

Optimal, Non-pipelined Reduce-scatter and Allreduce Algorithms

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Abstract

The reduce-scatter collective operation in which p processors in a network of processors collectively reduce p input vectors into a result vector that is partitioned over the processors is important both in its own right and as building block for other collective operations. We present a surprisingly simple, but non-trivial algorithm for solving this problem optimally in $\lceil \log_2 p \rceil$ communication rounds with each processor sending, receiving and reducing exactly $p-1$ blocks of vector elements. We combine this with a similarly simple, well-known allgather algorithm to get a volume optimal algorithm for the allreduce collective operation where the result vector is replicated on all processors. The communication pattern is a simple, $\lceil \log_2 p \rceil$ -regular, circulant graph also used elsewhere. The algorithms assume the binary reduction operator to be commutative and we discuss this assumption. The algorithms can readily be implemented and used for the collective operations `MPI_Reduce_scatter_block`, `MPI_Reduce_scatter` and `MPI_Allreduce` as specified in the MPI standard. We also observe that the reduce-scatter algorithm can be used as a template for round-optimal all-to-all communication and the collective `MPI_Alltoall` operation.

1 Introduction

Collective *combine* or *reduction operations* in which sets of processors (processes) cooperate to globally combine or reduce sets of input vectors and distribute the result in various ways across the processors are important algorithmic building blocks for applications on large-scale, parallel computing systems; for recent applications of mostly known algorithms, see, e.g., [9, 13, 14].

Given p consecutively ranked processors $r, 0 \leq r < p$ with input vectors V_r with the same number of elements and an associative, binary operator \oplus that can element wise combine two vectors, the global combine or reduction problem is to compute

$$W = \bigoplus_{r=0}^{p-1} V_r .$$

By the associativity of \oplus , brackets can be left out. If the operator is also commutative, the order of the input vectors does not matter. The result vector W can be stored at either a designated root processor, at all processors, or be partitioned into p blocks of elements with block $W[r]$ of the result stored at processor r . Blocks may have the same or different numbers of vector elements. These problems are solved by the MPI collectives `MPI_Reduce` (reduction to a designated root process), `MPI_Allreduce` (result vector replicated on all processes), `MPI_Reduce_scatter_block` (result vector partitioned into blocks having exactly the same number of

elements) and `MPI_Reduce_scatter` (result vector partitioned into blocks of possibly different sizes) [12]. The commonly used term *reduce-scatter* is somewhat unfortunate, since it suggests that the problem is solved in two stages as a reduction to a root processor followed by a scatter operation for partitioning the result vector. Good algorithms do not take this detour, but solve the problem directly. A better intuition is therefore to view the operation as p simultaneous, rooted reductions with each processor r being the root in a reduction of the blocks with index r . The reduce-scatter algorithm to be presented in the following follows this intuition, but the processors cooperate subtly in the reduction of the blocks. We will alternatively refer to the reduce-scatter operation as *partitioned all-reduce*.

Our algorithms work uniformly for any number of processors p . We assume the operator \oplus to be commutative. The processors communicate in a $\lceil \log_2 \rceil$ -regular circulant graph pattern where each processor has $\lceil \log_2 p \rceil$ incoming and $\lceil \log_2 p \rceil$ outgoing neighbor processors. Communication is assumed to be only one-ported (a processor can be engaged in one communication operation at a time), but to allow a processor to send a block to some processor and at the same time receive a block from some other processor [1, 8]. This simultaneous send/receive model corresponds to what the combined `MPI_Sendrecv` operation of MPI is meant to accomplish [12].

The reduce-scatter (partitioned all-reduce) and allreduce operations have been intensively researched and many algorithms and implementations, taking aspects of the communication system (different topologies, different, hierarchical organizations) into account have been proposed. A primary starting point for the algorithms of this paper is the well known and often used power-of-two, straight doubling, circulant graph, dissemination allgather (concatenation, all-to-all broadcast) algorithm by Bruck et al. [8]. The algorithms by Bar-Noy and others for allreduce (computing census functions) [2, 7] that use a cleverly adjusted doubling scheme have likewise been a starting point for subsequent algorithms and generalizations, both for the allreduce and for the reduce-scatter (partitioned all-reduce) operation [5, 22].

Well-known algorithms assuming either a ring or a fully connected communication network can solve the problem in $p - 1$ communication rounds, in which each processor sends and receives a partial block result $W[i]$ to and from a preceding and a succeeding processor and performs a reduction on the received partial result block, see for instance [10, 11, 15]. With a ring, the \oplus operator must be commutative whereas with a fully connected network, the algorithm can also work for non-commutative operators [11]. These algorithms are optimal in the number of blocks that are sent and received per processor, namely $p - 1$, but have a linear number of communication rounds which is very unattractive for small block sizes and large number of processors p . The lower bound on the number of communication rounds is clearly $\lceil \log_2 p \rceil$, as is well known [8].

The reduce-scatter problem can be solved in $\log_2 p$ communication rounds with the optimal number $p - 1$ of sent, received and reduced partial result blocks with a $\log_2 p$ -dimensional hypercube or butterfly communication pattern. Likewise, the allreduce problem can be solved with twice as many communication rounds, partial result blocks and send-receive operations. A drawback of these simple algorithms is that they do not readily extend to arbitrary numbers of processors (not only powers-of-two). This problem has often been addressed and extensions that are better than the trivial reduction to the nearest power-of-two have been proposed and implemented [16, 18]. Hypercube or butterfly pattern algorithms with some care work also for non-commutative operators.

For the reduce (reduction to root) and allreduce operations, pipelined fixed-degree (binary) trees are also used. Such algorithms are simple to implement and can work for any number of processors, sometimes also for non-commutative operators (depending on how trees are constructed and numbered), but have the disadvantage of losing effective bandwidth proportional to the arity of the trees. Likewise, there is a latency penalty proportional to the size of the

pipeline block size, which can in addition be difficult to select well. Some of these problems can be alleviated by using two trees simultaneously [17].

A standard observation is that allreduce can be accomplished by performing a reduce-scatter (partitioned all-reduce) operation followed by an allgather operation. Lower bound arguments in [3, 15] show that when the total number $p(p - 1)$ of required applications of the \oplus operator to blocks of elements are evenly shared by the processors, it is required to send and receive $2(p - 1)$ partial result blocks per processor. At least $\lceil \log_2 p \rceil$ communication rounds are required. Using the reduce-scatter (partitioned all-reduce) and allgather algorithm of the present paper, the bound on the number of blocks is achieved with $2\lceil \log_2 p \rceil$ communication rounds.

We finally observe that all-to-all communication can be accomplished by a (commutative) reduce-scatter operation by taking concatenation as the operator.

2 The Algorithms

We are given p consecutively ranked processors $r, 0 \leq r < p$ each of which can in a communication step simultaneously send a block and receive a block from two other, possibly different processors. The reduce-scatter (partitioned all-reduce) and allreduce algorithms uniformly follow a communication pattern in which each processor r in a communication round k sends a block of elements to a *to-processor* $(r + s_k) \bmod p$ and receives a block of elements from a *from-processor* $(r - s_k + p) \bmod p$ for certain skips (or jumps) s_k . A graph $C_p^{s_0, s_1, \dots, s_{q-1}}$ with vertices $r, 0 \leq r < p$ and directed edges $(r \pm s_k + p) \bmod p$ is called a *circulant graph* with *skips* (jumps) $s_k, k = 0, \dots, q - 1$ (sometimes a *loop network*, see [4]). The skips s_k are chosen by repeated halving of p with rounding up until $s_k = 1$, $s_k = \lceil s_{k+1}/2 \rceil$. The number of such roughly halving steps required is clearly $q = \lceil \log_2 p \rceil$.

2.1 A Simple, Uniform Reduce-scatter Algorithm

For the reduce-scatter problem, each processor takes an input vector V_r of elements and each V_r is partitioned in the same way into p disjoint blocks of elements such that each processor has p blocks of input each with a given, known number of elements. The number of elements per block may be the same (as in the `MPI_Reduce_scatter_block` operation) or may be different (as in the `MPI_Reduce_scatter` operation). The input blocks for processor $r, 0 \leq r < p$ are indexed as $V_r[i], 0 \leq i < p$. The reduce-scatter operation computes for each processor r the sum

$$W = \bigoplus_{i=0}^{p-1} V_i[r] .$$

A partial result block is any sum of input blocks for some subset of processors. A complete reduce-scatter (partitioned all-reduce) algorithm for processor r is shown as Algorithm 1. Each processor maintains partial result blocks $R[i]$ for some i that will contribute towards the final result W both for processor r itself and for other processors ranked after r (modulo p). The partial result blocks are maintained in the same way for all processors such that for processor r , $R[i], 0 \leq i < p$ is a partial result that will contribute to the final result at processor $(r + i) \bmod p$. This is achieved initially by a rotated copy of the input blocks $V[(r + i) \bmod p]$ into $R[i]$. In each communication round, a consecutive sequence of partial result blocks $R[s \dots s' - 1]$ is sent to the to-processor $(r + s) \bmod p$ and a consecutive sequence with the same number of blocks is received from the from-processor $(r - s + p) \bmod p$ and added into $R[0 \dots s' - s - 1]$ using the \oplus operator. Thus, for each $i, 1 \leq i < p$, the partial result for the block $R[i]$ is sent once as part of a consecutive sequence of blocks. Block $R[0]$ is kept as W and will eventually store the result of the reduction for block r .

Algorithm 1 The p -block reduce-scatter (partitioned all-reduce) algorithm for processor $r, 0 \leq r < p$. Each processor has an input vector V of p blocks of elements. Processor r receives in W the computed reduction over the r th input blocks, $W = \bigoplus_{i=0}^{p-1} V[i]$. The commutative operator for pairwise reduction of blocks is \oplus .

```

procedure PARTITIONEDALLREDUCE( $V[p], W$ )
   $W \leftarrow V[r]$ 
  for  $i = 1, \dots, p - 1$  do  $R[i] \leftarrow V[(r + i) \bmod p]$ 
  end for ▷  $R[0]$  will be kept in  $W$ 
   $s \leftarrow p$ 
  while  $s > 1$  do
     $s', s \leftarrow s, \lceil s/2 \rceil$  ▷ Halve and round up
     $t, f \leftarrow (r + s) \bmod p, (r - s + p) \bmod p$  ▷ To- and from processors
    Send( $R[s \dots s' - 1], t$ ) || Recv( $T[0 \dots s' - s - 1], f$ )
     $W \leftarrow W \oplus T[0]$ 
    for  $i = 1, \dots, s' - s - 1$  do  $R[i] \leftarrow R[i] \oplus T[i]$ 
    end for
  end while
end procedure

```

The sequence of skips (jumps) s_k for the circulant graph are computed incrementally by halving s from the previous iteration and rounding up. It can easily be seen that any i can be written as a sum of different such skips $s_k \leq i$, which means that for any processor r , there is a (at least one) path from any other processor $(r - i + p) \bmod p$ consisting of different edges s_k . The computation of partial results are performed along such paths with leaf processors contributing input block $V[r]$ and interior processors contributing a partial result including their own input block. For each processor r , there is a spanning tree directed towards r formed by combining certain such paths along which the result for processor r is computed. The decomposition of i into sums of different s_k is not necessarily unique, and depends on p . The spanning tree to r is built incrementally by hooking trees to roots with edges of length s in each iteration.

Theorem 1. *On p input vectors partitioned into p blocks, Algorithm 1 solves the reduce-scatter (partitioned all-reduce) problem in $\lceil \log_2 p \rceil$ send-receive communication rounds. Each processor sends and receives exactly $p - 1$ partial result blocks of elements and performs exactly $p - 1$ applications of the commutative reduction operator \oplus on partial result blocks.*

Proof. The communication round complexity is obvious, since $q = \lceil \log_2 p \rceil$ roughly halving steps are needed for the **while**-loop to terminate. Let s_k be the value of s before the k th iteration, $k = 0, 1, \dots, q - 1$. Starting with $s_0 = p$, by the repeated halving, clearly $p = s_0 > s_1 > \dots > s_{q-1} = 1$. In iteration k , each processor sends and receives $s_k - s_{k+1}$ blocks of elements and applies the \oplus operator also to this number of blocks. Since $\sum_{k=0}^{q-1} (s_k - s_{k+1}) = s_0 - s_{q-1} = p - 1$, the bounds on the communication and computation volume follows.

The algorithm maintains for each processor r the invariant that for $0 \leq i < s_k$, $R[i]$ (with $W = R[0]$) stores a partial result over a subtree T_i rooted at i with subtrees T_i and T_j being disjoint for $i \neq j$ but spanning all $i, 0 \leq i < p$. In other words, each processor r maintains a spanning forest over all $i, 0 \leq i < p$. The invariant holds before the first iteration of the **while**-loop since initially each T_i is a singleton storing the input $R[i] = V[(r + i) \bmod p]$. After the last iteration where $s_{q-1} = 1$ the invariant implies that for each processor r , $R[0] = W$ is the result of a reduction over a spanning tree T_0 of the blocks $V_{(r-i+p) \bmod p}[r]$.

In iteration k , subtrees T_j represented by $R[j], s_{k+1} \leq j < s_k$ are hooked into subtrees

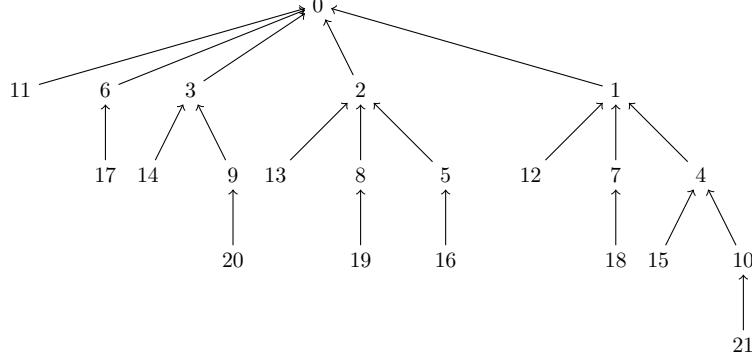


Figure 1: The tree implicitly constructed by each processor by Algorithm 1 for $p = 22$.

$T_i, 0 \leq i < s_k - s_{k+1}$, with $j = i + s_{k+1}$, $T_{i+s_{k+1}} \xrightarrow{s_{k+1}} T_i$, by an edge labeled with the skip s_{k+1} , and the partial sums represented by the subtrees $R[i], 0 \leq i < s_k - s_{k+1}$ updated by the partial sums $R[j]$ sent from processor $(r - s_{k+1} + p) \bmod p$. Partial results $R[j], 1 \leq j < p$ are sent once, and $W = R[0]$ never. Thus, the invariant is maintained, and in each iteration, the number of disjoint subtrees decreases by $s' - s$. \square

Example: It is illustrative to trace the way Algorithm 1 builds the reduction trees for the blocks. For instance, for $p = 22$, the skips are $s = 11, 6, 3, 2, 1$. In each communication round, a tree T_{i+s} is hooked into tree T_i for $0 \leq i < s' - s$ by an edge of length s . When the algorithm terminates with $s = 1$, a tree as depicted in Figure 1 has been constructed (implicitly). For any given processor, say $r = p - 1 = 21$, the order in which input blocks are reduced can be found by a depth-first traversal of this tree, subtracting the node label i from r (modulo p) to get the index of the input block $V[(r - i + p) \bmod p]$. Processor $r = 21$ receives partial results from processor $21 - 11 = 10, 21 - 6 = 15, 21 - 3 = 18, 21 - 2 = 19$ and finally $21 - 1 = 20$. Let x_i denote the input block of processor i for processor r , $x_i = V_i[r]$. Processor $r = 21$ then computes

$$\begin{aligned} W = \sum_{i=0}^{p-1} x_i &= x_{21} + x_{10} + \\ &\quad (x_{15} + x_4) + \\ &\quad (x_{18} + x_7 + (x_{12} + x_1)) + \\ &\quad (x_{19} + x_8 + (x_{13} + x_2) + (x_{16} + x_5)) + \\ &\quad (x_{20} + x_9 + (x_{14} + x_3) + (x_{17} + x_6 + (x_{11} + x_0))) \end{aligned}$$

where each line shows the received partial sums in the five communication rounds.

If we assign time costs to the bidirectional send-receive operations, the total time of the algorithm for p processors and vectors of m elements can be estimated.

Corollary 1. *In a homogeneous, linear-affine transmission cost model where concurrent, bidirectional sending and receiving blocks of m/p elements by all processors in a communication round can be charged $\alpha + \beta m/p$ time and pairwise reduction of two m/p -element vectors by the*

binary \oplus operator takes time $\gamma m/p$, the reduce-scatter (partitioned all-reduce) problem on input vectors of m elements uniformly partitioned into blocks of m/p elements is solved in time

$$T(m, p) = \alpha \lceil \log_2 p \rceil + \beta \frac{p-1}{p} m + \gamma \frac{p-1}{p} m$$

by Algorithm 1. The time for the initial copy of the m input elements into $R[i]$ adds another term of at most γm .

The proof of Theorem 1 did not use any particular properties of the roughly halving scheme for computing s except for the fact that it allows any $i, 0 \leq i < p$ to be written as a sum of different s_k values of s . The algorithm can therefore be adopted to other communication patterns leading to different number of communication rounds.

Corollary 2. *The reduce-scatter problem can be solved in q communication rounds on any circulant graph $C_p^{s_0, s_1, \dots, s_{q-1}}$ with skips $s_0 > s_1 > \dots > s_{q-1} = 1$ provided that any $0 < i < p$ can be written as a sum of different $s_k, 0 < k < q$.*

Different circulant graphs may be more or less suited to be embedded into a concrete, given communication network, and some may conceivably perform better than or different from the roughly halving scheme of Algorithm 1. It is an open, experimental question, which sequence of skips may perform best in practice on a concrete high-performance system.

Examples: The reduce-scatter problem is solved on a fully connected network in $p - 1$ communication steps by taking $s_k = p, p - 1, p - 2, \dots, 1$. This algorithm can easily be made to work also for non-commutative operators and corresponds to the folklore algorithm also stated in [11]. A straight power-of-two halving scheme, as used by Bruck et al. [8] will lead to another $\lceil \log_2 p \rceil$ round algorithm by taking $s_0 = p$ and letting $s_k, k > 0$ be the largest power-of-two smaller than s_{k-1} . We can get an algorithm running in a square root of p number of rounds by taking $s_k = p - k \lceil \sqrt{p} \rceil$ as long as $s_k > \lceil \sqrt{p} \rceil$ and for smaller p use either of the above schemes.

Algorithm 1 does not make any assumptions on the way input and result vectors are partitioned into disjoint blocks, except for requiring that all vectors are partitioned in same way. Thus, the number of elements in block $V_r[i]$ and block $V_r[j]$ may differ, but the algorithm will work correctly as long as the number of elements in $V_i[r]$ is equal to the number of elements in $V_j[r]$ for all r . Let m be the total number of elements over all blocks $V_r[i]$ (which is the same for all processors r). Since in the extreme case, all elements are concentrated in one block only, partial results of all m elements will be sent and/or received and reduced in every communication round. This leads to the following observation.

Corollary 3. *On p input vectors of m elements partitioned into p blocks of possibly different numbers of elements, Algorithm 1 solves the reduce-scatter (partitioned all-reduce) problem in time at most $\lceil \log_2 p \rceil(\alpha + \beta m + \gamma m)$, assuming a homogeneous, linear-affine transmission cost model with constant latency α and transmission and computation cost per unit β, γ , respectively.*

The algorithm can therefore be used also for `MPI_Reduce_scatter` as long as the sizes of the input blocks do not differ too much, and in the extreme case of only one block, also for `MPI_Reduce` (reduction to root) as long as the number of elements is not too large compared to p .

For large, irregular reduce-scatter problems where the sizes of the blocks for the processors can differ significantly, pipelined algorithms, also using a circulant graph communication pattern, can perform much better, depending only linearly on the total problem size m , see [20].

As the example showed, the applications of \oplus are not done in rank order, and the algorithm assumes and exploits heavily the commutativity of the \oplus operator. However, all processors perform the reductions in the same order, which depends on the skips arising by the repeated halving of p . If the input happens to be in the right order, the algorithm would work for also for a non-commutative operator. If this is not the case, the input blocks could be permuted into a suitable order, but this entails a much too expensive all-to-all redistribution step.

2.2 An Allreduce Algorithm

It is easy to see that the allreduce problem can be solved by a reduce-scatter operation followed by an allgather operation that gathers together all result blocks at all processors. An allgather operation can, as classically shown in [8], easily be implemented by a doubling scheme, essentially the reduce-scatter algorithm run in reverse. A variant which exactly reverses the sequence of skips is shown as Algorithm 2. To avoid recomputing the skips s , they are pushed on a stack during the reduce-scatter phase and popped in the allgather phase. This leads to the following result.

Algorithm 2 The allreduce algorithm for processor r , $0 \leq r < p$ derived from the reduce-scatter algorithm by addition of an allgather phase that collects all result block on all processors. Each processor has an input vector V that can be partitioned into p blocks of elements. Each processor r returns in W the resulting reduction over all input vectors. The commutative operator for pairwise reduction of blocks is \oplus .

```

procedure ALLREDUCE( $V, W$ )
    ▷ Assume  $V, W$  both partitioned into blocks  $V[i], W[i]$ 
    for  $i = 0, \dots, p - 1$  do  $R[i] \leftarrow V[(r + i) \bmod p]$ 
    end for
     $s, S \leftarrow p, \perp$  ▷ Empty stack
    while  $s > 1$  do
        PUSH( $s, S$ ) ▷ Partitioned all-reduce phase
         $s', s \leftarrow s, \lceil s/2 \rceil$  ▷ Push skip  $s$  on stack
         $t, f \leftarrow (r + s) \bmod p, (r - s + p) \bmod p$  ▷ Halve and round up
        Send( $R[s \dots s' - 1], t$ ) || Recv( $T[0 \dots s' - s - 1], f$ )
        for  $i = 0, \dots, s' - s - 1$  do  $R[i] \leftarrow R[i] \oplus T[i]$ 
        end for
    end while
    while  $S \neq \perp$  do ▷ Allgather phase
         $s' \leftarrow \text{POP}(S)$ 
         $f, t \leftarrow (r + s) \bmod p, (r - s + p) \bmod p$ 
        Send( $R[0 \dots s' - s - 1], t$ ) || Recv( $R[s \dots s' - 1], f$ )
         $s \leftarrow s'$ 
    end while
    for  $i = 0, \dots, p - 1$  do  $W[(r + i) \bmod p] \leftarrow R[i]$ 
    end for
end procedure

```

Theorem 2. *On p input vectors partitioned into p blocks, Algorithm 2 solves the allreduce problem in $2\lceil \log_2 p \rceil$ send-receive communication rounds. Each processor sends and receives exactly $2(p - 1)$ blocks of elements and performs exactly $p - 1$ applications of the commutative reduction operator \oplus on blocks of elements.*

The bound on the number of blocks communicated and the number of reductions is optimal [3, 15].

3 Implementation in and for MPI

Both Algorithm 1 and 2 can readily be implemented in MPI [12] with `MPI_Sendrecv` or `MPI_Isendrecv` for the bidirectional, combined `Send()` || `Recv()` operation. Standard considerations as when implementing the doubling allgather algorithm of Bruck et al. [8] apply, see for instance [6, 19]. In particular, the doubling and halving schemes lead to latency contention and communication redundancy when run as written on clustered, hierarchical systems with constrained per node bandwidth [21].

The algorithms compute the required skips in constant time per communication rounds. All partial result blocks are kept in consecutive buffers and no reordering of blocks is needed in the $\lceil \log_2 p \rceil$ communication rounds. Reduction and copy operations can therefore be done as bulk operations over many blocks. A property of the roughly halving scheme is that no sequence of blocks is longer than $\lceil p/2 \rceil$. This can be exploited to avoid half of the copy operations [22]. The standard, straight doubling scheme does not have this property [8]. Explicit copying could be avoided altogether by using the derived datatype mechanism of MPI [12], as done for all-to-all algorithms in [23]; however, copying is done only before and after the communication rounds, and therefore this is not likely to be a fruitful implementation choice.

4 Summary

This paper gave a very simple and easily implementable algorithm for the reduce-scatter (partitioned all-reduce) operation as found in message-passing frameworks like MPI [12]. The algorithm is optimal in number of communication rounds and in communication and computation volume. The algorithm was used as building block of an allreduce algorithm that is likewise optimal in communication and computation volume.

The circulant graph communication patterns that were used for reduce-scatter (partitioned all-reduce) and allreduce, can, with some craft, also be used to solve the all-to-all communication problem in the same number of communication rounds, similarly to the straight doubling all-to-all (indexing) algorithms given in [8], namely by taking the \oplus operator to be concatenation of element blocks. By specialization of the algorithms, likewise algorithms for the rooted, regular scatter and gather problems can easily be derived (`MPI_Scatter`, `MPI_Gather`). We also indicated that the algorithms can be used for reduction to root (`MPI_Reduce`), and by implication, for broadcast (`MPI_Bcast`), and may be attractive for small problem sizes. Circulant graphs are thus a universal scheme for collective operations as found in MPI and elsewhere [22].

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