Simulation/Modelling plans in RA3

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color meets flavor

Motivation

Will discuss 3 main areas (based on material I was sent):

- precision measurements limited by parton shower (PS) and hadronisation uncertainties
- deployment of new matrix-element generators and their expected improvements
- modelling in very specific phase-spaces (e.g. threshold region)

What are the limiting factors in the measurements?

Limiting factors in top mass analyses

	1D	2D
Uncertainty	Δm_{top} [GeV]	Δm_{top} [GeV]
Statistics	0.044 ± 0.000	0.046 ± 0.000
Method	0.008 ± 0.008	0.012 ± 0.008
Signal MC Generator	0.023 ± 0.020	0.031 ± 0.021
NNLO by 3D	0.058 ± 0.000	0.089 ± 0.000
LineShape	0.601 ± 0.023	0.591 ± 0.024
Hadronisation	0.067 ± 0.022	0.392 ± 0.023
ISR/FSR	0.600 ± 0.013	0.218 ± 0.014
Colour reconnection (CR1)	0.021 ± 0.048	0.043 ± 0.050
Underlying event	0.072 ± 0.032	0.040 ± 0.033
Parton density function	0.016 ± 0.000	0.014 ± 0.000
Single top modelling	0.077 ± 0.003	0.070 ± 0.004
Background-Norm	0.009 ± 0.000	0.007 ± 0.000
JES	0.688 ± 0.005	0.220 ± 0.004
JER	0.049 ± 0.003	0.081 ± 0.004
JVT	0.014 ± 0.000	0.002 ± 0.000
b-tagging	0.125 ± 0.001	0.118 ± 0.001
Lepton	0.058 ± 0.001	0.059 ± 0.001
MET	0.041 ± 0.000	0.037 ± 0.000
Pileup	0.096 ± 0.000	0.026 ± 0.000
Recoil effect	0.354 ± 0.024	0.353 ± 0.025
Tot syst (without recoil)	1.117 ± 0.015	0.802 ± 0.021
Tot syst (with recoil)	1.172 ± 0.016	0.877 ± 0.022
Total (with recoil)	1.172 ± 0.016	0.878 ± 0.022

Largest single effect:
* lineshape (hvq decay vs MadSpin decay),
* will be removed once we use bb4l as nominal
* full systematic model for bb4l developed by Katharina Voss (Siegen)

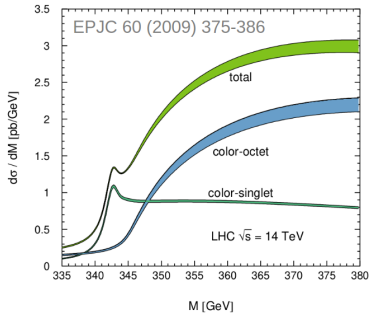
ATL-PHYS-PUB-2025-036

Hadronisation: Pythia vs. Herwig comparison, mainly from difference in W-boson mass here. Can be reduced by removing badly reconstructed events (cut on DNN output)

Recoil-to-b vs. recoil-to-top option in Pythia. Recoil-to-b is default setting (also used for b-tagging etc) in Run 2. Cannot be solved for ongoing mass analysis. Sherpa and Herwig also have similar settings

Mini-workshop Recoil

How does the threshold region look like at the LHC? EPJC 60 375-386,2009



- at threshold: non-perturbative regime, Coulomb-like interaction
  ↪ quark velocities low, described by non-relativistic QCD (NRQCD)
- colour singlet: ${}^1S_0^{[0]}$: attractive potential: $V(r) = -\frac{4}{3}\frac{\alpha_S}{r}$
  ↪ peak below production threshold
- colour octet: ${}^1S_0^{[8]}$: repulsive potential: $V(r) = \frac{1}{6}\frac{\alpha_S}{r}$
  ↪ little contribution below threshold

How can we model this pseudo-bound state? → CMS

arXiv:2507.05119

- non-relativistic Coulomb-like effects are not included in our normal simulation
- need a dedicated sample that simulates this process
- in first search from CMS: simple pseudo-scalar resonance η_t with MadGraph (LO):

  ↪ $m_\eta = 343$ GeV, $\Gamma_\eta = 7$ GeV
- updated by CMS after fitting simulation to calculation from Maria Garzelli et al:

  ↪ $m_\eta = 343$ GeV, $\Gamma_\eta = 2.8$ GeV
- colour singlet, no octet contribution

↪ will call this “simplified model” in the following

How can we model this pseudo-bound state? → ATLAS

arXiv:2601.11780

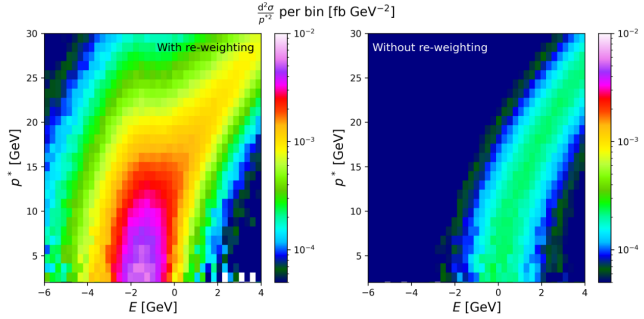
- use improved signal model developed by Fuks et al.:

  ↪ reweight matrix-elements from Madgraph (LO) using non-relativistic Greens function

$$|M|^2 \longrightarrow |M|^2 \left| \frac{\tilde{G}(E;p^*)}{\tilde{G}_0(E;p^*)} \right|^2$$

  ↪ terms $\propto$ first power in $\frac{\alpha_S}{v}$ are included in resummation

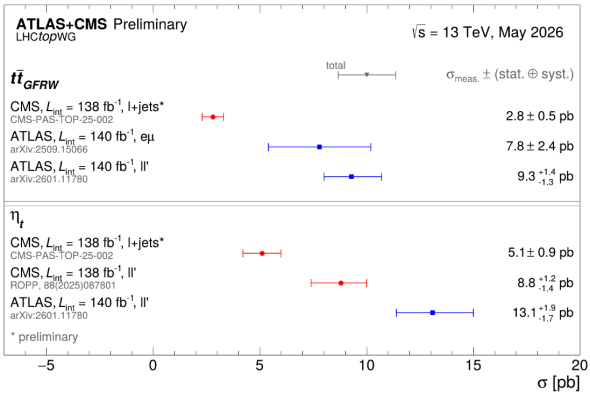
- include systematic uncertainties on NR-QCD process; $m = 173$ GeV and $\Gamma = 1.49$ GeV
- reweighting affects rate and shape:



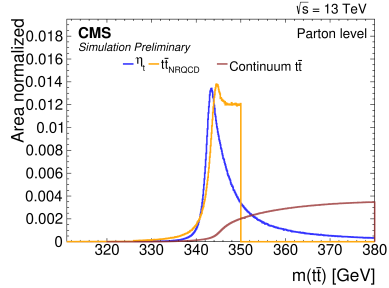
Publications Fuks et al:

- PRD 104, 034023 (2021)
- EPJC 85 (2025) 157
- arXiv:2505.03869
- arXiv:2509.03596
- arXiv:2511.02040

Comparison of “Toponium” results from ATLAS and CMS



➔ New single-lepton result by CMS included now also the GFRW: ▸ CMS-PAS-TOP-25-002

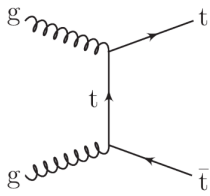


- observe smaller cross-sections for single-lepton channel than for dilepton
- observe smaller cross-sections when using Greens-function reweighting
  ↪ need to better understand phase space overlap
- what other effects play a role?

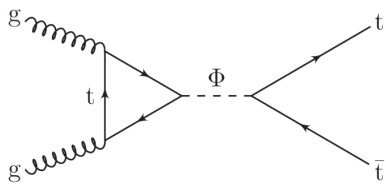
Why is region so important? → search for new physics

arXiv:2507.05119

SM top-pair production:



Potential heavy Higgs boson: decays also to $t\bar{t}$



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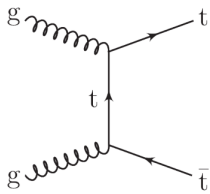

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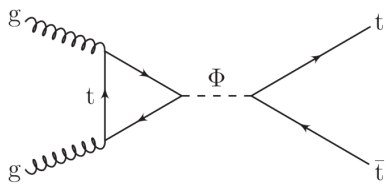
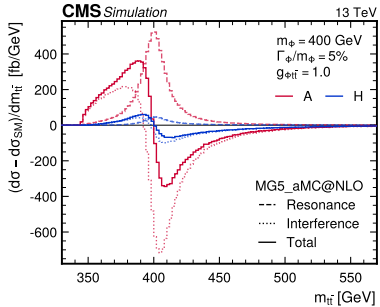
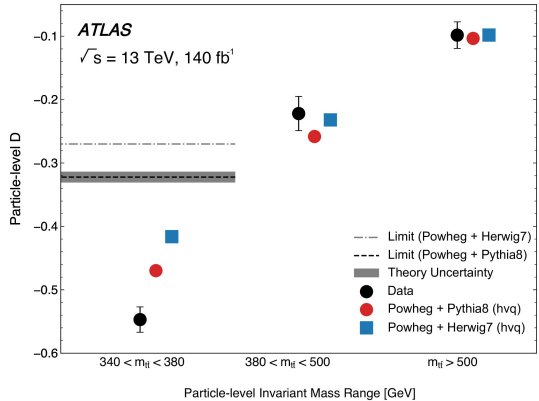


- heavy Higgs could be scalar/pseudo-scalar
  ↪ $t\bar{t}$ system would be in ${}^3P_0 / {}^1S_0$ state
- interferes with SM $t\bar{t}$ production
  ↪ causes peak-dip structure
- if SM modelling at low $m_{t\bar{t}}$ incomplete
  ↪ could misinterpret excess as new physics!



Why else is this region so important? → entanglement measurement

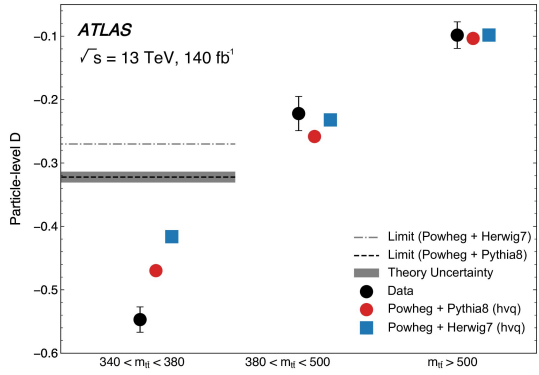
Nature 633 (2024) 542



Split dataset in 3 regions according to m(tt). Sign for entanglement: D < -⅓

Why else is this region so important? → entanglement measurement

Nature 633 (2024) 542

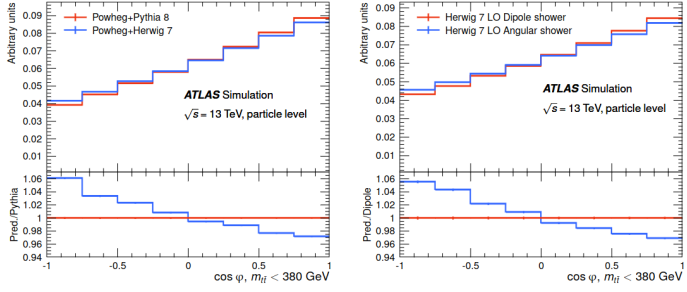


In threshold region:
observe entanglement, but see stronger effect in data than in simulation: are we missing something here?

Away from threshold,
no entanglement expected,
good agreement of simulation with data

What did we learn in this measurement?

- Simulation used is not optimal:
  - ↪ spin-correlation and top decays only simulated in leading order
  - ↪ spin correlation not propagated fully to the parton shower (when interfacing Powheg to PS)
  - ↪ larger difference between two algorithms Pythia 8 and Herwig 7
- Can be done potentially in the future in Herwig @NLO, would allow to fully propagate spin information to parton shower. Requires further development.



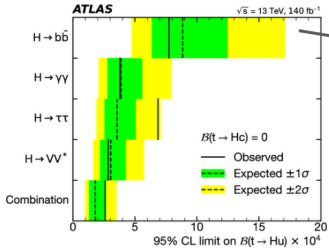
Slide from Carmen on $t\bar{t} + X$ modelling

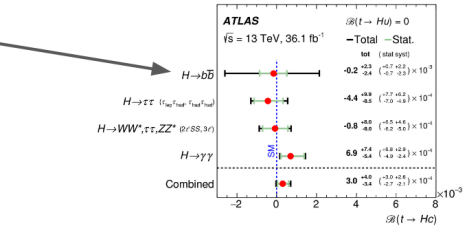
Link

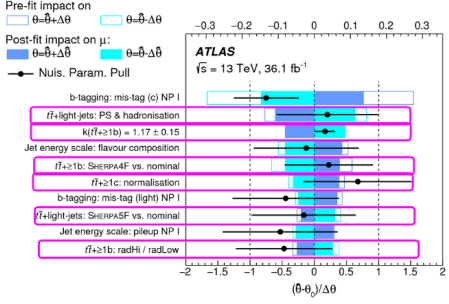
- Modelling of top+X crucial to improve measurements
  - ↪ Inclusive cross section measurements at 6% precision: refined uncertainty treatment unavoidable!
- Several MC generators used as nominal for $t\bar{t} + X$ processes:
  - ↪ $t\bar{t} + Z, t\bar{t} + \gamma$ (only 2 → 3 at NLO) and (LO): MadGraph5_aMC@NLO
  - ↪ $t\bar{t} + W$: Sherpa
  - ↪ Difficult to have a coherent set of uncertainties and correlate uncertainties in combined measurements
- $t\bar{t} + X, t + X$ EFT samples: Common samples with the same setup, UFO model!
- Caveats:
  - fixed QCD scales instead of dynamical scales like the SM samples
  - LO instead of NLO like most SM samples: (bin-by-bin) NLO/LO rescaling needed! (Assumes higher orders in EFT and SM scale similarly)
  - more see dedicated EFT talk later
- $t\bar{t}Z$ and $t\bar{t}\gamma$ processes: also need to handle the overlap with tWZ and $tW\gamma$

Search for FCNC in tHq (bb) in Siegen

Slides Ines Pinto







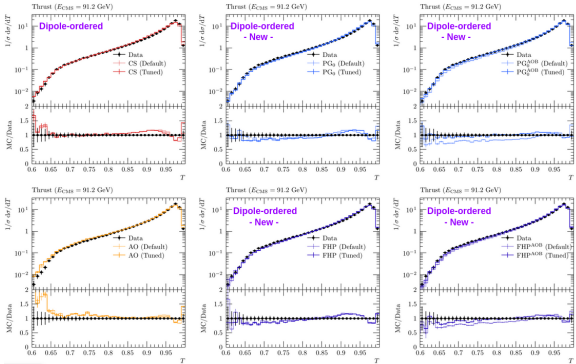
- Sensitivity of search limited by systematic uncertainty for H(bb) channel
- Systematic uncertainties strongly dominated by tt+HF and ttbar PS uncertainties

What are the theory developments in colour-meets-flavour?

Herwig generator: Group of Simon Plätzer (Siegen) – NLL PS and hadronisation

↪ higher accuracy in parton showers: need corresponding developments in hadronisation models

↪ relevant for RA3: top decays and jet-flavour tagging ▸ arXiv:2605.02622 ▸ Eur.Phys.J.C 85 (2025) 7, 796 ▸ JHEP 07 (2025) 005



Plot: two new dipole-shower algorithms with NLL accuracy: first tunes already performed

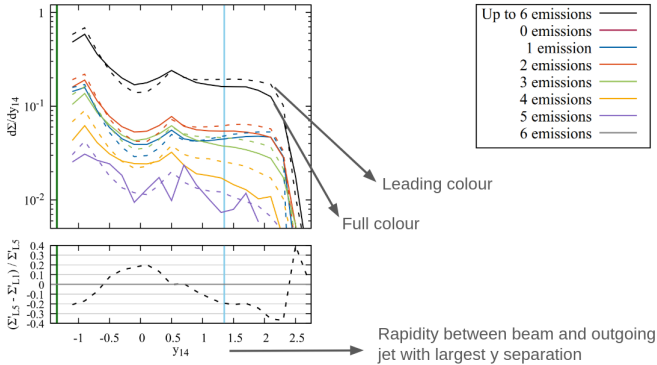
↪ further studies needed to understand the interplay between PS and hadronisation models

↪ room for collaboration with experiment also to understand effects on shower-ordering (example: spin/entanglement), recoil effects (example: top mass)

CVolver: Group of Simon Plätzer (Siegen) – Amplitude-level evolution

CVolver: simulation of parton showers at amplitude level

↪ can calculate cross-sections with exact colour evolution for jet observables [JHEP 02 (2026) 174] [JHEP 07 (2023) 126] [JHEP 09 (2025) 207]



↪ use jet x-sec where additional jets in defined phase-space are vetoed: study wide-angle, soft gluon radiation

↪ applications: vector-boson fusion, exclusive jet bins, etc

↪ currently purely a theory tool, will be made public this year

Whizard generator: Group of Wolfgang Kilian (Siegen)

Goal:

$\hookrightarrow$ produce Whizard predictions fo the LHC: $t\bar{t}$ and $t\bar{t} + X$ off-shell calculation and simulation at NLO + threshold

Already available for e^+e^- collisions JHEP 03 (2018) 184:

- complete description of the $t\bar{t}$ threshold
- off-shell events at NLO-QCD in the continuum, properly matched to the resummed NR-QCD result at threshold which results in toponium-like enhancement
- almost complete: validation of Whizard for off-shell $t\bar{t}$ production with shower matching at NLO-QCD, validated against $bb4\ell$ generator and LHC data
- NLO QCD and EW corrections

Started project theory/experiment (Siegen+Dortmund):

- complete the validation and fine-tune the current framework for top data
- adapt the existing e^+e^- top-threshold framework to the LHC environment
- apply the framework to $t\bar{t} + X$ processes ($t\bar{t} + \gamma$ and $t\bar{t} + Z$)

MiNNLOPS generator: Group of Marius Wiesemann (TU Dortmund)

New recursive parton-shower matching approach:

- NNLO+PS with NNLL
- inclusion of QCD and EW corretions
- N3LO+PS matching for Higgs production (and Drell Yan)

Relevant Processes for this subgroup (MiNNLO and new approach in future):

- $t\bar{t}$ @ NNLO+PS
- H @ NNLO+PS with complete mass effects (top exists, bottom and charm in progress)
- HH @ NNLO+PS with approximated mass effects
- ttH @ NNLO+PS
- other processes which exist for MiNNLO already: VH, $bb \to H$, bbH
- to be considered: ttZ, ttW, etc.

To-Do List for CmF topics

- What are the limiting factors in the Higgs sector and FCCee?
- Need a new FSR tune, current uncertainty too large when compared to recent measurements
  ↪ had a first study with Bachelor student at TU Dortmund, current efforts in ATLAS for new tune ongoing
- Need new tune for recoil-to-top (or any other new MC generator setup that is being developed in CmF):
  ↪ How are the tunes currently being handeled in the generator communities?
  ↪ Can we decide on a tuning setup together so we can make consistent comparisons?
- Are there specific measurements that the theorists would find most useful for tuning that we could measure?
- First efforts for theory+experiment collaborations already agreed upon (Whizard + LHC experiments)
- How can we work together on PS/hadronisation uncertainties that are limiting factors for many measurements?
- Spin/Interference/Off-shell/Threshold region are common themes in $t\bar{t}$ and $t\bar{t} + X$ analyses

Perfect time for CmF: large number of developments in Whizard, Herwig and MiNNLOPS, experiments currently planning new measurements, lets use this momentum!