Introduction to Monte Carlo generators - II (Fully exclusive modeling of high-energy collisions)

Andrzej Siódmok





CTEQ School - University of Pittsburgh, USA 18 - 28 July 2017

Thanks to: S. Gieseke, S.Höche, F. Krauss, L. Lonnblad, W. Placzek, S. Prestel, M. H. Seymour, T. Sjöstrand, P. Skands, M. Schönherr, B. Webber

Reminder: Building blocks of Monte Carlo Generators



taken from Stefan Gieseke®

The general approach is the same in different programs but the models and approximations used are different.



- ► 1st lecture
 - Monte Carlo methods why and how?
 - Parton Shower
- 1st tutorial
 - Build your own Parton Shower (in Python)!
- 2nd lecture
 - Hadronization
 - Multiple Parton Interaction
 - Tuning
- 2nd tutorial
 - Shower uncertainties (in Python) or
 - MC@NLO/POWHEG (see Marek's lecture) matching in Python
- 3rd tutorial
 - ▶ Real life example work with Herwig, Sherpa and Pythia!

Hadronization

Hadronization (non-perturbative semi-empirical models)



Two main models: Lund string model and Cluster model also older: Flux tube model and Independent fragmentation (Feynman-Field fragmentation '78)

- Hadronization factorizes from hard process (process-independent)
- Both main models contain many parameters to be determined from data, preferably LEP.

Lund String model

[Andersson, Gustafson, Ingelman, Sjostrand] Phys. Rept. 97(1983)31

Originally invented without parton showers in mind.



We start with 2-jet events in $e^+e^- \rightarrow$ hadrons. Lund string model: like rubber band that is pulled apart and breaks into pieces, or like a magnet broken into smaller pieces.

Lund model - Physical motivation

Self coupling of gluons ↔ "attractive field lines"

Linear static potential $V(r) \approx \kappa r$.



 $\kappa = 1 \text{ GeV/fm} \sim \text{potential energy gain lifting a 16 ton truck.}$ Flux tube uniform traversal shape (in the central region) $\rightarrow \text{simple}$ description as a 1+1 - dimensional object - a string Lund string: like rubber band that is pulled apart and breaks into pieces



Lund model - string motion

As a $q\bar{q}$ pair moves apart, they are slowed down and more and more energy is stored in the string.

If the energy is small, the $q\bar{q}$ pair will eventually stop and move together again. We get a "YoYo" - state which we interpret as a meson.

If high enough energy, the string will break as the energy in the string is large enough to create a new $q\bar{q}$ pair.



Assume negligibly small quark masses. Then linearity between space-time and energy-momentum gives:

$$\left|\frac{\mathrm{d}E}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}E}{\mathrm{d}t}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}t}\right| = \kappa$$

Combine yo-yo-style string motion with string breakings. Motion of quarks and antiquarks with intermediate string pieces.



A quarks from one string break combines with a antiquarks from an adjacent one.

How does the string break?

The quarks obtain a mass and a transverse momentum in the breakup through a tunneling mechanism



Probablity of tunneling:

$$\mathcal{P} \propto \exp\left(-rac{\pi m_{\perp \mathrm{q}}^2}{\kappa}
ight) = \exp\left(-rac{\pi p_{\perp \mathrm{q}}^2}{\kappa}
ight) \, \exp\left(-rac{\pi m_\mathrm{q}^2}{\kappa}
ight)$$

- Suppression of heavy quarks: $u\bar{u} : d\bar{d} : s\bar{s} : c\bar{c} \approx 1 : 1 : 0.3 : 10^{-11}$
- ▶ Diquark (qq qq̄ breakups) ~ antiquark ⇒ simple model for baryon production.

String model has very good energy-momentum picture however it is unpredictive in understanding of hadron mass effects \Rightarrow many parameters, 10-20 depending on how you count.

The Lund model - gluons



The Lund string model predicted the string effect measured by Jade. In a three-jet event there are more energy between the gq and $g\bar{q}$ jets than between $q\bar{q}$.

[Webber NPB238(1984)492]

What if we have PS (more perturbative input before hadronization). Can we get a simpler model? Cluster Model:



- QCD parton showers provide pre-confinement of colour:
- Planar approximation: gluon = colour-anticolour pair

[Webber NPB238(1984)492]

What if we have PS (more perturbative input before hadronization). Can we get a simpler model? Cluster Model:



- QCD parton showers provide pre-confinement of colour:
- Planar approximation: gluon = colour-anticolour pair
- colour-singlet pairs end up close in phase space and form highly excited hadronic states, the *clusters*
- Clusters (~ excited hadrons) decay into hadrons

Mass spectrum of colour-singlet pairs asymptotically independent of energy, production mechanism $_{13/63}$

Cluster model - Mass spectrum

Mass spectrum of primordial clusters independent of cm energy.



Peaked at low mass (1-10 GeV) typically decay into 2 hadrons. Project colour singlets onto continuum of high-mass mesonic resonances (clusters). Decay to lighter well-known resonances and stable hadrons.

- ► Although cluster mass spectrum peaked at small *m*, broad tail at high *m*.
- Small fraction of clusters too heavy for isotropic two-body decay to be a good approximation
- ► heavy cluster decay first (Longitudinal cluster fission) into lighter cluster, or radiate a hadron C → CC C → HC, it is rather



string-like.

 $\blacktriangleright ~ \sim 15\%$ of primary clusters get split but $\sim 50\%$ of hadrons come from them!

Hadronization - comparison of the model

Taken from T. Sjöstrand

B^0 B^0 K^+ g F^- G K^- K^- π^+ T^+ $\overline{\Lambda^0}$ D_s^-		
program	PYTHIA	Herwig
model	string	cluster
energy–momentum picture	powerful	simple
	predictive	unpredictive
parameters	few	many
flavour composition	messy	simple
	unpredictive	in-between
parameters	many	few

Multiple Particle Interaction



How do we know MPI exists? Data makes you smarter!

UA5 experiment at the SPS - proton-antiproton 540 GeV c.m.







FIG. 12. Charged-multiplicity distribution at 540 GeV, UA5 results (Ref. 32) vs multiple-interaction model with variable impact parameter: solid line, double-Gaussian matter distribution; dashed line, with fix impact parameter [i.e., $\bar{O}_0(b)$].

Sjöstrand & v. Zijl, Phys.Rev.D36(1987)2019

Direct observation of multiple interactions

Five studies: AFS (1987), UA2 (1991), CDF (1993, 1997), D0 (2009)

 $\begin{array}{l} \mbox{Order 4 jets } p_{\perp 1} > p_{\perp 2} > p_{\perp 3} > p_{\perp 4} \mbox{ and define } \varphi \\ \mbox{as angle between } p_{\perp 1} \mp p_{\perp 2} \mbox{ and } p_{\perp 3} \mp p_{\perp 4} \mbox{ for AFS/CDF} \end{array}$

Double Parton Scattering

Double BremsStrahlung





21 / 63

CDF Run II On event-by-event basis: π AWAY 1) Identify the leading object in the event 2) Build TRANSVERSE REGIONS w.r.t. it Leading-track TOWARDS 3) Compute Σp_T of charged particles (or multiplicity) in the different regions φ TOWARD SETTINGS: • pT > 0.5 GeV/c TRANSVERSE (tracks and leading-track) AWAY AWAY $-\pi$ · leading-track not included η in distributions

22 / 63

 $\Delta \phi$

TRANSVERSE

CDF Run II Good description of Run I Underlying event data ($\chi^2 = 1.3$).



Motivation:

- The minimum bias/underlying event is an unavoidable background to most collider observables and having good understand of it leads to more precise collider measurements!
- First LHC results are Minimum Bias and Underlying Event! Alice: [0911.5430], CMS [1002.0621], ATLAS [1003.3124] so it must be important ;)
- These will be particularly relevant for the LHC as, when it is operated at design luminosity, rare signal events will be embedded in a background of more than 20 near-simultaneous minimum-bias collisions.
- Any realistic experiment simulation event generator needs to be able to model these effects.
- "Don't worry, we will measure and subtract it" But... fluctuations and correlations on an event-by-event basis are crucial.

MPI model basics

Inclusive hard jet cross section in pQCD:

$$\sigma^{\rm inc}(s, p_t^{\rm min}) = \sum_{i,j} \int_{p_t^{\rm min^2}} dp_t^2 \int dx_1 dx_2 \ f_i(x_1, Q^2) f_j(x_2, Q^2) \ \frac{d\hat{\sigma}_{i_j}}{dp_t^2}$$



 $\sigma^{\rm inc} > \sigma_{\rm tot}$ eventually

Interpretation:

- σ^{inc} counts all partonic scatters in a single *pp* collision
- more than a single interaction

$$\sigma^{\rm inc} = \langle n_{\rm dijets} \rangle \sigma_{\rm inel}$$

MPI model basics (Herwig++)

Assumptions:

а

the distribution of partons in hadrons factorizes with respect to the b and x dependence \Rightarrow average number of parton collisions:

$$\begin{split} \bar{n}(\vec{b},s) &= L_{\text{partons}}(x_1, x_2, \vec{b}) \otimes \sum_{ij} \int dp_t^2 \frac{d\hat{\sigma}_{ij}}{dp_t^2} \\ &= \sum_{ij} \frac{1}{1 + \delta_{ij}} \int dx_1 dx_2 \int d^2 \vec{b}' \int dp_t^2 \frac{d\hat{\sigma}_{ij}}{dp_t^2} \\ &\times D_{i/A}(x_1, p_t^2, |\vec{b}'|) D_{j/B}(x_2, p_t^2, |\vec{b} - \vec{b}'|) \\ &= \sum_{ij} \frac{1}{1 + \delta_{ij}} \int dx_1 dx_2 \int d^2 \vec{b}' \int dp_t^2 \frac{d\hat{\sigma}_{ij}}{dp_t^2} \\ &\times f_{i/A}(x_1, p_t^2) G_A(|\vec{b}'|) f_{j/B}(x_2, p_t^2) G_B(|\vec{b} - \vec{b}'|) \\ &= A(\vec{b}) \sigma^{\text{inc}}(s; p_t^{\text{min}}) . \end{split}$$
at fixed impact parameter b, individual scatterings are independent (leads to the Poisson distribution)

Eikonal model basics

From assumptions:

- at fixed impact parameter b, individual scatterings are independent,
- the distribution of partons in hadrons factorizes with respect to the b and x dependence.

we get the average number of partonic collisions at a given b value is

$$\bar{n}(b,s) = A(b)\sigma^{inc}(s; p_t^{\min}) = 2\chi(b,s)$$

where A(b) is the partonic overlap function of the colliding hadrons



 \Rightarrow Two main parameters: μ^2 , p_t^{\min} .

Good description of Run I Underlying event data ($\chi^2 = 1.3$).



Hot Spot model

Extension to soft MPI, $p_t < p_t^{\min}$

Fix the two parameters μ_{soft} and $\sigma_{\mathrm{soft}}^{\mathrm{inc}}$ in

$$n_{\text{tot}}(\vec{b},s) = \left(A(\vec{b};\mu)\sigma^{\text{inc}}\text{hard}(s;p_t^{\min}) + A(\vec{b};\mu_{\text{soft}})\sigma^{\text{inc}}_{\text{soft}}\right)$$

from two constraints. Require simultaneous description of σ_{tot} and b_{el} (measured/well predicted),

$$\begin{split} \sigma_{\text{tot}}(s) &\stackrel{!}{=} 2 \int d^2 \vec{b} \left(1 - e^{-\chi_{\text{tot}}(\vec{b},s)} \right) \,, \\ b_{\text{el}}(s) &\stackrel{!}{=} \int d^2 \vec{b} \frac{b^2}{\sigma_{\text{tot}}} \left(1 - e^{-\chi_{\text{tot}}(\vec{b},s)} \right) \end{split}$$

٠

Extension to soft MPI, $p_t < p_t^{\min}$

Continuation of the differential cross section into the soft region $p_t < p_t^{\min}$ (here: p_t integral kept fixed)



Detailed look at observables: Transverse Region



Notice Jet pedestal effect.

Look at LHC results (900 GeV)

► ATLAS charged particles in Min Bias ($N_{ch} \ge 1$, $p_T > 500 MeV$, $|\eta| < 2.5$)



oops, not so nice...

- despite very good agreement with Rick Field's CDF UE analysis.
- choice of PDF set (CTEQ61l vs MSTW LO** (our default))
- Failure of a physically motivated model usually points to more, interesting physics ... colour structure?

Colour Structure of the Underlying Event

Colour Structure of the Underlying Event multiple interactions, even when soft, can cause non-trivial changes to the colour topology of the colliding system as a whole, with potentially major consequences for the particle multiplicity in the final state

Each MPI (or cut Pomeron) exchanges color between the beams

The colour flow determines the hadronizing string topology

· Each MPI, even when soft, is a color spark

Siöstrand & PS. IHEP 03(2004)053

• Final distributions <u>crucially</u> depend on color space



Colour Structure of the Underlying Event

Colour Structure of the Underlying Event multiple interactions, even when soft, can cause non-trivial changes to the colour topology of the colliding system as a whole, with potentially major consequences for the particle multiplicity in the final state

Each MPI (or cut Pomeron) exchanges color between the beams

The colour flow determines the hadronizing string topology

- Each MPI, even when soft, is a color spark
- Final distributions crucially depend on color space



Colour reconnection (CR) in Herwig++



Extending Herwig's hadronization model:

 ▶ QCD parton showers provide *pre-confinement* ⇒ colour-anticolour pairs form highly excited hadronic states, the *clusters*

Colour reconnection (CR) in Herwig++



Extending Herwig's hadronization model:

- ▶ QCD parton showers provide *pre-confinement* ⇒ colour-anticolour pairs form highly excited hadronic states, the *clusters*
- ► CR in the cluster hadronization model: allow *reformation* of clusters, *e.g.* (*il*) + (*jk*)
- Physical motivation: exchange of soft gluons during non-perturbative hadronization phase

Implementation

Allow CR if the cluster mass decreases,

$$M_{il} + M_{kj} < M_{ij} + M_{kl},$$

where $M_{ab}^2 = (p_a + p_b)^2$ is the (squared) cluster mass

► Accept alternative clustering with probability p_{reco} (model parameter) ⇒ this allows to switch on CR smoothly

MinBias ATLAS 900 GeV



MinBias ATLAS 900 GeV



Underlying event in Herwig++ - key components







Possibility of change of color structure (color reconnection)

[Gieseke, Röhr, AS, EPJC 72 (2012)]

The least understood part of modeling

Based on electromagnetic form factor (radius of the proton free parameter)

Main parameters:

- μ^2 inverse hadron radius squared (parametrization of overlap function)
- ▶ p_t^{\min} transition scale between soft and hard components $\Rightarrow p_t^{\min} = p_{t,0}^{\min} \left(\frac{\sqrt{s}}{F_0}\right)^b$
- *p_{reco}* colour reconnection

Underlying event in Herwig++ - key components



Based on electromagnetic form factor (radius of the proton free parameter)

Pythia:

- Many options including double Gaussian (similar shape to EE)

- x-depended overlap [Corke,

Sjostrand, JHEP 1105:009]



Pythia:

Regularise cross section with p_t^{\min} as

free parameter:

$$\frac{d\sigma}{lp_T^2} \propto \frac{\alpha^2(p_T^2)}{p_T^4} \rightarrow \frac{\alpha^2(p_T^2 + p_t^{\min^2})}{(p_T^2 + p_t^{\min^2})^2}$$





Possibility of change of color structure (color reconnection) [Gieseke, Röhr, AS, EPJC 72 (2012)] The least understood part of modeling (very active area research)

Pythia:

Recent development: String

Formation Beyond Leading Colour J.

Christiansen, P. Skands

[arXiv:1505.01681]

Herwig++ MPI model with independent hard and soft processes, showered and with colour reconnection. Just few parameters. Min bias without integrated diffraction (work in progress).

Pythia MPI interleaved with showering. MPI ordered in p_T . The most sophisticated model. Many options and parameters (Pythia has strong emphasis on NP physics) \Rightarrow many tune families.

Sherpa New model - SHRiMPS with integrated diffraction based on KMR (Khoze-Martin-Ryskin model). Model in development currently not suitable for UE studies (work in progress - this winter?). Currently for UE there is "cheap version of Pythia's UE model" (F. Krauss)

UE measurements - Energy Overview



Run II results - UE [ATL-PHYS-PUB-2015-019]



Many LHC UE observables (not tuned since not available) and well described by most of the models!

Problems - very soft MinBias ATLAS



Need of the colour reconnection.

Problems - very soft MinBias ATLAS



Need of the colour reconnection. MB 7000 TeV, problem at low p_T , high Nch (CMS ridge)

Problems - Identified particles



More plots: mcplots.cern.ch



- MC models have parameters such as pT cutoff, energy evolution, colour-reconnection... + many parameters of hadronization models
- ► Tuning (fixing) of parameters required to constrain models
- No unique way of tuning: which data samples should be used? Divide and conquer (split parameters in subgroups which can be tune separately) ...
- "manual" tunning hard and inefficient lots of man and CPU power needed.
- new tools help to automatize this process -> however still you need to think it is not "Fire-and-forget"

Tuning

Rivet and Professor



Rivet and Professor

TUNING PROCEDURE IN PROFESSOR (1D, 1BIN)

- **()** Random sampling: *N* parameter points in *n*-dimensional space
- 2 Run generator and fill histograms
- For each bin: use N points to fit interpolation (2nd or 3rd order polynomial)
- Construct overall (now trivial) $^2 \approx \sum_{bins} \frac{(interpolation-data)^2}{error^2}$
- o and Numerically minimize pyMinuit, SciPy





4/16

NOnet

Tuning

Tuning

Rivet and Professor





Rivet and Professor Observables and Weights

- This is what Professor minimises: $\chi^2(\vec{p}) = \sum_{\mathcal{O}} \sum_{b \in \mathcal{O}} \frac{W_b}{W_b} \frac{(f^{(b)}(\vec{p}) \mathcal{R}_b)^2}{\Delta_k^2}$
- Slightly more art than science
- Garbage in, garbage out
- Use weights wb to:
 - emphasize certain observables
 - emphasize certain bins of an observable
 - switch off single bins (e.g. MinBias region for Jimmy Herwig)
- No MinBias physics in Jimmy Herwig
- Cannot get first 3 bins or so right
- Transition from MinBias to UE type physics
- ⇒ Exclude these bins from Professor minimisation



Semi hard underlying event

Taken from Peter Skands:





🏠 🛇 🔿 🕂 🧭 🛱 🔚

10 pperp (leading track) [GeV] 15



10 pperp (leading track) [GeV] 15



🏠 🔘 🕀 🗲 👘 🔚

Obs 1: /ATLAS_2010_S8	894728/d02-x01-y01 🛟 🗌 logx 🗌 logy	Ratio	/ATLAS_2010_S8894728/d04-x01-y01 🛟 🗌 logx 🗌 logy 🛛				Ratio	
ColourDisrupt		0.4826		Limits 1:		Limits 2:		Show GoF
InverseRadius		1.9990	Set params	AMIN	None	AMIN	None	🗹 Show ref data
KtMin		3 8907	Precision:	XMax	None	XMax	None	Nil
ReconnectionProbability		0.0001	÷.	. YMin	None	YMin	None	
int Dt		0.4753	Reset limits	1 YMax	None	YMax	None	
intert		2.3710	Dense Kouite (
			Reset limits .					

Colour reconnections in Herwig++ [Gieseke, Röhr, AS, Eur.Phys.J. C72 (2012) 2225]

$$f_a(m_{cut}) \equiv N_a(m_{cut}) / \sum_{b=h,i,n} N_b(m_{cut}) = \frac{N_a(m_{cut})}{N_{cl}},$$
 (1)



Since these n-clusters can lie at very different rapidities (the extreme case being the two opposite beam remnants), the strings or clusters spanned between them can have very large invariant masses (though normally low pT), and give rise to large amounts of (soft) particle production.

Colour reconnections in Herwig++ [Gieseke, Röhr, AS, Eur.Phys.J. C72 (2012) 2225]

$$f_a(m_{cut}) \equiv N_a(m_{cut}) / \sum_{b=h,i,n} N_b(m_{cut}) = \frac{N_a(m_{cut})}{N_{cl}},$$
 (1)



Since these n-clusters can lie at very different rapidities (the extreme case being the two opposite beam remnants), the strings or clusters spanned between them can have very large invariant masses (though normally low pT), and give rise to large amounts of (soft) particle production.







Summary:

- Tremendous amount of new developments in GPMCs.
- Parton showers well established.
- Hard matrix element "NLO revolution" and more see Marek's lectures.
- Hadronization crucial to obtain fully exclusive simulation of the collisions. Two main models: string and cluster.
- MPI models under constant improvement (new MPI model Shrimps in Sherpa, improvements in Pythia and Herwig, for LHC)!
- Good first round of LHC data well described...
- ... but still a lot space for improvements.
- Not-too-soft not-too-high-multiplicity physics under good control (if you use modern models with modern tunes).

- Event generators crucial since the start of LHC studies.
- Qualitatively predictive already 25 years ago
- Quantitatively steady progress, continuing today:
 - continuous dialogue with experimental community,
 - more powerful computational techniques and computers,
 - new ideas.
- As LHC needs to study more rare phenomena and more subtle effects, generators must keep up by increased precision.

Thank you for the attention!

MCnet Short-term studentships



3-6 month fully funded studentships for current PhD students at one of the MCnet nodes. An excellent opportunity to really understand and improve the Monte Carlos you use!

Application rounds every 3 months.



MCnet projects Pythia Herwig Sherpa MadGraph Ariadne CEDAR

Enjoy the rest of the school!

