Faster Parton Distribution Evaluation in Monte Carlos

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(Dated: March 4, 2004)

Abstract

I recommend a few trivial changes to the routines that evaluate CTEQ parton distribution functions. These changes allow modern compilers to optimize the evaluation routines, while having no quantitative effect on the results. Computation time is reduced by a factor of 2 in matrix-element calculations, and by 1.3–1.5 in the showering Monte Carlo event generators with fast detector effects included. The results suggest that additional time should be invested in optimizing these routines.
I. INTRODUCTION

A significant amount of time and computing resources are spent on calculating events at hadron colliders. Whether a theoretical calculation of matrix elements, or an experimental simulation of events with detector effects, one common element is the evaluation of parton distribution functions (PDFs). In profiling FORTRAN versions of code \[1, 2\] written to simulate single-top-quark production, it has become apparent that much of the execution time of real production code is spent acquiring these PDFs. Upon close examination of the CTEQ PDFs \[3\], a handful trivial optimizations arise that can cut this time in half. I list specific recommendations that are simple to implement, but which can have large consequences for efficiency.

Profiling a FORTRAN version of the code for fully differential next-to-leading order single-top-quark production \[1, 2\] indicates that at least 75% of the running time is spent in acquiring PDFs. Furthermore, most of that time is spent inside the subroutine POLINT. POLINT is a routine designed to perform a polynomial fit of degree \(n - 1\) to a data set of \(n\) points based on Neville’s algorithm \[4\]. This subroutine is used by the CTEQ Collaboration \[3\] to interpolate smoothly between the values of \(x\) and \(Q^2\) that are read in from a table of best-fit values. Clearly any increase in speed in evaluating POLINT will translate directly into decreased execution time for the program.

One approach to increasing speed would be to replace POLINT outright with alternate interpolations, or functional fits to the PDFs. While these are reasonable choices, I wish to retain the same method to ensure that any results are numerically identical to results obtained previously. Therefore, I will limit my recommendations to trivial modifications of POLINT itself. Two useful changes to the coding are:

1. Remove the line: IF(DEN.EQ.0.)PAUSE.

2. Write different versions of POLINT for 3- and 4-point interpolation, and call them directly. E.g., replace POLINT(XA,YA,N,X,Y,DY) with POLINT3(XA,YA,3,X,Y,DY), and explicitly set \(N\) to 3 in the code.

The first optimization is the most important as the line is never reached in the evaluation of the CTEQ PDFs, but it generally prevents the compiler from fully optimizing the loops. Beyond being an unnecessary comparison, the real problem is that allowing a break point
out of the loop can disallow some types of parallel instructions to be passed to the CPU. The second optimization mostly helps compilers to optimize the loops by defining the number of iterations at compile time, rather than dynamically.

II. OPTIMIZATION RESULTS

In order to assess the usefulness of these optimizations, I evaluate four programs. I consider a loop over PDFs, and three calculations of $t$-channel single-top-quark production: an analytic next-to-leading order calculation of jet distributions \[1, 2\], HERWIG 6.1 \[5\], and PYTHIA 6.2 \[6\]. The first two calculations are compiled with the GNU compiler g77 versions 2.95 and 3.1, and the Intel compiler ifc 6.0. The two showering event generators have only been considered with the Intel compiler because they were linked with a fast detector simulation called SHW \[7\] that requires additional libraries that would also have to be recompiled. While additional information might be gained by trying more compilers, there are program specific issues that would also have to be addressed. All numerical results are from execution on a 1.4 GHz Pentium 4 machine. Limited tests performed on Pentium 3 machines are completely consistent with the results described below.

A. Benchmark for PDFs

The most naive test of potential speed gains comes from looping over parton distribution functions. For this benchmark, values of $x$ are looped over, the scale is chosen to be $Q^2 = (x \times 1960 \text{ GeV})^2$, and all parton flavors are evaluated. These choices are both more representative of an actual program, and avoid any possibility of anomalous gains due to fast memory access in the level 2 cache. The most immediate observation is that there is less than a 5% difference between g77 2.95 and g77 3.1.\footnote{One exception is that specific Pentium 4 optimizations in g77 3.1 can increase the difference to 10%.

1} Furthermore, the fastest time I have been able to achieve using g77 is slower than unoptimized times I obtain by using ifc 6.0. Since this is true in all cases tested, I split the results by compiler.

Using g77, the running time ranges from 30–39 s. Removing IF(DEN.EQ.0.)\text{PAUSE} increases the speed by 10%. Using POLINT3 instead of POLINT increases speed by an additional
10%. The cumulative effect is a net 20% gain (30% if specialized instructions for the Pentium 4 are used).

The results for using the Intel compiler are more complicated, and lead to some general conclusions. First, the Intel compiler performs more analysis in generating assembly code and branch prediction. If poor choices of optimization flags are made, the code can run a factor of 2 slower. If default optimization is chosen, the base time of execution is 30 s. Using POLINT3 instead of POLINT increases speed by up to 20%. Interestingly, just removing IF(DEN.EQ.0.)PAUSE from POLINT increases the speed by 26%, and the combination of both is 30% faster. The fact that the optimization is not strictly multiplicative indicates there are subtle effects involved in how instructions and data are fed to the processor. By trying various compiler flags, it appears that generally the optimization is all or nothing. As we will see next, this artificial test code actually underestimates the potential speed gain for the Intel compiler.

B. Matrix element codes

Artificial benchmarks can be misleading. Therefore, I consider the effects of both changes on working production coding of single-top-quark production [1, 2]. The results using the g77 compiler are identical to the benchmark scenario above (10% increases in speed for each change, and if Pentium 4 specialization is used). With a net 30% improvement in speed, the program can run in 80 s when compiled with g77. This is a factor of 1.4 faster than without the changes.

The Intel compiler provides more interesting results. The default running time is 83 s. Typically there is a 20% increase in speed when using POLINT3 instead of POLINT. Dropping IF(DEN.EQ.0.)PAUSE alone increases the speed by 33%; and both optimizations together yield a net speed increase of 35% (execution times of about 54 s). It is interesting that the most efficient compiler options for the optimized code are actually 45% (1.8 times) faster than when using the same options in the original code (which runs in 98 s). It appears that adding both optimizations reduces the dependence on compiler options of the net execution time. Hence, a combination of both optimizations seems a desirable option.

Since matrix element calculations spend so much time calling PDFs it is prudent to make one additional recommendation:
3. Eliminate any unnecessary calls to the PDFs.

While this may seem obvious, it can be less simple to implement in practice. Both HERWIG and PYTHIA use the PDFLIB [8] interface STRUCTM from CERNLIB to access PDFs. The PDFLIB routines return a full (though not necessarily complete) set of unique PDFs — $g$, $u$, $d$, $\bar{u}$, $\bar{d}$, $s$, $c$, and $b$. In some matrix elements, not all PDFs are always needed. In particular, the leading order diagram for $t$-channel single-top-quark production requires only the $b$ or $\bar{b}$ PDFs from one of the incoming hadrons at a time. By eliminating calls to PDFs that are never used, execution time is cut by an additional 33%. Hence the net code is actually up to a factor of 2.6 faster than by default. If there is a clear way to eliminate extraneous calls to PDFs when coding matrix elements, it should be implemented.

C. HERWIG and PYTHIA

While many theoretical calculations are still only at the matrix-element level, experiments and careful phenomenological studies generally resort to using showering Monte Carlo event generators. These codes are significantly more complex, and we might expect to see less gain in efficiency as time is spent in showering, and detector simulation. In order to assess the impact on the two most common event generators, HERWIG [5] and PYTHIA [6], I use them to calculate $t$-channel single-top-quark production, including all showering effects, etc. I also run the output through the fast detector simulation SHW [7] in order to represent the most complicated calculation a phenomenologist is likely to perform.

The HERWIG event generator appears to spend just as much time evaluating PDFs as the matrix element example considered above. Using POLINT3 instead of POLINT improves the speed by 20%. Removing IF(DEN.EQ.0.)PAUSE alone improves the speed by 22%. As in the matrix-element case, adding both optimizations to the Intel ifc 6.0 compiler results in a combined gain of 25% (1.33 times faster). It is interesting to note that the gain can be as large as 33% (1.5 times faster) if non-optimal compiler flags are chosen, as is often the case when linking against precompiled libraries. If both recommended optimizations are used, however, the actual time of execution is less sensitive to compiling options.

The improvement in PYTHIA is not as large as in HERWIG, but it is still significant. Removing IF(DEN.EQ.0.)PAUSE or using POLINT3 independently reduce the time of computation by 15% (about 1.2 times faster). Including both optimizations appears to provide only a
percent or two in further improvement. PYTHIA provides internal routines for some CTEQ PDFs based on functional fits. By implementing these changes to POLINT, the more accurate table-based evaluation is actually a few percent faster than the supposedly optimized, but less accurate fits. This suggests that parameterizations may not really be needed any longer. At very least some profiling should be done before it is determined that hand-coded optimizations should be used over more general results.

III. CONCLUSIONS

Given recent improvements in compilers, it behooves us to reconsider where bottlenecks in computational speed arise. It appears that one source of significant loss of computational speed is in evaluating parton distribution functions. For users of the CTEQ PDFs I propose making three simple changes to the code that can cut total computational time by a factor of 2 or more. First, I recommend that unnecessary calls to the PDFs be removed. In the case of interface functions the $\bar{c}$, and $\bar{b}$ PDFs may directly set equal to the already evaluated $c$, and $b$ PDFs, respectively. This is already done in the PDFLIB functions STRUCTM and PFTOPDG. Note that the PDFLIB routines also set $\bar{s} = s$, which is an interface bug for PFTOPDG, since newer PDFs may not have the same value for both partons. Care must be taken to ensure that a given set of PDFs are consistently called.

The second recommendation is to make 2 trivial changes to the subroutine POLINT. Comment out the line \texttt{IF(DEN.EQ.0.)PAUSE}, and replace the general $n$-point fitting POLINT with versions specialized to 3- or 4-point fits. Depending on the exact compiler and program, gains of 20–30\% (factors of 1.25–1.4) are typical with, with gains up to a factor of 2 possible if the right compiler optimizations are chosen. These routines should be changed in the base CTEQ distribution [3], the PDFLIB routines in CERNLIB [8], and in the new Les Houches Accord compilation of PDFs LHAPDF [9].

Despite the large gains in speed obtained by the changes I propose, many programs will still spend most of their time calling PDF subroutines. This suggests two paths that should be followed. First, a systematic study of the CTEQ evolution code should be performed to determine whether there are places that the code could be rewritten to improve efficiency without changing the numerical output. This would allow universal improvements in code execution. Second, each Monte Carlo writer should be aware of these timing issues (and
potential bugs if $s$ is not the same as $\bar{s}$), and attempt to reduce unnecessary calls to the PDFs in their own code. Finally, it is interesting that these optimizations can remove the need for less accurate parameterizations.

Acknowledgments

This work was supported by the U. S. Department of Energy under Contract No. DE-AC02-76CH03000.

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