Active Libraries: Rethinking the roles of compilers and libraries

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Abstract

We describe Active Libraries, which take an active role in compilation. Unlike traditional libraries which are passive collections of functions and objects, Active Libraries may generate components, specialize algorithms, optimize code, configure and tune themselves for a target machine, and describe themselves to tools (such as profilers and debuggers) in an intelligible way. Several such libraries are described, as are implementation technologies.

1 Introduction

This paper attempts to document a trend toward libraries which take an active role in generating code and interacting with programming tools. We call these Active Libraries. They solve the problem of how to provide efficient domain-specific abstractions (Section 1.1): active libraries are able to define abstractions, and also control how they are optimized. Several existing libraries for arrays, parallel physics, linear algebra and Fast Fourier Transforms fit the description of active libraries (Section 2). These libraries take novel approaches to generating optimized code (Section 3). To implement active libraries, programming systems and tools which open up the development environment are needed (Section 4).

1.1 Why are active libraries needed?

To produce readable, maintainable scientific computing codes, we need abstractions. Every subdomain in scientific computing has its own requirements: interval arithmetic, tensors, polynomials, automatic differentiation,
sparse arrays, spinors, meshes, and so on. How should these abstractions be provided? The alternatives are:

**Extend mainstream languages.** In the past, syntax and efficiency concerns have encouraged building abstractions into languages and compilers. Fortran 95, for example, has built-in complex numbers and numerical arrays, and many intrinsic functions for common numerical operations. Efforts are underway to extend the Java language for scientific computing [18], and similar efforts in the past have extended C [25]. However, loading up these languages with features for the scientific market can meet with only limited success. The costs of compiler development are quite high, and scientific computing is a comparatively small segment of the market. Even Fortran, whose bread and butter is scientific computing, is showing signs of hitting economic limits to its size. A controversial 60-page proposal to add interval arithmetic to Fortran 2000 was eventually discarded after much debate. The committee had to balance the limited demand for interval arithmetic against the large implementation costs for vendors. Although we may succeed in getting mainstream languages to incorporate basic scientific features such as numeric arrays and complex numbers, the likelihood of these languages providing specialized features such as interval arithmetic and sparse arrays is small.

There are other disadvantages to building abstractions into mainstream languages: feature turnaround is very slow, since extensions require championing a proposal through years of standards committee meetings. Experimental features must be prematurely standardized, before experience can produce a consensus on the “right way” to implement them.

**Domain-Specific Languages (DSLs).** Dozens of DSLs for scientific computing have been produced to handle sparse arrays, automatic differentiation, interval arithmetic, adaptive mesh refinement, and so on. DSLs are often implemented as preprocessors for mainstream languages such as C, Fortran, C++, or Java. The growing availability of compiler construction tools has encouraged a proliferation of DSLs. Although DSLs are an attractive alternative, many people would prefer to work in mainstream languages for the wealth of tools support and libraries available. DSLs frequently have problems with portability and long-term support, since they tend to be research projects. It is also impossible to use multiple DSLs at once; for example, although separate Fortran-based DSLs are available for both sparse arrays and interval arithmetic, you cannot use the features of both DSLs in the same source file.

**Object-oriented language features.** An alternative to building abstractions into languages is to provide language features which allow library
developers to construct their own abstractions. In C++ and Fortran 90/95, we are seeing libraries for many applications (sparse arrays, interval arithmetic, data-parallel arrays) which were previously solved by domain-specific languages. Unfortunately, such libraries are hard to optimize. Compilers have difficulty because they lack semantic knowledge of the abstractions: instead of seeing array operations, they see loops and pointers. Libraries also tend to have layers of abstraction and side effects which confound optimizations. The heroic optimizers needed to overcome these problems may never appear, because the economics of the scientific market may not support their development. It is doubtful that the optimization problems admit a general-purpose solution, since every problem domain has its own tricks and peculiarities.

What we really need are language features which allow library developers to define their own abstractions, and also to specify how these abstractions are optimized. We call this solution Active Libraries. Active Libraries combine the benefits of built-in language abstractions (nice syntax and efficient code) with those of library-level abstractions (adaptability, quick feature turnaround, cheap to implement).

2 Examples of Active Libraries

In defining Active Libraries, we are not proposing a new concept, but rather trying to summarize what many people are already trying to do. In the following sections, we highlight existing software packages which illustrate the characteristics of Active Libraries.

2.1 Blitz++

The Blitz++ library \[32\] provides generic array objects for C++ similar to those in Fortran 90, but with many additional features. In the past, C++ array libraries have been 3-10 times slower than Fortran, due to the temporary arrays which result from overloaded operators. Blitz++ solves this problem using the expression templates technique \[30\] to generate custom evaluation kernels for array expressions. The library performs many loop transformations (tiling, reordering, collapsing, unit stride optimizations, etc.) which have until now been the responsibility of optimizing compilers. Blitz++ also generates different code depending on the target architecture.

For operations on small vectors and matrices, Blitz++ uses the template metaprogram technique \[31\] to generate specialized algorithms. This avoids
the performance penalty often associated with small objects by completely unrolling loops and inlining code.

2.2 POOMA

POOMA is a C++ library for parallel physics which uses many of the same techniques as Blitz++. Users write simple array expressions, such as “A=B+C”, which trigger the generation of data-parallel implementation routines using threads and message passing \[21\]. POOMA uses template techniques to generate components (such as Fields) using a variety of types, geometries, addressing schemes, data distribution and communication parameters.

2.3 Matrix Template Library

The Matrix Template Library (MTL) \[28\] is a C++ library which extends the ideas of STL \[24\] to linear algebra. MTL handles both sparse and dense matrices. For dense matrices, MTL uses template metaprograms to generate tiled algorithms. Tiling is a crucial technique for obtaining top performance from cache-based memory systems; MTL uses template metaprograms to tile on both the register and cache level. For register tiling, it uses template metaprograms to completely unroll loops. MTL provides generic, high-performance algorithms which are competitive with vendor-supplied kernels.

2.4 Generative Matrix Computation Library

The Generative Matrix Computation Library (GMCL) \[16\] provides heavily parameterized matrix classes. Users can specify the element type, whether the matrix is dense or sparse, the storage format (including several sparse formats), dynamic or static memory allocation, error checking, and several other parameters. The GMCL uses template metaprograms to examine the parameters and determine any interactions between them (for example, sparse matrices cannot use static memory allocation); it then instantiates a matrix class with the desired characteristics. The implementation is roughly 7500 lines of C++ code, yet covers more than 1840 different kinds of matrices. Despite this flexibility, the authors report performance on par with manually generated code.
2.5 FFTW: The Fastest Fourier Transform in the West

FFTW \cite{14} is a C library for Fast Fourier Transforms. It generates a collection of small “codelets,” each of which is a small step in the transform process. At installation, FFTW evaluates the performance of each codelet for the target architecture. At run-time, the codelets are dynamically stitched together to perform FFTs. FFTW records the ordering of these codelets using bytecode, which is generated and interpreted at run time. Based on extensive benchmarking, the authors report superior performance over all commonly used FFT packages.

2.6 PhiPAC, ATLAS

Obtaining top performance for matrix operations requires substantial expertise and hand-tuning. PhiPAC \cite{4} provides a methodology to achieve near-peak performance automatically. It uses parameterized code generators, whose parameters are related to machine-specific tuning. PhiPAC searches the parameter space to find the best implementation for a given target architecture. On dense matrix-matrix multiplication, PhiPAC performs better then vendor-supplied kernels on many platforms. The ATLAS package \cite{33} provides similar capabilities.

3 Optimization models

Active Libraries make it possible to approach code optimization in several new and exciting ways. In describing some of the new approaches to optimization being explored, it is useful to distinguish between two flavours of optimization, which we call low-level and high-level:

- **Low-level** optimizations can be applied without knowing what the code is supposed to do (copy propagation, dead code elimination, instruction scheduling, loop pipelining).

- **High-level** optimizations which require some understanding of the operation being performed. Examples: tiling for stencils; fusing loops over sparse arrays; iteration-space tiling.

3.1 Transformational optimization

Traditional approaches to optimization are *transformational*. In transformational optimization, low-level code is transformed into an equivalent (but
One of the difficulties with transformational optimization is that the optimizer lacks an understanding of the intent of the code. This makes it harder to apply high-level optimizations. For example, rather than seeing an array stencil operation, a transformational optimizer will just see loops, pointers, and variables. To apply interesting optimizations, the optimizer must recognize that this low-level code represents a stencil operation (or more accurately, that it possesses the sort of data dependencies which benefit from tiling). More generally, the optimizer must infer the intent of the code to apply higher-level optimizations. To this end, sophisticated optimizers employ algebraic reasoning, pattern recognition and matching techniques. However, such optimizers can still only apply radical optimizations in simple situations, and with limited success.

Another problem with transformational optimizers is the lack of extensibility. If the optimizer doesn’t recognize what your code is trying to do, you are probably out of luck. Optimizations for dense arrays are fairly reliable, because their use is very common; if you are working with sparse arrays or interval arithmetic, the likelihood of achieving optimal performance is smaller.

3.2 Generative optimization

Many environments which provide higher-level abstractions (for example, arrays in Fortran 90) can use generative optimization. Code written using higher-level abstractions can be regarded as a specification of what operation needs to be performed; an efficient implementation is then generated to fulfill the “specification”. This approach to optimization can be much simpler than transformational optimization, since the full semantics are available to whatever generates the optimized code. Generative optimization can make it simpler to apply radical, high-level optimizations.

While generative optimization can produce good code for individual operations, it tends to miss optimizations which depend on context. For example, one problem encountered in libraries which use expression templates (e.g. Blitz++, POOMA) is that while individual array statements can be optimized well, opportunities for between-statement optimizations are missed. For example, in the array statements \( A = B + C \); \( D = B - C \); there is a substantial gain if the two expressions are evaluated simultaneously, since they share the same operands. Attempts to solve this problem have focused on increasing granularity, so that code is generated for basic blocks of array statements,
3.3 Explorative optimization

For library developers, finding a near-optimal implementation of a routine is very difficult. Modern architectures can behave unpredictably due to pipeline and cache effects. Between the library writer and the hardware lies the compiler, a black box which transforms one's code in sometimes mysterious ways. Aside from some basic guidelines relating to cache reuse, performance tuning usually requires randomly adjusting code and measuring the result.

Explorative optimization gives up on the notion that performance is somehow predictable. The basic approach is to examine an algorithm and identify parameters which might affect performance (for example loop structures, tile sizes, and unrolling factors). One then writes a parameterized code generator which produces variants of the basic algorithm. The parameter space is then explored point by point, and the performance of each variant is measured until the best implementation is found. This approach was pioneered by FFTW (Section 2.4) and PhiPAC (Section 2.6). On dense matrix-matrix multiplication, PhiPAC performs better than vendor-supplied kernels on many platforms.

Explorative optimization is expensive in time, but is worth it if a near peak-performance kernel is required. So far, there is no way to automatically construct variants of a given piece of code; one must write the code generators manually.

3.4 Compositional optimization

Compositional optimization is useful when a problem can be decomposed into a sequence of calls to well-tuned kernels. The FFTW package (Section 2.4) uses this approach to decompose FFTs into a sequence of calls to high-speed kernels which were found using explorative optimization. FFTW records and interprets the sequence of calls using a bytecode. Compositional optimization has also been used in the context of compilers, to generate high-performance communication code [29].

For compositional optimization to be effective, the problem must be decomposable into coarse chunks, so that the overhead of composition is negligible.
4 Technologies for Active Libraries

In the following sections, we describe technologies relevant to Active Libraries. Some of these are already being used, for example generic programming and C++ templates; others are promising technologies still being explored.

4.1 Component generation

Traditional libraries define *concrete components*. We use the term *components* loosely here, to mean an algorithm, class, or collection of these things. By concrete, we mean that the behavior is fixed: the component operates on a fixed kind of data (for example, arrays of `double`), using a specific data structure, and handles errors in a fixed way. Concrete components might allow for some flexibility through configuration variables, but the code of the component is unchanging. Concrete components require a trade-off between flexibility and efficiency: if the library developer wants to provide a customizable component, this must be done through callbacks and runtime checking of configuration variables, which are often inefficient. To solve this problem, we need ways to *generate* customized components on demand. We contrast two approaches: Generic Programming and Generative Programming.

4.1.1 Generic Programming

The aim of Generic Programming can be summarized as “reuse through parameterization”. Generic components have parameters which customize their behaviour. When a generic component is *instantiated* using a particular choice of parameters, a concrete component is generated. This allows library developers to create components which are very customizable, yet retain the efficiency of statically configured code. Probably the greatest achievement of the Standard Template Library in C++ [24] was to separate algorithms from the data structures on which they operate, allowing them to be combined in a mostly orthogonal way. In C++, template parameters can effectively be types, data structures, or even pieces of code and algorithms. Other languages which support generic programming are Ada (via its *generics* mechanism), and Fortran 2000 (albeit in a limited way).

There are two main benefits of generic programming: (1) Library developers have to develop and maintain less code; (2) Application developers find it easier to find components which match their needs. There are some
4.2 C++ Templates

limitations of generic programming as currently supported: (1) Aggressive parameterization is quite ugly; providing more than 2-3 template parameters introduces serious usability problems. This can be alleviated somewhat by named template parameters. (2) Generic programming may result in code bloat, due to multiple versions of generic components. (3) Perhaps most importantly, generic programming limits code generation to substituting concrete types for generic type parameters, and welding together pre-existing fragments of code in fixed patterns. It does not allow generation of completely new code, nor does it allow computations to be performed at compile time.

4.1.2 Generative Programming

Generative Programming is a broader term which encompasses generic programming, code generation, code analysis and transformation, and compile-time computation. In general, it refers to systems which generate customized components to fulfill specified requirements.

A central idea in Generative Programming (and also in Aspect-Oriented Programming) is separation of concerns: the notion that important issues should be dealt with one at a time. In current languages, there are many aspects such as error handling, data distribution, and synchronization which cannot be dealt with in a localized way. Instead, these aspects are scattered throughout the code. One of the goals of Generative Programming is to separate these aspects into distinct pieces of code. These pieces of code are combined to produce a needed component. Doing so often requires more than cutting and pasting, and this is where the need for code generation, analysis, and transformation arises. Active Libraries can be viewed as a vehicle for implementing the goals of Generative Programming.

4.2 C++ Templates

In addition to enabling generic programming, the template mechanism of C++ unwittingly introduced powerful code generation mechanisms. Nested templates allow data structures to be created and manipulated at compile time, by encoding them as types. This is the basis of the expression templates technique, which creates parse trees of array expressions at

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1 Named template parameters can be listed in any order, with missing parameters assuming default values. Though not directly supported in C++, the technique can be faked (see [16]).

2 We regard techniques such as template metaprograms and expression templates to lie outside the domain of generic programming.
compile time, and uses these parse trees to generate customized kernels. Expression templates also provides a crude facility similar to the \texttt{lambda} operator of functional languages, which may be used to replace callbacks. 

Template metaprograms \cite{template-metaprograms} use the template instantiation mechanism to perform computations at compile-time, and generate specialized algorithms by selectively inlining code as they are executed. Although these techniques are powerful, the accidental nature of their presence has resulted in a clumsy syntax. Nonetheless, they provide a reasonable way to implement Active Libraries in C++, and several libraries based on these techniques (Blitz++, POOMA, MTL) are being distributed. Recently, a package which simplifies the construction of template metaprograms has been made available \cite{template-simplification}.

4.3 Extensible compilation, Reflection, and Metalevel Processing

In metalevel processing systems, library writers are given the ability to directly manipulate language constructs. They can analyze and transform syntax trees, and generate new source code at compile time. The MPC++ metalevel architecture system \cite{mpc++} provides this capability for the C++ language. MPC++ even allows library developers to extend the syntax of the language in certain ways (for example, adding new keywords). Other examples of metalevel processing systems are Xroma \cite{xroma}, Open C++ \cite{open-c++}, and Magik \cite{magik}. A potential disadvantage of metalevel processing systems is the complexity of code which one must write: modern languages have complicated syntax trees, and so code which manipulates these trees tends to be complex as well.

4.4 Run-Time Code Generation (RTCG)

RTCG systems allow libraries to generate customized code at run-time. This makes it possible to perform optimizations which depend on information not available until run-time, for example, the structure of a sparse matrix or the number of processors in a parallel application. Examples of such systems which generate native code are ‘C (Tick-C) \cite{tick-c}, and Fabius \cite{fabius}. Speeds as high as 6 cycles per generated instruction have been achieved. Recently, this technology has been extended to C++ \cite{rtcg-c++}.

4.5 Partial Evaluation

Code generation is an essential part of active libraries. Over the past two decades, researchers in the field of Partial Evaluation have developed an
4.6 Multilevel Languages

extensive theory and literature of code generation [19]. In its simplest form, a partial evaluator analyzes a program and separates its data into a static portion (values known at compile-time) and a dynamic portion (values not known until run-time). It then evaluates as much of the program as possible (using the static values) and outputs a specialized residual program. For example, a partial evaluator could take a dot-product routine, and produce a specialized version for a particular vector length. These techniques have been applied to scientific codes with promising results [2, 3, 22].

However, this just provides a taste of the field; partial evaluation has evolved into a comprehensive toolbox containing both theories and practical software. One of the most important theoretical contributions was that the concept of generating extensions [13] unifies a very wide category of apparently different program generators. Using partial evaluation, concrete components which check configuration variables at run-time can be transformed into component generators (or generating extensions in the terminology of the field [4, 10, 20]) which produce customized components (eliminating the run-time checking of configuration variables). Automatic tools for turning a general component into a component generator now exist for C and Scheme [20]. However, such tools are not yet available for C++.

4.6 Multilevel Languages

Another important contribution of Partial Evaluation is the concept of two-level (or more generally, multi-level) languages. Two-level languages contain static constructs (which are evaluated at compile-time) and dynamic code (which is compiled and later evaluated at run-time). Two-level languages provide a simpler notation for writing code generators (compared to systems which generate source code or intermediate representations). For example, consider a (fictional) two-level language based on C++, in which static variables and control flow are annotated with the @ symbol. A code generator for dot products of length N would be written as:

```c
double dot(double* a, double* b, int@ N) {
    double sum = 0;
    for@ (int@ i=0; i < N; ++i)
        sum += a[i] * b[i];
    return sum;
}
```

In this example, the @ symbol indicates that N and i are compile-time variables. The for@ loop is evaluated at compile time, and the residual code
is equivalent to $N$ statements of the form $\text{sum} += a[i] \cdot b[i]$, with $i$ replaced by appropriate integer literals. This dot-product generator is dramatically simpler than an equivalent implementation using template metaprograms or metalevel processing. Two-level languages have been used to generate customized run-time library code for parallel compilers [29].

4.7 Extensible Programming Tools

Libraries typically have two (or more) layers: there are user-level classes and functions, and behind them are one or more implementation layers. Using tools such as debuggers and profilers with large libraries is troublesome, since the tools make no distinction between user-level and implementation code. For example, a user who invokes a debugger on an array class library will be confronted with many irrelevant (and undocumented) private data members, when all they wanted to see was the array data. Using a profiler with such a library will expose many implementation routines, instead of indicating which array expressions were responsible for a slow program. This problem is compounded when template libraries are used, with their long symbol names and many instances.

The solution may be extensible tools, which provide hooks for libraries to define customized support for debugging, profiling, etc. An example of such interaction is Blitz++ and the Tau [27] profiling package. Tau is unique in that it allows libraries to instrument themselves. This allows Blitz++ to hide implementation routines, and only expose user-level routines. Time spent in the library internals is correctly attributed to the responsible user-level routine. Blitz++ describes array evaluation kernels to Tau using pretty-printing. When users profile applications, they do not see incomprehensible expression template types; rather, they see expressions such as “$A=B+C+D$”.

If debuggers provided similar hooks, users could debug scientific codes by looking at visualizations and animations of the array data. The general goal of such tool/library interactions is to provide a user-oriented view of libraries, rather than an implementation-oriented view.

5 Conclusions

Active Libraries are able to define domain-specific abstractions, and also control how these abstractions are optimized. This may involve compile-time computations, code generation, and even code analysis and transformation. It is no coincidence that all of the existing examples are libraries
for scientific computing: this is a field which requires many abstractions, and also demands high performance. Active libraries may be the best way to construct and deliver efficient, configurable abstractions.

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