_j)$ , MultiValue =  $(V_k, V_l, \text{NULL}, V_m, \dots)$ 
           if NULL exists in MultiValue:
             for each non-NULL  $V$  in MultiValue:
               Output: Key =  $(V_i, V_j, V)$ , Value = NULL

Output:
  MapReduce object  $G$  = triangles in graph: Key =  $(V_i, V_j, V_k)$ , Value = NULL

```

Fig. 5. MapReduce algorithm for triangle enumeration, using two MapReduce objects G and G_0 .

Note that if a graph has only a few components, the fourth **collate()**, which keys on the zone ID, may generate a few very large key/multivalued (KMV) pairs. For example, if the entire graph is fully connected, in the last iteration, a single KMV pair assigned to one processor will result, containing all vertices in the graph. This imbalance in memory and computational work can lead to poor parallel performance of the overall algorithm. To counter this effect, various operations in stages 3 and 4 include extra logic. The idea is to partition zones whose vertex count exceeds a user-defined threshold into P sub-zones, where P is the number of processors. The 64-bit integer that stores the zone ID also stores a bit flag indicating the zone has been partitioned and a set of bits that encode the processor ID.

During the third **map()**, if the zone has been partitioned, the vertex is assigned to a random processor and the processor ID bits are added to the zone ID, as indicated by the Z_i^+ notation in Fig. 6. Likewise, if Z_i has been partitioned, the fourth **map()** emits the **kV** pair for the zone ID as (Z_i^+, Z_{winner}) instead of as (Z_i, Z_{winner}) . In this case, (Z_i, Z_{winner}) is emitted not once, but $P + 1$ times, once for each processor, and once as if Z_i had not been partitioned (for a reason discussed below).

With this additional partitioning logic, the fourth **collate()** (which keys on zone IDs, some of which now include processor bits) collects only $1/P$ of the vertices in partitioned zones onto each processor. Yet the multivalued on each processor still contains all the zone-reassignments relevant to the unpartitioned zone. Thus, the fourth **reduce()** can change the zone ID (if nec-

Input:
 MapReduce object E = edges of graph: Key = (V_i, V_j) , Value = NULL
 MapReduce object V = zone assignments of vertices: Key = V_i , Value = $Z_i = V_i$
 MapReduce object W = workspace

Iterate:

- 1 Map W using E as input: Convert edges to vertices
 Input: Key = $E_{ij} = (V_i, V_j)$, Value = NULL
 Output: Key = V_i , Value = E_{ij}
 Output: Key = V_j , Value = E_{ij}
- 1 Add V to W
- 1 Collate W : Vertex as key
- 1 Reduce W : Emit edges of each vertex with zone of vertex
 Input: Key = V_i , MultiValue = $EEEE...Z$
 for each E in MultiValue:
 Output: Key = E_{ij} , Value = Z_i
- 2 Collate W : Edge as key
- 2 Reduce W : Emit zone re-assignments
 Input: Key = E_{ij} , MultiValue = $Z_i Z_j$
 $Z_{winner} = \min(Z_i, Z_j)$; $Z_{loser} = \max(Z_i, Z_j)$
 if Z_i and Z_j are different:
 Output: Key = Z_{loser} , Value = Z_{winner}
- 2 Exit: if W is empty (no output by Reduce 2)
- 3 Map V : Invert vertex/zone pairs
 Input: Key = V_i , Value = Z_i
 if Z_i is not partitioned:
 Output: Key = Z_i , Value = V_i
 else:
 Output: Key = Z_i^+ , Value = V_i for a random processor
- 4 Map V using W as input: Add zone reassignments in W to data in V
 if Z_i is not partitioned:
 Output: Key = Z_i , Value = Z_{winner}
 else:
 Output: Key = Z_i^+ , Value = Z_{winner} for every processor
 Output: Key = Z_i , Value = Z_{winner}
- 4 Collate V : Zone ID as key
- 4 Reduce V : Emit new zone assignment of each vertex
 Input: Key = Z_i or Z_i^+ , MultiValue = $VVVV...ZZZZ...$
 $Z_{new} = \min(Z_i \text{ or } Z_i^+, Z, Z, \dots)$
 partition Z_{new} if number of $V > \text{threshold}$
 for each V_i in MultiValue:
 Output: Key = V_i , Value = Z_{new}

Output:
 MapReduce object V = zone assignment of each vertex: Key = V_i , Value = Z_i

Fig. 6. MapReduce algorithm for connected component labeling, using 3 MapReduce objects E , V , and W .

essary) in a consistent manner across all P multivalues that contain the zone's vertices. When the fourth **reduce** () emits new zone assignments for each vertex, the zone retains its partitioned status; the partition bit is also explicitly set if the vertex count exceeds the threshold for the first time.

Note that this logic does not guarantee that the partition bits of the zone IDs for all the vertices in a single zone are set consistently on a given iteration. For example, an unpartitioned zone with a small ID may consume a partitioned zone. The vertices from the partitioned zone retain their partitioned status, but the original vertices in the small zone may not set the partition bit of their zone IDs. On subsequent iterations, the fourth **map** () emits $P + 1$ copies of new zone reassignments for both partitioned and unpartitioned zone IDs, to ensure all vertices in the zone will know the correct reassignment information.

```

Input:
  MapReduce object  $V$  = maximal independent set vertices, initially empty
  MapReduce object  $E$  = edges of graph: Key =  $(V_i, V_j)$  with  $V_i < V_j$ , Value = NULL
Map  $E$ : Assign random values consistently to each vertex  $V_i$  and  $V_j$  in  $E$ 
Clone  $E$ : Convert KV pairs in  $E$  directly to KMV pairs with MultiValue = NULL

while  $N_{edges}$  in  $E > 0$ :
  1 Reduce  $E$ : Determine WINNER/LOSER vertex of each edge
    Input: Key =  $E_{ij}$ , MultiValue = NULL or LOSER
    if MultiValue = LOSER, emit nothing
     $V_w$  = WINNER vertex,  $V_l$  = LOSER vertex
    Output: Key =  $V_w$ , Value =  $(V_l, WINNER)$ 
    Output: Key =  $V_l$ , Value =  $(V_w, LOSER)$ 
  1 Collate  $E$ : Vertex as key
  2 Reduce  $E$ : Find WINNER vertices
    Input: Key =  $V_i$ , MultiValue =  $VVVV...$ 
    if all  $V_j$  in MultiValue are flagged with WINNER,  $V_i$  is a WINNER
    for each  $V_j$  in MultiValue:
      Output: Key =  $V_j$ , Value =  $(V_i, WINNER)$ 
    else:
      for each  $V_j$  in MultiValue:
        Output: Key =  $V_j$ , Value =  $V_i$ 
  2 Collate  $E$ : Vertex as key
  3 Reduce  $E$ : Find LOSER vertices
    Input: Key =  $V_i$ , MultiValue =  $VVVV...$ 
    if any  $V_j$  in MultiValue is flagged with WINNER,  $V_i$  is a LOSER
    for each  $V_j$  in MultiValue:
      Output: Key =  $V_j$ , Value =  $(V_i, LOSER)$ 
    else:
      for each  $V_j$  in MultiValue:
        Output: Key =  $V_j$ , Value =  $V_i$ 
  3 Collate  $E$ : Vertex as key
  4 Reduce  $E$ : Emit WINNER vertices and LOSER edges
    Input: Key =  $V_i$ , MultiValue =  $VVVV...$ 
    if all  $V_j$  in MultiValue are flagged with LOSER,  $V_i$  is a WINNER
    Output: to  $V$ : Key =  $V_i$ , Value = NULL
    for each  $V_j$  in MultiValue:
      if  $V_j$  is flagged with LOSER:
        Output: to  $E$ : Key =  $E_{ij}$  with  $V_i < V_j$ , Value = LOSER
      else:
        Output: to  $E$ : Key =  $E_{ij}$  with  $V_i < V_j$ , Value = NULL
  4 Collate  $E$ : Edge as key

Output:
  MapReduce object  $V$  = maximal independent set vertices: Key =  $V_i$ , Value = NULL

```

Fig. 7. MapReduce algorithm for finding a maximal independent set of graph vertices via Luby's algorithm, using two MapReduce objects E and V .

4.4. Maximal independent set identification

An “independent” set of vertices from a graph is one where no pair of vertices in the set is connected by an edge. The set is “maximal” if no vertex can be added to it¹. Finding a maximal independent set (MIS) is useful in several contexts, such as identifying large numbers of independent starting vertices for graph traversals. Luby's algorithm [19] is a well-known parallel method for finding a MIS. Fig. 7 outlines a MapReduce version of Luby's algorithm, assuming an input graph of undirected edges (V_i, V_j) where $V_i < V_j$ for every edge, i.e. an upper-triangular R-MAT matrix.

¹ A maximal set is “maximum” if it is the largest maximal set. Finding a graph's maximum independent set is an NP-hard problem, which MapReduce is unlikely to help with.

Before the iterations begin, a random value is assigned to each vertex (stored consistently for all edges in E containing V_i), which is used to compare pairs of vertices. The vertex ID itself could be used as the random value, but since the vertices eventually selected for the MIS depend on the randomization, this may introduce an unwanted bias. Instead, a random number generator can be used to assign a consistent random value R_i to each vertex in each edge (via a `map()`), which is then carried along with the vertex ID through each stage of the algorithm. In the notation of Fig. 7, each V_i is then really two quantities, a vertex ID (1 to N) and R_i . Alternatively, the R_i can be used to relabel the vertices in a random manner, assigning each a new, unique vertex ID from 1 to N . In this case, V_i is simply the new vertex ID, and the vertices in the final MIS could be remapped to recover their original IDs. These operations can be performed with a few extra MapReduce steps, outside the iteration loop.

The pre-iteration `clone()` converts the initial list of edge key/value (kv) pairs stored in MapReduce object E to key/multivalued (KMV) pairs, with the edge as the key, and NULL as the value. Thus, the iterations can begin with a `reduce()`, without need for a `collate()`. A second empty MapReduce object V is also created, which will accumulate MIS vertices as the iterations proceed.

At each iteration, the current set of edges in E is examined to identify winning vertices. Vertices adjacent to winners are flagged as losers, and all edges that contain a loser vertex are marked for removal at the start of the next iteration. Vertices with all their edges marked as losers are also flagged as winners. At each iteration marked edges are removed from the graph, and winning vertices are added to the MIS. When the graph is empty, the MIS is complete.

The first `reduce()` flags the two vertices in each edge as a potential winner or loser. This is done by comparing the two random values for the vertices (or the randomized vertex IDs as explained above). The first `collate()` thus produces a multivalued for each vertex V_i which contains all the vertices it shares an edge with, and associated winner/loser flags.

In the second `reduce()`, if V_i won the comparison with all its neighbor vertices, then it becomes a “winner” vertex. All vertices connected to the winner are emitted with V_i tagged with a winner flag. If V_i is not an overall winner, its neighbor vertices are emitted without the winner flag on V_i . The second `collate()` collects this new information for each vertex.

In the third `reduce()`, if any neighbor of V_i was a winner in the previous `reduce()` (indicated by a winner flag), V_i becomes a “loser” vertex and emits all its neighbor vertices with V_i tagged with a loser flag. Otherwise it emits all its neighbor vertices without the loser flag on V_i .

In the fourth `reduce()`, some vertices have all their neighbor vertices flagged as losers; these vertices become winners. They are either the vertices identified as winners in the second `reduce()`, or vertices who would become singletons (having no edges) when edges containing a loser vertex are removed (on the next iteration). These winning vertices are emitted to the MapReduce object V that stores the accumulating MIS.

All edges of each vertex are also emitted, retaining the loser flag if they have it; they are emitted with $E_{ij} = (V_i, V_j)$ as their key, with $V_i < V_j$. This is to ensure both copies of the edge come together via the fourth `collate()`. The multivalued for each edge now has two values, each of which is either NULL or a loser flag.

In the first `reduce()` of the next iteration, any edge with a loser flag in its multivalued does not compare its two vertices; it is effectively deleted from the graph. The iterations end when all edges have been removed from the graph. At this point, the MapReduce object V contains a complete MIS of vertices.

4.5. Single source shortest path calculation

For a directed graph with weighted edges, the single-source shortest path (SSSP) algorithm computes the shortest weighted distance from a chosen source vertex to all other vertices in the graph. This calculation is straightforward when global graph information is available. The source vertex is labeled with distance zero. Then in each iteration, edge adjacencies of labeled vertices are followed, and adjacent vertices are relabeled with updated distances. When no distances change, the iterations are complete. Most importantly, only edges adjacent to modified vertices need be visited in each iteration.

For a distributed graph, global information about edge adjacencies and labeled vertices is not available. Instead, following the Bellman-Ford-style algorithm of [6,4,12], every edge of the graph is visited in each iteration and vertex distances are updated. A MapReduce formulation of this algorithm, described in Fig. 8, begins with a graph E of directed edges (V_i, V_j) . As generated by the R-MAT procedure discussed earlier, this may include self-edges (V_i, V_i) and loop edges (both (V_i, V_j) and (V_j, V_i)). These are handled as special cases within the algorithm to avoid spurious contributions to the shortest path distances. MapReduce object V stores the distance of each vertex V_i from the source vertex V_s .

To begin, the distance to all vertices is set to infinity, except a distance of 0 for V_s itself. At each iteration, a `map()` is performed using E as input to add edges and their weights to each vertex in V . After a `collate()`, each vertex V_i knows its outgoing edges and their weights, as well as its own current distance. It may also have one or more distances assigned to it from a previous iteration (from an inbound edge). In the `reduce()`, each vertex resets its distance to the minimum of these new distances and its current distance. If its distance changed, it emits new distance values d_j for the vertices associated with its outgoing edges, where $d_j = d_i + w_{ij}$. It also unsets a “done” flag, stored by each processor. When the `reduce()` is complete, an MPI.Allreduce is performed to check the “done” flag status on all processors. If any distance was changed, the iterations continue, and the distance updates propagate through the graph. Otherwise the algorithm is done.

As with PageRank and R-MAT generation, significant savings in communication and execution time can be achieved by pre-aggregating the data stored in MapReduce objects and by splitting the data appropriately across more than one MapReduce object. An enhanced SSSP algorithm is shown in Fig. 9. The MapReduce objects V and E which store vertices and edges

```

Input:
  MapReduce object  $E$  = graph edges with weights: Key =  $(V_i, V_j)$ , Value =  $w_{ij}$ 
  MapReduce object  $V$  = vertices with distances from source vertex  $V_s$ :
    Key =  $V_i$ , Value =  $\infty$ , except Value for  $V_s = 0$ 

while not done:
  done = 1
  Map  $V$  using  $E$  as input: Add edge weights in  $E$  to data in  $V$ 
    Input: Key =  $E_{ij}$ , Value =  $w_{ij}$ 
    Output: Key =  $V_i$ , Value =  $(V_j, w_{ij})$ 
  Collate  $V$ : Vertex is key
  Reduce  $V$ : Loop over edges of vertex to update distance from  $V_s$ 
    Input: Key =  $V_i$ , MultiValue =  $d_i$ , edges  $(V_j, w_{ij})$ , candidate distances  $d_j$ 
     $d_{min} = \min(d_i, d_j, d_j, \dots)$ 
    If  $d_{min} \neq d_i$ :
      done = 0
      Output: Key =  $V_j$ , Value =  $d_{min} + w_{ij}$  for each edge vertex  $V_j$ 
    Output: Key =  $V_i$ , Value =  $d_{min}$ 
  done = MPI_Allreduce(done, MPI_MIN)

Output:
  MapReduce object  $V$  = vertices with distances from source vertex  $V_s$ :
    Key =  $V_i$ , Value =  $d_i$ 

```

Fig. 8. MapReduce algorithm for single-source shortest path (SSSP) calculation, using two MapReduce objects V and E .

```

Input:
  Pre-aggregated MapReduce object  $E$  = graph edges with weights: Key =  $(V_i, V_j)$ , Value =  $w_{ij}$ 
  Pre-aggregated MapReduce object  $V$  = vertices with distances from source vertex  $V_s$ :
    Key =  $V_i$ , Value =  $\infty$ , except Value for  $V_s = 0$ 
  MapReduce object  $U$  = updates to distances, initially empty

while not done:
  done = 1
  Aggregate  $U$ 
  Add  $U$  to  $V$ ,  $U$  = empty
  Compress  $V$ : Compute best distance for each vertex
    Input: Key =  $V_i$ , MultiValue =  $d_i$ , candidate distances  $d_j$ 
     $d_{min} = \min(d_i, d_j, d_j, \dots)$ 
    If  $d_{min} \neq d_i$ :
      done = 0
      Output to  $U$ : Key =  $V_i$ , Value =  $d_{min}$ 
    Output to  $V$ : Key =  $V_i$ , Value =  $d_{min}$ 
  done = MPI_Allreduce(done, MPI_MIN)
  if not done:
    Add  $U$  to  $E$ ,  $U$  = empty
    Compress  $E$ : Generate candidate distances for neighbors of changed vertices.
      Input: Key =  $V_i$ , MultiValue = edges  $(V_j, w_{ij})$  and  $d_i$  if updated in previous step
      If updated  $d_i$  exists:
        Output to  $U$ : Key =  $V_j$ , Value =  $d_i + w_{ij}$  for each edge vertex  $V_j$ 

Output:
  MapReduce object  $V$  = vertices with distances from source vertex  $V_s$ :
    Key =  $V_i$ , Value =  $d_i$ 

```

Fig. 9. Enhanced MapReduce algorithm for single-source shortest path (SSSP) calculation, with an additional MapReduce object U . Pre-aggregating the vertices V and edges E , and storing only changed distances in U , reduces communication and execution time.

are aggregated across processors only once at the beginning of the computation, which means the communication portion of the `collate()` is performed to assign each key to a processor. The `collate()` of Fig. 8 can then be replaced with a `compress()` which requires no communication.

In each iteration of SSSP, typically only a small number of new distances are generated. The enhanced algorithm uses MapReduce object U to store these updates. Only the updates in U are communicated; they are aggregated to the same processor that permanently stores the corresponding vertex and its edges. Thus, the total amount of required communication is smaller than in the original algorithm, which communicated all graph edges at each iteration. Updated vertex distances are stored in MapReduce object V , as before.

5. Performance Results

In this section, we present performance results for the graph algorithms of the preceding section, implemented as small C++ programs calling our MR-MPI library. The benchmarks were run on a medium-sized Linux cluster of 2 GHz dual-core AMD Opteron processors connected via a Myrinet network. Most importantly for MR-MPI, each node of the cluster has one local disk, which is used for out-of-core operations. To avoid contention for disk I/O, we ran all experiments with one MPI process per node. For comparisons with other implementations, we used either the same cluster or, where noted, Sandia's Cray XMT, a multi-threaded parallel computer with 500 MHz processors and a 3D-Torus network.

We ran the algorithms on three R-MAT graphs of different sizes, each for a varying number of processors. Details of the input data are shown in Table 1. The *small* problem (around 8M edges) can typically be run on a single processor without incurring out-of-core operations. The *medium* problem (around 134M edges) can be run on a single processor with out-of-core operations; larger processor configurations, however, do not necessarily require out-of-core operations. The *large* problem (around 2B edges) requires out-of-core operations on our 64-node cluster. These are edge counts before pre-processing steps used in some of the algorithms, e.g. to eliminate self-edges or convert the matrix to upper-triangular form.

All data sets used R-MAT parameters $(a, b, c, d) = (0.57, 0.19, 0.19, 0.05)$ and generated eight edges per vertex (on average). These parameters create a highly skewed degree distribution, as indicated by the maximum vertex degree in Table 1.

The resulting timings give a sense of the inherent scalability of the MapReduce algorithms as graph size grows on a fixed number of processors, and of the parallel scalability for computing on a graph of fixed size on a growing number of processors. Where available, we compare the MapReduce algorithm with other parallel implementations, including more traditional distributed-memory algorithms and also multi-threaded algorithms in the Multi-Threaded Graph Library (MTGL)

Table 1
Characteristics of R-MAT input data for graph algorithm benchmarks.

Data Set	# of vertices	# of edges	Maximum vertex degree
RMAT-20 (small)	$2^{20} \approx 1M$	$2^{23} \approx 8M$	$\approx 24K$
RMAT-24 (medium)	$2^{24} \approx 17M$	$2^{27} \approx 134M$	$\approx 147K$
RMAT-28 (large)	$2^{28} \approx 268M$	$2^{31} \approx 2B$	$\approx 880K$

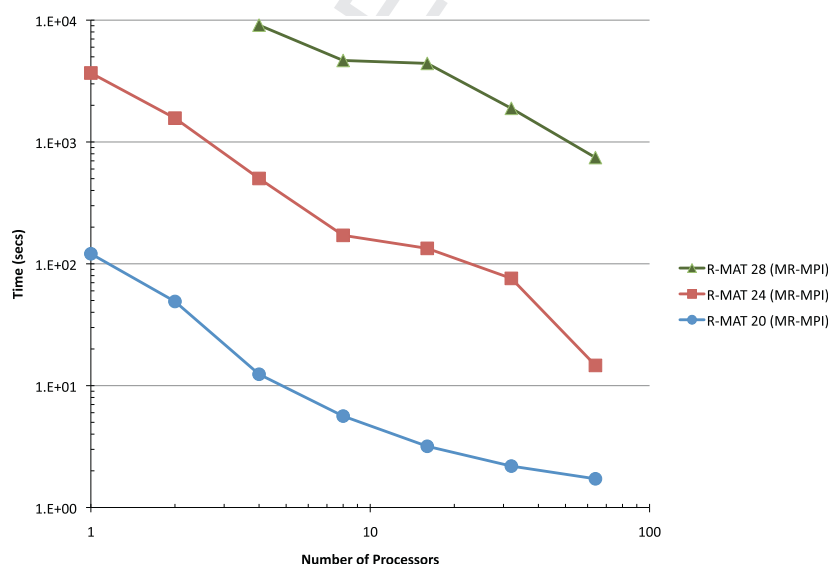


Fig. 10. Performance of the MR-MPI R-MAT generation algorithm. (Fig. 3)

[5] on the Cray XMT. We compute parallel efficiency on P processors as $(time_M \times M) / (time_P \times P)$ where M is the smallest number of processors on which the same graph was run, and $time_P$ is the execution time required on P processors.

5.1. R-MAT generation results

In Fig. 10, we show the scalability of the R-MAT generation algorithm (Fig. 3) for RMAT-20, RMAT-24 and RMAT-28. For RMAT-20 and RMAT-24, the algorithm exhibits superlinear speed-up. This is due to the decreased amount of file I/O needed with greater numbers of processors; with a larger total memory, a fixed-size problem requires less I/O as processors are added. For RMAT-28, which requires significant out-of-core operations, parallel efficiency ranges from 52% to 97%. For these problems the enhanced algorithm of Fig. 3 ran about 10% faster than the algorithm of Fig. 2.

5.2. PageRank results

In Fig. 11, we show the performance of the PageRank algorithm (Fig. 4) compared to a distributed-memory matrix-based implementation using the linear algebra toolkit Trilinos [14]. The Trilinos implementation of PageRank uses Epetra matrix/vector classes to represent the graph and PageRank vectors and requires the matrix and associated vectors fit in the aggregate memory of the processors used. Rows of matrix A and the associated entries of the PageRank vector x are uniquely assigned to processors; a random permutation of the input matrix effectively load balances the non-zero matrix entries across processors. Interprocessor communication gathers x values for **matrix-vector** multiplication and sums partial products into the y vector. Most communication is point-to-point communication, but some global communication is needed for computing residuals and norms of x and y .

Fig. 11 shows the execution time per PageRank iteration for R-MAT matrices RMAT-20, RMAT-24 and RMAT-28. Converging the PageRank iterations to tolerance 0.002 requires five or six iterations. Several R-MAT matrices of each size were generated for the experiments; the average time over the set of matrices is reported here. The Trilinos implementations show near-perfect strong scaling for RMAT-20 and RMAT-24. The MR-MPI implementations also demonstrate good strong scaling. However, MR-MPI's execution time is more than an order of magnitude slower than the Trilinos implementation. The benefit of MR-MPI's out-of-core implementation is seen, however, with the RMAT-28 data set, which could be run on smaller processor sets than the Trilinos implementation, which required 64 processors for RMAT-28.

A more detailed analysis of the performance of the MR-MPI PageRank algorithm is shown below. We perform the analysis using RMAT-20, which is small enough to fit in memory and thus does not need out-of-core operations, and RMAT-28, which requires out-of-core operation in MR-MPI. Table 2 shows the amount of time spent in each step of Fig. 4 for the MR-MPI implementation and the equivalent Trilinos implementation on 64 processors. For both implementations, the **matrix-vector** multiplication (Step 2) is the most costly step. However, the MR-MPI algorithm is consistently slower than the Trilinos implementation in each step. This effect is more pronounced for RMAT-28, where MR-MPI performs out-of-core operations.

To understand where MR-MPI spends its effort during the PageRank computation, we break down the operation times further for Step 2, the most expensive step of the PageRank computation; the results are in Table 3. In the table, we divide the **collate ()** operation into its two parts: an **aggregate ()** that involves parallel communication and a **convert ()** that gathers

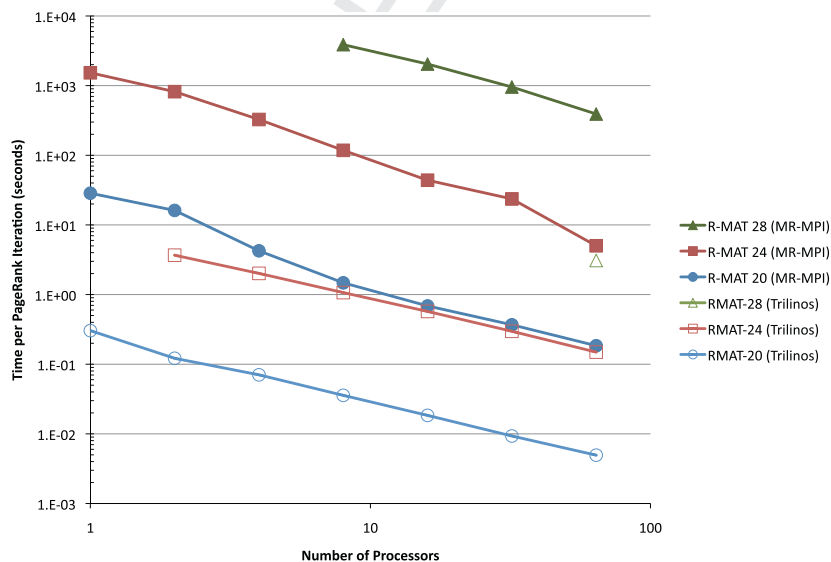


Fig. 11. Comparison of PageRank implementations using MR-MPI (Fig. 4) and Trilinos' matrix/vector classes on R-MAT data sets.

Table 2

Detailed execution times (in seconds) per PageRank iteration on 64 processors for each stage of the algorithm in Fig. 4 using MR-MPI and Trilinos.

	RMAT-20		RMAT-28	
	MR-MPI	Trilinos	MR-MPI	Trilinos
Step 1 (Compute adjustment)	0.0203	0.00030	17.53	0.0838
Step 2 (Multiply $A^T x$)	0.1377	0.00455	341.26	2.9239
Step 3 (Apply adjustment)	0.0015	0.00015	2.14	0.0494
Step 4 (Scale y)	0.0013	0.00014	1.74	0.0359
Step 5 (Compute residual)	0.0207	0.00014	21.20	0.0457

Table 3

Percentage of execution time in each operation of Step 2 of the MR-MPI PageRank algorithm in Fig. 4; experiments used 64 processors.

PageRank Step 2	RMAT-20	RMAT-28
Copy x to y	1.1%	0.4%
Add A to y	3.0%	14.3%
Convert y	23.5%	43.6%
Reduce y	7.7%	5.8%
Aggregate y (first part of collate)	24.9%	6.8%
Convert y (second part of collate)	38.2%	27.4%
Reduce y	1.6%	1.7%

local key/value (kV) pairs with matching keys into a key-multivalue (KMV) pair. All interprocessor communication occurs in the `aggregate()`. While the time spent in `aggregate()` is significant, it is small compared to the time spent in the two `convert()` operations. When out-of-core operations are required for RMAT-28, the communication cost in the `aggregate()` is a smaller percentage of total time for Step 2, as other data manipulation operations such as `convert()` and `add()` require a relatively larger percentage of the total time. Further experimentation is needed to determine whether reorganizing the MapReduce data, as described in Section 4.1, would reduce the execution time of Step 2. Organizing the data such that both the matrix A and vectors x and y are in the same MapReduce object would eliminate the `copy()` and `add()` functions, as well as the first `convert()`. However, to update the y values at the completion of Step 2, either an additional `convert()` or `aggregate()` with greater amounts of data would be needed.

Similarly, in Table 4, we show the execution times required for each operation in Step 5 of Fig. 4, for the residual computation. Clearly the time to convert kV pairs to KMV pairs dominates this computation. Reorganization of the vectors x and y into a single MapReduce object (as described in Section 4.1) would benefit this step of the computation, as the `add()`, `convert()`, and `reduce()` could be replaced by a single `map()`, with execution time comparable to the vector-scaling operation of Step 4.

5.3. Triangle finding results

In Fig. 12, we show the performance of the triangle finding algorithm (Fig. 5). Execution times for this algorithm were too large to allow the problem to be easily run with RMAT-28 on our cluster. Parallel efficiencies for RMAT-20 ranged from 80% to 140%; for RMAT-24, they ranged from 50% to 120%. The RMAT-20 matrix contained about 100 million triangles; the RMAT-24 contained 2.1 billion.

5.4. Connected components

In Fig. 13, we show the performance of the connected component identification algorithm (Fig. 6). A comparison is made with a hybrid “Giant Connected Component” implementation using both Trilinos and MR-MPI. Power law graphs often have one or two very large components and many very small components. The hybrid algorithm exploits this feature by using an inexpensive breadth-first search (BFS) from the vertex with highest degree to identify the largest components one at a time,

Table 4

Percentage of execution time in each operation of Step 5 of the MR-MPI PageRank algorithm in Fig. 4; experiments used 64 processors.

PageRank Step 5	RMAT-20	RMAT-28
Add y to x	2.2%	9.8%
Convert x	95.1%	84.9%
Reduce x	2.5%	5.3%
MPI_Allreduce	0.2%	0.0%

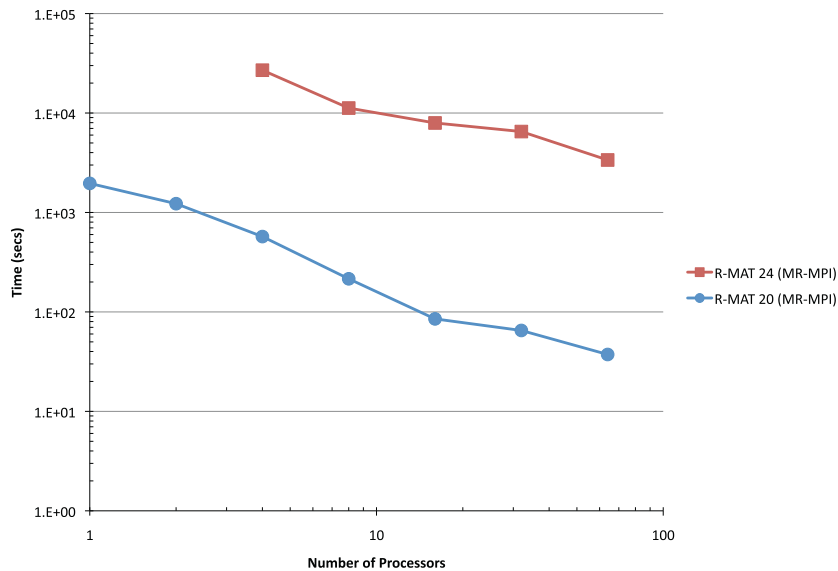


Fig. 12. Performance of the MR-MPI triangle-finding algorithm (Fig. 5).

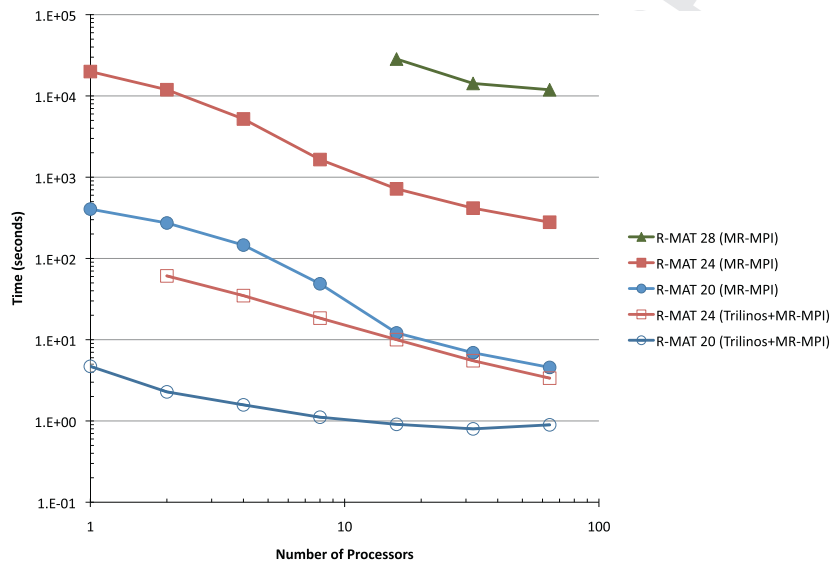


Fig. 13. Performance of the MR-MPI connected components algorithm (Fig. 6) compared with a hybrid "Giant Connected Component" algorithm based on Trilinos.

followed by a more expensive algorithm to identify the small components in the remainder of the graph. In our hybrid implementation, we initially perform **matrix-vector** multiplications in Trilinos to perform a BFS, finding a handful of components that include 70% or more of the vertices (for these R-MAT matrices). We then apply our MapReduce algorithm to the remaining graph to identify the small components. This hybrid approach is quite effective, reducing the execution time to identify all components in RMAT-20 and RMAT-24 by 80–99%, as shown in Fig. 13. For RMAT-28, where the graph is too large to fit into memory, Trilinos cannot perform the initial BFS, so only the MapReduce algorithm was used. The total number of components identified were roughly 498K, 9.37M, and 169M for the three increasing R-MAT sizes; five or six iterations were required by the algorithm.

5.5. Maximally independent set results

The execution times for the maximal independent set (MIS) algorithm (Fig. 7) are shown in Fig. 14. Like the R-MAT generation results, superlinear speed-up of the algorithm occurs for RMAT-20 and RMAT-24, as more of the graph fits into pro-

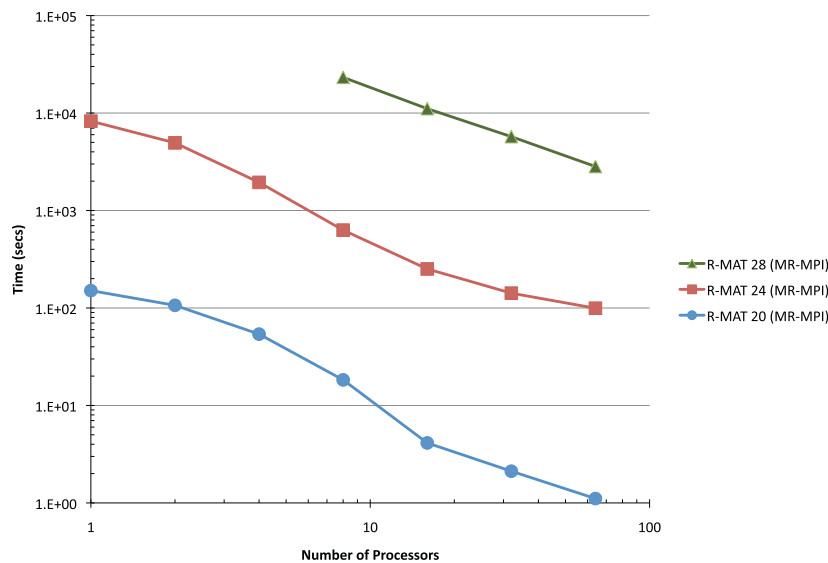


Fig. 14. Performance of the MR-MPI maximal independent set algorithm (Fig. 7).

cessor memory and less file I/O is needed. For RMAT-28, the algorithm requires significant out-of-core operations. In this case, parallel efficiency is nearly perfect going from 8 to 64 processors. The number of vertices in the resulting MIS were 368K, 5.18M, and 72.4M for the three increasing R-MAT sizes; the number of iterations required by the algorithm ranged from five for RMAT-20 to nine for RMAT-28.

5.6. Single-source shortest path results

The execution times for the SSSP algorithms of Figs. 8 and 9 are shown in Fig. 15. The results show the benefit of using the enhanced algorithm, which gave at least a 17% (and often greater) reduction in execution time due to reduced communication; only the updated distances are communicated throughout most of the enhanced algorithm. However, the execution times are still large compared to multi-threaded implementations; for example, Madduri et al. [20] report execution times of only 11s on 40 processors for a multithreaded implementation on a Cray MTA-2 (the predecessor of the XMT) on graphs with one billion edges. Seven to ten iterations were required in the MapReduce algorithms to find the SSSP to all vertices.

To compare our MR-MPI implementation with a wider set of algorithms, we performed experiments comparing MR-MPI, Hadoop, PBGL (Parallel Boost Graph Library) [13] and a multi-threaded implementation on the Cray XMT using two web

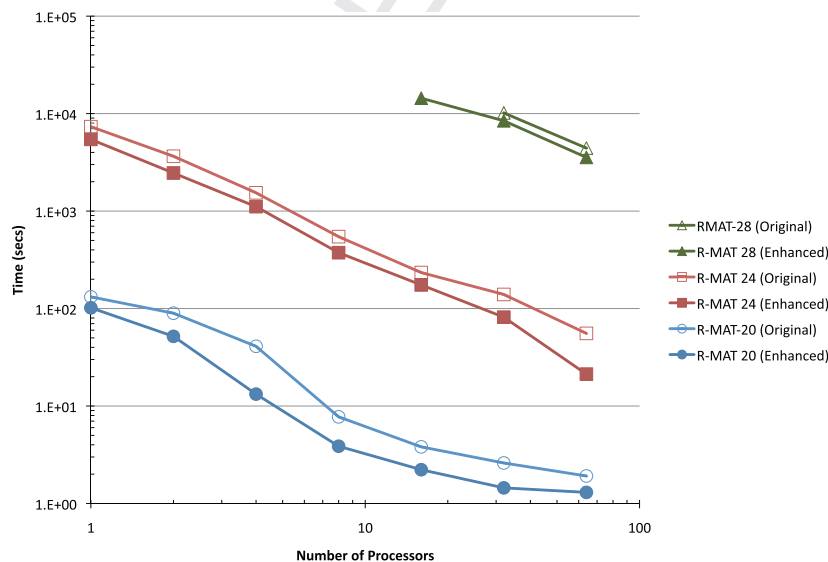


Fig. 15. Execution times for SSSP using MR-MPI with R-MAT matrices. Both the original algorithm (Fig. 8) and the enhanced algorithm (Fig. 9) are included.

graphs: WebGraphA with 13.2M vertices and 31.9M edges, and WebGraphB with 187.6M vertices and 531.9M edges. In Fig. 16, we show execution times for the SSSP algorithm using WebGraphA. Like our MR-MPI implementation, the Hadoop implementation is a Bellman-Ford-style [4,12] algorithm. The XMT and PBGL implementations are based on delta-stepping [21], and do not require full iterations over the entire edge list to advance a breadth-first search. We observe that the MR-MPI implementation runs in less time than the Hadoop implementation, but requires significantly more time than the XMT and PBGL implementations. In experiments with WebGraphB, the benefit of the enhanced algorithm (Fig. 9) is clearly shown, with a 40% reduction in execution time compared to the original SSSP algorithm (Fig. 8). But the Bellman-Ford-style iterations are especially costly in the MR-MPI and Hadoop implementations for WebGraphB, which required 110 iterations to complete; execution times for this data set are shown in Table 5.

5.7. Implementation effort

To give a rough sense of the effort involved to implement the various MapReduce algorithms described in this section, we list in Table 6 the line counts of the C++ codes used to perform the benchmarks. Each code makes calls to the MR-MPI library and implements the algorithm in the indicated figure. The line counts exclude comments and blank lines which typically add about 30% to the total. They also exclude the routines used to generate the R-MAT matrix input (except in the case of the two R-MAT algorithms themselves) or process it into upper-triangular form, since that is common to several of the benchmarks.

For comparison, we wrote a parallel distributed-memory R-MAT generation code with explicit MPI calls using a different (non-MapReduce) algorithm than that of Figs. 2 and 3. It required 845 lines of code, mainly because it must implement the parallelism explicitly, whereas the codes of this section relegate that task to the MR-MPI library. A similar all-MPI implementation of the PageRank algorithm required 718 lines. By contrast an implementation of PageRank using the Trilinos parallel linear algebra library (discussed in Section 5.2) required only 153 lines of code, since entire dot-products and **matrix-vector** multiplications can be invoked by single function calls to Trilinos. Our collaborators (see Acknowledgments) have a Hadoop implementation of the SSSP algorithm of Fig. 8. It required 697 lines of Java.

5.8. Scalability to large numbers of processors

Finally, we demonstrate the scalability of our MR-MPI library to large numbers of processors. The library was used on Sandia's Redstorm and Thunderbird parallel computers. Redstorm is a large Cray XT3 with 2+ GHz dual/quad-core AMD

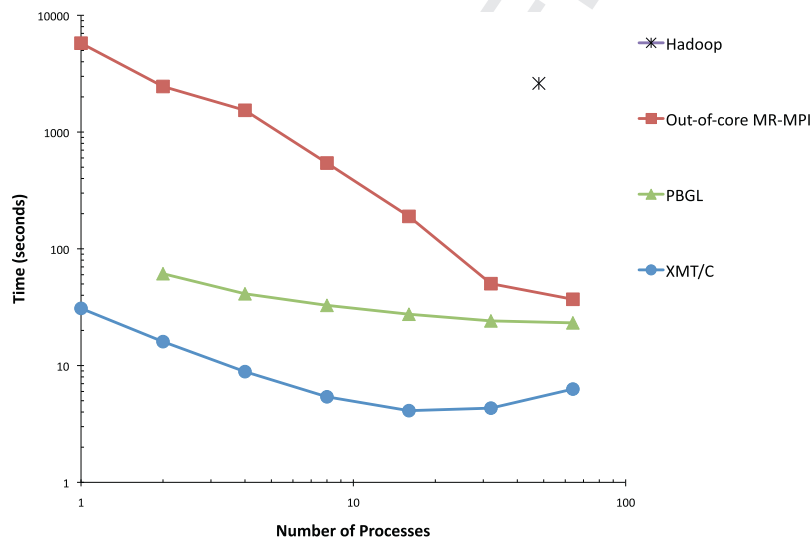


Fig. 16. SSSP using MR-MPI for WebGraphA with 13.2M vertices and 31.9M edges. Run times using Hadoop and PBGL are also shown.

Table 5
Execution times for SSSP with WebGraphB.

Implementation	Number of processes	SSSP Execution time
Hadoop	48	38,925 s.
MR-MPI original (Fig. 8)	48	13,505 s.
MR-MPI enhanced (Fig. 9)	48	8,031 s.
XMT/C	32	37 s.

Table 6

Lines of code to implement each of the graph algorithms in the associated figures.

Algorithm	R-MAT	R-MAT++	PageRank	Tri	CC	MIS	SSSP	SSSP++
Lines of code	208	216	603	367	453	393	394	448
Figure	2	3	4	5	6	7	8	9

Table 7

Characteristics of R-MAT input data for PageRank and Connected Components scalability experiments.

Data set	R-MAT a	R-MAT b	R-MAT c	R-MAT d	# of vertices	# of edges	Maximum vertex degree
Nice	0.45	0.15	0.15	0.25	2^{25}	2^{28}	1108
Nasty	0.57	0.19	0.19	0.05	2^{25}	2^{28}	230,207

Opteron processors and a custom interconnect providing 9.6 GB/s of interprocessor bandwidth. Thunderbird is a large Linux cluster with 3.6 GHz dual-core Intel EM64T processors connected by an Infiniband network. Because these systems do not have local disks for each processor, we selected a data set and page sizes that fit in memory, so out-of-core operations were not needed. For these experiments, we used two R-MAT data sets with 2^{25} vertices and 2^{28} edges, with parameters given in Table 7. The “nice” parameters produce a less-skewed sparsity pattern in the matrix than the “nasty” parameters, as indicated by the maximum degree metric. We ran both the PageRank and Connected Components algorithms on these matrices.

Fig. 17 shows the performance of the various PageRank implementations on distributed memory and multi-threaded architectures. The MR-MPI and Trilinos implementations are described in Sections 4.1 and 5.2, respectively. In the multi-threaded MTGL implementation, rank propagates via adjacency list traversal in a compressed sparse-row data structure. To maintain its scalability, code must be written so that a single thread spawns the loop that processes all in-neighbors of a given vertex; this detail enables the compiler to generate hotspot-free code.

The MR-MPI implementation demonstrated good scalability up to 1024 processors; however, as before, it required an order-of-magnitude more execution time than the matrix-based implementations on Redstorm. The Trilinos implementation is competitive with the multi-threaded implementation in MTGL on the Cray XMT, when both are run on the same number of processors.

Similar results were obtained for the Connected Components algorithm, as shown in Fig. 18. As with PageRank, the MR-MPI implementation showed good scalability up to 1024 processors, but required significantly more time than the hybrid algorithm using Trilinos and MR-MPI or the MTGL algorithm.

6. Lessons learned

We conclude with several observations about performing MapReduce operations on distributed-memory parallel machines via MPI.

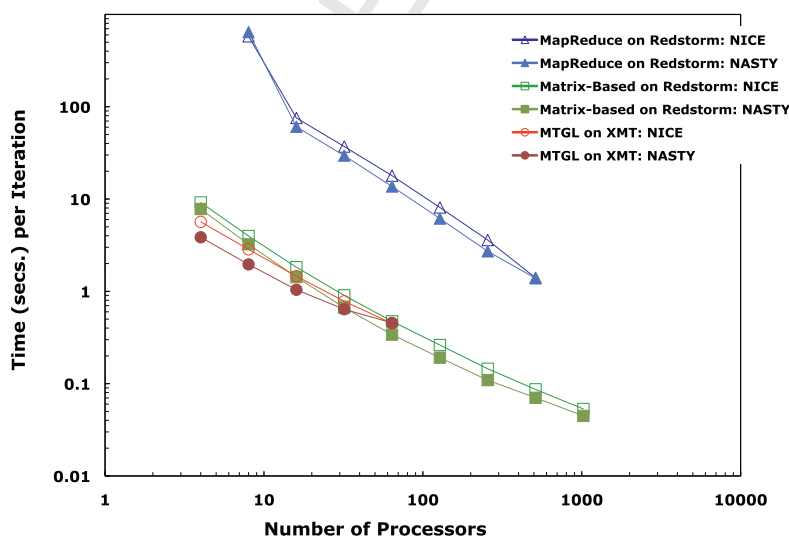


Fig. 17. Scalability comparison of PageRank using MapReduce (MR-MPI), matrix-based (Trilinos), and multi-threaded (MTGL) implementation on the R-MAT data sets in Table 7.

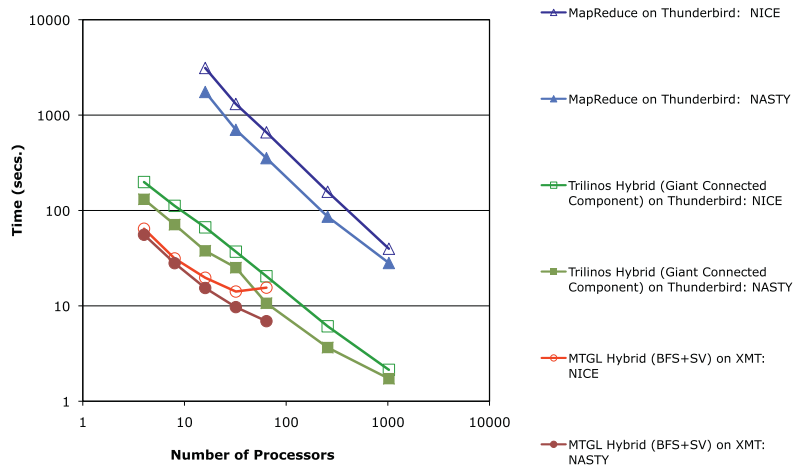


Fig. 18. Scalability comparison of Connected Components algorithms using MapReduce (MR-MPI), matrix-based/MapReduce hybrid (Trilinos/MR-MPI), and MTGL implementations on the R-MAT data sets in Table 7.

MapReduce achieves parallelism through randomizing the distribution of data across processors, which often intentionally ignores data locality. This translates into maximal data movement (during a data shuffle or `collate()` operation) with communication between all pairs of processors. But the benefit is often good load-balance, even for hard-to-balance irregular data sets, such as those derived from sparse graphs with power-law degree distributions. By contrast, MPI-based parallel algorithms, e.g. for matrix operations, or grid-based or particle-based simulation codes, typically work hard to localize data and minimize communication. To do this they often require application-specific logic and parallel communication coding to create and maintain a data decomposition, generate ghost copies of nearby spatially-decomposed data, etc.

MapReduce algorithms can be hard to design, but are often relatively easy to write and debug. Thinking about a computational task from a MapReduce perspective is different from traditional distributed-memory parallel algorithm design. For example, with an MPI mindset, it often seems heretical to intentionally ignore data locality. However, writing small `map()` and `reduce()` functions is typically easy. And writing an algorithm that involves complex parallel operations without needing to write application-specific code to communicate data via MPI calls or to move data between out-of-core disk files and processor memory is often a pleasant surprise. By contrast, extending a library like Trilinos (or other in-core MPI applications) to enable it to perform its suite of linear algebra operations in out-of-core mode on large data sets would be a considerable effort. Moreover, if a MapReduce algorithm is initially coded so that it runs correctly on one processor, it often works out-of-the-box on hundreds or thousands of processors, without the need for additional debugging.

Performing MapReduce operations on a fixed allocation of processors on a traditional MPI-based parallel machine is a somewhat different conceptual model than performing MapReduce operations on a cloud computer using (for example) Hadoop. In the former case, one can potentially control which processor owns which data at various stages of an algorithm. This is somewhat hidden from the user in a typical cloud-computing model, where data simply exists somewhere in the cloud and Hadoop ensures data moves where it is needed and is operated on by some processor. The cloud model is a nice data-centric abstraction which allows for fault tolerance both to data loss (via redundant storage) and to processor failure (via reassignment of work), neither of which is typically possible on current MPI-based parallel machines.

However, since the MPI implementation of MapReduce as described in this paper is processor-centric, one can sometimes fruitfully exploit the possibility for processors to maintain “state” over the course of multiple map and reduce operations. By controlling where data resides for maps and reduces (e.g. via a user-specified hash function), and by assuming that processor will always be available, more efficient operations with less data movement are sometimes possible. The discussion of enhanced graph algorithms in Section 4 illustrated this. To fully exploit this idea for large data sets, mechanisms and data structures are needed for processors to store, retrieve, and efficiently find needed datums on local disk (e.g. static edges of a graph), so that archived state can be used efficiently during subsequent map and reduce operations.

Finally, though this paper focuses on graph algorithms expressed as MapReduce operations, there is nothing about the MR-MPI library itself that is graph specific. We hope the library can be generally useful on large-scale monolithic or cloud-style parallel machines that support MPI, for a variety of data-intensive or compute-intensive problems that are amenable to solution using a MapReduce approach.

Acknowledgments

The MR-MPI library is open-source software, which can be downloaded from <http://www.sandia.gov/sjplimp/mapreduce.html>. It is freely available under the terms of a BSD license. Benchmark programs that implement the algorithms in Section 4 are included in the distribution. We thank the following individuals for their contributions to this paper: Greg Bayer

and Todd Plantenga (Sandia) for explaining Hadoop concepts to us, and for the Hadoop implementations and timings of Section 5; Jon Cohen (DoD) for fruitful discussions about his MapReduce graph algorithms [8]; Brian Barrett (Sandia) for the PBGL results of Section 5; Jon Berry (Sandia) for the MTGL results of Section 5, and for his overall support of this work and many useful discussions. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

References

- [1] Apache Hadoop WWW site: <<http://www.hadoop.apache.org/>>.
- [2] Titan Informatics Toolkit WWW site: <<http://www.titan.sandia.gov/>>.
- [3] S. Balay, W.D. Gropp, L.C. McInnes, B.F. Smith, Efficient management of parallelism in object oriented numerical software libraries, in: E. Arge, A.M. Bruaset, H.P. Langtangen (Eds.), *Modern Software Tools in Scientific Computing*, Birkhäuser Press, 1997, pp. 163–202.
- [4] R. Bellman, On a routing problem, *Quart. Appl. Math.* 16 (1) (1958) 87–90.
- [5] J.W. Berry, B. Hendrickson, S. Kahan, P. Konecny, Software and algorithms for graph queries on multithreaded architectures, in: *Proceedings of the 21st International Parallel and Distributed Processing Symposium*, 2007.
- [6] C. Bisciglia, A. Kimball, S. Michels-Slettvet, Lecture 5: Graph algorithms and PageRank, 2007. <<http://www.code.google.com/edu/submissions/mapreduce-minilecture/lec5-pagerank.ppt>>.
- [7] D. Chakrabarti, Y. Zhan, C. Faloutsos, R-MAT: a recursive model for graph mining, in: *SIAM Data Mining*, 2004.
- [8] J. Cohen, Graph twiddling in a mapreduce world, *Comput. Sci. Eng.* 11 (2009) 29–41.
- [9] J. Dean, S. Ghemawat, MapReduce: simplified data processing on large clusters, in: *OSDI04: sixth Symposium on Operating System Design and Implementation*, 2004.
- [10] J. Dean, S. Ghemawat, Mapreduce: simplified data processing on large clusters, *Commun. ACM* 51 (1) (2008) 107–113.
- [11] J. Ekanayake, G. Fox, High performance parallel computing with clouds and cloud technologies, in: *First International Conference on Cloud Computing (CloudComp09)*, 2009.
- [12] L.R. Ford, D.R. Fulkerson, *Flows in Networks*, Princeton University Press, 1962.
- [13] D. Gregor, A. Lumsdaine, The parallel BGL: a generic library for distributed graph computations, *Parallel Object-Oriented Scientific Computing*, 2005.
- [14] M. Heroux, R. Bartlett, V.H.R. Hoekstra, J. Hu, T. Kolda, R. Lehoucq, K. Long, R. Pawlowski, E. Phipps, A. Salinger, H. Thornquist, R. Tuminaro, J. Willenbring, A. Williams, An overview of Trilinos, Technical Report SAND2003-2927, Sandia National Laboratories, 2003.
- [15] T. Hoeftler, A. Lumsdaine, J. Dongarra, Towards efficient mapreduce using mpi, in: M. Ropo, J. Westerholm, J. Dongarra (Eds.), volume 5759 of *Lecture Notes in Computer Science*, Springer, 2009, pp. 240–249.
- [16] U. Kang, C. Tsourakakis, C. Faloutsos, PEGASUS: a peta-scale graph mining system - implementation and observations, in: *ICDM: IEEE International Conference on Data Mining*, 2009.
- [17] A.N. Langville, C.D. Meyer, A survey of eigenvector methods for web information retrieval, *SIAM Rev.* 47 (1) (2005) 135–161.
- [18] J. Lin, C. Dyer, *Data-Intensive Text Processing with Mapreduce*, Morgan & Claypool, 2010.
- [19] M. Luby, A simple parallel algorithm for the maximal independent set problem, *SIAM J. Comput.* 15 (4) (1986) 1036–1055.
- [20] K. Madduri, D.A. Bader, J.W. Berry, J.R. Crobak, An experimental study of a parallel shortest path algorithm for solving large-scale graph instances, in: *ALENEX, SIAM*, 2007.
- [21] U. Meyer, P. Sanders, Delta-stepping: a parallel single source shortest path algorithm, in: *ESA '98: Proceedings of the 6th Annual European Symposium on Algorithms*, Springer-Verlag, 1998, pp. 393–404.
- [22] T. Tu, C.A. Rendleman, D.W. Borhani, R.O. Dror, J. Gullingsrud, M.O. Jensen, J.L. Klepeis, P. Maragakis, P. Miller, K.A. Stafford, D.E. Shaw, A scalable parallel framework for analyzing terascale molecular dynamics simulation trajectories, in: *SC '08: Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, IEEE Press, Piscataway, NJ, USA, 2008, pp. 1–12.