## Pythia

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Pythia
（ピューティアー）
PART $1\left\{\begin{array}{l}\text { 1．Introduction to Event Generators } \\ \text { 2．Constraining Pythia at LEP } \longleftrightarrow q \bar{q} \text { continuum } \\ \text { 3．Pythia for B Decays }\end{array}\right.$
PART $2\left\{\begin{array}{l}\text { 4．Tuning Approaches } \\ \text { 5．The MCPLOTS event－generator validation resource }\end{array}\right.$


## Event Generators: Divide and Conquer

Model full event structure by repeated/nested factorizations
$\rightarrow$ Split the problem into many ~ simple pieces

$$
\mathscr{P}_{\text {event }}=\mathscr{P}_{\text {Hard }} \otimes \mathscr{P}_{\text {Res }} \otimes \mathscr{P}_{\text {FSR }} \otimes \mathscr{P}_{\text {Had }} \otimes \mathscr{P}_{\text {Dec }} \otimes \ldots
$$

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


Hard Process \& Decays:
Process-specific (N)LO matrix elements $\rightarrow$ Sets "Hard" scale: Qmax


Accelerated Charges $\rightarrow$ Perturbative Bremsstrahlung:
Differential evolution, dP/dQ², from $Q_{\text {max }}$ to Qhadronization ~ 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

$$
\rightarrow \text { collinear: }
$$

$$
\begin{gathered}
\left|\mathcal{M}_{F+1}(\ldots, a, b, \ldots)\right|^{2} \stackrel{a| | b}{\rightarrow} g_{s}^{2} \mathcal{C} \frac{P(z)}{2\left(p_{a} \cdot p_{b}\right)}\left|\mathcal{M}_{F}(\ldots, a+b, \ldots)\right|^{2} \\
P(z)=\text { DGLAP splitting kernels", with } z=E_{a} /\left(E_{a}+E_{b}\right)
\end{gathered}
$$

$$
\underset{\rightarrow \text { soft: }}{\underset{\text { Gluon j }}{ }}\left|\mathcal{M}_{F+1}(\ldots, i, j, k \ldots)\right|^{2} \xrightarrow{j_{g} \rightarrow 0} g_{s}^{2} \mathcal{C} \frac{\left(p_{i} \cdot p_{k}\right)}{\left(p_{i} \cdot p_{j}\right)\left(p_{j} \cdot p_{k}\right)}\left|\mathcal{M}_{F}(\ldots, i, k, \ldots)\right|^{2}
$$

$$
\text { Coherence } \rightarrow \text { Parton } \mathrm{j} \text { really emitted by ( } \mathrm{i}, \mathrm{k} \text { ) "dipole" or "antenna" (eikonal factors) }
$$

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

## Parton Showers rely on Factorisations in Soft/Collinear Limits

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

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

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

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, 1605.08352
Can vary renormalisation scale and non-singular terms independently
ee $\rightarrow$ hadrons 91.2 GeV


Note: ME corrections were switched off for illustration. Would reduce red band, but not blue.

## 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- $\mathrm{N}_{\mathrm{C}}$ ) "colour flow" $\rightarrow$ determine between which partons to set up confining potentials

"Linear confinement"


Map to Strings: Quarks $\Rightarrow$ string endpoints; gluons $\Rightarrow$ "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: $E_{\mathrm{CM}} \gtrsim 10 \mathrm{GeV}$
$\mathcal{B}$ Belle II could provide extremely accurate constraints at the lower endpoint of the dynamical range?
$\mathcal{B}+$ test for small-system modifications $\longleftrightarrow$ eg non-universal best-fit tune parameters


## String Breaking

In "unquenched" QCD
$g \rightarrow q \bar{q} \Longrightarrow$ The strings will "break"
Non-perturbative so can't use $P_{g \rightarrow q \bar{q}}(z)$
Model: Schwinger mechanism


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

## Schwinger Case: the String Fragmentation Function

Schwinger $\Longrightarrow$ 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, $f\left(z, Q_{\text {HAD }}^{2}\right)$


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

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

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

IR Safe 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 $g \rightarrow g g$ or $g \rightarrow q \bar{q}$ splitting, or a $\rho \rightarrow \pi \pi$ decay, in limit of zero opening angle.
$\rightarrow$ Hadronization and hadron decays suppressed by powers of $\Lambda_{\mathrm{QCD}} / Q$

## 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.

## Constraining PYTHIA: IR Safe Observables (main examples) (at $\sqrt{ } \sim m_{\mathcal{D}}$

Top Row: from PS et al., "Tuning PYTHIA 8.1: the Monash 2013 Tune", Eur.Phys.J.C 74 (2014) 8

$\mathcal{B}$ Question: could Belle II separate $e^{+} e^{-} \rightarrow \gamma^{*} \rightarrow c \bar{c}$ out from $d \bar{d}, u \bar{u}, s \bar{s}$ ?





Bottom Row: from mcplots.cern.ch

## 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: $x_{p}=\frac{2|p|}{E_{\mathrm{CM}}}$
But, even at $\mathrm{E}_{\mathrm{CM}} \sim 10 \mathrm{GeV}$, these hadrons are produced in jets;
Jets have longitudinal and transverse axes:
More information: rapidity spectra (along primary event/jet axis) : $d n_{\mathrm{ch}} / d y, d n_{\mathrm{PID}} / d y$
And momentum transverse to $\mathrm{it}, d \mathrm{n} / d p_{\perp} ;+$ Let $2^{\text {nd }}$ axis define a plane $\Longrightarrow p_{\perp \text { in }} p_{\perp \text { out }}$

## Main Examples of IR Sensitive Observables

Top Row: from PS et al., "Tuning PYTHIA 8.1: the Monash 2013 Tune", Eur.Phys.J.C 74 (2014) 8










Bottom Right Plots: from "String Fragmentation with a Time-Dependent Tension", N. Hunt-Smith \& PS, Eur.Phys.J.C 80 (2020) 11

## $30 \%$ 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 ...?
$\mathcal{B}$ 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 $\Longrightarrow$ matching, merging, ...
Would this be interesting to Belle II?

## QED Multipole Radiation Patterns

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

$\begin{gathered}\text { Soft Photon Emission: } \\ \text { [Dittmaier, 2000] }\end{gathered}\left|M_{n+1}\left(\{p\}, p_{j}\right)\right|^{2}=-8 \pi \alpha \sum_{x, y}^{n} \sigma_{x} Q_{x} \sigma_{y} Q_{y} \frac{s_{x y}}{s_{x j} s_{y j}}\left|M_{n}(\{p\})\right|^{2}$ ——— Opposite-charge pairs $>$ positive terms
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 $M C$ generator response and $\chi^{2}$ minimization $2^{\text {nd }}$-order polynomials account for parameter correlations.

Modern Python Package with much more functionality, tutorials, etc.
https://professor.hepforge.org/
(1) Random sampling: $N$ parameter points in $n$-dimensional space
(2) Run generator and fill histograms
(3) For each bin: use $N$ points to fit interpolation (2 $2^{\text {nd }}$ or $3^{\text {rd }}$ order polynomial)
(4) Construct overall (now trivial) $\chi^{2} \approx \sum_{\text {bins }} \frac{(\text { interpolation-data) })^{2}}{e_{\text {error }}{ }^{2}}$
(5) and Numerically minimize pyMinuit, SciPy


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

## Some Dangers:

Overfitting: very precisely measured data points can generate large $\chi^{2}$ values even if MC gets within what one would naively consider "reasonable" agreement Fit reacts by sacrificing agreement elsewhere (typically in tails) to improve $\chi^{2}$ 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 $\chi_{5 \%}^{2}$ values $\sim$ 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 $\chi^{2}$ 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
I won't have time to discuss that today, but I think it looks promising
I encourage you to study it and use it

Variance reduction to semi-automate how to weight observables \& bins

## Practical Example: Uncertainties on Dark-Matter Annihilation Spectra

## 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: $\qquad$


| Parameter | without $5 \%$ | with $5 \%$ |
| :--- | :---: | :---: |
| StringPT:Sigma | $0.3151_{-0.00010}^{+0.0010}$ | $0.3227_{-0.0028}^{+0.0028}$ |
| StringZ: aLund | $1.028_{-0.031}^{+0.031}$ | $0.976_{-0.054}^{+0.052}$ |
| StringZ: avgZLund | $0.5534_{-0.0010}^{+0.0010}$ | $0.5496_{-0.0026}^{+0.0026}$ |
| $\chi^{2} /$ ndf | $5169 / 963$ | $778 / 963$ |



## Practical Example: Uncertainties on Dark-Matter Annihilation Spectra



Same done tor antiprotons, positrons, antineutrinos

Weighted Average: good consistency across observables

$$
\text { 10-point variations }>\text { Fairly }
$$ convincing uncertainty bands?



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 ( $w^{\prime}>1$ )? Or less likely ( $w^{\prime}<1$ )
Crucially: maintaining unitarity $\Longrightarrow$ 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 (Lund Symmetric FF)


$f(z) \sim$ scaled light-cone hadron momentum fraction

$$
\propto \frac{1}{z^{1+r_{Q} b m_{Q}^{2}}}(1-z) \exp \left(-\frac{b m_{\perp}^{2}}{z}\right)
$$

variations

## Reweighting Methodology:

Accept-Reject Algorithm (analogous to shower variations):

$$
w^{\prime}=w \prod_{i \in \text { accepted }} R_{i, \text { accept }}^{\prime}(z) \prod_{j \in \text { rejected }} R_{j, \text { reject }}^{\prime}(z)
$$

with

$$
R_{\text {accept }}^{\prime}(z)=\frac{P_{\text {accept }}^{\prime}(z)}{P_{\text {accept }}(z)} \quad R_{\text {reject }}^{\prime}(z)=\frac{P_{\text {reject }}^{\prime}(z)}{P_{\text {reject }}(z)}=\frac{1-P_{\text {accept }}^{\prime}(z)}{1-P_{\text {accept }}(z)}
$$




## From Data Analysis $\boldsymbol{m} \rightarrow$ Validation of (current \& future) MC Event Generators

Experimental Measurement
Data Preservation (for HEP): HEPData
HEPData is funded by the UK STFC and is
based at the IPPP at Durham U.


Analysis Preservation (for HEP): Rivet

## 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!

## 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 mcplots.cern.ch

## Preview at mcplots-dev.cern.ch

## MCPLOTS

Online repository of Monte Carlo plots compared to experimental data
783667
plots

Plots by analyses

## Preview at mcplots-dev.cern.ch



Plots by beams : pp


## MCPLOTS - New Look Coming Soon

Plots by analyses

## Preview at mcplots-dev.cern.ch



## MCPLOTS - New Look Coming Soon



EEC Asymmetry
M(Heavy Hemisph)
M(Light Hemisph)
$\Delta \mathrm{M}$ (Heavy-Light)
Planarity
Sphericity
Thrust
1-Thrust
Thrust Major
Thrust Minor
Thrust Oblateness
Charm and Bottom .
$f_{\text {weak }}$
Mean of $f_{\text {weak }}$
B multiplicity
D multiplicity
D* multiplicity
$\Lambda_{b}$ multiplicity
D* spectrum

## MCPLOTS = Gitlab repositoty

You can clone it, implement new analyses, etc.
Could be adapted with suite of Belle II comparisons?

Main contact: natalia.korneeva@cern.ch


Download as: .pdf .eps .png .script.tgz OPAL experiment: data | article paper Herwig 7 (Def): data Igenerator card Pythia 8 (Def): data |generator card Sherpa (Def): data |generator card Vincia (Def): data Igenerator card

Direct access to all generator cards, data points, MC points, journal paper, etc

Extra Slides

## Examples with Pythia 8

## Transverse Fragmentation Function (Gaussian)



## Simple case:

neutral scalar $\rightarrow 2$ charged fermions = A single OED dipole

$$
\begin{gathered}
\text { LO QED } \propto \frac{2 s_{e^{-} e^{+}}}{s_{e^{-} \gamma} s_{\gamma e^{+}}} \\
\text {eikonal term }
\end{gathered}+\frac{1}{M_{0}^{2}}\left(\frac{s_{\gamma e^{+}}}{s_{e^{-} \gamma}}+\frac{s_{e^{-} \gamma}}{s_{\gamma e^{+}}}+2\right)
$$



## 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) $>$ 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 OED; includes spin dependence
l.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 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?

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



Sectorize phase space: for each possible photon emission kinematics $p_{\gamma^{\prime}}$ find the 2 charged particles with respect to which that photon is softest > "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.

## Further Details

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 $\gamma \rightarrow e^{+} e^{-}, \mu^{+} \mu^{-}, \ldots$ 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

