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- PART 11. Introduction to Event Generators2. Constraining Pythia at LEP $\leftrightarrow q\bar{q}$ continuum3. Pythia for B Decays
- PART 24. Tuning Approaches5. The MCPLOTS event-generator validation resource

THE ROYAL















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Event Generators: Divide and Conquer

Model full event structure by repeated/nested factorizations

→ Split the problem into many ~ simple pieces



Quantum mechanics \rightarrow **Probabilities** \rightarrow Make **Random Choices** (as in nature) → Markov-Chain Monte Carlo → "Event Generators"



Hard Process & Decays:

Process-specific (N)LO matrix elements → Sets "Hard" scale: QMAX





Accelerated Charges → **Perturbative Bremsstrahlung**: Differential evolution, dP/dQ^2 , from Q_{MAX} to $Q_{Hadronization} \sim 1$ GeV

Hadronization (and hadron decays) Non-perturbative model of color-singlet parton systems \rightarrow hadrons

1) Bremsstrahlung via Parton Showers

Most bremsstrahlung is

driven by divergent propagators \rightarrow simple structure



Mathematically, gauge amplitudes factorize in singular limits

Partons ab collinear:
$$|\mathcal{M}_{F+1}(\dots,a,b,\dots)|^2 \xrightarrow{a||b}{\rightarrow} g_s^2 \mathcal{C} \frac{P(z)}{2(p_a \cdot p_b)} |\mathcal{M}_F(\dots,a+b,\dots)|^2$$

P(z) =**DGLAP splitting kernels**", with $z = E_a/(E_a + E_b)$

Gluon j

$$\rightarrow$$
 soft: $|\mathcal{M}_{F+1}(\ldots,i,j,k\ldots)|^2 \xrightarrow{j_g \to 0} g_s^2 \mathcal{C} \frac{(p_i \cdot p_k)}{(p_i \cdot p_j)(p_j \cdot p_k)} |\mathcal{M}_F(\ldots,i,k,\ldots)|^2$

Coherence \rightarrow Parton j really emitted by (i,k) "dipole" or "antenna" (eikonal factors)

These are the **building blocks of parton showers** (DGLAP, dipole, antenna, ...) (+ running coupling, unitarity, and explicit (E,p) conservation.)

see e.g PS, Introduction to QCD, TASI 2012, arXiv:1207.2389

Shower Uncertainties: Non-Singular Variations in Pythia 8

Parton Showers rely on Factorisations in Soft/Collinear Limits

$$M_{n+1}|^2 \rightarrow \sum_{\text{radiators } \uparrow} a_{\text{sing}} |M_n|^2$$

Approximations based on universal singular structures of gauge theories. Driven by $1/Q^2$ poles from propagators, with spin-dependent numerators Renormalization-scale variations only produce terms \propto to these "kernels"

But genuine matrix elements also have "non-singular terms"

Our solution

[Vincia 1102.2126; Pythia 1605.08352]

Non-singular variations

$$a_{\rm sing} \rightarrow a_{\rm sing} + \Delta a_{\rm non-sing}$$

Can also be helpful to estimate need for higher matching/merging

Non-Singular Variations: Example

Example from Mrenna & **PS**, Automated Parton-Shower Variations in Pythia 8, <u>1605.08352</u>

Can vary renormalisation scale and non-singular terms independently



2) Hadronization and Jets

Consider a quark and anti-quark produced in e+e- annihilation



i) Initially Quarks separate at high velocity

ii) Colour flux tube forms between quarks

iii) Energy stored in the flux tube sufficient to produce new $\bar{q}q$ pairs

> iv) Process continues \Longrightarrow Jets of colourless hadrons

Confinement in PYTHIA: The Lund String Model

Simplified (leading-N_C) "colour flow" -> determine between which partons to set up confining potentials



Map to Strings: Quarks = string endpoints; gluons = "kinks" System then evolves as a string world sheet

+ String breaks via spontaneous $q\bar{q}$ pair creation ("Schwinger mechanism") \rightarrow hadrons

Baseline string model formulated in continuum limit of asymptotically "long" strings: $E_{\rm CM} \gtrsim 10 \, {\rm GeV}$ Belle II could provide extremely accurate constraints at the lower endpoint of the dynamical range? 4 + test for small-system modifications $\leftrightarrow \rightarrow$ eg non-universal best-fit tune parameters



String Breaking



Assume probability of string break constant per unit world-sheet area

Schwinger Case: the String Fragmentation Function

Schwinger \implies Gaussian p_{\perp} spectrum (transverse to string axis) & Prob(d:u:s) \approx 1 : 1 : 0.2 The meson M takes a fraction z of the quark momentum, Probability distribution in $z \in [0,1]$ parametrised by **Fragmentation Function**, $f(z, Q_{HAD}^2)$



Observation: All string breaks are **causally disconnected**

- Lorentz invariance \implies string breaks can be considered in any order. Imposes "left-right symmetry" on the FF
- \implies **FF** constrained to a form with **two free parameters**, *a* & *b*: constrained by fits to measured hadron spectra

Lund Symmetric Fragmentation $f(z) \propto \frac{1}{z}(1-z)^{a} \exp\left(-\frac{b(m_{h}^{2}+p_{\perp h}^{2})}{t}\right)$ **Function**

Supresses high-z hadrons

Supresses low-z hadrons

Constraining PYTHIA (in the $q\bar{q}$ continuum)

We use a combination of Infrared Safe* and Infrared Sensitive observables

 \implies Stereo Vision on perturbative and nonperturbative QCD respectively Some overlap / interplay: IR Safe becomes Sensitive at low scales & IR Sensitive seeded by IR Safe.

<u>IR Safe</u> Observables satisfy two simultaneous conditions

1) Soft Safe: observable does not change when adding soft partons/particles E.g., adding infinitely soft gluons (perturbative), or soft pions (non-perturbative) 2) Collinear Safe: observable does not change when splitting a particle collinearly E.g., doing a $g \to gg$ or $g \to q\bar{q}$ splitting, or a $\rho \to \pi\pi$ decay, in limit of zero opening angle. \rightarrow Hadronization and hadron decays suppressed by powers of $\Lambda_{
m OCD}/Q$

Full Set of IR Safe Observables:

Event Shapes: typically Thrust Family, Linearised Sphericity Family, EECs, Angularities Jet Rates: typically Durham kT resolutions (but other clustering algorithms also interesting) Jet Structure: Jet Masses, Jet Broadenings, Jet Shapes Sometimes done using Charged Tracks only, for best experimental resolution.







IR Sensitive Observables

Multiplicities, Spectra, and Correlations

- Inclusive charged particles
- Identified particles (rates and ratios).
- + correlations, with event multiplicity, with rapidity along jet axis, with ...?
- Strangeness correlations, baryon correlations, ...

Spectra

- Conventional absolute momentum fraction: $x_p = \frac{2|p|}{E_{CM}}$
- But, even at $E_{CM} \sim 10$ GeV, these hadrons are produced in jets; Jets have longitudinal and transverse axes:
 - **More information: rapidity spectra** (along primary event/jet axis) : dn_{ch}/dy , dn_{PID}/dy
 - And momentum **transverse to it**, dn/dp_{\perp} ; + Let 2nd axis define a plane $\implies p_{\perp in}, p_{\perp out}$



 $(at \sqrt{s} \sim m_Z)$

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PYTHIA & B Decays — Recent collaboration with EVTGEN (M. Kreps, Warwick)

30% of B meson decays modelled as partonic transitions, with spectator

Passed back to PYTHIA for re-hadronisation (with same string parameters as at LEP). How reliable is this modelling really? Not aware anyone has looked at that since org papers. These tend to be high-multiplicity (multi-prong) modes Rarely used as signals. But enter as backgrounds, and tagging modes? Experimental constraints on these? Belle II, LHCb, ALICE ... ? Would like to discuss, if there is interest, what Belle II could do here?

QED Radiative Corrections in B Decays

HERWIG and SHERPA have dedicated modules, based on "YFS" formalism For PYTHIA, QED in hadron decays is normally done with **PHOTOS** Now: looking at adapting the QED Multipole Shower Module from VINCIA Native C++ and built-in in PYTHIA \rightarrow thread-safe and trivial to parallelise May be superior to YFS in some ways + modern shower formalism \implies matching, merging, ... Would this be interesting to Belle II ?

QED Multipole Radiation Patterns



Soft Photon Emission: [Dittmaier, 2000]

$$|M_{n+1}(\{p\}, p_j)|^2 = -8\pi \alpha$$

Same-charge pairs ➤ negative terms







PART 2 Tuning

Tuning: **PROFESSOR** — a powerful tool for (semi)automated tuning

Inspired by idea pioneered by DELPHI (Hamacher et al., 1995):

Bin-wise interpolation of MC generator response and χ^2 minimization 2nd-order polynomials account for parameter correlations.

Luning procedure Professo

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





Modern Python Package with much more functionality, tutorials, etc. https://professor.hepforge.org/

Random sampling: N parameter points in *n*-dimensional space



PROFESSOR — Caveats

A. Buckley et al., Eur. Phys. J.C 65 (2010) 331

I would (by now) recommend using PROFESSOR. Wisely.

Some Dangers:

Overfitting: very precisely measured data points can generate large χ^2 values even if MC gets within what one would naively consider "reasonable" agreement Fit reacts by sacrificing agreement elsewhere (typically in tails) to improve χ^2 in peaks. PROFESSOR now has facility to include a "sanity limit" (e.g., 5%) "theory uncertainty" > Fit not rewarded (much) for improving agreement beyond that point. More freedom in tails. Also tends to produce $\chi^2_{5\%}$ values ~ unity \rightarrow better uncertainty bands?

Incompatibilities: model may be unable to agree with (some part of) a given measurement

Fit reacts by desperately trying to reduce order-of-magnitude differences in bins it shouldn't have been asked to fit in the first place, at cost of everything else > total garbage. Choose measurements carefully — within domain of applicability of physics model

+ PROFESSOR now has facility to not penalise χ^2 beyond some max deviation.

Some Helper Tools

Wouldn't it be nice if there was a tool:

- That could automatically detect correlations between parameters and observables. And tell you which "groups" they fall into naturally : which parameter sets you should ideally tune together, and which are more nicely factorised.
- This is (at least partly) what the tool AutoTunes does Bellm, Gellersen, Eur. Phys.J.C 80 (2020) I won't have time to discuss that today, but I think it looks promising I encourage you to study it and use it
- You may also be interested in Apprentice Krishnamoorthy et al., EPJ Web Conf. 251 (2021) 03060 Variance reduction to semi-automate how to weight observables & bins

Practical Example: Uncertainties on Dark-Matter Annihilation Spectra

Based on A. Jueid et al., <u>1812.07424</u> (gamma rays, *eg for GCE*) and <u>2202.11546</u> (antiprotons, *eg for AMS*) + <u>2303.11363</u> (all)

Compare different generators?

- E.g., HERWIG PYTHIA
- Problem: tuned to ~ same data
- Difference not guaranteed to span genuine uncertainties

Instead, did parametric refittings of LEP data within PYTHIA's modelling

- Simple sanity limit / overfit protection / tension resolution:
 - Add blanket 5% baseline uncertainty
- (+ exclude superseded measurements)
- + Universality Tests:



Practical Example: Uncertainties on Dark-Matter Annihilation Spectra

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Same done tor antiprotons, positrons, antineutrinos Main Contact: adil.jueid@gmail.com Tables with uncertainties available on request. Also the spanning tune parameters of course.



New: Automated Hadronization Uncertainties

Problem:

Given a colour-singlet system that (randomly) broke up into a specific set of hadrons:



What is the **relative probability** that same system would have resulted, if the fragmentation parameters had been **different?** Would this particular final state become **more likely** (w' > 1)? Or **less likely** (w' < 1)Crucially: **maintaining unitarity** \implies inclusive cross section remains unchanged!

August 2023: Bierlich, Ilten, Menzo, Mrenna, Szewc, Wilkinson, Youssef, Zupan
 [Reweighting MC Predictions & Automated Fragmentation Variations in Pythia 8, 2308.13459]
 Method is general; demonstrated on variations of the 7 main parameters governing longitudinal and transverse fragmentation functions in PYTHIA 8
 https://gitlab.com/uchep/mlhad-weights-validation

Examples with Pythia 8

Longitudinal Fragmentation Function (Lur 0.1



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From Data Analysis Individuation of (current & future) MC Event Generators



Data Preservation (for HEP): HEPData

(HEPData is funded by the UK <u>STFC</u> and is based at the <u>IPPP</u> at Durham U.)

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Analysis Preservation (for HEP): Rivet

(Rivet is developed by the CEDAR project, also based in the UK)

When showing plots from the original paper:

• • •



"Yes but this has been corrected in version X of that generator" "But this other tune or MC that you didn't compare to does better" "Does the model shown there also describe correctly this **other** important observable?"

Instant answers would be convenient for faster & better informed discussions!

LHC@home/Test4Theory

2010: LHC@home developers approached the CERN Theory Group

Could we propose a simple test application for embedding physics applications in a Virtual Machine (CernVM) for running on the LHC@home volunteer cloud?

PYTHIA: simple to build (no external libs), small footprint, ...

Would not previously have been able to run on a volunteer-cloud environment: No native Windows support, nor much interest (or manpower) to develop that Small group of physicists; main (only) goal (& grant funding) = physics research

Virtualisation factorised the problem:

Physics application just saw a (configurable) standard Linux environment (now CentOS)

Became the Test4Theory project, the world's first virtual volunteer cloud

Run event generators \rightarrow RIVET and display results at <u>mcplots.cern.ch</u>



Preview at mcplots-dev.cern.ch

MCPLOTS

Online repository of Monte Carlo plots compared to experimental data



126 generators



783667 plots







LHC@HOME ABOUT PLOTS -COMPARISON -











ABOUT

Select between all available MC generators & versions

HOME

\approx

 $\Delta B(Max-Min)$

C parameter

D parameter

EEC

EEC Asymmetry

M(Heavy Hemisph)

M(Light Hemisph)

ΔM(Heavy-Light)

Planarity

Sphericity

Thrust

1-Thrust

Thrust Major

Thrust Minor

Thrust Oblateness

Charm and Bottom .

fweak

Mean of fweak

B multiplicity

D multiplicity

D^{*} multiplicity

 $\Lambda_{\rm b}$ multiplicity

D^{*} spectrum



Extra Slides

Examples with Pythia 8

Transverse Fragmentation Function (Gauss



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1. Types of (QED) Showers



Note: this is (intentionally) oversimplified. Many subtleties (recoil strategies, gluon parents, initial-state partons, and mass terms) not shown.

$$+\frac{s_{e^-\gamma}}{s_{\gamma e^+}}+2
ight)$$

Beyond 2-body Systems: QED Multipoles

PYTHIA QED

Determines a "best" set of dipoles. No genuine multipole effects. I.e., interference beyond dipole level only treated via "principle of maximal screening" Works as a parton shower evolution (+ MECs) \succ interleaved with QCD, MPI, ...

YFS QED [Yennie-Frautschi-Suura, 1961 > several modern implementations]

Allows to take full (multipole) soft interference effects into account "Scalar QED"; no spin dependence.

I.e., starts from purely soft approximation; collinear terms not automatic Is not a shower; works as pure afterburner, adding a number of photons to a final state with predetermined kinematics; no interleaving

VINCIA QED [Kleiss-Verheyen, 2017 > Brooks-Verheyen-PS, 2020]

Allows to take full (multipole) soft interference effects into account Not limited to scalar QED; includes spin dependence

I.e., starts from antenna approximation; including collinear terms Works as a parton shower evolution; can be interleaved (+ MECs).

What's the problem?

Example: Quadrupole final state (4-fermion: $e^+e^+e^-e^-$)



Why was this not done as a shower before?

The orange terms are negative \succ negative weights (+ big cancellations) YFS gets around that by not being formulated as a shower (& no spin dependence) Utilises that the sum is always non-negative.

What does VINCIA do differently?



Sectorize phase space: for each possible photon emission kinematics p_{γ} , find the 2 charged particles with respect to which that photon is softest \succ "Dipole Sector"

Use dipole *kinematics* for that sector, but sum **all** the positive and negative antenna terms (w spin dependence) to find the **coherent emission** probability.

Antenna phase-space factorisation is exact, also for massive particles

+ Universal mass corrections are included in the eikonals > Should have extremely faithful representation of "dead cone" effect (radiation from massive particles strongly damped for $\theta_{\gamma} \lesssim E/m$ [Gehrmann-de Ridder, Ritzmann, PS, 2012]

Also automatically includes $\gamma \rightarrow e^+e^-, \mu^+\mu^-, \dots$ splittings (not in PHOTOS? YFS?)

First steps towards application of VINCIA QED to Hadron Decays Honours project of Giacomo Morgante (Monash, 2023, in collaboration with Warwick)

+ Can incorporate Matrix-Element Corrections [Giele, Kosower, PS, 2011, + more recent] Not implemented yet. Techniques known; worked out focusing on QCD Will affect tails of hard radiation (process-dependent non-singular terms), so this is potentially an important still missing feature. Also: Form Factors, VMD contributions, BRs, ...

+ Can be interleaved with event evolution, e.g., with Resonance Decays