Automated Calculation and Simulation Systems

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I briefly summarize the parallel sessions on Automated Calculation and Simulation Systems for high energy particle physics phenomenology at ACAT 2002 (Moscow State University, June 2002) and present a short overview over the current status of the field and try to identify the important trends.

1. Introduction

Future particle colliders—planned or already under construction—will explore a new frontier in energy and precision. Final states with more tagged particles and better defined jets will become available for physics analysis.

If there is low energy supersymmetry, the determination of the quantum numbers of the predicted particles will require comprehensive studies of complicated cascade decays, taking advantage of spin correlations. If there is no low energy supersymmetry, physics beyond the standard model will contribute to processes like $W/Z$, $\nu e\bar{\nu} e$, $t\bar{t}$ production, and $WW/\tau\bar{\tau}$ scattering, but the effects will be very small and can only be observed in precision measurements of these processes—and complementary processes at hadron colliders—that must be compared to precision calculations in the standard model, effective field theories and specific models for physics beyond the standard model.

Therefore, we will need reliable predictions, implemented in precision simulation tools to unleash the full potential of future colliders. Since the primary objective of the next generation of colliders is the determination of the nature of electroweak symmetry breaking, particular care must be taken to obtain gauge invariant predictions. Polarization will be important to focus on longitudinal gauge bosons and for measuring quantum numbers of supersymmetric particles.

It will be qualitatively more complicated to reach reliable high precision predictions for these multi particle final states than for the two particle final states that have dominated physics at LEP1: 1) the parameter space of models beyond the standard model is much larger, 2) the number of Feynman diagrams contributing to a process explodes combinatorially, 3) algebraic expressions become much more complicated with the growing number of building blocks (i.e. independent momenta and polarization vectors), 4) gauge cancellations become numerically hazardous, and 5) phase space also becomes much more intricate.

Therefore, even if we had enough graduate students and postdocs, we should not waste them on repetitive “assembly line” calculations. Instead, efforts must be directed toward formalizing the calculations so that the repetitive part can be delegated to computers, which are more patient with and particularly reliable for repetitive work. Of course, this is not a new observation and has formed the rationale for the AIHEP workshops starting in 1990, which were the precursor of the present ACAT conferences.

In a bird’s eye’s view, the status and trends at ACAT 2002 were: 1) tree-level calculations in the standard model for $2\rightarrow 4$ and $e^+e^-\rightarrow 6$ have been well under control for some time now and can readily be used by non-experts, 2) the support for general $2\rightarrow 6$ and $2\rightarrow 8$ processes is coming along, but not completely usable for production yet (systems with already complete physics support do not scale optimally, while optimally scaling systems have not been implemented
2. Automated Calculation and Simulation Systems

Fully Automated Calculation and Simulation Systems (ACSS) in particle physics aim to produce cross sections and event samples for a given physics model and scattering process

\[
\begin{align*}
\text{model} & : \mathcal{L} \\
\text{parameters} & : m, g, \ldots \\
\text{process} & : e^+e^- \rightarrow \nu_e e^+ \nu_\mu d\bar{u} \\
\text{cuts} & : p_{T \text{min}}, E_{\text{min}}, \ldots \\
\end{align*}
\]

with as little as possible human intervention (ideally without any, of course). The job of ACSS can roughly be be divided into two steps

1. calculate the matrix element \( T \) (i.e. generate Feynman diagrams, derive arithmetical expression and generate executable code)

2. integrate \(|T|^2\) with a phase space measure \(d\mu\) or generate events according to \(|T|^2d\mu\) (the efficiency of this step can be improved significantly by using information on the structure of \( T \)).

In a third step, the partonic final states have to be transformed into hadronic final states. This fragmentation and hadronization is typically delegated to the established players in this field like Pythia and HERWIG.

Still, an ACSS is a complex piece of software and can only be constructed and maintained if broken into several components. As a typical example, the structure of WHIZARD is displayed in figure 1. Indeed, some systems are complete and self-contained, while some provide components of complete systems\(^1\): CompHEP is a complete system (two talks and two posters at ACAT 2002), CalcHEP is a CompHEP clone (one talk), GRACE is a complete system (one talk and additional talks in the sessions on numerical integration and sampling), O’Mega calculates efficient matrix elements for many particle final states, WHIZARD calculates efficient matrix elements for many particle final states and integrates other components into a complete system, HELAC/PHEGAS calculates efficient standard model matrix elements and performs phase space integration, Madgraph calculates standard model matrix elements and integrates other components into a complete system.

\(^1\)Lack of space makes it impossible to provide complete references. The ordering proceeds from complete systems to components and is alphabetical in each group.

Figure 1. Components of the WHIZARD ACSS. WHIZARD can use different components for generating matrix elements and relies on the VAMP library for adaptive multi channel sampling of phase space parameterizations matching the matrix element’s dominant peaking structures. The other ACSS are structured in a similar way.

The main challenges lie beyond the standard model (in the MSSM in particular) and virtual radiative corrections. Regarding the former, progress has been reported at the conference and regarding the latter, there is growing evidence, concern and consensus that the classic analytical approach “does not scale”. Recently, several projects have started to work on different (semi-)numerical approaches and progress by one group has been reported at this conference.\(^2\)

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matrix elements\footnote{A companion program \texttt{MadEvent} for event generation was introduced not too long after the conference.}. \texttt{Alpha} calculates efficient standard model matrix elements for many particle final states, \texttt{FeynArts/FeynCalc/FormCalc} calculates standard model and MSSM loop diagrams, \texttt{CalcPHEP} (now \texttt{SANC}) calculates standard model $2 \rightarrow 2$ processes at one-loop (two talks and two posters).

3. Trends at ACAT 2002

3.1. Supporting More General Models

Currently, all ACSS use a set of Feynman rules (i.e. a set of propagators and vertices) as input. This is mathematically equivalent to the Lagrangian describing the model. However, the derivation of the Feynman rules derivation from a Lagrangian—even if straightforward—can be extremely tedious and error-prone (e.g. there are many thousand different vertices in the MSSM).

In two talks\footnote{\texttt{CompHEP}’s special purpose C-routines for the symbolic evaluation of squared diagram are being replaced by calls to the general purpose \texttt{form} system.}, tools for the derivation of Feynman rules in complicated models—the MSSM in particular—have been discussed at ACAT 2002. Such tools need to be able to expand lagrangians in terms of component fields and momenta and simultaneously handle mixing from non-diagonal mass matrices. These operations must use a very natural notation in order to minimize the potential for human errors.

Therefore, such tools\footnote{\texttt{Pythia7} is not an ACSS in the strict sense, but all ACSS have to talk to \texttt{PYTHIA} or \texttt{HERWIG} for fragmentation and hadronization of hard events. \texttt{Pythia7} is a project to completely rewrite the Lund event generators in \texttt{C++}. It will provide a general structure for implementing models for event generation, not only the Lund Model (in fact, \texttt{HERWIG++} has joined the effort). Today, \texttt{Pythia7} exists as a proof-of-concept version (some basic $2 \rightarrow 2$ matrix elements, remnant handling and Lund string fragmentation. A new pre-release with the first \texttt{HERWIG} contributions is planned for 2002 and a usable generator is planned for the following year. \texttt{Pythia7} should be available as the standard generator at the LHC start-up.} evolve quickly into fully developed symbolic manipulation languages, with some special features: 1) transparent notation for objects from mutually commutative, but non-commutative algebras, like non-simple gauge groups (this is poorly supported in general purpose computer algebra systems) and 2) support for the dual role played by covariant derivatives as operators and field components. Soon there will be several \textit{independently} derived sets of machine readable Feynman rules for the MSSM.

In addition, moving beyond the standard model requires that some systems have to relax assumptions that were useful for implementing the Standard Model in the first generation of ACSS: Majorana spinors have to be supported in addition to Dirac spinors, vertices of degree higher than four, more complicated momentum dependence in higher dimensional operators, non-local vertices factors (e.g. in non-commutative field theories), non Feynman diagram contributions (e.g. K-matrix unitarization), etc.

One solution is to replace previously hard-coded subsystems making special assumptions by general purpose components. One poster reported how \texttt{CompHEP}’s special purpose C-routines for the symbolic evaluation of squared diagram are being replaced by calls to the general purpose \texttt{form} system.

3.2. Component Architecture and Persistence

The components in an ACSS have to communicate across a variety of boundaries: abstraction layers (subroutines, objects, modules, etc.), address spaces (processes, networks, etc.), and time (data storage, persistency). These issues were addressed by two talks\footnote{External representations of event samples are required for communicating partonic events to soft QCD Monte Carlos and to detector simulations. External representations are also useful for saving both intermediate and final results. The latter can be useful if reading the stored events is faster than re-generation. However, there will always be a gain for reweighting processed data and one must also not underestimate the value of external representations for debugging.}

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A proposal of a text based data description language for event samples and the implementation
of the accompanying toolkit \[6\] was welcomed, but during the discussion there was demand for replacing the concrete syntax by XML, while retaining the toolkit interface, was voiced.

### 3.3. Loops

In two talks \[7,8\] and two posters, the project of a re-implementation of the complete standard model one-loop radiative corrections (incl. soft bremsstrahlung) for \(e^+e^- \rightarrow ff\) from scratch was presented.

One motivation for such a re-implementation lies in the need to preserve the body of knowledge for future generations by providing a consistent and systematic option for redoing the calculations. An application will be the relaxation of Z-pole assumptions for applications to off-resonance physics at a linear collider.

The calculational procedure starts by a decomposition into form factors, followed by the calculation of the form factors using a collection of \texttt{form3} procedures for symbolic calculation, renormalization and generating numerical Fortran code. Currently, the \(t\)-channel neutral current processes and the \(s\)-channel processes are done and show very good agreement with existing codes. Interference contributions and decays are in progress.

### 4. Outlook

If we would ever manage to produce a fully general and efficient ACSS, that is even easy to use for non-experts, we would risk to make ourselves obsolete as phenomenological theorists. Fortunately, we will never get there because theoretical theorists will always come up with new features that we have not anticipated and experimentalists will always push the frontiers in energy and precision, calling for ever more precise calculations of ever more complicated processes.

Currently there is a vast uncharted territory (figure 2) and a systematic exploration of the high energy/high precision region with many legs and many loops will require the development of new semi-numerical methods.

Finally, variety is good, since we need to be able to cross check our results. Communication among developers and among programs—using pluggable components in the ideal case—is necessary for this.

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