Prior Art for Linear Algebra

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Contents

1 Brief History of Linear Algebra Libraries in C++

1.1 Object-Oriented Numerics in the 1990s

Linear algebra libraries in C++ at first evolved from the general category of "object-oriented programming." For example, the First annual Object-Oriented Numerics Conference (OON-SKI) took place in 1993.[1] Rogue Wave, a C++ compiler company, sponsored OON-SKI, so the conference logically focuses on work in C++. "Numerics" here means "numerical computation" or "scientific computing": computations on large arrays of floating-point numbers, doing things like discretizing differential equations or statistical data analysis.[2] The introduction to the corresponding journal special issue described the phenomenon of "object-oriented numerics" as follows:

> ... [W]e are observing the emergence of a subdiscipline: the use of object-oriented techniques in numerics. But what we are really seeing is something even more profound: finally rejoining of scientific computing with the science of computers. Traditionally, programming has been done by engineers, physicists and mathematicians with little or no training in computer science. Now, however, we are seeing an infusion of ideas coming from computer science world into the scientific computing world, brining along modern ideas on how to structure complex numerical code. Object-oriented techniques is merely one of many such ideas [VC93].

The introduction talks about the issues like needing to teach compilers how to fuse loops and avoid temporaries when doing overloaded-operator arithmetic on arrays in C++. It also shows the existence of C++ libraries for a variety of applications, including a library of multidimensional arrays, and the integration of C++ with distributed-memory parallel computation.

One can see the explosion of interest in "object-oriented numerics" by the large variety of conferences that sprang up in the mid-1990's.[3] Interest died down later, but this perhaps reflects the stage in mathematical software development where users came to accept externally developed libraries as part of their applications. In the United States, this may correspond to the Department of Energy's Accelerated Strategic Computing Initiative (ASCI) program, which was founded in 1996.[4] An important part of ASCI was "[s]oftware design and development" for complicated "multi-physics scientific applications." Before ASCI, experience with such software development was "limited to a few isolated projects." ASCI aimed to "carry out multiple substantial simulation projects that will provide proofs of principle, at scale, of software development methodologies and frameworks that provide portability, extensibility, modularity, and maintainability while delivering acceptable performance."

Another contribution to the development of C++ linear algebra libraries may have been the "killer micros" revolution of the early 1990's. Killer micros were consumer-grade, low-cost microprocessors

[1] `https://www.hindawi.com/journals/sp/si/250702/`

[2] Authors use adjectives like "numerical" to describe scientific and engineering computation.

[3] See e.g., `http://www.math.unipd.it/~michela/OP.htm#conferences`.

[4] [Mes99]

whose performance threatened and eventually overtook that of expensive vector supercomputers.[5] This revolution disrupted Fortran's dominance and let developers write more complicated codes. Vector supercomputers like the Cray 1 depended on custom vectorizing Fortran compilers for good performance. "Scalar" code ran much more slowly on the Cray 1 than vectorized code, and getting code to vectorize took careful dialog with the compiler. Killer micros had less optimized hardware, but also had performance less sensitive to software design. Hardware performance improvements tracked the 18-month Moore's Law curve, so users could just wait for the next processor generation, instead of expensively optimizing their code. This gave developers more freedom to use languages other than Fortran, and to write more complicated codes that depended less on vectorization. Simultaneously, new distributed-memory parallel computers emerged, along with new languages to program them. For example, the technical report describing Connection Machine's CM-1 only mentions one programming language: *Lisp, an ANSI Common Lisp derivative.[6] Applications running on CM-2 also used C*, a parallel superset of ANSI C. Other distributed-memory parallel computers of the era favored C and offered C++ compilers. Library-oriented approaches to parallel computing, like PVM and MPI, came with C as well as Fortran bindings. The switch from Fortran and the increasing complexity of software made C++ and richer library abstractions more attractive.

1.2 Templates

C++ had a reputation for poor performance compared with Fortran. Even developers willing to write C++ in "numerical" codes considered it better to use C++ has a high-level coordination language, and reserve lower-level languages like C for tight loops.[7] Developers saw C++ templates, in particular expression templates, as an optimization technique that could close the performance gap. Expression templates would let developers write compact, abstract code that "looks like math," yet optimizes by fusing loops and avoiding temporaries. For example, the Dr. Dobbs article[8] on the Blitz++ library,[9] written by the library's author, focuses on expression templates for vector operations.

Developers also recognized the cost of virtual method calls in C++, especially in inner tight loops, and used templates to reduce the cost of run-time polymorphism. For example, the Bernoulli Generic Matrix Library uses the "Barton-Nackman trick,"[10] a special case of the "Curiously Recurring Template Pattern," to turn run-time polymorphism into compile-time polymorphism.[11]

Early libraries that relied on templates suffered due to incomplete compiler implementations. For example, Blitz++'s installation process exercises the compiler to test language feature compliance. Its User's Guide recommends that if the compiler "doesn't have member templates and enum computations, just give up."[12] A comparable library, POOMA (Parallel Object-Oriented Methods and Applications),[13] pushed the boundaries of what the available C++ compilers could handle. Chris Luchini, a POOMA developer, recalls that the project exposed many compiler bugs.[14] Many compilers lagged behind the C++ standard, only implemented a subset of features, and generated slow code.[15]

[5] [Mar91]
[6] [KH89]
[7] [Arg+97]
[8] [Vel97]
[9] [Vel05]
[10] [BN94]
[11] In [MPS00], authors cite [Vel00]
[12] See Section 1.4.3 of [Vel05].
[13] `http://www.nongnu.org/freepooma/tutorial/introduction.html`
[14] [Hoe18]
[15] [MPS00]

Software for scientific computing may need to build with several different compilers and run on different kinds of hardware. Lack of consistently complete implementations of templates challenged portability requirements and restricted adoption. For example, in the Trilinos software project, a requirement to support a C++ compiler with incomplete template support drove the project to forbid templates in its foundational linear algebra library, Epetra.[16]

1.3 POOMA

The POOMA (Parallel Object-Oriented Methods and Applications) project was most active 1998-2000. POOMA's goal was to support structured grid and dense array computations. As per oral history[17] and POOMA's documentation, the team had a particular interest in SGI Origin shared-memory parallel computers. POOMA shares features with more recently linear algebra libraries, such as polymorphism on storage layout and parallel programming model, so it is worth studying for historical lessons.

POOMA's main data structure is Array. Array has three template parameters: the rank (the number of dimensions), the entry type (e.g., `double`), and the "engine." Engines are about storage of data. They correspond somewhat to the Accessor policy in the `mdspan` multidimensional array proposal.[18] An engine implements access to entries of the Array. Entries could actually exist in some storage somewhere, or they could be computed from indices and not actually stored. Engines also describe parallel distribution somewhat – e.g., through the MultiPatch engine.[19]

POOMA's Internals and Ranges let users construct possibly strided multidimensional index ranges. These features let users write very general indexed loops, like in the ZPL programming language.[20] However, POOMA users had to work a bit harder on distributed-memory parallel systems, to expose "guard regions" with redundant storage on process boundaries.[21]

The POOMA project had to "discover" experimentally how C++ templates work, and develop their own idioms. For example, the developers learned that C++ does not permit templating on return type and then deducing the return type.[22] As mentioned above, POOMA developers also had to explore the limits of compiler correctness and performance.

1.4 C++ for More Radical Optimizations

As experience with C++ templates increased, some developers applied them to more radical code optimizations. For example, the Bernoulli Generic Matrix Library used templates to generate optimized sparse matrix codes from a high-level specification.[23] Bernoulli used a kind of relational algebra (described in detail in the PhD dissertation) that is somewhat analogous to the C++ Ranges

[16] [Hoe18]

[17] See [Hoe18].

[18] [Edw+18]

[19] `http://www.nongnu.org/freepooma/tutorial/tut-04.html`

[20] [Cha+98]

[21] This essentially means that POOMA did not do implicit boundary exchange. High-performance computing experts like to expose and reify the parallel distribution, and any redistribution operations. This helps them avoid communication and data movement, and makes parallel synchronization semantics clear. This is also a bit of a reaction to High-Performance Fortran, where even copying from one array to another could require parallel synchronization.

[22] `http://www.nongnu.org/freepooma/tutorial/tut-03.html`

[23] [AMP00] By the time, I (Mark Hoemmen) encountered the Bernoulli project, it had abandoned C++ code generation in favor of OCaml (or some other ML derivative)-based code generation framework. My guess is that avoiding intermediate high-level C++ step improved run-time performance and avoided compiler correctness issues.

proposal [NCB18], in that it gives users a general way to describe operations over sequences, while optimizing by avoiding storage of temporary intermediate sequences.

1.5 Lessons Learned from Efforts in Other Programming Languages

1.5.1 LINPACK

Dongarra[24] gives an oral history of standardization of popular Fortran linear algebra libraries, including EISPACK and LINPACK. LINPACK came later. Here is a longer quote from this oral history explaining LINPACK's choice to rely on the BLAS:

> Since linear systems have perhaps a broader impact, LINPACK was going to a wider audience, and we felt that it would have a larger acceptance. This package was designed at a time when the biggest computers available were the vector computers. The vector supercomputers were just coming onto the scene, and the package was designed with vector computers in mind, so the package was designed to rely on an underlying set of routines called the BLAS (the Basic Linear Algebra Subprograms). The BLAS are a set of kernels which form the computational core of LINPACK; they are the vector operations that are going to be done over and over again in the package. The BLAS were a set of standard routines which were formed right before LINPACK was really kicked off, and we made a decision to use them.

In so far as possible, the project wrote one version of the algorithms for four different data types (two different real precisions and two different complex precisions), and generated Fortran code for each of the four data types from this "abstract" representation.

1.5.2 High Performance Fortran

The High Performance Fortran (HPF) programming language[25] inherited Fortran's native support for multidimensional arrays. It added support for parallel arithmetic operations on these multidimensional arrays, that might be distributed in parallel over multiple processors. Compare also to the 2-D block cyclic data distributions that ScaLAPACK[26] supports for dense matrices. 2-D block cyclic distributions include block and cyclic layouts, both 1-D and 2-D, as special cases.

1.6 Vector Spaces and Parallel Data Distributions

How can I tell if I'm allowed to add two vectors together, or multiply two matrices? Is it enough for their dimensions to be compatible? Mathematicians would point out that two vector spaces might still differ, even if they have the same dimension or are otherwise isomorphic. I can't add a coordinate in 3-D Euclidean space to a quadratic polynomial with real coefficients, just like I can't add meters to seconds. Like a physical unit, a vector space is a kind of "metadata." Equating all isomorphic vector spaces strips off their metadata.

[24] [Don05]
[25] [KKZ07; KKZ11]
[26] [Bla+97]

A distributed-memory parallel data distribution is very much like a vector space. It takes an N-dimensional vector space and imposes a two-dimensional index $(p, I(p))$ on it, Here $p \in [0, P)$ is the parallel process index (the "rank," in MPI terms), and $I(p)$ is the set of indices that live on Process p. The only thing that would make this a finite-dimensional vector space is the field over which the entries of a vector are defined. Even if two vectors x and y have the same dimension N, if the two vectors have different parallel distributions, I can't add them together without communication. "Communication" here may mean different things on different parallel computers, but this generally means some combination of moving data between processors (either through a memory hierarchy, or across a network), and synchronization between processors. Communication is expensive relative to floating-point arithmetic.[27] It also affects correctness, because it may introduce deadlock, depending on what surrounding code does. Thus, programmers like to see communication made explicit, even if it is hidden behind a convenient interface.

Linear algebra libraries can make this easier for programmers through the abstract language of vector spaces. For example, the library can let users construct and pass around a parallel distribution using the two-dimensional indexing structure $(p, I(p))$ mentioned above. Users then create matrices and vectors using distribution objects created in this way. The library can forbid implicit arithmetic operations between different vector spaces, but can make data redistribution and/or "communicating" arithmetic operations explicit. Users can also get the data distributions out of a matrix or vector, and check themselves whether two different distributions are the same. It's easier to explain all this to users in the abstract language of vector spaces.

Even if I don't care about distributed-memory parallelism, I may still care about shared-memory parallelism (threads) and memory affinity.

1.7 A Matrix has Four Vector Spaces

Matrices fulfill two different roles. First, matrices are 2-D data containers. Their rows have a data distribution, and their columns do also. Second, I can do matrix-vector products with a matrix. This makes a matrix a function from its domain vector space to its range vector space.

[27] [WM95; Bla+97]

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