Computing the R of the QR factorization of tall and skinny matrices using MPI_Reduce

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This work was supported by NSF-CCF (grant #881520).

Abstract. A QR factorization of a tall and skinny matrix with \( n \) columns can be represented as a reduction. The operation used along the reduction tree has in input two \( n \)-by-\( n \) upper triangular matrices and in output an \( n \)-by-\( n \) upper triangular matrix which is defined as the R factor of the two input matrices stacked the one on top of the other. This operation is binary, associative, and commutative. We can therefore leverage the MPI library capabilities by using user-defined MPI operations and MPI_Reduce to perform this reduction. The resulting code is compact and portable. In this context, the user relies on the MPI library to select a reduction tree appropriate for the underlying architecture.

1 Background

In [5,6], we introduced the so-called “Communication-Avoiding algorithms” for performing the QR factorization of a dense matrix. These algorithms minimize the number of communications between computing units (parallel case) and/or minimize the number of communications between computing unit and main memory (sequential case).

Communication-Avoiding algorithms fall in the class of (panel factorization)/(update) algorithms. For an \( m \)-by-\( n \) matrix, the algorithm perform the factorization of the first \( p \) columns (called the “panel”) and then update the remaining \( n - p \) columns, and so on. We note that, since \( p \) is small with respect to \( m \), the panel is tall and skinny. This mechanism is standard and is for example widely used in LAPACK’s subroutines. The Communication-Avoiding algorithms differs from LAPACK ones by the way they handle panel factorizations. The main idea is to reformulate the Householder QR factorization algorithm of a tall and skinny matrix as a reduction operation (see [5,6]). The mathematics behind these algorithms is slightly different from the textbook ones however they are stable. Incidentally we note that actually they are slightly more stable than the previous algorithm [2].

The Communication-Avoiding algorithms encompass a wide family of algorithms depending on which reduction tree is chosen. For example, the “Tile Algorithms” are Communication-Avoiding algorithms with a flat reduction tree. They are polylogarithmically optimal in the sequential case [5,6]. They have
been successfully used in the out-of-core context where I/O time between disk and processor is predominant \cite{9}. (We note that the work in \cite{9} predates our work of three years.) The tile algorithm also provides a large parallelism which makes them very suitable in the multicore context \cite{3,4,13}. They have been implemented on the IBM Cell Broadband Engine \cite{11} and on parallel distributed machines \cite{14}.

The “Tall and Skinny QR” (TSQR) algorithm is a Communication-Avoiding algorithm with a binary reduction tree, it is optimal in the parallel case (see \cite{5,6}), it has been used on tall and skinny matrices in parallel distributed in \cite{14} and in the multicore context \cite{10} on more square matrices.

Recent experiments on the grid \cite{1} have used more original trees in order to account for the topology of the underlying network.

The motivations for this paper are two folds. First, we present the reduction operation of our communication avoiding algorithms in the context of MPI\_reduce, we believe this is a pedagogical example that illustrates this reduction in its all generality. A binary reduction tree is an option, a flat reduction tree is another one, but actually any reduction tree is suitable. (This simply stems from the associativity of the binary operation we are using.) This demonstrates the generality of the approach. The second goal is to present the MPI community with a new and useful reduction operation. MPI currently supports our reduction and the two implementations we have tested (MPICH and Open MPI) behave correctly. Nevertheless we believe this is an interesting performance optimization problem.

## 2 A reduction operation

Figure 1 illustrates the algorithm when a binary tree is used. At the start, we need to perform the local QR factorization of our matrices. This is the computational step 1 (red circles). Then we “reduce” the four R factors to obtain the final R factor. We use a binary reduction tree where communications are shown in blue and reduction operations are done with computational step 2 (red circles). At each level of the tree, we want to reduce two upper triangular matrices with the reduction operation:

$$R := \text{qr}(R_1, R_2),$$

where the \text{qr} operator represents the QR factorization of the two input matrices stacked the one on top of the other. The C code to perform this operation is given in Table 3.

This operation is binary. (Trivial: take two upper triangular matrices in input, get one upper triangular matrix in output.) We can also prove it is associative, that is

$$\text{qr}(\text{qr}(R_1, R_2), R_3) = \text{qr}(\text{qr}(R_1, R_2), R_3).$$

This is less obvious and we need to warn the reader that the equal sign above needs to be understood as “essentially equal”. This comes from the fact that the R factor of a QR factorization is essentially unique meaning that it is unique.
up to multiplication of each row by +1 or -1 (for the real arithmetic case). In other words, we have an associativity as good as our QR factorization definition. This is therefore completely justified. We note that one can actually impose the diagonal of the R factor to have positive signs \[7\], in which case we have (strict) uniqueness of the The associativity allows us to construct various reduction trees.

This binary operation is also (essentially) commutative. (We can specify this additional property to MPI and MPI can take advantage of it.)

Independently of the reduction tree used, the stability and the number of operations performed remains the same.

We note that, if each triangular matrix is \(n\)-by-\(n\), our reduction operation performs \(O(n^3)\) operations for \(O(n^2)\) data communicated. Reduction operations in general have the same number of operations as data communicated.

## 3 Implementation

We have implemented the reduction operation using the MPI\_reduce and MPI\_Allreduce functions. This enables us to have a two-line-long code, see Table 1.

```c
lapack_dgeqrf( mloc, n, A, lda, tau, work, lwork, &info );
MPI_Allreduce( MPI_IN_PLACE, R, 1, mpidatatype_matrixR, LILA_MPIOP_QR_UPPER, mpi_comm);
```

Table 1. Code for performing QR factorization when only the R-factor is needed. We use MPI\_Allreduce to perform the reduction.

The first step is to perform the local QR factorization (the first blue computational step in Figure 1). This is done by calling the LAPACK routine DGEQRF. The second step is to perform the reduction with MPI\_Allreduce. We use a user-defined datatype for upper triangular matrix (mpi\_datatype\_matrixR). The reduction operation is provided to MPI as a user-defined operation (LILA\_MPIOP\_QR\_UPPER) that implements the C code provided in Table 3. The difference between MPI\_reduce and MPI\_Allreduce is that, at the end of MPI\_reduce, the R factor is on the root process only whereas in MPI\_Allreduce the R factor is redistributed all the way down to each process participating in the reduction. The end result of MPI\_allreduce is equivalent to the one of MPI\_reduce followed by MPI\_Bcast.

The QR factorization of two triangular matrices one on top of the other as implemented by LILA\_qr\_uppers in Table 3 as two outputs. The first output is a triangular matrix \(R\) which is stored in place of \(R_1\) which contains the R factor of the QR factorization, the second output is a triangular matrix \(V\) which is stored in place of \(R_2\) and which contains the Householder vectors used to create the unitary transformation that transforms \([R_1; R_2]\) in \([R; 0]\).

The present discussion considers the binary operation \(R := qr(R_1, R_2)\).

We essentially disregard the need for further use of the Householder vectors \(V\).
When only the R factor is needed, this is indeed appropriate. V is not needed any longer.

If we want to compute the Q factor of the QR factorization, we apply the transpose of the Householder transformation to the identity matrix. If we want to update the trailing matrix during a blocked QR factorization, we apply the Householder transformation to the trailing matrix. In these two cases, we need to be able to recreate the unitary transformation (or its transpose) used during the reduction. This means that we need to store the Householder vectors at each step of the reduction tree and we also need to store the shape of the reduction tree. Currently MPI does not allow us to do this easily. The MPI community might be interested in rendering these operations more straightforward.

4 Experimental Results

Experiments are performed on the Blue Gene/L System (frost.ucar.edu). Each compute node and I/O node is a dual-core chip, containing two 700MHz PowerPC-440 CPUs, 512MB of memory, and two floating-point units (FPUs) per core. Each processor has a peak of 2.8 GFlop/sec.

For the experiments, instead of using LAPACK DGEQRF as shown in Table 1, we have been using a recursive variant named DGEQR3 [8] since this latter performs better on this infrastructure.

Experimental results are presented in Table 2. We compare three implementations. The first row represents TSQR with hand made reduction tree (we use a binary tree), the second row represents TSQR with reduction performed by MPI_Allreduce (so this is the exact same code as in Table 1), the third row is ScaLAPACK Householder QR factorization (PDEGQR: best of PDGEQR2 and PDGEQRF). (All three codes return numerically correct results.)

We present the performance in MFlop/sec/proc of the operation. (The number of floating point operations is taken as $2mn^2$.) This is a strong scalability experiment, the matrix size is kept constant ($m = 1,000,000$ and $n = 50$) and the number of processors is increased from 32 to 256.

We observe that TSQR with MPI_Allreduce behaves nicely. It outperforms the ScaLAPACK Householder QR factorization (PDGEQRx) quite significantly. This is due to the fact that we are comparing a Communication Avoiding algorithm (TSQR) with a non communication avoiding one (PDGEQRx). However our hand coded binary tree reduction TSQR outperforms the MPI_Allreduce implementation. (In the future we would like to see which tree the MPI_Allreduce is selecting.)

5 Conclusion

Using high level language is important for the portability of our codes. The two-line code presented in this manuscript describes at a high level an algorithm to compute the R of the QR factorization of tall and skinny matrices using a
Table 2. Performance in MFlop/sec/proc to compute the R factor of the QR factorization. The number of floating point operations is taken as $2mn^2$ for all operations. The matrix has dimension $m = 1,000,000$ and $n = 50$. This is a strong scalability experiment, the matrix size is kept constant while the number of processors is increased.

| # of processors | 32  | 64  | 128 | 256 |
|-----------------|-----|-----|-----|-----|
| 1. TSQR         | 690 | 666 | 662 | 610 |
| 2. TSQR with MPI Reduce | 420 | 411 | 414 | 392 |
| 3. ScaLAPACK Householder QR | 193 | 190 | 206 | 184 |

reduction tree. This code can be ported on many architectures and still keeps it efficiency providing that the middleware layer (MPI) is able to select the appropriate reduction tree for the underlying infrastructure (cluster of multicore node, grid, etc.) and the reduction operation.

In the tall and skinny context, there is one reduction involved total. In the general case, however, it is important to realize that each reduction is followed by an update, itself followed by a reduction, etc. The choice of the reduction tree impacts dramatically subsequent operations. A flat tree for example enables a pipeline of tasks and, for that reason, the flat tree is often preferred in the parallel square case.

Communication algorithms encompasses a wide variety of algorithms that are now actively studied. It is important to understand that they derive from the same formulation (given in [5,6,12]): panel factorization with reduction tree and update.

The optimization of the reduction tree for the Householder QR factorization for various matrix shapes, various network topologies, various memory hierarchies is currently a research problem.

Note. The content of this manuscript was initially presented in [12] but never published. The introduction and conclusion have been adapted to reflect recent research work.

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Fig. 1. AllReduce Householder Algorithm for four processes when only the R-factor is requested.
int LILA_qr_uppers (int n, double *R1, double *R2, double *tau, double *work)
{
    /*
    * The cost of this operation is 2/3 n^3 to compare with
    * 10/3n^3 (=2mn^2-2/3*n^3, with m=2n) using a standard Householder code
    *
    * We exploit the fact that:
    * - the two matrices R1 and R2 are triangular
    * - the matrix H is lower triangular
    * The cost comes mainly from step (j.2): 2*(n-j)*j and (j.4): 2*(n-j)*j
    * that you integrate from j=1:n.
    * Purpose
    * ========
    *
    * Consider the (2N)-by-N matrix:
    * W = [ R1 ]
    *     [ R2 ]
    *
    * LILA_qr_uppers performs the QR factorization of W.
    *
    * The output are stored in
    * TAU, the scalars to apply the Householder transformation
    * for further use
    * R2, the upper triangular matrix that holds the Householder
    * vectors. They are represented as:
    *     [ I ]
    *     [ R2 ]
    *
    * R1, the upper triangular matrix that holds the R factor
    *
    * J. Langou, 2007.
    */
    int j;
    for (j=0; j<n; j++)
    {
      lapack_dlarfg( j+2, &(R1[j*n+j]), &(R2[j*n]), 1, &(tau[j]));
      if ((j<n-1) && (tau[j] != 0.0e+00))
      {
        /*
         * w := R2(1:j,j+1:n)' * v(1:j) + R1(j,j+1:n)
         */
        cblas_dgemv( CblasColMajor, CblasTrans, j+1, n-j-1, 1.0e+00,
                    &(R2[(j+1)*n]), n, &(R2[j*n]), 1, 0.0e+00, work, 1 );
        cblas_daxpy( n-j-1, 1.0e+00, &(R1[(j+1)*n+j]), n, work, 1 );
        /*
        * R1(j,j+1:n) = R1(j,j+1:n) - tau * w
        * R2(1:j,j+1:n) = R2(1:j,j+1:n) - tau * v(1:j) * w
        */
        cblas_daxpy( n-j-1, -tau[j], work, 1, &(R1[(j+1)*n+j]), n);
        cblas_dger( CblasColMajor, j+1, n-j-1, -tau[j], &(R2[j*n]), 1,
                    work, 1, &(R2[(j+1)*n]), n );
      }
    }
    return 0;
}

Table 3. Code for Householder QR factorization of two upper triangular matrices.