Deriving Correct High-Performance Algorithms
FLAME Working Note #86

Devangi N. Parikh
Margaret E. Myers
Robert A. van de Geijn
The University of Texas at Austin
Austin, Texas 78712
{dnp,myers,rvdg}@cs.utexas.edu

October 13, 2017

Abstract

Dijkstra observed that verifying correctness of a program is difficult and conjectured that derivation of a program hand-in-hand with its proof of correctness was the answer. We illustrate this goal-oriented approach by applying it to the domain of dense linear algebra libraries for distributed memory parallel computers. We show that algorithms that underlie the implementation of most functionality for this domain can be systematically derived to be correct. The benefit is that an entire family of algorithms for an operation is discovered so that the best algorithm for a given architecture can be chosen. This approach is very practical: Ideas inspired by it have been used to rewrite the dense linear algebra software stack starting below the Basic Linear Algebra Subprograms (BLAS) and reaching up through the Elemental distributed memory library, and every level in between. The paper demonstrates how formal methods and rigorous mathematical techniques for correctness impact HPC.

1 Introduction

A typical approach to the porting of functionality to a new architecture is to retarget an existing implementation. Along the way, a software developer may use a profiler to identify the compute-intensive part of the code, which then becomes the first step in a long optimization process. Sometimes (often?), after a lot of effort, it is discovered that an entirely new algorithm should be used instead.

As an example, let us consider an important step when computing the solution of the generalized Hermitian eigenvalue problem. This problem can be formulated mathematically as $Ax = \lambda Bx$, where $A$ is Hermitian and $B$ is Hermitian and positive-definite. The positive definiteness of $B$ can be exploited by computing its Cholesky factorization ($B = LL^H$ where $L$ is lower triangular) and transforming the problem into a standard Hermitian eigenvalue problem: $L^{-1}AL^{-H}z = \lambda z$ where $z = L^Hx$.

While high-performance implementation of Cholesky factorization is a well-studied topic \cite{1}, the computation $A = L^{-1}AL^{-H}$, also called two-sided triangular solve with multiple right-hand sides (two-sided TRSM) since it can also be reformulated as solving $CL^H = A$, where $C$ overwrites $A$, is an important operation that is a bit more off the beaten track.

The distributed memory parallel implementation of this operation appears to have started with the direct translation of the LAPACK \cite{11} routine $[\text{sdcz}]\text{SYGST}$ into the ScalAPACK routine $P[\text{SDCZ}]\text{SYGST}$. Since much of the computation in $[\text{SDCZ}]\text{SYGST}$ involves a triangular solve with multiple right-hand sides operation $[\text{SDCZ}]\text{TRSM}$, which

---

1This is an example that we encountered many years ago. We consider it a convenient example to make our point. What we describe about the history of this operation should not be taken to be criticism of current implementations. The performance graphs we use were taken from a technical report written many years ago. The point of this paper is to answer the question of how to make the discovery of algorithms systematic. The performance graphs used are merely there for illustration. The focus of the reader should be on how deriving correct algorithms helps discover high-performance solutions.
is known not to parallelize well, the resulting performance was extremely poor, as illustrated in Figure 1 (the performance curve is among those at the very bottom). A better implementation, which uses a totally different algorithmic variant, proposed by Sears et al. [32], yields much better performance (given by the curve \texttt{pdsyngst}) and is also available in ScaLAPACK. The associated paper describes the new algorithm, but does not describe how to systematically find it: It is due to the special skill of a few experts that a better algorithm was found. The technique is special enough that the better algorithm was instantiated for the case where (due to symmetry) only the lower triangular part of matrix $A$ is updated, but not for the case where the upper triangular part is targeted instead.

In Figure 1, we also show performance curves for five more algorithms. They are implemented using the Elemental library for distributed memory parallel dense matrix computations. The point is that there are many algorithms, among which is an algorithm that best translates to distributed memory architectures. The details of the optimization of the chosen algorithm are secondary to the choice of that algorithm. Our approach is captured by a quote attributed to Dijkstra: “Always design your program as a member of a whole family of programs, including those that are likely to succeed it.”

2 Deriving from specification

“The only effective way to raise the confidence level of a program significantly is to give a convincing proof of its correctness. But one should not first make the program and then prove its correctness, because then the requirement of providing the proof would only increase the poor programmer’s burden. On the contrary: the programmer should let correctness proof and program grow hand in hand.” - Edsger W. Dijkstra (1972) [9]

In this section, we show how goal-oriented programming, advocated by Dijkstra and others, can be made practical for HPC. The methodology was first proposed in a dissertation by Gunnels [20] and a related paper [21]. It was refined into the “worksheet” that is explained in this section, in [4].

We focus on the two-sided TRSM as the driving example: Solve

$$LCL^H = A,$$

overwriting $A$ with the solution $C$.

Since $A$ is symmetric, we will only use and update its lower triangular part.

We give the information required so that those familiar with the FLAME methodology [22] [1] [8] [33] [29] [30] can understand how the algorithms were derived while others will at least appreciate the high level ideas.
2.1 Derivation of a family of algorithms

We reformulate the computation $A := L^{-1}AL^{-H}$ as the constraint $A = C \land LCL^H = \hat{A}$ where $\land$ denotes the logical AND operator. This constraint expresses that $A$ is to be overwritten by matrix $C$, where $C$ satisfies the given constraint in which $\hat{A}$ represents the input matrix $A$. This constraint is known as the postcondition in the FLAME methodology. Details, such as the fact that $A$ is symmetric and that only the lower triangular part is to be updated, are kept implicit in our discussion. Deriving algorithms now becomes an eight step process, captured in Figure 3. This “worksheet” is filled in the order indicated in the left column marked “Step.”

Step 1: Precondition and postcondition. We start by entering the precondition (the state of the variables at the start) and postcondition (the state of the variables upon completion) in the worksheet.

Step 2: Derivation of the loop-invariants. Key to proving a loop correct is an assertion known as the loop-invariant. By showing that if it holds before an iteration, then it holds again after the iteration, mathematical induction tells us it holds for all iterations. The question is how to systematically derive the loop-invariant so it can be used to derive the loop. A recursive definition of the operation, which we call the Partitioned Matrix Expression (PME), provides the answer.

We form the PME by partitioning the matrices so that

$$A \rightarrow \begin{pmatrix} A_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix}, C \rightarrow \begin{pmatrix} C_{TL} & * \\ C_{BL} & C_{BR} \end{pmatrix}, \text{ and } L \rightarrow \begin{pmatrix} L_{TL} & 0 \\ L_{BL} & L_{BR} \end{pmatrix},$$

where $A_{TL}, C_{TL},$ and $L_{TL}$ are square submatrices and $*$ denotes the parts of the Hermitian matrices that are neither stored nor updated. Partitioning captures that algorithms inherently “march” through matrices in a way that identifies regions that have or have not been (partially) updated and/or which computation has been performed.

Substituting these partitioned matrices into the postcondition yields

$$\begin{pmatrix} A_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix} \land \begin{pmatrix} C_{TL} & * \\ C_{BL} & C_{BR} \end{pmatrix} \land \begin{pmatrix} L_{TL} & 0 \\ L_{BL} & L_{BR} \end{pmatrix}^H = \begin{pmatrix} \hat{A}_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix} \land \begin{pmatrix} L_{TL}C_{TL}L_{TL}^H = \hat{A}_{TL} \\ L_{BR}C_{BL} = A_{BL}L_{TL}^H - L_{BL}C_{TL} \\ L_{BR}C_{BR}L_{BR}^H = A_{BR} - L_{BL}C_{TL}L_{BL}^H - L_{BL}C_{BL}L_{BR}^H - L_{BR}C_{BL}L_{BL}^H \end{pmatrix}.$$

This expresses all conditions that must be satisfied upon completion of the computation, in terms of the submatrices. The bottom-right quadrant can be further manipulated into

$$L_{BR}C_{BR}L_{BR}^H = \hat{A}_{BR} - L_{BL}C_{TL}L_{BL}^H - L_{BL}C_{BL}L_{BR}^H - L_{BR}C_{BL}L_{BL}^H = \hat{A}_{BR} - L_{BL} + \frac{1}{2}C_{BL}L_{BL} + \frac{1}{2}C_{BL}L_{BL}^H - W_{BL}^H \wedge W_{BL} = L_{BL}C_{BL} \land W_{BL} = L_{BR}C_{BL} - \frac{1}{2}Y_{BL}$$

using a standard trick to cast three rank-$k$ updates into a single symmetric rank-$2k$ update. Thus, the PME can be rewritten as

$$\begin{pmatrix} A_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix} \land Y_{BL} = L_{BL}C_{TL} \land W_{BL} = L_{BR}C_{BL} - \frac{1}{2}Y_{BL} \land \begin{pmatrix} L_{TL}C_{TL}L_{TL}^H = \hat{A}_{TL} \\ L_{BR}C_{BL} = A_{BL}L_{TL}^H - Y_{BL} \\ L_{BR}C_{BR}L_{BR}^H = \hat{A}_{BR} - (L_{BL}W_{BL}^H + W_{BL}L_{BL}^H) \end{pmatrix}.$$

We are now ready to identify loop-invariants for algorithms. In the case of this operation, there are many such loop invariants. However, careful consideration for maintaining symmetry in the intermediate update and avoiding unnecessary computation leaves the five tabulated in Figure 2. What would have made Dijkstra happy with us is that we determine loop invariants a priori.
To now derive a specific algorithm, one picks one of the loop invariants for the remainder of the steps. In our discussion, we pick the simplest, Invariant 1.

**Steps 3 and 4: Loop guard and initialization.** The next step is to determine under what condition, the loop guard, execution of the loop is not yet finished. Determining this condition means reasoning as follows: After the loop completes, the loop guard is false and the loop invariant still holds. This must imply that we have completed the correct result. It is not hard to see that when $A_{TL}, C_{TL}, \ldots$ become all of $A, C, \ldots$ (respectively), the loop invariant implies the postcondition.

Similarly, before we start the loop, the loop invariant must hold. Thus, we need to partition the matrices in such a way that the precondition implies the loop invariant. Step 4 in Figure 3 has this property.

**Step 5: Progress.** Next we observe that progress must be made through the matrices. In other words, the top-left quadrants $A_{TL}, C_{TL}, \ldots$ must expand. We denote this by repartitioning, exposing submatrices (in order to derive high-performance blocked algorithms) that are taken from some of the quadrants at the top of the loop and added to other quadrants at the bottom of the loop.

**Step 6: State after repartitioning.** The algorithm must have the property that it maintains Invariant 1. We know what the state of the various quadrants of $A$ is at the top of the loop. The repartitioning step is really an indexing step: it exposes submatrices without updating their contents. Some of these submatrices will need to be updated in order to maintain the loop invariant. Step 6 answers the question “What is the state of the matrix $A$ at the top of the loop in terms of the exposed blocks?” The answer can be systematically determined by reasoning through how the exposed submatrices are related to the quadrants that appear in the loop invariant.

**Step 7: State after moving the computation forward.** Again, the algorithm must have the property that it maintains Invariant 1. We know what the state of the various quadrants of $A$ is at the bottom of the loop. The continue with step is again an indexing step: it consolidates submatrices into quadrants without updating their contents. Step 7 answers the question “What is the state of the matrix $A$ at the bottom of the loop in terms of the exposed blocks?” Again, the answer can be systematically determined by reasoning through how the exposed submatrices are related to the quadrants that appear in the loop invariant.
| Step | Annotated Algorithm: $A = C \land LCL^H = \hat{A}$ |
|------|--------------------------------------------------|
| 1a.  | $\{ A = \hat{A} \}$ |
| 2.   | \[
\left\{ \begin{array}{c}
A_{TL} \star \hat{A}_{BL} \\
A_{BR}
\end{array} \right\} = \left( \begin{array}{c}
C_{TL} \\
A_{BL}
\end{array} \right) \land L_{TL}C_{TL}L_{TL}^{-1} = \hat{A}_{TL}
\]
| 3.   | while $m(A_{TL}) < m(A)$ do |
| 5a.  | Determine blocksize $b$ |
| 5b.  | Continue with |
| 6.   | \[
\begin{array}{c}
A_{00} \\
A_{10} \\
A_{20}
\end{array} = \left( \begin{array}{c}
C_{00} \\
A_{10} \\
A_{20}
\end{array} \right) \land L_{00}C_{00}L_{00}^{-1} = \hat{A}_{00}
\]
| 8.   | \[
Y_{10} := L_{10}A_{00} \quad \text{(HEMM)}
\]
|      | $A_{10} := A_{10}L_{10}^H \quad \text{(TRSM)}$
|      | $A_{11} := A_{11} - \frac{1}{2}Y_{10}$
|      | $A_{11} := L_{11}^{-1}A_{11}L_{11}^H$
|      | $A_{10} := L_{10}^{-1}A_{10}$
|      | $A_{10} := L_{11}^T A_{10}$
| 7.   | \[
\begin{array}{c}
L_{00}C_{00}L_{00}^{-1} = A_{00} \\
L_{10}C_{00}L_{00}^{-1} = A_{10} \\
L_{11}C_{10}L_{11}^H = A_{11}
\end{array}
\]
| 2.   | \[
\left\{ \begin{array}{c}
A_{TL} \star \hat{A}_{BL} \\
A_{BR}
\end{array} \right\} = \left( \begin{array}{c}
C_{TL} \\
A_{BL}
\end{array} \right) \land L_{TL}C_{TL}L_{TL}^{-1} = \hat{A}_{TL}
\]
| 1b.  | $A = C \land LCL^H = \hat{A}$

Figure 3: Derivation of blocked Variant 1.
Algorithm: $A := L^{-1}AL^{-H}$

Partition $A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix}$, $L \rightarrow \begin{pmatrix} L_{TL} & L_{TR} \\ L_{BL} & L_{BR} \end{pmatrix}$, $Y \rightarrow \begin{pmatrix} Y_{TL} & Y_{TR} \\ Y_{BL} & Y_{BR} \end{pmatrix}$

where $A_{TL}$, $L_{TL}$, and $Y_{TL}$ are $0 \times 0$.

while $m(A_{TL}) < m(A)$ do

Determine block size $b$

Repartition

$$\begin{pmatrix} A_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} Y_{TL} & 0 \\ Y_{BL} & Y_{BR} \end{pmatrix}, \quad \begin{pmatrix} A_{00} & * & * \\ A_{10} & A_{11} & A_{21} \\ A_{20} & A_{21} & A_{22} \end{pmatrix}, \quad \begin{pmatrix} L_{TL} & 0 \\ L_{BL} + L_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} L_{00} & 0 \\ L_{10} & L_{11} & 0 \\ L_{20} & L_{21} & L_{22} \end{pmatrix},$$

where $A_{11}, L_{11},$ and $Y_{11}$ are $b \times b$

| Variant 1 |
|---|
| $Y_{10} := L_{10}A_{00}$ (HEMM) |
| $A_{10} := A_{10}L_{00}^{-H}$ (TRSM) |
| $A_{10} := W_{10} = A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{11} := A_{11}$ |
| $-(A_{10}L_{10}^{-H} + L_{10}A_{10}^{H})$ |
| $A_{11} := L_{11}^{-1} A_{11} L_{11}^{-H}$ |
| $A_{10} := A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{10} := L_{11}^{-1} A_{10}$ |

| Variant 2 |
|---|
| $Y_{10} := L_{10}A_{00}$ (HEMM) |
| $A_{10} := W_{10} = A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{11} := A_{11}$ |
| $-(A_{10}L_{10}^{-H} + L_{10}A_{10}^{H})$ |
| $A_{11} := L_{11}^{-1} A_{11} L_{11}^{-H}$ |
| $A_{21} := 2A_{21} - A_{20}L_{10}^{H}$ (GEMM) |
| $A_{21} := A_{21}L_{11}^{-H}$ |
| $A_{10} := A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{10} := L_{11}^{-1} A_{10}$ |

| Variant 3 |
|---|
| $Y_{10} := L_{10}A_{00}$ (HEMM) |
| $A_{10} := W_{10} = A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{11} := A_{11}$ |
| $-(A_{10}L_{10}^{-H} + L_{10}A_{10}^{H})$ |
| $A_{11} := L_{11}^{-1} A_{11} L_{11}^{-H}$ |
| $A_{21} := 2A_{21} - A_{20}L_{10}^{H}$ (GEMM) |
| $A_{21} := A_{21}L_{11}^{-H}$ |
| $A_{10} := A_{10} - \frac{1}{2} Y_{10}$ |
| $A_{10} := L_{11}^{-1} A_{10}$ |

| Variant 4 |
|---|
| $A_{10} := L_{11}^{-1} A_{10}$ |
| $A_{20} := A_{20} - L_{21}A_{10}$ (GEMM) |
| $A_{11} := L_{11}^{-1} A_{11} L_{11}^{-H}$ |
| $Y_{21} := L_{21}A_{11}$ |
| $A_{21} := A_{21}L_{11}^{-H}$ |
| $A_{21} := W_{21} = A_{21} - \frac{1}{2} Y_{21}$ |
| $A_{22} := A_{22}$ |
| $-(L_{21}A_{21}^{H} + A_{21}L_{21}^{H})$ (HER2K) |
| $A_{21} := A_{21} - \frac{1}{2} Y_{21}$ |
| $A_{21} := L_{22}^{-1} A_{21}$ (TRSM) |

| Variant 5 |
|---|
| $A_{11} := L_{11}^{-1} A_{11} L_{11}^{-H}$ |
| $Y_{21} := L_{21}A_{11}$ |
| $A_{21} := A_{21}L_{11}^{-H}$ |
| $A_{21} := W_{21} = A_{21} - \frac{1}{2} Y_{21}$ |
| $A_{22} := A_{22}$ |
| $-(L_{21}A_{21}^{H} + A_{21}L_{21}^{H})$ (HER2K) |
| $A_{21} := A_{21} - \frac{1}{2} Y_{21}$ |
| $A_{21} := L_{22}^{-1} A_{21}$ (TRSM) |

Continue with

$$\begin{pmatrix} A_{TL} & * \\ A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & * & * \\ A_{10} & A_{11} & A_{21} \\ A_{20} & A_{21} & A_{22} \end{pmatrix}, \quad \begin{pmatrix} L_{TL} & 0 \\ L_{BL} + L_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} L_{00} & 0 \\ L_{10} & L_{11} & 0 \\ L_{20} & L_{21} & L_{22} \end{pmatrix},$$

endwhile

Figure 4: All five blocked variants for computing $A := L^{-1}AL^{-H}$.  

6
Step 8: Updating the exposed submatrices. Finally, we recognize that the contents of the submatrices must be updated from the state indicated in Step 6 to the state indicated in Step 7.

The algorithms. The eight steps now yield the algorithmic variant, blocked Variant 1, that corresponds to Invariant 1. All the assertions in the grey boxes in the worksheet provide the proof of correctness, which has been created hand-in-hand with the derivation of the algorithm. After eliminating those grey boxes, we are left with the algorithm, as shown in Figure 4. In that figure, we also give Variants 2-5, which result from applying the same steps to Invariants 2-5.

2.2 Not all algorithms are created equal

All algorithms in Figure 4 incur a cost of about $n^3$ floating point operations (flops) when $n$ is the matrix size. A quick way to realize where the algorithms spend most of their time is to consider the partitionings

\[
\begin{pmatrix}
A_{00} & * & * \\
A_{10} & A_{11} & * \\
A_{20} & A_{21} & A_{22}
\end{pmatrix}
\quad \begin{pmatrix}
L_{00} & 0 & 0 \\
L_{10} & L_{11} & 0 \\
L_{20} & L_{21} & L_{22}
\end{pmatrix}
\quad \begin{pmatrix}
C_{00} & * & * \\
C_{10} & C_{11} & * \\
C_{20} & C_{21} & C_{22}
\end{pmatrix}
\]

and to note that operations that involve at least one operand that is highlighted contribute to an $O(n^3)$ (highest order) cost term while the others contribute to at most an $O(bn^2)$ term. Thus, first and foremost, it is important that the highlighted operations in Figure 4 attain high performance.

On sequential and shared memory parallel architectures, all of the operations highlighted in Figure 4 can be implemented with level-3 BLAS (matrix-matrix) calls, which in principle can attain high performance [10, 16, 17]. In practice, there are some differences. These differences become very pronounced on parallel architectures, as illustrated in Figure 4

As was already pointed out in a paper by Sears et al. [32], and is explored in more detail in [31], it is the parallel triangular solves with $b$ right-hand sides (TRSM), $A_{10} := A_{10}L_{00}^H$ in Variant 1 and $A_{21} := L_{22}^{-1}A_{21}$ in Variant 5, that inherently do not parallelize well yet account for about 1/3 of the flops for Variants 1 and 5. The reason is that inherent dependencies exist within the TRSM operation, the details of which go beyond the scope of this paper. All of the other highlighted operations can, in principle, asymptotically attain near-peak performance when correctly parallelized on an architecture with reasonable communication [33, 8, 19, 34]. Thus, Variants 1 and 5 cast a substantial fraction of computation in terms of an operation that does not parallelize well, in contrast to Variants 2, 3, and 4. Variant 3 has the disadvantage that intermediate result $Y_{BL}$ must be stored. An expert knows that (general of Hermitian) rank-k updates (the case of matrix-matrix multiplication where the “k” dimension is small) inherently parallelizes well. It is for this reason that Variant 4 comes out on top. Variant 2 might be a good choice when implementing an out-of-core algorithm, since the highlighted computations for it require the bulk of data ($A_{00}$ and $A_{20}$) to be read but not written. In other words, different circumstances call for different algorithmic variants.

3 Questions and answers

3.1 How broadly has it been applied?

The methodology has been applied to a broad set of operations that are part of the BLAS and LAPACK, as well as BLAS-like and LAPACK-like operation. All in all, given how many special cases there are for each operation (e.g., whether the upper or lower triangular part of a matrix is to be updated in the two-sided TRSM), this means it has been applied to hundreds of operations, yielding families of algorithms for each.

Over the years, a number of question have been raised about the scope: Does it apply to common but more difficult operations like LU with partial pivoting and Householder transformation based QR factorization? The answer is “yes” [35]. Does it apply to eigenvalue problems? The answer is “no yet” since it has been proven that, in general, there is no algorithm for solving such problems in a finite number of computations. As the example in Section 2 shows, important steps encountered along the way do lend themselves to the technique. It may be that the iterative methods that underlie eigenvalue problem solvers can also be developed, but this is an open question.
3.2 What is the practical impact?

These algorithms have been incorporated, in one form or another, in our BLAS-like Library Instantiation Software (BLIS) [38, 37] and libflame libraries [36, 39]. Many have also made their way into the Elemental library for distributed memory dense matrix operations.

3.3 Can formal derivation be easily mastered?

Proving simple programs correct and deriving such simple programs was long a core part of computer science curricula (but less so more recently) [18]. For almost two decades, we have taught the practical techniques at the core of this paper in an upper division undergraduate course titled “Programming for Correctness and Performance.” We have frequently drawn undergraduates (often as early as in their freshman year) into research on scientific computing by introducing them to these techniques. More recently, we have taught these techniques as part of a Massive Open Online Course (MOOC) titled “LAFF-On Programming for Correctness” [30, 29]. In our experience, it is easier to get novices than experienced scientific software developers to embrace formal derivation. As such, the described methodology democratizes the development of linear algebra algorithms and libraries.

3.4 If it is systematic, can it be made automatic?

Computer science is in part about taking knowledge and making it systematic to the point where a computer can perform related tasks. Given that the methodology we described in Section 2 is systematic, can it be automated? The answer is that it can, and that it has been. As soon as we formulated the described eight steps as the “worksheet” given in Figure 3, we recognized it could be automated. A first prototype was given in the dissertation of Bientinesi [2] and the latest efforts in the dissertation of Fabregat [12], including an open source tool, Cl1ck [2]. A number of papers also describe their efforts [14, 13].

3.5 How do we choose the best?

For the example used in Section 2, we discussed how a distributed memory implementation should ideally cast most computation in terms of (general or Hermitian) rank-k updates. The reason is that these operations parallelize well. In other situations, casting most computation in terms of other operations (e.g., matrix-panel multiplication, for which the bulk of data is read but not written) may be more appropriate. One strategy is to derive and implement all algorithms and to then choose the one that attains the best performance. A good case study for this focuses on inversion of a symmetric positive-definite (SPD) matrix [5]. Another strategy is to leverage expert knowledge.

In yet another dissertation, Low [24] shows that a property of the resulting algorithm can be an input to the derivation process. In this case, he shows, the loop invariant for the algorithm with the desired property can be recognized from the PME, making it only necessary to derive the corresponding algorithm with the described techniques. In the dissertation, it is argued that this side-steps the so-called phase ordering problem for compilers.

Our own approach to implementation of high-performance linear algebra operations breaks the process up into phases. The first phase is to derive a family of algorithms. These tend to be loop-based so that the algorithmic block size naturally matches the cache sizes in a hierarchical memory. The second phase is to optimize the loop body. For this, we often merge data movements required to implement the various updates in the loop body.

The operations in a loop body can be viewed as a directed acyclic graph (DAG) where nodes represent computation and/or data movement and edges represent data dependencies. Optimizations that an expert applies can then be viewed as taking subgraphs and replacing them with alternative, equivalent subgraphs, in an effort to reduce overhead. Each step preserves correctness. The process defines a design space that can be explored for the best implementation.

As part of a dissertation [25] and related papers [26, 27], this has been formalized as a methodology called Design by Transformation (DxT). The approach is systematic enough that it has been automated in a prototype system, DxTer. Details go beyond the scope of this paper. What is important is that in a study that explores the design space that is created [28], it is shown that the design decision that has the greatest impact on performance is what algorithm from the family of algorithms to use.

Source code for Cl1ck available from [https://github.com/dfabregat/Click](https://github.com/dfabregat/Click)
3.6 What about roundoff error?

Correctness for scientific computing has a different meaning due to the presence of roundoff error when floating point arithmetic is employed. If the algorithm is not correct in exact arithmetic, it likely has problems when floating point arithmetic is used. Thus, the methodology yields a family of algorithms that are candidates.

An algorithm is numerically stable if the computed solution is the exact solution to a slightly modified (perturbed) problem. Since there tends to already be error in data and/or entering data as floating point numbers itself introduced error, the best one can hope for is the solution to a slightly changed input. The goal for numerical algorithms thus is deriving numerically stable algorithms.

A backward error analysis is often the vehicle by which it is shown that an algorithm is numerically stable. In the dissertation of Paolo Bientinesi [2] and a related paper [7], it has been shown that the methodology for deriving algorithms in Section 2 can be extended to systematically derive the backward error analysis of matrix algorithms. The process of deriving numerically stable algorithms is pursued in two steps: first identify algorithms that are correct in exact arithmetic and then derive their backward error analyses. The methodology is simple enough that it has been successfully taught to undergraduates and beginning graduate students using a technical report version [6] of [7] that includes exercises.

3.7 Does it apply beyond dense linear algebra?

The methodology has been successfully applied to the Krylov subspace methods that underlie (sparse) iterative methods for solving linear systems [11]. The key there is that by thinking of the vectors that are computed as columns in a matrix, the problem can again be formulated to involve dense matrices. Very recently, the method has been applied to the computation of all triangles in a graph [23]. Again, the key is to reformulate this as a matrix computation. In [24], it is argued that the methodology should be applicable to the class of primitive recursive functions.

The general insights are as follows: The likely target domain should inherently benefit from casting computation as a loop-based algorithm rather than a recursive computation. In this case: Start with a notation that captures how one reasons at a high level (in our case, it is the partitioning of the matrices that is captured by the notation); Cast the operation to be computed in terms of a recursive definition over an inductively defined data structure. (In our case, this is the PME.); Extract from this recursive definition one or more loop invariants. If the methodology applies, the loop should now naturally follow.

4 Conclusion

Had someone told us two decades ago that it was possible to apply goal-oriented programming techniques to dense linear algebra operations, we would have been skeptical. Only further research can help explore how far the approach can be pushed. Thus, one novel contribution of this paper is that it gives evidence that formal derivation of programs is important to software correctness for HPC applications [15].

Acknowledgments. This research was supported in part by NSF Award ACI-1550493. We would like to thank our many collaborators who have contributed to this research over the years.

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.
References

[1] E. Anderson, Z. Bai, C. Bischof, L. S. Blackford, J. Demmel, Jack J. Dongarra, J. Du Croz, S. Hammarling, A. Greenbaum, A. McKenney, and D. Sorensen. LAPACK Users’ guide (third ed.). Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1999.

[2] Paolo Bientinesi. Mechanical Derivation and Systematic Analysis of Correct Linear Algebra Algorithms. PhD thesis, Department of Computer Sciences, The University of Texas, 2006. Technical Report TR-06-46. September 2006.

[3] Paolo Bientinesi, John A. Gunnels, Margaret E. Myers, Enrique S. Quintana-Ortí, Tyler Rhodes, Robert A. van de Geijn, and Field G. Van Zee. Deriving dense linear algebra libraries. Formal Aspects of Computing, 25(6):933–945, Nov 2013.

[4] Paolo Bientinesi, John A. Gunnels, Margaret E. Myers, Enrique S. Quintana-Ortí, and Robert A. van de Geijn. The science of deriving dense linear algebra algorithms. ACM Trans. Math. Soft., 31(1):1–26, March 2005.

[5] Paolo Bientinesi, Brian Gunter, and Robert A. van de Geijn. Families of algorithms related to the inversion of a symmetric positive definite matrix. ACM Trans. Math. Softw., 35(1):3:1–3:22, July 2008.

[6] Paolo Bientinesi and Robert A. van de Geijn. The science of deriving stability analyses. FLAME Working Note #33. Technical Report AICES-2008-2, Aachen Institute for Computational Engineering Sciences, RWTH Aachen, November 2008.

[7] Paolo Bientinesi and Robert A. van de Geijn. Goal-oriented and modular stability analysis. SIAM J. Matrix Anal. Appl., 32(1):286–308, March 2011.

[8] Almadena Chtchelkanova, John Gunnels, Greg Morrow, James Overfelt, and Robert A. van de Geijn. Parallel implementation of BLAS: General techniques for level 3 BLAS. Concurrency: Practice and Experience, 9(9):837–857, Sept. 1997.

[9] Edsger W. Dijkstra. The humble programmer. Turing Award lecture; published as Edsger W. Dijkstra. The humble programmer. Commun. ACM, 15(10):859–866, 1972. Turing Award lecture, 1972.

[10] Jack J. Dongarra, Jeremy Du Croz, Sven Hammarling, and Iain Duff. A set of level 3 basic linear algebra subprograms. ACM Trans. Math. Soft., 16(1):1–17, March 1990.

[11] Victor Eijkhout, Paolo Bientinesi, and Robert van de Geijn. Towards mechanical derivation of krylov solver libraries. Procedia Computer Science, 1(1):1805 – 1813, 2010. ICCS 2010.

[12] Diego Fabregat-Traver. Knowledge-Based Automatic Generation of Linear Algebra Algorithms and Code. PhD thesis, RWTH Aachen, April 2014.

[13] Diego Fabregat-Traver and Paolo Bientinesi. Automatic generation of loop-invariants for matrix operations. In Computational Science and its Applications, International Conference, pages 82–92, Los Alamitos, CA, USA, 2011. IEEE Computer Society.

[14] Diego Fabregat-Traver and Paolo Bientinesi. Knowledge-based automatic generation of partitioned matrix expressions. In Vladimir Gerdt, Wolfram Koepf, Ernst Mayr, and Evgenii Vorozhtsov, editors, Computer Algebra in Scientific Computing, volume 6885 of Lecture Notes in Computer Science, pages 144–157, Heidelberg, 2011. Springer.

[15] Ganesh Gopalakrishnan, Paul D. Hovland, Costin Iancu, Sriram Krishnamoorthy, Ignacio Laguna, Richard A. Lethin, Koushik Sen, Stephen F. Siegel, and Armando Solar-Lezama. Report of the HPC correctness summit, jan 25-26, 2017, washington, DC. CoRR, abs/1705.07478, 2017.

[16] Kazushige Goto and Robert van de Geijn. Anatomy of high-performance matrix multiplication. ACM Trans. Math. Soft., 34(3: Article 12, 25 pages), May 2008a.
[17] Kazushige Goto and Robert van de Geijn. High-performance implementation of the level-3 BLAS. *ACM Trans. Math. Soft.*, 35(1):1–14, 2008b.

[18] David Gries. *The Science of Programming*. Springer-Verlag, 1981.

[19] John Gunnels, Calvin Lin, Greg Morrow, and Robert van de Geijn. A flexible class of parallel matrix multiplication algorithms. In *Proceedings of First Merged International Parallel Processing Symposium and Symposium on Parallel and Distributed Processing (1998 IPPS/SPDP ’98)*, pages 110–116, 1998.

[20] John A. Gunnels. *A Systematic Approach to the Design and Analysis of Parallel Dense Linear Algebra Algorithms*. PhD thesis, Department of Computer Sciences, The University of Texas, December 2001.

[21] John A. Gunnels, Fred G. Gustavson, Greg M. Henry, and Robert A. van de Geijn. FLAME: Formal Linear Algebra Methods Environment. *ACM Trans. Math. Soft.*, 27(4):422–455, December 2001.

[22] John A. Gunnels, Fred G. Gustavson, Greg M. Henry, and Robert A. van de Geijn. FLAME: Formal Linear Algebra Methods Environment. *ACM Trans. Math. Soft.*, 27(4):422–455, 2001.

[23] Matthew Lee and Tze Meng Low. A family of provably correct algorithms for exact triangle counting. 2017. submitted to Correctness2017.

[24] Tze Meng Low. *A Calculus of Loop Invariants for Dense Linear Algebra Optimization*. PhD thesis, The University of Texas at Austin, Department of Computer Science, December 2013.

[25] Bryan Marker. *Design by Transformation: From Domain Knowledge to Optimized Program Generation*. PhD thesis, The University of Texas at Austin, Department of Computer Science, May 2014.

[26] Bryan Marker, Don Batory, and Robert van de Geijn. A case study in mechanically deriving dense linear algebra code. *International Journal of High Performance Computing Applications*, 27(4):439–452, November 2013.

[27] Bryan Marker, Don Batory, and Robert van de Geijn. Code generation and optimization of distributed-memory dense linear algebra kernels. In *International Workshop on Automatic Performance Tuning (iWAPT’13)*, 2013.

[28] Bryan Marker, Don Batory, and Robert van de Geijn. Understanding performance stairs: Elucidating heuristics. In *29th IEEE/ACM International Conference on Automated Software Engineering (ASE 2014)*, 2014.

[29] Margaret E. Myers and Robert A. van de Geijn. Laff-on programming for correctness, 2017. Massive Open Online Course on edX.

[30] Margaret E. Myers and Robert A. van de Geijn. *LAFF-On Programming for Correctness*. ulaff.net, 2017.

[31] Jack Poulson, Robert van de Geijn, and Jeffrey Bennighof. Parallel algorithms for reducing the generalized hermitian-definite eigenvalue problem. FLAME Working Note #56. Technical Report TR-11-05, The University of Texas at Austin, Department of Computer Sciences, February 2011.

[32] Mark P. Sears, Ken Stanley, and Greg Henry. Application of a high performance parallel eigensolver to electronic structure calculations. In *Proceedings of the 1998 ACM/IEEE conference on Supercomputing (CDROM)*, Supercomputing ’98, pages 1–1, Washington, DC, USA, 1998. IEEE Computer Society.

[33] Robert van de Geijn and Jerrell Watts. SUMMA: Scalable universal matrix multiplication algorithm. *Concurrency: Practice and Experience*, 9(4):255–274, April 1997.

[34] Robert A. van de Geijn. *Using PLAPACK: Parallel Linear Algebra Package*. The MIT Press, 1997.

[35] Robert A. van de Geijn and Enrique S. Quintana-Ortí. *The Science of Programming Matrix Computations*. http://www.lulu.com/content/1911788, 2008.

[36] Field G. Van Zee. *libflame: The Complete Reference*. www.lulu.com, 2009.
[37] Field G. Van Zee, Tyler M. Smith, Bryan Marker, Tze Meng Low, Robert A. van de Geijn, Francisco D. Igual, Mikhail Smelyanskiy, Xianyi Zhang, Michael Kistler, Vernon Austel, John A. Gunnels, and Lee Killough. The blis framework: Experiments in portability. *ACM Trans. Math. Softw.*, 42(2):12:1–12:19, June 2016.

[38] Field G. Van Zee and Robert A. van de Geijn. Blis: A framework for rapidly instantiating blas functionality. *ACM Trans. Math. Softw.*, 41(3):14:1–14:33, June 2015.

[39] Field G. Van Zee, Ernie Chan, Robert A. van de Geijn, Enrique S. Quintana-Orti, and Gregorio Quintana-Orti. The libflame library for dense matrix computations. *IEEE Des. Test*, 11(6):56–63, November 2009.