Bandicoot: C++ Library for GPU Linear Algebra and Scientific Computing

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Abstract

This report provides an introduction to the **Bandicoot** C++ library for linear algebra and scientific computing on GPUs, overviewing its user interface and performance characteristics, as well as the technical details of its internal design. Bandicoot is the GPU-enabled counterpart to the well-known Armadillo C++ linear algebra library, aiming to allow users to take advantage of GPU-accelerated computation for their existing codebases without significant changes. Adapting the same internal template meta-programming techniques that Armadillo uses, Bandicoot is able to provide compile-time optimisation of mathematical expressions within user code. The library is ready for production use and is available at https://coot.sourceforge.io. Bandicoot is distributed under the Apache 2.0 License.

1 Introduction

A number of recent significant advancements in scientific computing have been enabled by the use of graphics accelerators / graphics processing units (GPUs), notably in the fields of machine learning [6, 19], HPC and supercomputing [14, 33], healthcare and life sciences [25, 38], as well as modeling and simulation [16]. GPUs are built on the concept of SIMT (single instruction, multiple threads) and are thus capable of performing the same operation on separate chunks of data in parallel. Often, modern GPUs are extremely parallel: Nvidia's recent mainstream consumer-focused GeForce RTX 4090 GPU contains 16,384 cores, leading to a throughput of around 80 TFLOPS for 32-bit floating point data.

A large part of the reasons for the significant speedups and advancements in the fields listed above is the core accelerations that GPUs provide to linear algebra operations. The nature of most linear algebra computations is very well-suited to SIMT-like approaches: for instance, the common axpy vector-scalar product task, (e.g. $\mathbf{y} \leftarrow \mathbf{y} + \alpha \mathbf{x}$) is embarrassingly parallel and clearly suited for SIMT processing on a GPU.

However, from a user perspective, writing scientific code that properly exploits GPUs is cumbersome and not portable. The CUDA framework [21] is specific to Nvidia devices, and thus any CUDA code cannot directly work on AMD or Intel GPUs, or any other GPU-like devices such as Google's tensor processing units [18]. Even higher-level toolkits such as MATLAB [35] and R [24] typically need special setup to use GPUs, and that setup is typically limited to a certain type of GPU. Standardization efforts like OpenCL [32], which promise code that works on any GPU-like device, are often not well-supported by vendors. Balkanization has occurred in the space, with numerous incompatible efforts like Apple's Metal¹ and AMD's ROCm², in addition to Nvidia's CUDA.

From a non-expert user's perspective, this situation is abysmal: scientists and developers operating at a higher level do not want to spend time digging into low-level implementation details of their GPUs, but instead want to be able to simply write linear algebra and have it work efficiently on their GPU. This is, after all, the reason that linear algebra libraries and interfaces like LAPACK and BLAS [3, 4] were originally written: to provide an interface in order to abstract away the implementation details.

High-level interfaces have seen massive amounts of success over the years, specifically because they allow developers and scientists to maximize productivity by focusing on their higher-level task. In this vein, toolkits like MATLAB and Mathematica [44] have been extremely successful, in large part because of the simple and intuitive interface they provide. In the

https://developer.apple.com/metal/

²https://www.amd.com/en/graphics/servers-solutions-rocm

field of machine learning, Python [39] and its linear algebra abstraction NumPy [15] have become dominant in large part for the same reason. However, these higher-level languages often come with a cost; for instance, MATLAB and Python have high amounts of overhead, and require large runtime environments that depend on numerous additional packages.

Motivated by high-level MATLAB-style expressive syntax, the well-known Armadillo C++ linear algebra library [30] was created to satisfy the need for a high-level and intuitive linear algebra interface while maximizing runtime performance. Armadillo uses template meta-programming [40] in order to optimise linear algebra expressions at program compilation time; this can provide significant and demonstrable speedups over other solutions [28, 31, 29, 27]. Its clear interface and flexibility has led to widespread adoption, including via bindings to other languages like R [11] and Python [37, 26].

However, Armadillo is only able to use CPUs and CPU-specific libraries such as OpenBLAS [20, 41] and Intel's Math Kernel Library (MKL) for its linear algebra operations. Therefore, practitioners cannot make use of the GPUs that they likely have available to accelerate their linear algebra programs. This motivated us to develop the **Bandicoot** C++ GPU linear algebra library.

Bandicoot is aiming to provide an API that closely matches Armadillo's API, with the primary difference being that linear algebra operations are performed on the GPU instead of the CPU, and the memory used for matrices is GPU memory instead of system RAM. Bandicoot abstracts away the vendor-specific technologies that are used for GPU programming, and can run on virtually any GPU via its support for both CUDA and OpenCL backends. Users do not need to learn low-level details about their devices, as Bandicoot will automatically try to configure and use the most appropriate device.

Higher-level libraries are already beginning to use Bandicoot, with work underway to adapt the *ensmallen* numerical optimisation library [8] and the *mlpack* machine learning library [9] to use Bandicoot and provide GPU-accelerated algorithms.

The rest of this report is dedicated to describing the user interface of Bandicoot (Section 2), detailing differences from Armadillo that are important to know when converting Armadillo code to use GPUs (Sections 3 and 4), demonstrating speedups gained by using Bandicoot (Section 5), defining the upcoming roadmap of features to be implemented (Section 6), and documenting the internal design and details of the library (Section 7).

2 Overview of Functionality

Bandicoot aims to provide an API that closely matches the API of the Armadillo C++ linear algebra library [30]. This means that Bandicoot's interface is the same as Armadillo's intuitive and readable interface, so far as is possible (see Section 3). The following example Bandicoot program may therefore look familiar to Armadillo users:

```
#include <bandicoot>
using namespace coot;
int main()
{
  fmat X(1000, 1000, fill::randu);
  fmat Y(1000, 2000, fill::randu);
  // (X + I)' (Y + 2)
  fmat Z = (X + eye<fmat>(1000, 1000)).t() * (Y + 2);
}
```

The basic type in Bandicoot is the Mat (matrix) class, which as a template parameter takes the element type to be held in the matrix. That is, the Mat<float> class is a matrix that holds 32-bit float values. Bandicoot provides convenient typedefs for various matrix types; thus, the fmat class is equivalent to Mat<float>, and umat class is equivalent to Mat<uword>, where uword is the unsigned integer type provided by Bandicoot—generally equivalent to size_t.

Similar to the Mat class, Bandicoot provides the Col and Row classes for row and column vectors, respectively. Convenience typedefs are also provided: fvec and fcolvec for Col<float>, and frowvec for Row<float>.

When Bandicoot code is run, linear algebra operations are performed on the GPU. Bandicoot supports both a CUDA backend and an OpenCL backend. Details of which backend to be used and which device to use can optionally be controlled via the coot_init() function, meant to be used at the beginning of the program:

```
// Use only one of the following in your program, or omit entirely for automatic selection
coot_init("opencl", true /* print information */);
coot_init("opencl", false, 0 /* OpenCL platform ID */, 1 /* OpenCL device id */);
coot_init("cuda", true, 2 /* CUDA device ID */);
```

Of course, device initialisation will fail if neither OpenCL nor CUDA is available on the system.

More complicated linear algebra operations, such as matrix multiplication and decompositions (LU, SVD, eigen, etc.), use external support libraries whenever possible. The support libraries that are used depend on which backend is enabled:

- The CUDA backend uses cuBLAS, cuRand, and cuSolver, which are parts of the CUDA Toolkit³.
- The OpenCL backend uses clBLAS [1] and internal adaptations of MAGMA [36] and clMAGMA [12].

This is similar to Armadillo's use of external support libraries such as OpenBLAS [41] or other BLAS/LAPACK replacements.

A condensed overview of the functionality of Bandicoot is given in Tables 1 through 7:

- Table 1 briefly describes the main members of the Mat class.
- Table 2 lists the overloaded C++ operators that can be used with Bandicoot objects.
- Table 3 lists a subset of currently available decomposition techniques.
- Table 4 lists a subset of functions that generate matrices and vectors.
- Table 5 lists a subset of functions for Bandicoot objects that return scalar values.
- Table 6 lists a subset of functions for Bandicoot objects that return vectors (Col/Row).
- Table 7 lists a subset of functions for Bandicoot objects that return matrices (Mat).

The full documentation is available online at https://coot.sourceforge.io/docs.html.

Function/Variable	Description
.n_rows	number of rows (read-only)
.n_cols	number of columns (read-only)
.n_elem	total number of elements (read-only)
	Note: individual element access is inefficient; see Section 3.
(i)	access the i-th element, assuming a column-by-column layout
[i]	access the i-th element with no bounds check
(r, c)	access the element at row r and column c
.at(r, c)	access the element at row r and column c, but with no bounds check
.get_dev_mem()	get raw GPU memory (returns object with .cuda_mem_ptr/.cl_mem_ptr members)
.reset()	set the number of elements to zero
.set_size(rows, cols)	set the size to the specified dimensions, without preserving data
.reshape(rows, cols)	set the size to the specified dimensions, while preserving data
.fill(k)	set all elements to be equal to k
.ones(rows, cols)	set all elements to one, optionally first resizing to specified dimensions
.zeros(rows, cols)	set all elements to zero, optionally first resizing to specified dimensions
.eye(rows, cols)	set to the identity matrix, optionally first resizing to specified dimensions
.randu(rows, cols)	set to uniformly distributed random values in $[0, 1]$ with optional resize
.randn(rows, cols)	set to Gaussian random values (~ $N(0, 1)$) with optional resize
.t()	return transpose of object
.is_empty()	test whether there are no elements
.is_square()	test whether the matrix is square
.is_vec()	test whether object is a vector
.print(header)	print elements to the cout stream, with an optional header
.raw_print(header)	as above, but with no formatting of the output stream
submatrix views:	
.diag(k)	read/write access to the k-th diagonal
.row(i)	read/write access to the i-th row
.col(j)	read/write access to the j-th column
.rows(a, b)	read/write access to the submatrix spanning from row a to row b
.cols(c, d)	read/write access to the submatrix spanning from column c to column d
.submat(p, q, r, s)	read/write access to the submatrix starting at element (p, q) and ending at (r, s)
.submat(span(p, r), span(q, s))	same as above

Table 1: Member functions and variables of the Mat class (subset).

Operation	Description
A - k	subtract scalar k from all elements in A
k - A	subtract each element in A from scalar k
A + k, k + A	add scalar k to all elements in A
A * k, k * A	multiply matrix A by scalar k
A + B	add matrices A and B
A - B	subtract matrix B from A
A * B	matrix multiplication of A and B
A % B	element-wise multiplication of A and B
A / B	element-wise division of A by B

Table 2: Matrix operations involving overloaded C++ operator functions (subset).

Function	Description
lu(L, U, P, X)	Lower-upper decomposition of X such that $P * X = L * U$ and $X = P.t() * L * U$
lu(L, U, X)	Same as above, but with permutation matrix combined with L: $X = L * U$
chol(X)	Cholesky decomposition of X, returns R such that $X = R.t() * R$
svd(X)	Singular value decomposition of X
eig_sym(X)	Eigendecomposition of X
pinv(X)	Moore-Penrose pseudo-inverse of X
solve(A, B)	Solve a system of linear equations $A * X = B$, where X is unknown

Table 3: Matrix decompositions and related functions (subset).

Function	Description
eye(rows, cols)	matrix with the elements along the main diagonal set to one;
	if rows == cols, an identity matrix is generated
ones(rows, cols)	matrix with all elements set to one
zeros(rows, cols)	matrix with all elements set to zero
randu(rows, cols)	matrix with uniformly distributed random values in the interval $[0,1]$
randn(rows, cols)	matrix with random values from the normal distribution with $\mu = 0$ and $\sigma = 1$
linspace(start, end, n)	vector with n elements, linearly increasing from start up to (and including) end
repmat(A, p, q)	replicate matrix A in a block-like fashion, resulting in p by q blocks of A

Table 4: Functions for generating matrices (subset).

Function	Description
accu(A)	accumulate (sum) all elements of A
as_scalar(expr)	evaluate an expression that results in a 1×1 matrix, convert the result to a scalar
det(A)	determinant of square matrix A
dot(A, B)	dot product of A and B, assuming they are vectors with equal numbers of elements
norm(A, p)	p-norm of A, with $p = 1, 2, \cdots$ or $p = "inf", "-inf", "fro"$
trace(A)	sum of the diagonal elements of square matrix A
all(A)	check whether all elements in A are nonzero
all(A < x)	check whether all elements in A are less than scalar x
	(note that other relational expressions may also be used)
any(A)	check whether any elements in A are nonzero
any(A < x)	check whether any elements in A are less than scalar x
	(note that other relational expressions may also be used)

Table 5: Scalar valued functions (subset).

Function	Description
max(A, dim)	find the maximum in each column of A (dim = 0),
	or each row of A (dim = 1) (default: dim = 0)
min(A, dim)	as above, but find the minimum
sum(A, dim)	as above, but find the sum
statistics:	
mean(A, dim)	as above, but find the average
median(A, dim)	as above, but find the median
stddev(A, dim)	as above, but find the standard deviation
var(A, dim)	as above, but find the variance
diagvec(A, k)	extract the k-th diagonal from matrix A (default: $k = 0$)

Table 6: Vector valued functions (subset).

Function	Description
cor(A, B)	the element at (i, j) in the result will be the the correlation
	between the i-th variable in A and the j-th variable in B,
	where each row of A and B is an observation and each column is a variable
cov(A, B)	as per cor(A, B), but calculate the covariance
conv(A, B)	one-dimensional convolution of A and B, assuming they are vectors
conv2(A, B)	two-dimensional convolution of matrices A and B
cross(A, B)	cross product of A and B, assuming they are 3-dimensional vectors
find(A)	find the indices of non-zero elements of A
find(A < k)	find the indices of elements of A with values less than scalar k
	(note that other relational expressions may also be used)
<pre>find_finite(A)</pre>	find the indices of finite elements of A
<pre>find_nonfinite(A)</pre>	find the indices of nonfinite elements of A
find_nan(A)	find the indices of elements of A with value nan (not a number)
join_rows(A, B)	append each row of B to its respective row of A
join_cols(A, B)	append each column of B to its respective column of A
reshape(A, r, c)	copy A with dimensions set to r rows and c columns
sort(A, dim)	copy A with the elements sorted in each column (dim = 0)
	or row (dim = 1)
<pre>sort_index(A)</pre>	assuming A is a vector, generate a vector that describes the
	sorted order of A's elements (i.e. the indices)
trans(A)	Hermitian transpose of A
diagmat(A)	interpret matrix A as a diagonal matrix
	(this can save computation time during multiplication)
misc(A)	apply a miscellaneous function to each element of A, where misc can be:
	pow, exp, log, log10, sqrt, square,
trig(A)	apply a trigonometric function to each element of A, where trig can be:
	cos, sin, tan, acos, asin, atan,

Table 7: Matrix valued functions (subset).

3 Fundamental Differences from Armadillo

Although Bandicoot aims to be API-compatible with Armadillo wherever possible, major differences in the computational designs of CPUs and GPUs mean that Bandicoot and Armadillo have some fundamental differences, as elucidated below.

The first and most important difference is the location where data is stored: in Armadillo, elements of a matrix are stored in CPU (host) memory; that is, system RAM. In Bandicoot, elements of a matrix are instead stored in device (GPU) memory. Because Bandicoot users are writing control code that runs on the host, this means that accessing the individual elements of a matrix requires a transfer from GPU memory to CPU memory. For a single element, this can be very expensive!

To demonstrate the difference by counterexample, consider the following example code:

```
fmat A(1000, 1000, fill::randu);
// count the number of elements greater than 0.3 (inefficient version)
size_t count = 0;
for (size_t i = 0; i < A.n_elem; ++i)
        {
        if (A[i] > 0.3) // WARNING: in Bandicoot, this causes a time-consuming CPU/GPU transfer!
        ++count;
     }
```

When A is an Armadillo matrix, the matrix's elements are already in system memory and no transfer is necessary. However, when A is a Bandicoot matrix, a transfer from GPU memory is performed. On the same system used for benchmarks in Section 5, this particular code snippet takes 0.0004s with Armadillo and 13s with Bandicoot's CUDA backend!

For this reason, **C++ iterators over Bandicoot matrices are not provided**. This is an intentional design decision to prevent users from accidentally writing slow code. Instead of iterating individually over elements in a Bandicoot matrix, users should strive to use linear algebra expressions instead. The code above can be more efficiently expressed as the equivalent operation:

```
fmat A(1000, 1000, fill::randu);
// count the number of elements greater than 0.3 (efficient version)
size_t count = size(find(A > 0.3)).n_rows;
```

Compared to the previous program, this rewrite is more efficient (and more readable), with speed comparable to Armadillo.

The second fundamental difference between Bandicoot and Armadillo is related to the amount of parallelism that GPUs provide. The main avenue to speedup with a GPU is provided by the extreme level of parallelism (SIMT). For instance, Nvidia's recent GeForce RTX 4090 GPU contains 16,384 cores, whereas recent AMD Epyc (x86-64 compatible) CPUs contain up to 128 cores (i.e. about 2 orders of magnitude difference). The clear implication of this is that keeping all of the cores in the GPU busy is of the utmost importance to get speedup.

For this reason, Bandicoot is ill-suited to calculations on small matrices. For instance, performing an operation like A += 3 where A is a 10×10 matrix only makes use of at most 100 GPU cores. Thus, if a program makes use of many small matrices, conversion to Bandicoot may not give any speedup. For this reason, fixed-size matrices (e.g. arma::mat::fixed<>) do not provide tangible benefit and are not currently implemented as a feature in Bandicoot. As observed in our empirical evaluations shown in Section 5, Bandicoot typically becomes noticeably faster than the CPU for matrices sized about 1000×1000 or larger; the specific trade-off point will depend on the workload, CPU, and GPU, so this 'rule of thumb' above may not always apply.

The third fundamental difference between Bandicoot and Armadillo is that GPUs tend to provide higher performance for lower-precision numeric types [13]. Some older GPUs, in fact, do not have support for 64-bit floating point types [43]. For this reason, when using Bandicoot, it is generally recommended to use 32-bit floating point numbers (e.g. float) instead of 64-bit (e.g. double); that is, the use of coot::fmat matrix type is generally recommended instead of coot::mat matrix type. If coot::mat is used but Bandicoot detects that the GPU does not support 64-bit precision, a std::runtime_error exception will be thrown.

The last major fundamental difference between Bandicoot and Armadillo is the fact that individual GPU kernels must be compiled at runtime for each specific device. With Armadillo, all operations can be compiled entirely at compile time (e.g. in the g++ compilation call). In contrast, when any Bandicoot program is run, the first step is to compile all GPU kernels for the device that is found. Bandicoot caches the compiled kernels (by default in ~/.bandicoot on Linux and macOS systems), so on most systems this startup step is a one-time cost that typically takes between 3 and 5 minutes. At the current time, compilation of custom kernels for operations such as Armadillo's transform() function are not available, but future releases aim to include this support (see Section 6).

For situations where mixed use of Armadillo and Bandicoot is appropriate, the conv_to() function can be used to convert back and forth, as below:

```
using namespace coot;
fmat X_gpu(1000, 1000, fill::randu);
// transfer matrix from GPU to CPU
arma::fmat X_cpu = conv_to<arma::fmat>::from(X_gpu);
// transfer back from CPU to GPU
X_gpu = conv_to<fmat>::from(X_cpu);
```

4 Linking Bandicoot Programs

Like Armadillo, Bandicoot provides a *wrapper library* to ease the linking process. Linking to GPU libraries (especially in the CUDA framework) can be cumbersome, with Nvidia even going so far as providing the nvcc compiler wrapper to simplify the process⁴. Bandicoot's library obviates the need for this complexity, and a typical program using Bandicoot can be compiled with a command as simple as

g++ prog.cpp -o prog -O2 -lbandicoot

This links against the Bandicoot wrapper library (libbandicoot.so on Linux and libbandicoot.dylib on macOS), which is itself dynamically linked against all of Bandicoot's dependencies. All of the functions in the Bandicoot wrapper library are simply wrapper functions that in turn call the external library functions Bandicoot depends on. Therefore, via transitive linking, a user can link against only the Bandicoot wrapper library.

An important note is that while Bandicoot and Armadillo are interoperable and meant to be compatible, Bandicoot does not depend on Armadillo. Thus, there is only need to link against Armadillo (-larmadillo) if Armadillo is explicitly being included and used in the program.

In some situations, it is preferable to not link against the wrapper library and instead link directly against Bandicoot's dependencies. This situation could occur if a user wants to use Bandicoot without installing the library, or wants to use Bandicoot as a standalone header-only library. If this is desired, the COOT_DONT_USE_WRAPPER macro must be set (e.g. #define COOT_DONT_USE_WRAPPER), Then, the libraries that must be linked against are detailed below.

• Regardless of which backend is enabled, the following libraries must be linked against.

-lblas (CPU BLAS support; can use -lopenblas instead)

-llapack (CPU LAPACK support; can use -lopenblas)

• If the OpenCL backend is enabled (e.g. COOT_USE_OPENCL is defined), the following libraries are required.

-10penCL (core OpenCL support)

-lclBLAS (clBLAS for BLAS operations)

• If the CUDA backend is enabled (e.g. COOT_USE_CUDA is defined), the following libraries are required.

4https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/index.html

-lcuda (core CUDA support)

- -lcudart (CUDA runtime library)
- -lnvrtc (runtime compilation of CUDA kernels)
- -lcublas (cuBLAS for BLAS operations)
- -lcusolver (cuSolverDn for decompositions and factorisations)
- -lcurand (cuRand for random number generation)

5 Empirical Speed Comparison

We performed several tests in order to demonstrate the speedups that can be seen when using Bandicoot. The speedups that are observed are not simply due to underlying speedups from the use of GPUs instead of CPUs: internally, Bandicoot uses delayed evaluation [42], where C++ template meta-programming techniques apply optimisations at compile time [40]. Where applicable, the order of operations is optimised, while redundant or unnecessary operations are removed entirely, and inefficiently-expressed operations are rewritten efficiently. This technique is also used in Armadillo and has been shown to provide significant speedups over alternate linear algebra libraries [23, 27].

Our timing comparisons focus on the speedups Bandicoot can provide over Armadillo due to the use of GPUs instead of CPUs. These comparisons also shed light on the situations where Bandicoot is more appropriate than Armadillo. All comparisons were done on a system with an Intel Core i9-10920X (3.5 GHz, 12 cores, 19.25MB cache), an Nvidia RTX 2080Ti GPU (1350 MHz, 4352 cores, 11GB RAM) with Nvidia driver version 525.105.17, and 128GB system RAM, with Linux kernel 6.1.0 and GCC 12.2.0. For completeness, comparisons were performed using both 32-bit floating-point precision (float) and 64-bit floating-point precision (double). (See Section 3 for more details on precision on GPUs.)

For these comparisons, we use Bandicoot's OpenCL backend, Bandicoot's CUDA backend, and Armadillo on the CPU.

Task 1. Accumulate elements of a vector. The inner loop of the code used for timing is shown below.

```
// N is specified externally
// when using Armadillo, 'using namespace arma' is used
// when using Bandicoot, 'using namespace coot' is used
fvec f(N);
f.randu();
coot_synchronise(); // applicable only to Bandicoot
```

wall_clock c;

```
c.tic();
float result = accu(c);
coot_synchronise(); // applicable only to Bandicoot
const double time = c.toc();
```





(b) accu() performance for doubles.



Figure 1 shows results for the accu() task. The observations about matrix size from Section 3 are validated: Bandicoot is faster only for larger vector sizes. The CUDA backend is more effective than the OpenCL backend, which is not particularly surprising on an Nvidia device. For large enough vector sizes, Bandicoot can outperform Armadillo by roughly two orders of magnitude.

Task 2. Scalar vector multiply-add (axpy). The inner loop of the code used for timing is shown below.

```
// N is specified externally
// when using Armadillo, 'using namespace arma' is used
// when using Bandicoot, 'using namespace coot' is used
fvec A(N, fill::randu);
fvec B(N, fill::randu);
coot_synchronise(); // applicable only to Bandicoot
```

wall_clock c;

c.tic(); B += 3 * A; coot_synchronise(); // applicable only to Bandicoot const double time = c.toc();





(b) *axpy* performance for doubles.



The axpy results in Figure 2 match the observations from the accu() experiment: Bandicoot is only faster for larger vector sizes.

Task 3. Matrix multiplication. The inner loop of the code used for timing is shown below.

```
// N is specified externally
// when using Armadillo, 'using namespace arma' is used
// when using Bandicoot, 'using namespace coot' is used
fmat A(N, N, fill::randu);
fmat B(N, N, fill::randu);
coot_synchronise(); // applicable only to Bandicoot
```

wall_clock c;

c.tic(); fmat C = A * B; coot_synchronise(); // applicable only to Bandicoot const double time = c.toc();





(b) Matrix multiplication performance for doubles.

Figure 3: Matrix multiplication performance for Bandicoot and Armadillo with square matrices as a function of matrix size.

The results in Figure 3 highlight some additional differences between CPUs and GPUs: the performance differences for float and double element types, discussed in Section 3, are clear in this benchmark. 32-bit performance significantly exceeds 64-bit performance, and for 64-bit types, on this system, arguably no speedup is seen. Note that because Bandicoot and Armadillo wrap other libraries where possible, this comparison is really a comparison between clBLAS [1], cuBLAS, and OpenBLAS [20, 41].

Task 4. LU decomposition. The inner loop of the code used for timing is given below.

```
// N is specified externally
// when using Armadillo, 'using namespace arma' is used
// when using Bandicoot, 'using namespace coot' is used
fmat A(N, N, fill::randu);
coot_synchronise(); // applicable only to Bandicoot
```

wall_clock c;

c.tic(); fmat L, U; lu(L, U, A); coot_synchronise(); // applicable only to Bandicoot const double time = c.toc();



(a) lu() performance for floats.



Figure 4: LU decomposition performance for Bandicoot and Armadillo with square matrices as a function of matrix size.

Due to the more complex nature of decompositions, they are not as easily parallelized onto the GPU as operations like accu() and *axpy*, and Figure 4 shows that speedups may be more limited in this case. Nonetheless, Bandicoot is still able to provide up to a 10x speedup for float matrices, and up to a 5x speedup for double matrices, for matrices that are sufficiently large.

6 Roadmap

So far as is possible, the primary medium-term goal for Bandicoot is to be fully API-compatible with Armadillo, to ease conversion of Armadillo programs. However, Bandicoot opens numerous possibilities to go beyond Armadillo. Some of the roadmap goals of the development team are listed and detailed below, in approximate priority order. (Note that priorities may change over time; the development team does not intend to address this list sequentially.)

- Additional decompositions. Bandicoot does not currently implement the qr(), eig_gen(), qz(), or schur() decompositions. Bandicoot also lacks some of the more complex options of Armadillo's solve() [29].
- **Support for** Cube. Bandicoot does not currently implement the 3-dimensional matrix class Cube. This class is especially useful for higher-order operations that operate on collections of matrices.
- **Complex number support**. Bandicoot does not currently allow complex element types for matrices, e.g., Mat< std::complex<float> >. It is a near-term goal to support this, as this is important and highly-used functionality in Armadillo.
- Use of CLBlast instead of clBLAS. The clBLAS project [1] has not been updated in years and there are some bugs that are likely to remain unfixed. The newer CLBlast project [22] provides an appealing alternative. Like Armadillo's support for any BLAS/LAPACK replacement, the goal for Bandicoot is to allow the use of either library with the OpenCL backend.
- Additional backends. The balkanization of the GPU space is a real concern, as OpenCL is effectively being replaced by proprietary frameworks from multiple vendors. Although OpenCL is likely to work as a backend for many years, better performance will be obtained with vendor-specific backends due to the amount of effort those vendors put into optimising their specific backends. A few examples of backends that would be useful to add are listed below.
 - *Metal*. The Apple Metal framework⁵ is Apple's new accelerator framework for hardware acceleration.
 - ROCm. AMD has an accelerator platform tuned for its GPUs called ROCm⁶.
 - oneAPI. Intel has its own competing framework called oneAPI7.
 - SYCL. The SYCL framework⁸ is not vendor-specific, and could be considered a spiritual successor to OpenCL.
- Low-precision type support. Especially in the field of machine learning, low-precision floating-point types are often used to increase computational performance and/or energy efficiency [17, 34]. Types such as 'brain floating point' have also been gaining widespread adoption [5]. As CUDA supports precisions down to 8-bit (fp8), and OpenCL extensions support half-precision floating-point (fp16), it is an important development goal to allow Bandicoot to seamlessly support these types whenever they are available in hardware.
- **Integration into higher-level libraries**. With the first release of Bandicoot now complete, work is underway to adapt higher-level libraries that use Armadillo to also be capable of using Bandicoot. Two important examples are the *ensmallen* C++ numerical optimisation library [8] and the *mlpack* C++ machine learning library [9]. Other possibilities being considered for development also include an Rcpp binding [10] for Bandicoot to allow users of R to GPU-accelerate their RcppArmadillo code [11].

More development details and plans can be found on the Gitlab development website, found at https://gitlab.com/ conradsnicta/bandicoot-code/.

⁵https://developer.apple.com/metal/

%https://www.khronos.org/sycl/

⁶https://www.amd.com/en/graphics/servers-solutions-rocm

⁷https://www.intel.com/content/www/us/en/developer/tools/oneapi/overview.html
8https://www.khspnos.org/ovel/

7 Internal Design

Internally, Bandicoot is built on a template meta-programming framework similar to Armadillo's template meta-programming framework. The idea of this framework is to provide significant compile-time optimisations of mathematical expressions given in user code. This is accomplished by collecting (at compile time) the structure of a linear algebra expression as a type, and then, when possible, using techniques such as SFINAE [40] and template specialisation to restructure the expression into an equivalent but more efficient form. Importantly, to keep Bandicoot user-friendly, this entire template meta-programming framework is internal to the library, and therefore invisible to the user.

In this section, we give an overview of that framework and show some simple examples of how optimisations can be applied in this manner. We also discuss differences between the internal designs of Bandicoot and Armadillo. The discussion is aimed to be useful to those who are curious about the internal details, or those who are interested in contributing to Bandicoot development. Knowledge of C++ and template meta-programming concepts is helpful. This section is not necessary reading for Bandicoot users: the documentation in earlier sections of this report and on the Bandicoot website is sufficient for that use case.

The base type in Bandicoot, which is the base type that all matrix and vector objects as well as all linear algebra expressions inherit from, is the template type Base<eT, T1> where eT refers to the *element type* and takes values float, double, int, etc., and T1 refers to the actual type of the Bandicoot linear algebra expression itself. This is a form of static polymorphism (that is, polymorphism without runtime virtual-table lookups) modeled after the "Curiously Recurring Template Pattern" (CRTP) [2, 7].

User-facing classes include the Mat<eT>, Col<eT>, and Row<eT> classes, which represent matrices, column vectors, and row vectors, respectively. A number of predefined convenience typedefs are given, allowing users to use, e.g., the more concise fmat type instead of Mat<float>.

Expressions in Bandicoot are built up as C++ types using the Op<eT, T1, op_type>, Glue<eT, T1, T2, glue_type>, mtOp<out_eT, T1, mtop_type>, eOp<eT, T1, eop_type>, and eGlue<eT, T1, T2, eglue_type> template classes. Each of these classes represents a specific type of linear algebra operation:

- Op<T1, op_type>: unary operation of type op_type that will operate on T1
- mtOp<out_eT, T1, mtop_type>: a multi-type operation of type mtop_type on T1 that produces an output that has different element type out_eT
- e0p<T1, eop_type>: an element-wise operation of type eop_type on T1
- Glue<T1, T2, glue_type>: binary "glue" operation of type glue_type that will operate on T1 and T2
- eGlue<T1, T2, eglue_type>: an element-wise "glue" operation of type eglue_type on two operands of types T1 and T2

Here, the operation types (op_type, glue_type, etc.) are placeholder types that represent the operation to be performed: for instance, Bandicoot contains types such as op_sum, glue_times, mtop_conv_to, op_vectorise, op_repmat, and so forth.

Expressions are assembled as users call functions. Bandicoot's functions do not return types such as Mat<eT>, but instead return any of the expression types listed above, which capture (as a type) the expression to be performed. As an example, the function signature for Bandicoot's trans() function is as follows:

```
// Note: the actual version in the library may differ slightly.
template<typename eT, typename T1>
inline
const Op<T1, op_htrans>
trans(const Base<eT, T1>& X);
```

The important observations here are that trans() does not require a matrix or vector object as input—instead, it can receive any Bandicoot expression; and, instead of returning a Mat<eT> that holds the transposed result, the function returns an Op<T1, op_htrans> indicating that computing the value of the expression will require taking the transpose of T1.

Before considering how such expressions are evaluated, we can easily demonstrate how some compile-time optimisations can be performed. Observe the following additional overload of the trans() function that Bandicoot includes:

This more complicated overload is for situations where a user passes a diagonal matrix (signified as an op_diagmat; this is produced by e.g. the diagmat() function). Because the transpose of a diagonal matrix is equivalent to the diagonal matrix itself, we do not even need to add an op_htrans to the expression type, and so we can simply return the given Op<T1, op_diagmat> completely unchanged. Note that the enable_if2<> is an SFINAE restrictor on the return type [40] that will not allow the function to be selected unless the given T1 is a Bandicoot type (e.g. it must inherit from Base<eT, T1> for some eT).

Bandicoot contains multiple optimisations of this form, where user-level functions will greedily apply optimisations during the construction of the full expression type.

As an example of how compound expressions are represented internally, let us consider the following expression:

A * trans(diagmat(V)) + 4 * B

where A and B have type mat, and V has type vec. Abusing notation to replace individual operations with their resulting type, the type expression formed by the compiler for the input above is

```
A * trans(diagmat(V)) + 4 * B
A * trans(Op<vec, op_diagmat>) + 4 * B
A * Op<vec, op_diagmat> + 4 * B
Glue<mat, Op<vec, op_diagmat>, glue_times> + 4 * B
Glue<mat, Op<vec, op_diagmat>, glue_times> + eOp<mat, eop_scalar_times>
eGlue<Glue<mat, Op<vec, op_diagmat>, glue_times>, eOp<mat, eop_scalar_times>, eglue_plus>
```

While this type is quite intimidating in its textual representation (especially when encountered as an error message during Bandicoot development), it is a complete description of the operation to be performed. Further, with most compilers, these types are ephemeral and can be completely optimised out of the program. Each operation type (Op, Glue, etc.) simply holds a reference to its operands, and possibly one or two primitives (int, etc.) of metadata, and thus may be easily optimised out of the program entirely.

Next, let us consider how expressions like this are evaluated and the results stored in specified output matrices. The expression above may appear in a program like this:

mat C = A * trans(diagmat(V)) + 4 * B;

The evaluation of Bandicoot expressions is delayed until an assignment operator is encountered. In this case, the function that will actually cause the expression to be evaluated is Mat<double>::operator=(const Base<eT, T1>&) where T1 will be the full type of the expression, given above.

The majority of the work that operator=(const Base<eT, T1>&) performs is handled by the unwrap<T1> meta-programming struct. unwrap uses partial template specialisations, each dependent on the outer type of the given expression. The simplest unwrap specialisation is for a Mat object:

```
// Note: this is a conceptual simplification
template<typename eT>
struct unwrap< Mat<eT> >
    {
    const Mat<eT>& M;
    unwrap(const Mat<eT>& in) : M(in) { }
};
```

When operator=(...) is called on a Mat<eT> argument, unwrap only stores a reference to the matrix via the .M member, followed by operator=(...) accessing this result.

More complicated unwrapping behavior is performed for expressions. For instance, the unwrap struct specialised for a given type named as Op<T1, op_type> will call the static function op_type::apply(Mat<eT>&, Op<T1, op_type>&), which is expected to compute the result of the operation on the input T1 and store it in the given output matrix; for example, op_diagmat will generate a diagonal matrix from a given vector expression. The specific apply() function implemented for op_type will then also use the unwrap struct on the given T1 type, which in turn may result in follow-on calls to other apply() functions which use partially specialised unwrap structs. Additional optimisations via partial specialisations of the arguments of the apply() function may also be applied.

One optimisation that is unique to Bandicoot is its ability to fuse type conversions into operations. Consider the following example code:

```
fmat B = conv_to<fmat>::from(resize(A, 5, 6));
```

Assuming that A has type imat (i.e. integer matrix), the type of this expression is

```
mtOp<float, Op<Mat<int>, op_resize>, mtop_conv_to>
```

As with all other operations, unwrap will first call the function mtop_conv_to::apply() with B as the output matrix. However, instead of first evaluating the inner operation and then converting the result, Bandicoot will *fuse* the inner operation with the type conversion. This is accomplished at the top level by allowing each apply() function to output into a matrix of a different element type. So, in this example, the function op_resize::apply(Mat<float>&, Op<Mat<int>, op_resize>&), which has different output and input element types, will be called.

Subsequently, op_resize::apply(), when actually performing the resize operation (merely a copy of the elements), will call a "two-way" GPU kernel, where the input element type is allowed to differ from the output element type, and the conversion between input and output types is performed as part of the computation. The use of this two-way kernel thus prevents an additional copy of elements after the original resizing operation. In this example, fusing the conversion cuts the operation time in half.

Many operations in Bandicoot are implemented with support for fused conversions. The motivation for this is to reduce the number of separate GPU operations necessary to evaluate an expression. Whereas Armadillo is able to generate code specific to each individual expression, Bandicoot is not (currently) able to generate GPU code specific to each individual expression; therefore, reducing the number of GPU operations as much as possible is a priority.

Typically, after template meta-programming optimisations and fused conversions are applied to the expression in the manners described above, an individual operation's apply() function will call at least one GPU kernel using either the OpenCL or CUDA backend. This has conceptual similarity to Armadillo, whose "backend" includes direct calls to LAPACK and BLAS functions.

Since Bandicoot supports multiple backends, which can be configured at runtime, a singleton object exists as an interface layer between the apply() functions and the GPU. The object is called coot_rt_t and is obtained with coot_rt_t::get_rt(). coot_rt_t provides numerous static functions that take direct GPU memory as input. Thus, a typical apply() function implementation may contain calls such as, e.g., coot_rt_t::acquire_memory<eT>(n_elem) to allocate memory, or coot_rt_t::accu(X.get_dev_mem(), X.n_elem) to accumulate all the elements in a given object X.

The coot_rt_t object also serves as an implementational firewall between high-level Bandicoot objects and the GPUs. All CUDA-specific code is contained entirely within the coot_rt_t::get_rt().cuda_rt object, and all OpenCL-specific code, including calls to supporting libraries such as clBLAS, is contained entirely within the coot_rt_t::get_rt().cl_rt object. This separation makes it easy to enable or disable a backend at compile time, as well as to add an entirely new backend (as alluded to in Section 6).

This architectural overview provides the basics of the internal structure of Bandicoot. We note that it is a cursory look at the details of Bandicoot's implementation, and hence it is intended as a starting point for further exploration of the codebase.

8 Conclusion

In this report we provided an overview of the Bandicoot C++ GPU linear algebra library. Bandicoot aims to provide an API that is compatible with Armadillo's API, allowing users to take advantage of GPU-accelerated computation for their existing codebases without significant changes. Empirical evaluations show that Bandicoot can provide significant speedups over CPU-only computation, depending on the nature of the workload and the size of the data. Bandicoot can use either an OpenCL or CUDA backend.

Bandicoot's open-source nature enables extensions and customisation, and we hope that the community will find it useful. Contributions (especially towards goals in the given roadmap of Section 6) are more than welcome and can be made on the Bandicoot Gitlab code repository: https://gitlab.com/conradsnicta/bandicoot-code/. More details about the library, including frequently asked questions and comprehensive documentation of user-accessible functions can be found on the publicly accessible website at https://coot.sourceforge.io.

References

- [1] clBLAS. https://github.com/clMathLibraries/clBLAS. Accessed: 2023-07-17.
- [2] A. Alexandrescu. Modern C++ Design: Generic Programming and Design Patterns Applied. Addison-Wesley, 2001.
- [3] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LAPACK Users' Guide*. SIAM, 1999.
- [4] L. S. Blackford, A. Petitet, R. Pozo, K. Remington, R. C. Whaley, J. Demmel, J. Dongarra, I. Duff, S. Hammarling, G. Henry, et al. An updated set of basic linear algebra subprograms (BLAS). ACM Transactions on Mathematical Software, 28(2):135–151, 2002.
- [5] N. Burgess, J. Milanovic, N. Stephens, K. Monachopoulos, and D. Mansell. Bfloat16 processing for neural networks. In Symposium on Computer Arithmetic, pages 88–91, 2019.
- [6] D. C. Ciresan, U. Meier, J. Masci, L. M. Gambardella, and J. Schmidhuber. Flexible, high performance convolutional neural networks for image classification. In *International Joint Conference On Artificial Intelligence (IJCAI)*, pages 1237–1242, 2011.
- [7] J. O. Coplien. Curiously recurring template patterns. In C++ Gems, pages 135–144. 1996.
- [8] R. R. Curtin, M. Edel, R. G. Prabhu, S. Basak, Z. Lou, and C. Sanderson. The ensmallen library for flexible numerical optimization. *Journal of Machine Learning Research*, 22(1):7552–7557, 2021.
- [9] R. R. Curtin, M. Edel, O. Shrit, S. Agrawal, S. Basak, J. J. Balamuta, R. Birmingham, K. Dutt, D. Eddelbuettel, R. Garg, et al. mlpack 4: a fast, header-only C++ machine learning library. *Journal of Open Source Software*, 8(82):5026, 2023.
- [10] D. Eddelbuettel and R. François. Rcpp: Seamless R and C++ integration. Journal of Statistical Software, 40(8):1-18, 2011.
- [11] D. Eddelbuettel and C. Sanderson. RcppArmadillo: Accelerating R with high-performance C++ linear algebra. *Computational Statistics & Data Analysis*, 71:1054–1063, 2014.
- [12] A. Haidar, C. Cao, I. Yamazaki, J. Dongarra, M. Gates, P. Luszczek, and S. Tomov. Performance and Portability with OpenCL for Throughput-Oriented HPC Workloads Across Accelerators, Coprocessors, and Multicore Processors. In 5th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA 14), New Orleans, 2014.
- [13] A. Haidar, S. Tomov, J. Dongarra, and N. J. Higham. Harnessing GPU tensor cores for fast FP16 arithmetic to speed up mixed-precision iterative refinement solvers. In SC18: International Conference for High Performance Computing, Networking, Storage and Analysis, pages 603–613. IEEE, 2018.
- [14] T. Hamada, T. Narumi, R. Yokota, K. Yasuoka, K. Nitadori, and M. Taiji. 42 TFlops hierarchical N-body simulations on GPUs with applications in both astrophysics and turbulence. In *High Performance Computing Networking, Storage and Analysis*, pages 1–12, 2009.

- [15] C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, et al. Array programming with NumPy. *Nature*, 585(7825):357–362, 2020.
- [16] M. J. Harris, W. V. Baxter, T. Scheuermann, and A. Lastra. Simulation of cloud dynamics on graphics hardware. In ACM Conference on Graphics Hardware, pages 92–101, 2003.
- [17] I. Hubara, M. Courbariaux, D. Soudry, R. El-Yaniv, and Y. Bengio. Quantized neural networks: Training neural networks with low precision weights and activations. *The Journal of Machine Learning Research*, 18(1):6869–6898, 2017.
- [18] N. P. Jouppi, C. Young, N. Patil, D. Patterson, G. Agrawal, R. Bajwa, S. Bates, S. Bhatia, N. Boden, A. Borchers, R. Boyle, et al. In-datacenter performance analysis of a tensor processing unit. In *International Symposium on Computer Architecture*, pages 1–12, 2017.
- [19] A. Krizhevsky, I. Sutskever, and G. E. Hinton. ImageNet classification with deep convolutional neural networks. In F. Pereira, C. Burges, L. Bottou, and K. Weinberger, editors, *Advances in Neural Information Processing Systems*, volume 25, pages 1097–1105. Curran Associates, Inc., 2012.
- [20] M. Kroeker and Z. Xianyi. OpenBLAS: an optimized BLAS library, 2023. https://github.com/xianyi/OpenBLAS.
- [21] J. Nickolls, I. Buck, M. Garland, and K. Skadron. Scalable parallel programming with CUDA. Queue, 6(2):40-53, 2008.
- [22] C. Nugteren. CLBlast: A tuned OpenCL BLAS library. In Proceedings of the International Workshop on OpenCL, pages 1–10, 2018.
- [23] C. Psarras, H. Barthels, and P. Bientinesi. The linear algebra mapping problem: Current state of linear algebra languages and libraries. *ACM Transactions on Mathematical Software*, 48(3), 2022.
- [24] R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2021.
- [25] D. Ravì, C. Wong, F. Deligianni, M. Berthelot, J. Andreu-Perez, B. Lo, and G.-Z. Yang. Deep learning for health informatics. *IEEE Journal of Biomedical and Health Informatics*, 21(1):4–21, 2016.
- [26] J. Rumengan, T. Y. Zhuo, and C. Sanderson. PyArmadillo: a streamlined linear algebra library for Python. Journal of Open Source Software, 66(6), 2021.
- [27] C. Sanderson and R. Curtin. Armadillo: C++ template metaprogramming for compile-time optimization of linear algebra. In *Platform for Advanced Scientific Computing (PASC) Conference, Switzerland*, 2017.
- [28] C. Sanderson and R. Curtin. A user-friendly hybrid sparse matrix class in C++. In *Lecture Notes in Computer Science (LNCS)*, Vol. 10931, pages 422–430, 2018.
- [29] C. Sanderson and R. Curtin. An adaptive solver for systems of linear equations. In International Conference on Signal Processing and Communication Systems (ICSPCS), pages 1–6. IEEE, 2020.
- [30] C. Sanderson and R. R. Curtin. Armadillo: a template-based C++ library for linear algebra. *Journal of Open Source Software*, 1(2):26, 2016.
- [31] C. Sanderson and R. R. Curtin. Practical sparse matrices in C++ with hybrid storage and template-based expression optimisation. *Mathematical and Computational Applications*, 24(3), 2019.
- [32] J. E. Stone, D. Gohara, and G. Shi. OpenCL: A parallel programming standard for heterogeneous computing systems. *Computing in Science & Engineering*, 12(3):66, 2010.
- [33] J. E. Stone, K. L. Vandivort, and K. Schulten. GPU-accelerated molecular visualization on petascale supercomputing platforms. In Proceedings of the 8th International Workshop on Ultrascale Visualization, pages 1–8, 2013.
- [34] G. Tagliavini, S. Mach, D. Rossi, A. Marongiu, and L. Benini. A transprecision floating-point platform for ultra-low power computing. In *Design, Automation & Test in Europe Conference & Exhibition*, pages 1051–1056, 2018.
- [35] The MathWorks Inc. MATLAB version 9.13.0 (r2022b), 2022.
- [36] S. Tomov, J. Dongarra, and M. Baboulin. Towards dense linear algebra for hybrid GPU accelerated manycore systems. *Parallel Computing*, 36(5-6):232–240, June 2010.
- [37] R. Urlus. CARMA: bidirectional conversions between NumPy and Armadillo, 2023. https://github.com/RUrlus/carma.
- [38] J. Vamathevan, D. Clark, P. Czodrowski, I. Dunham, E. Ferran, G. Lee, B. Li, A. Madabhushi, P. Shah, M. Spitzer, and S. Zhao. Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery*, 18(6):463–477, 2019.
- [39] G. Van Rossum and F. L. Drake. Python 3 Reference Manual. CreateSpace, Scotts Valley, CA, 2009.
- [40] D. Vandevoorde, N. Josuttis, and D. Gregor. C++ Templates: The Complete Guide. Addison-Wesley, 2nd edition, 2017.
- [41] Q. Wang, X. Zhang, Y. Zhang, and Q. Yi. AUGEM: automatically generate high performance dense linear algebra kernels on x86 CPUs. In *International Conference on High Performance Computing, Networking, Storage and Analysis*, pages 1–12, 2013.

- [42] D. A. Watt. Programming Language Design Concepts. Wiley, 2006.
- [43] N. Whitehead and A. Fit-Florea. Precision & performance: Floating point and IEEE 754 compliance for NVIDIA GPUs. White paper, NVIDIA Corp, 2011.
- [44] S. Wolfram. The MATHEMATICA® book, Version 4. Cambridge University Press, 1999.