Formal Linear Algebra Methods Environment (FLAME) Overview*

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Abstract

Since the advent of high-performance distributed-memory parallel computing, the need for intelligible code has become ever greater. The development and maintenance of libraries for these architectures is simply too complex to be amenable to conventional approaches to coding and attempting to employ traditional methodology has led to the production of an abundance of inefficient, anfractuous code that is difficult to maintain and nigh-impossible to upgrade.

Having struggled with these issues for more than a decade, we have arrived at a conclusion that is somewhat surprising to us: the answer is to apply formal methods from Computer Science to the development of high-performance linear algebra libraries. The resulting approach has consistently resulted in aesthetically-pleasing, coherent code that greatly facilitates performance analysis, intelligent modularity, and the enforcement of program correctness via assertions. Since the technique is completely language-independent, it lends itself equally well to a wide spectrum of programming languages (and paradigms) ranging from C and FORTRAN to C++ and Java to graphical programming languages like those used for LabView. In this paper, we illustrate our observations by looking at the development of the Formal Linear Algebra Methods Environment (FLAME) for implementing linear algebra algorithms on sequential architectures. This environment demonstrates that lessons learned in the distributed memory world can guide us toward better approaches to coding even in the sequential world.

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1 Introduction

When considering the unmanageable complexity of computer systems, Dijkstra recently made the following observations [7]:

(i) When exhaustive testing is impossible –i.e., almost always– our trust can only be based on proof (be it mechanized or not).
(ii) A program for which it is not clear why we should trust it, is of dubious value.
(iii) A program should be structured in such a way that the argument for its correctness is feasible and not unnecessarily laborious.
(iv) Given the proof, deriving a program justified by it, is much easier than, given the program, constructing a proof justifying it.

The core curriculum of any first-rate undergraduate Computer Science department includes at least one course that focuses on the formal derivation and verification of algorithms [12]. Many of us in scientific computing may have, at some point in time, hastily dismissed this approach, arguing that this is all very nice for small, simple algorithms, but an academic exercise hardly applicable in "our world." Since it is often the case that our work involves libraries comprised of hundreds of thousands or even millions of lines of code, the knee-jerk reaction that this approach is much too cumbersome to take seriously is understandable. Furthermore, the momentum of established practices and "traditional wisdom" do little if anything to dissuade one from this line of reasoning. Yet, as the result of our search for superior methods for designing and constructing high-performance parallel linear algebra libraries, we have come to the conclusion that it is *only* through the systematic approach offered by formal methods that we will be able to deliver reliable, maintainable, flexible, yet highly efficient matrix libraries even in the relatively well-understood area of (sequential and parallel) dense linear algebra.

While some would immediately draw the conclusion that a change to a more modern programming language like C++ is at least highly desirable, if not a necessary precursor to writing elegant code, the fact is that most applications that call packages like LAPACK [3] and ScaLAPACK [6] are still written in FORTRAN and/or C. Interfacing such an application with a library written in C++ presents certain complications. However, during the mid-nineties, the Message-Passing Interface (MPI) introduced to the scientific computing community a programming model, object-based programming, that possesses many of the advantages typically associated with the intelligent use of an object-oriented language [26]. Using objects (e.g. communicators in MPI) to encapsulate data structures and hide complexity, a much cleaner approach to coding can be achieved. Our own work on the Parallel Linear Algebra PACKage (PLAPACK) borrowed from this approach in order to hide details of data distribution and data mapping in the realm of parallel linear algebra libraries [28]. The primary concept also germane to this paper is that PLAPACK raises the level of abstraction at which one programs so that indexing is essentially removed from the code, allowing the routine to reflect the algorithm as it is naturally presented in a classroom setting. Since our initial work on PLAPACK, we have experimented with similar interfaces in such seemingly disparate contexts as (parallel) out-of-core linear algebra packages and a low-level implementation of the sequential BLAS [14].

FLAME is the latest step in the evolution of these systems. It facilitates the use of a programming style that is equally applicable to everything from out-of-core, parallel systems to single-processor systems where cache-management is of paramount concern.

Over the last seven or eight years it has become apparent that what makes our task of library development more manageable is this systematic approach to deriving algorithms coupled with the abstractions we use to make our code reflect the algorithms thus produced. Further, it is from these experiences that we can confidently state that this approach to programming greatly reduces the complexity of the resultant code and does not sacrifice high performance in order to do so.

Indeed, it is exactly the formal techniques that we may have at one time dismissed as merely academic or impractical which make this possible, as we will attempt to illustrate in the following sections.

2 The Case for a More Formal Approach

Ideally, an implementation should clearly reflect the algorithm as it is presented in a classroom setting. Even better, some of the derivation of the algorithm should be apparent in the code and different variants of an algorithm should be recognizable as slight perturbations to an algorithmic "skeleton" or base code. If the code is just a mechanically-realizable, straightforward translation of the algorithm presented in class, there should be no opportunity for the introduction of logical errors or coding bugs. Presumably, it should be possible to prove the algorithms correct, thus ensuring that the code is correct. Previewing the next sections, algorithms for blocked variants of LU factorization of a matrix are presented in Fig. 2. In Fig. 5 we show how this can be translated into an skeleton for a code. By entering different updates of submatrices into this skeleton, given in Section 6.2, different variants of the LU factorization algorithm are realized.

Typically, it is difficult to prove code correct precisely because one is unsure that the code truly mirrors the algorithm. With our approach, the chasm is largely bridged by the simple yet crucial fact that some very simple syntactic rewrite rules can produce the code from an algorithm expressed as one might in a classroom, using mathematical formulae and stylized matrix depictions. Since we can prove the correctness of the algorithm we wish to employ (the proof is generally constructive in nature, but that is of little consequence) and because the correctness of the translation from algorithm to code is at least as reliable as compiler technology, the complexity of the task at hand is greatly ameliorated. Namely, components are expected to live up to certain "contractual obligations" [1, 4, 11]. In the case of a library constructed entirely through the methodology presented here, these components would be composed in like manner so as to make this task manageable. This is largely due to the fact that the approach presented here leads to a software architecture layered in such a way so as to require one to rely on the correctness of a very small number of base-level modules. Since those units are small, their correctness can be established through the application of standard formal methods. It is true that, in practice, one must accept that an application will need to interface with other libraries (for example, the vendor-supplied BLAS) that are not built in a "proof-friendly" format. However, it may still be possible to establish the correctness of a program if one is careful to impose minimal obligations on these, presumably time-tested and well-documented, pieces of code.

Having said this, let us clarify through a simple example.

3 A Case Study: LU Factorization

We illustrate our approach by considering LU factorization without pivoting. Given $n \times n$ matrix A we wish to compute $n \times n$ lower triangular matrix L with unit main diagonal and $n \times n$ upper triangular matrix U so that $A = LU$. The original matrix A is overwritten by L and U in the process.

3.1 A simple derivation

The usual derivation of an algorithm for the LU factorization proceeds as follows:

Partition

$$A = \left(\begin{array}{c||c} \alpha_{11} & a_{12}^T \\ \hline\hline a_{21} & A_{22} \end{array}\right), L = \left(\begin{array}{c||c} 1 & 0 \\ \hline\hline l_{21} & L_{22} \end{array}\right), \text{ and } U = \left(\begin{array}{c||c} \upsilon_{11} & u_{12}^T \\ \hline\hline 0 & U_{22} \end{array}\right)$$

Now $A = LU$ translates to

$$\left(\begin{array}{c||c} \alpha_{11} & a_{12}^T \\ \hline\hline a_{21} & A_{22} \end{array}\right) = \left(\begin{array}{c||c} 1 & 0 \\ \hline\hline l_{21} & L_{22} \end{array}\right) \left(\begin{array}{c||c} \upsilon_{11} & u_{12}^T \\ \hline\hline 0 & U_{22} \end{array}\right) = \left(\begin{array}{c||c} \upsilon_{11} & u_{12}^T \\ \hline\hline l_{21}\upsilon_{11} & l_{21}u_{12}^T + L_{22}U_{22} \end{array}\right)$$

so that the following equalities must hold:

$$\begin{array}{rcl||rcl} \alpha_{11} & = & \upsilon_{11} & a_{12}^T & = & u_{12}^T \\ \hline\hline a_{21} & = & \upsilon_{11} l_{21} & A_{22} & = & l_{21}u_{12}^T + L_{22}U_{22} \end{array}$$

Finally, we arrive at the following algorithm

- Overwrite α_{11} and a_{12}^T with υ_{11} and u_{12}^T, respectively (no-op).
- Update $a_{21} \leftarrow l_{21} = a_{21}/\upsilon_{11}$.
- Update $A_{22} \leftarrow A_{22} - l_{21}u_{12}^T$.
- Recursively factor $A_{22} \rightarrow L_{22}U_{22}$.

While the algorithm is formulated as tail-recursive, it is usually implemented as a loop.

3.2 But what intermediate value is in the matrix?

In order to prove correctness, one question we must ask is what intermediate value is in A at any particular stage of the algorithm. To answer this, partition

$$A = \left(\begin{array}{c||c} A_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right), L = \left(\begin{array}{c||c} L_{TL}^{(k)} & 0 \\ \hline\hline L_{BL}^{(k)} & L_{BR}^{(k)} \end{array}\right), \text{ and } U = \left(\begin{array}{c||c} U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline 0 & U_{BR}^{(k)} \end{array}\right) \quad (1)$$

where $A_{TL}^{(k)}$, $L_{TL}^{(k)}$, and $U_{TL}^{(k)}$ are all $k \times k$ matrices. Notice that "T", "B", "L", and "R" stand for Top, Bottom, Left, and Right, respectively. Notice that

$$\left(\begin{array}{c||c} A_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c} L_{TL}^{(k)} & 0 \\ \hline\hline L_{BL}^{(k)} & L_{BR}^{(k)} \end{array}\right) \left(\begin{array}{c||c} U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline 0 & U_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c} L_{TL}^{(k)}U_{TL}^{(k)} & L_{TL}^{(k)}U_{TR}^{(k)} \\ \hline\hline L_{BL}^{(k)}U_{TL}^{(k)} & L_{BL}^{(k)}U_{TR}^{(k)} + L_{BR}^{(k)}U_{BR}^{(k)} \end{array}\right)$$

so the following equalities must hold when the algorithm has completed:

$$A_{TL}^{(k)} = L_{TL}^{(k)}U_{TL}^{(k)} \quad (2)$$

$$A_{TR}^{(k)} = L_{TL}^{(k)}U_{TR}^{(k)} \quad (3)$$

$$A_{BL}^{(k)} = L_{BL}^{(k)}U_{TL}^{(k)} \quad (4)$$

$$A_{BR}^{(k)} = L_{BL}^{(k)}U_{TR}^{(k)} + L_{BR}^{(k)}U_{BR}^{(k)} \quad (5)$$

Finally, let $\hat{A}_k$ equal a matrix that holds the current intermediate result of a given algorithm for computing the LU factorization. In the following pages we will show that different conditions on the contents of $\hat{A}_k$ logically dictate different variants for computing the LU factorization, and these different conditions can be systematically generated. Previewing this, notice that to compute the LU factorization, the submatrices of L and U must be computed. We assume that $\hat{A}_k$ must contain partial results towards that goal. Here are some possibilities:

Condition	$\hat{A}_k$ contains
Only (2) is satisfied.	$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right)$
Only (2) and (3) have been satisfied.	$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right)$
Only (2) and (4) have been satisfied.	$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline L_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right)$
Only (2), (3), and (4) have been satisfied.	$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline L_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right)$
(2), (3), and (4) have been satisfied and as much of (5) has been computed *without computing any part of* $L_{BR}^{(k)}$ *or* $U_{BR}^{(k)}$.	$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline L_{BL}^{(k)} & A_{BR}^{(k)} - L_{BL}^{(k)} U_{TR}^{(k)} \end{array}\right)$

Here we use the notation $\{L\backslash U\}$ to denote a lower and upper triangular matrix that are stored in a square matrix by overwriting the lower and upper triangular parts of that matrix. (Recall that L has ones on the diagonal, which need not be stored.)

In the subsequent subsections, we describe how to derive algorithms in which the desired conditions hold. Note that in this paper we will not concern ourselves with the question of whether the above conditions exhaust all possibilities. However, they do give rise to all commonly discussed algorithms. For example, they yield all algorithms depicted on the cover of and discussed in G.W. Stewart's recent book on matrix factorization [27].

3.3 Lazy Algorithm

This algorithm is often referred to as a bordered algorithm in the literature. Stewart, [27] rather colorfully, refers to it as Sherman's march.

Unblocked Algorithm

Let us assume that only (2) has been satisfied. The question becomes how to compute $\hat{A}_{k+1}$ from $\hat{A}_k$. To answer this, repartition

$$A = \left(\begin{array}{c\|\|c} A_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c\|\|c\|c} A_{00}^{(k)} & a_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline a_{10}^{(k)\,T} & \alpha_{11}^{(k)} & a_{12}^{(k)\,T} \\ \hline A_{20}^{(k)} & a_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

where $A_{00}^{(k)}$ is $k \times k$ (and thus equal to $A_{TL}^{(k)}$), and $\alpha_{11}^{(k)}$ is a scalar. Repartition L, U, and $\hat{A}_k$ conformally. Notice that we wish to change the contents of the current matrix from $\hat{A}_k$ to $\hat{A}_{k+1}$ or

$$\left(\begin{array}{c\|\|c} L\backslash U_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c\|\|c\|c} L\backslash U_{00}^{(k)} & a_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline a_{10}^{(k)\,T} & \alpha_{11}^{(k)} & a_{12}^{(k)\,T} \\ \hline A_{20}^{(k)} & a_{21}^{(k)} & A_{22}^{(k)} \end{array}\right) \text{ to } \left(\begin{array}{c\|\|c} \hat{A}_{TL}^{(k+1)} & \hat{A}_{TR}^{(k+1)} \\ \hline\hline \hat{A}_{BL}^{(k+1)} & \hat{A}_{BR}^{(k+1)} \end{array}\right) = \left(\begin{array}{c\|c\|\|c} L\backslash U_{00}^{(k)} & u_{01}^{(k)} & A_{02}^{(k)} \\ \hline l_{10}^{(k)\,T} & \upsilon_{11}^{(k)} & a_{12}^{(k)\,T} \\ \hline\hline A_{20}^{(k)} & a_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

Thus, it suffices to compute $u_{01}^{(k)}$, $l_{10}^{(k)}$, and $\upsilon_{11}^{(k)}$.

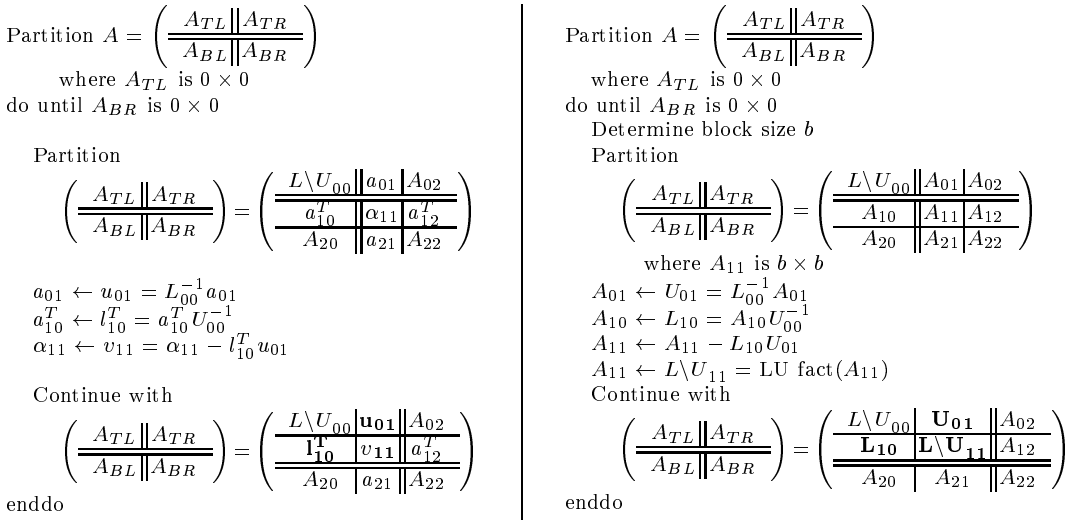


Figure 1: Unblocked and blocked versions of the lazy variant for computing the LU factorization of a square matrix A (without pivoting).

To derive how to compute these quantities, consider

$$\begin{array}{rcl} \left(\begin{array}{c||c|c} A_{00}^{(k)} & a_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline a_{10}^{(k)\,T} & \alpha_{11}^{(k)} & a_{12}^{(k)\,T} \\ \hline A_{20}^{(k)} & a_{21}^{(k)} & A_{22}^{(k)} \end{array}\right) & = & \left(\begin{array}{c||c|c} L_{00}^{(k)} & 0 & 0 \\ \hline\hline l_{10}^{(k)\,T} & 1 & 0 \\ \hline L_{20}^{(k)} & l_{21}^{(k)} & L_{22}^{(k)} \end{array}\right) \left(\begin{array}{c||c|c} U_{00}^{(k)} & u_{01}^{(k)} & U_{02}^{(k)} \\ \hline\hline 0 & v_{11}^{(k)} & u_{12}^{(k)\,T} \\ \hline 0 & 0 & U_{22}^{(k)} \end{array}\right) \\ & = & \left(\begin{array}{c||c|c} L_{00}^{(k)} U_{00}^{(k)} & L_{00}^{(k)} u_{01}^{(k)} & L_{00}^{(k)} U_{02}^{(k)} \\ \hline\hline l_{10}^{(k)\,T} U_{00}^{(k)} & l_{10}^{(k)\,T} u_{01}^{(k)} + v_{11}^{(k)} & l_{10}^{(k)\,T} U_{02}^{(k)} + u_{12}^{(k)\,T} \\ \hline L_{20}^{(k)} U_{00}^{(k)} & L_{20}^{(k)} U_{01}^{(k)} + l_{21}^{(k)} v_{11}^{(k)} & L_{20}^{(k)} U_{02}^{(k)} + l_{21}^{(k)} u_{12}^{(k)\,T} + L_{22}^{(k)} U_{22}^{(k)} \end{array}\right) \end{array}$$

From this equality we find that the following equalities must hold:

$$(6) \qquad \begin{array}{c|c|c} A_{00}^{(k)} = L_{00}^{(k)} U_{00}^{(k)} & a_{01}^{(k)} = L_{00}^{(k)} u_{01}^{(k)} & A_{02}^{(k)} = L_{00}^{(k)} U_{02}^{(k)} \\ \hline\hline a_{10}^{(k)\,T} = l_{10}^{(k)\,T} U_{00}^{(k)} & \alpha_{11}^{(k)} = l_{10}^{(k)\,T} u_{01}^{(k)} + v_{11}^{(k)} & a_{12}^{(k)\,T} = l_{10}^{(k)\,T} U_{02}^{(k)} + u_{12}^{(k)\,T} \\ \hline A_{20}^{(k)} = L_{20}^{(k)} U_{00}^{(k)} & a_{21}^{(k)} = L_{20}^{(k)} U_{01}^{(k)} + l_{21}^{(k)} v_{11}^{(k)} & A_{22}^{(k)} = L_{20}^{(k)} U_{02}^{(k)} + l_{21}^{(k)} u_{12}^{(k)\,T} + L_{22}^{(k)} U_{22}^{(k)} \end{array}$$

Thus, to compute $u_{01}^{(k)}$ we must solve the triangular system $L_{00}^{(k)} u_{01}^{(k)} = a_{01}^{(k)}$. The result can overwrite $a_{01}^{(k)}$. To compute $l_{10}^{(k)}$ we must solve the triangular system $l_{10}^{(k)\,T} U_{00}^{(k)} = a_{10}^{(k)\,T}$. The result can overwrite $a_{10}^{(k)\,T}$. To compute $v_{11}^{(k)}$ we merely compute $v_{11}^{(k)} = \alpha_{11}^{(k)} - l_{10}^{(k)\,T} u_{01}^{(k)} = \alpha_{11}^{(k)} - a_{10}^{(k)\,T} \hat{a}_{01}^{(k)}$. The result can overwrite $\alpha_{11}^{(k)}$. This motivates the algorithm in Fig. 1 (left) for overwriting given $n \times n$ matrix A with its LU factorization.

To show that indeed there is a possibility of proving the algorithm correct, consider the following result:

Theorem 1 *Consider the algorithm in Fig. 1 (left). This algorithm overwrites given $n \times n$ matrix A with its LU factorization.*

Proof: Realize that, by design, at the top of the loop during the kth iteration of the loop A contains the matrix $\hat{A}_k$ from the previous discussion. The derivation of the algorithm is such that it proves that given

that the contents of $\hat{A}_k$ are as desired, the contents of $\hat{A}_{k+1}$ are as desired which proves the inductive step. Since $\hat{A}_0 = A$ we conclude that $\hat{A}_n = L\backslash U$. $\square$

It is possible to similarly prove the correctness of the remainder of the variants.

Blocked Algorithm

For performance reasons it becomes beneficial to derive a blocked version of the above-presented algorithm. The derivation closely follows that of the unblocked algorithm: Again assume that only (2) has been satisfied. The question is now how to directly compute $\hat{A}_{k+b}$ from $\hat{A}_k$ for some small block size b (i.e. $1 < b \ll n$). To answer this, repartition

$$A = \left(\begin{array}{c||c} A_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c|c} A_{00}^{(k)} & A_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline A_{10}^{(k)} & A_{11}^{(k)} & A_{12}^{(k)} \\ \hline A_{20}^{(k)} & A_{21}^{(k)} & A_{22}^{(k)} \end{array}\right) \tag{7}$$

where $A_{00}^{(k)}$ is $k \times k$ (and thus equal to $A_{TL}^{(k)}$), and $A_{11}^{(k)}$ is $b \times b$. Repartition L, U, and $\hat{A}_k$ conformally. Notice that our assumption is that $\hat{A}_k$ holds

$$\hat{A}_k = \left(\begin{array}{c||c} L\backslash U_{TL}^{(k)} & A_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c|c} L\backslash U_{00}^{(k)} & A_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline A_{10}^{(k)} & A_{11}^{(k)} & A_{12}^{(k)} \\ \hline A_{20}^{(k)} & A_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

The desired contents of $\hat{A}_{k+b}$ are given by

$$\hat{A}_{k+b} = \left(\begin{array}{c||c} \hat{A}_{TL}^{(k+b)} & \hat{A}_{TR}^{(k+b)} \\ \hline\hline \hat{A}_{BL}^{(k+b)} & \hat{A}_{BR}^{(k+b)} \end{array}\right) = \left(\begin{array}{c|c||c} L\backslash U_{00}^{(k)} & U_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline L_{10}^{(k)} & L\backslash U_{11}^{(k)} & A_{12}^{(k)} \\ \hline A_{20}^{(k)} & A_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

Thus, it suffices to compute $U_{01}^{(k)}$, $L_{10}^{(k)}$, $L_{11}^{(k)}$, and $U_{11}^{(k)}$.

To derive how to compute these quantities, consider

$$\begin{array}{rcl} A & = & \left(\begin{array}{c||c|c} A_{00}^{(k)} & A_{01}^{(k)} & A_{02}^{(k)} \\ \hline\hline A_{10}^{(k)} & A_{11}^{(k)} & A_{12}^{(k)} \\ \hline A_{20}^{(k)} & A_{21}^{(k)} & A_{22}^{(k)} \end{array}\right) = \left(\begin{array}{c||c|c} L_{00}^{(k)} & 0 & 0 \\ \hline\hline L_{10}^{(k)} & L_{11}^{(k)} & 0 \\ \hline L_{20}^{(k)} & L_{21}^{(k)} & L_{22}^{(k)} \end{array}\right) \left(\begin{array}{c||c|c} U_{00}^{(k)} & U_{01}^{(k)} & U_{02}^{(k)} \\ \hline\hline 0 & U_{11}^{(k)} & U_{12}^{(k)} \\ \hline 0 & 0 & U_{22}^{(k)} \end{array}\right) \\ & = & \left(\begin{array}{c||c|c} L_{00}^{(k)}U_{00}^{(k)} & L_{00}^{(k)}U_{01}^{(k)} & L_{00}^{(k)}U_{02}^{(k)} \\ \hline\hline L_{10}^{(k)}U_{00}^{(k)} & L_{10}^{(k)}U_{01}^{(k)} + L_{11}^{(k)}U_{11}^{(k)} & L_{10}^{(k)}U_{02}^{(k)} + L_{11}^{(k)}U_{12}^{(k)} \\ \hline L_{20}^{(k)}U_{00}^{(k)} & L_{20}^{(k)}U_{01}^{(k)} + L_{21}^{(k)}U_{11}^{(k)} & L_{20}^{(k)}U_{02}^{(k)} + L_{21}^{(k)}U_{12}^{(k)} + L_{22}^{(k)}U_{22}^{(k)} \end{array}\right) \end{array}$$

This yields the equalities

$$\begin{array}{c||c|c} A_{00}^{(k)} = L_{00}^{(k)}U_{00}^{(k)} & A_{01}^{(k)} = L_{00}^{(k)}U_{01}^{(k)} & A_{02}^{(k)} = L_{00}^{(k)}U_{02}^{(k)} \\ \hline\hline A_{10}^{(k)} = L_{10}^{(k)}U_{00}^{(k)} & A_{11}^{(k)} = L_{10}^{(k)}U_{01}^{(k)} + L_{11}^{(k)}U_{11}^{(k)} & A_{12}^{(k)} = L_{10}^{(k)}U_{02}^{(k)} + L_{11}^{(k)}U_{12}^{(k)} \\ \hline A_{20}^{(k)} = L_{20}^{(k)}U_{00}^{(k)} & A_{21}^{(k)} = L_{20}^{(k)}U_{01}^{(k)} + L_{21}^{(k)}U_{11}^{(k)} & A_{22}^{(k)} = L_{20}^{(k)}U_{02}^{(k)} + L_{21}^{(k)}U_{12}^{(k)} + L_{22}^{(k)}U_{22}^{(k)} \end{array} \tag{8}$$

Thus,

1. To compute $U_{01}^{(k)}$ we must solve the triangular system $L_{00}^{(k)}U_{01}^{(k)} = A_{01}^{(k)}$. The result can overwrite $A_{01}^{(k)}$.

2. To compute $L_{10}^{(k)}$ we must solve the triangular system $L_{10}^{(k)} U_{00}^{(k)} = A_{10}^{(k)}$. The result can overwrite $A_{10}^{(k)}$.

3. To compute $L_{11}^{(k)}$ and $U_{11}^{(k)}$ we must update $A_{11}^{(k)} \leftarrow A_{11}^{(k)} - L_{10}^{(k)} U_{01}^{(k)} = A_{11}^{(k)} - A_{10}^{(k)} A_{01}^{(k)}$ after which the result can be factored into $L_{11}^{(k)}$ and $U_{11}^{(k)}$ using the unblocked algorithm. The result can overwrite $A_{11}^{(k)}$.

The above discussion motivates the algorithm in Fig. 1 (right) for overwriting the given $n \times n$ matrix A with its LU factorization. A careful analysis shows that the blocked algorithm does not incur even a single extra computation relative to the unblocked algorithm.

3.4 Row-Lazy Algorithm

As a point of reference, Stewart [27] calls this algorithm Pickett's charge south.

Let us assume that only (2) and (3) have been satisfied. We will now discuss only a blocked algorithm that computes $\hat{A}_{k+b}$ from $\hat{A}_k$ while maintaining these conditions.

Repartition A, L, U, and $\hat{A}_k$ conformally as in (7). Notice that our assumption is that $\hat{A}_k$ holds

$$\hat{A}_k = \left(\begin{array}{c||c} L\backslash U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline A_{BL}^{(k)} & A_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c|c} L\backslash U_{00}^{(k)} & U_{01}^{(k)} & U_{02}^{(k)} \\ \hline\hline A_{10}^{(k)} & A_{11}^{(k)} & A_{12}^{(k)} \\ \hline A_{20}^{(k)} & a_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

The desired contents of $\hat{A}_{k+b}$ are given by

$$\hat{A}_{k+b} = \left(\begin{array}{c||c} \hat{A}_{TL}^{(k+b)} & \hat{A}_{TR}^{(k+b)} \\ \hline\hline \hat{A}_{BL}^{(k+b)} & \hat{A}_{BR}^{(k+b)} \end{array}\right) = \left(\begin{array}{c|c||c} L\backslash U_{00}^{(k)} & U_{01}^{(k)} & U_{02}^{(k)} \\ \hline\hline L_{10}^{(k)} & L\backslash U_{11}^{(k)} & U_{12}^{(k)} \\ \hline\hline A_{20}^{(k)} & A_{21}^{(k)} & A_{22}^{(k)} \end{array}\right)$$

Thus, it suffices to compute $L_{10}^{(k)}$, $L\backslash U_{11}^{(k)}$, and $U_{12}^{(k)}$. Recalling the equalities in (8) we notice that

1. To compute $L_{10}^{(k)}$ we must solve the triangular system $L_{10}^{(k)} U_{00}^{(k)} = A_{10}^{(k)}$. The result can overwrite $A_{10}^{(k)}$.

2. To compute $L_{11}^{(k)}$ and $U_{11}^{(k)}$ we must update $A_{11}^{(k)} \leftarrow A_{11}^{(k)} - L_{10}^{(k)} U_{01}^{(k)} = A_{11}^{(k)} - A_{10}^{(k)} A_{01}^{(k)}$ after which the result can be factored into $L_{11}^{(k)}$ and $U_{11}^{(k)}$. The result can overwrite $A_{11}^{(k)}$.

3. To compute $U_{12}^{(k)}$ we must update $A_{12}^{(k)} \leftarrow A_{12}^{(k)} - L_{10}^{(k)} U_{02}^{(k)}$ after which we must solve the triangular system $L_{11}^{(k)} U_{12}^{(k)} = A_{12}^{(k)}$, overwriting the original $A_{12}^{(k)}$.

These steps and the preceding discussion lead one directly to the algorithm in 2(c).

3.5 Column-Lazy Algorithm

This algorithm is referred to as a left-looking algorithm in [10] while Stewart [27] calls it Pickett's charge east.

Let us assume that only (2) and (4) have been satisfied. Now it suffices to compute $U_{01}^{(k)}$, $L\backslash U_{11}^{(k)}$, and $L_{21}^{(k)}$. Using the same techniques as before derives the algorithm in Fig. 2 (d). Again, this algorithm overwrites given $n \times n$ matrix A with its LU factorization.

Partition $A = \left(\begin{array}{c||c} A_{TL} & A_{TR} \\ \hline\hline A_{BL} & A_{BR} \end{array}\right)$
where A_{TL} is 0×0
do until A_{BR} is 0×0

Repartition

$$\left(\begin{array}{c||c} A_{TL} & A_{TR} \\ \hline\hline A_{BL} & A_{BR} \end{array}\right) = \left(\begin{array}{c|c||c} A_{00} & A_{01} & A_{02} \\ \hline\hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

where A_{11} is $b \times b$

(a) Eager:
$A_{11} \leftarrow \{L\backslash U\}_{11} = LU(A_{11})$
$A_{12} \leftarrow U_{12} = L_{11}^{-1} A_{12}$
$A_{21} \leftarrow L_{21} = A_{21} U_{11}^{-1}$
$A_{22} \leftarrow A_{22} - L_{21} U_{12}$

(b) Lazy:	**(c) Row-lazy:**
View A_{00} as $\{L\backslash U\}_{00}$ $A_{01} \leftarrow L_{01} = L_{00}^{-1} A_{01}$ $A_{10} \leftarrow L_{10} = A_{10} U_{00}^{-1}$ $A_{11} \leftarrow \{L\backslash U\}_{11} = LU(A_{11} - L_{10}U_{01})$	View A_{00} as $\{L\backslash U\}_{00}$ $A_{10} \leftarrow L_{10} = A_{10} U_{00}^{-1}$ $A_{11} \leftarrow \{L\backslash U\}_{11} = LU(A_{11} - L_{10}U_{01})$ $A_{12} \leftarrow U_{12} = L_{11}^{-1}(A_{12} - L_{10}U_{02})$
(d) Column-lazy:	**(e) Row-column-lazy:**
View A_{00} as $\{L\backslash U\}_{00}$ $A_{01} \leftarrow U_{01} = U_{00}^{-1} A_{01}$ $A_{11} \leftarrow \{L\backslash U\}_{11} = LU(A_{11} - L_{10}U_{01})$ $A_{21} \leftarrow L_{21} = (A_{21} - L_{20}U_{01})U_{11}^{-1}$	$A_{11} \leftarrow \{L\backslash U\}_{11} = LU(A_{11} - L_{10}U_{01})$ $A_{12} \leftarrow U_{12} = L_{11}^{-1}(A_{12} - L_{10}U_{02})$ $A_{21} \leftarrow L_{21} = (A_{21} - L_{20}U_{01})U_{11}^{-1}$

Continue with

$$\left(\begin{array}{c||c} A_{TL} & A_{TR} \\ \hline\hline A_{BL} & A_{BR} \end{array}\right) = \left(\begin{array}{c|c||c} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline\hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

enddo

Figure 2: Blocked versions of LU factorization without pivoting for all five commonly encountered variants. The different variants share the same skeleton that partitions and repartitions the matrix. Executing the operations in one of the five boxes yields a specific algorithm.

3.6 Row-Column-Lazy Algorithm

This algorithm is often referred to as Krout's methods in the literature.

Let us assume that only (2), (3), and (4) have been satisfied. This time, it suffices to compute $L\backslash U_{11}^{(k)}$, $U_{12}^{(k)}$, and $L_{21}^{(k)}$, yielding the algorithm in Fig. 2 (e). Again, this algorithm overwrites given $n \times n$ matrix A with its LU factorization.

3.7 Eager algorithm

This algorithm is commonly known of as classical Gaussian elimination.

Finally, let us assume that (2), (3), and (4) have been satisfied, and as much of (5) as possible without completing any more of the factorization $L_{BR}U_{BR}$. Repartition A, L, U, and $\hat{A}_k$ conformally as in (7). Notice that our assumption is that $\hat{A}_k$ holds

$$\hat{A}_k = \left(\begin{array}{c||c} L\backslash U_{TL}^{(k)} & U_{TR}^{(k)} \\ \hline\hline L_{BL}^{(k)} & \hat{A}_{BR}^{(k)} \end{array}\right) = \left(\begin{array}{c||c|c} L\backslash U_{00}^{(k)} & U_{01}^{(k)} & U_{02}^{(k)} \\ \hline\hline L_{10}^{(k)} & A_{11}^{(k)} - L_{10}^{(k)}U_{01}^{(k)} & A_{12} - L_{10}^{(k)}U_{02}^{(k)} \\ \hline L_{20}^{(k)} & A_{21}^{(k)} - L_{20}^{(k)}U_{01}^{(k)} & A_{22}^{(k)} - L_{20}^{(k)}U_{02}^{(k)} \end{array}\right)$$

The desired contents of $\hat{A}_{k+b}$ are given by

$$\hat{A}_{k+b} = \left(\begin{array}{c||c} \hat{A}_{TL}^{(k+b)} & \hat{A}_{TR}^{(k+b)} \\ \hline\hline \hat{A}_{BL}^{(k+b)} & \hat{A}_{BR}^{(k+b)} \end{array}\right) = \left(\begin{array}{c|c||c} L\backslash U_{00}^{(k)} & U_{01}^{(k)} & U_{02}^{(k)} \\ \hline L_{10}^{(k)} & L\backslash U_{11}^{(k)} & U_{12}^{(k)} \\ \hline\hline L_{20}^{(k)} & L_{21}^{(k)} & A_{22}^{(k)} - L_{20}^{(k)}U_{02}^{(k)} - L_{21}^{(k)}U_{12}^{(k)} \end{array}\right)$$

Thus, it suffices to compute $L\backslash U_{11}^{(k)}$, $L_{21}^{(k)}$, $U_{12}^{(k)}$, and updating $\hat{A}_{22}^{(k)} = A_{22}^{(k)} - L_{20}^{(k)}U_{02}^{(k)} - L_{21}^{(k)}U_{12}^{(k)}$. Recalling the equalities in (8) we notice that

1. To compute $L_{11}^{(k)}$ and $U_{11}^{(k)}$ we must factor $\hat{A}_{11}^{(k)}$ which already contains $A_{11}^{(k)} - L_{10}^{(k)}U_{01}^{(k)}$. The result can overwrite $\hat{A}_{11}^{(k)}$.

2. To compute $U_{12}^{(k)}$ we must update $\hat{A}_{12}^{(k)}$ which already contains $A_{12}^{(k)} - L_{10}^{(k)}U_{02}^{(k)}$ by solving $L_{11}^{(k)}U_{12}^{(k)} = \hat{A}_{12}^{(k)}$, overwriting the original $\hat{A}_{12}^{(k)}$.

3. To compute $L_{21}^{(k)}$ we must update $A_{21}^{(k)}$ which already contains $A_{21}^{(k)} - L_{20}^{(k)}U_{01}^{(k)}$ by solving $L_{21}^{(k)}U_{11}^{(k)} = \hat{A}_{21}^{(k)}$, overwriting the original $\hat{A}_{21}^{(k)}$.

4. We must update $\hat{A}_{22}^{(k)}$ which already contains $A_{22}^{(k)} - L_{20}^{(k)}U_{02}^{(k)}$ with $\hat{A}_{22}^{(k)} - L_{21}^{(k)}U_{12}^{(k)}$ overwriting the original $\hat{A}_{22}^{(k)}$.

The resulting algorithm is given in Fig. 2(a). **Notice** that this final algorithm is equivalent to the algorithm derived in Section 3.1.

4 A Recipe for Deriving Algorithms

Note that the derivations of the different algorithms detailed above are extremely systematic. Indeed, the following recipe can be used:

1. State the operation to be performed.

2. Partition the operands. Notice that some justification is needed for the particular way in which they are partitioned. For the LU, this has to do with the fact that blocks of zeroes must be isolated in L and U. Details go beyond the scope of this paper.

3. Multiply out the partitioned matrices.

4. By equating submatrices on the left and right of the equal sign of the equality generated in Step 3, derive the equalities that must hold.

5. Pick a loop invariant from the set of possible loop invariants that satisfy the equalities given in Step 4.

6. From that loop invariant derive the steps required to maintain the loop invariant while moving the algorithm forward in the desired direction. This requires the following substeps:

   (a) Repartition so as to expose the boundaries after they are moved.

   (b) Indicate the current contents for the repartitioned matrices.

   (c) Indicate the desired contents for the repartitioned matrices such that the loop invariant is maintained.

   (d) Derive the steps required to achieve the desired contents.

7. Update the partitioning of the matrices.

8. State the algorithm.

9. Classify the algorithm. We have developed a systematic way of classifying the derived algorithms. While we use this classification in the labeling of the algorithms in the previous section, we will not go into detail here.

5 So Many Algorithms, So Little Time

So, why should we be concerned with a spectrum of algorithms for a given operation rather than picking the first one that yields good performance? The primary motivating force behind developing a systematic framework for deriving algorithms is that, depending on architecture and/or matrix dimensions, different algorithms exhibit different performance characteristics. An algorithm that performs admirably on one architecture and/or a particular problem size may prove to be an inferior algorithm when implemented on another architecture or applied to a problem with dissimilar dimensions.

In [14] we show that the efficient, transportable implementation of matrix multiplication on a sequential architecture with a hierarchical memory requires a hierarchy of matrix algorithms whose organization, in a very real sense, mirrors that of the memory system under consideration. Perhaps surprisingly, this is necessary even when the problem size is fixed. In that same paper we describe a methodology for composing these routines. In this way, minimal coding effort is required to attain superior performance across a wide spectrum of algorithms and problem sizes. Analogously, in [15] we demonstrate that an efficient implementation of parallel matrix multiplication requires both multiple algorithms and a method for selecting the appropriate algorithm for the presented case if one is to handle operands of various sizes and shapes. In [23, 24] we came to a similar conclusion in the context of out-of-core factorization algorithms.

A second reason for a systematic approach is that it may well be that we require specialized matrix kernels for which efficient implementations do not exist (as part of libraries like the BLAS or LAPACK). In [22] we show how such specialized matrix kernels speed up computations in control theory.

Finally, in [21] we show how the approach outlined above can be used to show that seemingly different algorithms for matrix inversions are actually equivalent and therefore share stability properties.

6 Coding the Algorithm

In this section we briefly discuss how dense linear algebra algorithms can be translated to code. We first show a more traditional approach, as it appears in popular packages like LAPACK. Next, we present an alternative that allows coding at a level of abstraction that mirrors how we naturally present the algorithms. This second approach has been successfully used in PLAPACK. FLAME represents a refinement of this methodology.

6.1 Classic implementation with the BLAS

Let us consider the blocked eager algorithm for the LU factorization presented in Fig. 2 (a). This algorithm requires an LU factorization of small matrix to factor $A_{11} \leftarrow L\backslash U_{11} = \text{LU fact.}(A_{11})$, triangular solves with multiple right-hand-sides to update $A_{12} \leftarrow U_{12} = L_{11}^{-1}A_{12}$ and $A_{21} \leftarrow L_{21} = A_{21}U_{11}^{-1}$, and a matrix-matrix multiply to update $A_{22} \leftarrow A_{22} - L_{21}U_{12}$. The triangular solves and matrix-matrix multiply are part of the Basic Linear Algebra Subprograms (BLAS) as calls to the routines `DTRSM` and `DGEMM`, respectively. The resultant code is given in Fig. 4. To understand this code, it helps to consider the partitioning of the matrix for a typical loop index j, as illustrated in Fig. 3: A_{11} is `B` by `B` and starts at element `A(J,J)`, A_{21} is `N-(J-1)-B` by `B` and starts at element `A(J+B,J)` , A_{12} is `B` by `N-(J-1)-B` and starts at element `A(J,J+B)`, and A_{22} is `N-(J-1)-B` by `N-(J-1)-B` and starts at element `A(J+B,J+B)`.

Given this picture, it is relatively easy to determine all of the parameters that must be passed to the appropriate BLAS routines.

6.2 The algorithm *is* the code

We would argue that it is relatively easy to generate the code in Fig. 4 given the algorithm in Fig. 2(a) and the picture in Fig. 3. However, the translation of the algorithm to the code is made tedious and error-prone by the fact that one has to very carefully think about indices and matrix dimensions. While this is not much of a problem if one were to implement just one algorithm, it becomes a major headache when implementing all possible variants for a given operation or, in the case of a library such as LAPACK, implementing even a single variant of a number of operations. One becomes even more acutely aware of these issues when distributed memory architectures enter the picture.

In an effort to make the code look as much like the algorithms given in Fig. 2 as is possible within the confines of C and FORTRAN, we have developed the Formal Linear Algebra Methods Environment (FLAME). The skeleton that is shared by all five variants of LU factorization is given in Fig. 5. To understand the code, it suffices to realize that A is being passed to the routine as a data structure `A` that describes all attributes of this matrix, such as dimensions and method of storage. Inquiry routines like `FLA_Obj_length` are used to extract information such as the row dimension of the matrix. Finally, `ATL`, `A00`, etc. are simply references into the original array described by `A`. If one is familiar with the alphabet soup used to name the BLAS kernels, it is clear that the following code segments, when entered in the appropropriate place in the code in 5, implement the different variants of the LU factorization:

Lazy algorithm

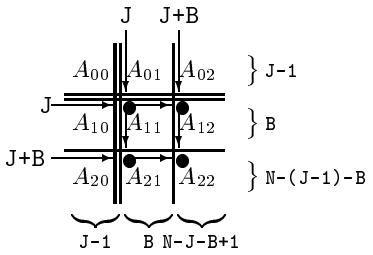
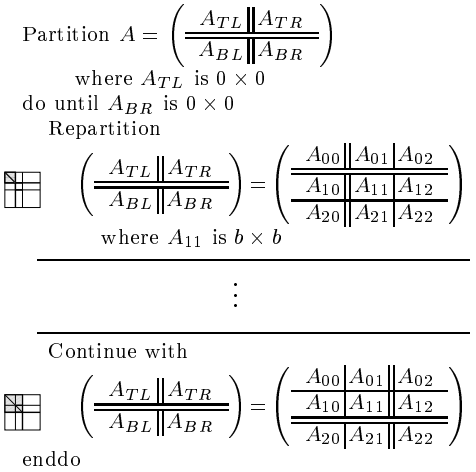


Figure 3: Partitioning of matrix A with all dimensions annotated when $A_{00} = A_{TL}$ is $(j-1) \times (j-1)$.

```
1         SUBROUTINE LU_EAGER_LEVEL3( N, A, LDA, NB )
2
3         INTEGER           N, LDA, NB, J, B
4         DOUBLE PRECISION  A( LDA, * ), ONE, NEG_ONE
5         PARAMETER         ( ONE = 1.0D00, NEG_ONE = -1.0D00 )
6
7         DO J=1, N, NB
8            B = MIN( N-J+1, NB )
9   C                                                        A11 <- L\U11 = LU fact( A11 )
10           LU_EAGER_LEVEL2( B, A( J,J ), LDA )
11
12           IF ( J+B .LE. N ) THEN
13
14  C                                                        A12 <- U12 = inv( L11 ) * A12
15
16              DTRSM( "LEFT",  "LOWER TRIANGULAR", "NO TRANSPOSE", "UNIT DIAGONAL",
17        $             ONE, B, N-(J-1)-B, A( J,J ), LDA, A( J, J+B ), LDA )
18
19  C                                                        A21 <- L21 = A21 * inv( U11 )
20
21              DTRSM( "RIGHT", "UPPER TRIANGULAR", "TRANSPOSE",    "NONUNIT DIAGONAL",
22        $             ONE, N-(J-1)-B, B, A( J,J ), LDA, A( J+B, J ), LDA )
23
24  C                                                        A22 <- A22 - A21 * A12
25
26              DGEMM( "NO TRANSPOSE", "NO TRANSPOSE", N-(J-1)-B, N-(J-1)-B, B,
27        $             NEG_ONE, A( J+B, J ), LDA, A( J, J+B ), LDA, ONE, A( J+B, J+B), LDA )
28           ENDIF
29        ENDDO
30
31        RETURN
32        END
```

Figure 4: FORTRAN implementation of blocked eager LU factorization algorithm using the BLAS.




```
1   #include "FLA.h"
2
3   void FLA_LU_nopivot_skeleton( FLA_Obj A, nb_alg )
4   {
5     FLA_Obj     ATL, ATR,   A00, A01, A02,
6                 ABL, ABR,   A10, A11, A12,
7                             A20, A21, A22;
8
9     FLA_Part_2x2( A,  &ATL, /**/ &ATR,
10                  /* ************** */
11                    &ABL, /**/ &ABR,
12              /* with */ 0, /* by */ 0, /* submatrix */ FLA_TL );
13
14    while ( b=min(min(FLA_Obj_length( ABR ), FLA_Obj_width( ABR )), nb_alg) != 0 ){
15
16      FLA_Repart_2x2_to_3x3( ATL, /**/ ATR,       &A00, /**/ &A01, &A02,
17                           /* ************* */   /* ******************** */
18                                  /**/            &A10, /**/ &A11, &A12,
19                             ABL, /**/ ABR        &A20, /**/ &A21, &A22,
20              /* with */ b, /* by */ b, /* A11 split from */ FLA_BR );
21      /* ************************************************************* */
                                        ⋮
35      /* ************************************************************* */
36      FLA_Cont_with_3x3_to_2x2( &ATL, /**/ &ATR,      A00, A01, /**/ A02,
37                                      /**/            A10, A11, /**/ A12,
38                               /* ************** */ /* ****************** */
39                                 &ABL, /**/ &ABR,     A20, A21, /**/ A22,
40              /* with A11 added to submatrix */ FLA_TL );
41    }
42  }
```

Figure 5: An skeleton for the implementation of any of the blocked LU factorization algorithms in C using FLAME.

```
23      FLA_Trsm( FLA_RIGHT, FLA_UPPER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_NONUNIT_DIAG,
24                ONE, A00, A10 );
25
26      FLA_Trsm( FLA_LEFT,  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
27                ONE, A00, A01 );
28
29      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A01, ONE, A11 );
30
31      FLA_LU_nopivot_level2( A11 );
```

Row-lazy algorithm

```
23      FLA_Trsm( FLA_RIGHT, FLA_UPPER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_NONUNIT_DIAG,
24                ONE, A00, A10 );
25
26      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A10, ONE, A11 );
27
28      FLA_LU_nopivot_level2( A11 );
29
30      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A02, ONE, A12 );
31
32      FLA_Trsm( FLA_LEFT,  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
33                ONE, A11, A12 );
```

Column-lazy algorithm

```
23      FLA_Trsm( FLA_LEFT,  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
24                ONE, A00, A01 );
25
26      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A10, ONE, A11 );
27
28      FLA_LU_nopivot_level2( A11 );
29
30      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A20, A10, ONE, A21 );
31      FLA_Trsm( FLA_RIGHT, FLA_UPPER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_NONUNIT_DIAG,
32                ONE, A11, A21 );
```

Row-column-lazy algorithm

```
23      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A01, ONE, A11 );
24      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A20, A01, ONE, A21 );
25      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A10, A02, ONE, A12 );
26
27      FLA_LU_nopivot_level2( A11 );
28
29      FLA_Trsm( FLA_RIGHT, FLA_UPPER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_NONUNIT_DIAG,
30                ONE, A11, A21 );
31
32      FLA_Trsm( FLA_LEFT,  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
33                ONE, A11, A12 );
```

Eager algorithm:

```
23      FLA_LU_nopivot_level2( A11 );
24
25      FLA_Trsm( FLA_RIGHT, FLA_UPPER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_NONUNIT_DIAG,
26                ONE, A11, A21 );
27
28      FLA_Trsm( FLA_LEFT,  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
29                ONE, A11, A12 );
30
31      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A21, A12, ONE, A22 );
```

6.3 Proving the code correct

In Section 3.3 we showed how the correctness of the lazy algorithm can be proved and argue that the correctness of the other algorithms can be similarly derived. *If* the routines called by the described FLAME code correctly implement the operations in the algorithm, then it can be argued that the code itself is correct. Indeed, debugging is not necessary.

6.4 But is this really a better approach?

Naturally, one can argue that determining which of the two approaches to coding the algorithm might be deemed "superior" is simply a matter of taste. However, contemplate the following questions:

- What if a bug were introduced into the FORTRAN implementation? For example, suppose that one of the `N-(J-1)-B` were accidentally changed to a `N-(J+1)-B`. This kind of bug is extremely hard to track down since the only clue is that the code produces the wrong answer or causes a segmentation fault. A similar bug cannot as easily be introduced into the code implemented using FLAME. Furthermore, with this approach to coding it is easy to perform a run-time check to determine if the dimensions of the different references into A are conformal.
- When coding all variants of the LU factorization one inherently has to derive all algorithms, leading to descriptions like those given in Fig. 2. However, translating those to code like that given in Fig. 4 would require careful consideration of the picture in Fig. 3. Moreover, due to the intricate indexing involved in that approach to coding, considerable testing would be required before one could declare the code bug-free. By contrast, given the algorithms, it has been demontrated that generating all variants using FLAME is straightforward. As already mentioned, since the code closely resembles the algorithm, one can be much more confident about its correctness even before the code is ever tested.
- What if we wished to parallelize the given code? Notice that parallelizing a small subset of the functionality of LAPACK as part of the ScaLAPACK project has taken considerable effort. The FLAME code can be transformed into PLAPACK code essentially by replacing `FLA_` by `PLA_`.
- What if we needed an out-of-core parallel version of the code? In principle, the FLAME code can be transformed into Parallel Out-of-Core Linear Algebra PACKage (POOCLAPACK) code by replacing `FLA_` by `POOCLA_`

6.5 But what about FORTRAN?

Again using MPI as an inspiration, a FORTRAN interface is available for FLAME. Examples of FORTRAN code are available on the FLAME web page.

6.6 But what about pivoting?

In Fig. 6 we show that pivoting can be easily added to, e.g., the eager LU factorization algorithm. Notice that in that implementation we also add recursion without much ado. We deem the code self-explanatory.

7 Performance

To illustrate that elegance does not necessarily come at the expense of performance, we measured the performance of the LU factorization with pivoting given in Fig. 6 followed by forward and backward substitution.

```
1   void FLA_LU( FLA_Obj A, FLA_Obj ipiv, int nb_alg )
2   {
3     < declarations >
4
5     FLA_Part_2x2( A,  &ATL, /**/ &ATR,
6                   /* ************** */
7                     &ABL, /**/ &ABR,
8                  /* with */ 0, /* by */ 0, /* submatrix */ FLA_TL );
9
10    FLA_Part_2x1( ipiv, &ipivT,
11                     /* ****** */
12                     &ipivB,
13                 /* with */ 0, /* length submatrix */ FLA_TOP );
14
15    while ( b = min( min( FLA_Obj_length( ABR ), FLA_Obj_width( ABR ) ), nb_alg ) ){
16      FLA_Repart_2x1_to_3x1( ipivT,                 &ipiv0,
17                          /* ***** */             /* ***** */
18                                                    &ipiv1,
19                             ipivB,                 &ipiv2,
20                  /* with */ b, /* length ipiv1 split from */ FLA_BOTTOM );
21      /* ************************************************************************ */
22      FLA_Part_1x2( ABR,   &ABR_1, &ABR_2, /* with */ b, /* width submatrix */ FLA_LEFT );
23
24      if ( nb_alg <= 4 ) FLA_LU_level2( ABR_1, ipiv1 );
25      else               FLA_LU       ( ABR_1, ipiv1, nb_alg/2 );
26
27      FLA_Apply_pivots( FLA_SIDE_LEFT, FLA_NO_TRANSPOSE, ipiv1, ABL );
28      FLA_Apply_pivots( FLA_SIDE_LEFT, FLA_NO_TRANSPOSE, ipiv1, ABR_2 );
29      /* ************************************************************************ */
30      FLA_Repart_2x2_to_3x3( ATL, /**/ ATR,         &A00, /**/ &A01, &A02,
31                          /* ************* */    /* ******************** */
32                                 /**/              &A10, /**/ &A11, &A12,
33                             ABL, /**/ ABR,         &A20, /**/ &A21, &A22,
34                  /* with */ b, /* by */ b, /* A11 split from */ FLA_BR );
35      /* ************************************************************************ */
36      FLA_Trsm( FLA_SIDE_LEFT, FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE, FLA_UNIT_DIAG,
37                ONE, A11, A12 );
38
39      FLA_Gemm( FLA_NO_TRANSPOSE, FLA_NO_TRANSPOSE, MINUS_ONE, A21, A12, ONE, A22 );
40      /* ************************************************************************ */
41      FLA_Cont_with_3x3_to_2x2( &ATL, /**/ &ATR,         A00, A01, /**/ A02,
42                                      /**/               A10, A11, /**/ A12,
43                             /* ************** */    /* ***************** */
44                               &ABL, /**/ &ABR,         A20, A21, /**/ A22,
45                  /* with A11 added to submatrix */ FLA_TL );
46
47      FLA_Cont_with_3x1_to_2x1( &ipivT,                 ipiv0,
48                                                        ipiv1,
49                             /* ***** */             /* ***** */
50                               &ipivB,                  ipiv2,
51                  /* with ipiv1 added to */ FLA_TOP );
52    }
53  }
```

Figure 6: FLAME recursive LU factorization with partial pivoting.

For comparison, we also measured the performance of the equivalent operations provided by ATLAS release R3.1 [29].

Some details: Performance was measured on a Pentium III based laptop with a 256K L2 cache running the Linux (Redhat 6.2) operating system. All computation was performed in 64-bit (double precision) arithmetic. For both implementations the same compiler options were used.

In Fig. 7 we report performance for four different implementations, indicated by the curves marked

`ATLAS:` This curve reports performance for the LU factorization provided by ATLAS R3.1, using the BLAS provided by ATLAS R3.1.

`ATL-FLAME:` This curve reports the performance of our LU factorization coded using FLAME built upon BLAS provided by ATLAS R3.1. The outer-most block size used for the LU factorization is 160 for these measurements. (Notice that multiples of 40 are optimal for the ATLAS matrix-matrix multiply on this architecture.)

`ITX-FLAME:` Same as the previous implementation, except that we optimized the matrix-matrix multiply (ITXGEMM). Details of this optimization are the subject of another paper [14]. This time the outer-most block size was 128. (Notice that multiples of 64 are optimal for the ITXGEMM matrix-matrix multiplication routine on this architecture.)

`ITX-FLAME-opt:` Same as the previous implementation, except that we optimized the level-2 BLAS based LU factorization of an intermediate panel as well as the pivot routine by not using the FLAME approach for those operations. For these routines we call `dscal`, `dger`, and `dswap` directly.

For all implementations, the forward and backward substitutions are provided by the ATLAS R3.1 `dtrsv` routine. The graph on the bottom shows the same data for smaller matrices is more detail.

Notice that for small matrices the unoptimized FLAME implementations perform somewhat worse, due to the overhead for manipulating the objects that encode the information about the matrices. When the level-2 BLAS based LU factorization is coded without this overhead, the performance is comparable even for small matrices. The better performance when the ITXGEMM matrix-matrix multiply is used is entirely due to the better performance of this matrix-matrix multiply.

It is important to realize that the performance difference between the implementation offered as part of ATLAS R3.1 and our own implementation is not the point of this paper: With some effort either implementation can be improved to match the performance of the other. Our primary point is that markedly less effort is required to implement these algorithms using FLAME while attaining performance comparable to that of what are widely considered to be high-performance implementations.

8 Future directions

Many aspects of the approach we have described are extremely systematic: the generation of the loop-invariants, the derivation of the algorithm as well as the translation to code. Not discussed is the fact that the analysis of the run-time of the resulting algorithm on sequential or, for that matter, parallel, architectures is equally systematic. We are pursuing a project that exploits this systematic approach in order to automatically generate entire (parallel) linear algebra libraries as well as run-time estimates for the generated subroutines [13]. The goal is to create a mechanism that will automatically choose between different algorithms based on architecture and/or problem parameters.

A considerably less ambitious project, already nearing completion, allows the user to program in a language-independent manner (i.e. by writing an ASCII version of the algorithms presented in this paper). Since it is our central thesis that the level of abstraction presented in this paper is the correct one, it seems an