GRANIITTI MC

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Reference; models, formulas
arXiv:1910.06300 [hep-ph], 80 pp

Code
github.com/mieskolainen/graniitti
35k+ lines of C++17, a few thousand in Python3 (tools)

Overview
mieskolainen.github.io

To automatically reproduce[1] **plots and tables, see scripts**:
.github/workflows/graniitti-install-generate-test.yml
and folder /**tests**

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[1] Modulo e.g. the soft tune differences between versions.

Alternatives for MC event generators?

No other way to do experimentally realistic (cuts included), *fiducial* simulations of arbitrary observables. Quantum computing (exponentially more efficient, in principle) not feasible yet, perhaps one day, but that will also include random sampling. Before that, Monte Carlo and deep learning enhanced Monte Carlo!

Which experiments?

Central exclusive (diffraction) measurements in

LHC: ATLAS+ALFA, CMS+TOTEM with forward protons; ALICE, LHCb without forward protons → forward veto aka 'Babinet's complement' ($\sqrt{s} = 7, 13$ TeV)

RHIC: STAR with forward protons ($\sqrt{s} = 0.2, 0.5$ TeV)

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LHC semi-exclusive $\pi^+\pi^-$ data

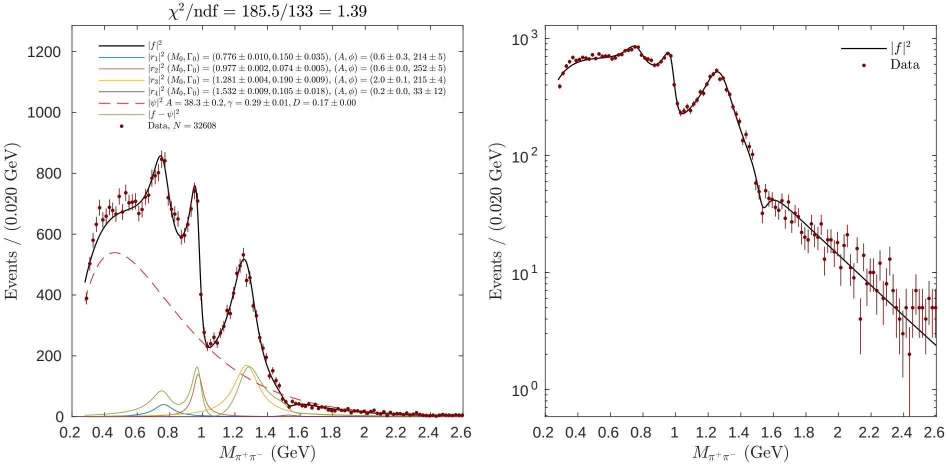


Figure: Semi-exclusive $\pi^+\pi^-$ data with forward veto at $\sqrt{s} = 7$ TeV in ALICE, and a simple analytical full spectrum fit (linear and log-scale). See details in my thesis CERN-THESIS-2020-152.

LHC semi-exclusive K^+K^- data

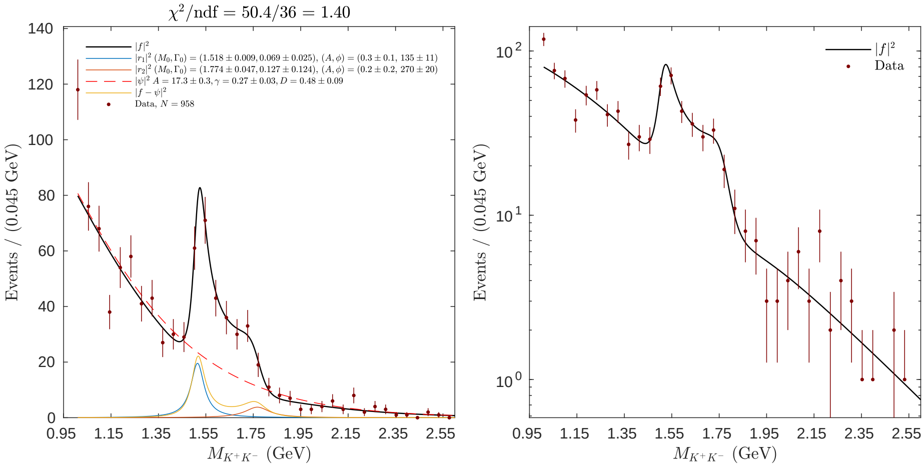


Figure: Semi-exclusive K^+K^- data with forward veto at $\sqrt{s} = 7$ TeV in ALICE, and a simple analytical full spectrum fit (linear and log-scale). See details in my thesis CERN-THESIS-2020-152.

How to do optimal efficiency corrections?

Maximally MC event generator independent efficiency corrections, especially suitable for exclusive measurents.

DeepEfficiency: a neural network, fully differential high-dimensional method over phase-space
MM, arXiv:1809.06101

Demonstrated in my thesis using full ALICE GEANT-simulations.

The philosophy can be extended further to do resolution (unfolding) type corrections. A grand challenge are purely data-driven neural corrections.

GRANIITTI physics scope

Designed for $pp \to p^{(*)} + X + p^{(*)}$, especially in Regge domain $|t_1|, |t_2| \ll s$ etc. Special emphasis on the non-perturbative production of system X (low-mass system) $\sim$ glueball domain physics.

Currently for proton-proton initial states. The software architecture easily generalizes to hadron-ion, lepton-hadron ... – future reservation.

Technology Overview

Written in C++17. Fully multithreaded code (max CPU core utilization). Standard grid computing support (pre-computed integration arrays, different random seeds). HepMC3(2) event output format.

- Standard methods: MC sampling in VEGAS (Lepage; dim-by-dim factorized importance sampling) & basic massive RAMBO (Kleiss, Stirling, Ellis; conformal transform based). Cutting edge development towards neural non-factorized chained Jacobian transforms [via so-called 'normalizing flows'] instead of e.g. manual 'multichannel' phase-space engineering.
- Soft Pomeron screening loop integrals computed numerically (interleaved within MC) event-by-event in the transverse momentum plane with exact momentum conservation in the vertices. Also, numerical integrals used for 2D-Fourier transforms between impact parameter $\vec{b} \leftrightarrow$ transverse momentum $\vec{p}_T$-space.
- Standard QFT kinematics x dynamics conventions followed, thus e.g. $\gamma\gamma$-driven scattering amplitudes can be imported from MadGraph 5 in C++ format.

Kinematics

- Kinematics of $2 \to N$ is first constructed to be exact for $2 \to 3$ process [lengthy polynomial expression due to three variable final masses, i.e. forward dissociation allowed] and sampled with VEGAS together with suitable analytic Jacobians.
- The central system phase space $1 \to N - 2$ is then further treated exactly with RAMBO, due to exact (recursive) phase space factorization. Alternatively, direct $2 \to N$ exact kinematic sampling via VEGAS, but mostly suitable for certain special amplitudes (not efficient enough).
- Arbitrary (cascaded) decay channels can be also generated according to Breit-Wigner × phase space. For $1 \to 2$ (+ sequential) spin dynamics is provided according to Jacob-Wick helicity amplitudes and user adjustable couplings.

Soft amplitudes / models available

All processes can be generated either with elastic or inelastic forward protons and screening/absortion loop on or off.

- "Eikonal Pomeron" ∼ (elastic 2 → 2 and all CEP screening/absorption loops)
- "Minimal Pomeron" ∼ (meson/baryon pair amplitudes, DIME MC like continuum amplitudes + Jacob-Wick helicity amplitudes for resonance decay + forward proton spin correlations, using numerical Wigner 3j algebra machinery, all spin combinations)
- "Tensor Pomeron" ∼ (fully covariant 2 → 4 amplitudes for meson/baryon pairs, continuum + resonances, using C++ template based Lorentz algebra [from numerical General Relativity, up to rank-4 + custom higher rank tensors] + Dirac spinor algebra)
- "Gribov/sliding helicity Pomeron" ∼ (technical prototype, implementation lacking unknown 3-point vertex-functions)

Model references

Harland-Lang, Khoze, Martin, Ryskin | Ewerz, Maniatis, Nachtmann | Lebiedowicz, Nachtmann, Szczurek ...

Example: 'Eikonal Pomeron' driven elastic scattering $\rightarrow$ used for the screening loops

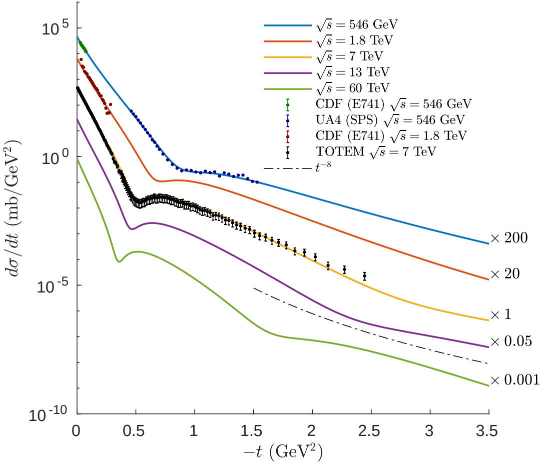


Figure: Mandelstam t-spectrum. See GRANIITTI paper for details.

Some 2-body processes

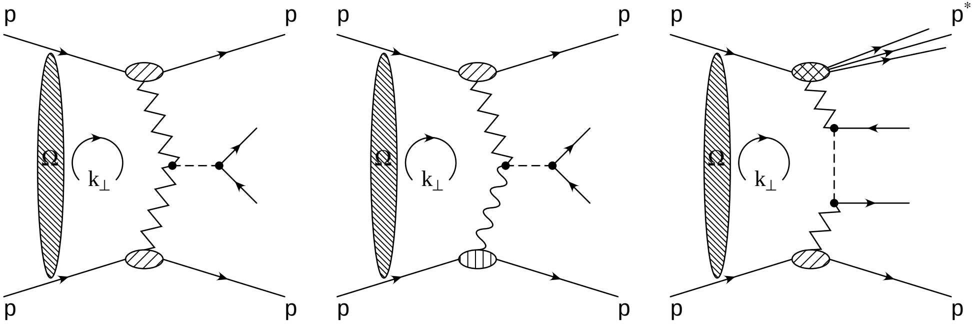


Figure: Pomeron-Pomeron-Resonance, Pomeron-Gamma-Resonance, Pomeron-Pomeron $\rightarrow$ central hadron pair + one excited forward proton p^*. k_T is the screening loop $2D$-momentum. See details in GRANIITTI paper.

Some 4-body processes

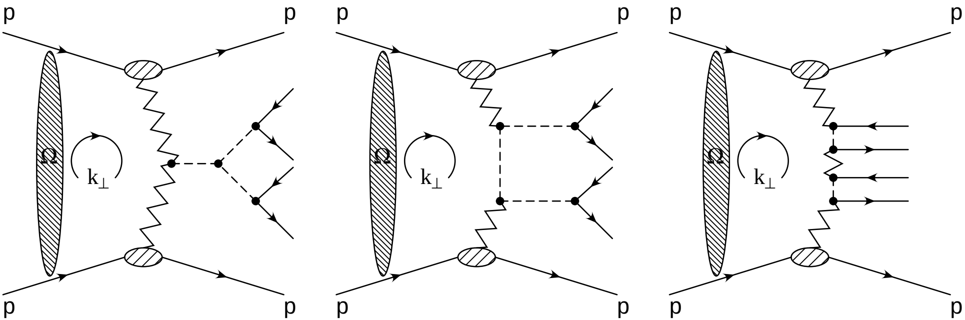


Figure: See details in GRANIITTI paper.

Example: 'Minimal Pomeron' driven resonances (Jacob-Wick helicity amplitudes)

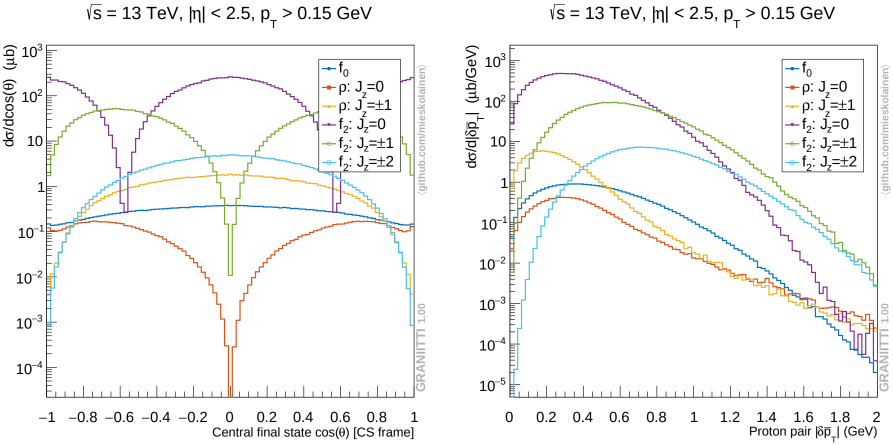


Figure: Angular distribution $\cos(\theta)$ of π^+ in the Collins-Soper frame for different (diagonal) spin polarization density components (left). Forward proton p_t-vector difference (right).

Example: 'Tensor Pomeron' driven spin-2 resonance components

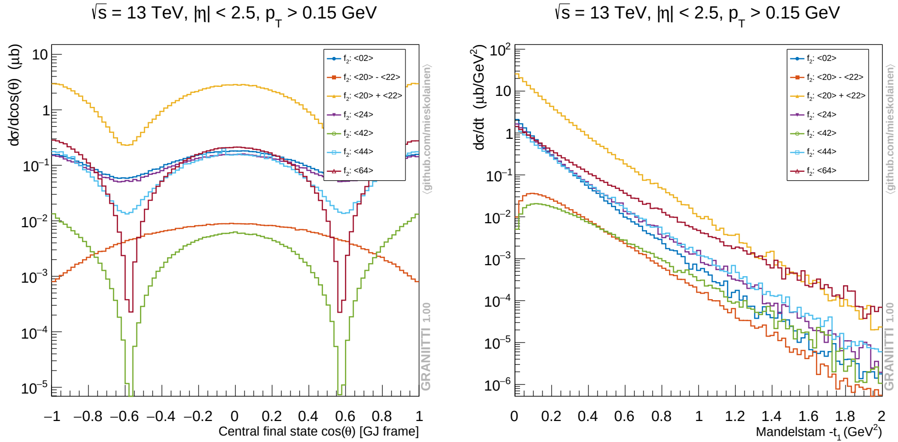


Figure: Angular distribution $\cos(\theta)$ of π^+ in the Gottfried-Jackson frame (left) and Mandelstam $-t_1$ for 7 different spin-2 couplings of the Tensor Pomeron model.

Free soft input parameters – Continuum

Eikonal Pomeron [elastic, and screening loop integral]

1. Proton (strong) form factor parameters [needed in all processes]
2. Non-linear Pomeron trajectory (α, α', pion loop form factor)
3. Proton-Pomeron coupling

Continuum sub-amplitude of Pomeron-Pomeron fusion to a hadron pair

1. Linear (affine) Pomeron trajectory (α, α')
2. Pomeron-Pion (Kaon, ...) couplings
3. Pion (Kaon) off-shell form factor choice (exponential, Orear, power-law ...) and its free parameters (1-2)

Free soft input parameters – Resonances

Pomeron-Pomeron-Resonance amplitude parameters [Minimal Pomeron]

1. Complex coupling (amplitude, phase)
2. Breit-Wigner propagator parameters (mass, width)
3. Leading structure of the polarization spin-density matrix [for example $J_z = 0$ vs $J_z = \pm 2$]

Pomeron-Pomeron-Resonance amplitude parameters [Tensor Pomeron]

1. Couplings [2 param for scalar/pseudoscalar/vectors, 7 param for spin-2 tensors]
2. Breit-Wigner propagator parameters (mass, width)

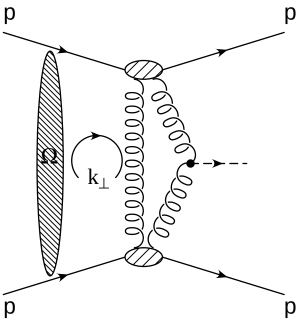
Branching Ratios

1. A given resonance BR to $\pi^+\pi^-, K^+K^-, \rho\rho$ etc. (using values from PDG)

And, briefly speaking, you can multiple the total number of parameters at least by 1.5 if you start adding other exchanges (Reggeons) than just Pomeron-Pomeron fusion.

Hard amplitudes available

- k_T-EPA $\gamma\gamma$-fluxes + Standard Model EW: $\gamma\gamma \to \ell^+\ell^-, W^+W^-$ ... (MadGraph 5 C++ amplitude export)
- Durham QCD $gg \to$ gluon/quark pair, meson pair production. Sudakov suppression integral factor and 'Shuvaev transformed' gluon pdfs based on numerical integral transforms; differential grids created automatically, cashed and hashed to disk and interpolated during the event-generation.



Model references

Durham QCD model

Elastic, single, double dissociative production of $pp \to p^{(*)} + \pi^+\pi^- + p^{(*)}$

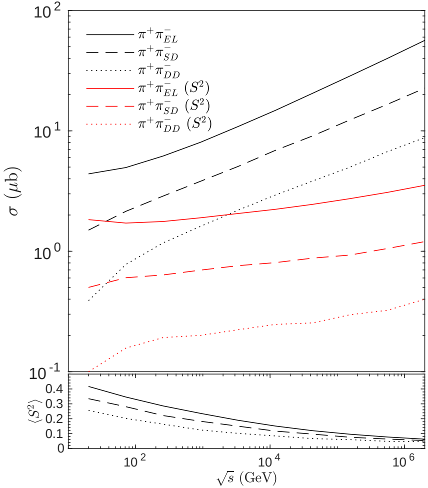


Figure: Integrated fiducial cross-sections without and with differential screening/absorption (S^2). See GRANIITTI paper for details.

Overview of cross-sections

			MEASUREMENT	GRANIITTI		
	$\sqrt{s}$	PHASE SPACE CUTS	value ± stat ± syst	σ_S	σ_0	$\langle S^2 \rangle$
gg	13	$\lvert y\rvert < 2.5$, $p_t > 20$ GeV		0.872	14.1 nb	0.06
$\pi^+\pi^-_{EL}$	7	$\lvert\eta\rvert < 0.9$, $p_t > 0.15$ GeV		3.84	19.6 μb	0.20
$\pi^+\pi^-_{SD}$	7	$\lvert\eta\rvert < 0.9$, $p_t > 0.15$, $M_1 < 5$ GeV		1.25	9.34 μb	0.13
$\pi^+\pi^-_{DD}$	7	$\lvert\eta\rvert < 0.9$, $p_t > 0.15$, $M_{1,2} < 5$ GeV		0.269	3.13 μb	0.09
$\pi^+\pi^-$	7	$\lvert Y_X\rvert < 0.9$		9.27	45 μb	0.21
$\pi^+\pi^-$	0.2	$\lvert\eta\rvert < 0.7$, $p_t > 0.2$ GeV		1.85	6.5 μb	0.28
W^+W^-	7	Full 4π		29.6	39 fb	0.76
e^+e^-	7	ATLAS [?]	0.428 ± 0.035 ± 0.018	0.462	0.494 pb	0.94
$\mu^+\mu^-$	7	ATLAS [?]	0.628 ± 0.032 ± 0.021	0.738	0.789 pb	0.94
$\pi^+\pi^-$	13	ATLAS (Thesis) [?]	18.75 ± 0.048 ± 0.770	20	106 μb	0.19
$\mu^+\mu^-$	13	ATLAS [?]	3.12 ± 0.07 ± 0.14	3.35	3.49 pb	0.96
e^+e^-	1.96	CDF [?]	1.6 ± 0.5 ± 0.3	1.65	1.74 pb	0.95
e^+e^-	1.96	CDF [?]	2.88 ± 0.57 ± 0.63	3.24	3.37 pb	0.96
$\pi^+\pi^-$	1.96	CDF [?]	† ± † ± †	1.93	8.96 μb	0.22
$\mu^+\mu^-$	7	CMS [?]	3.38 ± 0.58 ± 0.21	3.88	4.09 pb	0.95
$\pi^+\pi^-_{EL}$	7	CMS [?]	26.5 ± 0.3 ± 5.12	11.5	57 μb	0.20
$\pi^+\pi^-_{SD}$	7	$\lvert y\rvert < 2$, $p_t > 0.2$, $M_1 < 5$ GeV		3.77	28.6 μb	0.13
$\pi^+\pi^-_{DD}$	7	$\lvert y\rvert < 2$, $p_t > 0.2$, $M_{1,2} < 5$ GeV		0.851	9.4 μb	0.09
$\pi^+\pi^-_{EL}$	13	CMS [?]	19.0 ± 0.6 ± 3.2	14.6	80.2 μb	0.18
$\pi^+\pi^-_{SD}$	13	$\lvert\eta\rvert < 2.4$, $p_t > 0.2$, $M_1 < 5$ GeV		4.22	34.2 μb	0.12
$\pi^+\pi^-_{DD}$	13	$\lvert\eta\rvert < 2.4$, $p_t > 0.2$, $M_{1,2} < 5$ GeV		0.903	11 μb	0.08

Table: See GRANIITTI paper for details.

GRANIITTI vs STAR comparison of $pp \rightarrow p + \pi^+\pi^- + p$ *at* $\sqrt{s} = 0.2$ *TeV*

"Measurement of the central exclusive production of charged particle pairs in proton-proton collisions at 200 GeV with the STAR detector at RHIC." HEPData 1792394

Fiducial cuts as described in the STAR paper.

Partial tuning of GRANIITTI parameters done with ICETUNE (see details in Appendix).

MC comparison from the STAR paper

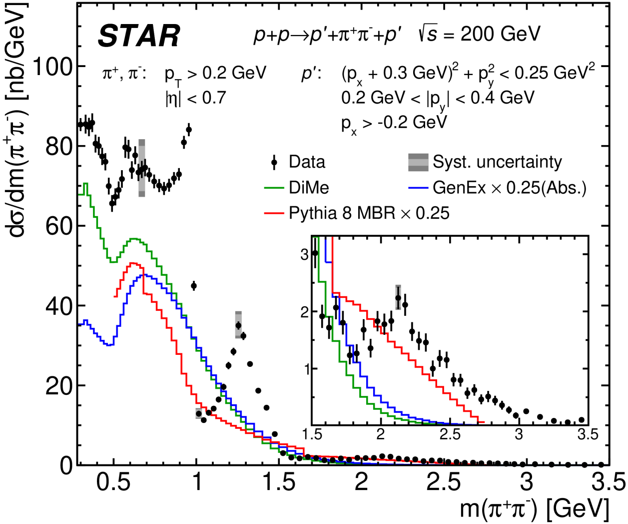


Figure: DIME MC, Pythia 8 MBR (×0.25), GenEx MC (×0.25) and STAR data.

GRANIITTI results

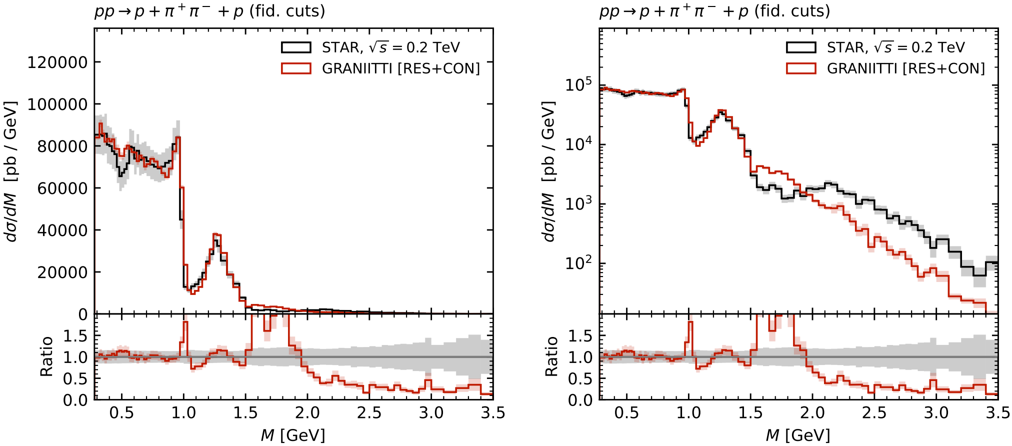


Figure: Central system invariant mass; linear-scale (left) and log-scale (right). Data includes statistical, systematic and luminosity uncertainties summed in quadrature. GRANIITTI results include statistical MC uncertainties.

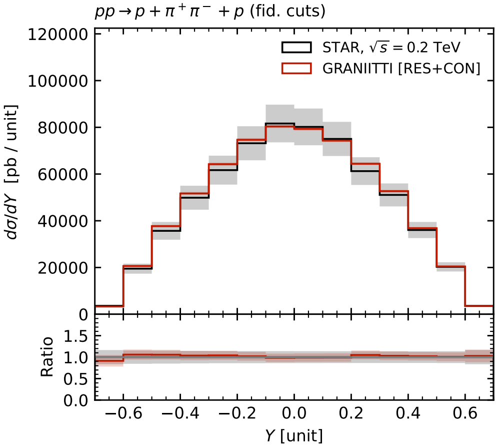


Figure: Central system rapidity.

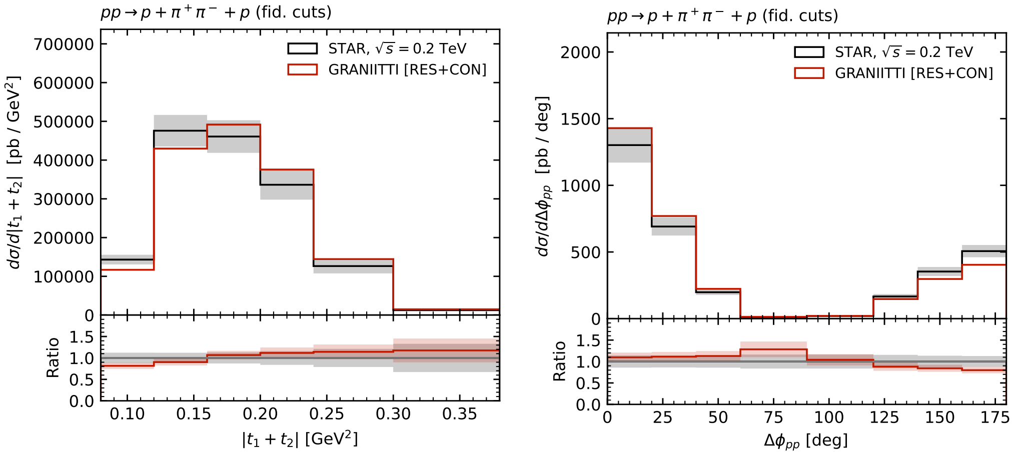


Figure: Absolute sum of Mandelstam t_1 and t_2 (left) and forward proton transverse angle separation (right).

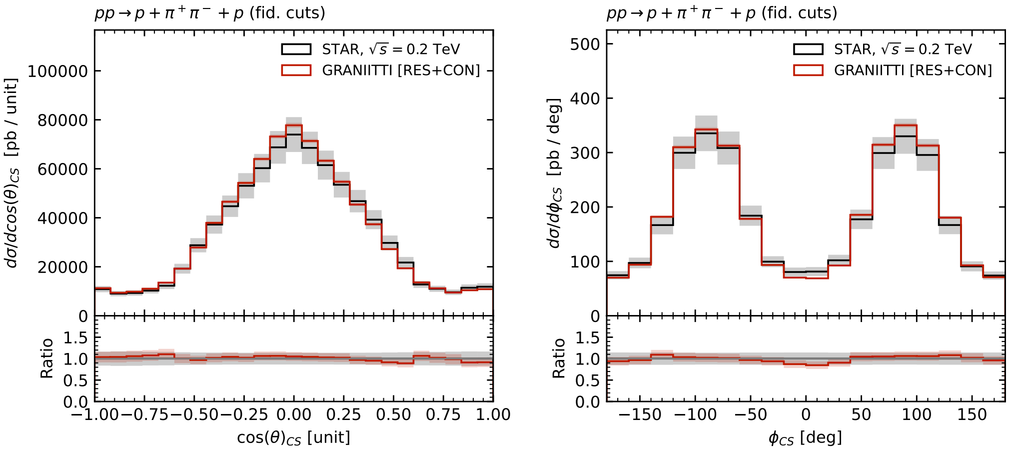
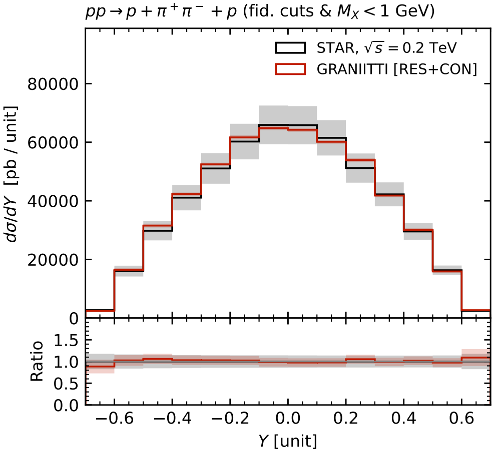


Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of π^+.

$pp \to p + \pi^+\pi^- + p$

with fid. cuts & $M_X < 1$ GeV



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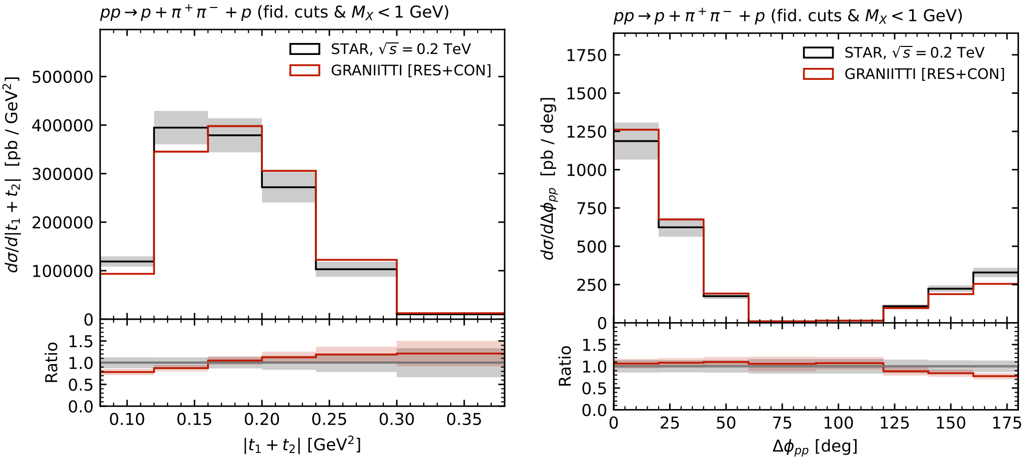


Figure: Absolute sum of Mandelstam t_1 and t_2 (left) and forward proton transverse angle separation (right).

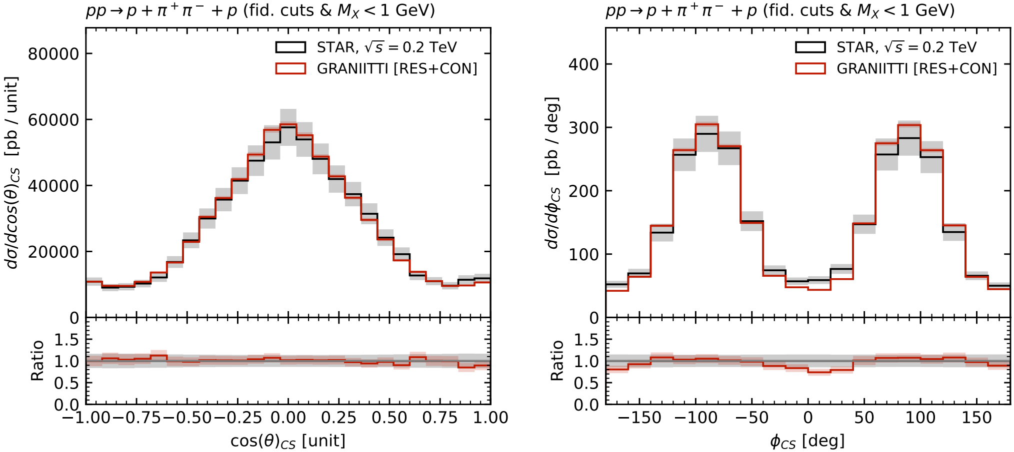
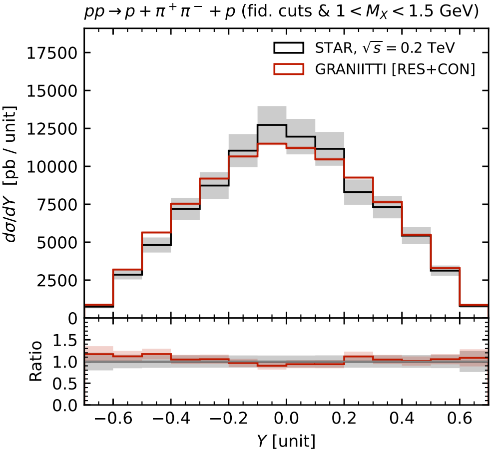


Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of π^+.

$pp \to p + \pi^+\pi^- + p$ with fid. cuts & $1 < M_X < 1.5$ GeV



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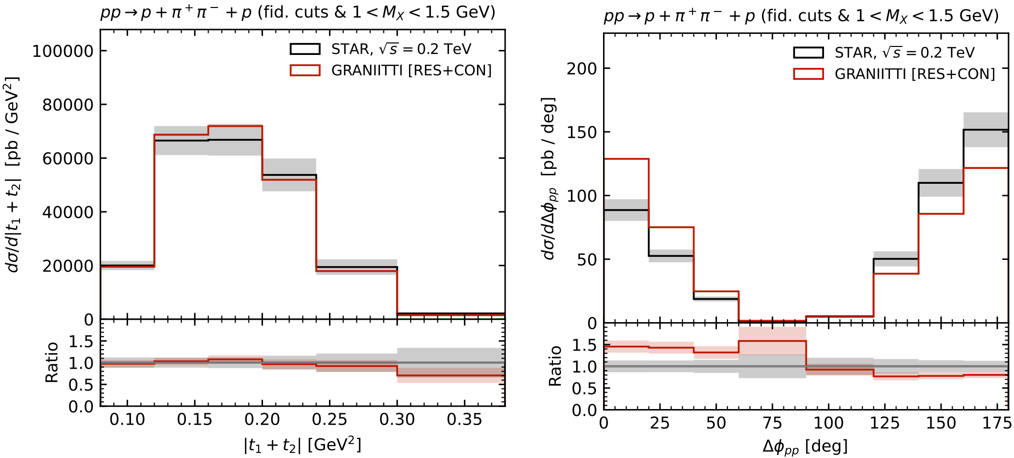

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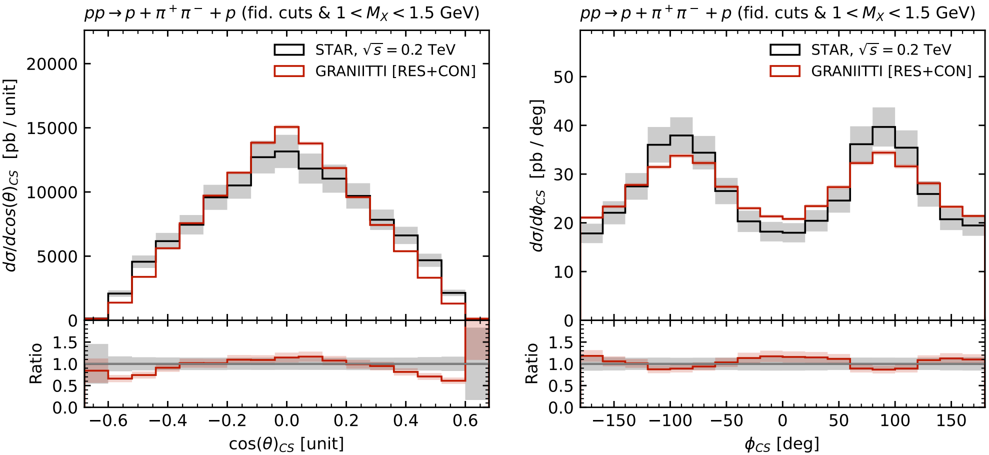
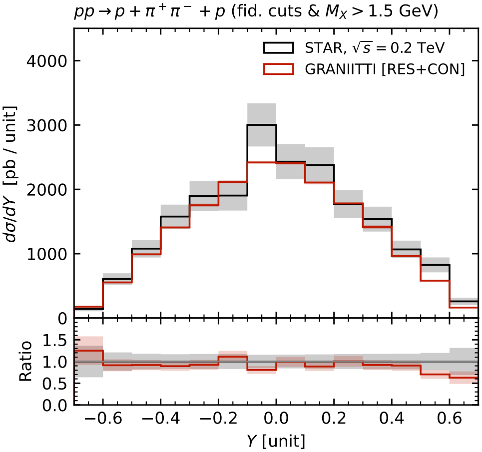


Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of π^+.

$pp \to p + \pi^+\pi^- + p$
with fid. cuts & $1.5 < M_X$ GeV



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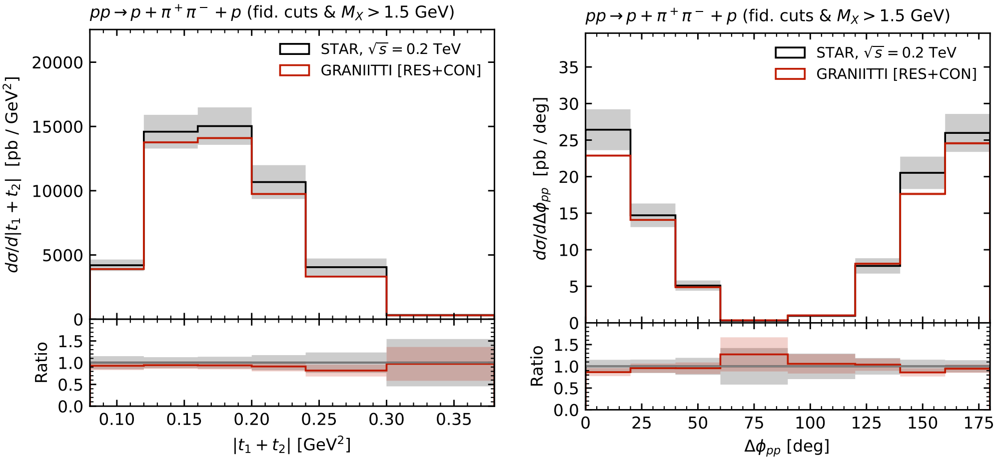

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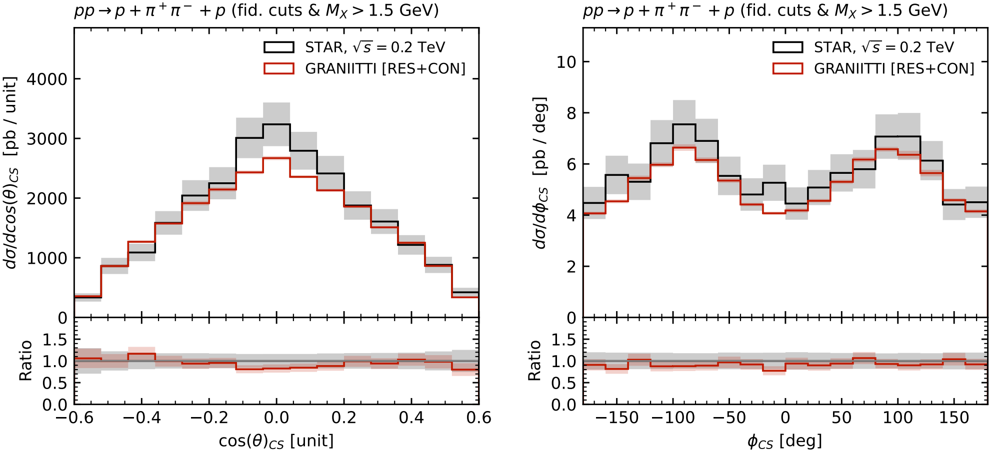


Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of π^+.

$pp \rightarrow p + \pi^+\pi^- + p$ with fid. cuts & $\Delta\phi_{pp} < 90^\circ$

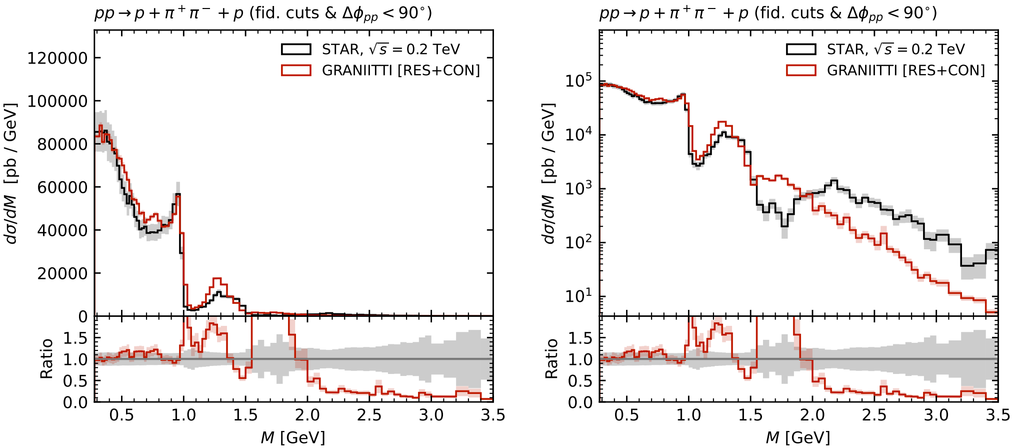


Figure: Central system invariant mass; linear y-scale (left) and log y-scale (right).

$pp \to p + \pi^+\pi^- + p$ with fid. cuts & $\Delta\phi_{pp} > 90^\circ$

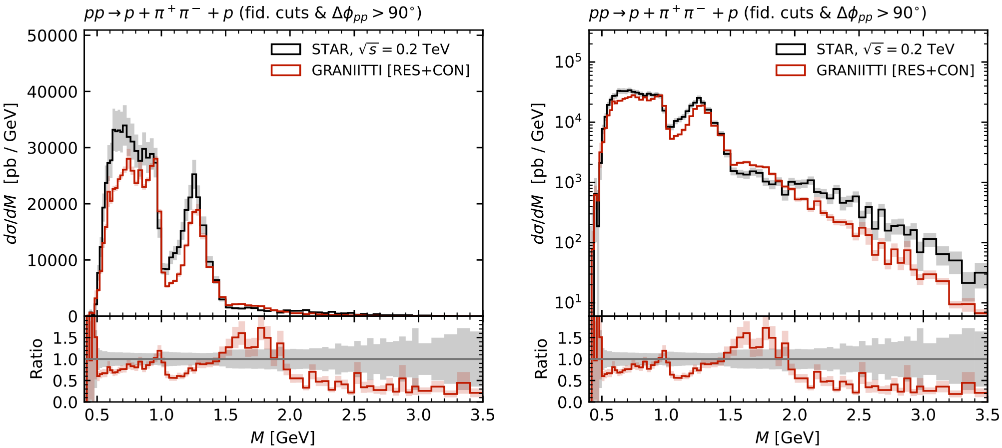
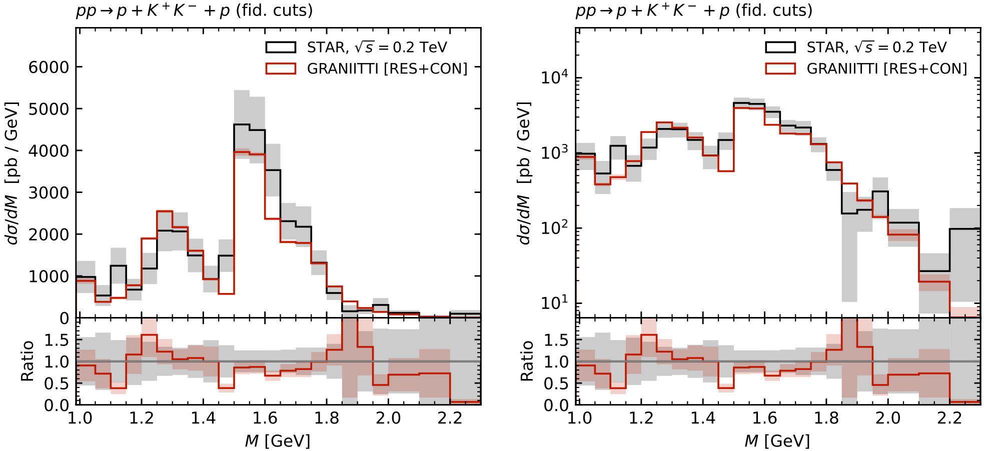


Figure: Central system invariant mass; linear y-scale (left) and log y-scale (right).

$pp \to p + K^+K^- + p$

with fid. cuts



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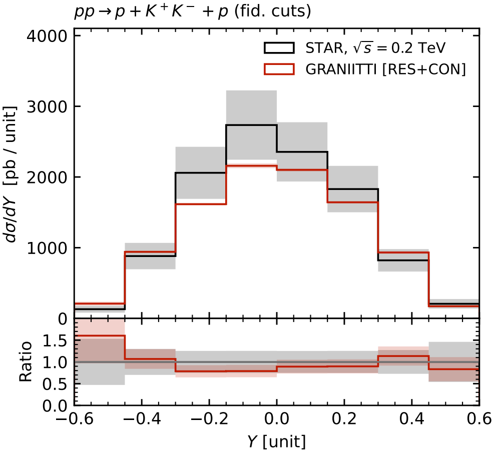

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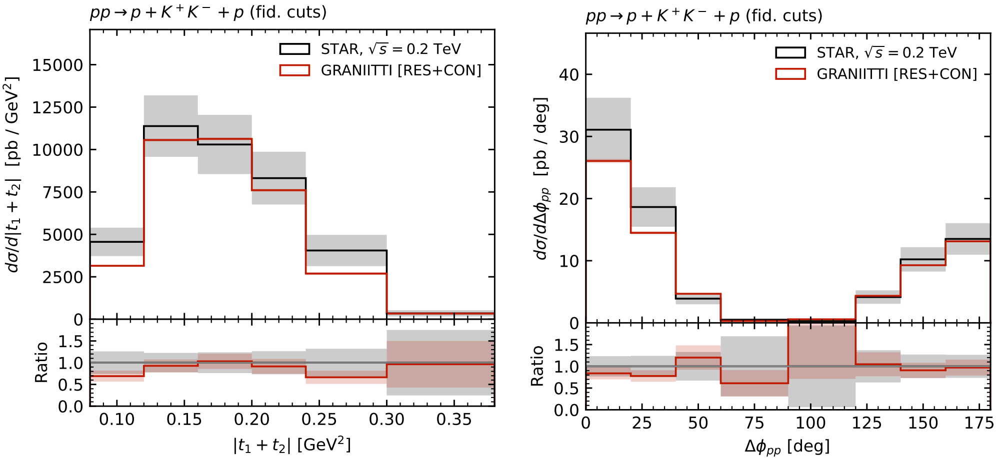

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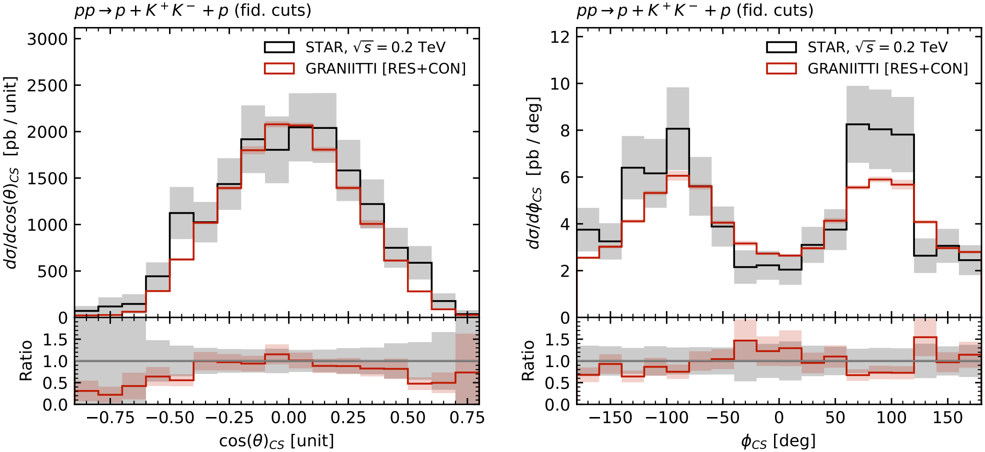
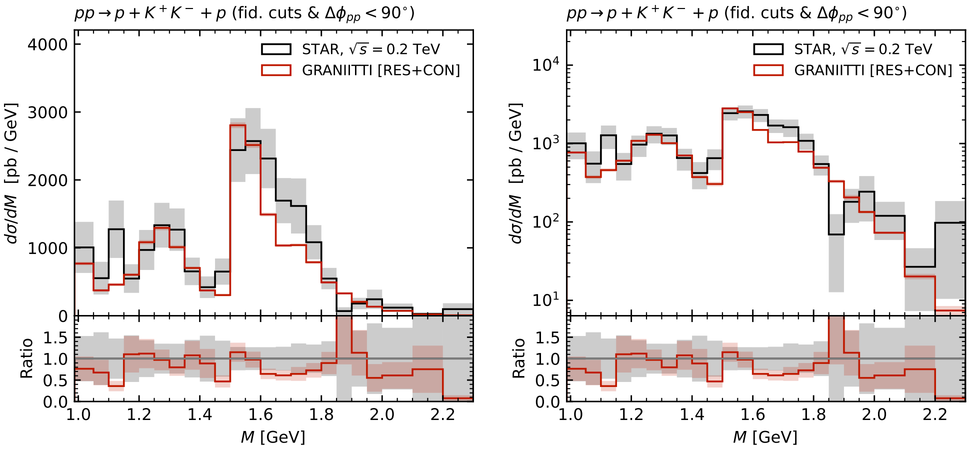


Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of K^+.

$pp \rightarrow p + K^+K^- + p$

with fid. cuts & $\Delta\phi_{pp} < 90^\circ$



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$pp \to p + K^+K^- + p$ with fid. cuts & $\Delta\phi_{pp} > 90^\circ$

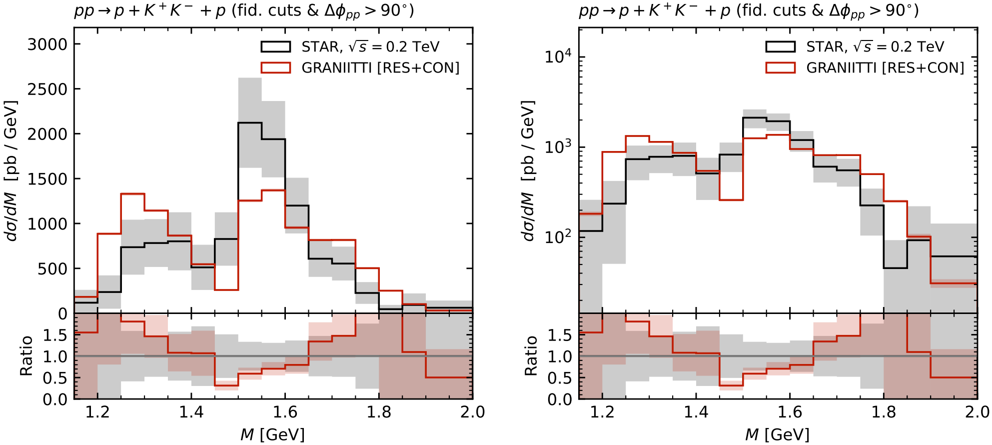
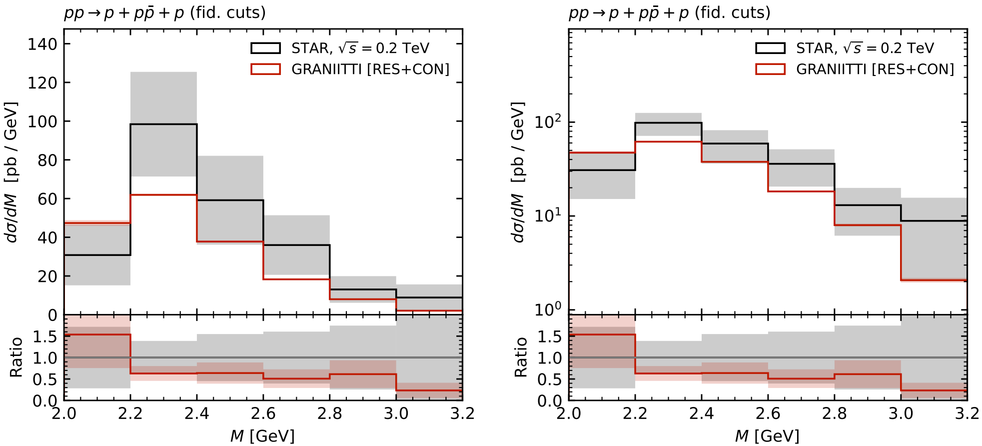


Figure: Central system invariant mass; linear y-scale (left) and log y-scale (right).

$pp \rightarrow p + p\bar{p} + p$ with fid. cuts (low stats)



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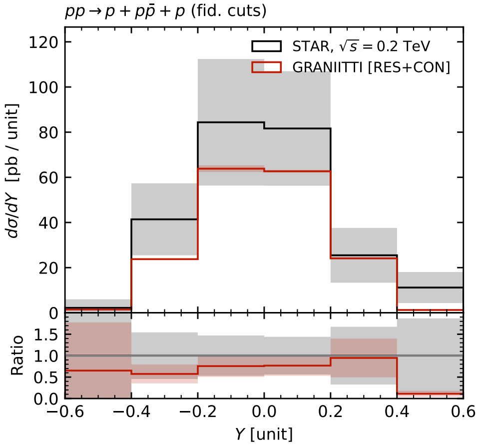

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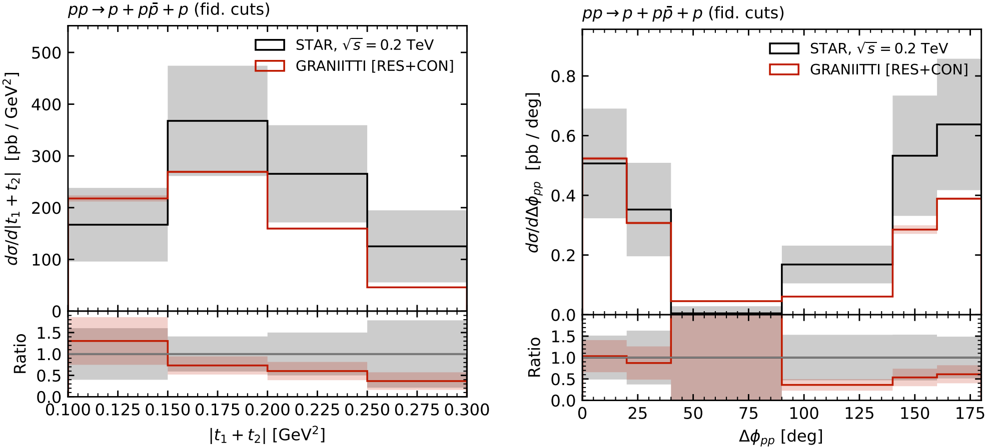

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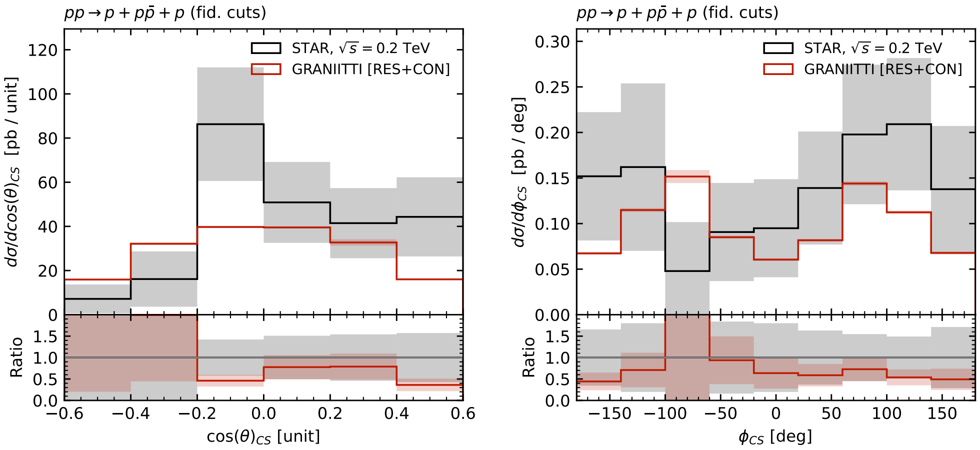

Figure: Collins-Soper frame angles $(\cos(\theta), \phi)$ of p.

$pp \to p + p\bar{p} + p$
with fid. cuts & $\Delta\phi_{pp} < 90^\circ$

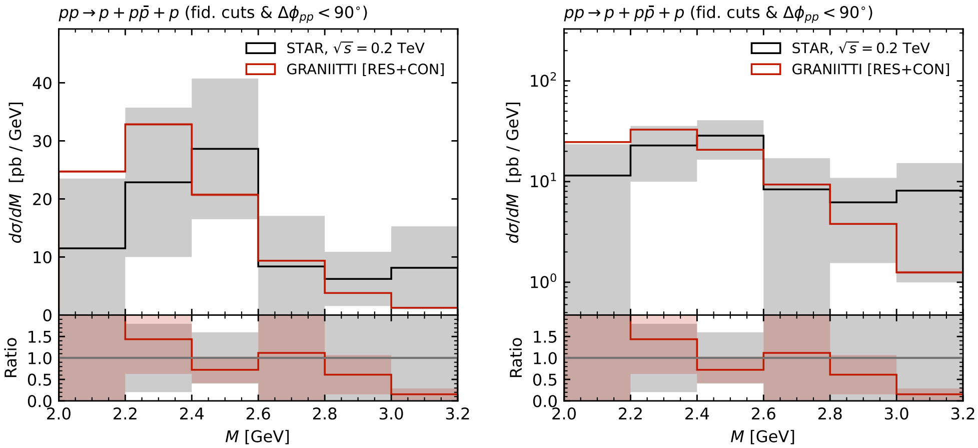

Figure: Central system invariant mass; linear y-scale (left) and log y-scale (right).

$pp \to p + p\bar{p} + p$
with fid. cuts & $\Delta\phi_{pp} > 90^\circ$

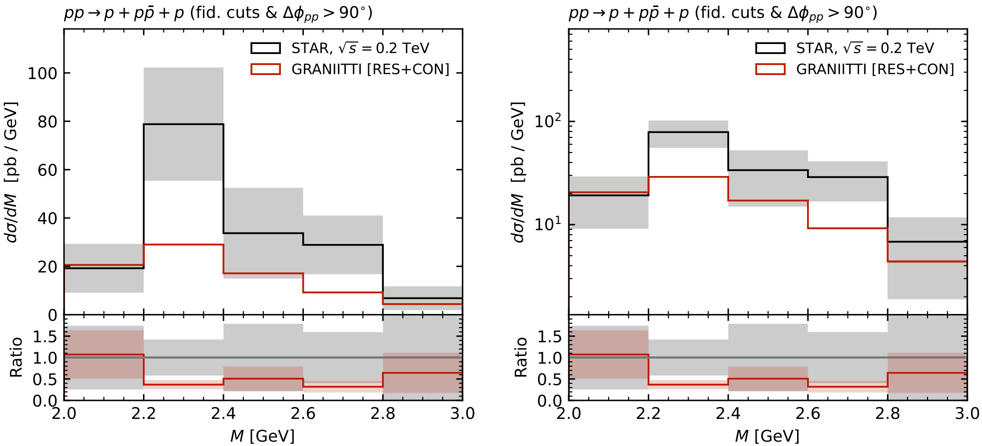

Figure: Central system invariant mass; linear y-scale (left) and log y-scale (right).

Observations based on STAR data

- While the low mass regime is OK, the high mass tail is off in $\pi^+\pi^- \to$ continuum off-shell form factor should be re-considered (extra 'suppression log' terms, pions vs kaon etc). Remember: # Data Features - # Model Degrees of Freedom = zero sum game ...?
- CS-frame here $\sim$ 'natural frame' (with minimal p_T effects), i.e. a diagonal and fixed spin polarization matrix seems approximately OK for the data, iff

$$f_0(500) \text{ is a scalar, seems to be needed for the fit} \tag{1}$$

$$\rho(770) \text{ with } J_z = \pm 1 \text{ (photoproduction)} \tag{2}$$

$$f_0(980) \text{ is a scalar} \tag{3}$$

$$f_2(1270) \text{ with } J_z = \pm 2 \tag{4}$$

$$f_0(1500) \text{ is a scalar} \tag{5}$$

$$f_2(1525) \text{ with } J_z \simeq 0 \tag{6}$$

$$f_0(1710) \text{ is a scalar} \tag{7}$$

However, more angular distributions would be needed (event-by-event data even better). Tensor Pomeron model could be compared next time. Ps. which J_z should a spin-2 glueball predominantly have in CEP?

Deep learning towards GRANIITTI v2

Coherent fluctuations & interactions + deep learning $\sim$ 'Deep Pomeron'

For the proton structure fluctuations, would be interesting to have something like parton densities, but suitable for soft diffraction (especially quasi-coherent/dissociative).

One suitable deep learning tech-tool for this could be 'deep diffusion models', which are powerful generative deep networks *inspired*[2] by non-equilibrium thermodynamics (Langevin stochastics)

→ A major challenge for fluctuation / lattice specialists is to formulate a suitable formulation. Then plug that into generative deep learning. Extract crucial input from measurements like pdfs are extracted → beneficial to have event-by-event data of type CERN Open Data – 1D-histogram cross-section measurements do not catch the high dimensional correlation structure maximally ...

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[2] The actual data generating process for these can be arbitrary, a quantum process or some macroscopic. They are neural nets, after all.

Equivariant (covariant) Deep Learning

"A neural network architecture that is fully equivariant with respect to transformations under the Lorentz group[3]". Let Q be a Lorentz transform acting on the Lorentz group $SO(1,3)$ (rotations and boosts). By definition

$$\text{Equivariance}: Q\,\phi(v) = \phi(Qv) \tag{8}$$

$$\text{Invariance}: \;\phi(v) = \phi(Qv), \tag{9}$$

where v is a 4-vector and ϕ is the learned neural function.

As a novel application, this could be used to learn the unknown soft 3-point functions $\phi(q_1^\mu, q_2^\nu)$ of the Pomeron-Pomeron-Resonance vertex from data. Assuming the learned vertex function set is finite and universal (one for a given resonance species with specific quark/glue content; meson, glueball) → can recycle it and obtain predictive power.

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[3] One example: An efficient Lorentz equivariant graph neural network for jet tagging, Gong et al. JHEP 30 (2022)

Deep Normalizing Flows for Importance Sampling

- Beyond factorized VEGAS by chaining invertible and diffentiable neural layers to obtain D-dimensional change of variables transform → normalizing flow (the word ‘normalizing’ means density evaluation, which is required for importance sampling)

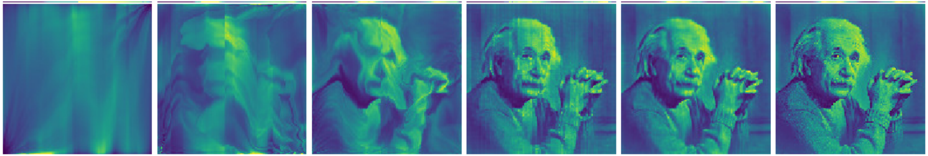

Figure: Sequential normalizing flow from a base to the target density. [arxiv:1808.03856]

- Deep learning and computer graphics ray tracing communities have done much progress on this, also in HEP [PhysRevD.101.076002].

- The challenge is to invent "flow layers" which are expressive, have a very fast analytical $\log(\det(J))$ and can handle sharp phase space boundaries (due to generation cuts).

Summary

- Introduced GRANIITTI, the first public fully open source event generator attacking the full $pp \rightarrow p + X + p$ resonance spectrum modelling in the low mass ‘glueball domain’ of central production, relevant at the LHC and RHIC. Compared the simulations against STAR measurements → quite promising results.

- New neural ideas towards GRANIITTI v2 – such as data-driven Pomeron-Pomeron-Resonance vertex functions – towards the first deep learning enhanced diffractive Monte Carlo event generator.

- I emphasize that event-by-event data (+ simulations propagated through GEANT) would be nice to have in the future (CERN OpenData repository) → optimal input data for learning e.g. soft neural scattering amplitudes.

Appendix

ICETUNE: Integrated HPC-tuning machinery in GRANIITTI

Python steered plotting and HPC-cluster distributable soft parameter tuning suite for all free parameters: general soft eikonal Pomeron, soft Pomeron-Pomeron amplitudes, resonance couplings & polarization etc.

Because the numerical screening loop integral increases computational cost by factor 10-100, HPC-distribution is very beneficial.

Raytune library allows to use the latest gradient free meta-optimization algorithms (Bayesian optimization, Evolutionary algorithms ...)

Tuning/fit receipt via ICETUNE

ICETUNE HPC-launch example

```
ray start –head –temp-dir=/tmp/ray; python python/icetune –tuneset default
```

FIXED

- All (eikonal / screening loop) non-linear Pomeron and Proton form-factor parameters are pre-fitted according to the elastic scattering data
- Pomeron[Reggeon]-Meson couplings for the continuum amplitude untouched (originating from Donnachie-Landshoff fits)
- CEP-amplitude linear Pomeron trajectory [$\alpha = 1.09, \alpha' = 0.2$ GeV^{-2}]
- Resonance branching ratios set from PDG / ansatz (not all known)

FREE

- Continuum amplitude off-shell meson form factor and its parameters (Orear chosen here, 2 parameters)
- Resonance (complex) couplings [except photoproduced $\rho(770), \phi(1020)$ from literature]
- Diagonal polarization elements for spin-2 resonances

Reproducability and automated test

Github actions based ‘Continuous Integration’ (CI)

Github server bot install Linux (Ubuntu), compiles GRANIITTI C++, generates events and tests the generator output. See the workflow: github.com/mieskolainen/graniitti/blob/master/.github/workflows/graniitti-install-generate-test.yml

Algorithms x-checked with another one

Following are (a part) of the automated testing (a growing suite of tests ...):

1. Single threaded C++ $\rightleftharpoons$ multithreaded C++ execution
2. Naive flat MC sampling $\rightleftharpoons$ VEGAS importance MC sampling
3. M-body generator $\rightleftharpoons$ RAMBO generator
4. Recursive Phase-Space $\rightleftharpoons$ Non-recursive Phase-Space division
5. Analytical (massless) phase space volume $\rightleftharpoons$ RAMBO computed MC volume
6. Screened amplitudes $\rightleftharpoons$ Non-screened (bare) amplitudes
7. k_T-EPA $\gamma\gamma$ + MadGraph $2 \to 2$ $\rightleftharpoons$ Full $\gamma\gamma$-QED $2 \to 4$ amplitude
8. Minimal Pomeron (Jacob-Wick sub-amplitudes) $\rightleftharpoons$ Tensor Pomeron (fully covariant Feynman rules)
9. Weighted output $\rightleftharpoons$ Unweighted (acceptance-rejection) event output
10. Elastic $d\sigma/dt$-measurements for various energies $\rightleftharpoons$ GRANIITTI elastic $d\sigma/dt$
11. LHC/RHIC/Tevatron CEP x-section measurements $\rightleftharpoons$ GRANIITTI CEP x-sections