MC’s for top physics:
Matrix Elements and NLO with Parton Showers

Fabio Maltoni
Center for Particle Physics and Phenomenology
Université Catholique de Louvain
Why top?
Top as a link to BSM

Definition of naturalness: less than 90% cancellation:

\[ \Lambda_t \lesssim 3 \text{ TeV} \quad \Lambda_W \lesssim 9 \text{ TeV} \quad \Lambda_H \lesssim 12 \text{ TeV} \]

* One can actually prove that this case in model independent way, i.e. that the scale associated with top mass generation is very close to that of EWSB.
Our AIM is twofold:

I. Measure all properties (mass, couplings, spin) to establish indirect evidence for SM and BSM physics.

Examples: precision EW and QCD ($m_{\text{top}}, \sigma(tt), \sigma(t)$);
Rare decays and anomalous couplings. CP violation.

II. Use top as direct probe of the EWSB sector and BSM physics

Examples: SM $ttH$; BSM: $Z'$ and $W'$ resonances; SUSY: $tH^+$ and $t \rightarrow bH^+$ or stop $\rightarrow t X$. 
Top as a template

Both involve production of heavy colored states decaying through a chain into jets, leptons and $E_T$. 
Top as a template

Both involve production of heavy colored states decaying through a chain into jets, leptons and $E_T$. 
Top as background

At the LHC, many measurements will need a good understanding and control of $t\bar{t}$ and single top events.

A few examples:

- $gg \rightarrow H$ and $qq \rightarrow Hqq$ with $H \rightarrow WW$
- $t\bar{t}$ in single top measurements
- $t\bar{t}+jets$ and $t\bar{t}bb$ in $t\bar{t}H$
- $t\bar{t}+jets$ in SUSY/UED searches (gluino pairs, stop pairs, $tH^+$,....)
- .....
Why MC’s?
The role of MC’s in the path to discovery

1. Fully exclusive description for rich and energetic final states (multi-jets + EW and QCD particles (W,Z, photon,b,t) with flexible MC to be validated and tuned to control samples. Accurate predictions (NLO,NNLO) for standard candles SM cross sections.

2. Inverse problem tools (Ex: OSET)

3. Simulation of any BSM signature: from models to events in an easy and fast way.

4. Accurate predictions for cross sections of selected models (Ex: SUSY) to identify couplings. Accurate predictions for primary couplings (Ex: spectra calculators).

5. Accurate ME based description for final state distributions which keeps all the relevant information (Ex. decay chain with spin).

6. Off-shell effects, Matrix Element methods, Global fits (Ex: Sfitter)
Plan

- Overview
- Matrix Element + Parton Shower
- NLO + Parton Shower
- MC for New Physics
- Conclusions
1. High-$Q^2$ Scattering

2. Parton Shower

3. Hadronization

4. Underlying Event
1. High-$Q^2$ Scattering

where new physics lies

- process dependent

- first principles description

- it can be systematically improved

2. Parton Shower

3. Hadronization

4. Underlying Event
1. High-$Q^2$ Scattering

QCD - "known physics"
- universal/ process independent
- first principles description

2. Parton Shower

3. Hadronization

4. Underlying Event
1. High-$Q^2$ Scattering
2. Parton Shower

- low $Q^2$ physics
- model dependent

3. Hadronization
4. Underlying Event
How we (used to) make predictions?

First way:

• Include higher order terms in our fixed-order calculations (LO→NLO→NNLO...)

  \[ \hat{\sigma}_{ab \rightarrow X} = \sigma_0 + \alpha_S \sigma_1 + \alpha_S^2 \sigma_2 + \ldots \]

• Just us the tree-level results for many partons final states

Comments:

1. The theoretical errors systematically decrease.
2. Pure theoretical point of view.
3. A lot of new techniques and universal algorithms are developed.
4. Final description only in terms of partons and calculation of IR safe observables ⇒ not directly useful for simulations
How we (used to) make predictions?

Second way:

- Describe final states with high multiplicities starting from $2 \rightarrow 1$ or $2$ procs, using parton showers, and then an hadronization model.

Comments:

1. Fully exclusive final state description for detector simulations.
2. Normalization is very uncertain
4. Improvements are only at the model level.
How to improve our predictions?

New trend: TH & EXP

Match fixed-order calculations and parton showers to obtain the most accurate predictions in a detector simulation friendly way!

Two directions:

1. Get fully exclusive description of many parton events correct at LO (LL) in all the phase space.

2. Get fully exclusive description of events correct at NLO in the normalization and distributions.
MC tools for top physics in a nutshell

- ME+PS
  - Herwig
  - Pythia
  - SingleTop, TopRex
  - Phantom
  - AcerMC
  - GRAPPA
  - CompHEP

- ME+PS+merging
  - Alpgen
  - MadGraph
  - Sherpa

- NLO+PS
  - MC@NLO
  - POWHEG
Always the FIRST tools. Main purpose is to provide an easily tunable description of the data.

Complete exclusive description of the events: hard scattering, showering & hadronization, underlying event

Significant and intense progress in the development of new showering algorithms with the final aim to go at (N?)NLO [Bauer, Schwartz, 2006; Giele, Kosower, Skands, 2007; Krauss, Schumman, 2007; Bauer, Tackman, Thaler, 2008]. Example: Working implementation for ARIADNE based on dipoles.

N.B. Apart from SHERPA, which provides its own PS, all other ME codes rely on Pythia or HERWIG for PS, hadro and UE. This is true also for NLO codes (MC@NLO and POWHEG).
MC tools for top physics in a nutshell

Optimized for a few or several processes. Based on a library of matrix elements (analytic or numeric). Limited in breath but easy to use, and optimal for specific studies. For example, pp>tt>6f studies. Some of them are localized in a specific exp collaboration.
Multipurpose Matrix Element creators and generators. Calculations are automatic at tree level. Matching is performed with the parton shower to produce inclusive multi-jet samples. Some codes (Alpgen) are optimized for multi-parton ME. Some codes are suitable for BSM physics.
MC tools for top physics in a nutshell

- ME+PS
  - Herwig
  - Pythia
  - SingleTop, TopRex
  - Phantom
  - AcerMC
  - GRAPPA
  - CompHEP

- ME+PS+merging
  - Alpgen
  - MadGraph
  - Sherpa

- NLO+PS

- MC@NLO
  - POWHEG

Combine NLO accuracy in normalization and shapes of hard radiation with parton shower. “Best” tools when NLO calculation is available (i.e. low jet multiplicity). Current limitation is manual work ⇒ small libraries. Only SM.
Matrix Element based MC's

Includes all possible subprocess leading to a given multi-jet final state automatically or manually (done once for all)

"Automatically" generates a code to calculate $|M|^2$ for arbitrary processes with many partons in the final state.

Most use Feynman diagrams w/ tricks to reduce the factorial growth [MadGraph, SHERPA], others have recursive relations to reduce the complexity to exponential [Alpgen, HELAC, Comix].

\[
\begin{align*}
d\bar{d} & \rightarrow a\ a\ u\ u\ g \\
d\bar{d} & \rightarrow a\ a\ c\ c\ g \\
s\bar{s} & \rightarrow a\ a\ u\ u\ g \\
s\bar{s} & \rightarrow a\ a\ c\ c\ g 
\end{align*}
\]
Integrate the matrix element over the phase space using a multi-channel technique and using parton-level cuts.

Events are obtained by unweighting. These are at the parton-level. Information on particle id, momenta, spin, color and mother-daughter is given in the Les Houches format.
Events in the LH format are passed to the showering and hadronization ⇒ high multiplicity hadron-level events

Parton-Jet merging (MLM or CKKW) happens here!

Events in stdhep format are passed through fast or full simulation, and physical objects (leptons, photons, jet, b-jets, taus) are reconstructed.
ME/PS matching

Approaches are complementary!

Two recipes available: CKKW and MLM
Available Codes with ME+PS matching

Hard scale Physics

- ALPGEN
- HELAC
- MG/ME
- AMEGIC++

Matching Schemes

MLM “family”
- Event rejection after PS
- Cone or Kt clustering

CKKW “family”
- Sudakov reweighting
- Veto on showers
- Kt clustering

Showering

- HERWIG
- PYTHIA
- ARIADNE
- SHERPA
$W^\pm + \text{jets}$ comparison plots: Jet $E_T$ for LHC

[J. Alwall et al., arXiv:0706.2569]
Sanity checks: differential jet rates

\[ \text{tt} + 2 \text{ partons} + \text{PS} \]
\[ D(2 \to 1) > Q_{\text{cut}} \]

\[ \text{tt} + 1 \text{ parton} + \text{PS} \]
\[ D(2 \to 1) < Q_{\text{cut}} \]
Sanity checks: differential jet rates

Jet rates are:
* smooth at the cutoff scale
* independent of the cutoff scale
Sanity checks: differential jet rates

Jet rates are:
* smooth at the cutoff scale
* independent of the cutoff scale
Sanity checks: differential jet rates

Jet rates are:
* smooth at the cutoff scale
* independent of the cutoff scale
A MC Shower like Pythia is by construction a highly tunable tool. Consider for instance the pt distribution of the second jet with different settings:
A MC Shower like Pythia is by construction a highly tunable tool. Consider for instance the $p_T$ distribution of the second jet with different settings:

In a matched sample these differences are irrelevant since the behaviour at high $p_T$ is described by the matrix element ⇒ more predictive power (= less flexibility...)

Uncertainties in the matching itself not included.
Comparisons: 1st jet rapidity

[Mangano, Moretti, Piccinini, Treccani, 2007]

\[ P_{T}^{>20 \text{ GeV}} \]

\[ P_{T}^{>50 \text{ GeV}} \]

\[ P_{T}^{>150 \text{ GeV}} \]

[Alwall, de Visscher, 2007]

\[ P_{T}^{>20 \text{ GeV}} \]

\[ P_{T}^{>50 \text{ GeV}} \]

\[ P_{T}^{>150 \text{ GeV}} \]
Comparisons: 1st jet rapidity

[Graph 1: Distribution of jet rapidity vs. transverse momentum (pt) for 'CKKW 1+1+1 jet', 'Apacic++ 2.0', and 'no int. shower'.]

[Graph 2: Distribution of non-heralded jet rapidity (\eta_{non-b-jet}) vs. rapidity (\eta) for 'CKKW 1+1+1 jet', 'Apacic++ 2.0', and 'no int. shower'.]
It seems that indeed both Pythia and Herwig develop a deep in the central rapidity region for high-pt jets, which is filled by ME+PS. Hard radiation in MC@NLO is not able to fill it, while POWHEG as a similar behaviour as ME+PS. It will be interesting to see what tt+1jet at NLO predicts (ongoing...)

Still a lot to learn by comparing different approaches!
To remember about the ME-PS matching

- It provides an algorithm to generate multi-jet inclusive samples, that are accurate in all the areas of the phase space avoiding double-counting.

- The matching (à la CKKW) has been rigorously proved in e+e- collisions and it is believed to be true also in pp collisions. The MLM matching is problematic in e+e- and just a prescription in pp, where, however, seems to work really well.

- At this stage there is a fair amount of tuning/checking/validation to make it work and evaluation of the systematics is still subject study.

- Since no exact virtual contributions are included the normalization of the cross section for each jet multiplicity is formally LO and therefore uncertain. Normalization has to be obtained from a NLO calculation.

- On the other hand, shapes and often jet rates are (so far) in very good agreement with NLO.

- Fast progress: new studies/proposals/developments every day.
NLOwPS
Problem of double counting becomes even more severe at NLO
* Real emission from NLO and PS has to be counted once
* Virtual contributions in the NLO and Sudakov should not overlap

Current available (and working) solutions:

**MC@NLO** [Frixione, Webber, 2003; Frixione, Nason, Webber, 2003]
- Matches NLO to HERWIG angular-ordered PS.
- “Some” work to interface an NLO calculation to HERWIG.
  - Uses only FKS subtraction scheme.
- Some events have negative weights.
- Sizable library of procs now.

**POWHEG** [Nason 2004; Frixione, Nason, Oleari, 2007]
- Is independent from the PS. It can be interfaced to PYTHIA or HERWIG.
- Can use existing NLO results.
- Generates only positive unit weights.
- For top only ttbar (with spin correlations) is available so far.
* Soft/Collinear resummation of the $p_T^{(tt)} \to 0$ region.
* At high $p_T^{(tt)}$ it approaches the $tt+$parton (tree-level) result.
* When $\Phi^{(tt)} \to 0$ the emitted radiation is hard and $tt$-parton result.
ttbar: MC@NLO vs POWHEG

Good agreement for all the observables. Sometimes noticeable differences appear that can be ascribed to the different treatment of the higher terms. More exhaustive studies would be welcome.
**m_{tt} spectrum: low mass**

Tree-level production with a dynamical scale reproduces the shape MC@NLO result extremely well. Very stable observable.

It is always important to validate the MC used in an analysis with the best tool available so far!
MC challenges in single top

* All three processes available in MC@NLO, for arbitrary CKM matrix.

* At NLO t- and s-channel become interwined:

However, since the interference vanishes, their definition as independent procs poses no problems at NLO. Notice that (1) and (4) are not generated by a standard (=Pythia or Herwig) PS approach.

* Wtb coupling might hide interesting BSM physics [see Aguilar-Saavedra’s talk yesterday] => very important to keep spin correlations between production and decay

* Accurate description of the softer b in the t-channel and tW associated production is extremely important.
Spin correlation effects are non-negligible even in observables that are not specifically designed to measure them!
t-channel: pt of the 2\textsuperscript{nd} b

A correct prediction for the shape of the 2\textsuperscript{nd} b is extremely important to reject \(t\bar{t}b\) events, by imposing a jet veto.

Observation:

* Collinear gluon splitting better handled by the shower (explicit resummation)
* high pt tail better described by the ME 2→3

Pragmatic solution: [Boos et al., 2000]
t-channel: pt of the 2\textsuperscript{nd} b

A correct prediction for the shape of the 2\textsuperscript{nd} b is extremely important to reject ttbar events, by imposing a jet veto.

However, this kind of “hard cutoff” matching is clearly very crude and theoretically inconsistent (strong cutoff dependence, other distributions affected,..)
MC@NLO provides a consistent matching between $2 \rightarrow 2$ and $2 \rightarrow 3$. This is done assuming the b initially massless.

Expected behaviour reproduced: small pt PS, high pt ME.
Alternative consistent approach (at LO) in AcerMC. [Hinchliffe and Keservan, 2006]

However, this procedure builds on the assumption that the massless PS describes well the IS collinear splitting into a massive quark pair at low pt....

On-going study on the $2 \rightarrow 3$ NLO massive calculation [see F. Tramontano’s talk]
tW in MC@NLO

[Frixione, Laenen, Motylinski, Webber, White, YESTERDAY]

b-initiated process like t-channel ⇒ same issue with the pt of the 2nd b.

Interference with tt at NLO ⇒ non trivial problem: definition of the process is at stake [Tim Tait: (2000), A. Belyaev & E. Boos (2001)].

First MC viable solution proposed [Campbell, FM, Willenbrock, LH 2005] and implemented in MCFM [Campbell, Tramontano, 2006].

However, interference is tamed with a (b-)jet veto ⇒ sensitivity to low pt partons ⇒ soft resummation
⇒ MC with PS and with NLO needed.

Result: tW can be defined in

* a MC-friendly way
* (de facto) non-ambiguous way.

First pheno consistent LHC study in progress.
To remember about the NLOwPS

MC@NLO [Frixione, Nason, Webber, 2003] is the standard code with a library of SM processes.

POWHEG [Frixione, Nason, Oleari, 2007] is a recent addition with a much smaller library at the moment.

“Best” tools when NLO calculation is available (i.e. low jet multiplicity).

Main points:
1. NLOwPS provide a consistent to include K-factors into MC’s
2. Scale dependence is meaningful
3. Allows a correct estimates of the PDF errors.
4. Non-trivial dynamics beyond LO included for the first time.

N.B. : The above is true for observables which are at NLO to start with!!!

Current limitations: Considerable manual work for the implementation of a new process and only SM.

$\mathcal{L} + ME + PS$
Preliminary observation

• For new physics associated to top, two approaches are possible:
  ▶ top-down (e.g., model parameter scanning)
  ▶ bottom-up (e.g., inverse problem, OSET)

• Different strategies lead to different MC tools.

• Some of the MC tools of the new generation (e.g. MadGraph and SHERPA) allow to tackle both by featuring:
  1. Main templates for BSM models available (MSSM, 2HDM, UED,...)
  2. Easy implementation of new models (from Feynman rules)
  3. Any tree-level process available* (automatic code creation).
  4. Multi-jets samples with matching for QCD background (and possibly BSM signals).

*within reason.
Add-on for BSM

Invent a model, renormalizable or not, with new physics. Write the Lagrangian and get the Feynman Rules.

The particles content, the type of interactions and the analytic form of the couplings in the Feynman rules define the model at tree level.

Parameters Calculator. Given the “primary” couplings, all relevant quantities are calculated: masses, widths and the values of the couplings in the Feynman rules.

Caution: tree-level relations have to be satisfied to avoid gauge violations and/or wrong branching ratios.

Les Houches interface

SUSY, Little Higgs, Higgsless, GUT, Extra dimensions (flat, warped, universal,...)

FeynHiggs, ISAJET, NMHDdecay, SOFTSUSY, SPHENO, SUSPECT, SDECAY...
From Lagrangians to Events

Tools exist to derive Feynman rules and couplings directly from the Lagrangian and effortless implement in any MC.

LanHEP [Semenov]: Interfaces to FeynArts (for theorists) and CompHEP/CalcHEP.

FeynRules [Duhr and Christensen]: New tool providing a complete model building development framework and interfaces to several MC's.
Decay chains

Beware that most of the MC’s* make some of or all the following simplifications:

1. production and decay are factorized.
2. Spin is ignored.
3. Chains proceed only through $1 \rightarrow 2$ decays.
4. The narrow width approximation is employed.
5. Non-resonant diagrams are ignored.

* Spin correlations between production and decay are correctly accounted for by HERWIG in the narrow width approximation [Richardson 2005; Gigg & Richardson, 2008]
Decay chains

\[ gg > (g o > t \sim (t_1 > c \ nu_1 )) (g o > b \sim (b_1 > (b (n_2 > \mu^+ (\mu^- > \nu_1)))) ) \]

Most matrix element based MC's*:

1. Full matrix element is obtained which includes correlations between production and decays.

2. Spin of the intermediate states is kept.

3. One can go beyond 1→2 decays.

4. Resonances have BW.

5. Non-resonant contributions can be systematically included only where relevant.

6. BW information passed to the event record.

* As for instance in SHERPA [Krauss et al.,] and in MadGraph [Alwall and Stelzer, 2007]
Example 1: SUSY

\[ \tilde{g}\tilde{g} \rightarrow t\tilde{t}_1\tilde{t}^*_1, \ t\tilde{t}^*\tilde{t}^*_1, \ \bar{t}\tilde{t}_1\tilde{t}_1 \]

\[ m_{\tilde{t}_1} < m_t \]

\[ pp \rightarrow \tilde{g}\tilde{g} \rightarrow bbl^\pm l^\pm + \text{jets} + E_{\text{miss}}^T \]

\[ \tilde{t} \rightarrow c\tilde{\chi}_1^0 \]

Same-sign top quarks as a signature of light stops.

Typical SUSY inclusive signature: need for a very good control of the SM backgrounds (here Pythia).

The whole analysis can be now performed within one MC including matched samples for the signal and backgrounds.
Example II: New resonances

In many scenarios for EWSB new resonances show up, some of which preferably couple to 3rd generation quarks.

Given the large number of models, in this case is more efficient to adopt a “model independent” search and try to get as much information as possible on the quantum numbers and coupling of the resonance.

To access the spin of the intermediate resonance spin correlations should be measured.

It therefore mandatory for such cases to have MC samples where spin correlations are kept and the full matrix element $pp > X > tt > 6f$ is used.
Example II: KK gluons with SHERPA

Model from [Agashe et al., hep-ph/0612015]:
Randall-Sundrum model, with different profiles for SM fermions.
Non-universal couplings to SM particles: suppressed to light quarks, $\sim 1$ to $t_L$, enhanced to $t_R$.

MC trivial

MC non-trivial
Conclusions

- New MC tools are available that can provide an accurate description of both SM and BSM signals and backgrounds involving top:
  - Impressive progress in fixed-order and parton-shower matching both at LO (inclusive tt+jets samples) and NLO (tt in MC@NLO and POWHEG). First systematics comparison available.
  - Progress in the simulation of basically any new physics scenario’s involving top (MSSM, new resonances, vector-like partners, anomalous couplings,...)
- New and exciting possibilities of interaction between TH’s and EXP’s...
Take a look around
At all people everywhere
So much energy and excitement in the air
And the time is right
To get together with the people you know
So sing out loud and clear don't be afraid
To let the LHC start

Chorus:

Are you ready for it?
Rockin' steady for it
Are you ready for it?
Rockin' steady for it
Are you ready for it?

Madonna
Credits

Many thanks for providing material, physics insights or both to this talk:

Simon de Visscher, Stefano Frixione, Stefan Hoeche, Frank Krauss, Carlo Oleari, Steffen Schuman