FERMILAB-SLIDES-23-298-T

From partons to jets and back
Simulating QCD interactions at highest energies

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50 Years of Quantum Chromodynamics
UCLA, 09/14/2023

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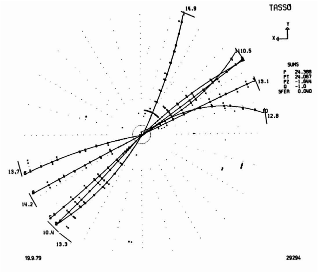
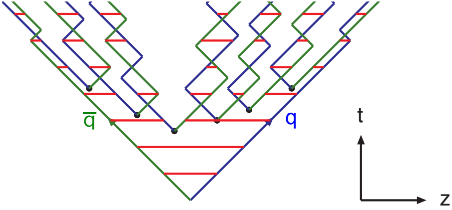
QCD simulations before PETRA

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





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

QCD simulations before PETRA

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

```
      SUBROUTINE JETGEN(N)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /PAR/ PUD, PS1, SIGMA, CX2, EBEG, WFIN, IFLBEG
      COMMON /DATA1/ MESO(9,2), CMIX(6,2), PMAS(19)
      IFLSGN=(10-IFLBEG)/5
      W=2.*EBEG
      I=0
      IPD=0
C 1 FLAVOUR AND PT FOR FIRST QUARK
      IFL1=IABS(IFLBEG)
      PT1=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI1=6.2832*RANF(0)
      PX1=PT1*COS(PHI1)
      PY1=PT1*SIN(PHI1)
  100 I=I+1
C 2 FLAVOUR AND PT FOR NEXT ANTIQUARK
      IFL2=1+INT(RANF(0)/PUD)
      PT2=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI2=6.2832*RANF(0)
      PX2=PT2*COS(PHI2)
      PY2=PT2*SIN(PHI2)
C 3 MESON FORMED, SPIN ADDED AND FLAVOUR MIXED
      K(I,1)=MESO(3*(IFL1-1)+IFL2,IFLSGN)
      ISPIN=INT(PS1+RANF(0))
      K(I,2)=1+9*ISPIN+K(I,1)
      IF(K(I,1).LE.6) GOTO 110
      TMIX=RANF(0)
      KM=K(I,1)-6+3*ISPIN
      K(I,2)=8+9*ISPIN+INT(TMIX+CMIX(KM,1))+INT(TMIX+CMIX(KM,2))
C 4 MESON MASS FROM TABLE, PT FROM CONSTITUENTS
  110 P(I,5)=PMAS(K(I,2))
      P(I,1)=PX1+PX2
      P(I,2)=PY1+PY2
      PMTS=P(I,1)**2+P(I,2)**2+P(I,5)**2
C 5 RANDOM CHOICE OF X=(E+PZ)MESON/(E+PZ)AVAILABLE GIVES E AND PZ
      X=RANF(0)
      IF(RANF(0).LT.CX2) X=1.-X**(1./3.)
      P(I,3)=(X*W-PMTS/(X*W))/2.
      P(I,4)=(X*W+PMTS/(X*W))/2.
C 6 IF UNSTABLE, DECAY CHAIN INTO STABLE PARTICLES
  120 IPD=IPD+1
      IF(K(IPD,2).GE.8) CALL DECAY(IPD,I)
      IF(IPD.LT.I.AND.I.LE.96) GOTO 120
C 7 FLAVOUR AND PT OF QUARK FORMED IN PAIR WITH ANTIQUARK ABOVE
      IFL1=IFL2
      PX1=-PX2
      PY1=-PY2
C 8 IF ENOUGH E+PZ LEFT, GO TO 2
      W=(1.-X)*W
      IF(W.GT.WFIN.AND.I.LE.95) GOTO 100
      N=I
      RETURN
      END


      SUBROUTINE LIST(N)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /DATA3/ CHA1(9), CHA2(19), CHA3(2)
      WRITE(6,110)
      DO 100 I=1,N
      IF(K(I,1).GT.0) C1=CHA1(K(I,1))
      IF(K(I,1).LE.0) IC1=-K(I,1)
      C2=CHA2(K(I,2))
      C3=CHA3((47-K(I,2))/20)
      IF(K(I,1).GT.0) WRITE(6,120) I, C1, C2, C3, (P(I,J), J=1,5)
  100 IF(K(I,1).LE.0) WRITE(6,130) I, IC1, C2, C3, (P(I,J), J=1,5)
      RETURN
  110 FORMAT(////T11,'I',T17,'ORI',T24,'PART',T32,'STAB',
     &T44,'PX',T56,'PY',T68,'PZ',T80,'E',T92,'M'/)
  120 FORMAT(10X,I2,4X,A2,1X,2(4X,A4),5(4X,F8.1))
  130 FORMAT(10X,I2,4X,1X,I2,2(4X,A4),5(4X,F8.1))
      END
```

```
      SUBROUTINE DECAY(IPD,I)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /DATA1/ MESO(9,2), CMIX(6,2), PMAS(19)
      COMMON /DATA2/ IDCD(12), CBR(29), KDP(29,3)
      DIMENSION U(3), BE(3)
C 1 DECAY CHANNEL CHOICE, GIVES DECAY PRODUCTS
      TBR=RANF(0)
      IDC=IDCD(K(IPD,2)-7)
  100 IDC=IDC+1
      IF(TBR.GT.CBR(IDC)) GOTO 100
      ND=(59+KDP(IDC,3))/20
      DO 110 I1=I+1,I+ND
      K(I1,1)=-IPD
      K(I1,2)=KDP(IDC,I1-I)
  110 P(I1,5)=PMAS(K(I1,2))
C 2 IN THREE-PARTICLE DECAY CHOICE OF INVARIANT MASS OF PRODUCTS 2+3
      IF(ND.EQ.2) GOTO 130
      SA=(P(IPD,5)+P(I+1,5))**2
      SB=(P(IPD,5)-P(I+1,5))**2
      SC=(P(I+2,5)+P(I+3,5))**2
      SD=(P(I+2,5)-P(I+3,5))**2
      TDU=(SA-SD)*(SB-SC)/(4.*SQRT(SB*SC))
      IF(K(IPD,2).GE.11) TDU=SQRT(SB*SC)*TDU**3
  120 SX=SC+(SB-SC)*RANF(0)
      TDF=SQRT((SX-SA)*(SX-SB)*(SX-SC)*(SX-SD))/SX
      IF(K(IPD,2).GE.11) TDF=SX*TDF**3
      IF(RANF(0)*TDU.GT.TDF) GOTO 120
      P(100,5)=SQRT(SX)
C 3 TWO-PARTICLE DECAY IN CM, TWICE TO SIMULATE THREE-PARTICLE DECAY
  130 DO 160 IL=1,ND-1
      I0=(IL-1)*100-(IL-2)*IPD
      I1=I+IL
      I2=(ND-IL-1)*100-(ND-IL-2)*(I+IL+1)
      PA=SQRT((P(I0,5)**2-(P(I1,5)+P(I2,5))**2)*
     &(P(I0,5)**2-(P(I1,5)-P(I2,5))**2))/(2.*P(I0,5))
  140 U(3)=2.*RANF(0)-1.
      PHI=6.2832*RANF(0)
      U(1)=SQRT(1.-U(3)**2)*COS(PHI)
      U(2)=SQRT(1.-U(3)**2)*SIN(PHI)
      TDA=1.-(U(1)*P(I0,1)+U(2)*P(I0,2)+U(3)*P(I0,3))**2/
     &(P(I0,1)**2+P(I0,2)**2+P(I0,3)**2)
      IF(K(IPD,2).GE.11.AND.IL.EQ.2.AND.RANF(0).GT.TDA) GOTO 140
      DO 150 J=1,3
      P(I1,J)=PA*U(J)
  150 P(I2,J)=-PA*U(J)
      P(I1,4)=SQRT(PA**2+P(I1,5)**2)
  160 P(I2,4)=SQRT(PA**2+P(I2,5)**2)
C 4 DECAY PRODUCTS LORENTZ TRANSFORMED TO LAB SYSTEM
      DO 190 IL=ND-1,1,-1
      I0=(IL-1)*100-(IL-2)*IPD
      DO 170 J=1,3
  170 BE(J)=P(I0,J)/P(I0,4)
      GA=P(I0,4)/P(I0,5)
      DO 190 I1=I+IL,I+ND
      BEP=BE(1)*P(I1,1)+BE(2)*P(I1,2)+BE(3)*P(I1,3)
      DO 180 J=1,3
  180 P(I1,J)=P(I1,J)+GA*(GA/(1.+GA)*BEP+P(I1,4))*BE(J)
  190 P(I1,4)=GA*(P(I1,4)+BEP)
      I=I+ND
      RETURN
      END
```

≈ 200 punched cards

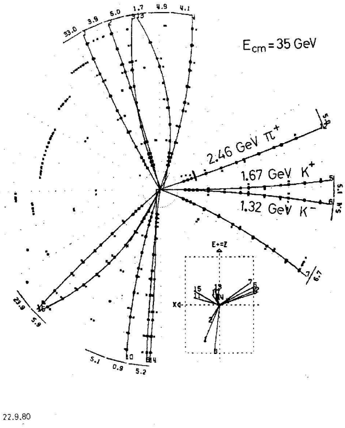
Fortran code

```
      SUBROUTINE EDIT(N)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /EDPAR/ ITHROW, PZMIN, PMIN, THETA, PHI, BETA(3)
      REAL ROT(3,3), PR(3)
C 1 THROW AWAY NEUTRALS OR UNSTABLE OR WITH TOO LOW PZ OR P
      I1=0
      DO 110 I=1,N
      IF(ITHROW.GE.1.AND.K(I,2).GE.8) GOTO 110
      IF(ITHROW.GE.2.AND.K(I,2).GE.6) GOTO 110
      IF(ITHROW.GE.3.AND.K(I,2).EQ.1) GOTO 110
      IF(P(I,3).LT.PZMIN.OR.P(I,4)**2-P(I,5)**2.LT.PMIN**2) GOTO 110
      I1=I1+1
      K(I1,1)=IDIM(K(I,1),0)
      K(I1,2)=K(I,2)
      DO 100 J=1,5
  100 P(I1,J)=P(I,J)
  110 CONTINUE
      N=I1
C 2 ROTATE TO GIVE JET PRODUCED IN DIRECTION THETA, PHI
      IF(THETA.LT.1E-4) GOTO 140
      ROT(1,1)=COS(THETA)*COS(PHI)
      ROT(1,2)=-SIN(PHI)
      ROT(1,3)=SIN(THETA)*COS(PHI)
      ROT(2,1)=COS(THETA)*SIN(PHI)
      ROT(2,2)=COS(PHI)
      ROT(2,3)=SIN(THETA)*SIN(PHI)
      ROT(3,1)=-SIN(THETA)
      ROT(3,2)=0.
      ROT(3,3)=COS(THETA)
      DO 130 I=1,N
      DO 120 J=1,3
  120 PR(J)=P(I,J)
      DO 130 J=1,3
  130 P(I,J)=ROT(J,1)*PR(1)+ROT(J,2)*PR(2)+ROT(J,3)*PR(3)
C 3 OVERALL LORENTZ BOOST GIVEN BY BETA VECTOR
  140 IF(BETA(1)**2+BETA(2)**2+BETA(3)**2.LT.1E-8) RETURN
      GA=1./SQRT(1.-BETA(1)**2-BETA(2)**2-BETA(3)**2)
      DO 160 I=1,N
      BEP=BETA(1)*P(I,1)+BETA(2)*P(I,2)+BETA(3)*P(I,3)
      DO 150 J=1,3
  150 P(I,J)=P(I,J)+GA*(GA/(1.+GA)*BEP+P(I,4))*BETA(J)
  160 P(I,4)=GA*(P(I,4)+BEP)
      RETURN
      END


      BLOCK DATA
      COMMON /PAR/ PUD, PS1, SIGMA, CX2, EBEG, WFIN, IFLBEG
      COMMON /EDPAR/ ITHROW, PZMIN, PMIN, THETA, PHI, BETA(3)
      COMMON /DATA1/ MESO(9,2), CMIX(6,2), PMAS(19)
      COMMON /DATA2/ IDCD(12), CBR(29), KDP(29,3)
      COMMON /DATA3/ CHA1(9), CHA2(19), CHA3(2)
      DATA PUD/0.4/, PS1/0.5/, SIGMA/350./, CX2/0.77/,
     &EBEG/10000./, WFIN/100./, IFLBEG/1/
      DATA ITHROW/1/, PZMIN/0./, PMIN/0./, THETA,PHI,BETA/5*0./
      DATA MESO/7,1,3,2,8,5,4,6,9,7,2,4,1,8,6,3,5,9/
      DATA CMIX/2*0.5,1.,2*0.5,1.,2*0.25,0.5,2*0.,1./
      DATA PMAS/0.,2*139.6,2*493.7,2*497.7,135.,548.8,957.6,
     &2*765.9,2*892.2,2*896.3,770.2,782.6,1019.6/
      DATA IDCD/0,1,6,11,12,13,15,17,19,21,22,25/
      DATA CBR/1.,0.381,0.681,0.918,0.969,1.,0.426,0.662,0.959,
     &0.980,1.,1.,1.,0.667,1.,0.667,1.,0.667,1.,0.667,1.,1.,
     &0.899,0.987,1.,0.486,0.837,0.984,1./
      DATA KDP/1,1,8,2,1,1,2,8,1,1,1,2,3,6,4,7,5,4,6,5,7,2,2,
     &1,2,4,6,2,1,1,1,8,3,2,1,3,8,17,18,1,8,8,2,8,3,8,3,8,2,8,
     &3,3,8,3,5,7,3,9,0,0,8,8,3,8,9,9,14*0,8,4*0,8,0/
      DATA CHA1/'UD','DU','US','SU','DS','SD','UU','DD','SS'/
      DATA CHA2/'GAMM','PI+','PI-','K+','K-','KO','KBO','PIO','ETA',
     &'ETAP','RHO+','RHO-','K*+','K*-','K*0','KB*0','RHO0','OMEG','PHI'/
      DATA CHA3/'    ','STAB'/
      END
```

- Implementation in a computer program – JETSET, later Pythia

The gluon changes everything



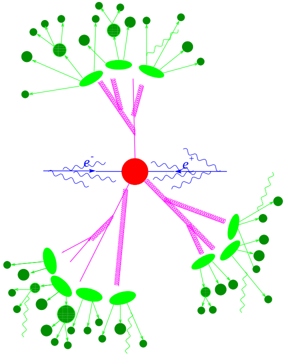
Neutrino ’79: Event 13177 makes history

Image credit: DESY, P. Duinker

The gluon changes everything

[Marchesini,Webber] Nucl.Phys.B238(1984)1, [Webber] Nucl.Phys.B238(1984)492
[Andersson,Gustafson,Ingelman,Sjöstrand] Phys.Rept.97(1983)31

- Short distance interactions
  - Signal process
  - QCD radiative corrections
- Long-distance interactions
  - Hadronization
  - Particle decays



Divide and Conquer

- Quantity of interest: Interaction rate
- Convolution of short & long distance physics

$$\sigma_{ee\to h+X} = \sum_{i\in\{q,g\}} \int \mathrm{d}x \, \underbrace{\hat{\sigma}_{ee\to i+X}(x,\mu_F^2)}_{\text{short distance}} \, \underbrace{D_i^{(h)}(x,\mu_F^2)}_{\text{long distance}}$$

Fourty years and many discoveries later ...

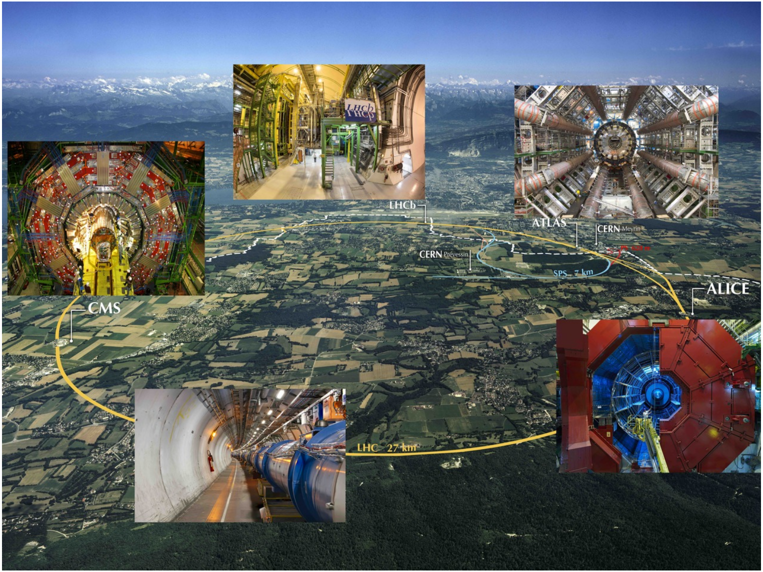
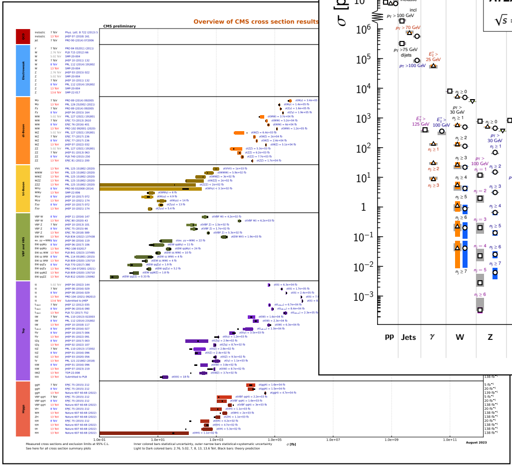
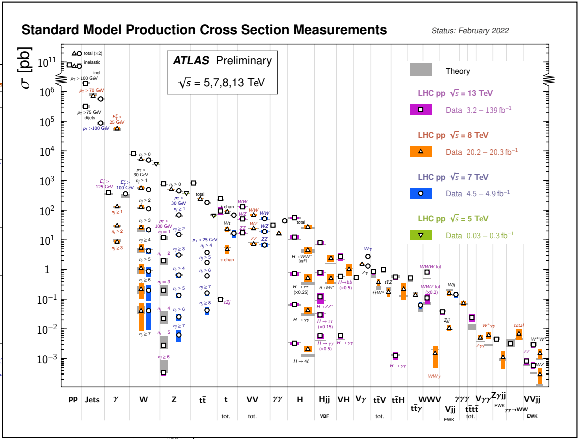


Image credit: CERN

... it's all about jets

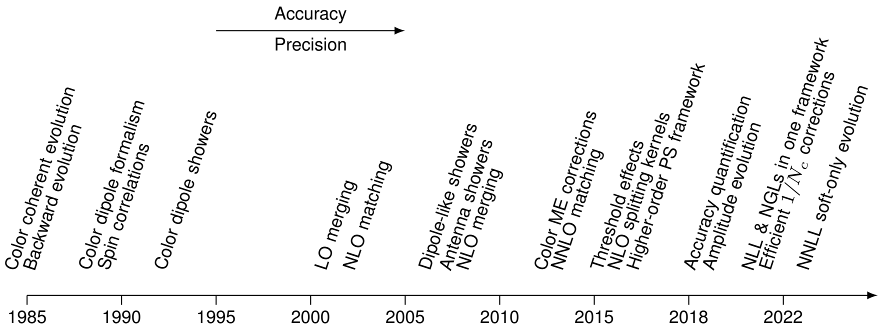


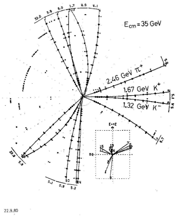


[ATLAS] https://twiki.cern.ch/twiki/bin/view/AtlasPublic/StandardModelPublicResults

[CMS] https://twiki.cern.ch/twiki/bin/view/CMSPublic/PhysicsResultsCombined

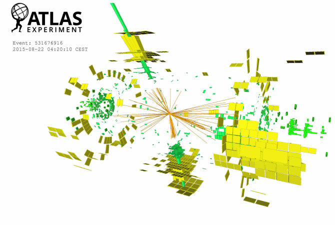
So we need to simulate jets ...





$\sqrt{s} \times 500$

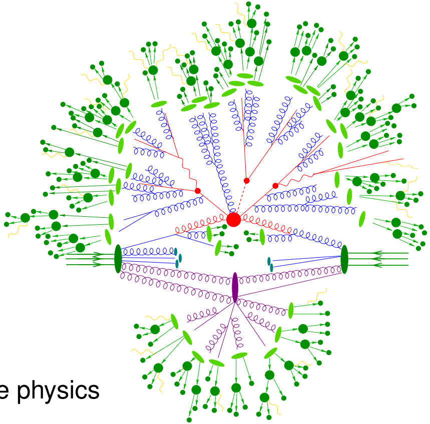
e^+e^- vs. pp



... lots of jets

[Buckley et al.] arXiv:1101.2599
[Campbell et al.] arXiv:2203.11110

- Short distance interactions
  - Signal process
  - Radiative corrections
- Long-distance interactions
  - Hadronization
  - Particle decays



Divide and Conquer

- Quantity of interest: Interaction rate
- Convolution of short & long distance physics

$$\sigma_{p_1 p_2 \to X} = \sum_{i,j \in \{q,g\}} \int \mathrm{d}x_1 \mathrm{d}x_2 \underbrace{f_{p_1,i}(x_1, \mu_F^2) f_{p_2,j}(x_2, \mu_F^2)}_{\text{long distance}} \underbrace{\hat{\sigma}_{ij \to X}(x_1 x_2, \mu_F^2)}_{\text{short distance}}$$

The connection to pQCD theory

- $\hat{\sigma}_{ij\to n}(\mu_F^2) \to$ Collinearly factorized fixed-order result at N^{x}LO

  Implemented in fully differential form to be maximally useful

  Tree level: $\mathrm{d}\Phi_n\; B_n$

  - Automated ME generators + phase-space integrators

  1-Loop level: $\mathrm{d}\Phi_n \left(B_n + V_n + \sum C + \sum I_n\right) + \mathrm{d}\Phi_{n+1}\left(R_n - \sum S_n\right)$

  - Automated loop ME generators + integral libraries + IR subtraction

  2-Loop level: It depends ...

  - Individual solutions based on SCET, q_T subtraction, P2B

- $f_i(x, \mu_F^2) \to$ Collinearly factorized PDF at N^{y}LO

  Evaluated at $O(1\mathrm{GeV}^2)$ and expanded into a series above $1\mathrm{GeV}^2$

  DGLAP: $\frac{\mathrm{d}x\, x f_a(x,t)}{\mathrm{d}\ln t} = \sum_{b=q,g}\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}z\, \frac{\alpha_s}{2\pi}\left[zP_{ab}(z)\right]_+ \tau f_b(\tau,t)\,\delta(x-\tau z)$

  - Parton showers, dipole showers, antenna showers, ...

  Matching: $\mathrm{d}\Phi_n\, \frac{S_n}{B_n} \leftrightarrow \frac{\mathrm{d}t}{t}\mathrm{d}z\, \frac{\alpha_s}{2\pi}\, P_{ab}(z)$

  - MC@NLO, POWHEG, Geneva, MINNLO$_{\mathrm{PS}}$, ...

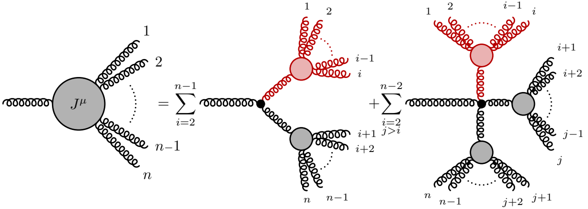
Fixed-order calculations – LO

[Berends,Giele] NPB306(1988)759

- Tree-level QCD a solved problem, but textbook methods unwieldy

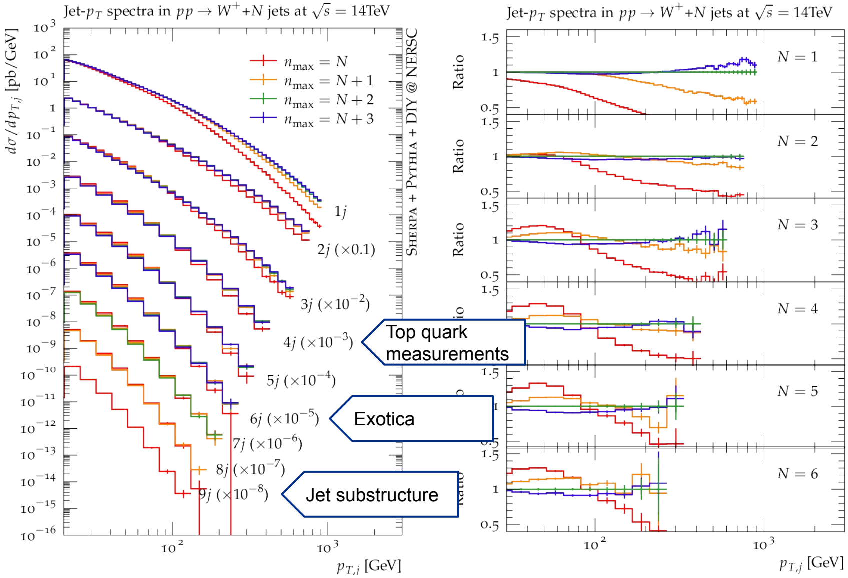
# of gluons	Min. # diagrams	Max. # diagrams
4	3	4
5	10	25
6	36	220
7	133	2485
8	501	34300
9	1991	559405
10	7335	10525900
11	28199	224449225
12	108281	5348843500

- Dynamic programming eliminates common subexpressions
  $\rightarrow$ Factorial scaling systematically reduced to exponential



Fixed-order calculations – LO

[Prestel,Schulz,SH] arXiv:1905.05120

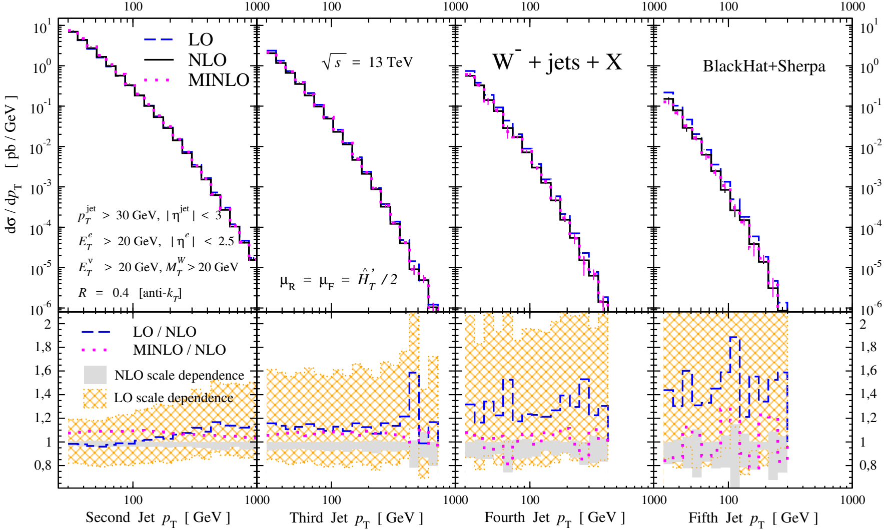


Fixed-order calculations – NLO

- General methods for regularization of IR singularities developed $\sim$25 years ago [Frixione,Kunszt,Signer] hep-ph/9512328 [Catani,Seymour] hep-ph/9605323, [Catani,Dittmaier,Seymour,Trocsanyi] hep-ph/0201036
- Generalized unitarity, advanced tensor reduction, reduction at integrand level led to industrialization of 1-loop computations $\sim$2010
  [Bern,Dixon,Dunbar,Kosower] NPB435(1995)59, NPB513(1998)3
  [Denner,Dittmaier] hep-ph/0509141, [Binoth,Guillet,Pilon,Heinrich,Schubert] hep-ph/0504267
  [Ossola,Papadopoulos,Pittau] hep-ph/0609007, arXiv:0802.1876, [Forde] arxiv:0704.1835
  [Ellis,Giele,Kunszt] arXiv:0708.2398, [Giele,Kunszt,Melnikov] arXiv:0801.2237, . . .
- Many highly challenging calculations as a community effort
  $\nearrow$ talks by R. Boughezal, T. Gehrmann
  - Automated tree-like components and phase space:
    HELAC, Herwig7, MadGraph5, MUNICH, Sherpa, Whizard, ...
  - Automated virtual corrections:
    BlackHat, Golem95, GoSam, HelacNLO, MadGolem,
    MadLoop, NJet, OpenLoops, Recola, Rocket, ...
  - Complete, dedicated codes: MCFM, NLOJet++, ...

Fixed-order calculations – NLO

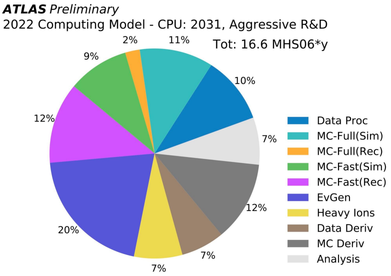
[Bern,Dixon,Febres Cordero,Ita,Kosower,Maître,Ozeren,SH] arXiv:1304.1253
[Anger,Febres-Cordero,Maître,SH] arXiv:1712.08621

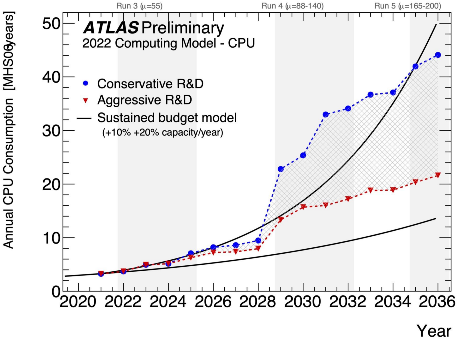


Fixed-order calculations – Computing bottlenecks

[HSF Generator WG] arXiv:2004.13687, arXiv:2109.14938

- Event generation will consume significant fraction of resources at LHC soon
- Need to scrutinize both generator usage and underlying algorithms
- Dedicated effort: HEP Software Foundation Generator Working Group



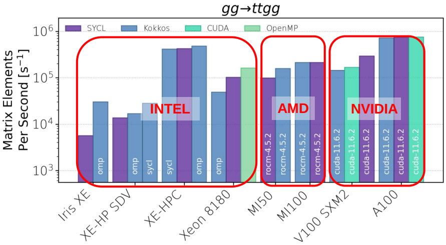


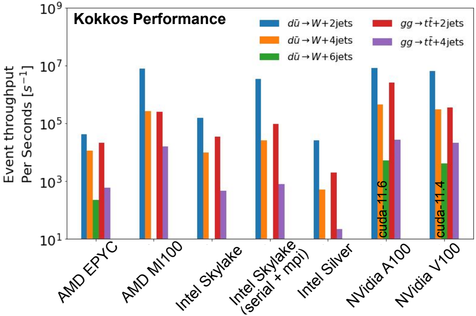
[ATLAS] CERN-LHCC-2022-005 / LHCC-G-182

Fixed-order calculations – Performance portability

[A. Valassi et al., ACAT ’22]

- Must keep up with rapidly developing & changing computing architectures
- Portability frameworks SYCL, Kokkos can target most modern platforms





[R. Wang et al., ACAT’22]

- Choice of algorithm must take theoretical, experimental & CS requirements into account
- New theory developments often useful for performance

Fixed-order calculations – AI-assisted integration

- Neural Networks used in many different ways to improve event generation
  [Butter et al.] arXiv:2203.07460

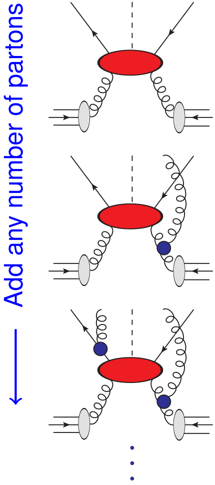
Surrogate model techniques

- Hit or miss w/ NN estimate
  - An order of magnitude faster
  - Insufficient training leads to large uncertainties, but no bias
  - Needs existing sample to train
- Generate events with GANs
  - Orders of magnitude faster
  - Needs existing sample to train
  - Bias if not trained right

Variabe transformation techniques

- Normalizing flows
  - Learn integrand to improve importance sampling
  - Insufficient training leads to large uncertainties, but no bias
  - Events generated from scratch no pre-existing sample required
  - Resulting events still need to be unweighted

Parton showers, dipole showers and all that



$$\sigma_{\mathrm{incl}}\Bigg[\Delta(t_c, Q^2)$$

$$+\int_{t_c}^{Q^2}\frac{\mathrm{d}t}{t}\int \mathrm{d}z\,\frac{\alpha_s}{2\pi}P(z)\;\Delta(t, Q^2)$$

$$+\frac{1}{2}\left(\int_{t_c}^{Q^2}\frac{\mathrm{d}t}{t}\int \mathrm{d}z\,\frac{\alpha_s}{2\pi}P(z)\right)^2\Delta(t, Q^2)$$

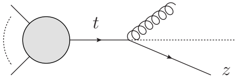
$$+\ldots$$

Radiative corrections as a branching process

[Marchesini,Webber] NPB238(1984)1
[Sjöstrand] PLB157(1985)321

- Probability for parton splitting in collinear limit

$$\lambda \to \frac{1}{\sigma_n}\int_t^{Q^2} \mathrm{d}\bar{t}\,\frac{\mathrm{d}\sigma_{n+1}}{\mathrm{d}\bar{t}} \approx \sum_{\text{jets}} \int_t^{Q^2} \frac{\mathrm{d}\bar{t}}{\bar{t}} \int \mathrm{d}z\,\frac{\alpha_s}{2\pi} P(z)$$



- Perturbative unitarity leads to a Markov process
  - Assume bosonic final state → naive probability for n emissions

$$P_{\text{naive}}(n,\lambda) = \frac{\lambda^n}{n!}$$

  - Probability conservation implies no-emission probability

$$P(n,\lambda) = \frac{\lambda^n}{n!}\exp\{-\lambda\} \qquad \longrightarrow \qquad \sum_{n=0}^{\infty} P(n,\lambda) = 1$$

$\Delta(t,Q^2) := \exp\{-\lambda\} \to$ Sudakov factor

- Practical challenges
  - Four-momentum conservation
  - On-shell conditions
  - Color conservation

Soft radiation and matching to collinear result

[Marchesini,Webber] NPB238(1984)1, NPB310(1988)461

- Eikonal can be written in terms of energies and angular "radiator" function

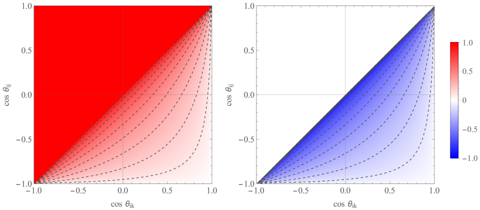
$$J_\mu J^\mu \to \frac{2p_i p_k}{(p_i p_j)(p_j p_k)} = \frac{W_{ik,j}}{E_j^2}\,, \qquad W_{ik,j} = \frac{1-\cos\theta_{ik}}{(1-\cos\theta_{ij})(1-\cos\theta_{kj})}$$

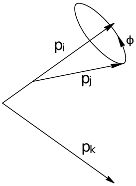
- Collinearly divergent as $\theta_{ij} \to 0$ and as $\theta_{kj} \to 0$

  $\to$ Expose individual singularities via $W_{ik,j} = \tilde{W}^i_{ik,j} + \tilde{W}^k_{ki,j}$

$$\tilde{W}^i_{ik,j} = \frac{1}{2}\left[\frac{1-\cos\theta_{ik}}{(1-\cos\theta_{ij})(1-\cos\theta_{kj})} + \frac{1}{1-\cos\theta_{ij}} - \frac{1}{1-\cos\theta_{kj}}\right]$$

- Azimuthal averaging yields famous angular ordering
  - Differential radiation pattern outside parent dipole more intricate
    Positive & negative contributions sum to zero

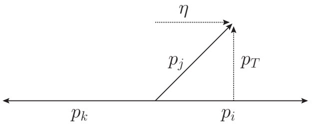




Dual description and the Lund plane

[Gustafson] PLB175(1986)453

- Compute everything in center-of-mass frame of fast partons



- Simple expressions for transverse momentum and rapidity

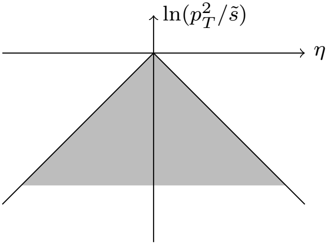
$$p_T^2 = \frac{2(p_i p_j)(p_k p_j)}{p_i p_k}\,, \qquad \eta = \frac{1}{2}\ln\frac{p_i p_j}{p_k p_j}$$

- In momentum conserving parton branching $(\tilde{p}_i, \tilde{p}_k) \to (p_i, p_k, p_j)$

$$-\ln \tilde{s}_{ik}/p_T^2 \le 2\eta \le \ln \tilde{s}_{ik}/p_T^2$$

Differential phase-space element $\propto \mathrm{d}p_T^2\,\mathrm{d}\eta$

- Visualized best in Lund plane
  - Gluon emission probability is constant
  - QCD evolution creates fractal structure
  - Recent revival in experimental analyses



Angular ordered parton showers

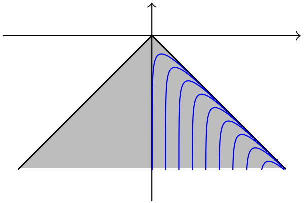
[Marchesini,Webber] NPB238(1984)1, ...

- Differential radiation probability

$$\mathrm{d}\mathcal{P} = \mathrm{d}\Phi_{+1}|M|^2 \approx \frac{\mathrm{d}\tilde{q}^2}{\tilde{q}^2}\,\mathrm{d}z\,\frac{\alpha_s}{2\pi}\,P_{\widetilde{ij}i}(z)$$

  - Ordering parameter $\tilde{q}^2 = \frac{2p_ip_j}{z(1-z)} \approx 4E_{\widetilde{ij}}^2 \sin^2\frac{\theta_{ij}}{2}$

- Lund plane filled from center to edges
  - Random walk in p_T^2
  - Color factors correct for observables insensitive to azimuthal correlations
  - Small dead zone at $\ln(p_T^2/\tilde{s}) \approx 0$



- Usually disfavored due to dead zones
  Not suitable to resum non-global logartihms

Dipole & antenna showers

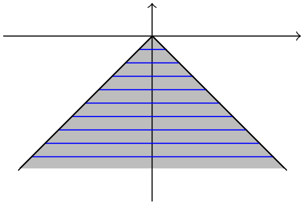
[Gustafson,Pettersson] NPB306(1988)746, ...

- Differential radiation probability for the dipole

$$\mathrm{d}\mathcal{P} = \mathrm{d}\Phi_{+1}|M|^2 \approx \frac{\mathrm{d}p_T^2}{p_T^2}\,\mathrm{d}\eta\,\frac{\alpha_s}{2\pi}\,\tilde{P}_{\widetilde{\imath\jmath}}(z)$$

  - Ordering parameter p_T^2

- Lund plane filled from top to bottom
  - Random walk in η
  - Color factors in CFFE approximation
  - Pairs of partons evolve simultaneously
  - No dead zones

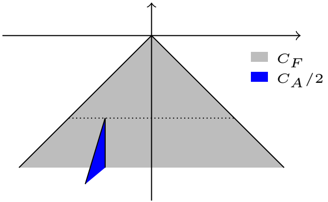


- Solves problem of dead zones
  Known issues with color coherence

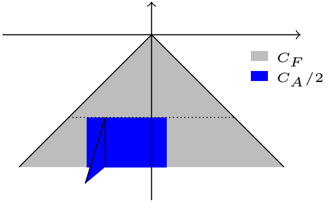
Getting color charges right on average

[Gustafsson] NPB392(1993)251

- In angular ordered showers angles are measured in the event center-of-mass frame $\rightarrow$ coherence effects modeled by angular ordering variable agree on average with matrix element



- In dipole-like showers angles effectively measured in center-of-mass frame of emitting color dipole $\rightarrow$ angular coherence not reflected by setting average QCD charge

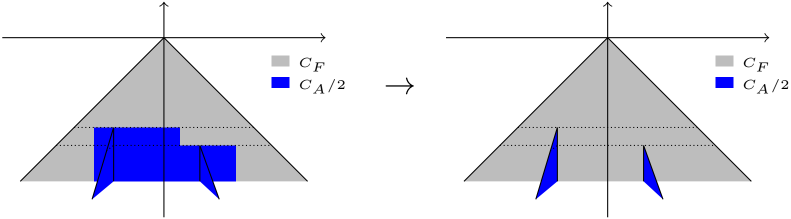


- Emission off "back plane" in Lund diagram should be associated with C_F, but is partly associated with $C_A/2$ in dipole showers

Getting color charges right on average

[Gustafsson] NPB392(1993)251

- Analyze rapidity of gluon emission in event center-of-mass frame
- Sectorize phase space, use color charge of parton closest to soft gluon



- Alternatively reweight to double-soft ME [Giele,Kosower,Skands] arXiv:1102.2126
  Algorithm scales as N^2 but can be simplified while retaining accuracy
  $\rightarrow$ Nested double-soft corrections in rapidity segments of parent dipole
  [Hamilton,Medves,Salam,Scyboz,Soyez] arXiv:2011.10054
- Starting with 4 emissions, there be "color monsters"
  [Dokshitzer,Troian,Khoze] SJNP47(1988)881, YF47(1988)1384
  - Quartic Casimir operators (easy)
  - Non-factorizable contributions (hard)

The problem of on-shell momentum mapping

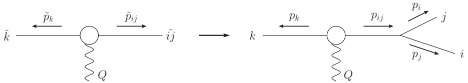
[Dasgupta,Dreyer,Hamilton,Monni,Salam] arXiv:1805.09327

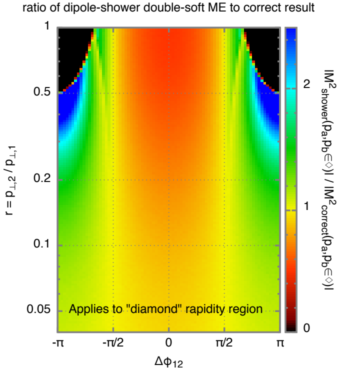
- Subtle problems in standard dipole, dipole-like and antenna mapping

$$p_k^\mu = \left(1 - \frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\right)\tilde{p}_k^\mu$$

$$p_i^\mu = \tilde{z}\,\tilde{p}_{ij}^\mu + (1-\tilde{z})\frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\tilde{p}_k^\mu + k_\perp^\mu$$

$$p_j^\mu = (1-\tilde{z})\,\tilde{p}_{ij}^\mu + \tilde{z}\frac{p_{ij}^2}{2\tilde{p}_{ij}\tilde{p}_k}\tilde{p}_k^\mu - k_\perp^\mu$$





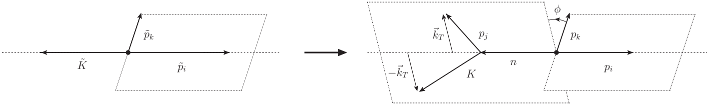
- Induces accidental angular correlations
  Spoils agreement w/ analytic resummation
- Good recoil schemes preserve logarithmic accuracy, but also impact phase-space coverage, especially for angular ordered evolution
  [Bewick,Ferrario-Ravasio,Richardson,Seymour] arXiv:1904.11866

NLL compatible on-shell momentum mappings

- Partitioning of antenna radiation pattern paired with suitable choice of evolution variable [Dasgupta,Dreyer,Hamilton,Monni,Salam,Soyez] arXiv:2002.11114

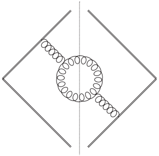
$$k_T = \rho v e^{\beta|\bar{\eta}|} \qquad \rho = \left(\frac{s_i s_j}{Q^2 s_{ij}}\right)^{\beta/2}$$

- Global transverse recoil, global longitudinal recoil gives analytic proof of NLL correctness for dedicated observables (thrust, multiplicity) [Forshaw,Holguin,Plätzer] arXiv:2003.06400
- Local transverse recoil, global longitudinal recoil allows analytic proof of NLL correctness, based on kinematics in $s \to \infty$ limit [Nagy,Soper] arXiv:2011.04773
- Keeping emitter along original direction & recoil vector arbitrary allows to match analytic resummation and prove NLL precision analytically [Herren,Krauss,Reichelt,Schönherr,SH] arXiv:2208.06057



Approximate soft NLO corrections

- Leading higher-order corrections to soft-gluon effects from collinear decay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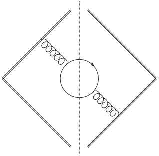


$$+ \ldots = \sum_{b=q,g} j_{ij,\mu}(p_{12}) j_{ij,\nu}(p_{12}) \, \frac{P_{gb}^{\mu\nu}(z_1)}{s_{12}}$$

- Add semi-classical contributions $\rightarrow$ 2-loop cusp anomalous dimension

$$\Gamma_{\rm cusp}^{(2)} = \left(\frac{67}{18} - \frac{\pi^2}{6}\right) C_A - \frac{10}{9} T_R n_f$$

- Soft splitting function with estimated higher-order corrections

$$P_{aa}(z) \xrightarrow{z\to 1} \frac{2C_a}{1-z}\left[1 + \frac{\alpha_s(\mu^2)}{2\pi}\left(-\beta_0 \ln\frac{k_T^2}{\mu^2} + \Gamma_{\rm cusp}^{(2)}\right)\right]$$

- Origin of CMW scheme [Catani,Marchesini,Webber] NPB349(1991)635
  De-facto standard in generator community for past $\sim$30 years

Complete soft NLO corrections at leading color

- Need a benchmark for parton shower to reproduce
  $\to$ soft-gluon resummed expression of Drell-Yan or DIS cross section

$$\frac{1}{\sigma}\frac{d\sigma(z,Q^2)}{d\log Q^2} = \mathcal{H}(Q^2)\,\widetilde{W}(z,Q^2)$$

  RGE governed by Wilson loop $\widetilde{W}$ ($Q(1-z)$ - total soft gluon energy)
- Non-abelian exponentiation theorem allows to expand as

$$\widetilde{W} = \exp\left\{\sum_{i=1}^{\infty} w^{(\mathrm{n})}\right\}$$

- One-loop result [Marchesini,Korchemsky] PLB313(1993)433, hep-ph/9210281

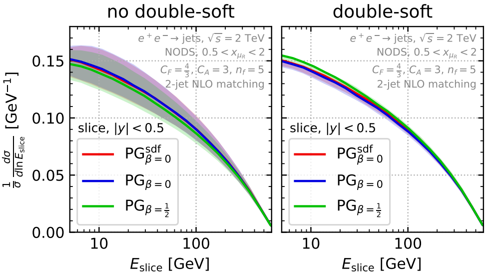
$$w^{(1)} = C_F\,\frac{\alpha_s(\mu)}{2\pi}\left[\ln^2 L + \frac{\pi^2}{6}\right]\,, \qquad L = -\frac{b_+ b_-}{b_0^2}\,, \qquad b_0 = \frac{2\,e^{-\gamma_E}}{\mu}$$

- Two-loop result [Belitsky] hep-ph/9808389

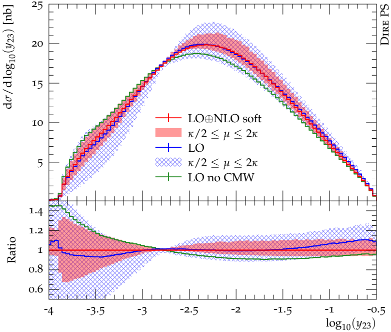
$$w^{(2)} = C_F\,\frac{\alpha_s^2(\mu)}{(2\pi)^2}\left[-\frac{\beta_0}{6}\ln^3 L + \Gamma^{(2)}_{\mathrm{cusp}}\ln^2 L + 2\ln L\left(\Gamma^{(2)}_{\mathrm{soft}} + \frac{\pi^2}{12}\beta_0\right) + \ldots\right]$$

Complete soft NLO corrections at leading color

[Ferrario Ravasio et al.] arXiv:2307.11142



[Dulat,Prestel,SH] arXiv:1805.03757



- Implementation in publicly available MC (Pythia)
- Uncertainty bands no longer just estimates, but perturbative QCD predictions for the first time
- Good agreement with CMW (leading soft effects)

Collinear higher-order corrections

[Prestel,SH] arXiv:1705.00742

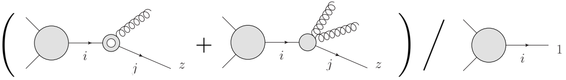
- DGLAP evolution kernels obtained from factorization

$$D_{ji}^{(0)}(z,\mu) = \delta_{ij}\delta(1-z) \qquad \leftrightarrow$$

$$D_{ji}^{(1)}(z,\mu) = -\,\frac{1}{\varepsilon}P_{ji}^{(0)}(z) \qquad \leftrightarrow$$

$$D_{ji}^{(2)}(z,\mu) = -\,\frac{1}{2\varepsilon}P_{ji}^{(1)}(z) + \frac{\beta_0}{4\varepsilon^2}P_{ji}^{(0)}(z) + \frac{1}{2\varepsilon^2}\int_z^1 \frac{\mathrm{d}x}{x}P_{jk}^{(0)}(x)P_{ki}^{(0)}(z/x)$$

$\leftrightarrow$



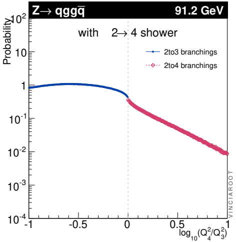
- $P_{ji}^{(n)}$ not probabilities, but sum rules hold ($\leftrightarrow$ unitarity constraint)
  In particular: Momentum sum rule identical between LO & NLO
- Can perform the NLO computation of $P_{ji}^{(1)}$ fully differentially
  using modified dipole subtraction, e.g.

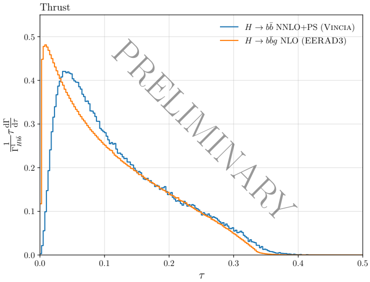
$$P_{qq'}^{(1)}(z) = \mathrm{C}_{qq'}(z) + \mathrm{I}_{qq'}(z) + \int \mathrm{d}\Phi_{+1}\Big[\mathrm{R}_{qq'}(z,\Phi_{+1}) - \mathrm{S}_{qq'}(z,\Phi_{+1})\Big]$$

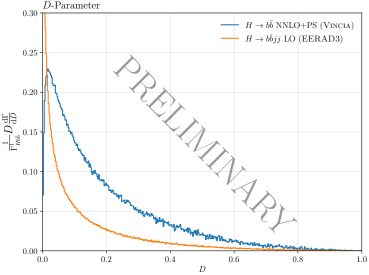
Combined soft & collinear higher-order corrections

[Hartgring,Laenen,Skands] arXiv:1303.4974
[Li,Skands] arXiv:1611.00013, [Campbell,Li,Preuss,Skands,SH] arXiv:2106.10987

- ME-corrected showers predict correct 2-emission pattern $\rightarrow$ possibility to extend to full NLO by including virtual corrections
- Can be turned into complete NLO-accurate emission generator by filling missing phase space with direct $2 \rightarrow 4$ transitions (hard corrections)

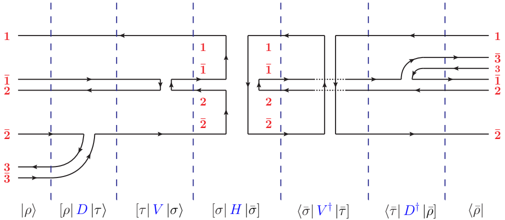


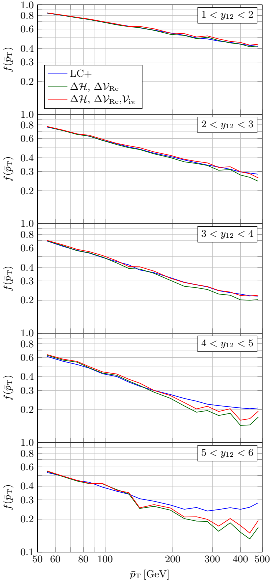




Parton showers beyond leading color accuracy

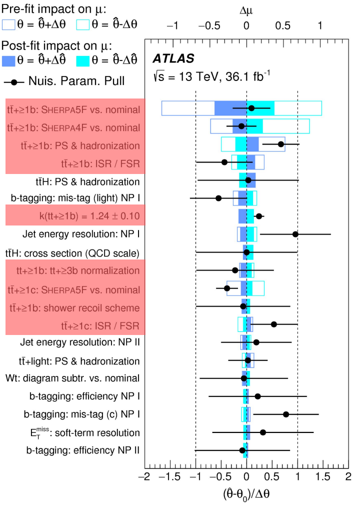
- Systematic expansion of shower operator
  [Nagy,Soper] arXiv:1902.02105, arXiv:1905.07176
  - Simplify soft insertion operators $T_i T_k \rightarrow T_i^2$ but retain bra/ket states exactly
  - Extend to higher number of terms in $1/N_c$ through additional operators
- Amplitude based evolution using color flow decomposition [DeAngelis,Forshaw,Plätzer] arXiv:2007.09648
  - Systematic expansion in $1/N_c$ terms related to number of swaps of color lines





Heavy flavor production & evolution

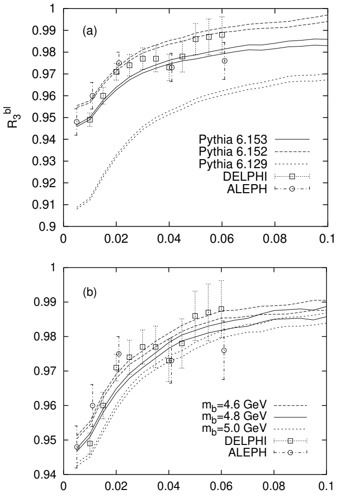
[ATLAS] arXiv:1712.08895



- Example $t\bar{t}b\bar{b}$: MC single largest source of uncertainty on signal strength
- Despite intense study of HF production
  - Fixed order, NLL, FONLL
    [Cacciari,Frixione,Houdeau,Mangano,Nason,Ridolfi,. . .] arXiv:1205.6344, hep-ph/0312132, hep-ph/9801375, NPB373(1992)295
  - In context of particle-level Monte Carlo
    [Norrbin,Sjöstrand], hep-ph/0010012, [Gieseke,Stephens,Webber] hep-ph/0310083, [Schumann,Krauss] arXiv:0709.1027, [Gehrmann-deRidder,Ritzmann,Skands] arXiv:1108.6172
- Recurring themes, not special to $t\bar{t}b\bar{b}$
  - PS uncertainties hard to judge and reduce
    [Cascioli,Maierhöfer,Moretti,Pozzorini,Siegert] arXiv:1309.591
  - Matching needed for inclusive predictions
    [Krause,Siegert,SH] arXiv:1904.09382, [Ferencz,Katzy,Krause,Pollard,Siegert,SH]

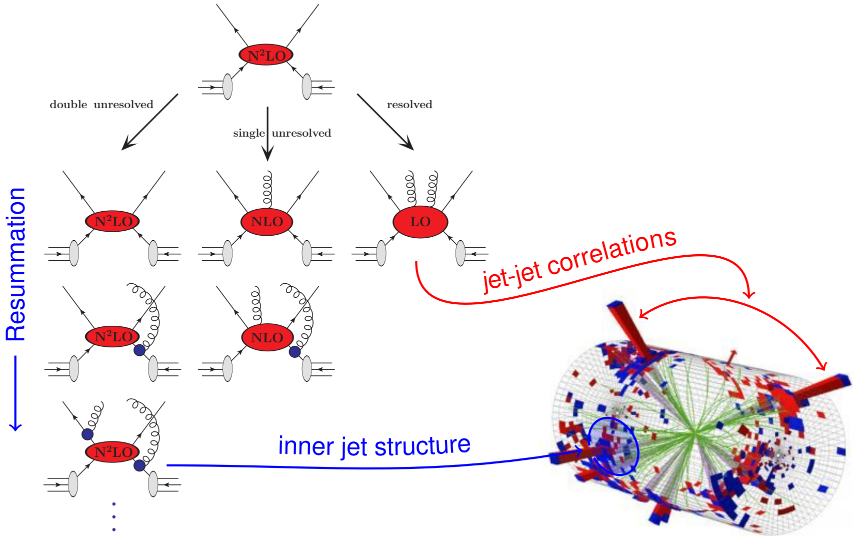
Heavy flavor production & evolution

- Both high-energy limit and threshold region should be described well, but
- Infrared finite prediction for $g \to Q\bar{Q}$ leaves splitting functions somewhat arbitrary
- Soft gluon emission off light/heavy quarks associated with $\alpha_s(k_T^2)$, i.e. "correct" scale is k_T^2 [Amati et al.] NPB173(1980)429, but no such argument to set scale for $g \to Q\bar{Q}$
  $\to$ HQ production rate not very stable w.r.t. parton shower variations
- A number of different prescriptions, e.g.
  [Norrbin,Sjöstrand], hep-ph/0010012,
  [Gieseke,Stephens,Webber] hep-ph/0310083,
  [Schumann,Krauss] arXiv:0709.1027,
  [Gehrmann-deRidder,Ritzmann,Skands] arXiv:1108.6172,
  [Assi,SH] arXiv:2307.00728
  varying success in describing expt. data



[Norrbin,Sjöstrand] hep-ph/0010021

Matching fixed-order calculations to parton showers



Matching fixed-order calculations to parton showers

Two major techniques to match NLO calculations and parton showers

Additive (MC@NLO-like)

[Frixione,Webber] hep-ph/0204244

- Use parton-shower splitting kernel as an NLO subtraction term
- Multiply LO event weight by Born-local K-factor including integrated subtraction term and virtual corrections
- Add hard remainder function consisting of subtracted real-emission correction

Multiplicative (POWHEG-like)

[Nason] hep-ph/0409146

- Use matrix-element corrections to replace parton-shower splitting kernel by full real-emission matrix element in first shower branching
- Multiply LO event weight by Born-local NLO K-factor (integrated over real corrections that can be mapped to Born according to PS kinematics)

Basis of matching – Modified subtraction

[Frixione,Webber] hep-ph/0204244

- NLO calculation of observable O

$$\langle O\rangle = \int \mathrm{d}\Phi_B \left\{\mathrm{B} + \tilde{V}\right\} O(\Phi_B) + \int \mathrm{d}\Phi_R\, \mathrm{R}\, O(\Phi_R)$$

- Parton-shower result until first emission ($\Delta^{(\mathrm{K})}(t) = \exp\left\{ -\int_t \mathrm{d}\Phi_1 \mathrm{K}(\Phi_1)\right\}$)

$$\langle O\rangle = \int \mathrm{d}\Phi_B\, \mathrm{B}\left[\Delta^{(\mathrm{K})}(t_c)\, O(\Phi_B) + \int_{t_c} \mathrm{d}\Phi_1\, \mathrm{K}(\Phi_1)\, \Delta^{(\mathrm{K})}(t(\Phi_1))\, O(\Phi_R)\right]$$

$$\stackrel{\mathcal{O}(\alpha_s)}{\to} \int \mathrm{d}\Phi_B\, \mathrm{B}\left\{1 - \int_{t_c} \mathrm{d}\Phi_1 \mathrm{K}(\Phi_1)\right\} O(\Phi_B) + \int_{t_c} \mathrm{d}\Phi_B \mathrm{d}\Phi_1\, \mathrm{B}\, \mathrm{K}(\Phi_1)\, O(\Phi_R)$$

- Overlap removal at $\mathcal{O}(\alpha_s)$ must be accurate for all IRC safe observables
  First solution in MC@NLO method, others are variants of this scheme

$$\langle O\rangle = \int \mathrm{d}\Phi_B\, \bar{\mathrm{B}}^{(\mathrm{K})}\, \mathcal{F}^{(0)}_{\mathrm{MC}}(\mu_Q^2, O) + \int \mathrm{d}\Phi_R\, \mathrm{H}^{(\mathrm{K})}\, \mathcal{F}^{(1)}_{\mathrm{MC}}(t(\Phi_R), O)$$

  MC events fall into categories, $\mathbb{S}$tandard and $\mathbb{H}$ard

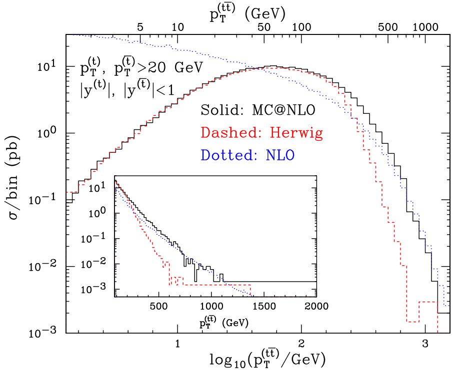
$$\mathbb{S} \;\to\; \bar{\mathrm{B}}^{(\mathrm{K})} = \mathrm{B} + \tilde{\mathrm{V}} + \mathrm{B}\int \mathrm{d}\Phi_1 \mathrm{K}(\Phi_1)$$

$$\mathbb{H} \;\to\; \mathrm{H}^{(\mathrm{K})} = \mathrm{R} - \mathrm{B}(\Phi_B(\Phi_R))\mathrm{K}(\Phi_1)$$

Fixed-order matching – NLO

[Nason,Webber] arXiv:1202.1251

$pp \to t\bar{t} + X$ @ 14 TeV

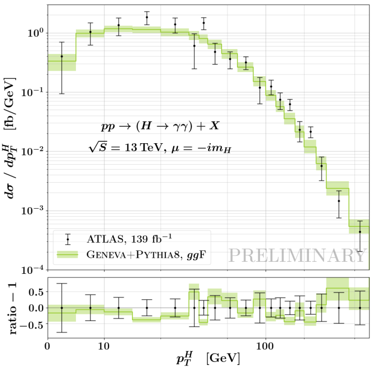


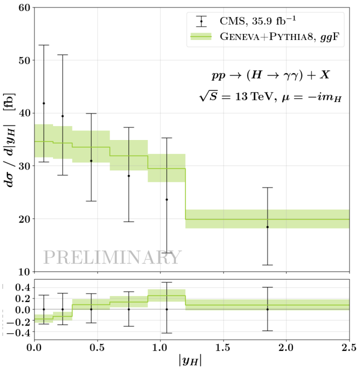
- Matching interpolates smoothly between fixed-order & resummation

Fixed-order matching – N^2LO

[Alioli et al.] arXiv:2301.11875

- In most cases excellent description of experimental data



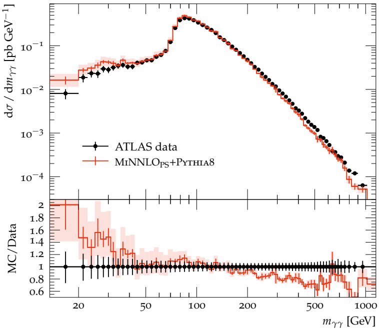


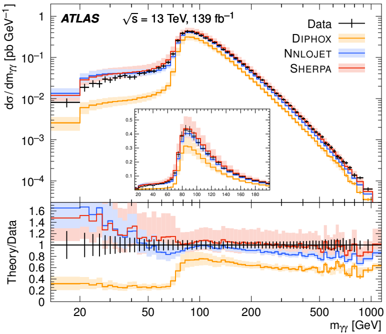
- $p_{T,H}$ and ATLAS data
- y_H and CMS data

Fixed-order matching – N^2LO

[Gavardi,Oleari,Re] arXiv:2204.12602

- Good description even of challenging multi-scale dynamics like in $\gamma\gamma + X$

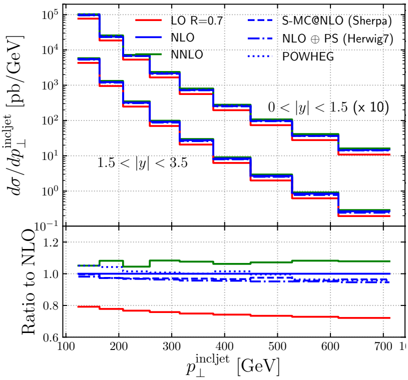


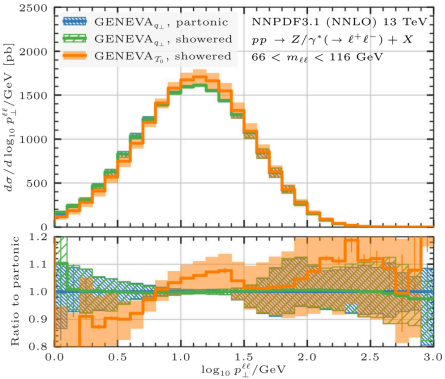


- Comparison between ATLAS data and MINNLO$_{PS}$
- Previous experimental analysis
  [ATLAS] arXiv:2107.09330

Residual uncertainties – N^{2}LO matching

[Bellm at al.] arXiv:1903.12563
[D. Napoletano] arXiv:2212.10489, [Alioli et al.] arXiv:2102.08390

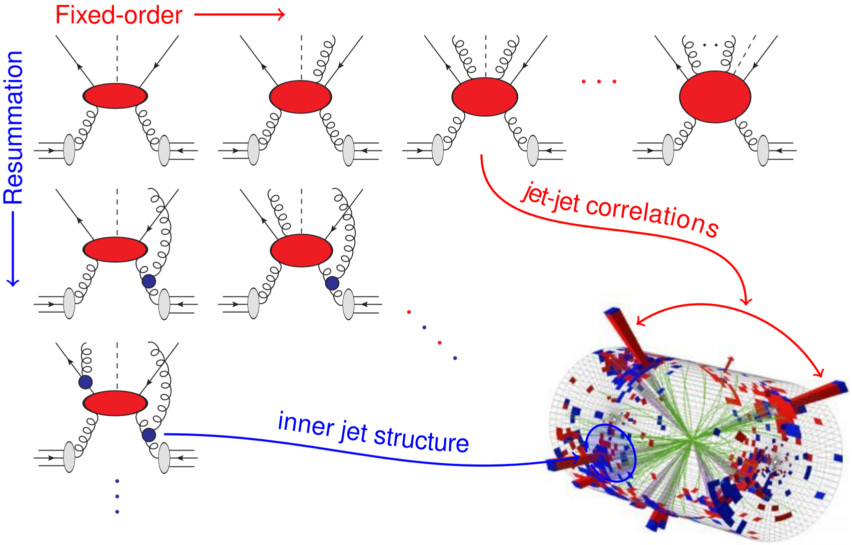




- NLO predictions for $pp \to jj$
- Choice of parton shower

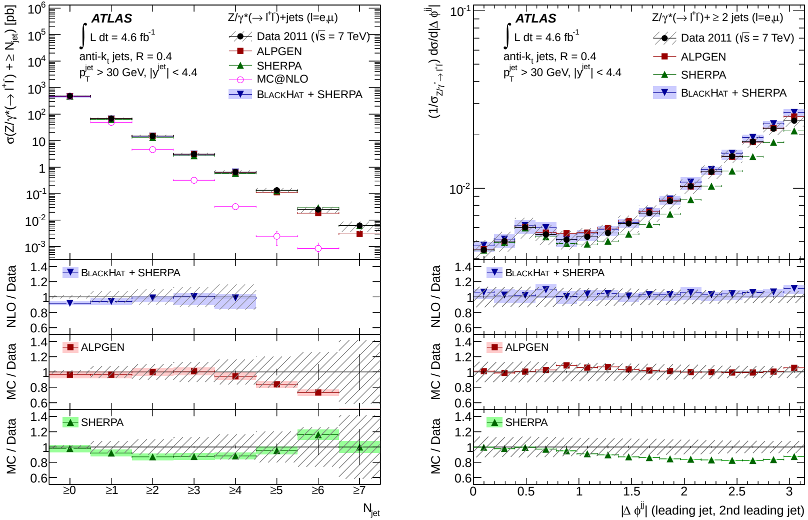
- N^{2}LO predictions for $pp \to Z$
- Choice of resolution variable

Merging calculations of varying jet multiplicity



QCD prediction of multi-jet dynamics

[ATLAS] arXiv:1304.7098



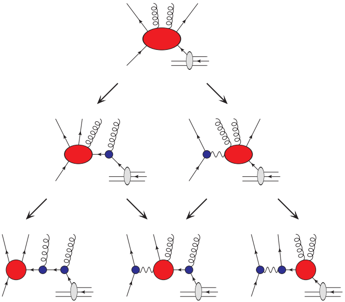
- Drell-Yan lepton pair plus multi-jet production at the LHC

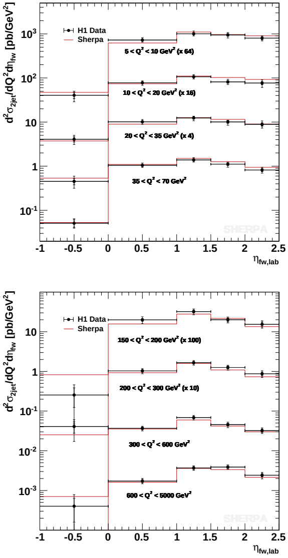
Lessons from HERA

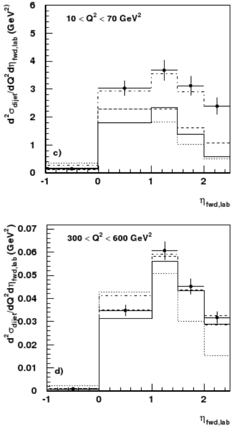
[Carli,Gehrmann,SH] arXiv:0912.3715

Simulation often too focused on resonant contributions

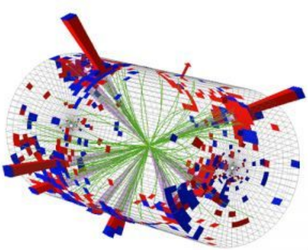
Need be inclusive to describe DIS, low-mass Drell-Yan or photon / diphoton production

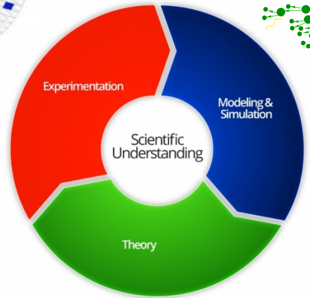


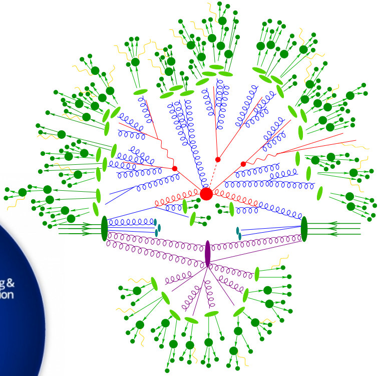




Half a century of teamwork ...







$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi} \not{D} \psi + h.c.$$

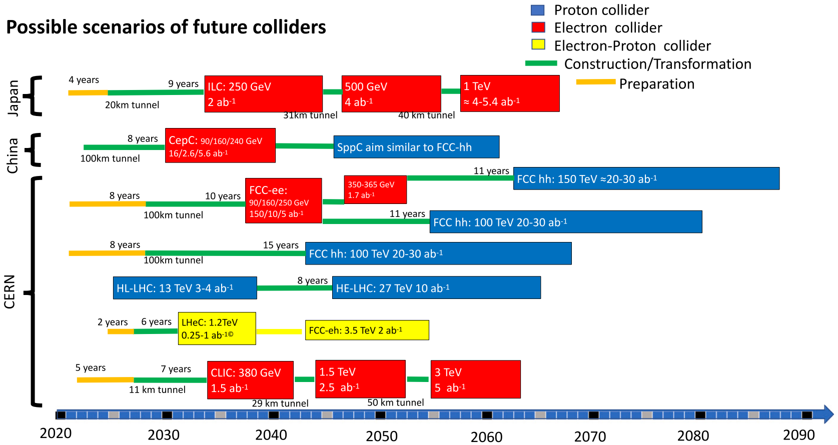
... and we're only getting started

- Fixed-order calculations
  - Higher-order matrix element calculations
  - Higher-order fully differential IR subtraction
  - Computing improvements
- Parton showers
  - Improved logarithmic precision
  - Higher-order splitting kernels
  - Interplay with analytic resummation
- Matching and merging
  - The role of unitarity constraints
  - Interplay with analytic resummation
  - Fully differential higher-order matching

Apologies for only selecting a small subset of topics
For a comprehensive overview: [Campbell et al.] arXiv:2203.11110

Whatever the future may hold ...

[Gray] Rev.Phys. 6 (2021) 100053



... nothing goes without QCD