Generators and Theory developments for HET physics

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3rd ECFA workshop on e⁺e⁻ Higgs, Electroweak & Top factories

Campus des Cordeliers, Paris, October 9-11, 2024

✓ Monte Carlo event generators became essential tools for data-theory comparison since the LEP era

FEATURE LEP'S PHYSICS LEGACY



A. Siódmok, I ECFA workshop on H/W/T factories, 2022, DESY

 Nowadays, all physics throughput from colliders (LHC, flavour factories) would be literally unthinkable without Monte Carlo generators Nowadays, all physics throughput from colliders (LHC, flavour factories) would be literally unthinkable without Monte Carlo generators

 Figuring out the physics potential (and foresee physics limitations) of a future machine impossible without Monte Carlo generators Nowadays, all physics throughput from colliders (LHC, flavour factories) would be literally unthinkable without Monte Carlo generators

 Figuring out the physics potential (and foresee physics limitations) of a future machine impossible without Monte Carlo generators

 Monte Carlo generators provide the best solution to extract meaningful results (test the SM, unveil BSM) by comparing theory predictions to complex and precise data ✓ Precision physics strongly demands including higher-order radiative corrections in the SM

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✓ Automated calculations are the standard for LHC

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 Interface through standard event formats is mandatory to interact with detector simulation and analysis software
 e.g. talks by Juraj Smieško and Alvaro Tolosa-Delgado Precision physics strongly demands including higher-order radiative corrections in the SM

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 Benchmarking and tuned comparisons essential to establish technical precision and estimate theoretical accuracy
 talk by Alan Price

MC needs for a future e^+e^- collider

Beamsstrahlung simulation (beam dynamics, luminosity spectra)



Thorsten Ohl (Univ. Würzburg

Luminosity Spectra Redux

e⁺e⁻ Higgs/EW/Top Factories, Paris, 10/24

RZBURG COM	bination Comp	arisons		S P
 e[±] energy spread beam energy spre 	from BS and a ad $\Delta E_{e^\pm}/E_{bean}$	verage photon $e_n \approx 0.15\%$ after	energy much smaller many bunch crossing	than gs:
FCC 2024	$\Delta_{BS}E_{e^\pm}/Gev$	$\langle E_{\gamma} \rangle_{BS}/Gev$	$0.15\% \cdot E_{e^{\pm}}/Gev$	
Z	0.0012	0.0016	0.07	
WW	0.0039	0.0059	0.12	
ZH	0.0140	0.0189	0.18	
Тор	0.0329	0.0531	0.27	
only visible for the	high energy de	esigns		

 nevertheless, already at LEP, on small-angle Bhabha scattering it induces a systematic bias on the acceptance



MC needs for a future e^+e^- collider

- QED RCs: soft and/or collinear resummation, YFS vs electron-PDFs, inclusive vs exclusive
- final state QCD showers, fragmentation and hadronisation
- fixed order RC in the full SM: NLO, NNLO
- on general grounds, the (impressive) O(0.1)% theoretical accuracy of LEP results needs to be pushed down for future e^+e^- machines.

This demands systematic improvements in the control of radiative corrections in the SM:

- at NLO (nowadays fully automatic) and at NNLO
- resummation techniques for leading higher-order corrections
- consistent combination of the two, following and possibly extending the example at hadron colliders (MC@NLO, POWHEG, MiNNLO_{PS}, UN2LOPS, ...)

Instead of focussing on calculating order-by-order exact corrections in α for a given process,
 ePDF, QED Parton Shower and Yennie-Fraustchi-Suura resummation take a different point of view as starting point:

they aim at calculating **approximate** and **"universal"** corrections **up to all orders**, by including (the important, leading) contributions arising from soft and/or collinear regions

- They rely on the general property of **factorization of soft/collinear divergencies** (enhancements) in QED, which leads to **exponentiation**
- Sometimes, in some phase-space regions, for some observables, for certain experimental cuts, you better have an approximate but resummed result than a fixed-order one

$$lpha < lpha^2 L^2$$
 somewhere, with $L = \log rac{s}{m^2}$

- ePDF (or Structure Functions at LL) solve the DGLAP equations in QED
- Their logarithmic accuracy can be improved by using NⁿLO splitting functions (e.g. $LL \rightarrow NLL$ [Frixione et al., 19, 21, 22])
- The formalism closely follows well established techniques in QCD
- · Resum collinear logs, valid in the stricity collinear limit (inclusive over radiation)

$$d\sigma(L,\ell) = \mathcal{K}_{coll}(L;\ell) \otimes d\hat{\sigma}(\ell)$$

$$\longrightarrow d\sigma_{kl} = \sum_{ij} \int dz_+ dz_- \Gamma_{i/k}(z_+,\mu^2,m^2) \Gamma_{j/l}(z_-,\mu^2,m^2)$$

$$\times d\hat{\sigma}_{ij}(z_+p_k,z_-p_l,\mu^2;p_X,\{k_i\}_{i=0}^n)$$

YFS resummation

- It's build upon the seminal paper YFS 61
- Naturally suited for exclusive radiation generation
- Resums infra-red logarithms
- After factorizing out all soft virtual and soft real corrections, the master formula is

$$\mathrm{d}\sigma = \sum_{n_{\gamma}=0}^{\infty} \frac{e^{Y(\Omega)}}{n_{\gamma}!} \,\mathrm{d}\Phi_{Q} \bigg[\prod_{i=1}^{n_{\gamma}} \mathrm{d}\Phi_{i}^{\gamma} \tilde{S}\left(k_{i}\right) \Theta(k_{i},\Omega) \bigg] \bigg(\tilde{\beta}_{0} + \sum_{j=1}^{n_{\gamma}} \frac{\tilde{\beta}_{1}(k_{j})}{\tilde{S}\left(k_{j}\right)} + \sum_{j=1}^{n_{\gamma}} \frac{\tilde{\beta}_{2}(k_{j},k_{k})}{\tilde{S}\left(k_{j}\right) \tilde{S}\left(k_{k}\right)} + \cdots \bigg)$$

where

 \dashrightarrow $e^{Y(\Omega)}$ resums all **soft** virtual and **soft** real emissions

- $\rightsquigarrow \tilde{S}(k_i)$ are eikonal factors
- $\rightsquigarrow \tilde{\beta}_n$ are IR-subtracted matrix elements remnants (with *n* photons)
- $ilde{eta}_n$ can be improved order-by-order to include exact NLO, NNLO, ...
- Comes with two "flavors": EEX (works at $|A|^2$ level) and CEEX (works at the A level)
- It can be improved to better include collinear logs [Ward]

Many MCs for LEP (and LHC) by Jadach and colleagues based on it

- It's an iterative MC solution of the (LL) DGLAP equations
- Kinematics of the emitted particles can be reconstructed \rightarrow exclusive generation
- As ePDF, it naturally resums collinear logs. It can be tweaked to include correct infrared limit of emitted radiation.
- It can be matched to NLO to improve accuracy, avoiding double counting
- Can it be extended to work at NLL?

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The availability of different QED resummation schemes gives the opportunity to check theoretical accuracy!

- process taylored
 - BHLUMI, KKMC[ee],KORALW/Z, YFSWW, RACOONWW, RACOON4F
 - BABAYAGA

- general purpose
 - HERWIG, PYTHIA
 - MadGraph5_aMC@NLO, SHERPA, WHIZARD

Jadach, Placzek, Skrzypek, Ward, Was

- Generators for $e^+e^- \rightarrow W^+W^- \rightarrow f_1f_2f_3f_4$ at LEP
- Based on YFS resummation of QED corrections, include NLO EW corrections
- Include Coulomb effect at threshold
- Now combined in KandY
- Interfaced to TAUOLA for τ decays

Jadach, Ward, Was, Yost, Siodmok

- Generator for $e^+e^- \rightarrow f\bar{f}$, with $f = \mu, \tau, q$
- It implements the CEEX YFS formalism for QED corrections
- It includes NLO EW corrections and collinear enhancement in resummation
- KKMCee is a port to C++ of the original Fortran code

- BabaYaga@NLO was developed to simulate Bhabha, $e^+e^- \rightarrow \mu^+\mu^-$ and $e^+e^- \rightarrow \gamma\gamma$ at flavour factories, with a 0.1% theoretical accuracy in mind
- QED Radiative Corrections are included by means of an (in-house) QED Parton Shower
- The QED PS is matched to NLO exact matrix elements
- Fully exclusive event generation
- · Although developed for low energies, it's being ported to high energies
 - $\rightarrow\,$ e.g. $e^+e^- \rightarrow \gamma\gamma(+n\gamma)$ with NLO EW corrections, as luminosity process for FCCee

PLB 798 (2019) 134976



MadGraph5 aMC@NLO

1,2, https://launchpad.net/mg5amcnlo

- MG5_aMC is an automatic event generator for any processes of the user's choice (in the SM and beyond)
- User input limited to run/model parameters, cuts, etc
- Unweighted events for PS matching can be generated at NLO QCD accuracy, possibly including multi-jet merging³
- NLO EW corrections can be computed as well², but only at fixed-order (no PS), either exactly or in the high-energy approximation⁴ (Sudakov)^{5a}
- In the Sudakov approximation, (the dominant part of) EW corrections can be included in NLO QCD-accurate events via reweighing^{5b}
- Several other features are available
- All this works for arbitrary processes and colliders

I Alwall, Frederix, Frixione, Hirschi, Maltoni, Mattelaer, Stelzer, Shao, Torrielli, MZ, <u>1405,0301</u> 2 Frederix, Frixione, Hirschi, Pagani, Shao, MZ, <u>1804,10017</u> 3 Frederix, Frixione, <u>1209,6215</u> 4 Denner, Pozzorini, <u>hep-ph/0010201</u>, <u>hep-ph/0104127</u> 5 a Pagani, MZ, <u>2110,03714</u>; 5b +Vitos, <u>2309,00452</u> 7 5 a Pagani, MZ, <u>2110,03714</u>; 5b +Vitos, <u>2309,00452</u> 1 b + Vitos, <u>2309,00452</u> 5 a Pagani, MZ, <u>2110,03714</u>; 5b +Vitos, <u>2309,00452</u> 5 a Pagani, MZ, <u>5110,03714</u>; 5b +Vitos, <u>2309,00452</u> 5 a Pagani, <u>510,0052</u> 5 a Pagani,

Marco Zaro, 12-10-2023



Capabilities of MG5 aMC at ete- colliders:



- NLO EW corrections can be included for (almost) all processes
- Through eMELA, ISR (possibly with beamstrahlung) in different ren/fact schemes can be employed
- The code automatically takes care to add to the short-distance xsection those terms necessary for consistency
 - \bullet Factorisation-scheme kernels included in the cross-section for Δ scheme and LL PDFs
 - Virtuals are corrected in order to account for different ren. scheme in model and PDFs ($\alpha(m_Z) \rightarrow MSbar$)
- For details and how-to, see <u>https://answers.launchpad.net/mg5amcnlo/+faq/3324</u>





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More results:



Marco Zaro, 12-10-2023

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talk by M. Zaro at 2nd Workshop on HET factories, Paestum, 2023





WIP in collaboration with Davide Pagani, Yang Ma



talk by M. Zaro at 2nd Workshop on HET factories, Paestum, 2023; Y. Ma, D. Pagani, M. Zaro, arXiv:2409.09129

The SHERPA framework

- ME generators for hard process
 - Comix, Amegic
 - + interfaces to loop libraries (OpenLoops, Recola, MCFM)
- Parton Showers
 - CSShower, Dire
- Underlying Event/MPI model
- Hadronisation
 - Cluster Fragmentation, + interface to Pythia
- QED radiation via YFS resummation



SHERPA 3 — multi-purpose event generation

- (Selected) Features:
 - Fixed Order
 - NLO QCD+EW,
 - NNLO QCD (selected processes)
 - Automated NLO (QCD) matching in S-MC@NLO
 - UN2LOPS matching to NNLO QCD
 - multi-jet merging in CKKW-L
 - Approximate EWcorrections in matching & merging (EWvirt/EWSud)
 - Photoproduction @ NLO QCD + PS

- YFS resummation of photon radiation
 - radiation from final state leptons
 - initial state radiation at *e*⁺*e*⁻ colliders
 - extended by $\gamma \to f\bar{f}$ splittings
 - Polarised
 - beams
 - intermediate particles
- MPI/MinBias and fragmentation modelling, including color reconnection

- External Interfaces:
 - HepMC 3
 - UFO 2 (including form factors)
 - RIVET 3/4
 - LHAPDF + several explicit pdf interfaces including various photon pdfs
 - OpenLoops/ Recola/MCFM/ MadLoops/ BlackHat
 - **Pythia 8** (string fragmentation)

QED initial state radiation

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1.005 0.00

- Soft photon resummation in Sherpa via YFS module [Krauss, Schönherr '08]
- **New:** real photon emission from • initial state [Krauss, Schönherr, Price '22]
- · replace simple electron pdf with explicit multi-photon emissions
- validated agains KKMC [Jadach, War, Was '99]



QE ion with $e^+e^- \gamma \rightarrow e^+e^-$

- Inal state QED radiation the above rachetion from first state options and schemer (from the state)
- New: supplemented with $\gamma \rightarrow e^+e^-$ splittings [Flower, Schönherr '22]
- Example: dilepton invariant mass in $pp \rightarrow e^+e^-$





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Outlook: more accurate parton showers

- New: Parton shower module ALARIC [Herren, Höche, Krauss, DR, Schönherr,'22]
 - explore connection between angular ordering and dipole showers
 - address NLL deficiencies found in recoil schemes of current dipole showers
- Multi-jet merging available now
 [Höche, Krauss, DR '24]
 - + first LHC phenomenology
- full NLO matching still WIP
- Basis for development towards higher accuracy showers



talk by D. Reichelt

Outlook: automated resummation

- accesible precise resummed calculations important
 - · predictions for experiments
 - references for parton showers
- CAESAR formalism provides convenient framework event/jet shape-type observables [Banfi, Salam, Zanderichi '04]
- CAESAR implementation in Sherpa [Gerwick, Höche, Marzani, Schumann '15] [Baberuxki, Preuss, DR, Schumann '19]
 - several studies already for LEP/ LHC/RHIC/FCC-ee (future lepton collider)



Example: event shapes in $H \rightarrow gg$ and and $H \rightarrow q\bar{q}$ decays using EERad in conjunction with Sherpa+CAESAR

[Gehrmann-de Ridder, Preuss, DR, Schumann '24]

talk by D. Reichelt

Outlook: performance updates/HPC

[arXiv:2209.00843] slide by E. Bothmann

- · MC event generation uses significant+increasing resources
- · (HL-)LHC measurements in danger of being limited by MC statistics
- Explore reduction of CPU footprint for heaviest use cases, e.g. ATLAS default setup Z + 0,1,2j@NLO + 3,4,5j@LO
 - 1. LHAPDF improvement
 - (LC)-MC@NLO: reduce matching accuracy to leading colour, neglect spin correlations, i.e. S-MC@NLO → MC@NLO also useful to reduce negative event fractions [Darger, Höche, Stiegert 2110.15211]
 - 3. pilot run: minimal setup until PS point accepted, then rerun full setup
 - 4. (LC)-MC@NLO-CSS: defer MC@NLO emission until after unweighting
 - use analytical loop library where available here: OPENLOOPS → MCFM via interface [Campbell, Höche, Preuss 2107.04472]
 - 6. pilot scale definition in pilot run that requires no clustering small weight spread by correction to correct scale
- · all new developments part of Sherpa 2.2.13 or later





talk by D. Reichelt



WHIZARD Overview(I)

- Complete MC event generator for all colliders: v3 released 27.4.2021 ÿ.
- ÿ. Hard matrix elements @ LO internally (0'Mega)
- ÿ. Hard matrix elements @ NLO externally (OpenLoops, Recola, GoSam....)
- ¥. Parton shower internal+external, hadronization external
- ş. Dedicated interfaces to Pythia6, Pythia8, Tauola, ...
- ÿ. Lepton collider beam simulations (Gaussian spread, parameterized fit, beam event files, 2d-histogram adapted, smoothened, photon collisions):









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WHIZARD **Overview(II)**

model = NMSSM
process susyprod = e1, E1 => stau1, Stau1
process staudec = stau1 => neu1, e3
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sqrts = 250 GeV beams = e1, E1 => circe2 => isr beams_pol_density = @(-1), @(+1) beams_pol_fraction = 80%, 30%

n_events = 10000
sample_format = lhef, stdhep, hepmc
simulate (susyprod)

- Collider setup: arbitrarily polarized beams, crossing angle, asymmetric beams
- Event formats available: LHA, LHE(v1-3), HepMC2, HepMC3(RootIO), LCIO, EDM4HEP (w.i.p.)!
- 👙 Factorized processes (unstable feature, NWA, specific decay helicity, polarized resonance decays)
- 🞍 Automated calculation of BRs of unstable particles, BRs can be set explicitly, e.g. to (N)NLO values
- BSM models through UFO interface (cf. later)
- Special treatment of top threshold physics (cf. later)
- Reweighting / recasting processes + multiple weights/observables
- Focus here new developments: Completion NLO automation, NLO matching, high-performance, revalidations, new physics implementations: long-lived particles, initial-state QED treatment, EW PDFs etc.



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WHIZARD NLO Automation: Loops & Legs

- 🖇 NLO SM automation for lepton-/hadron colliders completed 2022 👘 Chokoufé; Weiss 2017; Rothe 2021; Stienemeier; Bredt 2022
- 🞍 FKS subtraction, NLO matrix elements from OpenLoops/Recola/GoSam/...
- 着 also: resonance-aware FKS subtraction 🥂 cf. Ježo/Nason, arXiv:1509.09071; Chokoufé, 2017
- Setup for automatic differential fixed-order results (histogrammed distributions)
- Photon isolation, photon recombination, light-, b-, c-jet selection; loop-induced processes



NLO POWHEG-type matching

Matching NLO real emission from hard ME and parton shower (PS)

- POWHEG method: hardest emission first [Frixione/Nason et al.]
- Process-independent NLO matching in WHIZARD

LHC 13 TeV: NC Drell-Yan $pp \rightarrow \ell^+ \ell^-$ compared to CMS data





Available: all infrastructure for NLO QED/EW matching, needs to be completed/validated



Whizard in parallel

> 10^{-2} 10^{-3}

> > p = 1.0p = 0.9

 $e^+e^- \rightarrow \mu^+\mu^-$

 $e^+e^- \rightarrow \mu^+\mu^-\mu^+\mu^-$



Braß/Kilian/JRR, arXiv:1811.09711

- Parallelization of integration: OMP multi-threading for different helicities
- MPI parallelization (using OpenMPI or MPICH)
- Distributes workers over multiple cores, grid adaption needs non-trivial communication
- Speedups of 20 to 50, saturation at O(100) tasks [can do also parallel event generation]
- Load balancer / non-blocking communication [v3.0.0]



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 10^{2}

 $\frac{10}{8}$ 10¹

 $e^+e^- \rightarrow \mu^+\mu^-\mu^+\mu^-\bar{\nu}_{\mu}\nu_{\mu}$

 $\sigma \sigma \rightarrow W$

 $\sigma \sigma \rightarrow W \sigma$

 $gg \rightarrow Wgg$

16 64

CPUs

16 64

 $ii \rightarrow Wi$

 $ii \rightarrow Wii$

 $jj \rightarrow Wjjj$

CPUs

Whizard on GPUs



Preliminary:

Joint project with former Phd student; now works for NEC supercomputers

- Main core serial (or MPI-parallel) on CPU,
- 1. step: matrix elements as libraries off-loaded to GPU
- (Semi-) automatized ME generator exists for amplitudes on GPU
- Moderate speed-ups can be seen for more complicated processes
- 2. step: phase-space generation (SIMD paradigm) on the GPU
- $\frac{1}{2}$ W.i.p.: phase-space adaption on the GPU (w/ minimal data transfer CPU \leftrightarrow GPU)

Process	$t^{CPU}[s]$	$t^{GPU}[s]$
$e^+e^- ightarrow t \bar{t}$	0.98	4.28
$e^+e^- \rightarrow bW^+ \bar{b}W^-$	28.8	23.1
$e^+e^- ightarrow bW^+ ar b W^- H$	57.5	37.8
$e^+e^- \rightarrow b\bar{b}\bar{\nu}_e e^-\bar{\nu}_\mu\mu^+$	154	124
$e^+e^- \rightarrow 2j$	1.9	5.4
$e^+e^- ightarrow 3j$	45	65
$e^+e^- \rightarrow 4j$	870	608
$e^+e^- ightarrow 5j$	4106	978
$pp \rightarrow jj$	42	86
$pp \rightarrow W^+W^-W^+W^-$	670	192

Whizard MC Integrators:

- VAMP: adaptive multi-channel Monte Carlo integrator
- VAMP2: fully MPI-parallelized version, using RNG stream generator
- [VGPU: VAMP implementation on GPU]
- [VXInt: new adaptive generator + integrator based on INNs]

- (w.i.p first as a stand-alone tool)



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WHIZARD 2.8.3: Full UFO (1) support

Arbitrary Lorentz structures supported

Fermion-number violating interactions (3.0.0)

(N)LO matrix elements from UFO models (particularly SMEFTSim v3.x)

5-, 6-, 7-, 8-, ... point vertices (optimization for code generation pending)

Lots of bug reports and constructive feedback from many different users.

New paper on UFO 2.0: Darmé et al. arXiv: 2304.09883

News on the UFO / BSM in WHIZARD



I. Bozović-Jelizavčić, 2405.05820



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model = SM (ufo)

model = SM (ufo ("<my UEO path>"))



BSM @ NLO (QCD) with UFO

- [©] GoSam was the first OLP that kicked off NLO automation in Whizard in 2013
- Revived 2023 with NLO QCD for BSM models (e.g. SMEFT) for LHC J. Braun/P. Bredt/G. Heinrich/M. Höfer/JRR
- ⁹ End of 2023: full validation of NLO QCD processes for LHC within SM: $pp \rightarrow t\bar{t}, pp \rightarrow t\bar{t}H, pp \rightarrow \gamma\gamma, pp \rightarrow \gamma j \dots$
- [♀] Full support for Whizard⊕GoSam for MPI (Message Passing Interface) parallelization

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- GoSam UFO NLO interface allows support for almost any model
- W.i.p.: Note yet supported neither by the public Whizard nor GoSam versions
- Implementation and validation of resonance-aware subtraction for pp processes in Whizard
- 2024: First test runs for NLO QCD corrections for UFO BSM models

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Benchmarking



&Benchmark Aims

♦How to Benchmark

♦Future Plans and Outlook

talk by A. Price

Motivation: Philosophy

- ♦ Generators are generally trying to simulate the same physics
- ♦ Why not have one **master** input card that will work for all MC?
 - → Authors are unlikely to change or decide on a common input!
- Have python module which will create generator specific runcards from one master input
- This will help improve reproducibility and hopefully reduce input errors
- Preserve the "LEP era" MC, who may not have active authors on the timeline of a Higgs Factory

talk by A. Price

Reproducibility

- Provide "Add-on" to Key4Hep framework
- Should be simple enough that:
 - New process can be easily added
 - MC authors can update interfaces if needed
- ♦ Keep some public event records
 - ♦ Juggle usefulness vs Storage
- More dedicate test for new generator releases

We already have a sophisticated software system!



See Juraj Smieško <u>Talk</u>



Alan Price

Current Processes

We have input cards for all relevant $2 \rightarrow 2$ processes

We seeing excellent agreement in most cases, one or two effects (<5%) that requires more detailed study

Differential distributions are also in good agreement



- Editors: Carlo Carloni Calame, Juergen Reuter, Marco Zaro
- Preliminary outline:
 - (1) Hard processes: NLO QCD + NLO EW in the SM, NNLO
 - (2) Initial state radiation: LL/NLL ePDFs / YFS (coll. vs. soft resummation)
 - (3) Beam spectra: parameterized, simulated, Gaussian
 - (4) Parton showers and hadronization, incl. matching
 - (5) BSM simulations
 - (6) Dedicated processes with dedicated tools/implementations:

Bhabha, rad. Bhabha, $e^+e^- \rightarrow \gamma\gamma$, WW & $t\bar{t}$ thresholds

(7) Connection to software frameworks, event formats, and all that