Monte-Carlo Event Generators for Particle Physics in the 21st Century

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Monte-Carlo event generators

Theory: model $\rightarrow$ transition amplitudes $\rightarrow$ observables

Experiment: data (reconstructed events) $\rightarrow$ implications for assumed model?

Relation of event data to calculated observables?

1. Completely inclusive observables $pp \to X$: well defined

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4. Exclusive observables: event samples.
   Direct relation to data (w/ detector simulation), well defined problem but more work for theorists

   $\Rightarrow$ MC event generators

In this talk, I'll try to review all aspects of Monte-Carlo simulation.

The coverage is necessarily superficial, but I will try to

- sketch the state of the art
- mention important unsolved problems and desirable improvements

1. Fundamentals: Theory and Assumptions

Basic Idea of MC:

$$p(a \to b) = \int dx \, |\langle b(x)|a\rangle|^2$$

Evaluate by picking points x at random and compute the matrix element.

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Find mapping $x = f(y)$ such that, on statistical average

$$p(a \to b) = \text{const.} \times \int dy$$

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The problem can be easily solved if

1. there is only one parameter x: invert the function $|\langle b(x)|a\rangle|^2$, or:
2. the function varies only moderately: reject points based on the function value.

The Challenge

For particle physics, a complete event has dozens/hundreds/thousands of parameters (detected particles), and the function varies over many orders of magnitude (resonances), is exactly zero somewhere (cuts) and has algebraic (kinematics) singularities near the edge of parameter space.

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For the part that is accessible, the evaluation for millions of parameter points can become a huge effort in computing time.

Framework for Monte Carlo in High-Energy Elementary Particle Physics:

Quantum Theory

All calculations are based on a relativistic **quantum theory**.

Theoretically well defined: S matrix elements

$$S_{fi} = {}_{\text{out}}\langle q_1, q_2, \ldots | p_1, p_2, \ldots \rangle_{\text{in}}$$

between non-interacting asymptotic states (plane waves $\sim$ classical particles).

Observed: Scattering/production of (quasi)stable particles: leptons, photons, hadrons. Probability given by squared S matrix elements.

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(**caveat:** massless photons.

Well-known problem with solution: observables w/ infinite number of photons but finite energy. Separate treatment of Coulomb singularity. Technical difficulty for all implementations!)

Quantum Field Theory

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Model for S matrix elements.

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(**caveat:** Hadron physics is non-perturbative.

Believed to be derived from QCD Lagrangian, but partly non-calculable. Parton scattering can be sort-of proved as a deep-inelastic limit for the initial state.)

Lagrangian (perturbative) quantum field theory: just coincidence?

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- ??? New physics at high energies may be non-perturbative.
- ??? It need not be based on a local Lagrangian.
- ??? We don't know whether the S matrix can be derived from a quantum field theory.

Nevertheless, perturbation theory works for the Standard model, so...

- Completely automatic systems: from the Lagrangian to the event sample, to arbitrary precision

To Keep in Mind:

If there is anything that does not fall in the class of weakly interacting local quantum field theories, manual work is required again.

Elementary process at a hadron collider

We are particularly interested in **“hard”** processes. High p_T for all particles, all particles (jets) well separated.

- Expect at most one interesting, hard process per proton-proton interaction.
- All others are “soft”, boring, old-physics – but difficult to handle

Separating disparate energy scales:

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$\to$ hadrons, leptons, photons

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- But the experimental accuracy is a challenge for the theoretical description.

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Major Universal MC Projects

100s of MC projects. A few aim at covering all aspects, regularly used by experimental studies and analyses and actively supported

1. Started before 2000 and used **everywhere**
   - PYTHIA
   - HERWIG
2. Since 2000, frequently used for **LHC** analyses:
   - MadEvent (MadGraph)
   - Sherpa
3. Since 2000, standard for **ILC** studies:
   - WHIZARD

Disclaimer: many important projects mentioned neither in this short list, nor elsewhere in this talk!

2. Elementary Processes: Theory

Assume factorization.

We can start off by a module for elementary, perturbative processes in Lagrangian field theory

- described by Feynman rules
- evaluated for high energy and separation scales.

MC for the Standard Model

For the SM, the problem of generating the matrix elements for elementary processes (quarks, leptons, photons, gluons) is solved, in principle.

- everything is perturbative
- tree-level: automatic generation of amplitudes
- 1-loop level: automatic generation of virtual QCD corrections
- 1-loop level: programs exist that contain full SM corrections (not yet standard)
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Challenges: complexity.

Bookkeeping, flexibility, computational efficiency (speed and memory).

MC for the Standard Model: Setup

Choice of basis for external states: helicity amplitudes

$$\sum_{h=+1,-1} |p,\lambda\rangle\langle p,\lambda| = p_\mu\gamma^\mu$$

(don't use trace formalism)

- direct calculation of polarized observables
- total squared ME: sum over discrete intermediate states
- more efficient for high number of external fermions

Other choices?

MC for New Physics

Three classes:

1. Extended models, weakly interacting and perturbative: same methods, different Lagrangian (more complex)
   Automatic programs convert model $\rightarrow$ Feynman rules: FeynRules
   Computational challenges: factorize cascade processes?
2. Effective theory as extension: perturbative but problematic if cutoff scale within the accessible range.
   Matching to strongly interacting models. Requires matrix-element contributions not from Feynman rules.
3. Strongly interacting / non-QFT models: case-by-case handling still necessary

$\Rightarrow$ Automatic programs cover only class 1.

Unitarity Issues

Where class 2 arises:

Feynman perturbation theory violates basic principles: unitarity (optical theorem)

Normally not an issue (SM): corrections are small, phase-shifts are usually irrelevant
However: EW interactions at high energies, if slightly deviating from SM prediction:

- either undetectable
- or strongly interacting beyond some threshold

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Need to cope with *non-perturbative* high-energy asymptotics
$\Rightarrow$ model must preserve unitarity (beyond perturbation theory)

3. Elementary Processes: Calculation

Algorithms for Matrix Elements

Algorithms for constructing the amplitude

1. analytic expression, manually optimized (PYTHIA)
2. automatic generation of code based on Feynman graphs, some optimization afterwards (MadGraph)
3. string-inspired analytic methods (mainly QCD)
4. automatic generation of minimal code based on the Lagrangian/Feynman rules, skip generation of Feynman graphs (analytic/numeric) (WHIZARD, AlpGen, HELAC)

Tree level: $2 \to 6$ standard, $2 \to 8$ sometimes challenging

Phase-Space Handling

The amplitude varies over many orders of magnitude, is singular at some edges, and contains zero regions. Need suitable phase-space mappings, before applying rejections.

- The ultimate rejection efficiency is important. Ratio of average weight over maximum weight, after mapping.
- Many give up and return *weighted events*. The problem is deferred to the further (detector) simulation.

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In all interesting cases, there are many interfering graphs. The interference may be the dominant effect. No single parameterization preferred.

Multi-Channel Integration

1. Generic: phase-space separation, $\sum_i w_i = 1$ and $\int dx\, g_i(x) = 1$

$$\int dx\, |a(x)|^2 = \sum_i w_i \int dx \frac{g_i(x)}{\sum_k w_k g_k(x)} |a(x)|^2$$

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2. MadEvent: Feynman diagrams, $|a|^2 = |\sum_i a_i|^2$

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3. WHIZARD: Jacobians

$$\int dx\, |a(x)|^2 = \sum_i w_i \int dy_i \frac{g_i(y_i)}{\sum_k w_k \frac{g_k(y_i)}{|dx/dy_k|}} |a(y_i)|^2$$

   adapt: weights w_k and functions g_i (by discretization: VEGAS)

Cuts and Such

Cuts: necessary for

- Finite cross section (collinear/IR divergences)
- Realistic simulation

Cuts must be defined and evaluated event by event, based on kinematics.

Scale: energy scales influence factorization, renormalization, couplings, ...– also be evaluated event by event.

Weights: define particular observables, evaluated event by event.

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Programs should be able to accomodate user-defined cuts and scales

$\Rightarrow$ Challenge for the user interface.

4. Elementary Processes: Higher Orders

Radiative Corrections

Traditionally, matrix elements were available for lowest-order processes, often just $2 \to 2$.

If we have a perturbative expansion, we can calculate radiative corrections.

1. Radiation of extra particles, typically massless

   These are handled by tree-level matrix-element generation and phase space

2. Loop corrections to the lowest-order process

   There are stand-alone programs and libraries for these virtual corrections. Loop integrals are expanded in a combination of known functions, for which numerical routines are provided.

   The relation between input parameters and observables changes if virtual corrections are considered. There is some freedom in this, corresponding to the choice of a renormalization scheme.

Divergences

If massless particles are involved (photons, gluons), radiative corrections are divergent: IR (small energy) and collinear (small angle).

Divergences cancel in the sum for (IR-safe) observables. For initial-state radiation, this involves divergences in the PDFs.

Cancellation is pointwise in theory, but real and virtual corrections in practice are integrated separately.

Subtraction schemes: add and subtract a known function, for which the integral over the extra radiated particle phase space is known. This regulates singularities in both parts.

$$\begin{aligned}\sigma &= \int dq^n \, I_n^{\text{tree}}(q) \\ &\quad + \int dq^n \quad I_n^{\text{loop}}(q) \\ &\quad + \int dq^{n+1} \, dq' \quad I_{n+1}^{\text{tree}}(q, q')\end{aligned}$$

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1. Catani-Seymour scheme
2. Frixione-Kunszt-Signer scheme
3. Other approaches

⇒ Challenges: proliferation of subtraction terms, phase-space dependence, negative contributions to the result

Loop amplitudes

Loop momentum is not observable. Evaluate integrals before considering phase space for external momenta

Usual Procedure:

1. Construct all Feynman diagrams
2. Transform into algebraic expression
3. Regularization scheme (dim.reg.)
4. Algebraic reduction to master integrals
5. Evaluation of master integrals: library of special functions
6. Combination to complete amplitude (corrections)
7. Renormalization of UV divergences
8. Subtraction of IR divergences
9. Square, integrate, transform into MC and combine with (subtracted) tree-level processes

$\Rightarrow$ External, specialized programs: Golem, OpenLoops, BlackHat, etc.

Negative weights

Results computed in strict order in perturbation theory satisfy the optical theorem only if integrated over phase space

$\Rightarrow$ the weight of an exclusive event can be negative

This occurs for kinematics (soft-collinear) where the correction is enhanced, cancelling the perturbative suppression. Subtraction can make the problem more dramatic.

Approaches:

- Drop those events. May not work (large cancellation in sum)
- Only IR-safe observables. Can't be done exactly.
- Keep weighted events. Unrealistic.
- Reweight positive and negative events separately. Also unrealistic.
- Resum multiple soft radiation. Difficult in general.

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In principle, a realistic simulation should only produce positive weights (actually, uniform weights).

5. Multiple Radiation

Multiple Radiation

Perturbation theory can be truncated at fixed order, if the expansion parameter is small.

However, even for QED and QCD at high energies (small coupling), this does not work if

- the (exclusive) observable is enhanced by the logarithm of a large scale ratio, e.g., if the p_T cut is small, the expansion is in terms of

$$\alpha \log \frac{p_T}{E} \qquad \text{or even} \qquad \alpha \log^2 \frac{p_T}{E}$$

In some cases (single scale), this logarithm is absorbed in the running coupling $\alpha_s(\mu)$.

QED Case

In QED, multiple radiation is an issue for the initial state.

(Minor scale dependence of QED coupling!)

Photon emissions commute in QED (abelian coupling), so a resummation of soft photons to all orders is just an exponentiation.

Resummation of collinear photons (which carry substantial energy) is more difficult. Skrzypek/Jadach computed an effective structure function for electrons that includes this behavior up to third order.

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$\Rightarrow$ Challenge: For ILC precision physics, we should generate (part of) those photons explicitly: unfolding the all-order resummation.

QED Case

Final-state radiation of multiple photons:
$\Rightarrow$ simular methods for resummation (YFS).

Becomes important when considering precision measurements or very exclusive observables (high accuracy in energy and momentum resolution).

QCD Parton Shower

Multiple radiation of collinear and soft gluons:

The effective running coupling increases with decreasing resolution parameter, until QCD becomes strongly interacting and we have to match quarks and gluons to hadrons.

Soft-collinear kinematics allows us to neglect quantum interferences and switch to a quasi-classical description: Markov-chain probabilistic splitting.

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- Order parameter? Angle vs. p_T, etc.
- Systematic improvement - include quantum interferences?
- Apply Sudakov enhancement factors to parton-shower emission
- Matching/merging to matrix element including virtual corrections (NLO)
- Positivity of event weights?
- Radiation from massive unstable particles
- Initial-state parton shower interleaved with multiple hadronic interactions, matched to PDF
- Matching to hadronization models

Matching and Merging

Combine fixed-order (few partons, exact kinematics) with parton shower (many partons, soft-collinear kinematics

Many different algorithms, schemes, programs available. This field changes rapidly, new ideas and significant improvements appear frequently.

- CKKW matching
- MLM matching
- GenEvA
- MC@NLO
- POWHEG
- ...

Some programs have already managed to combine automatic tree-level and subtracted one-loop corrections with and parton-shower matching/merging.

The Les Houches Accord for communicating events was aimed at this problem. Works at leading order, what to do at higher orders?

Multi-Parton Interactions

Quantum mechanics: multiple partons interacting between the two beam hadrons.

- ⇒ Most extra interactions are **soft QCD**
- ⇒ For LHC and future hadron colliders, "soft" easily exceeds 10 GeV, even 100 GeV.

Participating partons interact with each other and with the hard process (if any).

⇒ interleaved parton shower

Problem: no solid theory for extracting multiple partons from a proton.

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This kind of physics involves ad-hoc models. They are based not on QCD but on more generic principles (momentum sum rules, etc.)

Multiple Electroweak Emission

At ultra-high energies, there is no fundamental distinction between photons, gluons, W, and Z bosons.

⇒ Need also consider **multiple emission of electroweak bosons**, interleaved with QCD and photon emission.

(First studies indicate that this is not a major issue.)

6. Unstable Particles

Unstable Particles

Some particles should be considered as stable partons (w.r.t. the TeV scale), but decay immediately (w.r.t. the hadronic scale)

- $W^\pm$, Z, t, H

or within the detector

- b, c (B and D hadrons)
- τ

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Different approaches:

- Exact as **resonances**

  Gauge invariance issues, significantly complicates the matrix-element and phase-space calculation, inapplicable for long decay cascades

- Factorized with **full spin and color correlation**

  Particle width inserted afterwards (if necessary), requires spin-density formalism, bookkeeping of decay chains

- Factorized neglecting spin and/or color correlation: **isotropic decay**

  Observables may depend on correlation

7. Initial and Final State

Hadron Beams: PDF

The operator-product expansion proves that

- some pp processes can be factorized into parton-distribution functions and partonic interactions.

??? There is no proof (but evidence) that this applies to hard processes in general.

??? There is no systematic way to incorporate the corrections to factorization.

Measuring and extracting PDFs is difficult and involves theory.

Applying PDFs requires applying conventions and schemes that have been used in the PDF determination.

Modern PDF sets come with error distributions, which should be understood by MC programs.

Standard package: LHAPDF.

Lepton Beams

ILC

- Beams are strongly collimated, classical Coulomb field has an effect on the interacting electrons.

$\Rightarrow$ Described by Monte-Carlo (GuineaPig, CAIN)

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Also: crossing angle

Hadronization

Parton-Hadron Duality

Ultimately, the quarks and gluons produced by the hard interaction (and the MC generator) must be replaced by mesons and baryons.

This is a non-perturbative dynamic process. Only basic guidelines: momentum conservation, parton-hadron duality, color coherence.

Two main classes of models:

- Cluster Model Partons combined to pseudo-hadrons which decay into actual hadrons
- String Model Partons organized by color connections which break up into hadrons

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Jet data at LHC and, in particular, ILC will allow for significant refinements.
More systematic understanding? Entirely new models?

8. Interfaces

Event Formats

A Monte-Carlo generator must make its generated events available to the outside.

Old-fashioned method: external linkage and COMMON block.

- This has become unfashionable with the introduction of C++ programs. COMMON blocks are also deprecated in Modern Fortran.

Modern way: event files.

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Have to agree on format. Many "standards" exist

- HEPEVT: actually common block definition, converted into ASCII files
- StdHEP: portable binary files, C/Fortran API
- HepMC: ASCII files, C++ interface for access
- LHEF: derived from HEPEVT, includes info for matching generator/shower
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(No format is able to fully specify the spin-density matrix of, e.g., a massive vector boson.)

Event Analysis

Experimentalist's view:

I can use my (common or experiment-specific) software for detector simulation and analysis. I just want event files.

Theorist's view:

I don't manage event samples. I want my generator to present cross sections and distributions

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- ⇒ Some MC generators have built-in capabilities for event analysis and visualization. Usually parton-level oriented (but applicable to full events).
- ⇒ Modern analysis methods use matrix-element reweighting, i.e., rerunning the matrix-element computation on an existing event sample.

User Interface

For universal event generators, the organization of input and workflow is often more complex than output (event samples).
Different stages of sophistication:

1. Workflow and all but few parameters predefined by the program author. (After all, we know the Standard Model.)
2. Program runs as subprogram/library. The workflow is determined by the calling program. Parameters are transferred via argument lists (or COMMON blocks, etc.)
3. Program runs stand-alone. Parameters and settings are defined on the command line or in input files. The workflow can be organized by running the program from a script (Shell, Python).
4. Program runs interactively, command-line or with a graphical interface. Workflow, parameters and switches are directly input by the user.
5. Program runs in either way. Workflow and parameters are determined in terms of a full-fledged steering language (DSL).

From the user's perspective:

- Steer by a GUI (easily accessible, quick) or file input (reproducible, long jobs)?
- Run stand-alone or linked to some other program?
- Requires a well-defined complex directory structure, or can be used from anywhere?
- Monolithic package or client-server (central installation) model?
- Which program languages do I need? Which compiler version? Which OS?
- Running locally, on a web server, on a batch system, or on the grid?

9. Computing Issues

All MCs operate **at the limit of numerical computability**. For the core programming language, the only reasonable choices are

- FORTRAN or Modern Fortran
- C or C++

Runtime management and intermediate analytical calculations may involve additional languages

$\Rightarrow$ Shell, Make, Perl, Python, OCaml, Mathematica, Form, ...

Free compilers are available and actively maintained.

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Modern Fortran and C++ are interoperable: can be freely combined via well-defined (C) interface.

Parallel Evaluation

MC event generation is trivially parallelizable. This fact is rarely exploited to the fullest.

Opportunities:

- OpenMP parallelization on multi-core processors
- MPI parallization on shared-memory machines
- batch-cluster distribution
- C++: parallelization via library methods
- Fortran: parallelization via coarrays
- GPU parallelization

Caveat: little support by Grid software

Software Development Issues

All MC projects are maintained by freelancers, many part-time, limited term (grad students, postdocs). Projects appear and disappear ad-hoc. Collaborations are informal.

Major, universal generators are at least medium-sized on commercial scale: 100k LOC and more

MC projects cannot fully implement professional software-development mechanism, but can borrow from those:

- Software versioning and repositories (Hepforge)
- Bug tracking and ticketing system
- Portable automatic configuration (autotools)
- Automatic test suites
- Continuous integration

Success of multi-billion dollar collider projects depends on the reliability of MC generators!

Our Project: WHIZARD

The WHIZARD project aims at covering all aspects

- either by providing algorithms, exchangeable where possible
- or by interfacing external programs and libraries

as a unified framework for physics simulation.

Project leaders: Wolfgang Kilian (U Siegen), Jürgen Reuter (DESY), Thorsten Ohl (U Würzburg)

+ postdocs ($\rightarrow$ Fabian Bach) + students.

Get involved:

- Website: `whizard.hepforge.org`
- 2nd WHIZARD Forum: Castle of Würzburg, March 16-18, 2015
- The collaboration is open for new contributions and participants

10. Concluding Remarks

Issues for Developers

- MC simulation issues span the whole range of theoretical particle physics + some experimental aspects
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- Nevertheless, physics coverage is incomplete.
- Continuous exchange between experimentalists and theorists is essential.
- New ideas are important and welcome even in subjects that are stone-age.
- Managing and funding major MC projects is difficult. Rapidly changing participation, undefined role between experimental collaborations and theory groups.

Issues for Users

- The subject is complicated. Some programs pretend to be usable as Black Boxes. Often, this is misleading.
- Some results may be improved by tuning parameters. For others, the problem is in the theory.
- Compare and combine different algorithms / program packages.

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