MC Challenges at high lumi/energy - LHC

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Main question

Will our MCs be up to the challenges of the HL-LHC in ten years from now?
Half-way of the MC4LHC activity

MC4LHC community got together and started to get ready 10 years in advance…

A good moment to start planning and identifying the most important challenges!
Predictive Monte Carlo Generators

\[ \sigma_X = \sum_{a,b} \int_0^1 dx_1 dx_2 f_a(x_1, \mu_F^2) f_b(x_2, \mu_F^2) \times \hat{\sigma}_{ab \rightarrow X}(x_1, x_2, \alpha_S(\mu_R^2), \frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2}) \]

A **predictive** MC associates an history to short-distance events obtained from a parton-level (at least) next-to-leading order calculation i) avoiding double counting, ii) keeping the formal fixed-order accuracy, iii) resumming collinear and soft enhanced effects, iv) deconstructing PDF and FF probabilities and v) providing hadronisation and an UE.
20 years ago

pp\rightarrow n \text{ particles}

<table>
<thead>
<tr>
<th>complexity [n]</th>
<th>accuracy [loops]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
</tr>
</tbody>
</table>

- Red circle: fully inclusive
- Orange circle: parton-level
- Green circle: fully exclusive
Progress in the past 20 years

- Merging and matching: ME+PS
- New Loop techniques
- BSM framework
- Automatic NLO+PS
- Merging at NLO
- NNLO+PS
- BSM at NLO+PS
- PS@NLL*
- Automatic NLOEW+PS

1999: First (LO) industrial revolution
2002
2008
2009
2011
2012
2013
2014
2015
2016: Second (NLO) industrial revolution
Present 2017

accuracy [loops]

- 3 (fully inclusive)
- 2 (parton-level)
- 1 (fully exclusive)
- 0 (fully exclusive and automatic)

QCD and EW

complexity [n]
It's hard to make predictions, especially about The Future

New Two Loop techniques

PS@NLL

MC@NNLO

Automatic MC@NNLO

AI MC

2017

Today

2027

2037

Third (NNLO) industrial revolution
The future (2027 circa)

QCD and EW

accuracy [loops]

fully exclusive
parton-level
fully exclusive and automatic

complexity [n]
MC Challenges

We can organise the MC challenges in three wide classes:

- Physics
- Technicalia
- Computing
Physics Goals of the HL LHC

1. Search for new resonant states, specific UV models or simplified ones, via non-SM final states or exotic signatures.

2. Search and quantification of deviations in the interactions among SM particles.

3. Precise determination of the fundamental parameters of the dim=4 SM Lagrangian, such as masses ($m_h$, $m_W$, $m_t$), and couplings.
Example #1: managing large rates

With 3 iab of luminosity expected at the end of the HL-LHC a large number of events for many interesting SM processes is expected in the bulk and a significant one also in the tails. This will challenge our mass production schemes with diverging needs: accuracy and precision (expensive) vs large samples vs statistically significant tails.

<table>
<thead>
<tr>
<th>Process</th>
<th>inclusive</th>
<th>pt&gt;X</th>
</tr>
</thead>
<tbody>
<tr>
<td>ttbar</td>
<td>3G</td>
<td>150K (pt&gt;1 TeV)</td>
</tr>
<tr>
<td>W</td>
<td>600G</td>
<td>200K (pt&gt;1 TeV)</td>
</tr>
<tr>
<td>Z</td>
<td>200G</td>
<td>70K (pt&gt;1 TeV)</td>
</tr>
<tr>
<td>H</td>
<td>150M</td>
<td>50K (pt&gt;300 GeV)</td>
</tr>
</tbody>
</table>
Example #2: managing small signals

Based on the full NLO computation of [Borowka et al. 1604.06447 and 1608.04798], [Heinrich et al. 1703.09252] (including a cutting edge two-loop computation) have implemented it in POWHEG and MG5aMC. NLO is significant improvement over LO. Genuine NLO observables are rather stable. However, still uncertainties due to shower scale choices.

Many other gg loop induced processes contribute to important SM final states at the LHC for which we do not have complete NLO+PS calculations/implementations: AA, AZ, ZZ, W+W-, HZ,..
Example #3: managing new ideas

Interesting suggestion to access the Yukawa $y_t t^4$ coupling from $ttt t$ final state [Cao et al., 1602.01934]] already picked up by the CMS collaboration:

Question is: is this result stable under radiative corrections?
Example #3: managing new ideas

A recent calculation [Frederix, Pagani, Zaro, to appear] can help understand the issue by computing all higher-order terms and finding an unexpected pattern of cancellations.

\[ \Sigma_{\text{LO}}(\alpha_s, \alpha) = \alpha_s^4 \Sigma_{4,0}^{\text{LO}} + \alpha_s^3 \alpha \Sigma_{4,1}^{\text{LO}} + \alpha_s^2 \alpha^2 \Sigma_{4,2}^{\text{LO}} + \alpha_s^3 \alpha \Sigma_{4,3}^{\text{LO}} + \alpha^4 \Sigma_{4,4}^{\text{LO}} \]

\[ = \Sigma_{\text{LO}_1} + \Sigma_{\text{LO}_2} + \Sigma_{\text{LO}_3} + \Sigma_{\text{LO}_4} + \Sigma_{\text{LO}_5} . \]

\[ \Sigma_{\text{NLO}}(\alpha_s, \alpha) = \alpha_s^5 \Sigma_{5,0}^{\text{NLO}} + \alpha_s^4 \alpha^1 \Sigma_{5,1}^{\text{NLO}} + \alpha_s^3 \alpha^2 \Sigma_{5,2}^{\text{NLO}} + \alpha_s^2 \alpha^3 \Sigma_{5,3}^{\text{NLO}} + \alpha_s^1 \alpha^4 \Sigma_{5,4}^{\text{NLO}} + \alpha^5 \Sigma_{5,5}^{\text{NLO}} \]

\[ = \Sigma_{\text{NLO}_1} + \Sigma_{\text{NLO}_2} + \Sigma_{\text{NLO}_3} + \Sigma_{\text{NLO}_4} + \Sigma_{\text{NLO}_5} + \Sigma_{\text{NLO}_6} . \]

<table>
<thead>
<tr>
<th>( \delta ) [%]</th>
<th>( \mu = H_T/8 )</th>
<th>( \mu = H_T/4 )</th>
<th>( \mu = H_T/2 )</th>
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</thead>
<tbody>
<tr>
<td>LO(_2)</td>
<td>-26.0</td>
<td>-28.3</td>
<td>-30.5</td>
</tr>
<tr>
<td>LO(_3)</td>
<td>32.6</td>
<td>39.0</td>
<td>45.9</td>
</tr>
<tr>
<td>LO(_4)</td>
<td>0.2</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>LO(_5)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.05</td>
</tr>
<tr>
<td>NLO(_1)</td>
<td>14.0</td>
<td>62.7</td>
<td>103.5</td>
</tr>
<tr>
<td>NLO(_2)</td>
<td>8.6</td>
<td>-3.3</td>
<td>-15.1</td>
</tr>
<tr>
<td>NLO(_3)</td>
<td>-10.3</td>
<td>1.8</td>
<td>16.1</td>
</tr>
<tr>
<td>NLO(_4)</td>
<td>2.3</td>
<td>2.8</td>
<td>3.6</td>
</tr>
<tr>
<td>NLO(_5)</td>
<td>0.12</td>
<td>0.16</td>
<td>0.19</td>
</tr>
<tr>
<td>NLO(_6)</td>
<td>&lt; 0.01</td>
<td>&lt; 0.01</td>
<td>&lt; 0.01</td>
</tr>
</tbody>
</table>

NLO\(_2\) + NLO\(_3\) = -1.7, -1.6, 0.9
MC Challenges: Physics

- (N)NLO+ fixed order precision & accuracy for QCD (tree-level and loop-induced)
- NLO+PS for EW and (two-loop) mixed QCD-EW corrections
- Accuracy and precision of the PS resummation (NLL and more)
- Modeling/measurements of non-perturbative effects (PDFs, fragmentation, UE)
- Bulk vs High-pT/boosted topologies
- Exclusive multi-jet final states at NLO
- New Physics modeling: new particles and interactions
- Dedicated developments for specific high precision measurements of in the SM ($m_W, m_t, ...$)
- Dedicated developments for new phenomena (e.g., long-lived particles)
- ...
Progress on PS@NLL

  Naturally, NLO DGLAP evolution must be part of the full solution
- NLO DGLAP splitting kernels known since long
- So far not implemented in parton showers because
  - Kernels are scheme dependent (easy)
  - Overlap with soft-gluon resummation (hard)
- Focus on purely collinear corrections (↔ B2) for a start
  - Redefine time-like Sudakovs to recover NLO DGLAP evolution
  - Negative NLO corrections require weighted veto algorithm
  - Flavor changing splitting functions require 2 → 4 transitions
- Flavor-changing case is simplest but requires all the technology

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Progress on PS@NLL

\[ P_{qq'}(z) = \left( I + \frac{1}{\varepsilon} \mathcal{P} - \mathcal{I} \right)_{qq'}(z) + \int d\Phi_{+1}(R - S)_{qq'}(z, \Phi_{+1}) \]

where

\[ I_{qq'}(z) = \int d\Phi_{+1} S_{qq'}(z, \Phi_{+1}) \]
\[ P_{qq'}(z) = \int z \frac{dx}{x} P_{qq}^{(0)}(x) P_{qq}^{(0)}(z/x) \]
\[ I_{qq'}(z) = 2 \int z \frac{dx}{x} C_F \left( \frac{1 + (1 - x)^2}{x} \ln(x(1 - x)) + x \right) P_{qq}(z/x) \]

**Basic layout of Dire** [Prestel,SH] arXiv:1506.05057
- Dipole-like parton shower, kernels as close as possible to DGLAP
- Partial fraction soft eikonal à la Catani-Seymour, evolve in dipole-\(k_T\)
- Two independent implementations (Pythia & Sherpa)
- Cross-validation at particle level

**New developments**
- MC counterterms implemented in Amegic & Comix [SH]
- MC@NLO matching & NLO subtraction in Sherpa [SH]
- UNLOPS / MEPS@NLO merging in Pythia / Sherpa [Prestel,SH]
Dedicated MC developments

POWHEG and MG5aMC

Resonance aware PS and NLO matching \( \rightarrow \) \( m_t \)

NLO QCD+EW corrections+PS (QCD and QED) \( \rightarrow \) \( m_W \)

POWHEG

Other dedicated implementations/efforts (for example in b radiation) will be needed.
NLO+PS with intermediate resonances

[Jezo and Nason, 2015]

Amplitudes squared are expressed in terms of sum of contributions from the BW’s. The cancellation between V and R happens only when \( m_b^2 < \Gamma \), A modified FKS method has been proposed that deals correctly with (spurious) double logs of \( \Gamma \) in POWHEG. Soft single logs \( \Gamma \) are left to cancel on their own in the \( \tilde{B} \) function.

Shift in the reconstructed top mass due to differences in the final state radiation treatment of the b quark. Implementation of WbWb available [Jezo et al. 2016]
**EW corrections**

- The development of automatic NLO includes the possibility of computing EW corrections (including real/virtual photons) fully automatically nowadays.

- A few automatic tools and several non-trivial results exist:
  - MG5aMC
  - Sherpa+OpenLoops
  - Sherpa+Recola

  giving consistent results. For example for ttH:

<table>
<thead>
<tr>
<th>Condition</th>
<th>Sherpa+Recola</th>
<th>MG5_AMC@NLO</th>
<th>Sherpa+OpenLoops</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{EW}^{NLO}$ [fb]</td>
<td>$\delta_{EW}$ [%]</td>
<td>$\delta_{EW}$ [%]</td>
<td>$\delta_{EW}$ [%]</td>
</tr>
<tr>
<td>inclusive</td>
<td>356.7(2)</td>
<td>$-1.2(2)$</td>
<td>$-1.4$</td>
</tr>
<tr>
<td>$p_T,t/\ell/H &gt; 200$ GeV</td>
<td>12.244(3)</td>
<td>$-8.5(1)$</td>
<td>$-8.5$</td>
</tr>
<tr>
<td>$p_T,t/\ell/H &gt; 400$ GeV</td>
<td>0.3435(3)</td>
<td>$-14.1(2)$</td>
<td>$-13.9$</td>
</tr>
<tr>
<td>$p_T,H &gt; 500$ GeV</td>
<td>1.7798(9)</td>
<td>$-11.7(1)$</td>
<td>$-11.6$</td>
</tr>
<tr>
<td>$</td>
<td>y_H</td>
<td>&gt; 2.5$</td>
<td>5.035(3)</td>
</tr>
</tbody>
</table>
**EW corrections**

Full automation ⇒ a wide spectrum of processes is available

[Frederix et al. 1711.XYWZ]

<table>
<thead>
<tr>
<th>Process</th>
<th>Syntax</th>
<th>LO Cross section (pb)</th>
<th>NLO Cross section (pb)</th>
<th>$\delta_{EW}(%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$pp \to e^+\nu_e$</td>
<td>$p \ p &gt; e^+ , \nu_e , QCD=0 , QED=2 , [QED]$</td>
<td>$5.2499 \pm 0.0006 \cdot 10^3$</td>
<td>$5.2113 \pm 0.0006 \cdot 10^3$</td>
<td>$-0.74 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+\nu_e j$</td>
<td>$p \ p &gt; e^+ , \nu_e , j , QCD=1 , QED=2 , [QED]$</td>
<td>$9.1468 \pm 0.0012 \cdot 10^2$</td>
<td>$9.0449 \pm 0.0014 \cdot 10^2$</td>
<td>$-1.11 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+\nu_e jj$</td>
<td>$p \ p &gt; e^+ , \nu_e , j , j , QCD=2 , QED=2 , [QED]$</td>
<td>$3.1557 \pm 0.0003 \cdot 10^2$</td>
<td>$3.0983 \pm 0.0006 \cdot 10^2$</td>
<td>$-1.82 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+e^-$</td>
<td>$p \ p &gt; e^+ , e^- , QCD=0 , QED=2 , [QED]$</td>
<td>$7.5370 \pm 0.0009 \cdot 10^2$</td>
<td>$7.5004 \pm 0.0011 \cdot 10^2$</td>
<td>$-0.49 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+e^- j$</td>
<td>$p \ p &gt; e^+ , e^- , j , QCD=1 , QED=2 , [QED]$</td>
<td>$1.5059 \pm 0.0001 \cdot 10^2$</td>
<td>$1.4909 \pm 0.0002 \cdot 10^2$</td>
<td>$-1.00 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+e^- jj$</td>
<td>$p \ p &gt; e^+ , e^- , j , j , QCD=2 , QED=2 , [QED]$</td>
<td>$5.1502 \pm 0.0004 \cdot 10^1$</td>
<td>$5.0482 \pm 0.0008 \cdot 10^1$</td>
<td>$-1.98 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+e^-\mu^+\mu^-$</td>
<td>$p \ p &gt; e^+ , e^- , \mu^+ , \mu^- , QCD=0 , QED=4 , [QED]$</td>
<td>$1.2353 \pm 0.0001 \cdot 10^2$</td>
<td>$1.1696 \pm 0.0003 \cdot 10^2$</td>
<td>$-5.32 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to e^+\nu_e\mu^-\nu\mu$</td>
<td>$p \ p &gt; e^+ , \nu_e , \mu^- , \nu , \mu , QCD=0 , QED=4 , [QED]$</td>
<td>$5.0649 \pm 0.0005 \cdot 10^{-1}$</td>
<td>$5.2511 \pm 0.0010 \cdot 10^{-1}$</td>
<td>$+3.68 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to H e^+\nu_e$</td>
<td>$p \ p &gt; h , e^+ , \nu_e , QCD=0 , QED=3 , [QED]$</td>
<td>$6.7736 \pm 0.0001 \cdot 10^{-2}$</td>
<td>$6.4979 \pm 0.0009 \cdot 10^{-2}$</td>
<td>$-4.07 \pm 0.01$</td>
</tr>
<tr>
<td>$pp \to H e^+ e^-$</td>
<td>$p \ p &gt; h , e^+ , e^- , QCD=0 , QED=3 , [QED]$</td>
<td>$1.4573 \pm 0.0001 \cdot 10^{-2}$</td>
<td>$1.3719 \pm 0.0002 \cdot 10^{-2}$</td>
<td>$-5.86 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to H jj$</td>
<td>$p \ p &gt; h , j , j , QCD=0 , QED=3 , [QED]$</td>
<td>$2.8270 \pm 0.0003 \cdot 10^{-2}$</td>
<td>$2.7076 \pm 0.0004 \cdot 10^{-2}$</td>
<td>$-4.22 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to W^+W^-W^+$</td>
<td>$p \ p &gt; W^+ , W^- , W^+ , QCD=0 , QED=3 , [QED]$</td>
<td>$8.2864 \pm 0.0005 \cdot 10^{-1}$</td>
<td>$8.8088 \pm 0.0013 \cdot 10^{-2}$</td>
<td>$+6.21 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to ZZW^+$</td>
<td>$p \ p &gt; Z , Z , W^+ , QCD=0 , QED=3 , [QED]$</td>
<td>$1.9872 \pm 0.0001 \cdot 10^{-2}$</td>
<td>$2.0188 \pm 0.0003 \cdot 10^{-2}$</td>
<td>$+1.59 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to ZZZ$</td>
<td>$p \ p &gt; Z , Z , Z , QCD=0 , QED=3 , [QED]$</td>
<td>$1.0763 \pm 0.0001 \cdot 10^{-2}$</td>
<td>$0.9743 \pm 0.0002 \cdot 10^{-2}$</td>
<td>$-9.47 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to H ZZ$</td>
<td>$p \ p &gt; H , Z , Z , QCD=0 , QED=3 , [QED]$</td>
<td>$2.1007 \pm 0.0003 \cdot 10^{-3}$</td>
<td>$1.9162 \pm 0.0003 \cdot 10^{-3}$</td>
<td>$-8.78 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to H ZW^+$</td>
<td>$p \ p &gt; H , Z , W^+ , QCD=0 , QED=3 , [QED]$</td>
<td>$2.4408 \pm 0.0000 \cdot 10^{-3}$</td>
<td>$2.4809 \pm 0.0005 \cdot 10^{-3}$</td>
<td>$+1.64 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to HHW^+$</td>
<td>$p \ p &gt; H , H , W^+ , QCD=0 , QED=3 , [QED]$</td>
<td>$2.7827 \pm 0.0001 \cdot 10^{-4}$</td>
<td>$2.4259 \pm 0.0027 \cdot 10^{-4}$</td>
<td>$-12.82 \pm 0.10$</td>
</tr>
<tr>
<td>$pp \to HHZ$</td>
<td>$p \ p &gt; H , H , Z , QCD=0 , QED=3 , [QED]$</td>
<td>$2.6909 \pm 0.0003 \cdot 10^{-4}$</td>
<td>$2.3921 \pm 0.0003 \cdot 10^{-4}$</td>
<td>$-11.10 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to t\bar{t}W^+$</td>
<td>$p \ p &gt; t , \bar{t} , W^+ , QCD=2 , QED=1 , [QED]$</td>
<td>$2.4108 \pm 0.0002 \cdot 10^{-1}$</td>
<td>$2.3013 \pm 0.0003 \cdot 10^{-1}$</td>
<td>$-4.54 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to t\bar{t}Z$</td>
<td>$p \ p &gt; t , \bar{t} , Z , QCD=2 , QED=1 , [QED]$</td>
<td>$5.0456 \pm 0.0006 \cdot 10^{-1}$</td>
<td>$5.0025 \pm 0.0007 \cdot 10^{-1}$</td>
<td>$-0.85 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to t\bar{t}H$</td>
<td>$p \ p &gt; t , \bar{t} , H , QCD=2 , QED=1 , [QED]$</td>
<td>$3.4481 \pm 0.0004 \cdot 10^{-1}$</td>
<td>$3.5098 \pm 0.0005 \cdot 10^{-1}$</td>
<td>$+1.79 \pm 0.02$</td>
</tr>
<tr>
<td>$pp \to jjj$</td>
<td>$p \ p &gt; j , j , j , QCD=0 , QED=0 , [QED]$</td>
<td>$7.9644 \pm 0.0010 \cdot 10^{0}$</td>
<td>$7.9479 \pm 0.0020 \cdot 10^{0}$</td>
<td>$-0.21 \pm 0.03$</td>
</tr>
<tr>
<td>$pp \to tj$</td>
<td>$p \ p &gt; t , j , QCD=0 , QED=2 , [QED]$</td>
<td>$1.0618 \pm 0.0001 \cdot 10^{2}$</td>
<td>$1.0543 \pm 0.0002 \cdot 10^{2}$</td>
<td>$-0.71 \pm 0.02$</td>
</tr>
</tbody>
</table>
Considerations and open issues:

• Knowledge of EW corrections is typically essential in high-pT tails ⇒ affects the accuracy of the predictions
• Evidence that real weak-boson radiation is well described by fixed-order computations
• Matching with the PS not available yet in general (it is for DY in POWHEG for example) but no road-block
• Computation of mixed QCD-EW corrections will be needed to reliably assess uncertainties
• Other open questions?
BSM simulations

- Well-tested and proven easy and robust path to BSM simulations: FeynRules → UFO → Matrix Element generator (MG5aMC, Sherpa, HW7) → LHEF → PS

- User-driven FeynRules Database of New Physics models continuously updated and enriched

- NLO+PS for BSM brings additional complications:
  - Renormalization of the $\mathcal{L}_{\text{NP}}$ needs to be performed and in case of use of numerical loop techniques the full set of counterterms is needed. Use NLOCT.
  - At NLO, processes mix with LO resonant contributions and in order to keep NLO accuracy in inclusive samples a MC friendly procedure to subtract real resonant diagrams must be in place (or a full off-shell computation should be available).
  - If non-renormalizable operators appear, such as in the EFT, higher-dimensional rank in the integrals appear as well as extra UV divergences and full mixing RGE are needed.

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Considerations and open issues:

- Most of the well-known NP signatures and simplified models can be achieved or are already available at NLO+PS with current technology.
- Models giving exotic signatures (see current long-lived particle searches) might need dedicated efforts. This will always be the case. *Should new physics models with special needs start to be addressed now?*
- “Precision” new physics searches and interpretations (such as EFT) builds up on SM accurate and precise predicition. Dedicated efforts to bring SMEFT to NLO accuracy in QCD. *Systematic effort for EW corrections needed.*
- Dark model searches (and the DMWG) are teaching us a lot on various MC issues too, such as the advantages of having common ATLAS and CMS NP samples.
- Fast and efficient parameter space scanning might become an issue.
MC Challenges : Technicalia

- Efficient generation for SM mass production (tails vs bulk)
- Built-in event-by-event reliable estimation of the uncertainties
- New techniques and improved accuracy/precision imply negative weights
- MVAs and New Analysis techniques
- New Physics parameter scanning (UV models, Simplified Models, EFT)
- Legacy and recasting tools
- …
Generating tails efficiently: bias functions

Usual technique used to generate samples over wide ranges, is to slice the phase space in $n$ mutually excluding domains (like $p_T$ intervals) and make $n$ independent generations.

1 nb * 3000 fb-1 = 3 billions top pairs in the full dataset
Generating tails efficiently: bias functions

An alternative approach is to bias the event generation directly at the start, with a suitable function.

These two plots were both obtained from 10k events, but for the right-hand side one, the matrix elements have been biased by the quantity. Now available at NLO accuracy in MG5aMC [Frederix, Hirschi, Mattelaer, 2017]. See documentation HERE.

Do other MCs have similar features? Are they general enough for all needs?
Uncertainties:

Short-distance cross section:
\( \mu_H, \mu_f^H, \text{PDF}^H, \alpha_s^H \)

Parton shower:
\( \mu_q^{PS}, \mu_T^{PS}, \mu_f^{PS}, \mu_{cut}^{PS}, \text{PDF}^{PS}, \alpha_s^{PS} \)

Multiple interactions:
\( \mu_q^{MPI}, \text{PDF}^{MPI}, \alpha_s^{MPI} \ldots \)

...correlated with:
\( \mu_f^H \) with shower starting scale
\( \mu_f^H, \text{PDF}^H \) with MPI
\( \mu_q^{PS}/\mu_f^H \) and \( \text{PDF}^{PS}/\text{PDF}^H \)
\( \mu_T^{PS}/\mu_T^H \) and \( \alpha_s^{PS}/\alpha_s^H \) for NLO+PS
\( \mu_{cut}^{PS} \) with “string \( p_\perp \)” & “primordial \( k_\perp \)”
\( \alpha_s^{MPI} \) and \( \alpha_s^{PS} \)
\( \alpha_s^{MPI} \) and “string tension”

Tough to describe all, let alone satisfactory uncertainty. Usual approach:
One set of scales \( \oplus \) one PDF \( \oplus \) one tune & **uncorrelated uncertainties**
Uncertainties: the power of reweighting

Goal:

Evaluate on the fly correlated and uncorrelated uncertainties (scales, PDF, parametric) on event-by-event basis by reweighting at no “extra” computing/storage cost.

Available Results:

aMC@NLO : Short distance scales + PDF uncertainties  [2011]
POWHEG : Short distance scales + PDF uncertainties     (available)
Sherpa: Short distance scales + PDF + Shower/alphas scale in PS [2015]
HW7: Shower/alphas scale in PS [2016]  [2016]
Pythia8: Shower/alphas scale in PS  [2016]
Uncertainties: the power of reweighting

reweighting the parton showers: $\alpha_S$ & PDF variations


- shower Sudakov depends on $\alpha_S$ & PDFs
- accept/reject probability
- need to reweight all acceptances/rejections
  
  $P_{\text{acc}} \rightarrow q P_{\text{acc}}$
  
  $P_{\text{rej}} = 1 - P_{\text{acc}} \rightarrow 1 - q P_{\text{acc}}$
  
  with $q \equiv \frac{\alpha'_S}{\alpha_S} \cdot \frac{f_2^I(x/z)/f_2^S(x)}{f_2^I(x/z)/f_2^B(x)}$

no shower emission reweighted

SHERPA NLOPS

pp $\rightarrow W[\text{jet}], \sqrt{s} = 13$ TeV

no emission reweighted

on-the-fly evaluation of ME & PS $\alpha_S$, PDF and scale uncertainties

takes only factor of $\mathcal{O}(1)$ more time wrt to standard single run
Uncertainties: the power of reweighting

**Reweighting the parton showers: \( \alpha_S \) & PDF variations**


- shower Sudakov depends on \( \alpha_S \) & PDFs
- \( \sim \) accept/reject probability
- need to reweight all acceptances/rejections
  
  \[ P_{\text{acc}} \rightarrow q P_{\text{acc}} \]
  \[ P_{\text{ rej}} = 1 - P_{\text{ acc}} \rightarrow 1 - qP_{\text{ acc}} \]
  
  with \( q \equiv \frac{\alpha'_S}{\alpha_S} \cdot \frac{f_a'(x/z)/f_b'(x)}{f_a(x/z)/f_b(x)} \)

\( \swarrow \) on-the-fly evaluation of ME & PS \( \alpha_S \), PDF and scale uncertainties

\( \swarrow \) takes only factor of \( \mathcal{O}(1) \) more time wrt to standard single run
Aside: Negative weights

- Negative weighted events have become a common feature of many techniques. A blessing (opened the door to NLO+PS) and a curse at the same time.
- POWHEG has been constructed to reduce to a minimum the relevance of negative weights. However, MC@NLO (used in Sherpa and MG5aMC) method, ALL NLO merging techniques (FxFx, MENLOPS,MINLO) feature negative events.
- In some cases, the fraction of negative events can become prohibitive (>30-40%) for large scale MC productions.
- PS@NLL also features negative weights.
- Problem could become even more serious at NNLO+PS@NLL…

Q3: Will this feature become a roadblock for mass production at the HL-LHC?
Possible improvement: reweight LHE events to different gluino masses.

Method: Use the conformal phase space mapping à la RAMBO [Kleiss, Stirling and Ellis, 1986] to generate weighted samples with different masses [being explored by O. Mattelaer, 2017]
Improving mass scans

Reduces the number of LHE files/events needed and facilitates the book-keeping.
MC Challenges : Computing

- Grid evolution
- Exploitation of new computing architectures (MIP, GPU’s, QC?)
- Exploitation of new ML techniques
- Efficient storage and retrieval of samples (going beyond the LHE format?)
- Common New Physics MC samples for both experiments
- ...

MCnet
New architectures

MadGraph (LO) on GPU

Sherpa and MG5aMC on HPC
- First steps for usage of general-purpose MC on HPC made
- Good experience with fixed-order calculations, which always repeat the same, simple computational task
- Current best performance at ~100 – 1000 cores per job (different at different orders, NNLO requires $O(10 – 100)$ more)
- Effort under way to design and write HPC-capable parton-level MC generator (recycling only algorithms)

Unweighted particle-level event generation more intricate, as program flow and memory usage both unpredictable (MC!)
- We’d appreciate an increase in L2 cache much more than an increase in the number of vector units
- But can still work well with what industry is giving us, No need to redesign particle-level part of simulation just combine with HPC-capable parton-level code when ready

[Hagiwara et al 200920092013]

Loss of gain when complexity increases.

Overall, quite limited experience. Should we think about a MC optimal architecture?

Talk by @StefanHoeche at CPAD
Using DNN to integrate over phase space

[J. Bendavid arXiv:1707.00028]

<table>
<thead>
<tr>
<th>Algorithm</th>
<th># of Func. Evals</th>
<th>$\sigma_w / &lt;w&gt;$</th>
<th>$\sigma_I / I$ (2e6 add. evts)</th>
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<tbody>
<tr>
<td>VEGAS</td>
<td>300,000</td>
<td>2.820</td>
<td>$\pm 2.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>Foam</td>
<td>3,855,289</td>
<td>0.319</td>
<td>$\pm 2.3 \times 10^{-4}$</td>
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<tr>
<td>Generative BDT</td>
<td>300,000</td>
<td>0.082</td>
<td>$\pm 5.8 \times 10^{-5}$</td>
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<tr>
<td>Generative BDT (staged)</td>
<td>300,000</td>
<td>0.077</td>
<td>$\pm 5.4 \times 10^{-5}$</td>
</tr>
<tr>
<td>Generative DNN</td>
<td>294,912</td>
<td>0.083</td>
<td>$\pm 5.9 \times 10^{-5}$</td>
</tr>
<tr>
<td>Generative DNN (staged)</td>
<td>294,912</td>
<td>0.030</td>
<td>$\pm 2.1 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 1. Performance comparison for integration of the 4-dimensional camel function between VEGAS, Foam, and the new BDT and DNN-based integration algorithms. The comparison shows the number of function evaluations required to train or construct grids for each algorithm, the resulting integration weight variance for further generated samples after training/grid construction, and the achievable integral precision with 2 million additional samples. The “staged” configurations refer to the case where integration is performed by sampling from the corresponding regression model, with the generative BDT or DNN used only to perform a secondary unweighting and integration of the regression approximation.
Conclusions and Outlook

• Challenges for the LHC will appear at three levels: Physics, Technicalia, Computing.

• From the physics point of view, a lot of progress is expected in hot topics such as NNLO computations in QCD and improving the shower accuracy to NLL. Expectations are high, yet breakthroughs will be necessary to achieve the goals.

• Event-by-event reweighting (LO and NLO) has imposed itself as the best way to maximise the information (from uncertainties to parameter scanning) contained in single samples and is already widely used.

• New computing technologies [hardware (parallel architectures) or software (ML, AI)] have the potential to change the way we simulate events at LHC and should be investigated.
Thanks

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