Monte Carlo and Tools

(Vitaliano Ciulli, Stefan Prestel, Emanuele Re)

"Physics at TeV colliders" 2019
Les Houches, 11 June 2019
MC generators: last 2 years

Color, spin, higher orders – and theoretical concerns

Heavy ions, collective effects & the ridge

Electroweak matching, multi-jets, resonance-aware generators
(our) thoughts for possible studies this year

- Matching and merging
  - top-pair: modeling of top $p_T$
  - $t\bar{t}b\bar{b}$: what is the status?

- Parton showers: accuracy, uncertainties, EW effects
  - multiple scales and uncertainties (follow up from LH '17)
  - EW corrections: find observables that highlight effects? Is modelling sufficient, do we need EW showers?

- Vector-bosons scattering / fusion
  - follow up from LH '17, this time at NLO (QCD+EW?)
  - impact of matching on distributions? Impact of recoil strategy in shower Sudakovs?

- Computing and formats
  - Negative weights: define a good metric for “bad” behavior
  - New formats/tools? (Need of) improvements of time-honored LHA?

- ...
LH 2019: first steps

► Wednesday morning (June 12th): kick-off meetings (10h30 - 12h00)

► We’ll keep the wikipage updated

► we’ve prepared a slack workspace which we plan to use once the activities are defined a bit better: click here for up-to-date information and discussions
matching and merging
Matching and merging: status and recent progress

- For color-singlet production, NNLO+PS is understood, at least 3 methods available (MiNLO, UNNLOPS, Geneva). So far, not yet clear how to go beyond this.

**WW @ NNLO+PS**

- For all other SM processes, NLO+PS (merging) is there, and used in several analyses

- Overall they work reasonably well, with exceptions, some of them quite notable...

**DIS @ NNLO+PS**
matching and merging: open issues

- long-standing discrepancies in description of inclusive $t\bar{t}$: e.g. top $p_T$
long-standing discrepancies in description of inclusive $t\bar{t}$: e.g. top $p_T$

(at least to me), not fully clear if this is understood: NNLO effect, scale choice, EW effects, MC-related issue, ATLAS vs. CMS...

[Czakon et al. '19]

[Cormier at al - HW7, '18]

can we make some progress here?
Matching and merging: open issues

- $t\bar{t}H(\to b\bar{b})$ needs MC simulation of $t\bar{t}b\bar{b}$: MC modeling is the largest source of uncertainties

Ongoing activities:

1. $t\bar{t}b\bar{b}$ at NLO+PS in the 4FS
2. Merging in a variable flavour number scheme
   - Large NLO perturbative uncertainties (20-30%)
   - Large discrepancies among different generators
   - Matching systematic + PS effects (recoils)
   - Tuned comparison ongoing in HXSWG, final outcome not yet clear
3. 2 samples: $tt+\text{jets}$ MEPS@NLO and $ttbb$ 4FS NLO+PS, overlap removal based on full PS history
   - Worked out for $Z+\bar{b}b$, ongoing for $t\bar{t}b\bar{b}$

$\tilde{V}+HF$ in the $VH$ signal region might also suffer from large MC uncertainties

$VH$ studies on these fronts (with Higgs WG)?
Matching and merging: open issues

- \( t\bar{t}H (\rightarrow b\bar{b}) \) needs MC simulation of \( t\bar{t}b\bar{b} \): MC modeling is the largest source of uncertainties

Ongoing activities:

1. \( t\bar{t}b\bar{b} \) at NLO+PS in the 4FS
   - Large NLO perturbative uncertainties (20-30%) + large discrepancies among different generators → matching systematic + PS effects (recoils)
   - Tuned comparison ongoing in HXSWG, final outcome not yet clear
.matching and merging: open issues

- $t\bar{t}H (\to b\bar{b})$ needs MC simulation of $t\bar{t}b\bar{b}$: MC modeling is the largest source of uncertainties

ongoing activities:

1. $t\bar{t}b\bar{b}$ at NLO+PS in the 4FS
2. merging in a variable flavour number scheme
   - 2 samples: $tt+jets\text{ MEPS@NLO} + t\bar{t}bb\text{ 4FS NLO+PS}$, overlap removal based on full PS history
   - worked out for $Z+b\bar{b}$, ongoing for $t\bar{t}bb$
matching and merging: open issues

- $t\bar{t}H(\rightarrow b\bar{b})$ needs MC simulation of $t\bar{t}b\bar{b}$: MC modeling is the largest source of uncertainties

ongoing activities:
1. $t\bar{t}b\bar{b}$ at NLO+PS in the 4FS
2. merging in a variable flavour number scheme

- $V+HF$ in the $VH$ signal region might also suffer from large MC uncertainties

- LH: studies on these fronts (with Higgs WG)?
parton showers
parton showers: status and recent progress

improving, or going beyond, existing shower algorithms:

▶ color correlations, spin correlations
  [Plätzer et al. // Prestel, Isaacson // Bellm // Webster, Richardson // Nagy, Soper '18-'19]

▶ evolution at the amplitude level
  [Angeles et al. '18] [Nagy, Soper '17-'18]

▶ first steps and tests towards evolution at next order
  [Höche, Prestel et al. '17-]

▶ dedicated studies to determine the actual logarithmic accuracy
  [Höche, Reichelt, Siegert '17, Dasgupta et al. '18, Bewick et al. '19]

<table>
<thead>
<tr>
<th>Observable</th>
<th>NLL_{ln \Sigma} discrepancy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 - T$</td>
<td>$0.116^{+0.004}_{-0.004} \bar{\alpha}^3 L^3$</td>
</tr>
<tr>
<td>vector $p_t$ sum</td>
<td>$-0.349^{+0.003}_{-0.003} \bar{\alpha}^3 L^3$</td>
</tr>
<tr>
<td>$B_T$</td>
<td>$-0.0167335 \bar{\alpha}^2 L^2$</td>
</tr>
<tr>
<td>$y_3^{\text{cam}}$</td>
<td>$-0.18277 \bar{\alpha}^2 L^2$</td>
</tr>
<tr>
<td>$FC_1$</td>
<td>$-0.066934 \bar{\alpha}^2 L^2$</td>
</tr>
</tbody>
</table>

- all the above quite difficult: some “easier” idea that could be interesting to explore here...
General-Purpose event generators cover many different phenomena through different models for

- hard scattering
- radiation cascade
- multiparton interactions
- hadronization and decay

Each model contains parameters & smooth matching introduces more.

Some (inter)dependences studied already… but we’re far from there yet.
general purpose generators: study of uncertainties

- LH is a good place for these studies
- LH is a good place for these studies

- aren’t these the studies usually kept for a “rainy day”? 

- variations in different shower algorithms
- variations vs. hadronization tuning.
- $\alpha_s (m_z)$ variations vs. PDF choices
- $\mu_r^2 - \mu_r^2 f$ correlation?
- $\mu_r^2 f$ vs. PDF member variations?
- $\mu_r^2$ variations vs. MPI tuning?
. LH is a good place for these studies

LH17
◇ $\mu^2_t$ variations in different shower algorithms
◇ $\mu^2_t$ variations vs. hadronization tuning.
◇ $\alpha_s(m_z)$ variations vs. PDF choices

I ideas for this time?
◇ PDF unfolding in different ISR algorithms?
◇ $\mu^2_t - \mu^2_f$ correlation?
◇ $\mu^2_f$ vs. PDF member variations?
◇ $\mu^2_t$ variations vs. MPI tuning?
EW effects are typically important at high energy & high precision.

Status at fixed-order is quite advanced; EW corrections in PS start to be implemented (e.g. in Sherpa, $t\bar{t}$+jets, ’18).

full EW shower evolution missing (but progress made e.g. on PDFs)

Possible points to discuss in LH:

- Status of EW effects in GPMCs satisfactory?
- EW evolution needed?
- Killer observables?
Vector-boson scattering will be a crucial process in the future.

- **Fixed-order calculations at impressive precision.**
  - NLO matching possible/available
  - **...**
  - WZ: NLO QCD+NLO EW [Denner et al. '19]
  - WW: NLO EW + PS [Chiesa et al. '19]

- **Is NLO matching fool-proof?**

- **Does parton shower recoil strategy deform results significantly?**

Possible study in LH: Comparison of calculations matched to PS, especially to understand deformation of fixed-order results by parton showers!
vector boson scattering
### VBS results

<table>
<thead>
<tr>
<th>channel</th>
<th>ATLAS</th>
<th>CMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^{\pm}W^{\pm}$</td>
<td>8,13 TeV</td>
<td>8,13 TeV</td>
</tr>
<tr>
<td></td>
<td>6.9 (4.6) σ</td>
<td>5.5 (5.7) σ</td>
</tr>
<tr>
<td>$WZ$</td>
<td>8,13 TeV</td>
<td>13 TeV</td>
</tr>
<tr>
<td></td>
<td>5.7 (3.3) σ</td>
<td>1.9 (2.7) σ</td>
</tr>
<tr>
<td>$Z\gamma$</td>
<td>8 TeV</td>
<td>8 TeV</td>
</tr>
<tr>
<td></td>
<td>2.0 (1.8) σ</td>
<td>3.0 (2.1) σ</td>
</tr>
<tr>
<td>$W\gamma$</td>
<td>-</td>
<td>8 TeV</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>2.7 (1.5) σ</td>
</tr>
<tr>
<td>ZZ fully leptonic</td>
<td>-</td>
<td>13 TeV</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>2.7 (1.6) σ</td>
</tr>
<tr>
<td>WV semi-leptonic</td>
<td>8 TeV</td>
<td>13 TeV</td>
</tr>
<tr>
<td></td>
<td>anomalous couplings</td>
<td>anomalous couplings</td>
</tr>
</tbody>
</table>
Some differences observed for WZ in the signal strengths:

<table>
<thead>
<tr>
<th>Process</th>
<th>Experiment</th>
<th>Obs. (fb)</th>
<th>Pred. (fb)</th>
<th>Obs. ratio</th>
<th>Region</th>
</tr>
</thead>
<tbody>
<tr>
<td>EW WZjj</td>
<td>ATLAS</td>
<td>0.57</td>
<td>+0.16</td>
<td>1.77</td>
<td>ATLAS SR</td>
</tr>
<tr>
<td></td>
<td>CMS</td>
<td>—</td>
<td>1.25</td>
<td>0.82</td>
<td>CMS tight SR</td>
</tr>
<tr>
<td>WZjj (EW+QCD)</td>
<td>ATLAS</td>
<td>1.68</td>
<td>+0.25</td>
<td>0.78</td>
<td>ATLAS SR</td>
</tr>
<tr>
<td></td>
<td>CMS</td>
<td>3.18</td>
<td>+0.71</td>
<td>0.98</td>
<td>CMS tight SR</td>
</tr>
<tr>
<td>QCD WZjj</td>
<td>ATLAS</td>
<td>—</td>
<td>—</td>
<td>0.56</td>
<td>ATLAS CR</td>
</tr>
<tr>
<td></td>
<td>CMS</td>
<td>—</td>
<td>18.6</td>
<td>~1.02</td>
<td>CMS tight CR</td>
</tr>
</tbody>
</table>

Fiducial regions however not easily comparable

MC predictions can differ significantly

Not clear if difference comes from data or MC!
## MC generators used

<table>
<thead>
<tr>
<th></th>
<th>$W_\gamma$ CMS</th>
<th>ZZ CMS</th>
<th>WZ ATLAS</th>
<th>WZ CMS</th>
<th>WV ATLAS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>EW</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EW</td>
<td>MG5 LO</td>
<td>MG5 LO</td>
<td>Sherpa NLO +jets</td>
<td>MG5 LO</td>
<td>Whizard LO</td>
</tr>
<tr>
<td></td>
<td>$k_F=1.2$ VBFNLO</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>QCD</strong></td>
<td>MG5 LO</td>
<td>MG5 NLO + FxFx</td>
<td>Sherpa NLO +jets</td>
<td>MG5 LO + MLM</td>
<td>Whizard LO</td>
</tr>
<tr>
<td><strong>aQGC</strong></td>
<td>MG5 LO</td>
<td>MG5 LO + ME reweigh</td>
<td>MG5 LO + ME reweigh</td>
<td>Sherpa LO + NLO XS</td>
<td></td>
</tr>
<tr>
<td>interf.</td>
<td>Neglected</td>
<td>Neglected</td>
<td>syst. (2%)</td>
<td>negligible</td>
<td>Neglected</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>ssWW ATLAS</th>
<th>ssWW CMS</th>
<th>$Z_\gamma$ ATLAS</th>
<th>$Z_\gamma$ CMS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>EW</strong></td>
<td>Sherpa LO +MEPS</td>
<td>MG5 LO</td>
<td>Sherpa LO NLO XS VBFNLO</td>
<td>MG5 LO kFactor 1.1</td>
</tr>
<tr>
<td><strong>QCD</strong></td>
<td>Sherpa LO +MEPS</td>
<td>MG5 LO</td>
<td>Sherpa LO</td>
<td>MG5 LO + MLM</td>
</tr>
<tr>
<td><strong>aQGC</strong></td>
<td>MG5 LO</td>
<td>MG5 LO</td>
<td>MG5 LO</td>
<td>MG5 LO</td>
</tr>
<tr>
<td>interf.</td>
<td>syst. (6%)</td>
<td>syst. (few %)</td>
<td>syst. (~10%)</td>
<td>syst. (~11%)</td>
</tr>
</tbody>
</table>
Les Houches 2017 study

Comparison of EW WZ production at fixed order

Very good agreement but only after a careful tuning of inputs, scales and PDFs

More studies/comparisons of theory predictions for same sign WW:

ATLAS study of generators
ATL-PHYS-PUB-2019-004

A. Ballestrero et al. (VBSCan)
https://arxiv.org/abs/1803.07943

Comparison of EW WZ production at fixed order

Table V.5: Fiducial cross sections at LO for the process

\[ \sigma [\text{fb}] / \text{bin} \]

<table>
<thead>
<tr>
<th>Scale choice</th>
<th>Signature</th>
<th>( \epsilon_{\text{ecola}} )</th>
<th>( \epsilon_{\text{MoCaNLO+Recola}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu )</td>
<td>( \bar{\mu} )</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>( \mu )</td>
<td>( \bar{\mu} )</td>
<td>7%</td>
<td>7%</td>
</tr>
</tbody>
</table>

Uncertainties are evaluated using the typical prescription of varying these, we compute the PDF uncertainty for the NNPDF3.0 set and the two scale choices considered.

This supports the findings of Ref. \[ VBFNLO \]

The predictions in the lower plot are normalised to the prediction of \( \text{M}+\text{R} \) at the LHC running at a centre-of-mass energy of 13 TeV.

The predictions are expressed in fb and are for \( \sigma_{\text{pp}} \).

The shaded bands indicate uncertainties.

The relative statistical uncertainty by bin for each sample. The statistical uncertainty on the predictions is shown in grey, other samples are indicated in the ratio with the predictions in the ecola.
Which tools for the comparison?

Both Les Houches and VBSCan comparison based on RIVET Routines available and being further developed (adding CR) here:

https://gitlab.cern.ch/lhcewkwg/lhcewkwg-multiboson/mc-comparison

Being used by LHCEEWG-MB to compare ATLAS and CMS generators setup: https://indico.cern.ch/event/826857/

e.g. number of jets in same sign WW with Powheg
Ideas for a LH 2019 project

Technical comparison of generators/theory at NLO?
  ▶ the most recently available is NLO EW WZjj in Powheg (Jager, Karlberg, Sheller [https://arxiv.org/abs/1812.05118])

Start looking at opposite sign WW?
  ▶ Experimentally more challenging, but sooner or later will come…
  ▶ How about the theory side?

Use EFT to extract more informations/combine the results?

Something else?
tools & formats
Weighted events are often unavoidable at some generation stage – sometimes physics-related, mostly due to limited person power/money/ recognition.

Wildly fluctuating or negative weights complicate MC error assessment, and require more resources.
Negative weights, performance metrics

Weighted events are often unavoidable at some generation stage – sometimes physics-related, mostly due to limited person power/money/recognition.

Wildly fluctuating or negative weights complicate MC error assessment, and require more resources.

These issues can be serious bottleneck for some analyses.

“Event generators computing” WS few months ago: find metric to define a “mutually acceptable level of weighting”?

- Fraction of negative-weight events :(
- Counter-event contribution to $d\sigma/d\sigma$ for reference $\sigma$?
High-Performance computing for the HL-LHC

In any case, HL-LHC may need better use of computing resources.

Example: (LO) merging at its limit

\[ N_{\text{jet}} \]

\[
\begin{array}{cccccc}
10^{-1} & 10^0 & 10^1 & 10^2 & 10^3 & 10^4 & 10^5 \\
\text{CPUh/Mevt} & \text{Sherpa / Pythia + DIY @ NERSC} & W^{\pm}+\text{jets, LHC@14TeV} & p_{T,j} > 20 \text{GeV}, |\eta_j| < 6 \\
\end{array}
\]

\[ W^{\pm}+\text{jets, LHC@14TeV} \]

\[ p_{T,j} > 20 \text{GeV}, |\eta_j| < 6 \]

\[ \sigma_{\text{lo}} \approx 0.5 pb \]

\( \Rightarrow \) Usable for analyses

Computation time dominated by fixed-order – for now, but not forever.

Is regeneration an option? Can we avoid I/O bottlenecks?
For LH: can we find/discuss suitable technologies for the future?
Updates of LHA/LHEF?

Les Houches Event Format has allowed to decouple ME generators and GPMCs. Bleeding-edge calculations may encourage updates.

Failed @ LH17 to agree on/implement suggested improvements.

Is it worth trying again? Should one make the format(s) also useful for other communities?

```
<event info="some non-standard attribute" npLO="-1" npNLO="0">
  4 81 1.00000E+00 2.779475E+02 7.861651E-03 1.08440E-01
  2 1 0 0 101 0 0.0000000000E+00 0.0000000000E+00 3.0163058970E+02 3.0163058970E+02 0.0000000000E+00
  -2 1 0 0 0 102 0.0000000000E+00 0.0000000000E+00 -2.9643457592E+02 2.9643457592E+02 0.0000000000E+00
  6 1 1 2 101 0 -1.358865269E+02 -1.6715922432E+02 1.1286978960E+02 3.0000000000E+02 1.7561597284E+02
  -6 1 1 2 0 102 1.358865269E+02 1.6715922432E+02 -1.0767377581E+02 2.9806466432E+02 1.7561597284E+02
</event>

<rwt>
<wgt id="1001">0.50109E+02</wgt>
<wgt id="1002">0.45746E+02</wgt>
<wgt id="1003">0.52581E+02</wgt>
</rwt>
<scales muf="90.1" mur="90.2" mups="90.3" newscale="90.4">comment</scales>
```
Legacy data


- **Raw data (level 4):** $O$(Petabyte)
- **Analysis level data (level 3):** sufficient for a complete re-analysis
- **Simplified event level data (level 2):** 4-vectors of detected particles
- **Published data (level 1):** for HEP, also available in HEPDATA

Focusing on published data, how can we allow testing the SM and performing searches for New Physics spanning over different experimental analyses?

The **MineHEP project** by Univ. of Florence, in collaboration with IPPP Durham, as a first step in this direction, is trying to organise the already available information in HEPDATA to easily extract as much information as possible with a search engine.

But other approaches are also possible/complementary (opendata, Rivet,…)

If people are interested, it is worth having a discussion on these items: feedback from this community is clearly most valuable!
No man is an island...

As usual, some projects will naturally overlap with the other working groups:

- New observables to test new showers $\rightarrow$ Jets WG
- Matching/merging crash tests with substructure $\rightarrow$ Jets WG
- GPMC Higgs modelling systematics $\rightarrow$ Higgs & SM WG
- …

After all, we hope new ideas will come from you, that’s what makes LH successful and useful!
Thanks for your attention!

First kick-off meetings tomorrow morning (June 12th).