

# High Energy Monte Carlo Generators

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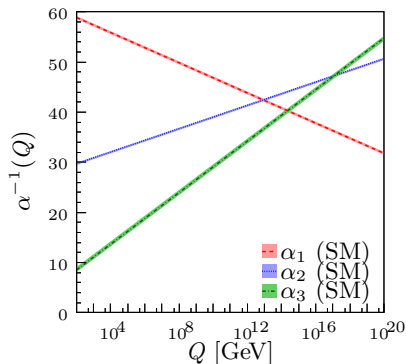
LHCb workshop on quantum interference effects, QCD measurements  
and generator tuning

# Introduction

# Monte Carlo Methods

- efficiently perform  $3n - 4$  dimensional integrals
- evolve from perturbative QFT to phenomenological models
- provides events for free

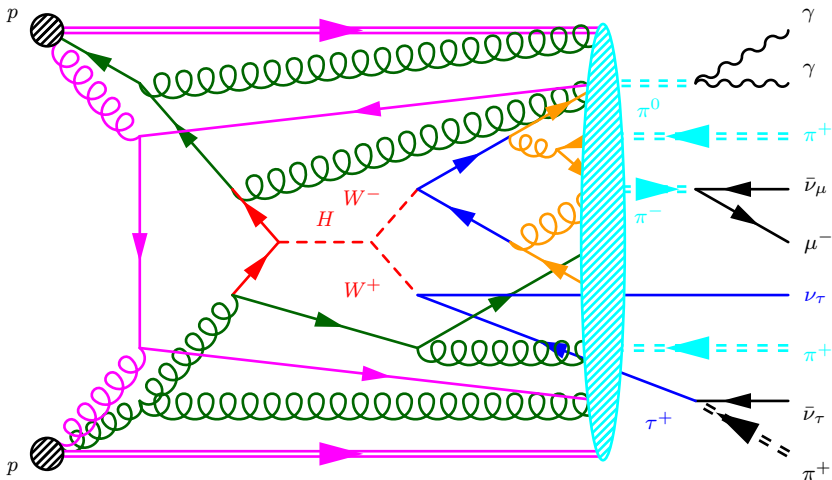
- ① generate perturbative hard process
- ② shower partons to lower energy with perturbative methods
- ③ apply phenomenological hadronization
- ④ decay particles



## Event Anatomy

1) hard process      3) ISR      5) underlying event      7) particle decays

2) resonance decays      4) FSR      6) hadronization



# Tuning Parameters

[T. Sjöstrand]

- **hard process**
  - PDFs, phase space cut-offs ( $\hat{p}_T$ ,  $\hat{m}$ ), renormalization scale, factorization scale, SM parameters (CKM,  $\alpha_s(M_Z)$ ,  $\sin \theta_W$ )
- **parton showers**
  - $\alpha_s(M_Z)$ , scales,  $p_T$  damping, matching parameters, ordering method
- **underlying event**
  - $\alpha_s(M_Z)$ , hard processes,  $p_T$  damping, beam profile (shape, impact parameter), color reconnection
- **hadronization**
  - longitudinal momentum sharing, transverse width, flavor composition, vector to pseudo-scalar composition, baryon and meson production ratios

# Observables

- test non-perturbative regimes of QCD
- tune multi purpose event generators
- look for new effects to refine models
- **hard process**
  - inclusive cross-sections
  - differential cross-sections
- **ISR**
  - light jet thrust ( $\alpha_s(M_Z)$ )
  - $p_T$  from  $Z \rightarrow \mu\mu$  (primordial  $k_T$ )
- **FSR**
  - similar to ISR
- **underlying event**
  - IR safe variables
  - energy flow
- **hadronization**
  - final state flavor composition
  - IR sensitive variables
  - charge density and multiplicity
- particle decays
  - branching fractions
  - angular and mass distributions, etc.

# Hard Processes

# Methods

- begin with rules from Lagrangian density

$$\mathcal{L}_{\text{QED}} = i\psi^\dagger \gamma_\mu \partial^\mu \psi - m\psi^\dagger \psi - iQg_e A_\mu \psi^\dagger \gamma^\mu \psi - (\partial^\mu A^\nu - \partial^\nu A^\mu) (\partial_\mu A_\nu - \partial_\nu A_\mu)$$

- build matrix element from diagrams

The diagram shows an annihilation process where an electron-positron pair ( $e^-$  and  $e^+$ ) annihilates into a virtual photon ( $\gamma$ ), which then decays into a tau-antitau pair ( $\tau^-$  and  $\tau^+$ ). The matrix element  $\mathcal{M}$  is given by:

$$\mathcal{M} = \bar{v}_{e^+} iQg_e \gamma^\mu u_{e^-} \frac{-ig_{\mu\nu}}{q^2} \bar{u}_{\tau^-} iQg_e \gamma^\nu v_{\tau^+}$$

- integrate over phase-space for partonic cross-section

$$\hat{\sigma} = \int \left( \frac{1}{8\pi} \right)^2 \frac{\langle |\mathcal{M}|^2 \rangle}{(E_{e^-} + E_{e^+})} \frac{|\vec{p}_{\mu^-}|}{|\vec{p}_{e^-}|} d\Omega$$



# Implementation

- convolute with PDFs for full cross-section

$$\sigma_{a_1 a_2 \rightarrow B} = \int \int x_{a_1}(x_{p_1}, Q^2, p_1) x_{a_2}(x_{p_2}, Q^2, p_2) \sigma_{p_1 p_2 \rightarrow B} dx_{p_1} dx_{p_2}$$

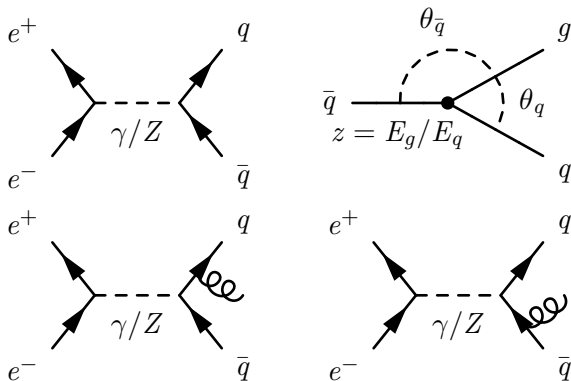
- can use a fully automated process given rules (MADGRAPH, BLACKHAT, etc.)
- in practice hard-coded averaged/summed cross-sections in  $d\hat{\sigma}/d\hat{t}$  are oftentimes used (PYTHIA, POWHEGBOX, etc.)

$$\begin{aligned} & \text{sigmagmgm} * \text{pow2}(e1 * e2) + \text{sigmagmZ} * e1 * e2 * \\ & (v1 * v2 * (1. + uH2/sH2) + a1 * a2 * \text{epsi} * (1. - uH2/sH2)) \\ & + \text{sigmaZZ} * ((v1 * v1 + a1 * a1) * (v2 * v2 + a2 * a2) \\ & * (1. + uH2/sH2) + 4. * v1 * a1 * v2 * a2 * \text{epsi} * (1. - uH2/sH2)) \end{aligned}$$

- $2 \rightarrow n$  for large  $n$  can challenge phase-space integrators

# Showers

## Example



$$d\sigma_{e^+e^- \rightarrow q\bar{q}g} \approx \sigma_{e^+e^- \rightarrow q\bar{q}} \left( \frac{2d\cos\theta_q}{\sin^2\theta_q} \right) \left( \frac{\alpha_s}{2\pi} \right) \left( \frac{N_c^2 - 1}{2N_c} \right) \left( \frac{1 + (1-z)^2}{z} \right) dz$$

## $q \rightarrow qg$ Splitting

- diverges for three scenarios
  - $z \rightarrow 0$  (soft)
  - $\theta \rightarrow 0$  (collinear to  $q$ )
  - $\theta \rightarrow \pi$  (collinear to  $\bar{q}$ )
- factorize collinear divergences as independent emissions

$$d\sigma_{e^+e^- \rightarrow q\bar{q}g} \approx \sigma_{e^+e^- \rightarrow q\bar{q}} \sum_i \left( \left( \frac{d\theta_{p_i}^2}{\theta_{p_i}^2} \right) \left( \frac{\alpha_s}{2\pi} \right) \left( \frac{N_c^2 - 1}{2N_c} \right) \left( \frac{1 + (1-z)^2}{z} \right) dz \right)$$

- generalize for all processes with splitting functions

$$d\sigma_{A \rightarrow Bb_j} \approx \sigma_{A \rightarrow B} \sum_i \left( \left( \frac{d\theta_{b_i}^2}{\theta_{b_i}^2} \right) \mathcal{P}_{b_j b_i}(z, \alpha_s) dz \right)$$

- parton  $b_i$  emits parton  $b_j$

# Splitting Functions

$$\mathcal{P}_{gq}(z, \alpha_s) = \left( \frac{\alpha_s}{2\pi} \right) \left( \frac{N_c^2 - 1}{2N_c} \right) \left( \frac{1 + (1 - z)^2}{z} \right) \quad (q \rightarrow gq)$$

$$\mathcal{P}_{gg}(z, \alpha_s) = \left( \frac{\alpha_s}{2\pi} \right) (2N_c) \left( \frac{1 - z}{z} + \frac{z}{1 - z} + z(1 - z) \right) \quad (g \rightarrow gg)$$

$$\mathcal{P}_{qg}(z, \alpha_s) = \left( \frac{\alpha_s}{2\pi} \right) \left( \frac{1}{2} \right) \left( z^2 + (1 - z)^2 \right) \quad (g \rightarrow q\bar{q})$$

$$\mathcal{P}_{qq}(z, \alpha_s) = \left( \frac{\alpha_s}{2\pi} \right) \left( \frac{N_c^2 - 1}{2N_c} \right) \left( \frac{1 + z^2}{1 - z} \right) \quad (q \rightarrow qq)$$

# Time and Spacelike Showers

- timelike showers (final state radiation)

$$\Delta_{ij}(q_1^2, q_2^2) = \exp \left( - \int_{q_2^2}^{q_1^2} \frac{1}{q^2} \int_{Q_0^2/q^2}^{1-Q_0^2/q^2} \mathcal{P}_{ji}(z, \alpha_s) dz dq^2 \right)$$

- solve for  $\Delta_{ij}(Q^2, q^2) = r \in [0, 1]$  for  $q^2$
  - if  $q^2 < Q^2$  (shower cut-off scale) terminate shower
- spacelike showers (initial state radiation)

$$\Delta_{ij}(q_1^2, q_2^2, x) = \exp \left( - \int_{q_2^2}^{q_1^2} \frac{1}{q^2} \int_{Q_0^2/q^2}^{1-Q_0^2/q^2} \mathcal{P}_{ij}(z, \alpha_s) \left( \frac{x}{zx} \right) \left( \frac{f(x/z, q^2, j)}{f(x, q^2, i)} \right) dz dq^2 \right)$$

- backwards evolution, evolve from high  $Q^2$  and small  $x$  to small  $q^2$  and large  $x$

# Matching and Merging

## Methods

LO  $n$ -jet Merging

CKKW(L)

MLM

Catani, Krauss,  
Kuhn, Webber  
hep-ph/0109231

Mangano, Moretti,  
Piccinini, Treccani  
hep-ph/0611129

- 1 calculate Sudakov factor on all lines
- 2 shower, reject emission using factor

- 1 perform shower and cluster jets
- 2 match jets to partons, reject if  $N_p \neq N_{\text{jets}}$

SHERPA

ALPGEN/HERWIG++

MADGRAPH/PYTHIA

MADGRAPH/PYTHIA

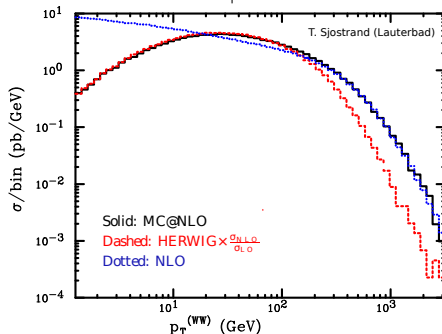
## NLO Merging

Mc@NLO

POWHEG

Frixione, Webber  
hep-ph/0402116

Frixione, Nason,  
Oleari  
0709.2092





## MC@NLO

- ① calculate NLO corrections to  $n$ -body process
- ② calculate first shower emission
- ③ break event into NLO  $\mathcal{ME}$  – first emission, remainder
- ④ apply showers to both parts of event

Advantages:

- NLO variables
- smooth matching with  $\mathcal{PS}$
- large number of processes

Disadvantages:

- negative weighting

$$pp \rightarrow (Z/\gamma^* \rightarrow) l_{\text{IL}} \bar{l}_{\text{IL}} + X$$

$$pp \rightarrow (W^+ \rightarrow) l_{\text{IL}}^+ \nu_{\text{IL}} + X$$

$$pp \rightarrow Z^0 + X$$

$$pp \rightarrow H^0 + X$$

$$pp \rightarrow t/\bar{t} + X$$

$$pp \rightarrow tW^-/\bar{t}W^+ + X$$

$$pp \rightarrow tH^-/\bar{t}H^+ + X$$

$$pp \rightarrow H^0 W^+ + X$$

$$pp \rightarrow H^0 (W^- \rightarrow) l_i^- \bar{\nu}_i + X$$

$$pp \rightarrow W^+ W^- + X$$

$$pp \rightarrow W^- Z^0 + X$$

$$pp \rightarrow (Z \rightarrow) l_{\text{IL}} \bar{l}_{\text{IL}} + X$$

$$pp \rightarrow (W^- \rightarrow) l_{\text{IL}}^- \bar{\nu}_{\text{IL}} + X$$

$$pp \rightarrow W^+ + X$$

$$pp \rightarrow b\bar{b} + X$$

$$pp \rightarrow \bar{t} + X$$

$$pp \rightarrow \bar{t} W^+ + X$$

$$pp \rightarrow \bar{t} H^+ + X$$

$$pp \rightarrow H^0 (W^+ \rightarrow) l_i^+ \nu_i + X$$

$$pp \rightarrow H^0 Z + X$$

$$pp \rightarrow Z^0 Z^0 + X$$

$$pp \rightarrow (\gamma^* \rightarrow) l_{\text{IL}} \bar{l}_{\text{IL}} + X$$

$$pp \rightarrow \gamma^* (\rightarrow \sum_i f_i \bar{f}_i) + X$$

$$pp \rightarrow W^- + X$$

$$pp \rightarrow t\bar{t} + X$$

$$pp \rightarrow t + X$$

$$pp \rightarrow tW^- + X$$

$$pp \rightarrow tH^- + X$$

$$pp \rightarrow H^0 W^- + X$$

$$pp \rightarrow H^0 (Z \rightarrow) l_i \bar{l}_i + X$$

$$pp \rightarrow W^+ Z^0 + X$$

# POWHEG

- ① pick largest  $p_T$  emission from NLO normalized  $\mathcal{M}\mathcal{E}$
- ② evolve shower downwards to  $p_T$  scale

Advantages:

- positive weights
- separation of shower

Disadvantages:

- designed for  $p_T$  ordered showers

HERWIG++		POWHEGBox
$pp \rightarrow H$	$pp \rightarrow W$	$pp \rightarrow Z$
$pp \rightarrow HW$	$pp \rightarrow W + \text{jet}$	$pp \rightarrow Z + \text{jet}$
$pp \rightarrow ZH$	$pp \rightarrow t$	$pp \rightarrow tW$
$pp \rightarrow W$	$gg \rightarrow H$	$pp \rightarrow VV \rightarrow H$
$pp \rightarrow Z$	$pp \rightarrow \text{jet} + \text{jet}$	$pp \rightarrow t\bar{t}$
	$pp \rightarrow WW + \text{dijet}$	$pp \rightarrow WW$
	$pp \rightarrow WZ$	$pp \rightarrow ZZ$
	$pp \rightarrow b\bar{b}WW$	

## More Methods

- UMEPS
  - unitarized matrix element and parton shower merging
  - tree-level  $n$ -leg merging without inclusive cross-section modification
- NL<sup>3</sup>
  - Nils Lavesson and Leif Lönnblad
  - $n$ -leg merging at NLO
- UNLOPS
  - unitarized next-to-leading-order parton shower
  - $n$ -leg merging at NLO but more generalized
- FxFX
  - R. Frederix and S. Frixione
  - merging and matching of MC@NLO

# Multi Parton Interactions

## Models

hard  $\rightarrow$  soft model (HEP)

- begin with  $t$ -channel  $2 \rightarrow 2$  QCD

$$d\hat{\sigma}_{2 \rightarrow 2} \propto dp_{\text{T}}^2 \frac{\alpha_s^2(p_{\text{T}}^2)}{p_{\text{T}}^4}$$

- divergent in  $p_{\text{T}}$ , cut-off or damp

$$\frac{\alpha_s^2(p_{\text{T}0}^2 + p_{\text{T}}^2)}{\alpha_s^2(p_{\text{T}}^2)} \frac{p_{\text{T}}^4}{(p_{\text{T}0}^2 + p_{\text{T}}^2)^2}$$

- models color screening and saturation effects
- number of interactions also depends on impact parameter

$$f(x, b) = f(x)g(b)$$

soft  $\rightarrow$  hard model (air-shower)

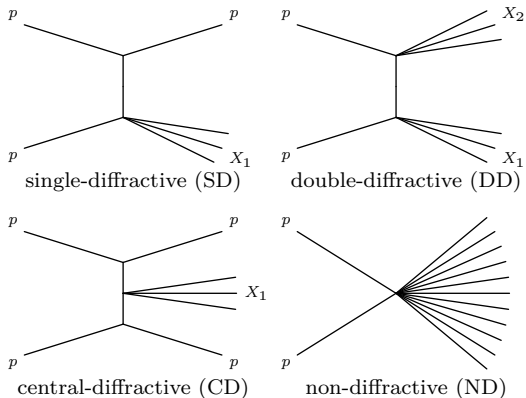
- begin with Regge effective field theory

$$d\sigma \propto \frac{dM^2}{M^2}$$

- $M$  is mass of the diffractive system
- exchange of color-singlet pomeron between hadrons
  - leading structure is  $f\bar{f}$  or  $gg$
  - at high energy primarily  $gg$
- include hard structure by resolving pomeron constituents
- requires some smooth transition between the two regimes

## Event Classification

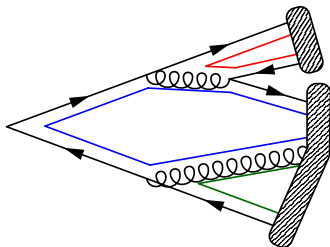
$$\sigma_{\text{inelastic}} = \sigma_{\text{SD}} + \sigma_{\text{DD}} + \sigma_{\text{CD}} + \sigma_{\text{ND}}$$



# Hadronization

## Models

string model (PYTHIA)

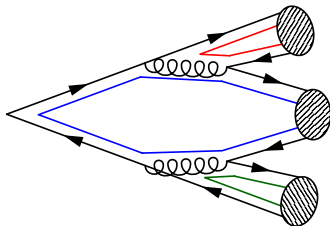


- linear confinement

$$V \approx \kappa r - \frac{4\alpha_s}{3r}$$

- split strings into hadrons
- kinematics well modeled
- poor final state flavor description

cluster model (HERWIG)



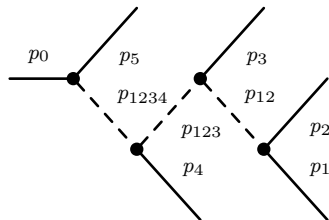
- pre-confinement
  - clusters independent of hard process scale
  - dependent on QCD and shower scale
- decay clusters into hadrons
- kinematics not as well modeled
- better final state flavor description



# Particle Decays

# Phase Space

- RAMBO
  - random momenta and boost
  - requires massless decay products
- $m$ -generator
  - mass generator
  - two-body decays through intermediate masses



$$\begin{aligned}
 d\Phi_2(q_0, q_1, q_2) &= \left( \frac{1}{(2\pi)^2 2^2} \right) \delta(q_0 - q_1 - q_2) \frac{d\vec{q}_1}{E_1} \frac{d\vec{q}_2}{E_2} \\
 d\Phi_3(q_0, q_1, q_2, q_3) &= \left( \frac{1}{(2\pi)^5 2^3} \right) \delta(q_0 - q_1 - q_2 - q_3) \frac{d\vec{q}_1}{E_1} \frac{d\vec{q}_2}{E_2} \frac{d\vec{q}_3}{E_3} \\
 &\quad \delta(q_{12} - q_1 - q_2) \delta(q_{12}^2 - m_{12}^2) dq_{12} dm_{12}^2 \\
 &= \left( \frac{2}{\pi} \right) d\Phi_2(q_0, q_{12}, q_3) m_{12} dm_{12} d\Phi_2(q_{12}, q_1, q_2)
 \end{aligned}$$

# Helicity Correlations

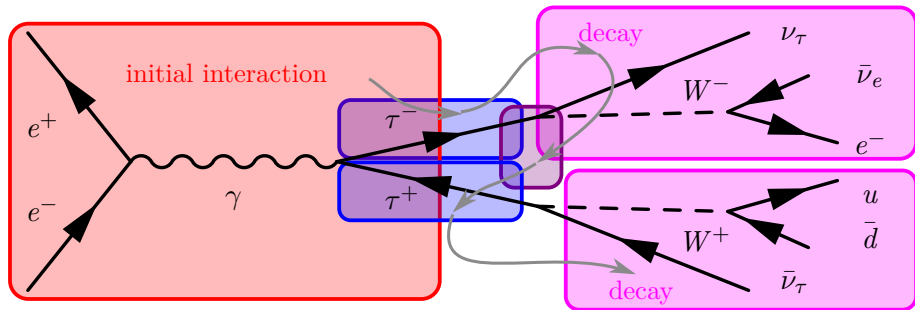
- algorithm by Collins and Knowles, expanded by Richardson
  - $D \equiv$  decay matrix for each particle,  $D_{\text{initial}} = \mathbb{I}$
  - $\mathcal{M} \equiv$  matrix element,  $\rho \equiv$  density matrix
- ① Calculate  $\mathcal{M}$  for the initial interaction.
  - ② Find  $\rho$  for an outgoing particle using the interaction  $\mathcal{M}$  and  $D$ 's of the remaining outgoing particles.
  - ③ Decay the particle using its  $\mathcal{M}$ ,  $\rho$ , and the  $D$ 's of its decay products.
  - ④ Repeat ② - ③ until all decay products are stable.
  - ⑤ Calculate  $D$  for the particle.
  - ⑥ Go up a decay and perform ② - ⑤ on the undecayed particles.
  - ⑦ Repeat ② - ⑥ until all particles are decayed.

## Example

$$\textcircled{2} \rho_{\lambda_j \lambda'_j}^j = \rho_{\kappa_1 \kappa'_1}^1 \rho_{\kappa_2 \kappa'_2}^2 \mathcal{M}_{\kappa_1 \kappa_2; \lambda_1 \dots \lambda_n} \mathcal{M}_{\kappa'_1 \kappa'_2; \lambda'_1 \dots \lambda'_n}^* \prod_{k \neq j} D_{\lambda_k \lambda'_k}^k$$

$$\textcircled{3} \mathcal{W}_{\text{decay}} = \rho_{\lambda_0 \lambda'_0} \mathcal{M}_{\lambda_0; \lambda_1 \dots \lambda_n} \mathcal{M}_{\lambda'_0; \lambda'_1 \dots \lambda'_n}^* \prod_{k=1, n} D_{\lambda_k \lambda'_k}^k$$

$$\textcircled{5} D_{\lambda_0 \lambda'_0} = \mathcal{M}_{\lambda_0; \lambda_1 \dots \lambda_n} \mathcal{M}_{\lambda'_0; \lambda'_1 \dots \lambda'_n}^* \prod_{l=1, n} D_{\lambda_l \lambda'_l}^l$$



# Tools

(by no means exhaustive)

# Resources

- HEPFORGE
  - <https://www.hepforge.org/>
  - collection of high energy physics tools
  - primarily MC related, not exhaustive but most complete available list
- *General-purpose event generators for LHC physics*
  - <http://arxiv.org/abs/1101.2599>
  - Buckley, Butterworth, Gieseke, Grellscheid, Höche, Hoeth, Krauss, Lönnblad, Nurse, Richardson, Schumann, Seymour, Sjöstrand, Skands, Webber
  - excellent review of current (relatively) MC techniques
- *QCD and Collider Physics* (the big pink book)
  - <http://www.hep.phy.cam.ac.uk/theory/webber/QCDupdates.html>
  - Ellis, Stirling, Webber
  - more detailed theoretical study of phenomenology

# Legacy General Purpose

- PYTHIA 6
  - <https://pythia6.hepforge.org/>
  - named after the oracle of Delphi
  - written in FORTRAN
  - most recent version is 6.4.28 released 05/09/2013
  - Lund string fragmentation model
  - no longer actively developed, now superseded by PYTHIA 8
- HERWIG
  - <http://www.hep.phy.cam.ac.uk/theory/webber/Herwig/>
  - Hadron Emission Reactions With Interfering Gluons
  - written in FORTRAN
  - most recent version is 6.5.21 released 11/03/2013
  - interface to MC@NLO
  - no longer actively developed, now superseded by HERWIG++

# Current General Purpose

- PYTHIA 8
  - <http://home.thep.lu.se/~torbjorn/Pythia.html>
  - written in C++
  - most recent version is 8.201 released 14/10/2014
  - comprehensive merging and matching schemes, interfaces well with most hard process generators
- HERWIG++ and THEPEG
  - <https://herwig.hepforge.org/>
  - written in C++
  - most recent version is 2.7.1/1.9.2 released 07/07/2014
  - fully automated LO BSM with helicity correlations
- SHERPA
  - <https://sherpa.hepforge.org>
  - written in C++
  - most recent version is 2.1.1 released 06/06/2014
  - automated LO  $n$ -leg hard processes with COMIX and AMEGIC



# Hard Coded Hard Process

- POWHEGBOX
  - <http://powhegbox.mib.infn.it/>
  - written in FORTRAN
  - most recent version is 2 released 29/03/2011 (but rolling in SVN)
  - structure for user written processes, large number of processes
- MC@NLO
  - <http://www.hep.phy.cam.ac.uk/theory/webber/MCatNLO/>
  - written in FORTRAN
  - most recent version is 4.10 released 17/07/2013
  - large number of processes, cohesive user interface
  - AMC@NLO focus of current development
- MCFM
  - <http://mcfm.fnal.gov/>
  - Monte Carlo for FeMtobarn processes
  - written in FORTRAN
  - most recent version is 6.8 released 26/04/2014

# Automated Hard Process

- BLACKHAT
  - <http://blackhat.hepforge.org/>
  - written in C++
  - still in beta
  - $n$ -leg with one-loop in QCD
- MADGRAPH 5
  - <http://madgraph.hep.uiuc.edu/>
  - written in FORTRAN, PYTHON, and C++
  - most recent version is 2.2.1 released 25/09/2014
  - $n$ -leg with one-loop in QCD and QED with AMC@NLO
  - can be showered with PYTHIA 8 using FxFx

# After-burners

- TAUOLA
  - <http://taulapp.web.cern.ch/taulapp/>
  - written in FORTRAN and C++
  - most recent version is 1.1.5 release 04/06/2014
  - tau decays
- PHOTOS
  - <http://photospp.web.cern.ch/photospp/>
  - written in FORTRAN and C++
  - most recent version is 3.65 released 03/05/2014
  - QED FSR emissions
- EVTGEN
  - <http://evtgen.warwick.ac.uk/>
  - written in C++
  - most recent version is 1.3.0 released 01/10/2014
  - $B$  and  $D$  decays

# Conclusions

# MC at LHCb

- generation was primarily through PYTHIA 6, migrated to PYTHIA 8
- use case very different from other experiments, care primarily about  $B$  and  $D$  decays
- mainly use minbias with EVTGEN on top
- focus not on hard processes, but do have POWHEGBOX and ALPGEN interfaced with PYTHIA 6 showers
- also have HERWIG++ interfaced

# Outlook

- very active MC community and development
- large variety of tools available
- pick your tools carefully!
- exciting developments in automated process calculation and shower matching/merging