CMS Monte Carlo Generators: Run II experience and needs for Run III

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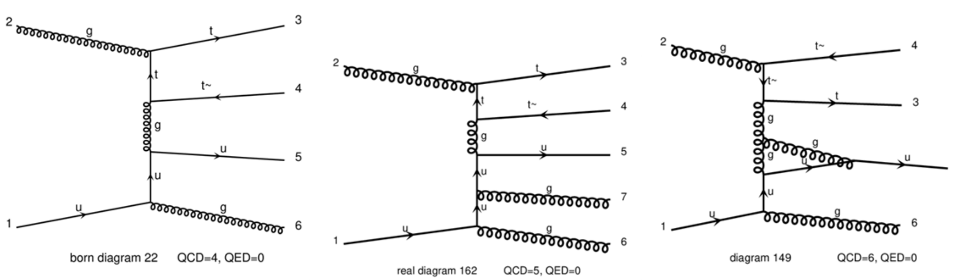
Introduction

- **CMS at LHC relies on detailed and large scale Monte Carlo production for modeling of the detector and underlying physics**

- **We are hitting several bottlenecks in term of cpu and disk space: robust software and computing infrastructure more and more essential to reach the physics goals**

- **Typical Monte Carlo workflow has a few distinct steps**
  - **Hard process/Matrix Element generation**: Generate kinematic configuration for a desired process up to parton level using perturbative QCD
  - **Parton Shower/Hadronization**: Adds additional QCD and QED emissions down to a low scale, and produces hadrons from QCD partons
  - **Detector Simulation(*) and Digitization**: Detailed Geant4 simulation of the interactions of the outgoing particles with the CMS detector, followed by simulation of detector electronics and creation of simulated raw data
  - **Reconstruction**: Reconstruction of simulated raw data into higher level physics objects
    - To a good approximation, identical code as runs on real data

- **Strong motivation for NLO and/or multi-leg/merged-multiplicity Monte Carlo generators whenever possible**
  - Achieve highest accuracy for final states with additional jets
  - Warning: large time/event required
  - Warning: NLO features negative weights, requiring up to x10 statistics wrt LO



tt+2-jet born | tt+2-jet real | tt+2-jet virtual

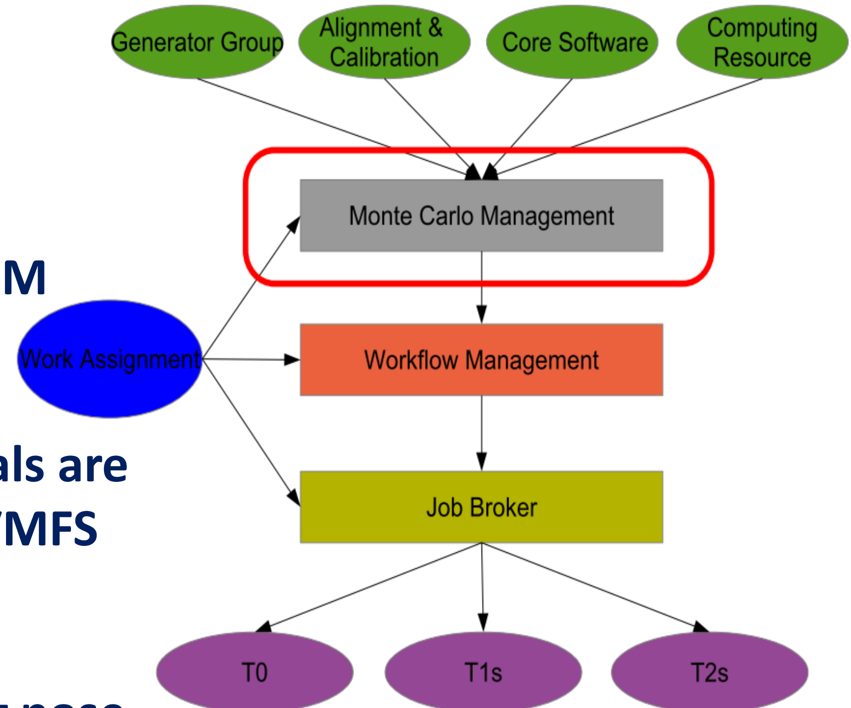
(*)cfr Talk "Current and Future Performance of the CMS Simulation" by K. Pedro

CMS Software Overview

- **Main CMS software application: CMSSW**
  - Modular C++ application which can be used for event generation, detector simulation, reconstruction, and analysis
- **Configuration of CMSSW runs steered with python files**
- **Input and output through ROOT-based Event Data Model (EDM) files**
  - Storing run-level, lumi-section-level (23s periods for real data), or event-level data products
- **CMSSW links directly to many externals**
  - Externally maintained C, C++, fortran, or python software which is either an indirect dependency or is directly called from within CMSSW
  - Externals are compiled with the same common libraries, compiler version as CMSSW and packaged together with a given release
  - Starting from either a tarball from the author's website, from GENSER, or from a cms-managed github mirror
- **Rapidly evolving software**
  - Swift change of compilers, OS versions, multi-thread support …
  - Difficult for the 'externals' to keep up

CMS Submission Infrastructure Overview

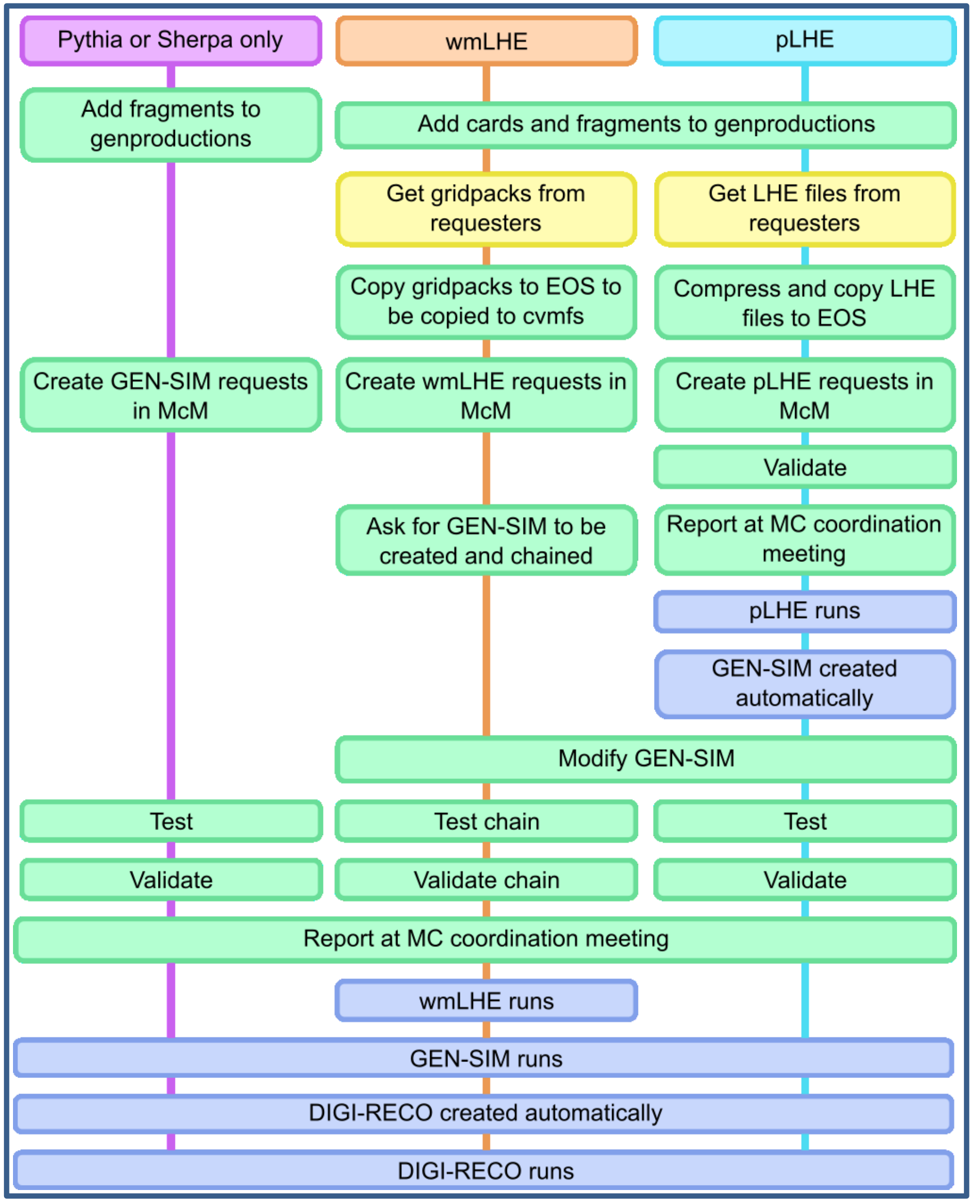
- **Large-scale submission of CMSSW jobs to grid resources managed with python-based tools**
  - For central production of Monte Carlo, data processing, etc
- **Jobs are assumed to run through CMSSW**
  - Configured by the corresponding python-based file
- **All inputs and outputs are assumed to be EDM files** (with a few special cases)
- **CMSSW software and corresponding externals are made available on worker nodes through CVMFS**
  - Distributes http-based read-only filesystem
- **CMS software evolution and multi-threading pose severe challenges to old/legacy MC software**
  - CMS has to produce MC events compatible to each collected dataset, even after many years the data was taken
  - Often ad-hoc "features" needed, difficult to mantain



(*)cfr CHEP 2016 talk "Software and Experience with Managing Workflows for the Computing Operation of the CMS Experiment" by J.-R. Vlimant

MC production workflows in CMS

- **Basic paradigm for event generation**
  - C++ module making calls to linked external generator code to produce, for each event, HepMC::GenEvent to be stored as EDM
- **Matrix element generators produce LHE files** (Madgraph, POWHEG, …)
  - Loosely coupled to CMSSW, calling of external generation script handled by CMSSW module "externalLHEProducer"
  - ASCII LHE files are transient and immediately packed into binary compressed format
- **Parton shower programs finalize the full event properties** (Pythia, Herwig, Sherpa)
  - Fully integrated as "externals" and packaged or linked directly from CMSSW interfaces



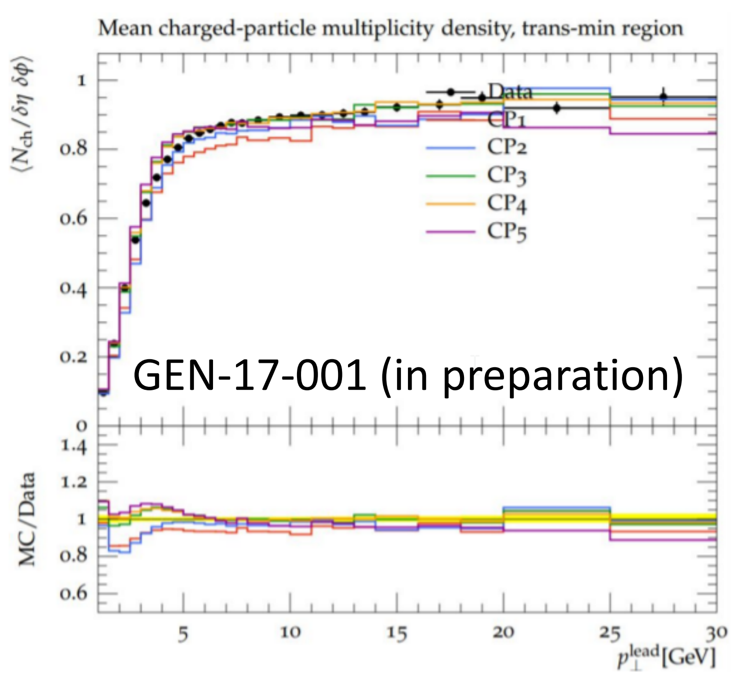
Gridpacks

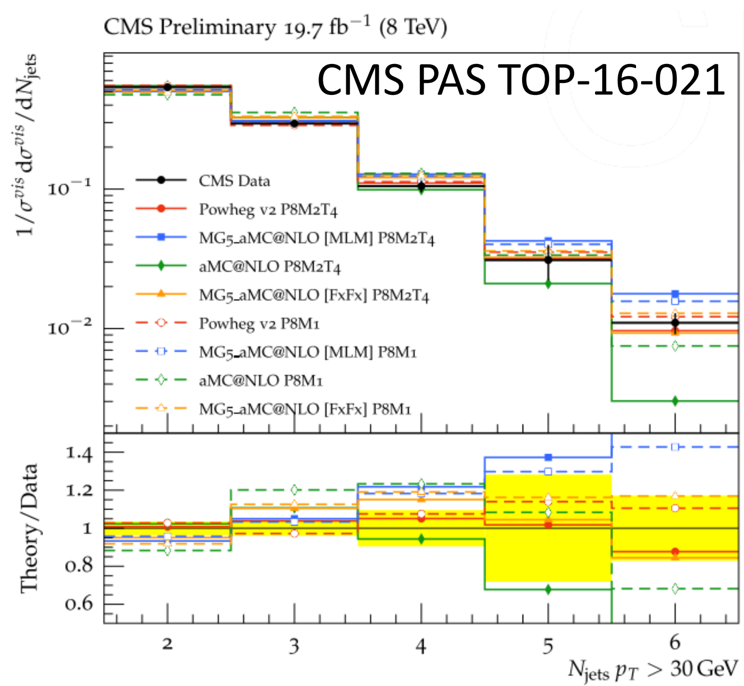
- **Matrix element generators typically have two discrete steps:**
  - Matrix element/code generation and phase space integration
  - Generation of events
- **Compiled code and results of the phase space generation stored into gridpacks**
  - For efficient generation of events on the grid
  - Largely self-contained tarballs prepared in advance and stored on CVMFS
  - Modeled on the built-in generator functionalities or through dedicated scripts
    - Maintaince of scripts for all the major generators (MG5 aMC, POWHEG, Sherpa, etc) can be quite heavy
  - Gridpack production is the default and most widely supported mechanism in CMS for Run 2
- **Gridpack preparation done exploiting batch-job parallelism (LSF or Condor)**
  - Compiling code on batch workers and long init time for event generation discouraged
  - Gridpack size can be an issue (>500MB for the tarball and 5GB decompressed)
  - Gridpack generation step needs reliability and reasonable run-time “as the physicist waits”
  - Recent and important developments through HTCondor Global Pool infrastructure(*)
- **Grid jobs using gridpacks from CVMFS can generate events with trivial process-level parallelization**

(*)cfr Poster “Producing Madgraph5_aMC@NLO gridpacks and using TensorFlow GPU resources in the CMS HTCondor Global Pool” by K.H. Anampa

Evolution of generators and tunes

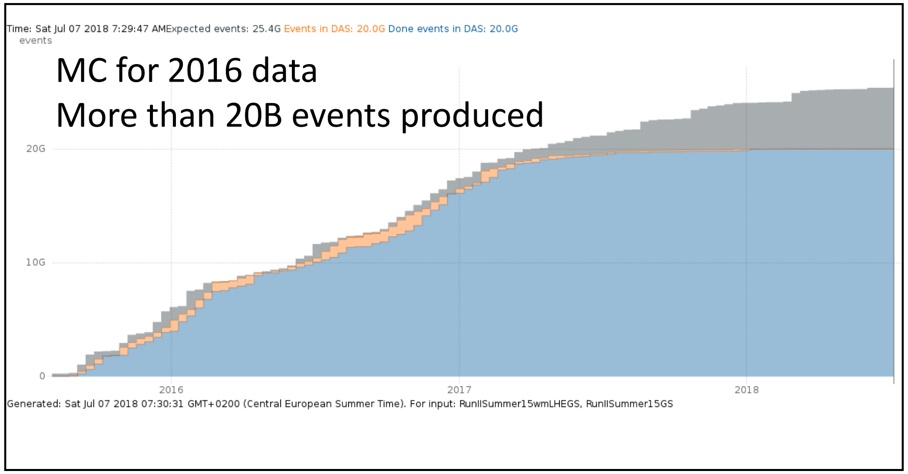
- **Major changes in generator releases, PDF versions and generator tunes for 2017 data**
  - New tunes (GEN-17-001, in preparation) and PDF (NNPDF3.1) derived to include 13 TeV data
    - Previous major update in 2014, based on 7 TeV data
  - Better Underlying event and jet multiplicity description
- **Such updates require careful planning and coordinated effort lasting several months**
  - Careful validation of generators and production setups
  - Large scale production of O(10K) gridpacks
- **Next major goal: coherent MC production with same settings for the full Run 2**

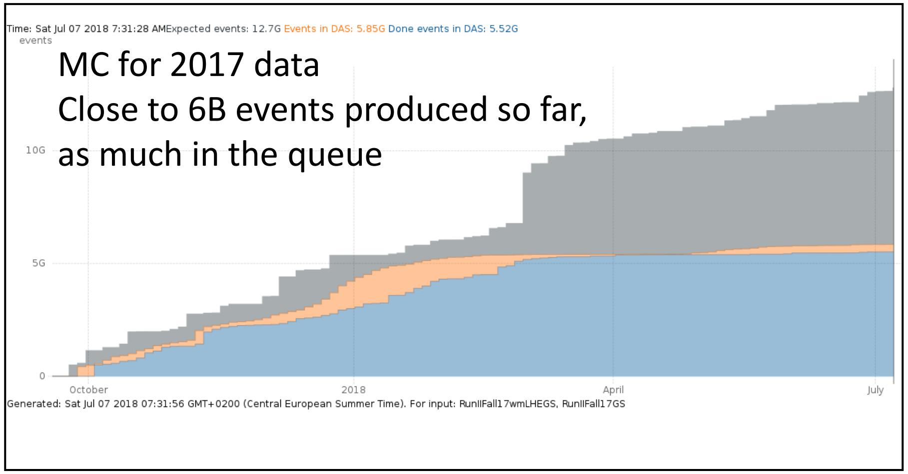




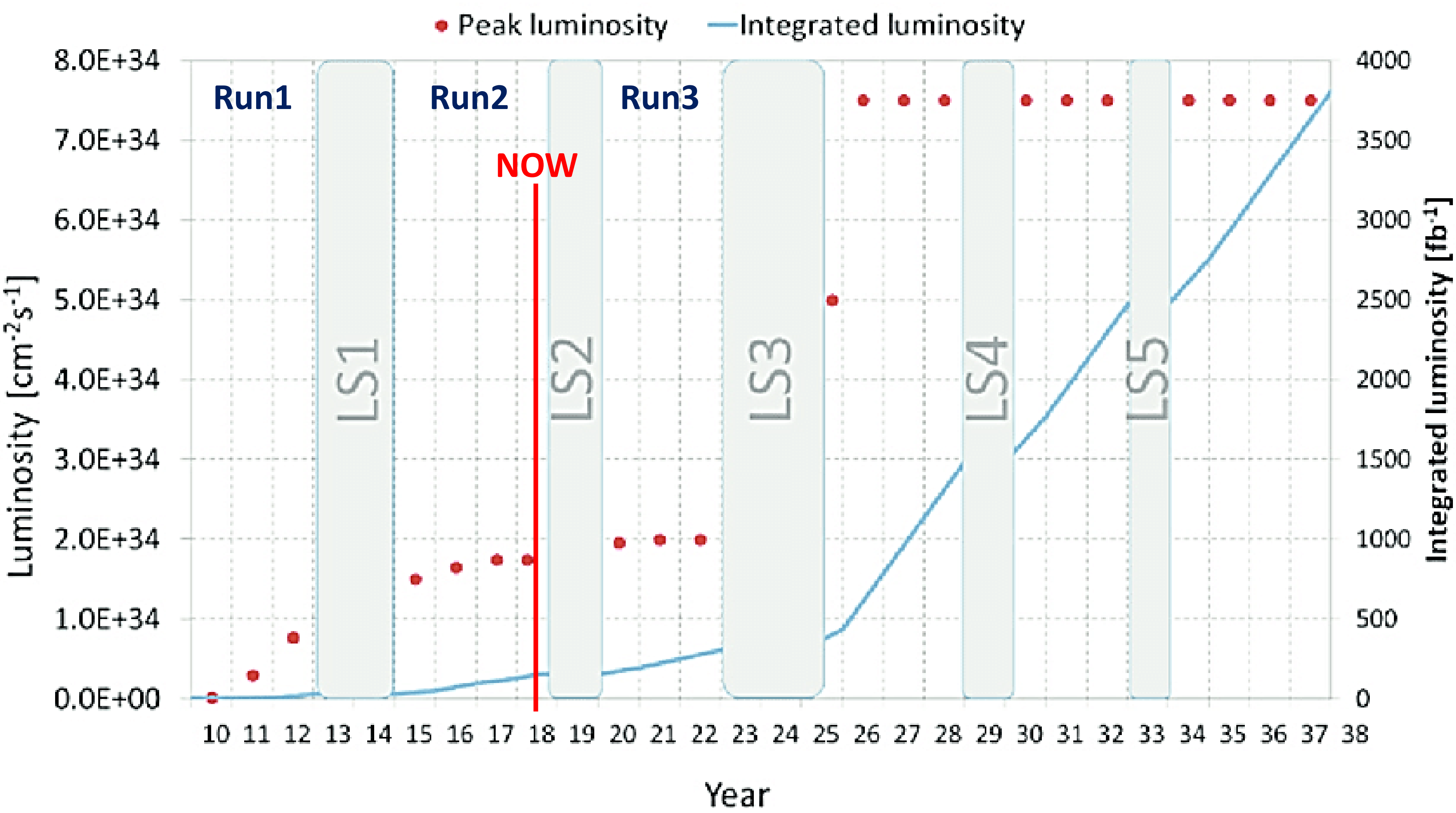
LHC Run2 experience in a nutshell

- **Computing resources planned ~1.5-2y in advance**
  - Current CMS MC budget is O(10-15B) events per year, O(10K) different requests
  - Competing resources with data taking, re-processing, upgrade and validation samples
  - Budgets do NOT scale linearly with LHC performance and effective integrated luminosity…
- **Start to plan each MC production campaigns O(6) months in advance**
  - Generator configurations and tunes, software version, reco conditions and corrections, production workflows need to be fully validated under time pressure
- **Moving more and more from fully inclusive datasets to fully exclusive datasets**
  - We'll have to make this work with more efficient slicing and weighting
  - Switching from search to precision: higher precision (NLO) requires higher resources…





Towards Run3 and beyond: it will only get worse



MC priorities and budgets from now to Run3

- **MC planning driven by physics priorities**
- **Physics priorities driven by machine conditions**
  - No major center of mass energy jumps
    - 13 to 14 TeV will not be a dramatic increase as from 8 to 13 TeV
  - Once "bulk of the distributions" explored, focus on "tails" of phase space
    - Notable exceptions are ultimate precision SM measurements
      - e.g. Weak mixing angle, top mass, W mass
- **Need to "fight" against conflicting requirements:**
  - (Much) larger datasets
  - Increased measurement precision
  - Need for alternative samples to estimate systematics uncertainties
    - Different generators or parameters
  - Flattening of computing resources (both cpu and disk space)
- **Need to find an evolution "model" that scales already for end of Run2**
  - Run2 is collecting >5 times data wrt Run1
  - Favor cpu (i.e. don't store LHE, "cheap" to reproduce) wrt disk occupancy
  - Store slimmed dataformats like MINIAOD and NANOAOD(*)

(*)cfr Talk "A further reduction in CMS event data for analysis: the NANOAOD format" by A. Rizzi

Generator technical developments: desiderata

- **A vast program of MC software improvement must be pursued in the next 5 years**
  - This can't be left on the shoulders of theorists and MC builders, and must be tackled community-wide
  - A community white paper has been issued to illustrate possible avenues[(*)]

- **Examples of needed technical improvements:**
  - Faster phase space integration
  - Drastic reduction of fraction of events with negative weights for NLO precision
    - E.g. folding of the integration phase space implemented in POWHEG
  - Drastic increase of the matching efficiency (currently ~30%)
  - Continue pursuing reduction of memory consumption to match higher jets and parallelization
    - Currently up to 4j at LO, up to 2j at NLO (expected more with low memomy multicore option)
  - Complete integration of process independent NLO QCD x EWK corrections
    - Up to high multiplicity final states , for both virtual and real contributions
    - Properly interfaced to parton shower
  - Bias weights for both LO and NLO
    - Produce inclusive samples with enriched statistics for specific phase spaces
  - Large flexibility for LHE level cuts for both LO and NLO
    - HT, VpT, number of additional jets, VBF-like, etc
  - Massive use of events weights for systematic uncertainties
    - Routinely used in Matrix Elements for PDF and perturbative QCD scales
    - Recent Pythia8 versions support weights for parton shower systematics
  - Single-gridpack parameter scan
    - Especially for BSM scans, so far very high number of gridpacks required

[(*)]cfr Talk "The HEP Software Foundation Community White Paper" by M. Jouvin

Conclusions

- **Monte Carlo Generators are an essential aspect of the Physics program of every experiment**
  - LHC is not an exception
- **Robust software and computing infrastructure essential to satisfy physics needs and goals**
  - Several challenges posed by the large amount of data collected and long timescale required for the MC to be available/reproducible
- **Need to find evolution "models" that scale for the future**
- **Experiments need to work in close contact with MC authors to improve program performance, precision and flexibility**
  - Community white paper issued recently

Backup slides

Multi-leg generators and gridpacks

- Several Monte Carlo generators have the capability to automatically generate matrix elements at LO for several jet multiplicities
- Results can be consistently combined across multiplicities when treated consistently in parton shower
- Most widely used configuration in CMS Run 2: Madgraph aMC@NLO (LO) + Pythia 8 with MLM matching
- Most complex processes with up to 4 additional jets
- CPU time up to about 10s per matrix element event (averaged over jet multiplicities), with O(10%) matching efficiency at the parton shower step → 100s cpu for matrix element per fully-simulated event

NLO Multi-leg generators

- A few Monte Carlo generators now have the capability to (semi)-automatically generate matrix elements at NLO in QCD for several jet multiplicites and consistently merge them
- Most widely used configuration in CMS Run2: Madgraph aMC@NLO (NLO) + Pythia 8 with FXFX merging
- At NLO in QCD, each multiplicity consists of born, real, and virtual contributions to the matrix element
- Most complex processes with up to two additional jets at NLO
- CPU time scaling up to to ~ 30 s per ME event with matching efficiencies of ~ 30% → 90 s of cpu time for matrix element per fully-simulated event
- Events are also accompanied by a possibly large fraction of negative weights (up to 40%) which reduces statistical precision and necessitates larger samples
- Diagram/code generation also very CPU and memory intensive → recent contribution to 2.4.x series to significantly improve (thread-level) parallelization and memory footprint of this step, eventually enabling more complex processes

Example CMSSW GEN Configuration Fragment

```
import FWCore.ParameterSet.Config as cms

from Configuration.Generator.Pythia8CommonSettings_cfi import *
from Configuration.Generator.Pythia8CUEP8M1Settings_cfi import *

generator = cms.EDFilter("Pythia8GeneratorFilter",
  maxEventsToPrint = cms.untracked.int32(1),
  pythiaPylistVerbosity = cms.untracked.int32(1),
  filterEfficiency = cms.untracked.double(1.0),
  pythiaHepMCVerbosity = cms.untracked.bool(False),
  comEnergy = cms.double(13000.0),

  crossSection = cms.untracked.double(1.92043e+07),

  PythiaParameters = cms.PSet(
    pythia8CommonSettingsBlock,
    pythia8CUEP8M1SettingsBlock,
    processParameters = cms.vstring(
      'HardQCD:all = on',
      'PhaseSpace:pTHatMin = 50  ',
      'PhaseSpace:pTHatMax = 80  ',
    ),
    parameterSets = cms.vstring('pythia8CommonSettings',
                                'pythia8CUEP8M1Settings',
                                'processParameters',
                               )
  )
)
```

CMS Software: LHE Input

- CMS maintains its own LHE parser (based on xerces-c xml library)
- An LHE file can be read as input to a CMSSW job and is converted on the fly to C++ classes LHERunInfoProduct and LHEEventInfoProduct which store the relevant information and can be stored/read from EDM files (support for per-event weights added to CMS lhe parser and classes)
- LHE information can be passed as input to a hadronizer as part of the event generation step in CMSSW (using for example the Pythia8::LHAup mechanism to pass the needed information on the fly in memory)
- LHE parsers included with Pythia, Herwig etc are not used
  - Advantage: Uniform hadronizer-independent storage and access to lhe information
  - Disadvantage: We have to maintain our own LHE parser
- CMS production tools do not work transparently with ascii LHE input (metadata not automatically available in data management system, skipping of events is inefficient, etc)
- It is possible to use privately produced LHE files for central production (user copies the files to eos and then a conversion step is run to produce EDM files containing the LHE products, which can then be used for further production steps for hadronization, simulation, etc)
- Disk space, file corruption, etc, are major issues when dealing with large sets of LHE files in this way

Parameter Scans

- Recently added some functionality in CMSSW for parameter scans (used so far for SUSY signal MC)
- SUSY signal production with MG5 aMC@NLO + Pythia 8 (LO MLM)
- Typical case: gluino/squark pair production (+0,1,2 jets LO) in MG5 aMC@NLO, decay in Pythia, steered by SLHA table
- Gridpack and pythia configuration+SLHA table for decays are randomly selected for each luminosity section ($\sim$ 200 events after matching)
- Resulting sample contains a mixture of all scan points
- High granularity of randomization ensures missing events from job failures are randomly and $\sim$ evenly distributed across scan points