QCD Simulation for LHC and Herwig++

Bryan Webber
University of Cambridge
Cavendish Laboratory

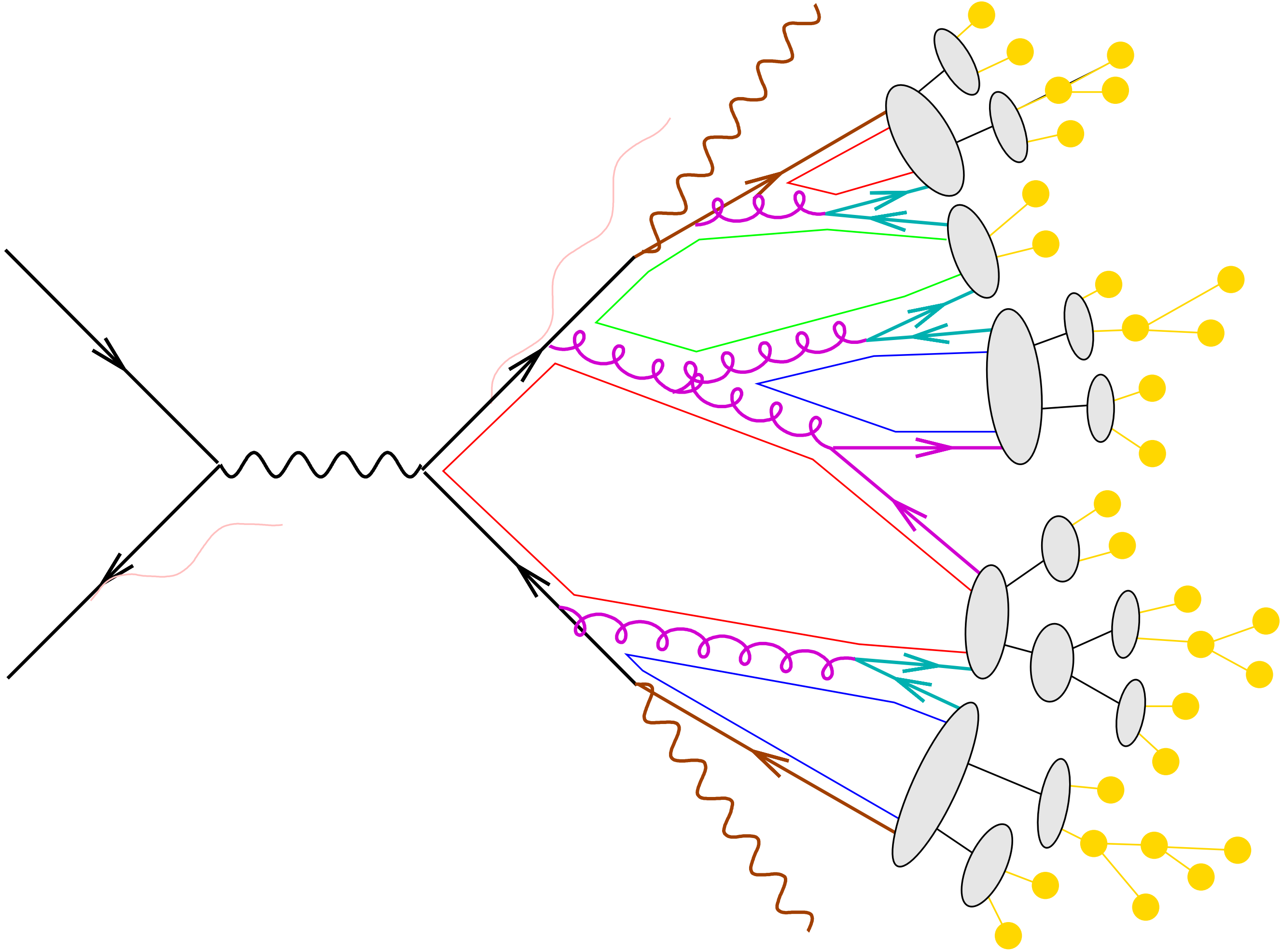
with Stefan Gieseke, Alberto Ribon, Mike Seymour & Phil Stephens (Cambridge, Manchester, CERN)

- Some issues in QCD simulation for LHC
  - Improving shower variables
  - Combining matrix elements and showers
  - Multiscale showering
- Herwig++
  - Overview
  - Hadronization model
  - Results (e^+e^-)
  - Outlook

S. Gieseke, P. Stephens and BW, JHEP **0312** (2003) 045 [hep-ph/0310083]

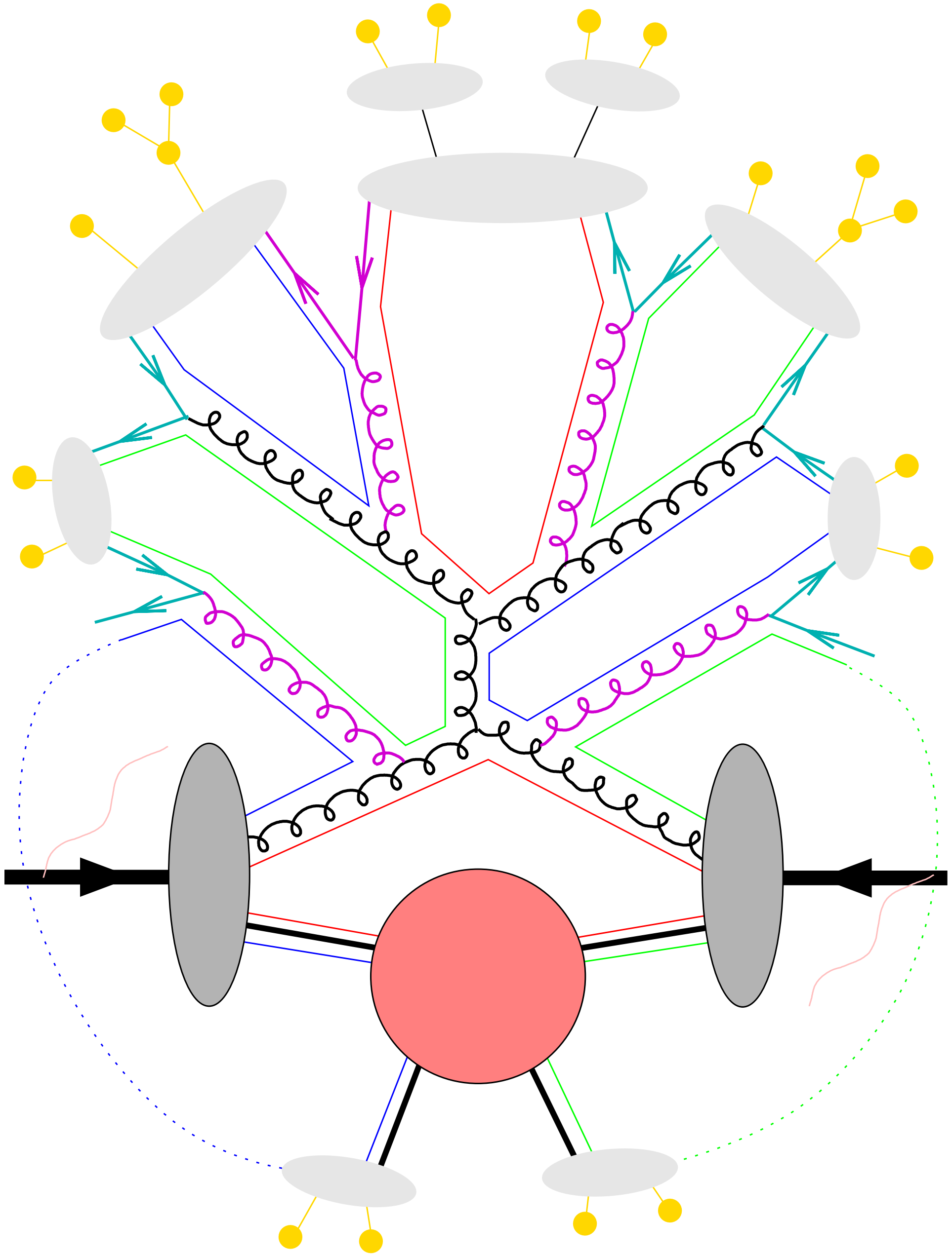
S. Gieseke, A. Ribon, M. H. Seymour, P. Stephens and BW, JHEP **0402** (2003) 005 [hep-ph/0311208]

e^+e^- Event Generator



- hard scattering
- (QED) initial/final state radiation
- partonic decays, e.g. $t \longrightarrow bW$
- parton shower evolution
- nonperturbative gluon splitting
- colour singlets
- colourless clusters
- cluster fission
- cluster $\longrightarrow$ hadrons
- hadronic decays

Additional Complications in pp

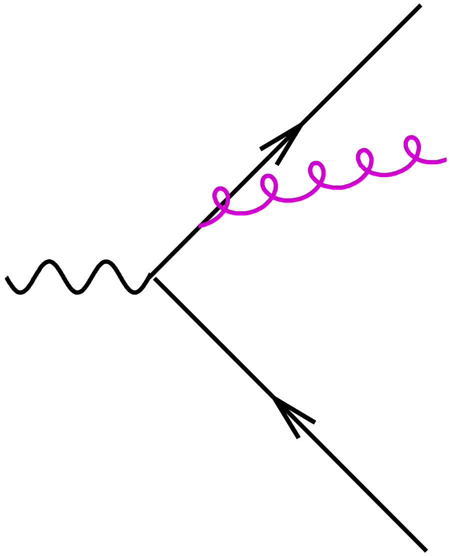


- backward parton evolution
- underlying event (Odagiri talk)

Collinear Enhancement (Light Partons)

ME involving $q \to qg$ (or $g \to gg$) strongly enhanced whenever emitted gluon is almost collinear. Propagator factor

$$\frac{1}{(p_q + p_g)^2} \approx \frac{1}{2E_q E_g (1 - \cos\theta_{qg})}$$



- soft+collinear divergences.
- dominant contribution to the ME.

Collinear factorization

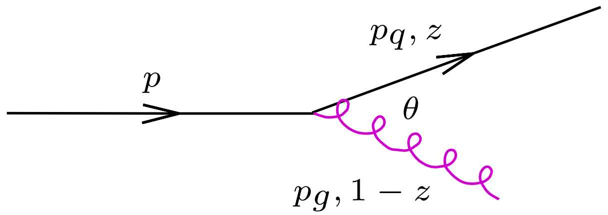
$$|M_{p+1}|^2 d\Phi_{p+1} \approx |M_p|^2 d\Phi_p \frac{dt}{t}\frac{\alpha_s}{2\pi} P(z)\, dz\, d\phi$$

$$P(z) = C_F \frac{1+z^2}{1-z}$$

⟶ Parton shower MC.

- Shower resums leading logarithmic contributions.

Quasi–Collinear Limit (Heavy Quarks)



- Sudakov basis p, n with $p^2 = m^2$ (‘forward’), $n^2 = 0$ (‘backward’), $p_\perp^2 = -\boldsymbol{p}_\perp^2$

$$\begin{aligned} p_q &= zp + \beta_q n - p_\perp \\ p_g &= (1-z)p + \beta_g n + p_\perp \end{aligned}$$

- Quasi-collinear limit (Catani et al.): for $|\boldsymbol{p}_\perp| \sim m \ll p_+$

$$\begin{aligned} P_{qq}(z, \boldsymbol{p}_\perp^2, m^2) &= C_F\left[\frac{1+z^2}{1-z} - \frac{2z(1-z)m^2}{\boldsymbol{p}_\perp^2 + (1-z)^2 m^2}\right] \\ &\equiv \frac{C_F}{1-z}\left[1 + z^2 - \frac{2m^2}{z\tilde{q}^2}\right] \end{aligned}$$

- Generalised angular variable: for $m \to 0\,,\quad \tilde{q} \sim |\boldsymbol{p}_\perp|/z(1-z) \sim E\theta$
- Collinear limit: for $p_\perp \to 0\,,\quad \tilde{q} \sim m/z\,,\quad P_{qq} \sim C_F(1-z)$

New evolution variables

- Adopt $\tilde{q}^2$ as new evolution variable: $\tilde{q}^2 = \frac{\boldsymbol{p}_\perp^2}{z^2(1-z)^2} + \frac{m^2}{z^2}$ for $q \to qg$
- Argument of running α_S chosen according to

$$\alpha_S\left(z^2(1-z)^2\tilde{q}^2 = \boldsymbol{p}_\perp^2 + (1-z)^2 m^2\right)$$

- Generalized angular ordering in $\tilde{q}_i \to \tilde{q}_{i+1} + \tilde{k}_{i+1}$:

$$\tilde{q}_{i+1} < z_i \tilde{q}_i \qquad \tilde{k}_{i+1} < (1-z_i)\tilde{q}_i$$

- Reinterpretation of evolution variables: branching probability for $a \to bc$ is still

$$dP(a \to bc) = \frac{d\tilde{q}^2}{\tilde{q}^2}\frac{\alpha_S}{2\pi} P_{ba}(z, \tilde{q})\, dz\, d\phi$$

$\longrightarrow$ Sudakov form factors etc. remain the same!

- Allows better treatment of heavy particles, avoiding collinear "dead cones" and overlapping regions in phase space, in particular for soft emissions.

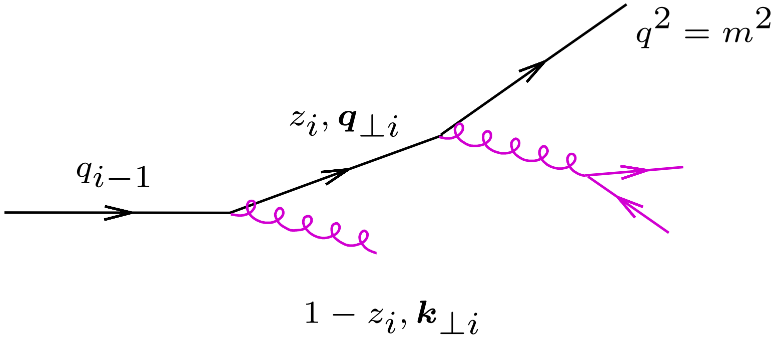
Kinematics

- Sudakov basis p, n with $p^2 = m^2$, $n^2 = 0$,

$$q_i = \alpha_i p + \beta_i n + q_{\perp i}$$

- Longitudinal splitting: $\alpha_i = z_i \alpha_{i-1}$
- Transverse momenta reconstructed from $\boldsymbol{p}_\perp$,

$$\boldsymbol{q}_{\perp i} = \boldsymbol{p}_{\perp i} + z_i \boldsymbol{q}_{\perp ,i-1} \qquad \boldsymbol{k}_{\perp i} = -\boldsymbol{p}_{\perp i} + (1 - z_i)\boldsymbol{q}_{\perp ,i-1}$$



- Recursive reconstruction of virtualities and β_i's from

$$\begin{aligned} q^2_{i-1} &= \frac{q_i^2}{z_i} + \frac{k_i^2}{1-z_i} + \frac{\boldsymbol{p}^2_{\perp i}}{z_i(1-z_i)} \\ \beta_i &= \frac{\boldsymbol{q}^2_{\perp i} + q_i^2 - \alpha_i^2 m^2}{2\alpha_i (p \cdot n)} \end{aligned}$$

- Azimuthal angle φ chosen randomly (now), or using *azimuthal spin correlations* (planned).

Universal cutoff parameter δ

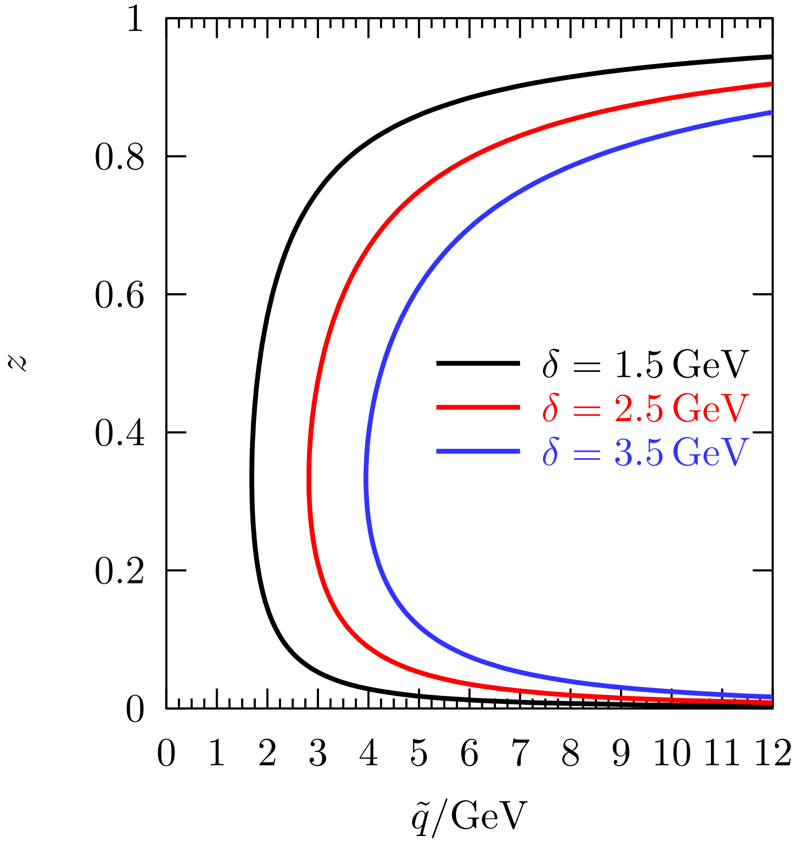
Require threshold in parton shower phase space.

$$\tilde{q} > Q_{\rm thr} = \beta m_q + \delta \qquad (\beta = 0.85)$$

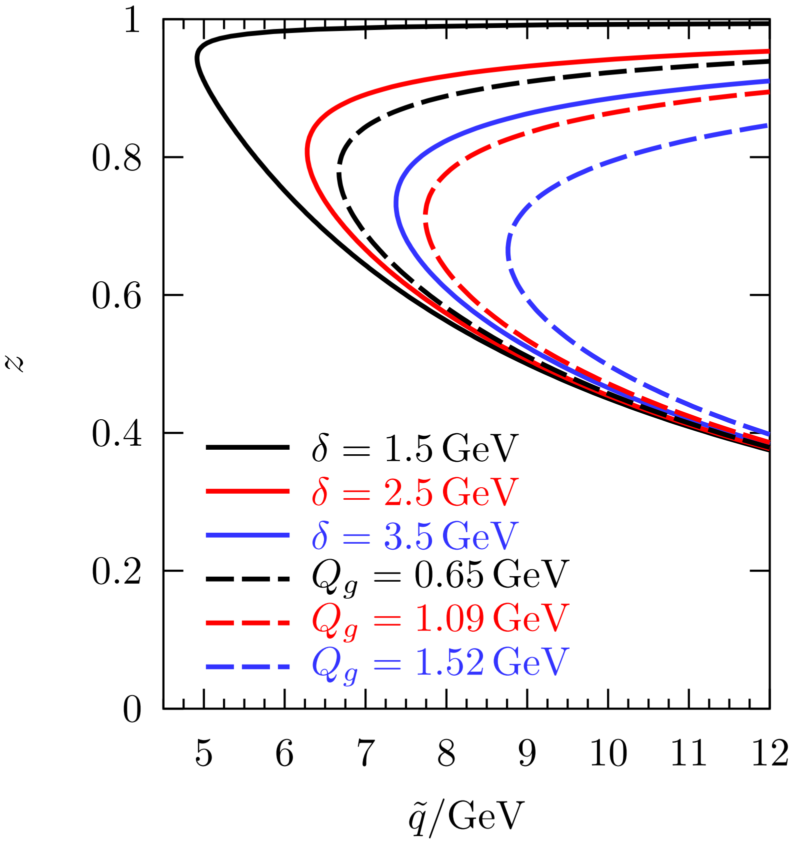
Parametrization of Q_g in terms of δ, m_q

$$Q_g = \frac{\delta - 0.3 m_q}{2.3}\,.$$

light quarks:

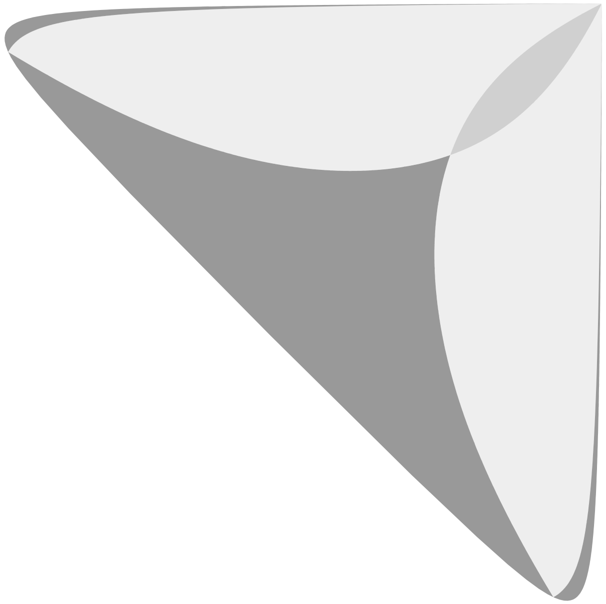


b quarks:

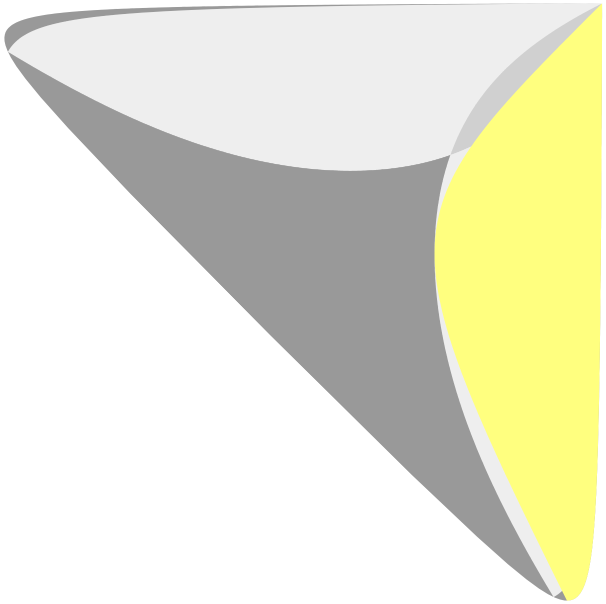


$q\bar{q}g$ phase space: old vs new variables

Herwig++



Fortran `HERWIG`

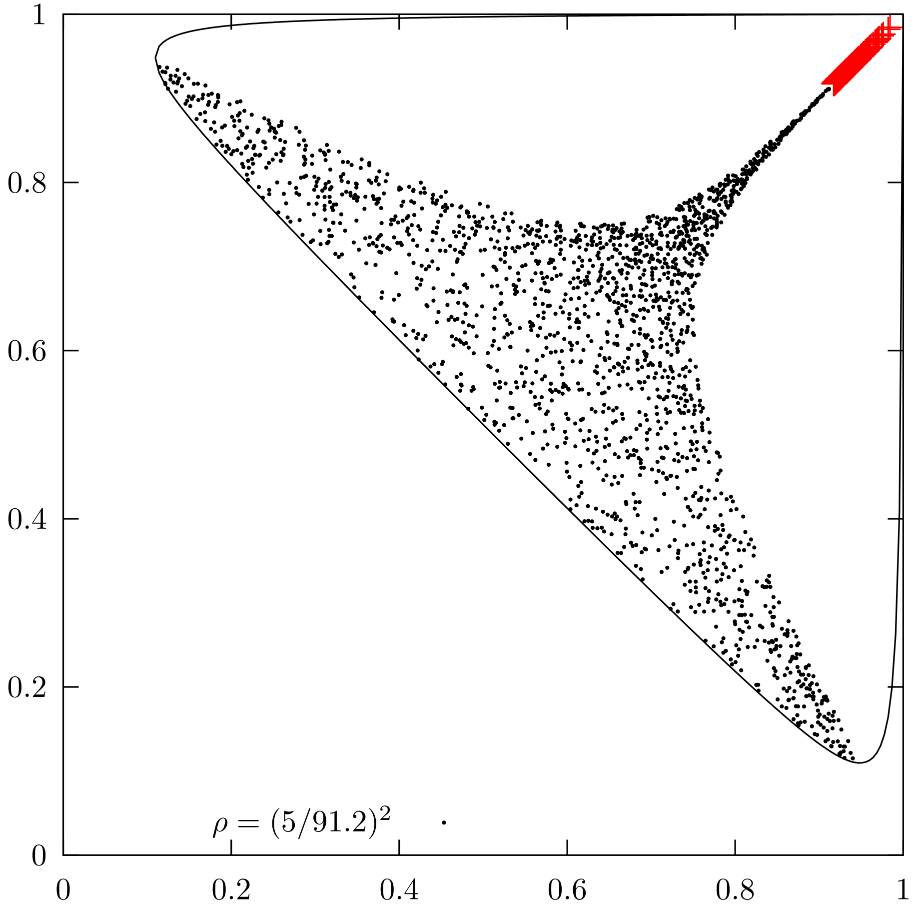


Comparison

- No overlapping regions in phase space.
- Smooth coverage of soft gluon region.
- No collinear dead cones.
- Larger non-collinear dead region.

Hard Matrix Element Corrections

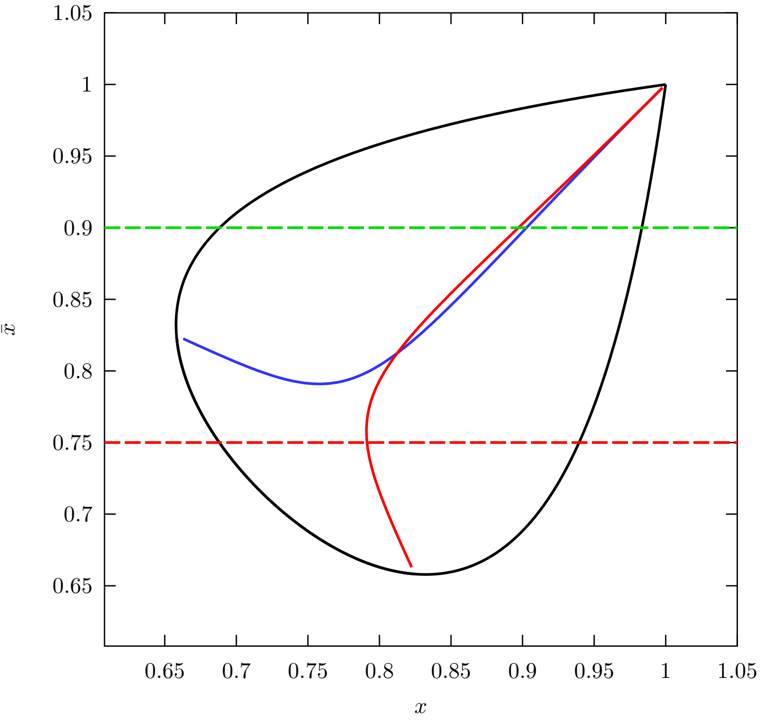
- Points $(x_q, x_{\bar{q}})$ in dead region chosen according to LO $q\bar{q}g$ matrix element and accepted according to ME weight.
- About 3% of all events are actually hard $q\bar{q}g$ events.
- Red points have weight > 1, practically no error by setting weight to one.
- Event oriented according to given $q\bar{q}$ geometry (Kleiss). Quark direction is kept with weight $x_q^2/(x_q^2 + x_{\bar{q}}^2)$.

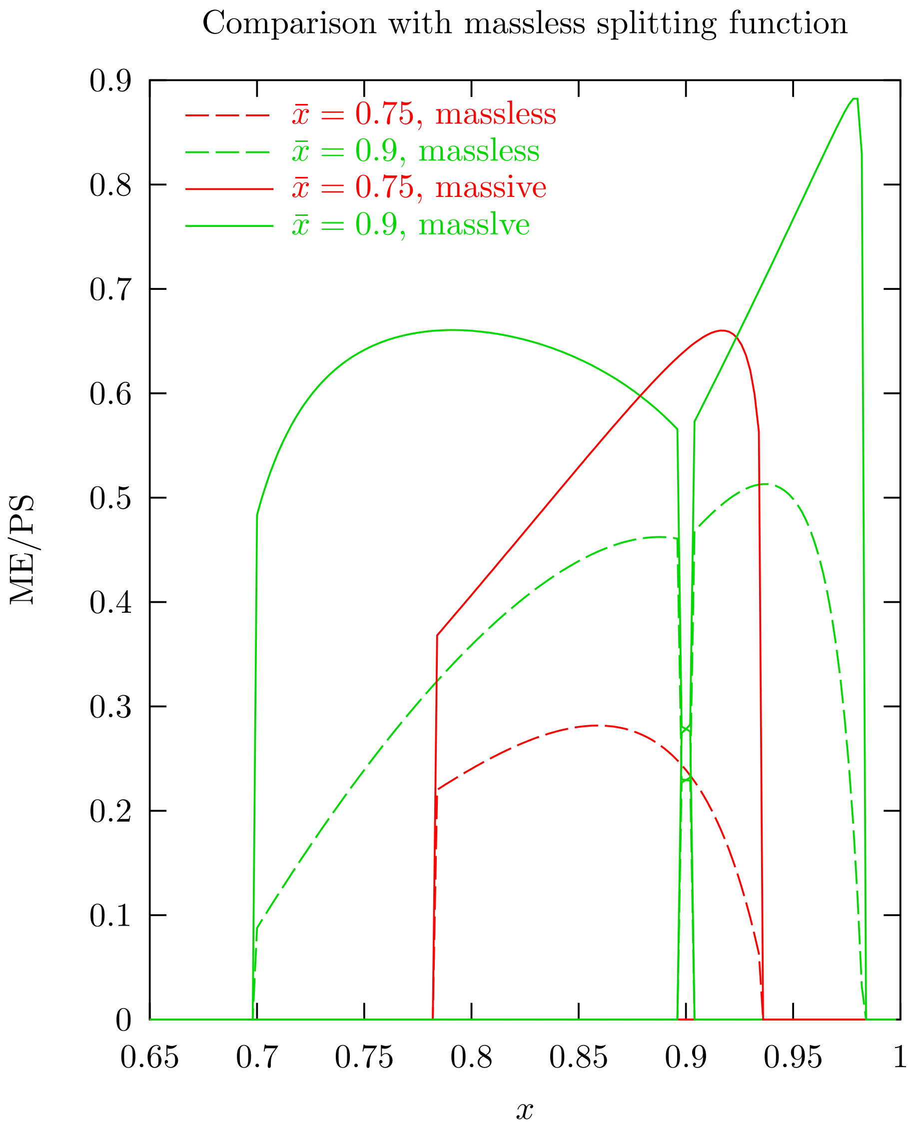


Soft Matrix Element Corrections

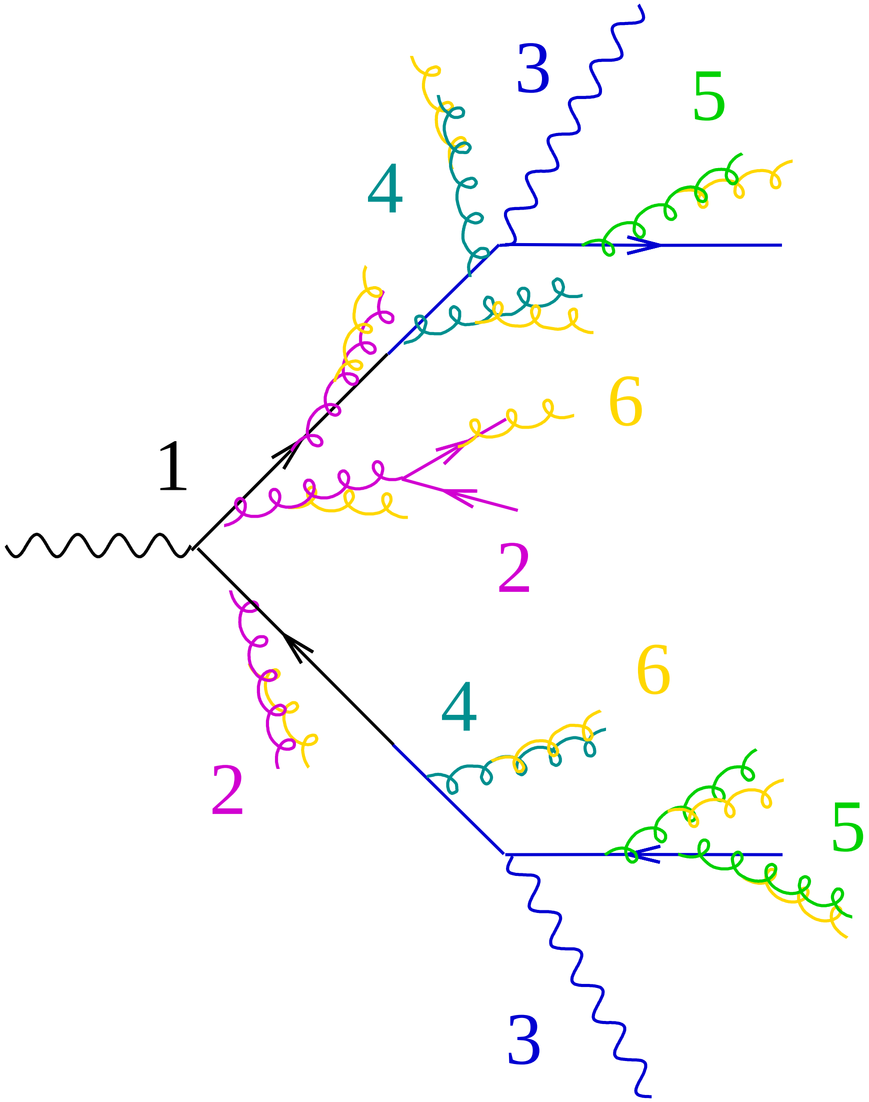
- Ratio ME/PS compares emission with result from true ME if slightly away from soft/collinear region.
- Veto on ‘hardest emission so far’ in $p_\perp$.
- Massive splitting function *very important*!

Example with heavy quark, $m^2/Q^2 = 0.1$ ($\approx t\bar{t}$ at 500 GeV)





Multiscale Showering



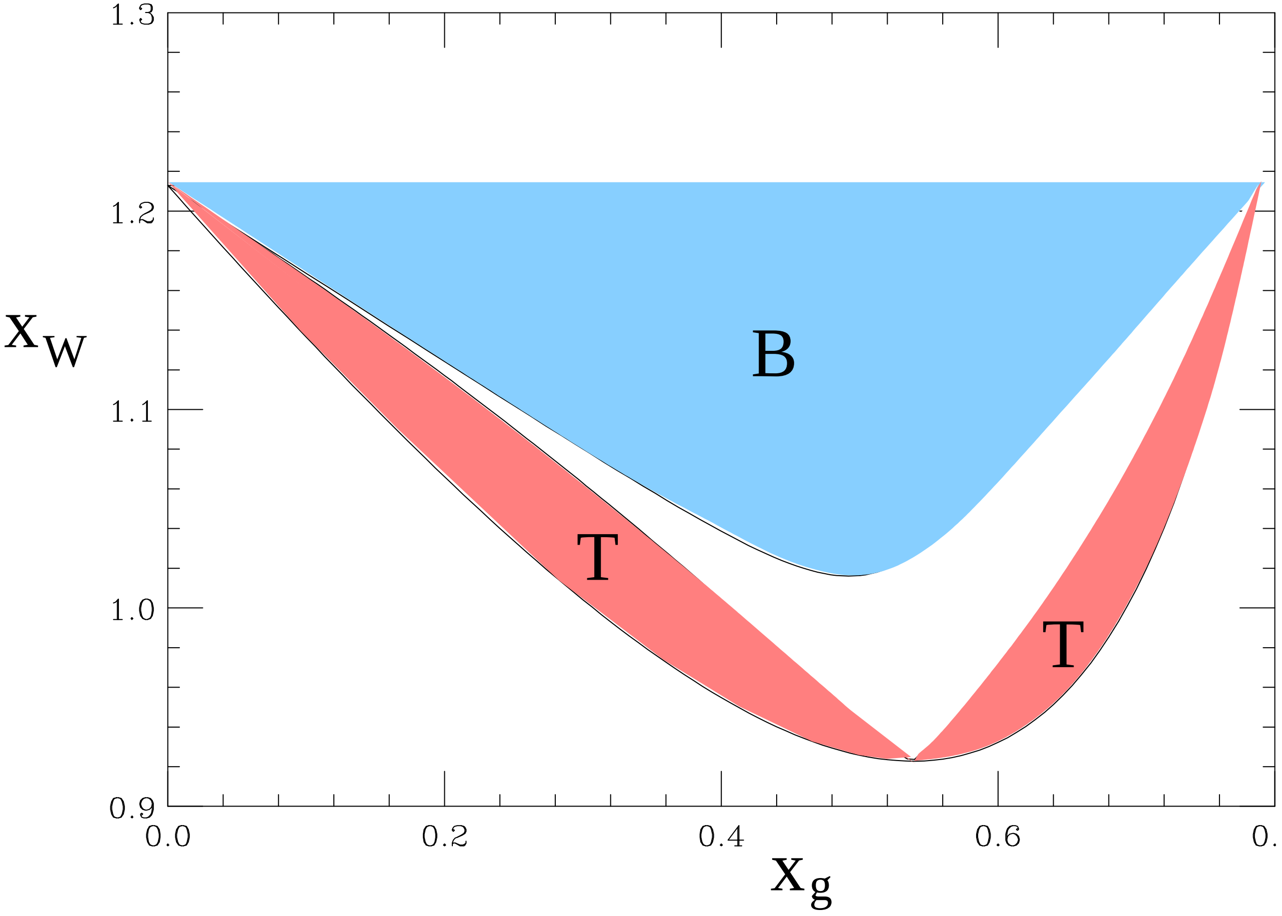
Example: $t\bar{t}$ production & decay

1. Hard process (scale $\sim \hat{s}$)
2. Showers from $t, \bar{t}$ $(\hat{s} \to \Gamma_t)$
3. Decays $t \to Wb$, $\bar{t} \to W\bar{b}$
4. ISR from $t, \bar{t}$ $(m_t \to \Gamma_t)$
5. FSR from $b, \bar{b}$ $(m_t \to \Gamma_t)$
6. Global showering $(\Gamma_t \to \Gamma_b)$

etc.

Heavy Quark Decay

- In $t \longrightarrow Wb$, ISR from t fills soft and collinear regions $\longrightarrow$ ME correction is finite.



- In Fortran `HERWIG`, ISR was missing $\longrightarrow$ infrared divergence in ME correction.

Combining Matrix Elements and Showers

Above method of hard+soft matrix element corrections is difficult to extend to NLO, or to more complicated processes.

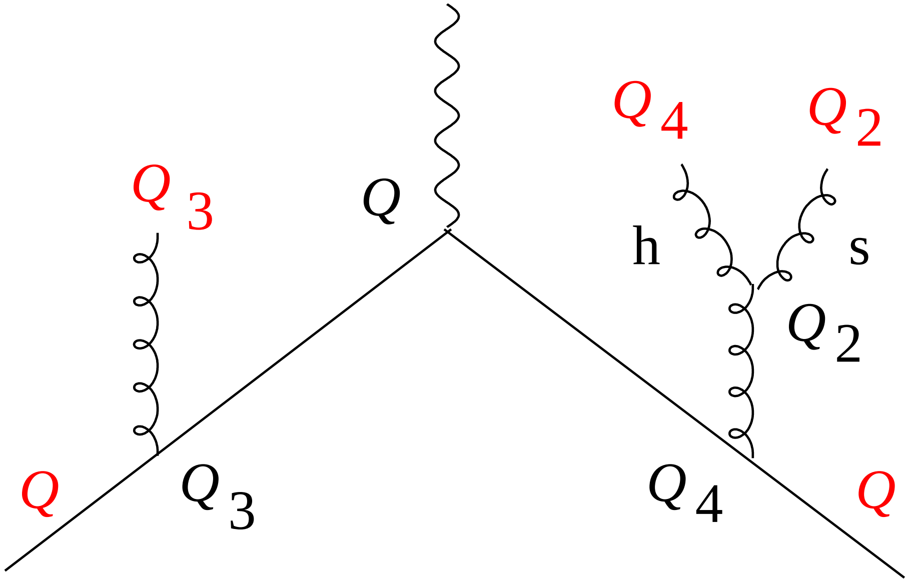
- MC@NLO: subtract approximate NLO contributions generated by showers from exact NLO matrix elements.
  - Regularizes divergences of NLO ME!
  - All NLO results formally reproduced
  - Shower resums soft & collinear divergences to all orders

  $\longrightarrow$ Frixione talk.
- CKKW (+ Krauss, Lönnblad, Mrenna & Richardson): generate ME with k_T-cutoff Q_1, apply corresponding Sudakov form factors, veto $k_T > Q_1$ in showers.
  - Q_1 dependence cancels to NLL
  - Can combine different multiplicity ME's without double counting jet rates (to NLL)

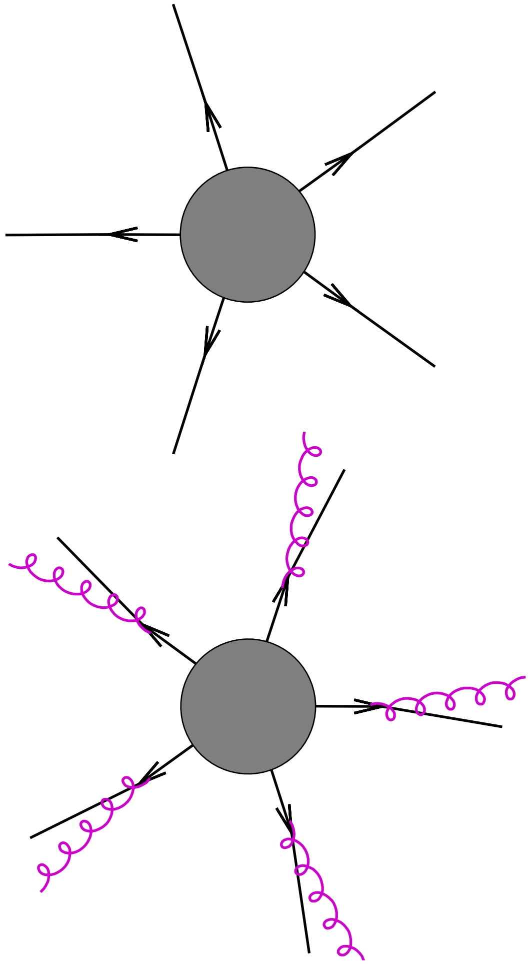
  $\longrightarrow$ Mrenna, Schumann talks.

Combining ME & PS: Scales

- Coherent branching $\longrightarrow$ evolution in angle, not k_T
- k_T-cutoff Q_1 on ME $\longrightarrow$ veto $k_T > Q_1$ in showers
- However, starting scale for showers is not $\tilde{q} = Q_1$
  - Showers must "fill in" radiation at larger angles, with $\tilde{q} > Q_1$ but $k_T < Q_1$
- Construct parton "histories" (gauge invariant) from clustering sequence
  - Each parton evolves from the $\tilde{q}$ scale at which it was "created" (shown in red)



Combining ME & PS: Kinematics



Formally subleading ⟶ important for MC@NLO.
After showering, hard partons have virtualities $q_i^2 \neq m_i^2$
⟶ boost/rescale jets.
Started with

$$\sqrt{s} = \sum_{i=1}^{n} \sqrt{m_i^2 + \boldsymbol{p}_i^2}$$

We can rescale 3-momenta with common factor K,

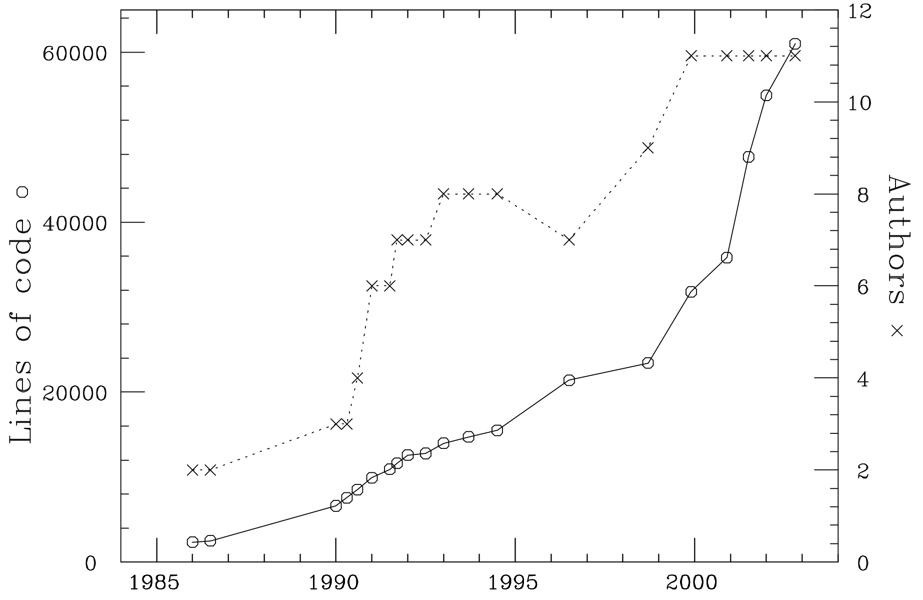
$$\sqrt{s} = \sum_{i=1}^{n} \sqrt{q_i^2 + K\boldsymbol{p}_i^2}$$

to preserve overall energy/momentum.
⟶ resulting jets are then boosted accordingly.

The new generator Herwig++

A completely new event generator in C++

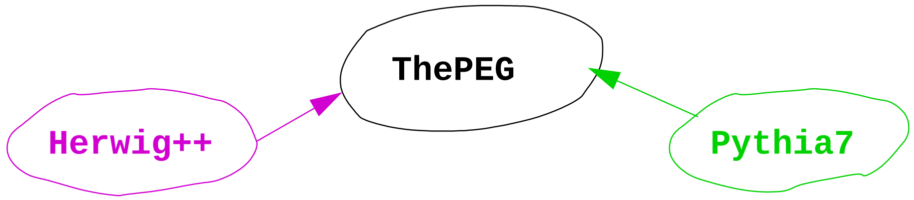
- Aiming at full multi–purpose generator for LHC and future colliders.
- Preserving main features of `HERWIG` such as
  - angular ordered parton shower
  - cluster hadronization
- New features and improvements
  - covariant shower formulation
  - improved parton shower evolution for heavy quarks
  - consistent radiation from unstable particles (multiscale evolution)



Growth of Fortran `HERWIG`

Use of ThePEG in Herwig++

ThePEG = Toolkit for high energy Physics Event Generation
Leif Lönnblad, http://www.thep.lu.se/ThePEG/



Share administrative overhead, common to event generators with Pythia7

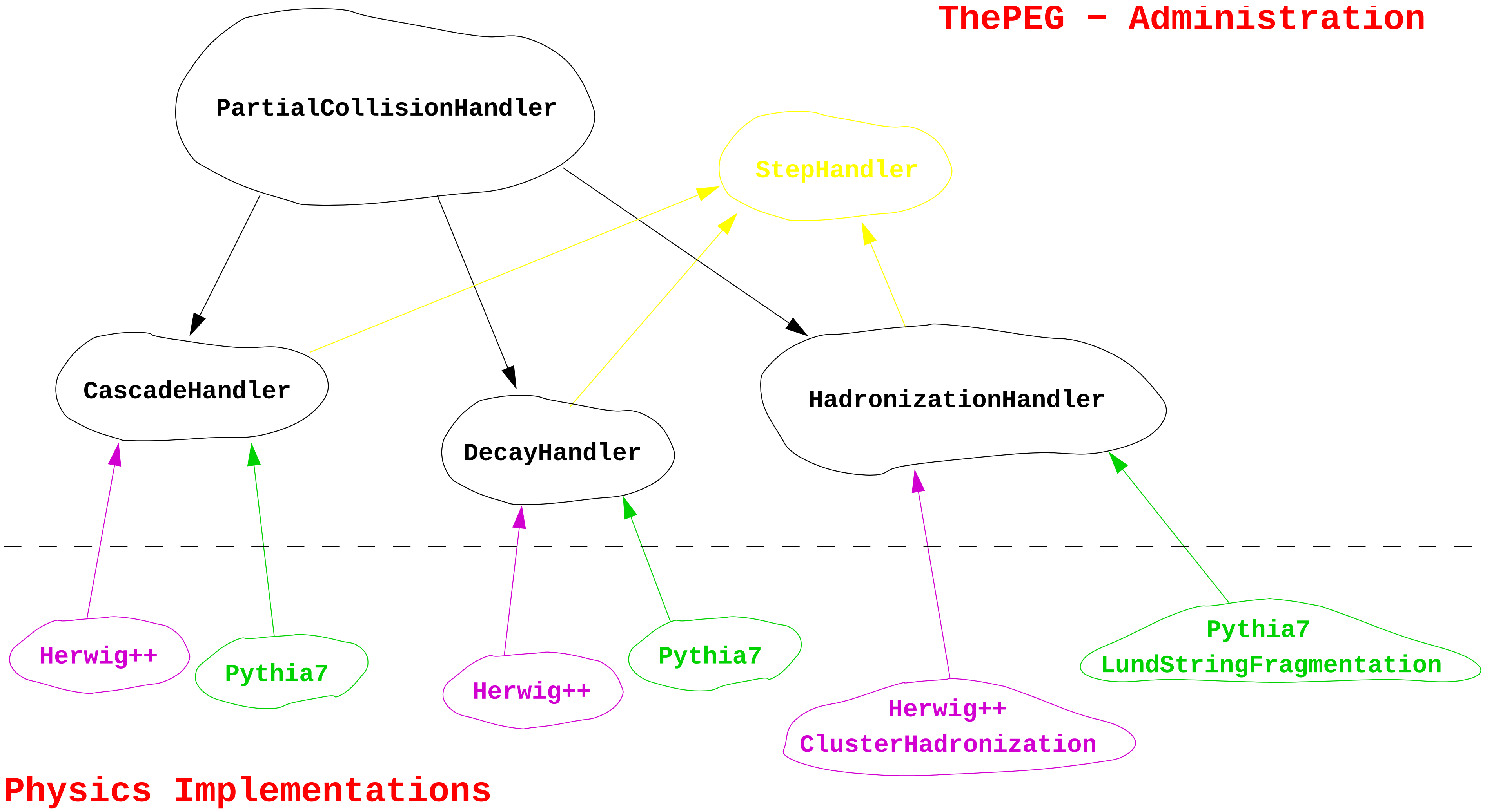
Independent *physics* implementation

Large but very flexible implementation

Common basis for Pythia7/Herwig++

- Lack of independence.
- Less possiblity to test codes against each other.
- Physics is still independent.
- Beneficial for the user to have the same framework.
- Running Herwig++ with Lund String Fragmentation from Pythia7 is very simple!

PartialCollisionHandlers



ThePEG – Administration

PartialCollisionHandler

StepHandler

CascadeHandler

DecayHandler

HadronizationHandler

Herwig++

Pythia7

Herwig++

Pythia7

Herwig++ ClusterHadronization

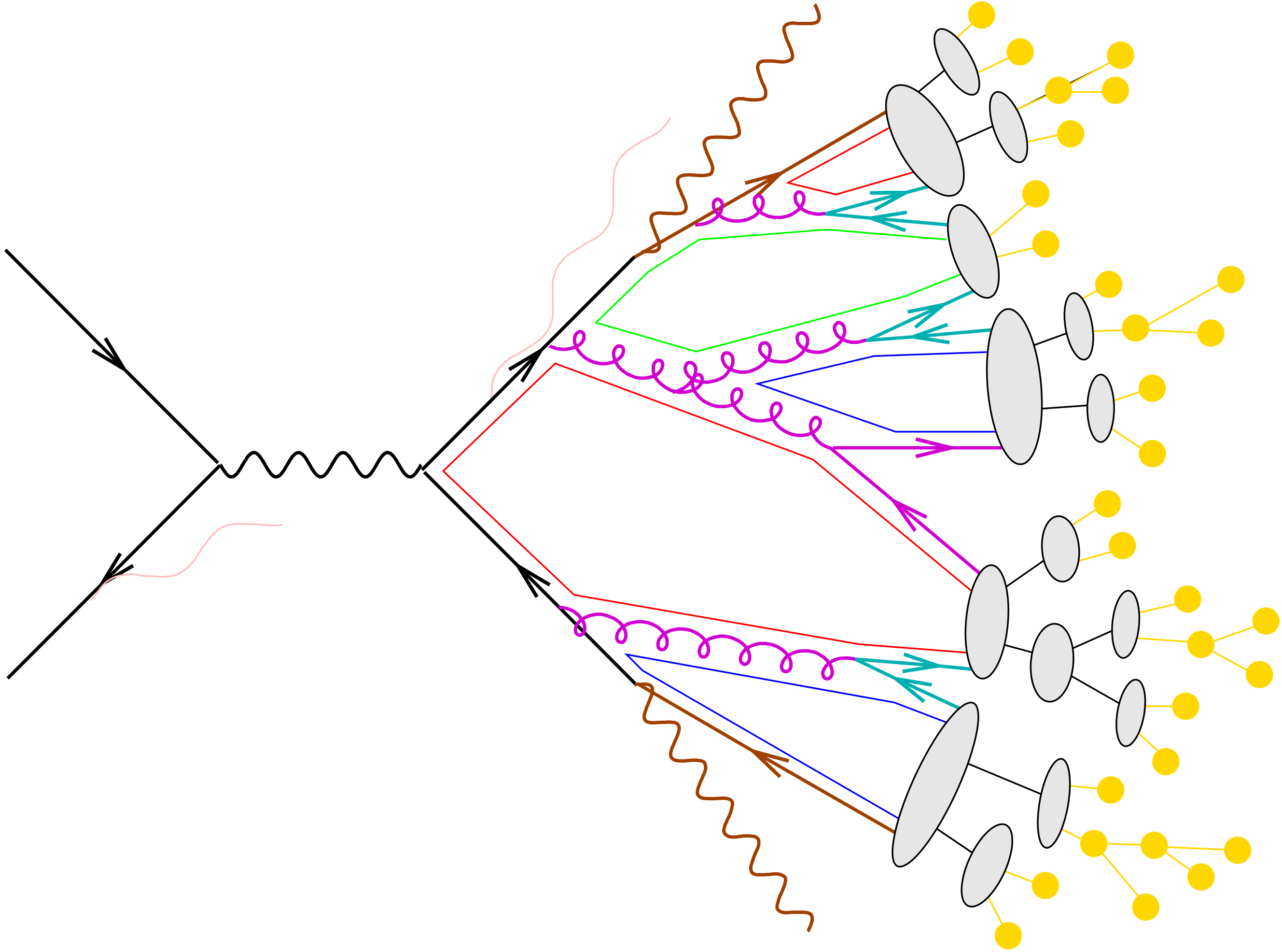
Pythia7 LundStringFragmentation

Physics Implementations

Hard interactions

- Basic ME's included in `ThePEG`, such as $e^+e^- \longrightarrow q\bar{q}$, QCD $2 \longrightarrow 2$: we use them.
- Soft and hard matrix element corrections implemented for $e^+e^- \longrightarrow q\bar{q}g$.
- `AMEGIC++` will provide arbitrary ME's for multiparton final states via `AMEGICInterface`.
- CKKW ME+PS foreseen.
- Other authors can easily include their own matrix elements (→ *safety* of OO code)

Cluster Hadronization Model



- hard scattering
- (QED) initial/final state radiation
- partonic decays, e.g. $t \longrightarrow bW$
- parton shower evolution
- nonperturbative gluon splitting
- colour singlets
- colourless clusters
- cluster fission
- cluster $\longrightarrow$ hadrons
- hadronic decays

Cluster hadronization in a nutshell

- Nonperturbative $g \to q\bar{q}$ splitting ($q = uds$) isotropically. Here, $m_g \approx 750\,\mathrm{MeV} > 2m_q$.
- Cluster formation, universal spectrum (see right)
- Cluster fission until

$$M^p < M^p_{\max} + (m_1 + m_2)^p$$

where masses are chosen from

$$M_i = \left[\left(M^P - (m_i + m_3)^P\right) r_i + (m_i + m_3)^P\right]^{1/P},$$

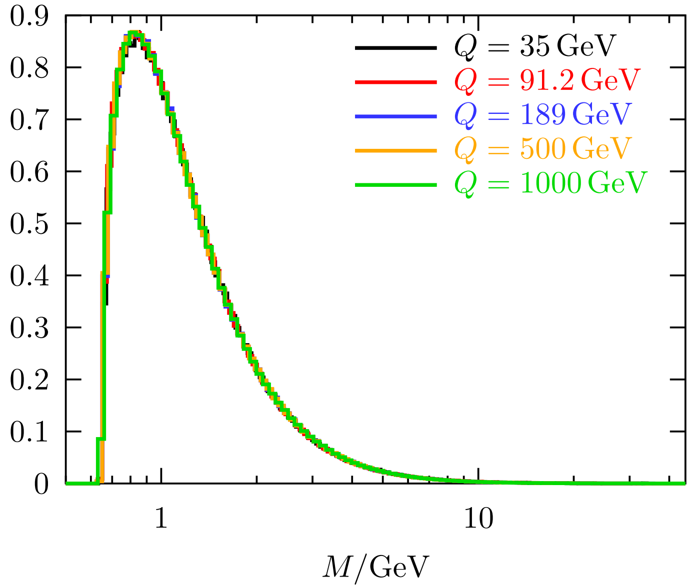
with additional phase space constraints. Constituents keep moving in their original directions.

- Cluster decay

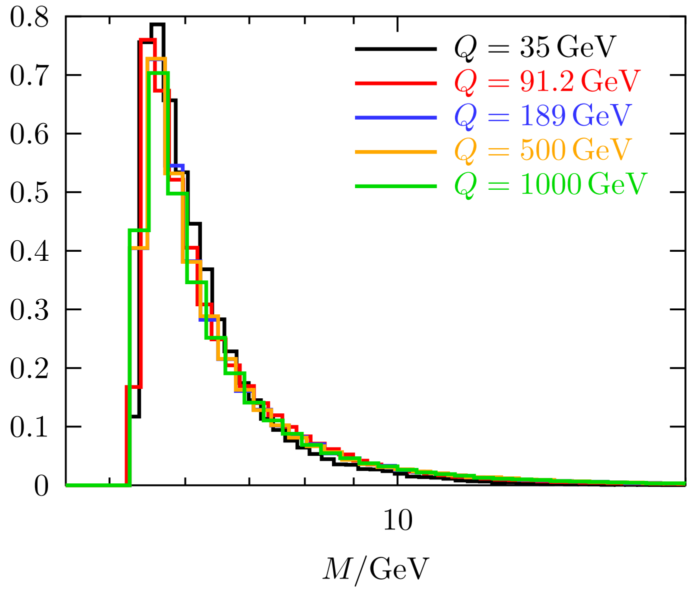
$$P(a_{i,q}, b_{q,j}|i,j) = \frac{W(a_{i,q}, b_{q,j}|i,j)}{\sum_{M/B} W(c_{i,q'}, d_{q',j}|i,j)}.$$

New! Meson/Baryon ratio is parametrized in terms of diquark weight. In Fortran `HERWIG` the sum ran over all possible hadrons.

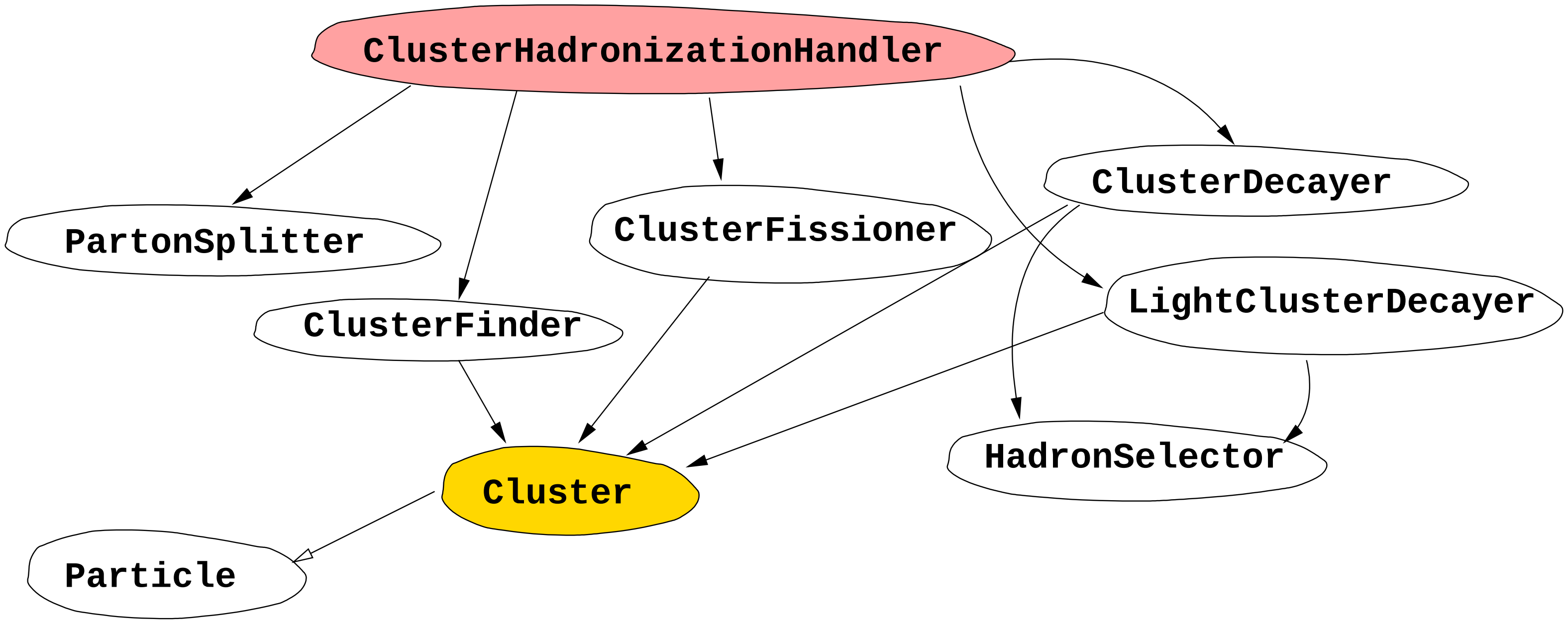
Primary Light Clusters



Primary b-Clusters

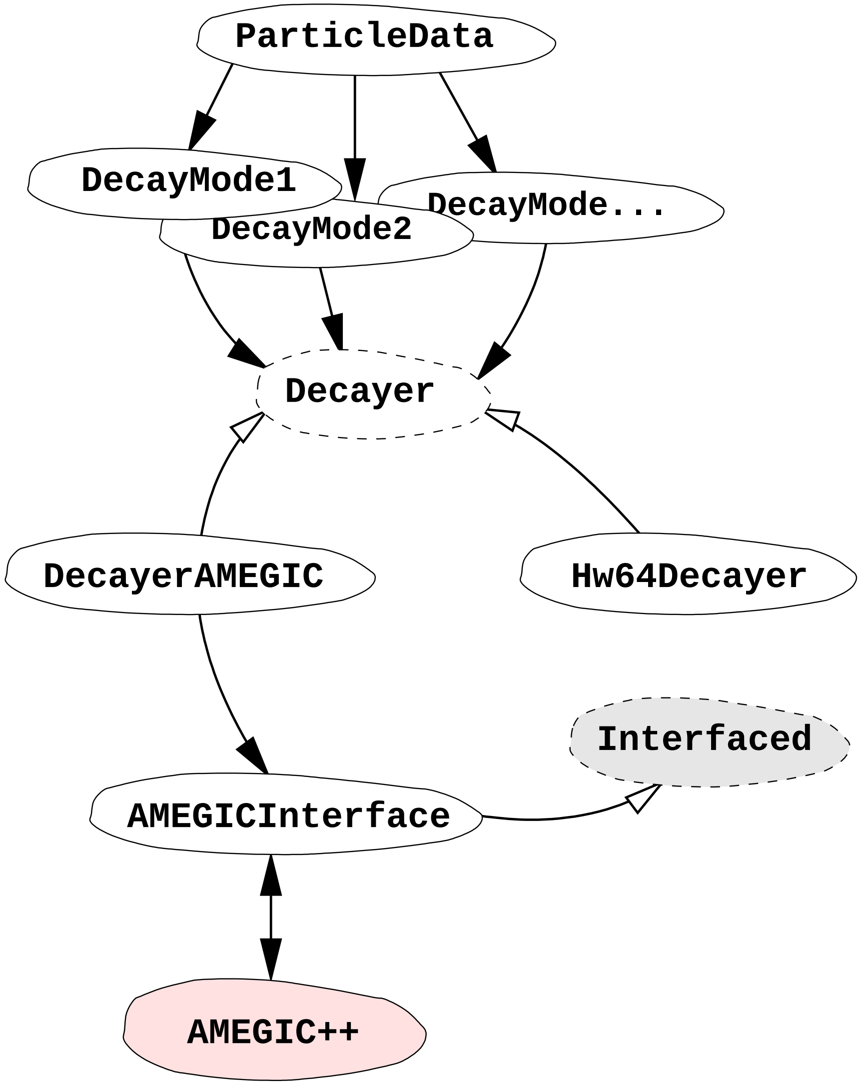


ClusterHadronization



- Cluster hadronization is designed, implemented and debugged.
- `HadronSelector`/ `ClusterDecayer` in different ways.
- Tests ongoing.
- Lund string model is implemented already in `Pythia7` and will work together with `Herwig++`.
- This requires that final state gluons are on-shell ⟶ foreseen in shower.

Particle Decays



- FORTRAN HERWIG is reproduced with Hw64Decayer using the same matrix element codes as before (used for hadronic decays right now).
- DecayerAMEGIC gets final states for a decay mode directly from AMEGIC++.
- Works fine in principle, further tests required.

$Z^0 \longrightarrow$ Hadron Multiplicities

Particle	Experiment	Measured	Old Model	Herwig++	Fortran
All Charged	M,A,D,L,O	20.924 ± 0.117	20.22*	20.814	20.532*
γ	A,O	21.27 ± 0.6	23.032	22.67	20.74
π^0	A,D,L,O	9.59 ± 0.33	10.27	10.08	9.88
$\rho(770)^0$	A,D	1.295 ± 0.125	1.235	1.316	1.07
$\pi^\pm$	A,O	17.04 ± 0.25	16.30	16.95	16.74
$\rho(770)^\pm$	O	2.4 ± 0.43	1.99	2.14	2.06
η	A,L,O	0.956 ± 0.049	0.886	0.893	0.669*
$\omega(782)$	A,L,O	1.083 ± 0.088	0.859	0.916	1.044
$\eta'(958)$	A,L,O	0.152 ± 0.03	0.13	0.136	0.106
K^0	S,A,D,L,O	2.027 ± 0.025	2.121*	2.062	2.026
$K^*(892)^0$	A,D,O	0.761 ± 0.032	0.667	0.681	0.583*
$K^*(1430)^0$	D,O	0.106 ± 0.06	0.065	0.079	0.072
$K^\pm$	A,D,O	2.319 ± 0.079	2.335	2.286	2.250
$K^*(892)^\pm$	A,D,O	0.731 ± 0.058	0.637	0.657	0.578
$\phi(1020)$	A,D,O	0.097 ± 0.007	0.107	0.114	0.134*
p	A,D,O	0.991 ± 0.054	0.981	0.947	1.027
Δ^{++}	D,O	0.088 ± 0.034	0.185	0.092	0.209*
Σ^-	O	0.083 ± 0.011	0.063	0.071	0.071
Λ	A,D,L,O	0.373 ± 0.008	0.325*	0.384	0.347*
Σ^0	A,D,O	0.074 ± 0.009	0.078	0.091	0.063
Σ^+	O	0.099 ± 0.015	0.067	0.077	0.088
$\Sigma(1385)^\pm$	A,D,O	0.0471 ± 0.0046	0.057	0.0312*	0.061*
Ξ^-	A,D,O	0.0262 ± 0.001	0.024	0.0286	0.029
$\Xi(1530)^0$	A,D,O	0.0058 ± 0.001	0.026*	0.0288*	0.009*
Ω^-	A,D,O	0.00125 ± 0.00024	0.001	0.00144	0.0009

$Z^0 \to$ Hadron Multiplicities (ctd')

Particle	Experiment	Measured	Old Model	Herwig++	Fortran
$f_2(1270)$	D,L,O	0.168 ± 0.021	0.113	0.150	0.173
$f_2'(1525)$	D	0.02 ± 0.008	0.003	0.012	0.012
$D^\pm$	A,D,O	0.184 ± 0.018	0.322^*	0.319^*	0.283^*
$D^*(2010)^\pm$	A,D,O	0.182 ± 0.009	0.168	0.180	0.151^*
D^0	A,D,O	0.473 ± 0.026	0.625^*	0.570^*	0.501
$D_s^\pm$	A,O	0.129 ± 0.013	0.218^*	0.195^*	0.127
$D_s^{*\pm}$	O	0.096 ± 0.046	0.082	0.066	0.043
J/Ψ	A,D,L,O	0.00544 ± 0.00029	0.006	0.00361^*	0.002^*
Λ_c^+	D,O	0.077 ± 0.016	0.006^*	0.023^*	0.001^*
$\Psi'(3685)$	D,L,O	0.00229 ± 0.00041	0.001^*	0.00178	0.0008^*

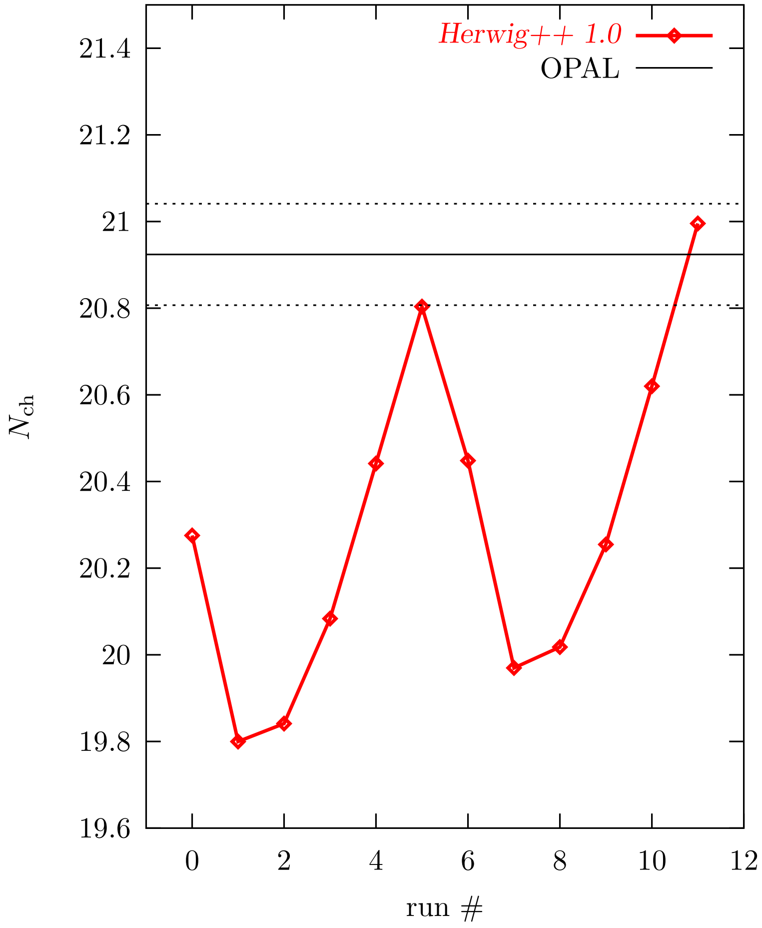
of $*$'s = observables with more than 3σ deviation:

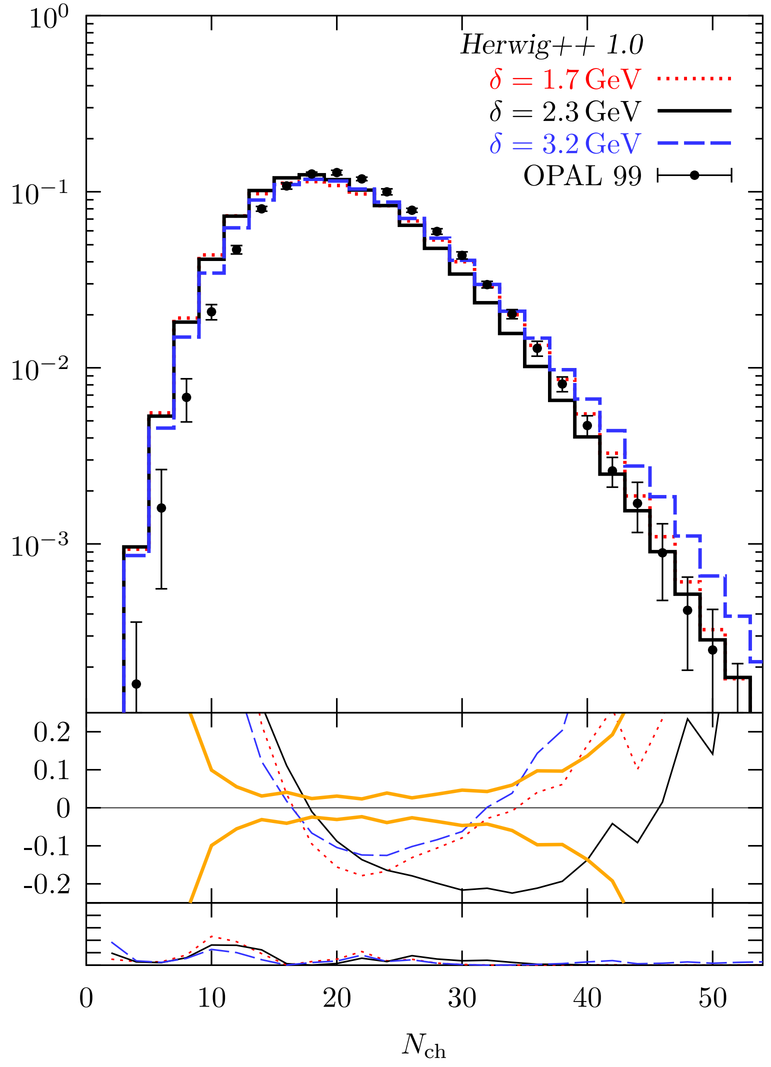
Old Model : Herwig++ : Fortran = 9 : 7 : 13

N.B. No systematic parameter tuning yet.

Charged Particle Multiplicity

Good indicator for quality of hadronization. Still very sensitive to shower cutoff:

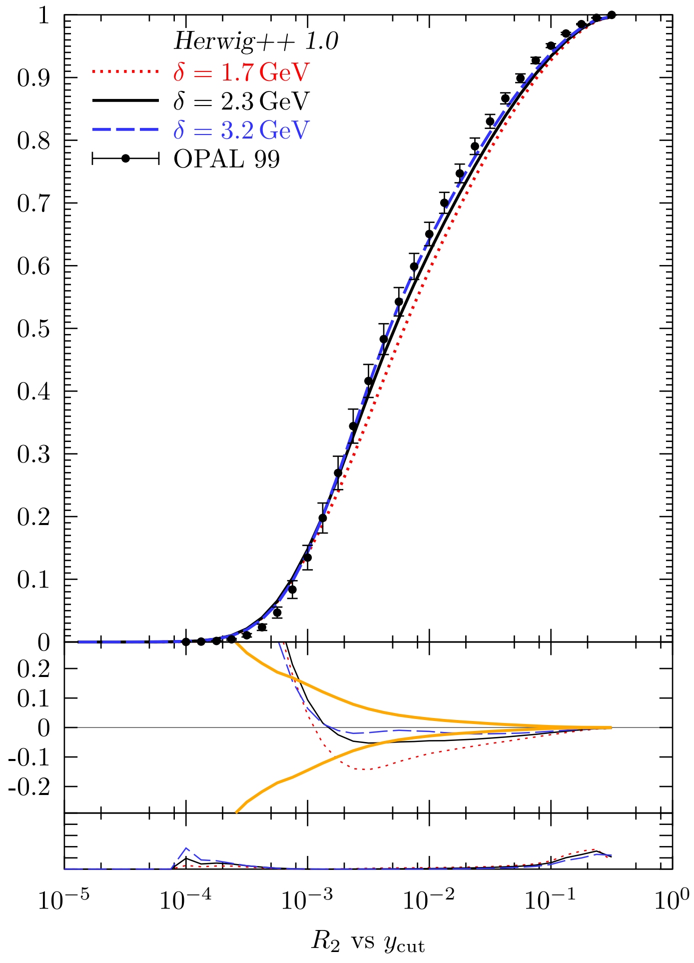


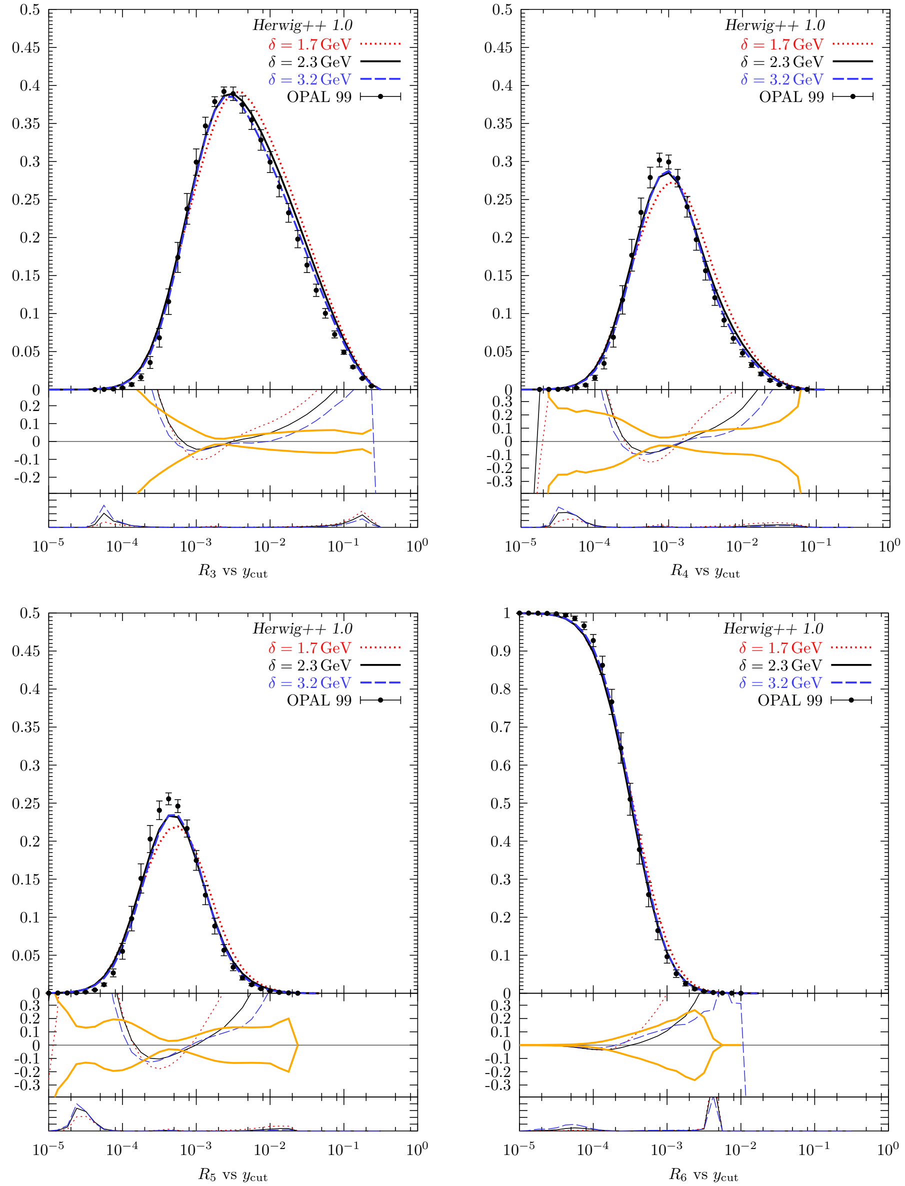


Jet Rates (Durham/k_T Algorithm)

$$R_n = \sigma(n\text{–jets})/\sigma(\text{jets}) \qquad (n = 2..5)$$

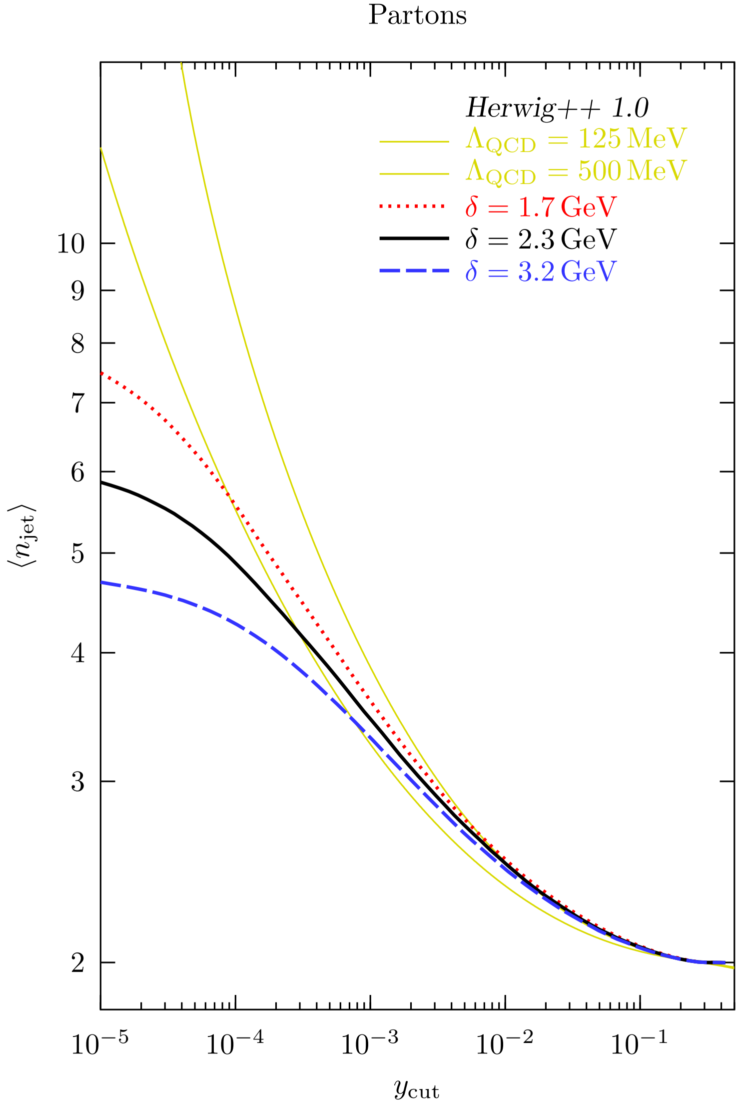
$$R_6 = \sigma(> 5\text{–jets})/\sigma(\text{jets})$$

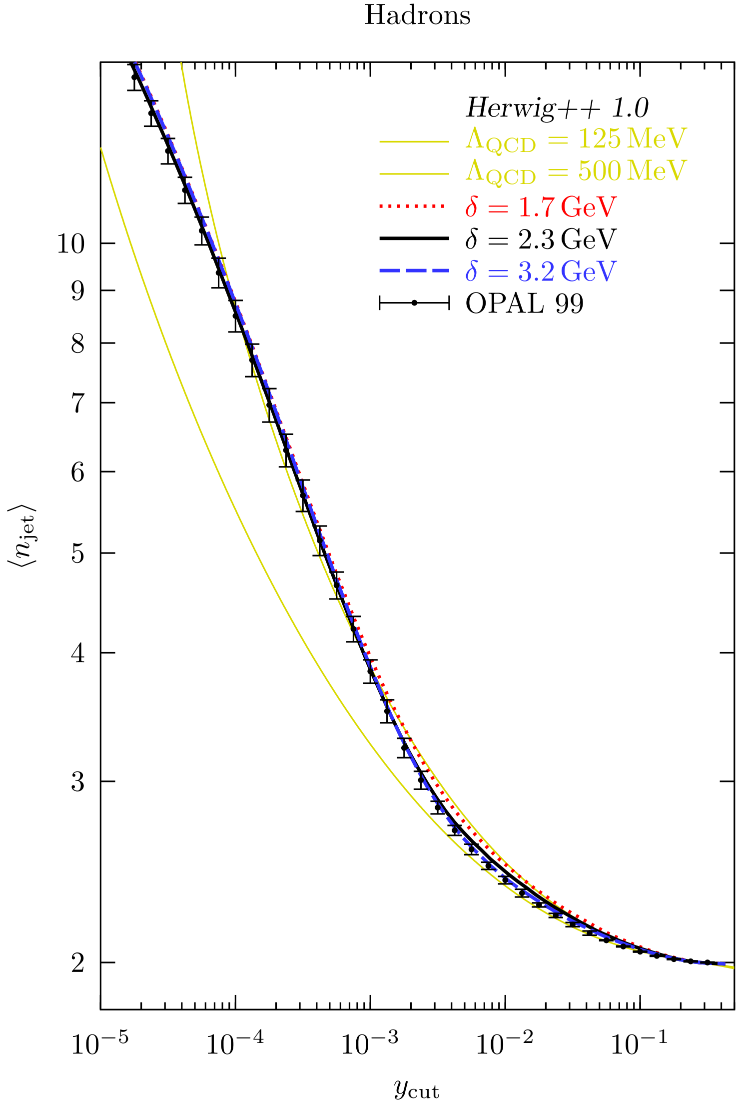




Jet Multiplicity

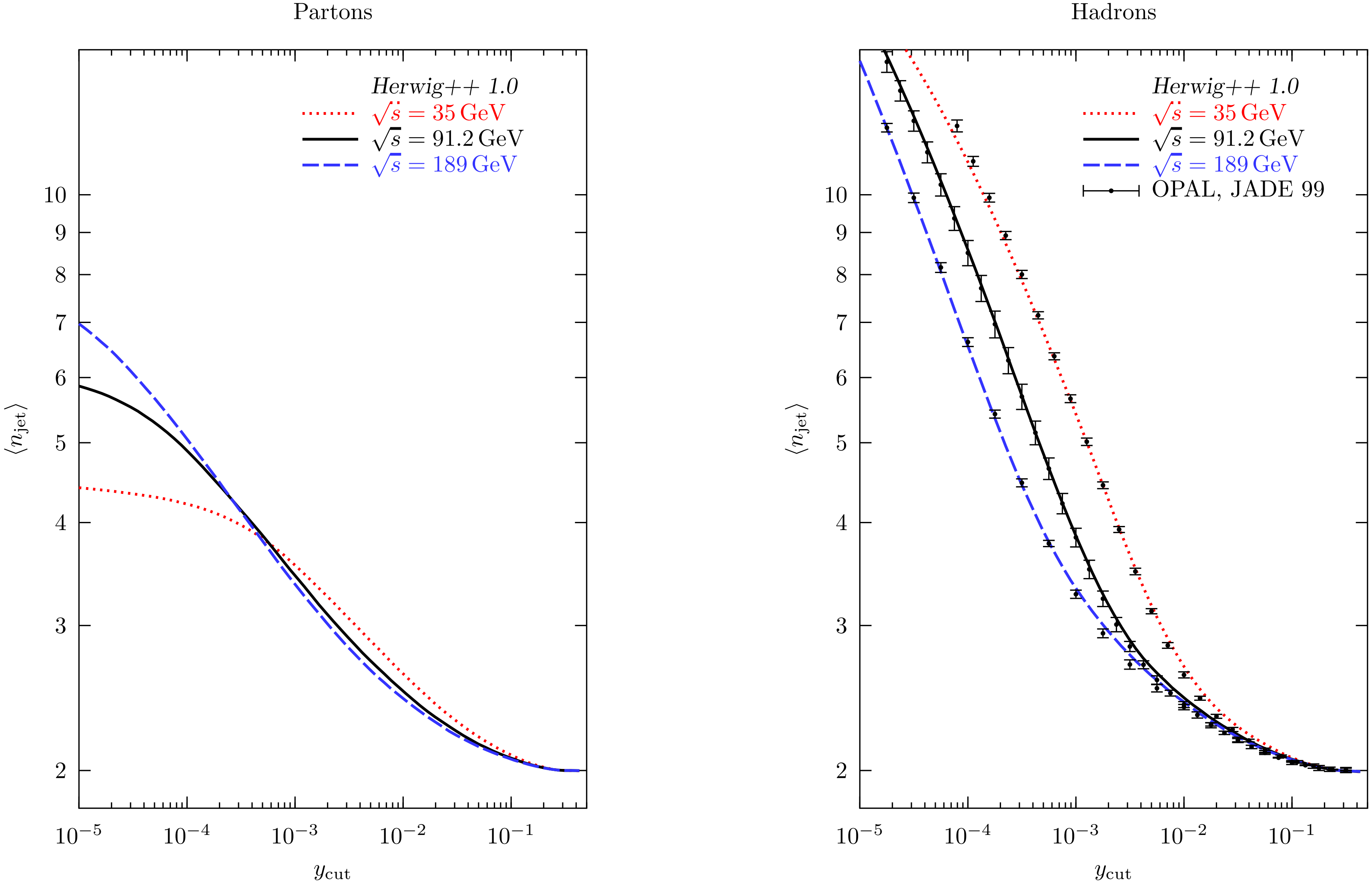
Cutoff dependence largely cancels between shower and hadronization.





Jet Multiplicity (PETRA, LEP, LEPII)

$\sqrt{s} = \{35, 91.2, 189\}$ GeV



Event Shape Variables, Definition

Thrust

$$F(\boldsymbol{n}) = \frac{\sum_\alpha |\boldsymbol{p}_\alpha \cdot \boldsymbol{n}|}{\sum_\alpha |\boldsymbol{p}_\alpha|}$$

Find $\boldsymbol{n}$, such that thrust

$$\begin{aligned} T &= \max_{\boldsymbol{n}} F(\boldsymbol{n}) \\ &= F(\boldsymbol{n}_T)\ , \end{aligned}$$

thrust major

$$\begin{aligned} M &= \max_{\boldsymbol{n} \perp \boldsymbol{n}_T} F(\boldsymbol{n}) \\ &= F(\boldsymbol{n}_M)\ , \end{aligned}$$

thrust minor

$$\begin{aligned} \boldsymbol{n}_m &= \boldsymbol{n}_T \times \boldsymbol{n}_M \\ m &= F(\boldsymbol{n}_m) \end{aligned}$$

Sphericity

$$Q_{ij} = \frac{\sum_\alpha (\boldsymbol{p}_\alpha)_i (\boldsymbol{p}_\alpha)_j}{\sum_\alpha \boldsymbol{p}_\alpha^2}$$

Diagonalize, eigenvalues

$$\lambda_1 > \lambda_2 > \lambda_3$$

$$\lambda_1 + \lambda_2 + \lambda_3 = 1$$

Then

$$\begin{aligned} S &= \tfrac{3}{2}(\lambda_2 + \lambda_3) \\ P &= \lambda_2 - \lambda_3 \\ A &= \tfrac{3}{2}\lambda_3 \end{aligned}$$

Eigenvector $\boldsymbol{n}_S$ sphericity axis etc.

C, D parameter

$$L_{ij} = \frac{\sum_\alpha (\boldsymbol{p}_\alpha)_i (\boldsymbol{p}_\alpha)_j / |\boldsymbol{p}_\alpha|}{\sum_\alpha |\boldsymbol{p}_\alpha|}$$

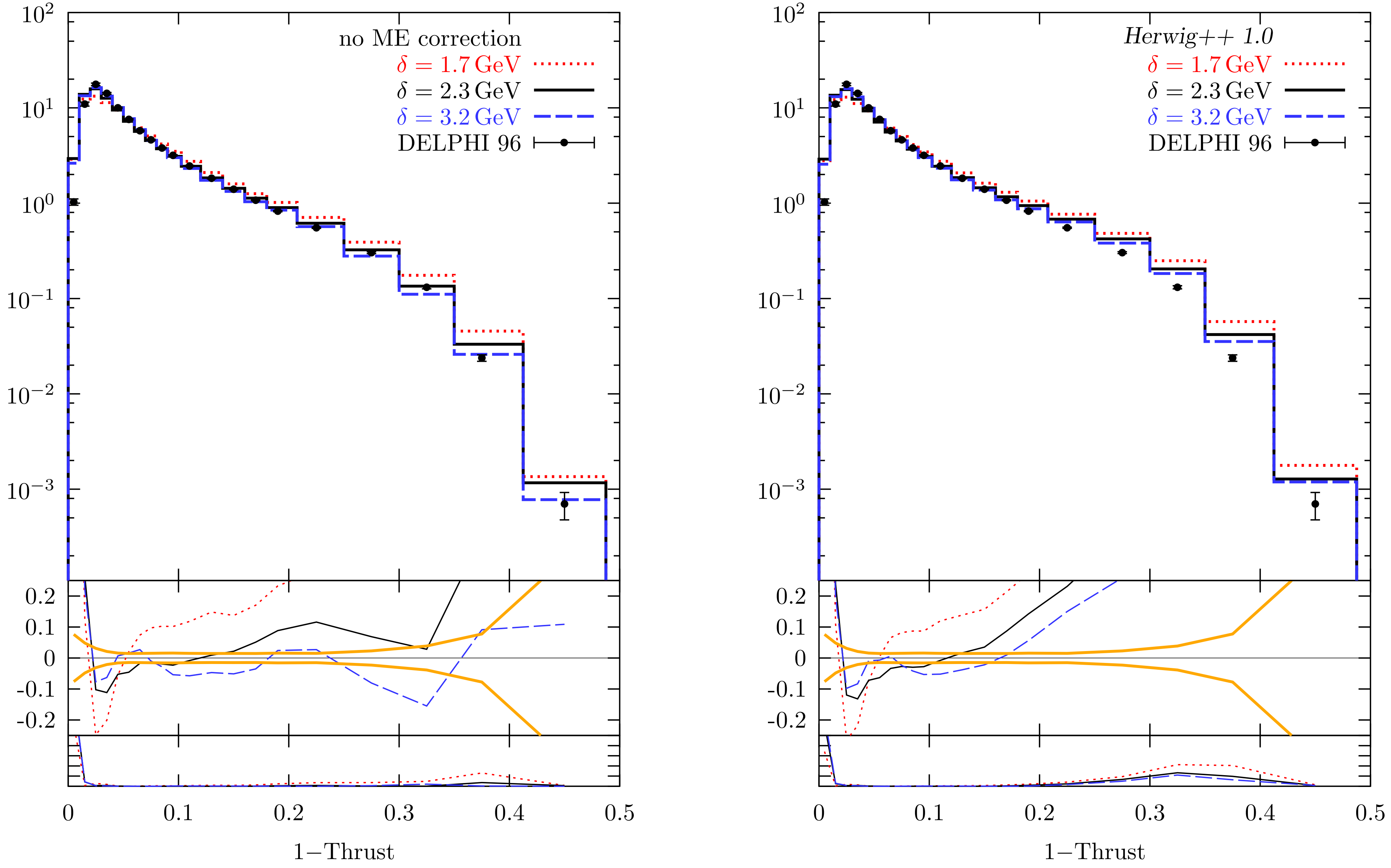
Diagonalize, eigenvalues

$$\lambda_1 + \lambda_2 + \lambda_3 = 1$$

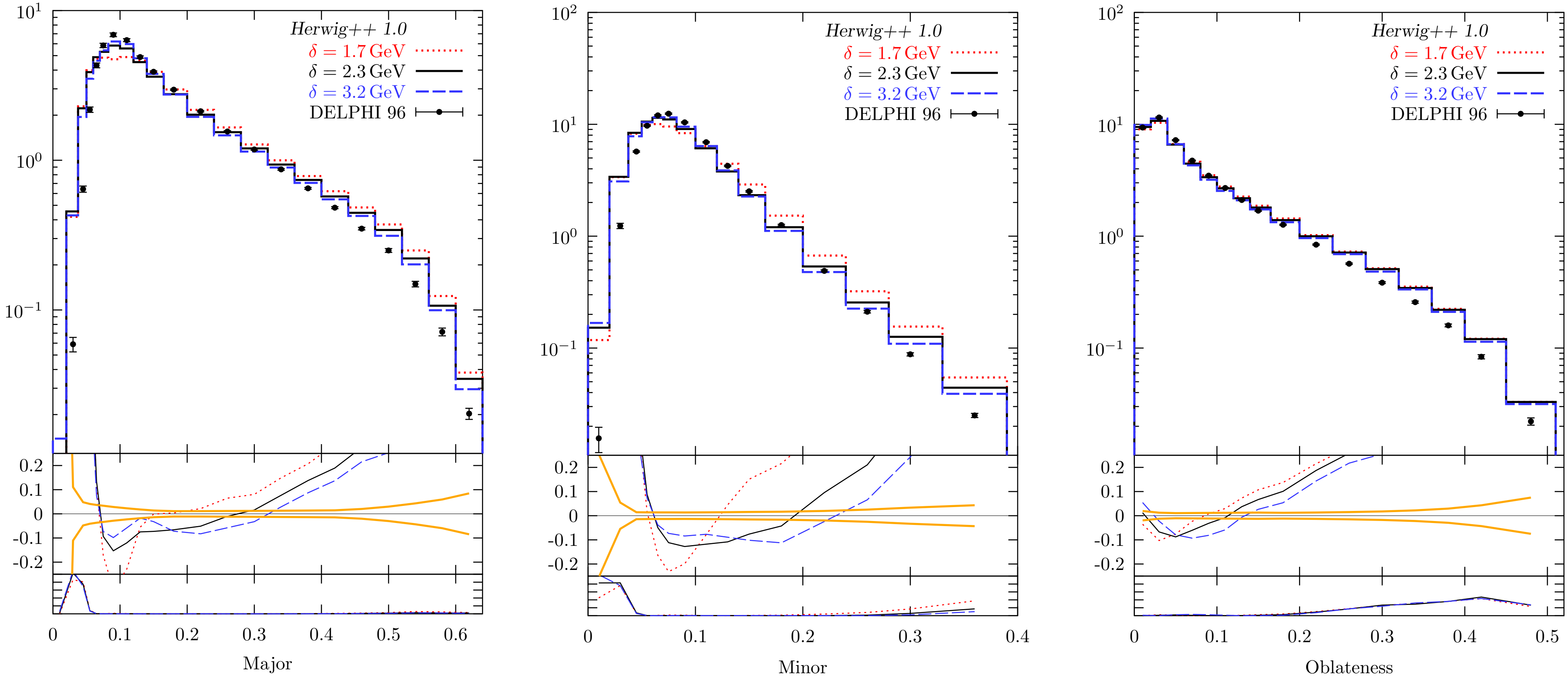
and define

$$\begin{aligned} C &= 3(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1) \\ D &= 27\lambda_1\lambda_2\lambda_3 \end{aligned}$$

Thrust — ME Corrections off/on

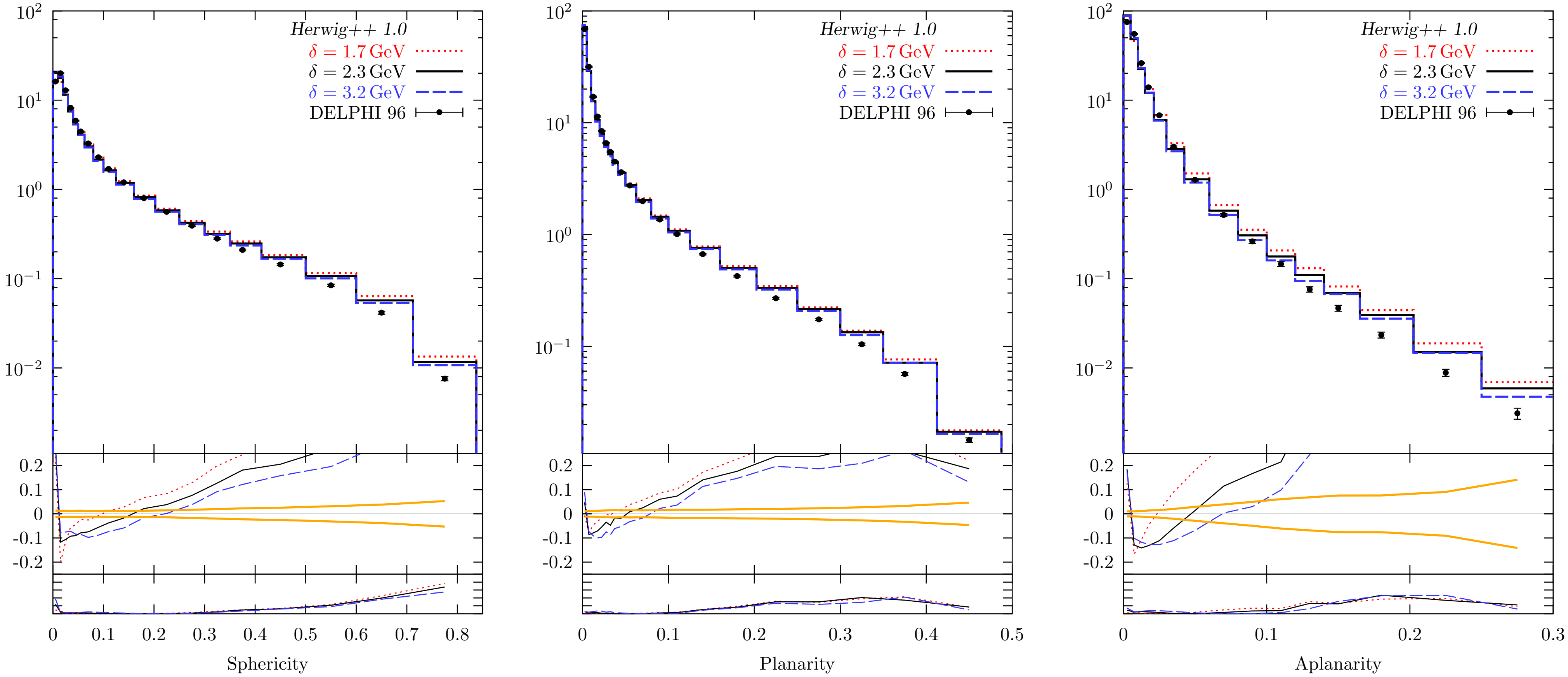


Major, Minor, Oblateness



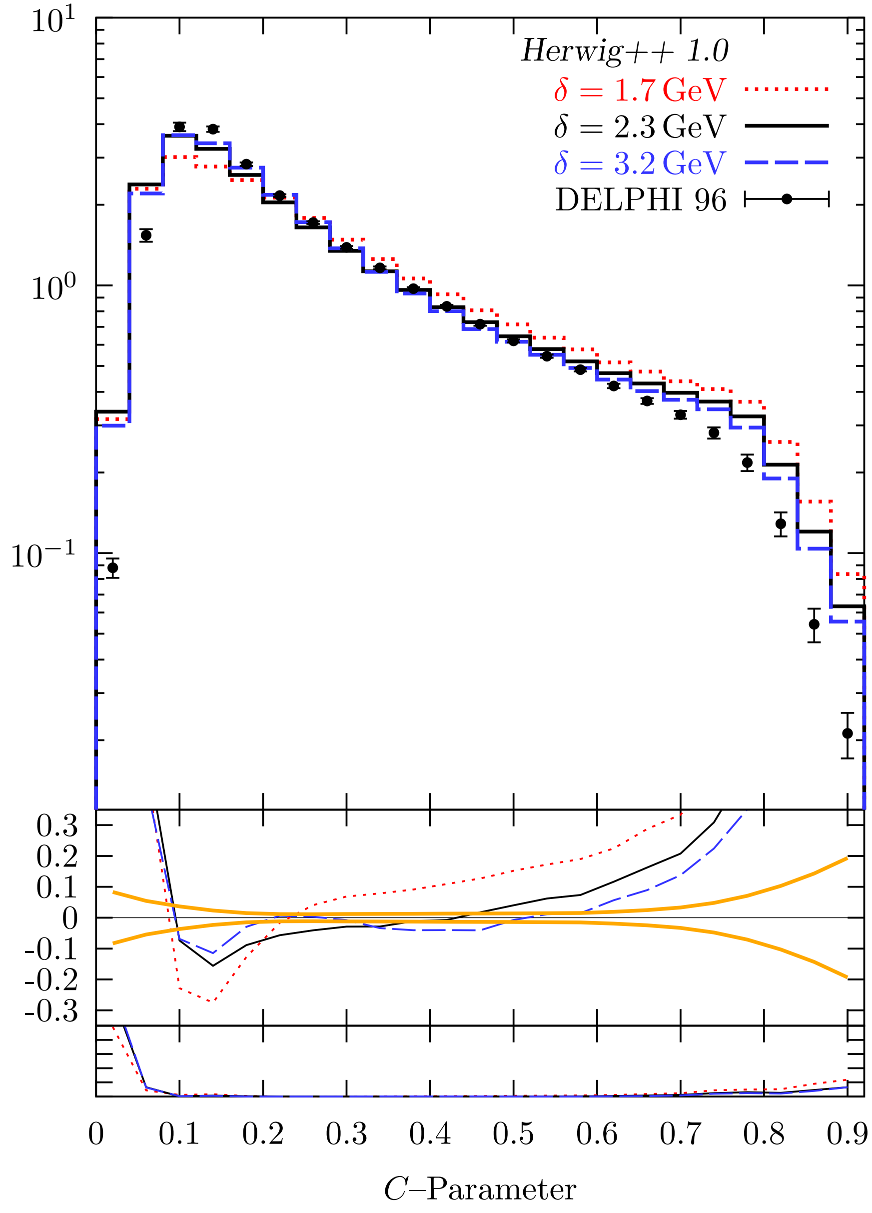
All Thrust–related distributions slightly wide, ie too many 2-jet like on one side and too many spherical events on the other side.

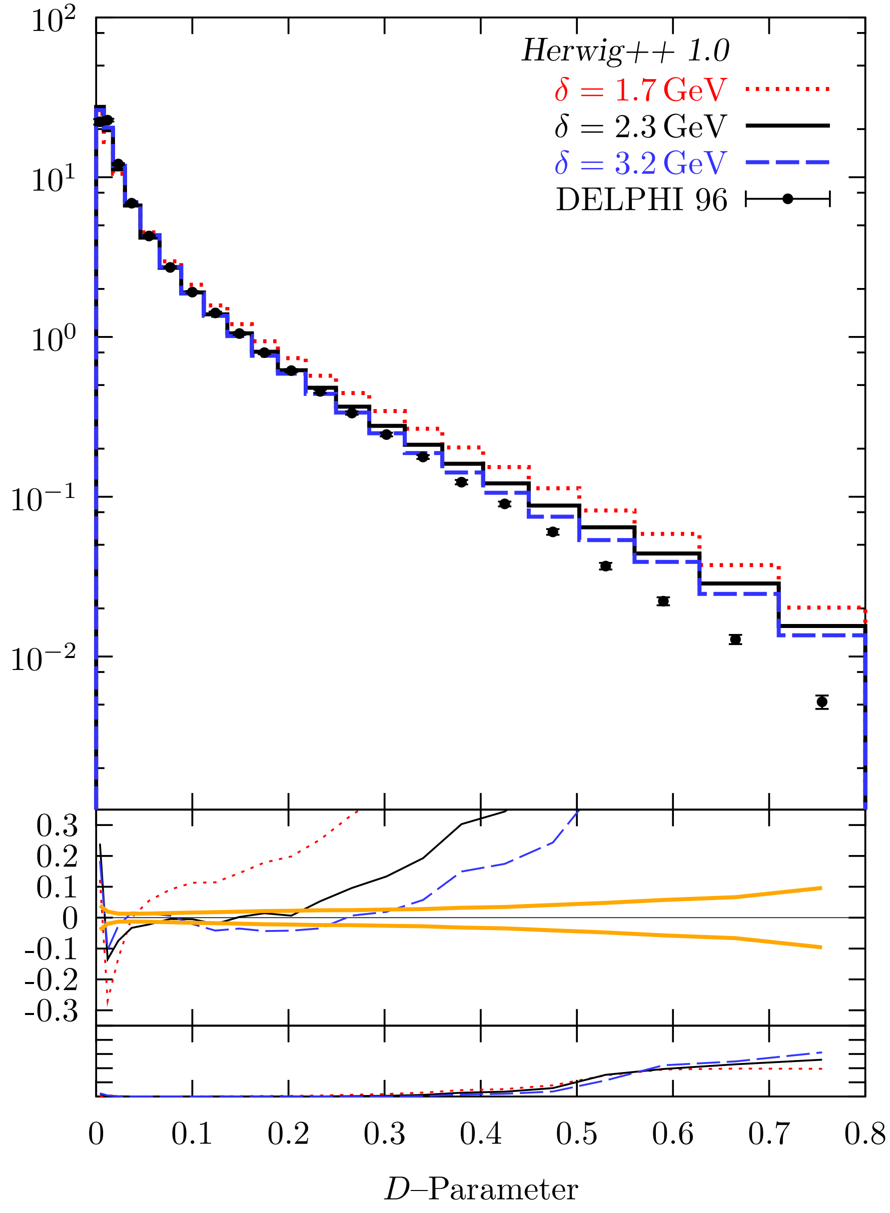
Sphericity, Planarity, Aplanarity



More emphasis on large momenta in quadratic tensor.

C and D parameter





Four–Jet Angles — Definitions

- Bengtsson–Zerwas angle

$$\chi_{BZ} = \angle(\boldsymbol{p}_1 \times \boldsymbol{p}_2, \boldsymbol{p}_3 \times \boldsymbol{p}_4)$$

- Körner–Schierholz–Willrodt angle

$$\Phi_{KSW} = \tfrac{1}{2}\left[\angle(\boldsymbol{p}_1 \times \boldsymbol{p}_3, \boldsymbol{p}_2 \times \boldsymbol{p}_4) + \angle(\boldsymbol{p}_1 \times \boldsymbol{p}_4, \boldsymbol{p}_2 \times \boldsymbol{p}_3)\right]$$

- (Modified) Nachtmann–Reiter angle

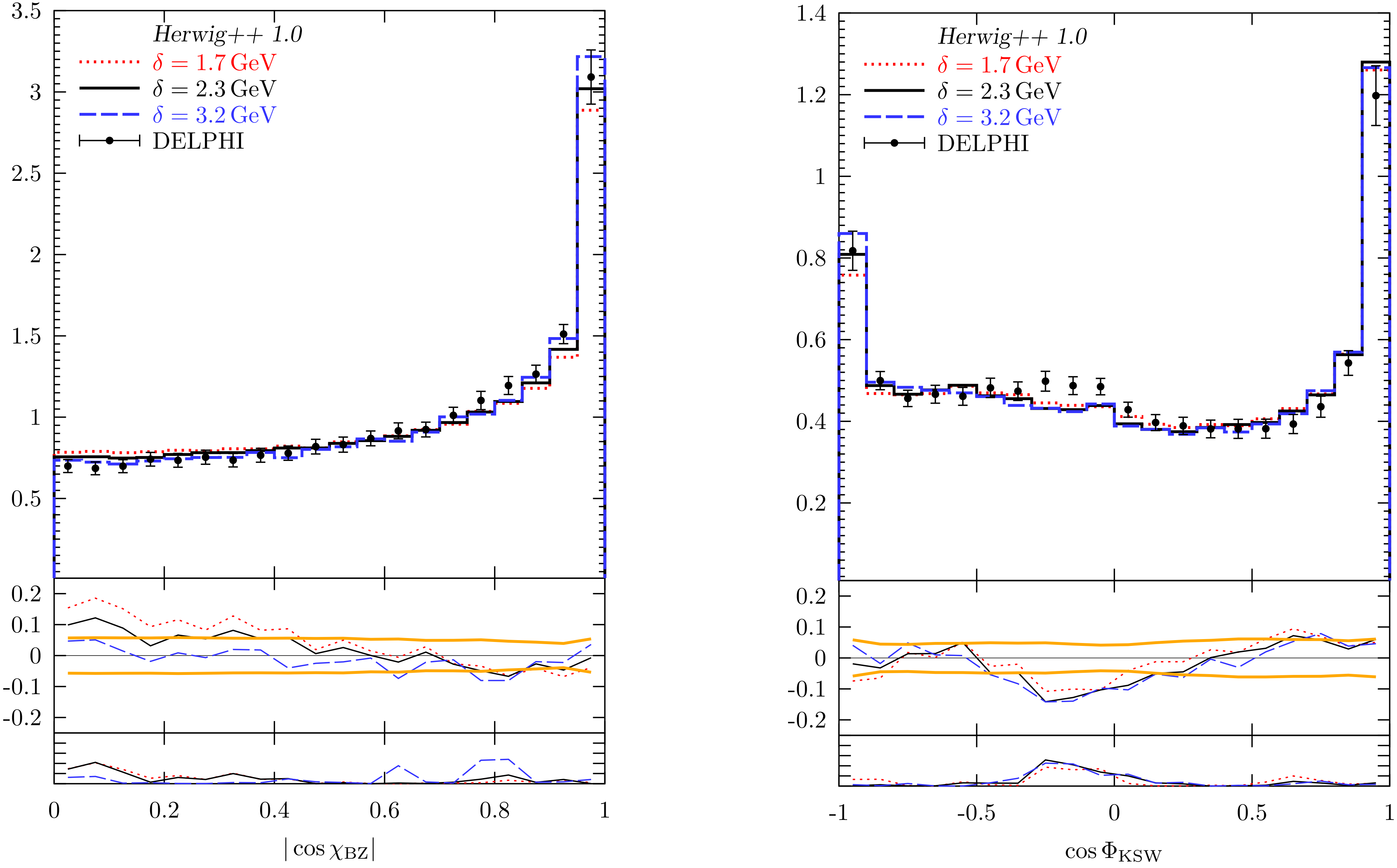
$$\theta^*_{NR} = \angle(\boldsymbol{p}_1 - \boldsymbol{p}_2, \boldsymbol{p}_3 - \boldsymbol{p}_4)$$

- Angle between softest jets

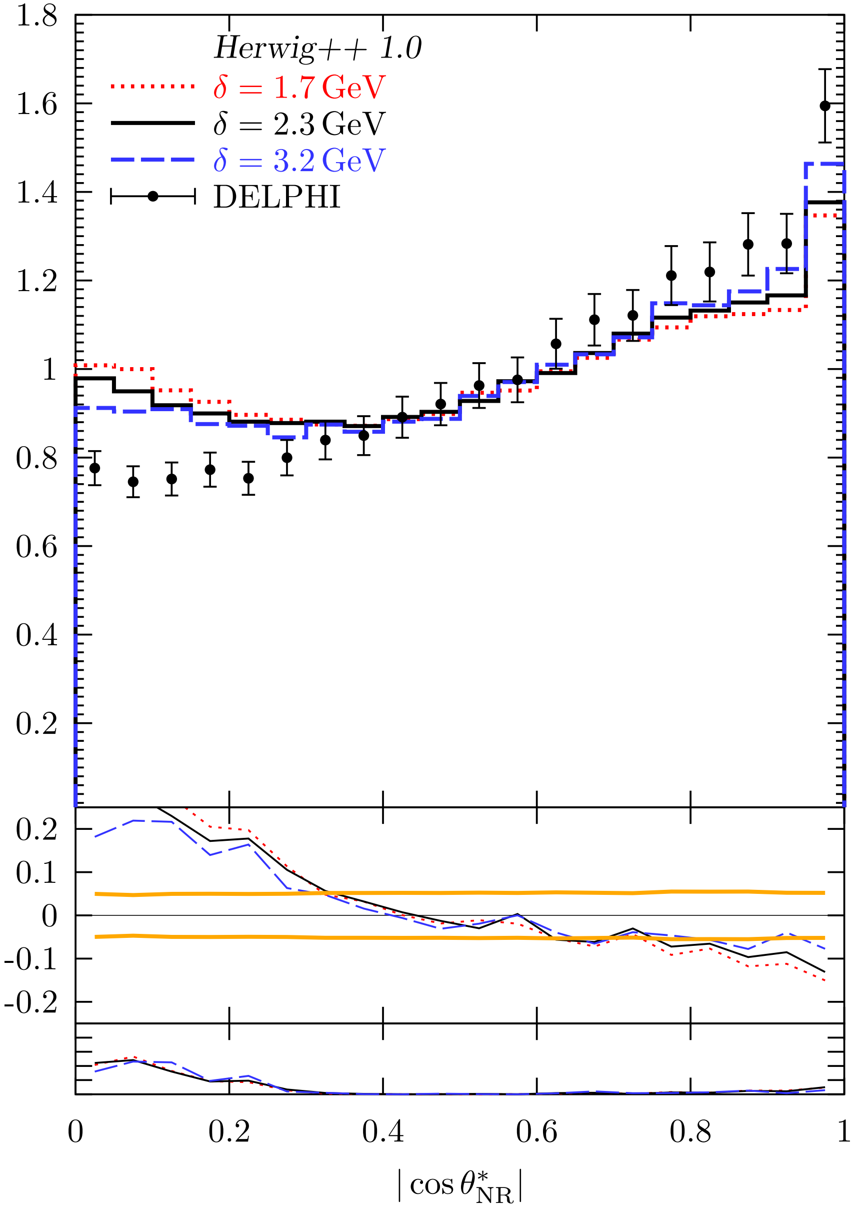
$$\alpha_{34} = \angle(\boldsymbol{p}_3, \boldsymbol{p}_4)$$

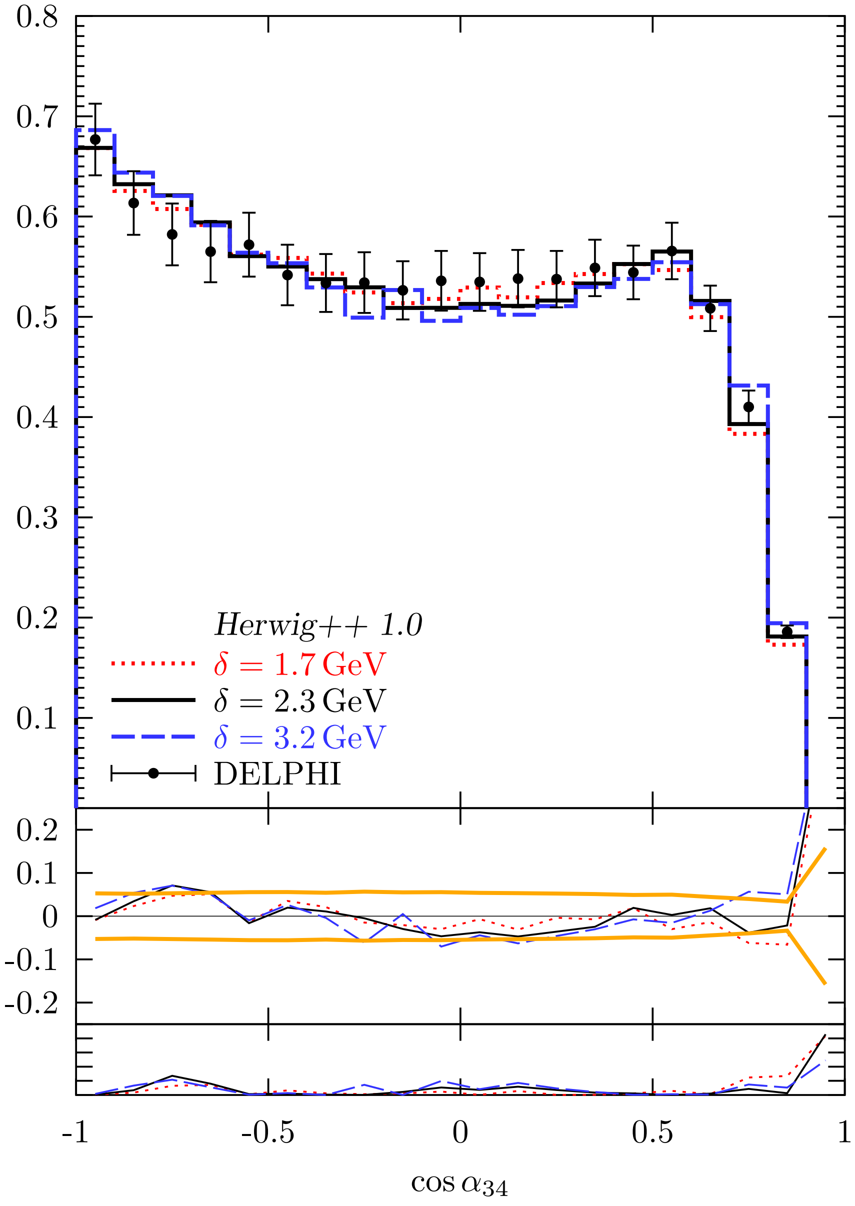
N.B. No four-parton ME in Herwig++ (yet).

Four–Jet Angles I

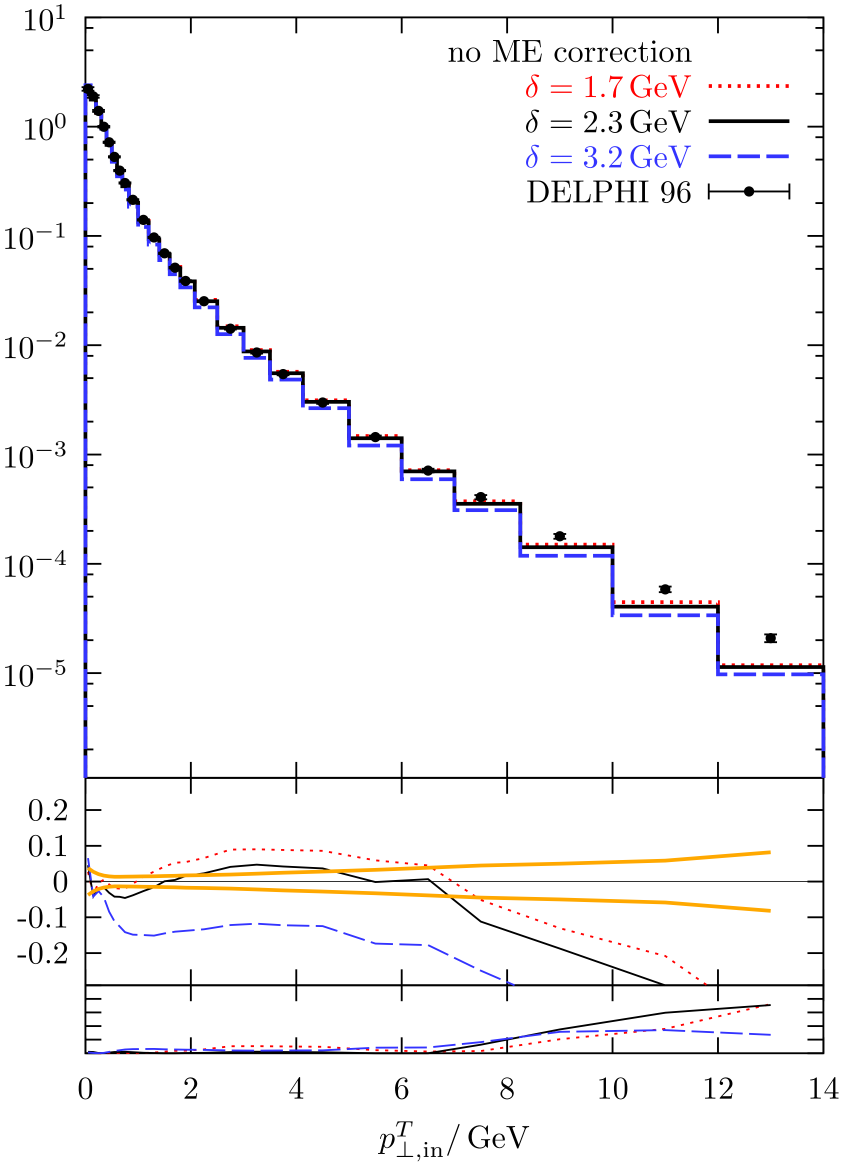


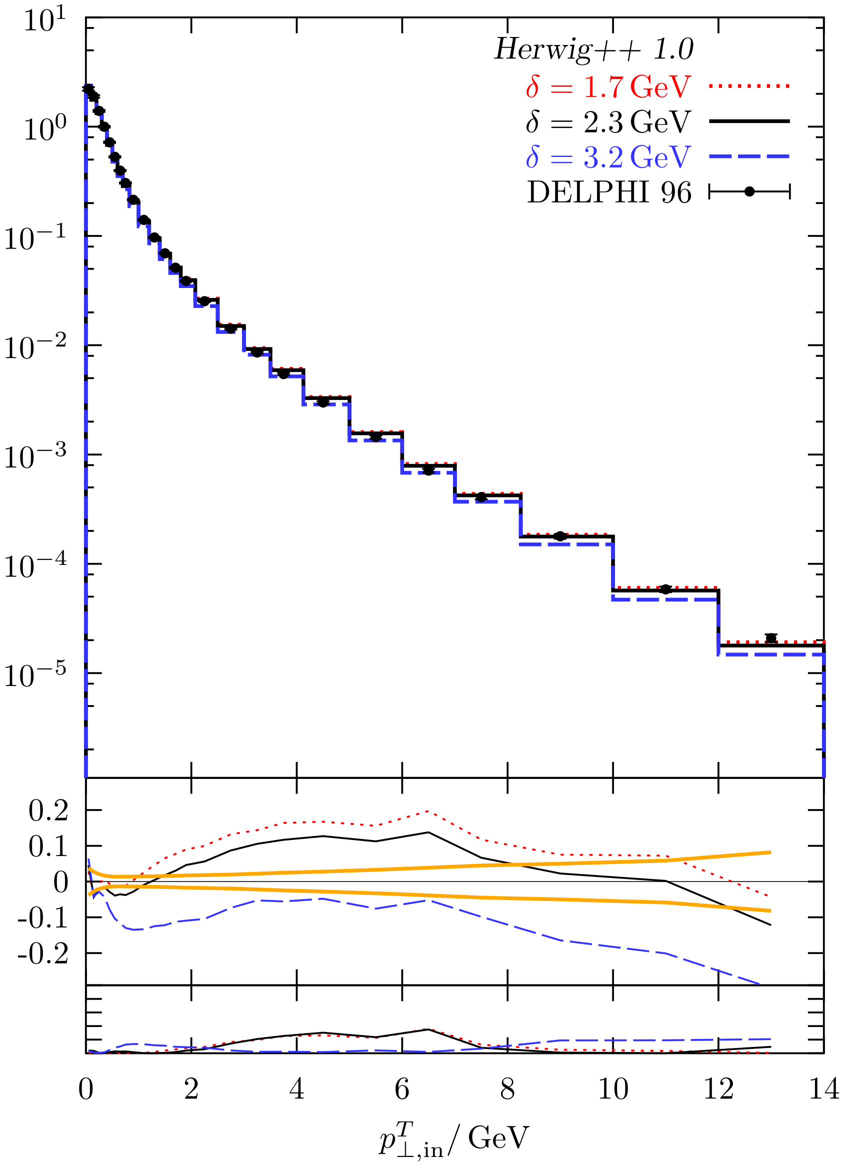
Four–Jet Angles II



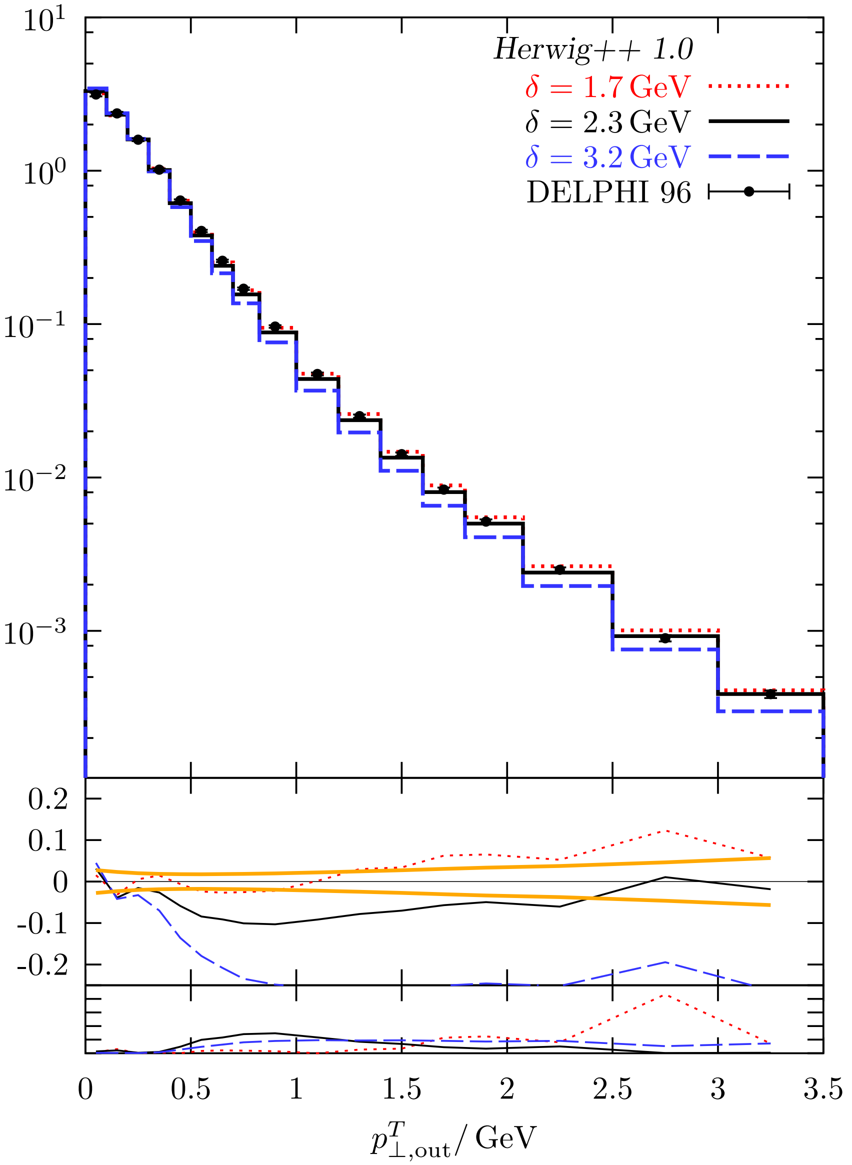


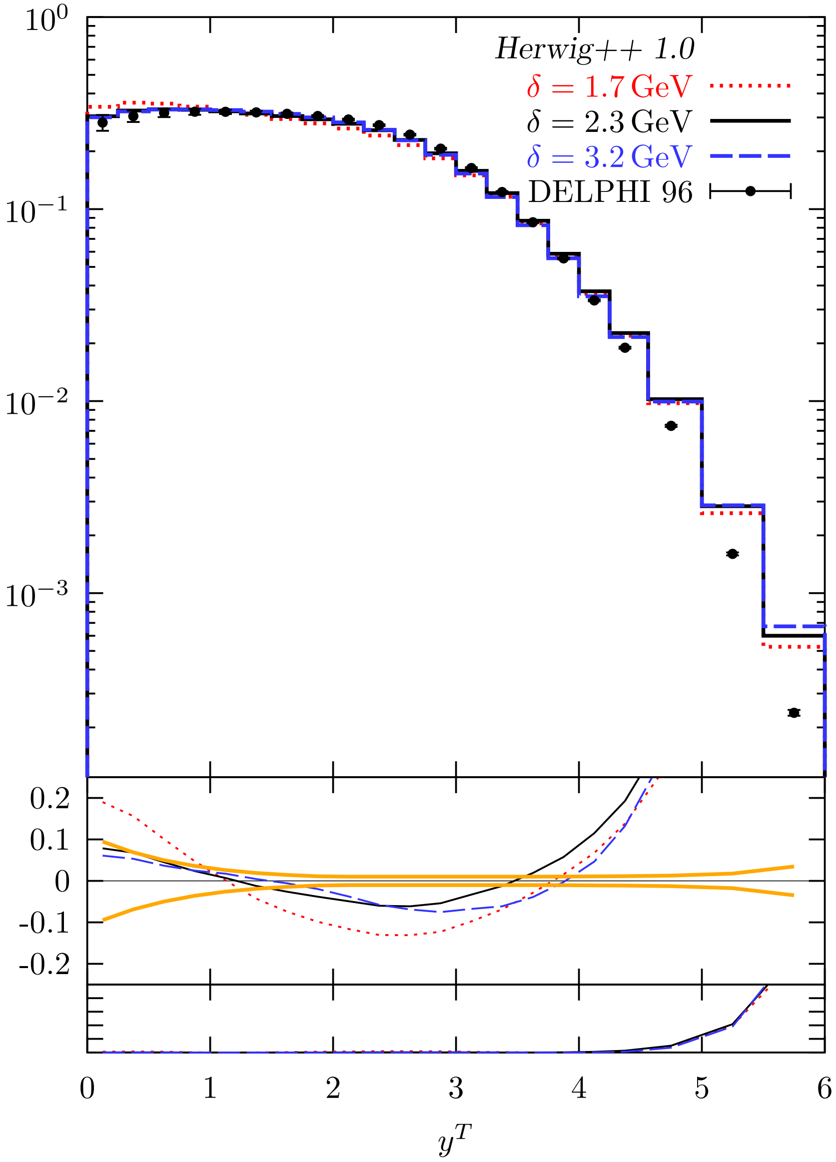
Single particle distributions: $p^T_{\perp,\mathrm{in}}$



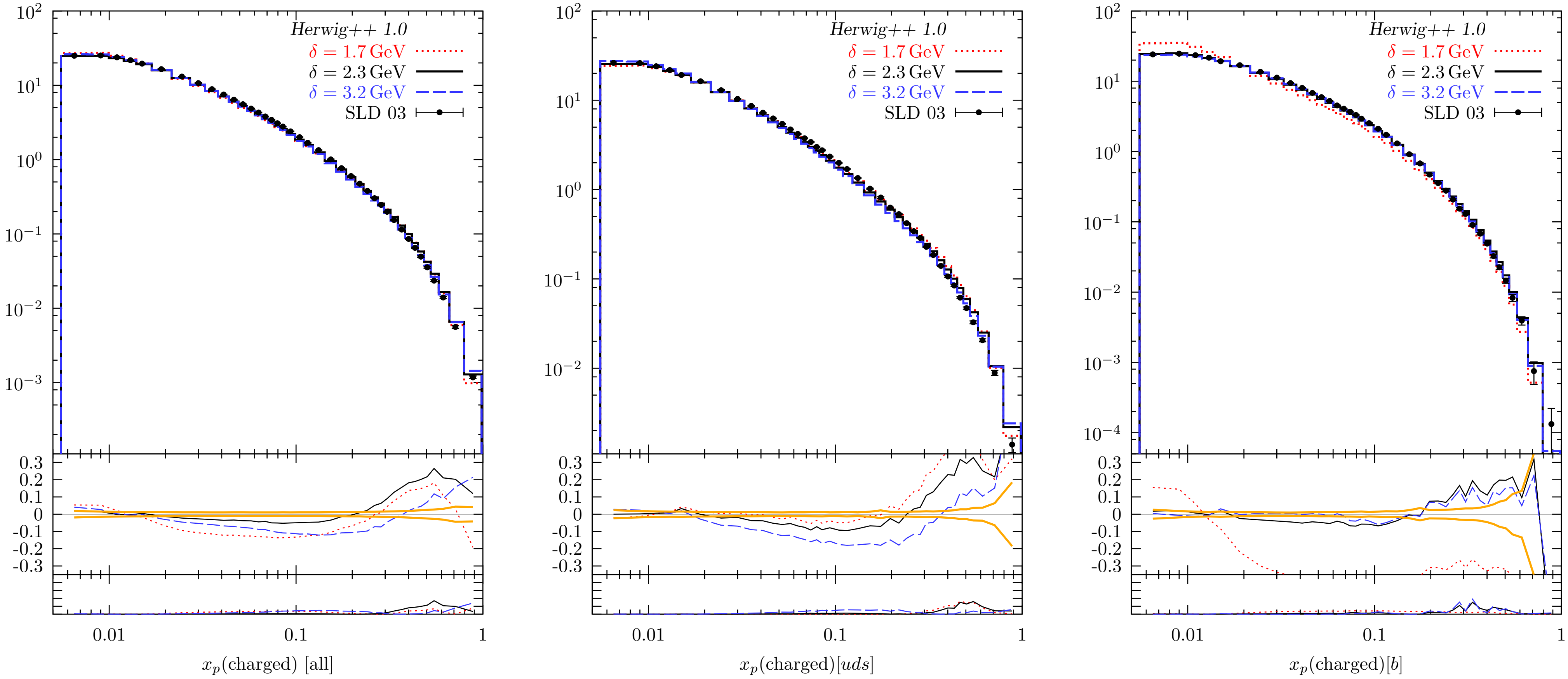


$p^T_{\perp,\mathrm{out}}$ and y^T

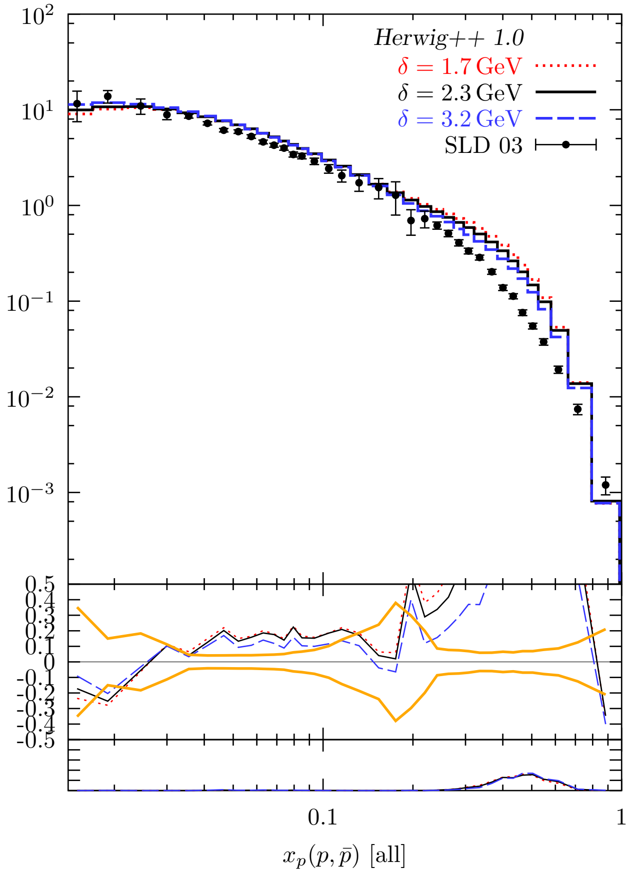


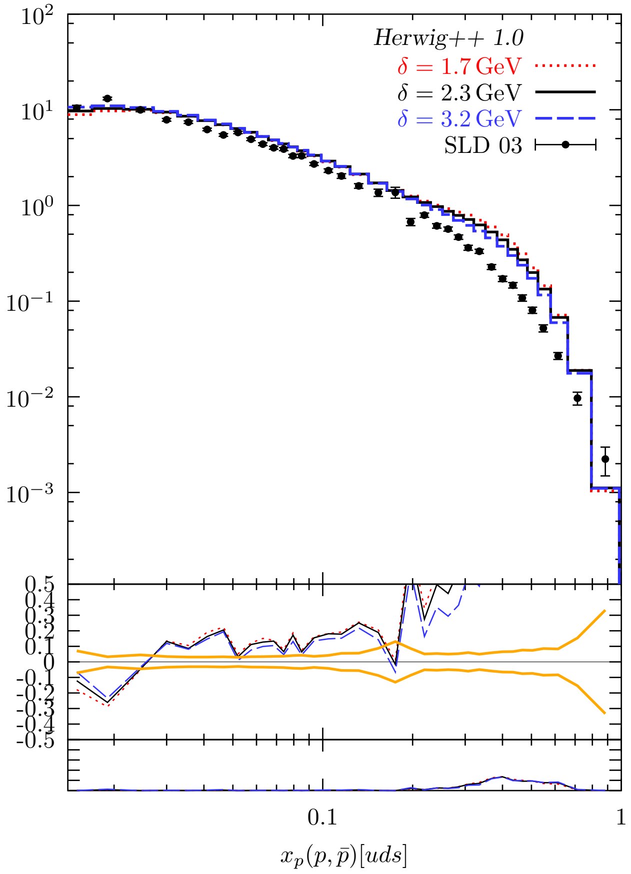


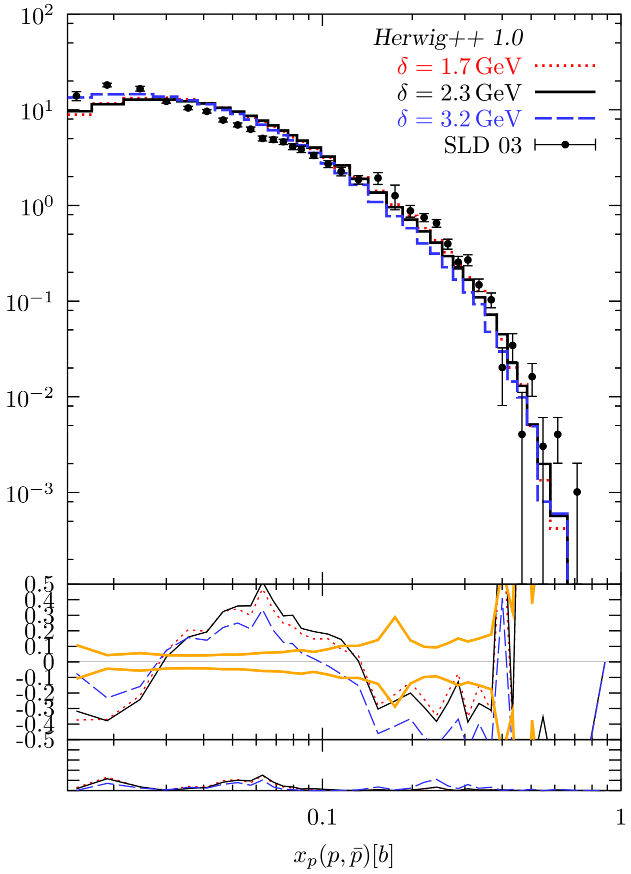
Scaled momentum (all, uds, b)



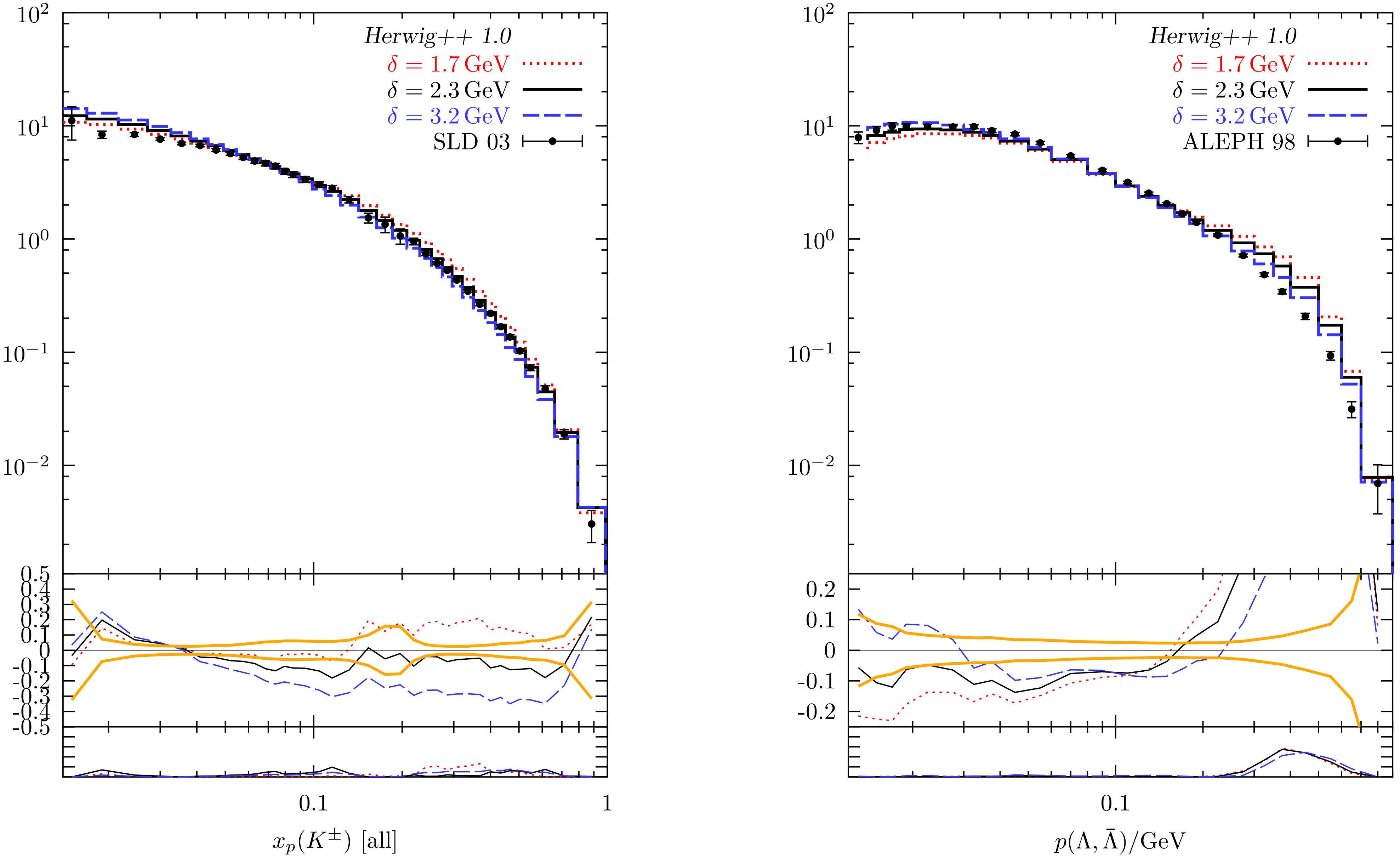
Proton momentum (all, uds, b)



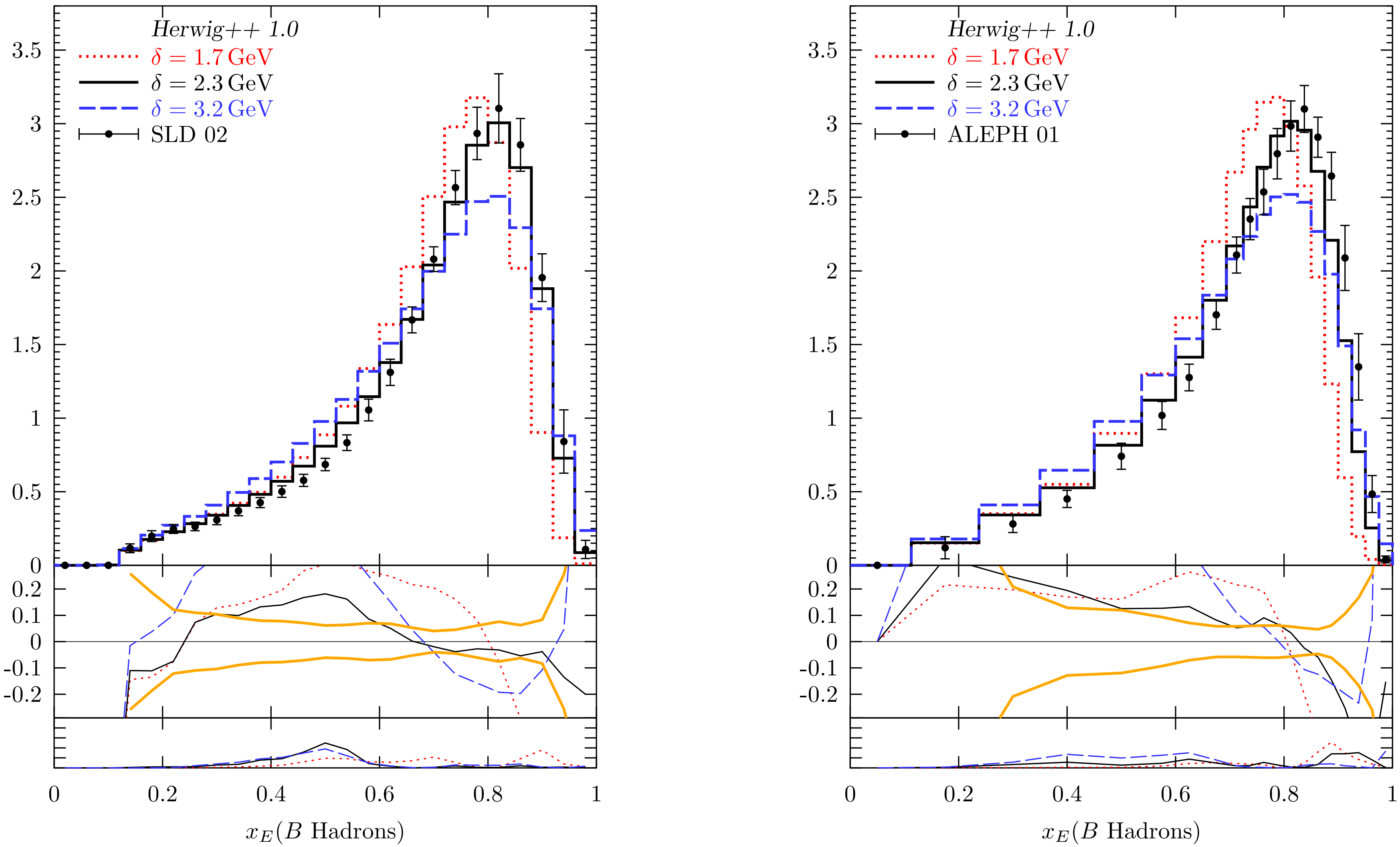




$K^{\pm}$, $(\Lambda, \bar{\Lambda})$ momentum



B-fragmentation function



Only parton shower parameters varied!

Recommended parameters

No systematic parameter tuning yet.

- Low cutoff preferred by event shapes, jet rates, differential jet rates.
- High cutoff preferred by single particle distributions along thrust or sphericity axis.
- Either high or low cutoff for y_n.
- High cutoff preferred by identified particle spectra, particularly for heavy flavour events.
- Intermediate cutoff preferred by B fragmentation function.

We recommend the intermediate value.

Parameter	Default	Initial
$\alpha_s(M_Z)$	0.118	0.114
δ/GeV	2.3	—
m_g/GeV	0.750	—
$Q_{\min}$/GeV in $\alpha_s(Q_{\min})$	0.631	—
ClMax/GeV	3.2	3.35
ClPow	2.0	—
PSplt1	1	—
PSplt2	0.33	—
B1Lim	0.0	—
ClDir1	1	—
ClDir2	1	—
ClSmr1	0.40	—
ClSmr2	0.0	—
Pwt_d	1.0	—
Pwt_u	1.0	—
Pwt_s	0.85	1.0
Pwt_c	1.0	—
Pwt_b	1.0	—
Pwt_{di}	0.55	1.0
Singlet Weight	1.0	—
Decuplet Weight	0.7	1.0

Status of Herwig++

S. Gieseke, A. Ribon, M.H. Seymour, P. Stephens, B.R. Webber
(Cambridge, Manchester, CERN)

`http://www.hep.phy.cam.ac.uk/theory/Herwig++`

Hard Matrix Elements

- Only simple $2 \longrightarrow 2$ ME so far.
- Hard and soft ME corrections for $e^+e^- \longrightarrow q\bar{q}g$.
- We have a working interface to AMEGIC++. For e^+e^- this will do the job for up to 6 jets.
- CKKW ME+PS matching algorithm will be implemented.
- More processes straightforward.
- Users can easily and safely include their own matrix elements.

Parton Shower

- New parton shower developed.
- Multiscale shower designed for treatment of unstable particles (no physics implementation yet).
- New evolution variables for better treatment of heavy quarks and smooth coverage of phase space.
- Extension to spacelike shower for pp and ep ongoing.

Status of Herwig++ (ctnd')

Hadronization

- Cluster hadronization is designed and implemented completely.
- Improved cluster decays implemented and tested.
- Works very well, further thorough tests ongoing.
- Lund string fragmentation model implemented in Pythia7 will work together with `Herwig++`.

Decays

- Fortran `HERWIG` decays are reproduced with class `Hw64Decayer` using the same ME's as before.
- `DecayerAMEGIC` gets final states for decays (eg. t decay, SUSY in future) directly from `AMEGIC++`
- Works very well, further thorough tests required.
- More to come (`EvtGen`,. . .)?

What's next?

Near Future. . .

- Initial state shower:
  - Complete implementation and tests.
- Refine e^+e^-:
  - Full CKKW ME+PS matching.
  - Precision tune to LEP data should be possible.
- With IS and FS showers running:
  - Can start to test Drell–Yan and jets in pp collisions.
  - Cross-check with Tevatron data and finally make predictions for the LHC.
- Underlying event.
- Hadronic decays: *NEW!* τ–decays, spin correlations (P Richardson).
- New ideas: NLO, multiscale, SUSY . . .

Schedule?

- Ready for LHC!