GPU acceleration and performance of the particle-beam-dynamics code Elegant

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(Dated: October 23, 2017)

Elegant is an accelerator physics and particle-beam dynamics code widely used for modeling and design of a variety of high-energy particle accelerators and accelerator-based systems. In this paper we discuss a recently developed version of the code that can take advantage of CUDA-enabled graphics processing units (GPUs) to achieve significantly improved performance for a large class of simulations that are important in practice. The GPU version is largely defined by a framework that simplifies implementations of the fundamental kernel types that are used by Elegant: particle operations, reductions, particle loss, histograms, array convolutions and random number generation. Accelerated performance on the Titan Cray XK-7 supercomputer is approximately 6-10 times better with the GPU than all the CPU cores associated with the same node count. In addition to performance, the maintainability of the GPU-accelerated version of the code was considered a key design objective. Accuracy with respect to the CPU implementation is also a core consideration. Four different methods are used to ensure that the accelerated code faithfully reproduces the CPU results.

PACS numbers: 07.05.Tp
Keywords: Particle-accelerator simulation, GPU acceleration

I. INTRODUCTION

Elegant is an open-source, multi-platform code used for design, simulation, and optimization of a wide variety of high-energy particle accelerators and accelerator-based systems, including free-electron laser (FEL) driver linear accelerators (“linacs”), energy recovery linacs (ERLs), and storage rings [1–3]. The parallel version, Pelegant [4, 5], uses MPI for parallelization and shares all source code with the serial version. In a number of settings that include accelerator design optimization, Elegant is used as the tracking component of fully scripted simulations. Elegant is fundamentally a lumped-element particle accelerator tracking code utilizing 6D phase space, and is written mostly in C. A variety of numerical techniques are used for particle propagation, including transport matrices (up to third order), symplectic integration, and adaptive numerical integration. Collective effects are also available, including space charge, coherent synchrotron radiation (CSR), wakefields, and resonant impedances.

In recent years, general purpose computing on graphics processing units (GPUs) has attracted significant interest from the scientific computing community because these devices offer unparalleled performance at low cost and at high performance per watt. Unlike general purpose processors, which devote significant on-chip resources to command and control, pre-fetching, caching, instruction-level parallelism, and instruction cache parallelism, GPUs devote a much larger amount of silicon to maximizing memory bandwidth and raw floating-point computation power. This comes at the expense of shifting the burden towards developers and away from on-chip command and control logic, and additionally requires relatively large problems with high levels of parallelism.

One of the challenges of accelerating a code such as Elegant is the sheer number and variety of kernels required to accelerate common use cases. Without reasonable accelerated coverage of the code the benefits of using the GPU may be severely reduced. This reduction occurs both from the time required to transfer the particles between the device and host memory when entering a stage of a simulation that cannot be performed on the GPU, as well as due to the fundamental limit in the form of Amdahl’s argument [6]. Amdahl’s argument states that if a runtime fraction, \( F \), of a code is accelerated (threaded) with \( n \) concurrent threads, then the maximum speedup is \( (F + (1 - F)/n)^{-1} \). Thus, the speedup from an accelerated portion of a code that covers a runtime fraction of 50% with infinite threads is only a factor of two, a rather modest

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acceleration. It has been our intent to accelerate a sufficient number of elements such that most beamline computations contain a significantly large runtime fraction of accelerated code. In addition, we intend the framework through which this acceleration is implemented to be extensible such that new beamline elements may be added as necessary.

The paper is organized as follows. Section II describes the acceleration framework. The vast majority of accelerated elements use a C++ templated class framework to greatly simplify implementation of per-particle operations. Depending on the element, the accelerated code may also use the framework routines to form histograms, perform array convolutions, evaluate reduction operations, and account for particle losses. In Section III, the performance of the accelerated functions is presented. We compare a NVIDIA Tesla K20c GPU with a single-core of a Intel Core i7-3770K CPU. This is inherently an unfair comparison as a workstation typically contains 4 to 16 cores. However, the speedup factors are not the focus of this section, rather we intend it as a discussion of the challenges of accelerating various functions and the scaling of the accelerated code with the number of particles. A fair comparison of full application speed-up is presented in Section IV for a realistic particle-accelerator simulation use case. Our implementation maintains Elegant’s existing MPI infrastructure to support CUDA-MPI hybrid parallelism. In this section we compare performance of the application on the Titan Cray XK-7 on both the CPUs and GPUs. Finally, in Section V we describe the multiple verification techniques used to ensure the GPU-accelerated code faithfully reproduces the original CPU-only implementation results.

II. COMPUTATIONAL INFRASTRUCTURE

The accelerated version of Elegant is programmed with the CUDA programming model; CUDA is NVIDIA’s programming model for GPU computing [7, 8]. In general, the organization of the accelerated Elegant code attempts to mirror the file organization of the CPU code as much as practical. For example, the code for the csbend, csr_csbend and drift_csbend elements [9] is located in the file csbend.c and the accelerated kernels used by these elements are located in the file gpu_csbend.cu (the file suffixes .c and .cu are used for files containing CUDA code).

Generally speaking, a particle tracking simulation with Elegant consists of the particle beam traversing a succession of so-called elements, each element representing a magnetic optics component, a physical effect, or a combination of the two [9]. Currently, not all elements have GPU-accelerated implementations; we have focused our efforts on the most commonly used elements. However, any beamline will run with the GPU-accelerated version of Elegant. Silent support is provided where the particles are transferred between the GPU and CPU if a beamline contains an element kernel which has only a CPU implementation.

We next describe aspects the GPU framework used to simplify the process of accelerating elements. There are three major barriers to acceleration: (1) the CPU code uses an array-of-structs data format whereas the GPU code must use a struct-of-arrays data format which permits coalesced memory transactions, (2) elements with collective effects require reduction, convolution and histogram operations, and (3) a sort operation is required in elements where particles are lost.

A. Template meta-programming

Compile-time polymorphism allows abstraction layers that can hide the more close-to-the-metal implementation details from application developers. We exploit compile-time polymorphism through template meta-programming with the following aims:

- To create extendible kernels that reduce both code maintenance and programming errors.
- To provide abstract interfaces that hide the CUDA-specific data-parallel implementation details.
- To ease the development workflow by avoiding CUDA-related boilerplate such as thread and block configurations, thread-index computations, and conversion between array-of-structures and structure-of-arrays data formats.

Central to this model is the GPU particle accessor class that behaves as though it were a CPU-style array of structs. Given such an accessor, a developer need only define a functor that acts on the individual particles by creating a basic class and overloading the proper operator. Any non-particle data needed by
the functor, such as physical constants and auxiliary arrays, is placed in the class member variables. The developer then passes the class to a template GPU driver function and thus replaces a complicated for-loop over particles with a small functor class and a call to a GPU driver. Minimal explicit CUDA code is written; instead, a developer writes per-particle update classes that encapsulate the data needed and algorithm to perform each particle update step.

Listing 1: The Elegant CPU exactDrift function.

```c
#define sqr(x) (x*x)

void exactDrift(double **part, long np, double length)
{
    long i;
    double *coord;
    for(i=0; i<np; i++) {
        coord = part[i];
        coord[0] += coord[1]*length;
        coord[2] += coord[3]*length;
        coord[4] += length*sqrt(1+sqr(coord[1])+sqr(coord[3]));
    }
}
```

Listing 2: The Elegant GPU exactDrift function.

```c
class gpuExactDrift{
public:
    gpuExactDrift(double len) : length(len) {}
    __device__ void inline operator()(gpuParticleAccessor& coord){
        coord[0] += coord[1]*length;
        coord[2] += coord[3]*length;
        coord[4] += length*sqrt(1+coord[1]*coord[1]+coord[3]*coord[3]);
    }
    double length;
};

void gpu_exactDrift(long np, double length){
    gpuDriver(np, gpuExactDrift(length));
}
```

For illustration, we consider the Elegant exactDrift kernel which has a CPU implementation as given in Code[1]. Note the GPU implementation, Code[2] only contains a single CUDA keyword, the __device__ keyword which instructs the compiler to compile the function operator() for the GPU. Even though the particle data is stored in struct-of-arrays format on the GPU, it is accessed through the GPU particle-accessor-class bracket operator just like the corresponding CPU data. The kernel as written is almost identical to that on the CPU although under the hood vastly different data structures are used. The GPU particle accessor class reads particle data from the struct-of-arrays format into the thread registers only if they are used. Upon destruction of the class (which is associated with a specific particle) particle data associated only with the indices used in the kernel are written. This workflow leads to nearly optimal global memory access patterns as the particle data can at most have a single read/write operation per kernel where the results of intermediate operations are stored within thread registers.

B. Histogram operations

Many of the beamline elements in Elegant that incorporate collective effects utilize a histogram-based approach. Histogram calculations on a GPU are challenging. In a straightforward GPU implementation, threads increment histogram bins that are present in shared memory. However, as multiple threads attempt to increment the same location in memory at the same time, this leads to thread contention issues that may cause performance degradation (if thread-safe atomic operations are used) or race conditions (otherwise).
Atomic operations to shared memory are not efficient, and the computational cost of such atomics roughly scales with the level of thread contention. For histogram kernels, the level of thread contention is largely determined by the number of bins and the resulting distribution (for example, a distribution that is localized to a few bins will create large thread contention). In order to minimize the computational cost of these atomic operations, the GPU Elegant histogram algorithm creates sub-histograms which reduce the thread contention but require an additional operation to subsequently combine the sub-histograms. This algorithm is illustrated pictorially in Fig. 1. The GPU histogram kernel is optimized to fit as many sub-histograms as possible per thread block while maintaining high block occupancy. The number of thread blocks is limited by the optimal block occupancy for a given device multiplied by the number of multiprocessors.

C. Convolution operations

Another potential barrier to achieving a good speedup on full beamline computations is array convolution operations (such as those present in wakefield elements). A serial implementation of this algorithm scales as $O(N_1 \times N_2)$, where $N_1$ and $N_2$ are the sizes of the arrays in the convolution. For typical operations, where arrays are histograms, the array size is several hundred to a few thousand. Given the convolution’s $O(N^2)$ scaling, we cannot afford to rely on the serial CPU calculation without negatively impacting performance of the simulation as a whole, even with millions of particles.

Our GPU kernel achieves good acceleration by buffering sub-sections of each array in shared memory while performing $O$(buffer size) computations. This operation computes part of the final result for a given array index. As the convolution is a linear operation, each thread block then applies an atomic addition operation to produce the final result of the convolution.

D. Reduction operations with asynchronous execution

Reductions of particle quantities to determine statistical beam properties are present in many Elegant beamline elements. We template standard reduction algorithms over the reduction operation (e.g. sum, minimum, maximum, etc.). In these algorithms thread blocks concurrently apply the reduction operation to subsections of the data array and place the result in global memory. The last block to finish the sub-reduction then reduces the results from the previous step.

Certain functions (i.e. accumulate_beam_sums and compute_centroids) compute the beam properties...
and may be called from multiple elements or the main Elegant do_tracking loop. These functions reduce quantities from separate data arrays, for example during computations of the mean and standard deviation of beam’s position and/or transverse velocity. By launching these functions asynchronously on separate CUDA streams we can take advantage of concurrency during the last reduction operation and the transfer of the reduction result(s), in addition to moving towards achieving the maximum device memory bandwidth during the concurrent reductions. Asynchronous reductions are 40% faster than their synchronous counterparts with data arrays of size one million on a NVIDIA Tesla K20c.

Listing 3: Part of the Elegant CPU compute_centroids code

```c
for (i_part=0; i_part<n_part; i_part++) {
    part = coordinates[i_part];
    for (i_coord=0; i_coord<6; i_coord++)
        #ifndef USE_KAHAN
            sum[i_coord] += part[i_coord];
        #else
            sum[i_coord] = KahanPlus(sum[i_coord], part[i_coord], &error[i_coord]);
        #endif
}
```

Listing 4: Part of the Elegant GPU compute_centroids code

```c
for (i_coord=0; i_coord<6; i_coord++)
    #ifndef USE_KAHAN
        gpuReduceAddAsync(d_particles+particlePitch*i_coord, n_part, &sum[i_coord]);
    #else
        gpuKahanAsync(d_particles+particlePitch*i_coord, &sum[i_coord], &error[i_coord], n_part);
    #endif
finishReductionStreams();
```

Our framework for these asynchronous reductions only requires the user to call the function finishReductionStreams before the result of the reduction is used. For illustration, consider the CPU code shown in Code 3 and the GPU code in Code 4. Aside from the different function calls, and the removal of the loop over particles which is placed inside the GPU reduction calls, the only other difference between these two sections of code is the addition of the finishReductionStreams call to the GPU code. The management of the CUDA streams, and allocation and use of pinned memory for the asynchronous memory transfer between the device and the host is generalized within the GPU Elegant computational framework.

E. Particle losses and sorting

Many beamline elements allow for particle losses (for example, a particle may collide with an aperture edge). When a particle is lost on the CPU, it is swapped with the particle at the end of the particle array and the particle count is decremented. This algorithm is not amenable to the GPU which performs concurrent particle-update operations. A straightforward GPU algorithm is to fill an array with the particle index plus the number of particles if the particle is lost, and just the particle index otherwise, and then sort the particle array by this key. However, this too is somewhat inefficient as sort algorithms are not amenable to the concurrency of the GPU. One can reasonably expect that the fraction of lost particles for any given element is small (<10%), otherwise the particular beamline configuration would not be of great interest. We use this property to create a more efficient algorithm than the straightforward sort-by-key algorithm. Relative to the sort-by-key algorithm, this optimized algorithm is $4 \times$ faster with 0.5% losses, $3 \times$ faster with 5% losses, $2.5 \times$ faster with 10% losses and roughly equivalent with 50% losses (benchmarking on an NVIDIA Tesla K20c).

Our particle-loss algorithm is illustrated in Fig. 2. A computational kernel must do two things to incorporate particle losses: it should return an unsigned integer (zero if the particle is lost and unity otherwise). It should also fill a particle-sort index with the particle index plus the number of particles if the particle
Figure 2: A pictorial representation of the GPU Elegant particle-loss sorting algorithm for a case with 20 total and four lost particles.

is lost, and the particle index otherwise. The particle-loss algorithm does a sum reduction over the return
value. If the result is equal to the number of particles, no particles are lost and the remainder of the loss
computation is skipped. If particles are lost, the end of particle array (size of the number of lost particles)
is sorted, and then sort index is converted to unity if the particle is lost, and zero otherwise. An inclusive
scan is performed which creates a particle linear index array. When subsequent elements of this array are
different, a particle is lost and the value of the second element, $i$, indicates that this is the $i^{th}$ particle lost.
This information is used to produce a contiguous particle loss map which contains indexing information on
the lost particles. A final step uses the particle loss map to swap particles to the end of the particle array,
and the particle count is decremented by number of lost particles. This final step is launched with a different
CUDA thread block decomposition that accounts for the sparsity of operations. Although the final two
steps of this algorithm contain uncoalesced reads and writes, it is still more efficient than a straightforward
sort-by-key algorithm given the sparsity of operations.

III. PERFORMANCE OF ACCELERATED ELEMENTS

Table I lists typical timings and speedup factors (columns 3-5) of accelerated Elegant functions (column
1) and the associated beamline element name(s) as used in the Elegant lattice input file (column 2) [9]. A
portion of the accelerated functions are not associated with one particular element, but rather are called
from Elegant’s main do_tracking loop. It is a requirement that these functions are accelerated in order
to avoid a transfer of the particles between the host and the device and thus to avoid an associated slow-
down from effects related to Amdahl’s argument [6]. For example, consider the accumulate_beam_sums
function, which computes properties of the beam distribution through a series of reductions. Depending on
the input parameters, these properties may be computed after each element in the beam line which would
be detrimental to an accelerated computation if this function were not accelerated.

Other beamline elements listed in Tab. I are the HKICK and VKICK, a horizontal and vertical steering
dipole elements implemented as a matrix, up to 2nd order; KICKER, a combined horizontal-vertical
steering magnet implemented as a matrix, up to 2nd order; SCRAPER, a collimating element that sticks a
limiter into one side of the beam; CENTER, an element that centers the beam; RCOL and ECOL, rectan-
gular and elliptical collimator elements; EDRIFT, an exact drift element; KQUAD, KSEXT, KOCT, and
KQUSE, a canonical kick quadrupole, sextupole, octupole, elements and an element combining quadrupole
and sextupole fields, using either 2nd or 4th order symplectic integration; QUAD and DRIFT, quadrupole
| function | elements | GPU time | CPU time | Accel Hist | Conv | Redu | Loss | Rand |
|----------|----------|----------|----------|------------|------|------|------|------|
| accumulate_beam_sums | main loop | 24.8 | 696 | 28.1 | X |
| addCorrectorRadiationKick | hkic, vkic, kicker | 0.066 | 3.97 | 60.4 | X | X |
| beam_scraper | scraper | 362 | 5249 | 14.5 | X | X |
| center_beam | center | 2.13 | 94.8 | 44.5 | X |
| elliptical_collimator | ecol | 2.63 | 78.9 | 30.0 | X | X |
| exactDrift | edrift | 0.835 | 17.8 | 21.3 |
| limit_amplitudes | main loop | 0.022 | 1.14 | 50.9 | X | X |
| multipole_tracking2 | koc, kquad, kquse, kext | 3.33 | 148 | 44.3 | X | X | X |
| rectangular_collimator | rcol | 1.23 | 59.3 | 48.1 | X | X |
| simple_rf_cavity | rfca | 3.51 | 164 | 46.6 | X |
| track_particles (M1) | drift, quad, sole | 1.98 | 69.9 | 35.3 |
| track_particles (M2) | drift, quad, sole | 0.087 | 13.3 | 152 |
| track_particles (M3) | quad, sole | 33.2 | 3450 | 104 |
| track_through_csbend | csbend | 53.4 | 1630 | 30.5 | X | X | X |
| track_through_csbendCSR | csrscsbend | 406 | 22k | 53.7 | X | X | X |
| track_through_driftCSR | csrdrift | 5.25 | 125 | 23.7 | X |
| track_through_lscdrift | lscdrift | 3.28 | 145 | 44.1 | X |
| track_through_matter | matter | 162 | 3716 | 23.0 | X | X |
| track_through_rfcw | rfcw | 181 | 7159 | 39.6 | X | X | X |
| track_through_trwake | trwake | 2.36 | 37.1 | 15.7 | X | X | X |
| track_through_wake | wake | 1.33 | 25.6 | 19.2 | X | X | X |

Table I: Elegant kernel performance with 3.2 million particles on a NVIDIA K20c GPU (CUDA 5.5) and Intel Core i7-3770K CPU, both using double precision. The element column indicates the element name(s) in beamline lattice input file name that will trigger a call of the kernel. The M# suffix on the track_particles functions indicates the order of the matrix. Times are reported in milliseconds. The last five columns list components of the framework used within each function: histograms, array convolutions, reductions, particle losses and random number generation.

Best performance, relative to the CPU code, is achieved with a large number of particles (hundreds of thousands and up). The computational code of most kernels scales as $O(N)$ where $N$ is the number of particles. When $N$ is large, other constant-scaling components (e.g. kernel launch overhead and array...
convolutions) are amortized over the large $O(N)$ number of computations and have little impact on the GPU performance. Fig. 3 plots the speed-up factors and efficiency scaling relative to the number of particles in the computations for selected accelerated functions. In general, good speed-up factors of 15-150x are obtained for these functions over a broad range of particles (100k-3.2M). The efficiency is measured relative to the case with 100k particles assuming constant-in-N scaling. As the number of particles is increased, the efficiency curves decrease in slope, indicating the increased amortization of the constant scaling components begins to have little effect. The `multipole_tracking2` and `track_particles_M2` functions do not use either histograms or reductions thus have a very small slope compared to the other functions that either use reductions or incorporate collective effects through histograms and convolutions.
Next we describe performance and scaling studies of the GPU-accelerated Elegant relative to the CPU-only version of the code. These studies are performed on the 18,688-node, hybrid-architecture, Titan Cray XK-7 supercomputer at the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory. We use the Linac Coherent Light Source (LCLS) [10] beam delivery system [11, 12] as our test lattice, such that the studies here represent end-to-end application performance in a realistic setting, as opposed to the kernel and function-specific descriptions from previous sections. In order to have a more balanced comparison of the GPU to CPU performance, the performance of two 8-core AMD Opteron CPUs is compared to the performance of a single NVIDIA Tesla K20x (as there are 16 CPU cores and a single GPU per Titan node). Both the CPU-only and GPU-enabled versions of the code are compiled with SDDS parallel (MPI) I/O enabled.

Results of the weak scaling studies (where the number of cores is increased in proportion to the problem size) are shown in Fig. 4. One can see that most beamline elements exhibit nearly perfect scaling over the explored range of the problem sizes (up to one billion macroparticles). The exception is the RFCW kernel, which is limited by the parallel scaling of its component transverse-wake kernel. One observation from these weak scaling studies is that, for the full LCLS test case, and relative to a job with 8 million particles, it takes the GPU-accelerated code only two and a half times longer to run a $256 \times$ bigger job to completion, a very good scaling performance in this important-in-practice range of problem sizes. In particular, the full LCLS beamline simulation was done within 18.5 minutes when using one billion ($10^9$) particles, which is comparable to the number of actual electrons in the beam.

Figure 5 shows the results of increasing the number of particles while running on only a single Titan node. The RFCW kernel is plotted independently as it dominates the run time, and all other elements are grouped as a single line (labeled “etc.”). The CPU-only (16 cores) and GPU-accelerated versions of the code are run for small-to-moderate particle counts. The scaling is linear as expected for ideal scaling and the GPU-accelerated version consistently outperforms the CPU-only version in terms of time to solution for a start-to-end simulation. For example, with 8 million particles the CPU-only version requires 64 minutes, whereas the GPU-accelerated version runs in 7 minutes, a speed-up of nearly a factor of 10.

Next, we present strong scaling studies on the CPUs (increasing the number of cores for a fixed problem size), once again using the LCLS driver linac’s lattice as a test case. Figures 6 and 7 show the scaling of total time spent in computationally expensive RFCW and in the rest of the elements, for 8M-particle runs (Fig. 6) and 128M-particle runs (Fig. 7). For comparison, dashed lines represent ideal scaling. The purpose of these CPU scaling studies is to enable comparison to the GPU results of Fig. 4 as described in the next paragraph. As can be seen from Figs. 6 and 7, strong scaling is nearly perfect when number of nodes is small, but there is a scaling bottleneck at approximately 4000 cores for this case. This scaling saturation for the CPU version is an indication that CPU-only simulations with one billion particles are difficult, and may not be practical in some cases. In this sense the accelerated Elegant can enable access to higher fidelity simulations that were previously unachievable.

As regards comparing the performance of the GPU-enabled Elegant to that of the parallel CPU-only
Figure 5: Scaling with the number of simulation particles for small to moderate particle counts on a single node of Titan for equivalent GPU (solid lines) and CPU (16 cores, dashed lines) runs. The RFCW kernel is plotted independently as it dominates the run time, all other elements are included in the etc. lines. Timings show I/O takes an order of magnitude less time than the plotted lines. The LCLS beam delivery system’s lattice is used as a test case.

Figure 6: Strong scaling results for 8 million particles with the CPU version of Elegant, with dashed lines representing ideal scaling. The LCLS driver linac’s lattice is used as a test case.

Version, one useful metric may be to compare the scaling of the number of cores needed for the two versions of the code to achieve approximately the same time to solution, as the problem size varies. For good performance by the accelerated code, a sufficiently large number of particles is required on the GPU. Thus, this metric is most relevant when large particle counts are necessary. We found that, for a 1M-particle simulation of the LCLS lattice, a simulation on 1 GPU takes the same time as a simulation on 16 CPUs, and an 8M-particle run on a single GPU takes roughly the same time as a 100-CPU run. Timing on Titan with 128M particles resulted in 16 K20 Kepler GPUs being equivalent to 1024 16-core AMD Opteron CPUs (again, in terms of time to solution). Thus, one could argue that, by this metric, a GPU cluster would be a more cost-efficient hardware choice for this type of simulation.

V. CODE VERIFICATION

Testing and verification of the CUDA implementation to ensure accuracy of the results has been an essential part of the work reported here. This is a complicated task, given that the potential Elegant use cases are widely varied, and full coverage of all cases is difficult. We describe four methods that are used to verify the GPU code: memory synchronization, unit tests, run-time CPU/GPU particle phase space coordinate comparisons after each element, and end-to-end distribution properties comparisons. We recommend that users of GPU Elegant employ these methods as appropriate to test new beamline setups with a modest number of particles before performing production runs.
A. Memory synchronization

A general consideration of any GPU/CPU implementation is synchronization and access limitations of data between the host and device memory. A logic error where both the CPU and GPU access and modify the particle data without synchronization would clearly have a detrimental effect on the simulation accuracy. In the worst case scenario, this logic error can lead to a situation where the application runs and produces a reasonable-looking but incorrect result. One mechanism for handling this problem is to accept that a run-time segmentation fault is better than producing the wrong result. Thus, when the particles are present on the device memory, the host particle array pointer is nullified. If any host operation dereferences the particle array pointer a segmentation fault is triggered. This provides the user with an indication that the result can not be trusted, and gives the developer detailed information on the location of the logic error.

B. Unit tests

Unit tests are designed to test a specific component of the code, have well-defined input and output, and run quickly. Ideally, unit tests should have full code coverage in the sense that if a mistake is introduced anywhere in the code during development, one or a set of the unit test should fail. It is also desirable for the unit test to have a hierarchical order such that the first unit test to fail should immediately point to the underlying problem that may cause the subsequent tests to fail. Our tests do not live up to this idealized standard, but instead are limited in scope to testing the GPU infrastructure described in Sec. II. These tests initialize a particle distribution, or general arrays of data and run the reduction, histogram, convolution, and particle-loss algorithms on both the CPU and GPU. A test is considered a failure if either the resulting output does not match or the GPU fails to outperform a single CPU core.

C. Run-time host/device element comparisons

In order to verify the code with a wide variety of beamline element use cases, runtime verification of the GPU routines can be enabled via a preprocessor flag (GPU_VERIFY=1) during compilation. Compilation with GPU verification is not intended for production runs, but rather it is to be used as an aid in development and as an option for the user to check the code.

With respect to programming details, the GPU function calls are embedded within the equivalent CPU routines, such that the GPU version is used when Elegant is compiled with GPU acceleration. When verification is enabled, timings are computed with the CUDA event timers where, in addition to the CUDA version of the routine, the CPU routine is also recursively called and timed. An example of the GPU and verification hooks is shown in Code 5. The result from both routines is then copied to the host memory and compared for accuracy. Warnings are printed if the resulting particle phase-space coordinates do not agree.
within a tolerance of $10^{-10}$. At the end of the Elegant run, aggregate timing statistics are displayed for each accelerated routine called.

Listing 5: GPU and verification callback hooks within the CPU `exactDrift` code.

```c
#ifdef HAVE_GPU
    if (getElementOnGpu()) {
        startGpuTimer();
        gpu_exactDrift(np, length);
    }
#endif

#ifdef GPU_VERIFY
    startCpuTimer();
    exactDrift(part, np, length);
    compareGpuCpu(np, "exactDrift");
#endif

return;
#endif
```

This run-time testing has several advantages and disadvantages relative to unit tests. Unit tests can be quickly run just after compilation and provide simple test cases for debugging, both advantages over the run-time testing. However, run-time testing allows for full coverage of possible use cases and can be more easily integrated within the existing Elegant regression testing system than unit tests. The implementation of the run-time testing is vastly more straightforward than unit testing, as all the element information is already present and does not need to be configured by the testing framework. One drawback to run-time tests is that some algorithms can generate significant false positives. For example, consider an algorithm used to center the beam at location $x_c$ via the operation $x_i = x_i - x_c$ for all particles, $i$, at locations $x_i$. For a large number of particles, some fraction of particles may already be almost at the centering location, $x_c$, and thus there will be a near-exact cancellation resulting in most of the floating-point significant digits to be filled with round-off values. This round-off error almost certainly does not agree during comparisons between the CPU and the GPU, and can produce spurious errors of order unity.

D. End-to-end verification

The final quality assurance test that we employ focuses on statistical properties of the particle beam distribution in start-to-end runs. For statistical tests to be meaningful, they should be applied either to the whole beam or to beam slices that constitute a large sample in terms of the macroparticle count (say, 50,000 particles or more). These tests are essential for kernels that use random numbers, as well as in simulation settings where accumulation of round-off is a concern.

There are a number of elements in Elegant that employ a random number generator (RNG) for simulation of one or more physical effects. For example, a Coulomb-scattering and energy-absorbing element `MATTER` that simulates material in the beam path uses an RNG for computing the probability of scattering for each particle and the scattering angle, and the `CSRCSBEND` and `CSBEND` elements’ incoherent synchrotron radiation model uses a random number to determine the number of photons emitted and then requires an additional random number for each emitted photon. For the GPU version of the code, we implement a random number generation framework which is based on the CUDA cuRAND library. Just as in the host CPU code, the random-number sequence generated in the GPU code is reproducible if the same seed is used in a subsequent run. However, the random number sequences themselves are not the same in the CPU and GPU code, which automatically causes particle-by-particle comparison tests to fail.

Statistical tests are facilitated by the simulation output data being in the SDDS format, so that one can make use of of several tools from the SDDS Toolkit for extracting, sorting, analyzing and visualizing the particle data. In addition, statistical tests can employ a variety of Elegant’s built-in capabilities for generating runtime beam phase-space distribution statistics.
VI. SUMMARY AND CONCLUSION

We developed a GPU-accelerated version of particle accelerator code Elegant. The new version demonstrates a greatly improved performance on hybrid platforms for computationally intensive simulations of the kind that frequently arises in the course of design and optimization of particle accelerator-based systems. A prominent feature of the computational infrastructure of the GPU-enabled Elegant is a C++ templated class framework. This framework facilitates the creation of extensible kernels and provides abstract interfaces that simplify the implementation of particle operations (e.g., by hiding the conversion between the array-of-structures and structure-of-arrays formats of the particle data).

We implemented optimized kernels for the reductions, convolution, histogram computation, and other operations that are at the core of modeling collective effects in Elegant and whose suboptimal performance can be the main limiting factor to the overall performance of the code. Our optimized histogram kernel creates sub-histograms in shared memory in such a way as to reduce the thread contention while maintaining high block occupancy, combining the sub-histograms from different blocks to produce the final histogram. The convolution computation kernel (required, e.g., in the computation of wakefield effects) relies on buffering sub-sections of each array in shared memory for computing part of the result for a given array index, with each thread block applying an atomic addition to produce the final result for the convolution. Reduction operations are central to the computation of the statistical properties of particle distributions. In our implementation, standard reduction algorithms are templated over the reduction operation. Our framework allows for launching asynchronously on separate CUDA streams of functions that reduce quantities from separate data arrays. We find asynchronous reductions to be about 40% faster than their synchronous counterparts on Tesla K20c GPUs with 1M-particle distributions. Finally, the modeling of beam particle loss in traversing the beamline necessitated a complete re-working for the GPU version of the CPU-based algorithm so as to accommodate concurrent particle-update operations. A specialized particle loss sorting algorithm described in this paper was optimized for the physically relevant case where the fraction of lost particles is small, and in our tests it was significantly faster than a straightforward sort-by-key algorithm, the ratio depending on the fraction of particles lost (e.g., 4× faster for the case of 0.5% particle loss).

The performance benefit from porting to the GPUs is, of course, only realized when the number of simulation particles is sufficiently large. In the case of GPU-accelerated Elegant, we find that the cost of kernel launches and constant-scaling components such as convolutions is well amortized for a particle count that is element-dependent, but generally in the range of 100k to about 3.2M. This range is well below the number of particles used in large-scale simulations with Elegant, and it should be kept in mind when allocating resources to a simulation with the GPU version of the code. Regarding the scaling behavior, in tests with up to one billion particles we see essentially ideal weak scaling for all elements except RFCW (which exhibited good scaling nonetheless, running only 2.5× slower for a 256× larger problem in what currently is a very common range of problem sizes).

From the perspective of the end user, of primary interest is not so much the speed-up data for individual kernels, but the performance of the code in start-to-end (S2E) simulations in realistic settings. We compared the performance of the GPU-enabled and CPU-only versions of Elegant by running S2E simulations of the LCLS beam delivery linac (fairly typical of an important class of accelerator systems) on Titan Cray XK-7 at ORNL. Focusing on the scaling of the two versions of the code in terms of the number of cores needed to achieve the same time to solution in S2E simulations, we found the GPU version to increasingly outperform the CPU-only version as the problem size grows larger: For example, performing a 1M-particle simulation of the LCLS lattice on Titan, a run on 1 K20 Kepler GPU takes as long as a run on 16 16-core AMD Opteron CPUs, while a 128M-particle run requires either 16 GPUs or 1024 CPUs to achieve the same time to solution.

In response to the evolving needs of the accelerator physics research community, new simulation capabilities are continually added to Elegant over time. To facilitate the maintainability and continued development of the code, the GPU version’s source code is organized in such a way that it can be easily related to the corresponding code in the CPU implementation. For quality assurance purposes we developed a testing and verification infrastructure that includes unit tests, runtime GPU/CPU phase space coordinate comparisons after individual elements, comparisons of the particle distribution statistical properties in end-to-end runs, and a mechanism for handling the memory synchronization problems. We made a heavy use of this testing and verification framework in the process of developing the GPU version of the code, and we expect it to be of value as new capabilities are added to Elegant in the future.
VII. ACKNOWLEDGEMENTS

This work was supported by the US DOE Office of Science, Office of Basic Energy Sciences under grant number DE-SC0004585, and in part by Tech-X Corporation, Boulder, CO. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. We would like to thank James Balasalle and Chris DeLuca for assistance with development.

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