Speeding up Madgraph5_aMC@NLO through CPU vectorization and GPU offloading: towards a first alpha release

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Abstract. The matrix element (ME) calculation in any Monte Carlo physics event generator is an ideal fit for implementing data parallelism with lockstep processing on GPUs and vector CPUs. For complex physics processes where the ME calculation is the computational bottleneck of event generation workflows, this can lead to large overall speedups by efficiently exploiting these hardware architectures, which are now largely underutilized in HEP. In this paper, we present the status of our work on the reengineering of the Madgraph5_aMC@NLO event generator at the time of the ACAT2022 conference. The progress achieved since our previous publication in the ICHEP2022 proceedings [1] is discussed, for our implementations of the ME calculations in vectorized C++, in CUDA and in the SYCL framework, as well as in their integration into the existing MadEvent framework. The outlook towards a first alpha release of the software supporting QCD LO processes usable by the LHC experiments is also discussed.

1. Introduction

Computing architectures designed for data parallelism, such as CPUs with vector registers and GPUs, are now ubiquitous in the computing resources used for the data processing of High Energy Physics (HEP) experiments, such as the High Performance Computing (HPC) centers available to the Large Hadron Collider (LHC) experiments and the sites of the Worldwide LHC Computing Grid (WLCG). The full compute power of GPUs and vector CPUs, however, is often underexploited in HEP processing, partly because the software is old and was designed before these architectures became mainstream, but also because many HEP workflows involve a lot of stochastic branching and are therefore intrinsically difficult to port to data parallel paradigms, one notable example being detector simulation. Monte Carlo (MC) matrix element generators, conversely, are an ideal fit to exploit these architectures. This is because the calculation of scattering amplitudes and matrix elements (MEs), which is the computational bottleneck of these programs for complex physics processes, involves the repeated execution of the same functions on different data items (the various "events" randomly generated by MC sampling), and it is possible to achieve a perfect lockstep processing in its data parallel execution.

Our work on the reengineering of the Madgraph5_aMC@NLO (MG5aMC) event generator [2] follows precisely this approach. As described in our previous proceedings of the vCHEP2021 [3] and ICHEP2022 [1] conferences, our new implementation of the ME calculation in CUDA and vectorized C++ achieves lockstep processing with 100% branch efficiency on NVidia GPUs and the maximum theoretically possible SIMD speedups (x8 and x16 in double and single floating point precision for AVX512/zmm) on vector CPUs. In this paper, we mainly document the results presented at the ACAT2022 conference (October 2022), where we had reported the process achieved in the few months since ICHEP2022 (July 2022). This includes in particular some performance tests of the vectorized C++ implementation using all cores of a CPU rather than a single CPU core, some performance improvements for the serial component of the overall workflow, the implementation of a new "mixed" precision mode where both single and double floating point precision are used for different parts of the ME calculation, and the full integration into the existing MadEvent framework of the ME calculation implemented using SYCL. We also briefly mention a few new results achieved since ACAT2022 at the time of writing (March 2023), some of which will be described in more detail in upcoming talks [4, 5].

As discussed in Ref. [3], our port of MG5aMC ME calculations to CUDA and NVidia GPUs, which is based on Feynman diagrams and helicity amplitudes, represents a restart from scratch of previous efforts [6, 7] in this direction in 2009, which unfortunately were never integrated into a production quality framework usable by HEP experiments. Other approaches for porting matrix element event generators to GPUs have also been suggested. The development of MadFlow [8, 9] is another project based on MG5aMC helicity amplitudes, which however is independent from our work and differs from it because it uses Python and the TensorFlow framework. Furthermore, a GPU port of ME calculations based on Berends-Giele recursion relations, which was initially prototyped [10] in 2010 as a way to achieve a better scalability with the number of external particles in the scattering process than one based on Feynman diagrams (polynomial rather than factorial), has recently been implemented into the new PEPPER simulation framework [11, 12].

2. Speeding up the serial component of the MadEvent framework

As we previously described in our ICHEP2022 proceedings [1], our strategy for delivering to the LHC experiments a software application that they can run to generate samples of events, with well-known user interfaces and identical physics output but at a fraction of current computational costs, is based on injecting one of our new data-parallel implementations (in CUDA/C++ or SYCL) of the ME calculation into the existing MadEvent framework, replacing only the previous scalar Fortran implementation of the same ME calculation. The "outer shell" of the MadEvent framework, which is also implemented in Fortran, takes care of all tasks other than the ME calculation, which we will collectively refer to as the "non-ME serial component" of MadEvent: this includes, amongst other things, the generation of pseudo-random numbers, their mapping to particle momenta using a well defined sampling strategy (based on the MadEvent singlediagram enhancement multichannel algorithm [13]), the merging of multi-jet final states (for instance using the so-called "MLM" scheme [14, 15]), the execution of the hit-or-miss unweighting algorithm, the calculation of cross sections and the I/O intensive writing of LHE event data files. While all these tasks only account for a few percent of the overall wall-clock time when the Fortran serial MEs are used, the situation changes dramatically when the much faster (one to three orders of magnitude) CUDA/C++ or SYCL data-parallel MEs based on CPU vectorization or GPUs are used, as the MadEvent non-ME serial component quickly becomes the bottleneck.

In the results presented at ICHEP2022 for the $gg \rightarrow t\bar{t}gg$ process, for instance, we had reported that generating 90k weighted events took 58.3 seconds overall (5.2s in the MadEvent non-ME serial component and 53.1s in the ME calculation, see Table 2 in Ref. [1]) using Fortran MEs, but only 6.1 seconds overall (5.7s non-ME and 0.36s MEs) using double-precision CUDA MEs. In other words, the factor ~200 speedup in the ME calculation only led to an overall speedup

		madevent				standalone	
CUDA grid size		8192				524288	
$gg \! \rightarrow \! t \bar{t} gg$	MEs	$t_{\rm TOT} = t_{\rm Mad} + t_{\rm MEs}$	$N_{\rm events}/t_{\rm TOT}$	$N_{ m events}/t_{ m MEs}$			
	precision	[sec]	[events/sec]	[MEs/sec]			
Fortran	double	55.4 = 2.4 + 53.0	1.63E3 (=1.0)	1.70E3 (=1.0)			
CUDA	double	2.9 = 2.6 + 0.35	3.06E4 (x18.8)	2.60 E5 (x152)	2.62E5	4.21 E5 (x 247)	
CUDA	float	2.8 = 2.6 + 0.24	3.24E4 (x19.9)	3.83E5 (x225)	3.96E5	8.77E5 (x516)	

Table 1. Processing times and throughputs for 90112 $gg \rightarrow t\bar{t}gg$ weighted events. One core of a CERN VM (Intel Silver 4216 CPUs, one NVidia V100 GPU), cuda11.7 and gcc11.2 builds. See Ref. [1] for further details, e.g. on the difference between the madevent and standalone columns.

by a factor ~10: this is the limit predicted by Amdahl's law [16] since the serial non-ME component was originally 5.2s/58.3s, i.e. approximately 10% of the overall processing time. Our new ACAT2022 results for the same process are given in Table 1: the generation workflow in the madevent executable now takes 55.4 seconds overall (2.4s non-ME and 53.0s MEs) using Fortran MEs, but only 2.9 seconds overall (2.6s non-ME and 0.35s MEs) using double-precision CUDA MEs, i.e. a factor two faster than in the ICHEP2022 results. The difference between the two sets of results is only in the MadEvent non-ME serial component, which is now a factor two faster, while the speed of the CUDA ME calculation is essentially unchanged. The overall speedup from Fortran to CUDA is now ~20, as predicted by Amdahl's law since the serial component was originally 2.4s/55.4s, i.e. approximately 5% of the overall processing time.

To explain this speed-up, we recal [1] that the original MadEvent framework, which was looping through individual events and executing the full processing chain (random sampling of momenta, computing MEs, unweighting, multi-jet merging etc.) one event at a time, had to be modified to allow the data-parallel calculation of MEs on a large batch of events at the same time: this naturally led to the introduction of large Fortran arrays to keep all relevant properties of all the events in that batch. In this particular case, the speedup of the serial non-ME component from 5.2s to 2.4s was obtained by rationalizing the handling of MLM multi-jet merging, and in particular by moving most of its processing before the ME calculation, which made it possible to completely get rid of some very large Fortran arrays that had been introduced in the initial transformation of MadEvent from a single-event to a multi-event processing framework.

Speeding up the MadEvent serial non-ME component is especially important when offloading the ME calculation to a GPU, but it remains relevant when MEs are computed on vector CPUs. For instance, our new results for generating 80k $gg \rightarrow t\bar{t}gg$ events on an Intel Gold 6148 CPU, which are given in Table 2, show that the overall workflow now takes 6.1 seconds (1.8s non-ME and 4.3s MEs) using our "512z" vectorization level (AVX512 with zmm registers [1]), while at ICHEP2022 we had reported that the same workflow on the same machine took 7.1 seconds (2.5s non-ME and 4.5s MEs, see Table 1 in Ref. [1]). Again, the difference between the two sets of results mainly comes from the MadEvent serial non-ME component, but the effect of Amdahl's law is less pronounced for C++ than for CUDA, as the ME calculation is still the bottleneck.

While this speed-up in MadEvent is already an important achievement, we think that this is just the first step and that there is still much potential for further performance improvements. Further rationalizations of the use of large Fortran arrays may still be possible. In addition, we are investigating ways to speed up the MadEvent serial non-ME component by parallelizing it at least in part. One idea, for instance, is to offload to the GPU (or vectorize on the CPU) some parts of the computation, such as the mapping from random numbers to momenta in the sampling algorithm, or the unweighting process. Another possible approach, which represents a truly heterogeneous processing scenario, would consist in running several copies of the madevent application in parallel on different CPU threads, while sharing the GPU amongst them for the ME calculation. In addition to speeding up the MadEvent non-ME component by parallelizing it amongst different CPU cores, another advantage of this approach is that it could allow a decrease in the RAM footprint of each madevent process on the CPU (which is problematic

			standalone		
$gg \rightarrow t\bar{t}gg$	MEs	$t_{\rm TOT} = t_{\rm Mad} + t_{\rm MEs}$ $N_{\rm events}/t_{\rm TOT}$ $N_{\rm events}$		$t_{\rm MEs}$	
$gg \rightarrow \iota\iota gg$	precision	[sec]	[events/sec]	[MEs/s	sec]
Fortran(scalar)	double	37.3 = 1.7 + 35.6	2.20E3 (=1.0)	2.30E3 (=1.0)	
C++/none(scalar)	double	37.8 = 1.7 + 36.0	2.17E3 (x1.0)	2.28E3 (x1.0)	2.37E3
C++/sse4(128-bit)	double	19.4 = 1.7 + 17.8	4.22E3 (x1.9)	4.62E3 (x2.0)	4.75E3
C++/avx2(256-bit)	double	9.5 = 1.7 + 7.8	8.63E3 (x3.9)	1.05E4 (x4.6)	1.09E4
C++/512y(256-bit)	double	8.9 = 1.8 + 7.1	9.29E3 (x4.2)	1.16E4 (x5.0)	1.20E4
C++/512z(512-bit)	double	6.1 = 1.8 + 4.3	1.35E4 (x6.1)	1.91E4 (x8.3)	2.06E4
C++/none(scalar)	float	36.6 = 1.8 + 34.9	2.24E3 (x1.0)	2.35E3 (x1.0)	2.45E3
C++/sse4(128-bit)	float	10.6 = 1.7 + 8.9	7.76E3 (x3.6)	9.28E3 (x4.1)	9.21E3
C++/avx2(256-bit)	float	5.7 = 1.8 + 3.9	1.44E4 (x6.6)	2.09E4 (x9.1)	2.13E4
C++/512y(256-bit)	float	5.3 = 1.8 + 3.6	1.54E4 (x7.0)	2.30E4 (x10.0)	2.43E4
C++/512z(512-bit)	float	3.9 = 1.8 + 2.1	2.10E4 (x9.6)	3.92E4 (x17.1)	$3.77\mathrm{E4}$

Table 2. Processing times and throughputs for $81952 \ gg \rightarrow t\bar{t}gg$ weighted events. One core of Juwels Cluster login node jwlogin07 (Intel Gold 6148 CPUs), gcc11.2 builds. See Ref. [1] for further details, e.g. on the five different vectorization levels (none, sse4, avx2, 512y, 512z).

as discussed in Ref. [1]), as it should be possible to achieve the same overall occupancy of the GPU while decreasing the number of events computed in parallel by a single madevent process, i.e. its CUDA grid size. The results of a preliminary test relevant to this approach are displayed in Fig. 1, which shows the variation of the combined ME throughput achievable from a single NVidia V100 GPU when this is shared by up to 8 processes running in parallel on different CPU threads. The notable effect that we were hoping to see, and which is indeed achieved, is that the throughput curve moves to the left as the number of CPU processes increases, while still reaching the same combined throughput plateau at the end: this means that the maximum GPU throughput may be reached by running many CPU applications with smaller CUDA grid sizes, rather than a single application with a very large grid size. Another positive result, which however we were not anticipating and will deserve more in-depth analysis, is the fact that the maximum combined GPU throughput actually increases by almost 50% when launching kernels from different CPU threads. It should be stressed that this plot, which was obtained using the infrastructure developed for the HEP-SCORE benchmarking project [17], refers to the "standalone" application [1] where the ME calculation is not yet integrated in the full MadEvent workflow: in the future, we plan to repeat similar studies using the full MadEvent workflows. which would represent a more realistic test of a production-like heterogeneous scenario.

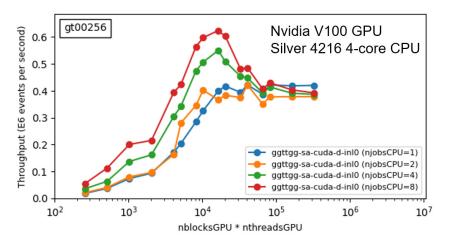


Figure 1. Total combined throughput for the $gg \rightarrow t\bar{t}gg$ process using 1, 2, 4 or 8 copies of our standalone application (see Ref. [1]), as a function of the CUDA grid size (number of blocks per grid times number of threads per block — "gt00256" indicates that the latter is fixed to 256).

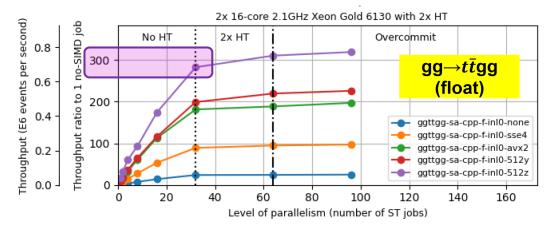


Figure 2. Total combined throughput for the $gg \rightarrow t\bar{t}gg$ process as a function of the number of copies of our single-threaded standalone application, in our five C++ vectorization scenarios. The y-axis represents the ratio of the achieved throughput to a reference with no vectorization and a single CPU process. For reference, the range of values of the absolute throughputs is also shown. The x-axis represents the number of simultaneous processes launched on the test node, which includes 32 physical CPU cores with Hyper-Threading enabled (64 logical cores in total).

3. Further performance tests and improvements in the ME calculation

In parallel to our efforts to understand and speed up the MadEvent serial non-ME component, we have also continued to pursue further improvements and analyses of the ME calculations.

To start with, based on the same benchmarking infrastructure that we used to produce Fig. 1 for the CUDA back-end, we analysed the performance of our vectorized C++ back-end when several CPU cores are used. This differs from the results that we presented in our previous papers as well as in Table 2 above, which all refer to a single CPU core. The results of this test are given in Fig. 2. One effect that is immediately visible is that the AVX512/zmm throughputs (purple line) continue to be significantly faster than the AVX512/ymm (red) and AVX2 (green) throughputs even when many cores are used, but not by a factor two. This may be due to a clock slowdown, but we have not verified it. With respect to non-vectorized throughput on a single core, the overall speedup of AVX512/zmm with 32 processes (the number of physical cores in these two Intel Gold 6130 CPUs) using single floating point precision is approximately 300, compared to a theoretical maximum of 512 (32 times 16), which seems quite satisfactory.

Another progress in the CUDA/C++ back-end has been the addition of a "mixed" floating precision mode, where Feynman diagrams are computed in double precision, while the "color algebra" part of the ME calculation is done in single precision. The rationale for this approach is that floats provide approximately a factor two speedup over doubles both in vectorized C++ (because twice as many floats as doubles fit into the same vector register) and in CUDA (because typical NVidia data center cards have twice as many FLOPs for FP32 as for FP64), but single precision does not provide enough numerical precision for the Feynman diagram part of the ME calculation. The idea was to test whether single precision could at least be used for the "color algebra": our tests confirmed that the same cross sections could be obtained within $\sim 10^{-5}$ in this case, which seems enough. Our throughput results for the $gg \rightarrow t\bar{t}ggg$ process are shown in

		madevent					standalone	
CUDA grid size		8192					16384	
$gg \rightarrow t\bar{t}ggg$	MEs	$t_{\rm TOT} = t_{\rm Mad} + t$	MEs	$N_{\rm events}/t_{\rm TOT}$	$N_{\rm events}/t_{\rm MEs}$			
	precision	[sec]		[events/sec]	[MEs/sec]			
Fortran	double	1228.2 = 5.0 + 1	223.2	7.34E1 (=1.0)	7.37E1 (=1.0)	—		
CUDA	double	19.6 = 7.4 +	12.1	4.61E3 (x63)	7.44E3 (x100)	9.10E3	9.51E3 (x129)	
CUDA	float	11.7 = 6.2 +	5.4	7.73E3 (x105)	1.66E4 (x224)	1.68E4	2.41E4 (x326)	
CUDA	mixed	16.5 = 7.0 +	9.6	5.45E3 (x74)	9.43E3 (x128)	1.10E4	1.19E4 (x161)	

Table 3. Processing times and throughputs for 90112 $gg \rightarrow t\bar{t}ggg$ weighted events. One core of a CERN VM (Intel Silver 4216 CPUs, one NVidia V100 GPU), cuda11.7 and gcc11.2 builds.

			standalone		
$gg \rightarrow t\bar{t}ggg$	MEs	$t_{\rm TOT} = t_{\rm Mad} + t_{\rm MEs}$	$N_{\rm events}/t_{\rm TOT}$	$N_{\rm events}/r$	$t_{\rm MEs}$
$gg \rightarrow iiggg$	precision	[sec]	[events/sec]	[MEs/sec]	
Fortran(scalar)	double	813.2 = 3.7 + 809.6	1.01E2 (=1.0)	1.01E2 (=1.0)	
C++/none(scalar)	double	986.0 = 4.3 + 981.7	8.31E1 (x0.8)	8.35E1 (x0.8)	9.82E1
C++/sse4(128-bit)	double	514.7 = 4.2 + 510.5	1.59E2 (x1.6)	1.61E2 (x1.6)	1.95E2
C++/avx2(256-bit)	double	231.6 = 4.0 + 227.6	3.54E2 (x3.5)	3.60E2 (x3.6)	4.41E2
C++/512y(256-bit)	double	208.6 = 3.9 + 204.8	3.93E2 (x3.9)	4.00E2 (x4.0)	$4.95\mathrm{E2}$
C++/512z(512-bit)	double	124.6 = 4.0 + 120.6	6.58E2 (x6.5)	6.79E2 (x6.7)	8.65 E2
C++/none(scalar)	float	936.1 = 4.3 + 931.8	8.75 E1 (x0.9)	8.79E1 (x0.9)	1.02E2
C++/sse4(128-bit)	float	228.9 = 3.9 + 225.0	3.58E2 (x3.6)	3.64E2 (x3.6)	4.30E2
C++/avx2(256-bit)	float	114.1 = 3.8 + 110.4	7.18E2 (x7.2)	7.43E2 (x7.4)	9.06E2
C++/512y(256-bit)	float	104.5 = 3.8 + 100.7	7.84E2 (x7.9)	8.14E2 (x8.1)	1.00E3
C++/512z(512-bit)	float	61.8 = 3.8 + 58.0	1.33E3 (x13.3)	1.41E3 (x14.1)	1.77E3
C++/none(scalar)	mixed	986.0 = 4.3 + 981.6	8.31E1 (x0.8)	8.35E1 (x0.8)	9.98E1
C++/sse4(128-bit)	mixed	500.4 = 3.9 + 496.5	1.64E2 (x1.6)	1.65E2 (x1.6)	2.00E2
C++/avx2(256-bit)	mixed	220.5 = 3.8 + 216.7	3.72E2 (x3.7)	3.78E2 (x3.8)	$4.55\mathrm{E2}$
C++/512y(256-bit)	mixed	195.6 = 3.7 + 191.8	4.19E2 (x4.2)	4.27E2 (x4.3)	$5.21\mathrm{E2}$
C++/512z(512-bit)	mixed	118.5 = 3.8 + 114.7	6.92E2 (x6.9)	7.15E2 (x7.2)	8.97E2

Table 4. Processing times and throughputs for $81952 \ gg \rightarrow t\bar{t}ggg$ weighted events. One core of Juwels Cluster login node jwlogin07 (Intel Gold 6148 CPUs), gcc11.2 builds.

Table 3 for CUDA and Table 4 for vectorised C++. While encouraging, these results are still preliminary and we plan to pursue further tests of this approach.

4. SYCL-based developments and C++ compiler studies

While all tables and plots presented so far in this paper refer to our original CUDA/C++ implementation, significant progress has also been achieved on various fronts in our parallel implementations using performance portability frameworks. Most recently, this work has focused on the SYCL implementation, while the developments using Kokkos have slowed down and those based on Alpaka have stopped. As noted in Ref. [1], the main interest of these APIs is that a single code base, with a few back-end-specific customizations, may be executed on many architectures, including GPUs from different vendors such as NVidia, AMD and Intel. This is shown in Fig. 3, which compares the performances of our CUDA, SYCL and Kokkos

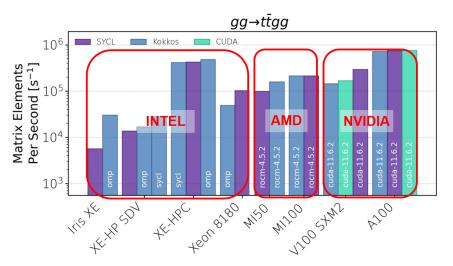


Figure 3. Comparison of the CUDA, Kokkos and SYCL ME engines for $gg \rightarrow t\bar{t}gg$ on many GPUs, using the standalone application (with optimal GPU grid sizes at the throughput plateau). "Xe-HP SDV" is a Software Development Vehicle for functional testing only, currently used at Argonne and at other customer sites to prepare their code for future Intel data centre GPUs. "XE-HPC" is an early implementation of the Aurora GPU. The throughput achieved on a full Xeon 8180 CPU using SYCL and Kokkos multi-threading is also shown for reference.

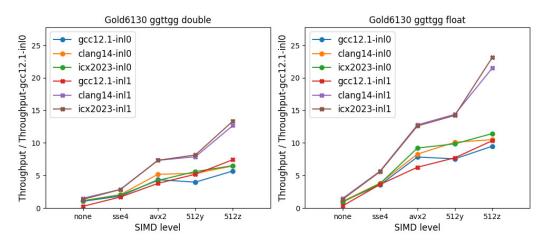


Figure 4. Comparison [18] of $gg \rightarrow t\bar{t}gg$ throughputs for different C++ builds, using five vectorization levels, three compilers (gcc12.1; clang14.0; icx2023, based on clang16.0) and two inlining approaches. The inl0 default build uses no inlining, the inl1 experimental build (which mimics some features of link time optimization) forces the inlining of helicity amplitude functions. Rather than absolute throughputs, all data points in each plot (left for double, right for single precision) represent the ratios to the throughput gcc12.1 inl0 build with no SIMD.

implementations on different systems; compared to previous results [1], this ACAT2022 plot is interesting because it also includes results on Intel XE-HPC, which is an early implementation of the Aurora GPU. A notable achievement reported at ACAT2022 is that the SYCL implementation of the ME calculation is now also fully integrated into MadEvent, which means for instance that we are able to produce cross-sections and LHE event data files by offloading the ME calculation to AMD or Intel GPUs, rather than using the Fortran CPU implementation.

A more recent development, which started well after ACAT2022, is that a vectorized SYCL implementation for CPU has also been prototyped. Preliminary tests indicate that this achieves a promising performance, with throughputs which sometimes exceed those of the gcc builds of the CUDA/C++ implementation: while this is not yet understood and will require further studies, it is likely that this may be due at least in part to the fact that the SYCL implementation is built using the clang-based icx Intel compiler. As shown in Fig. 4, in fact, which presents a recent [18] performance comparison between many builds of the CUDA/C++ implementation using different C++ compilers, we have observed that the performance of icx builds is almost the same as that of clang builds, which can be significantly better than that of gcc builds in some cases (more than a factor 2 faster with AVX512/zmm vectorization and agressive inlining); these results are however preliminary and will need more in-depth analysis. It is also interesting to note that, while our CUDA/C++ implementation of vectorization is based on gcc and clang compiler vector extensions, our SYCL version uses the sycl::vec type, which is itself implemented as a wrapper over clang vector extensions: in other words, compiler vector extensions are ultimately used for CPU vectorization in both of our CUDA/C++ and SYCL implementations.

5. Outlook: towards a first alpha release

Finally, the most important progress we achieved since ACAT2022 is that we completed the implementation of the event-by-event random choice of leading colors and helicities in LHE files. This was the last missing piece before we could provide in the CUDA/C++ MadEvent framework the full set of features needed by the LHC experiments for unweighted event generation. This functionality is now essentially complete, but we are still performing some final tests, also to understand its impact on performance; in particular, this feature introduces a minor level of stochastic branching in the ME workflow, degrading lockstep processing both on GPUs and on vector CPUs (it is possible that this effect is already visible in Fig. 4, which was prepared using this more recent code base). We are now working towards repackaging our work to provide a first alpha release of our work for the experiments, which we plan to achieve during Q2 2023.

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