Modernizing and improving simulators for HEP – Pythia, EvtGen

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MONASH University

Warwick RSE meeting
November 10, 2022

WARWICK
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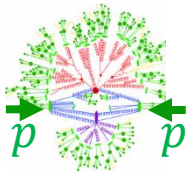
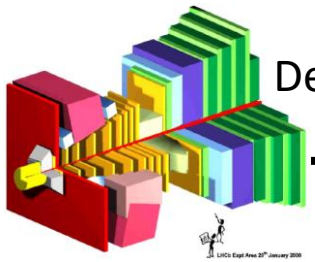
Overview

Simulation is essential since we interpret measurements by comparing simulation with collision data
⇒ Ideally, simulation should mirror data differing only by the knowledge of the “truth”.

Data

Collision





Detector

Electronics → Hardware trigger

Simplified conceptual sketch for LHCb Run I + II

Software trigger → Reconstruction → Stripping

Moore — Brunel — DaVinci

Turbo lines → Physics analysis

ROOT, Numpy, …

Simulation

Event generation → Interaction of particles with detector material → Detector response

Geant 4 — Boole

This talk

Collision and production → Decay

Pythia — EvtGen

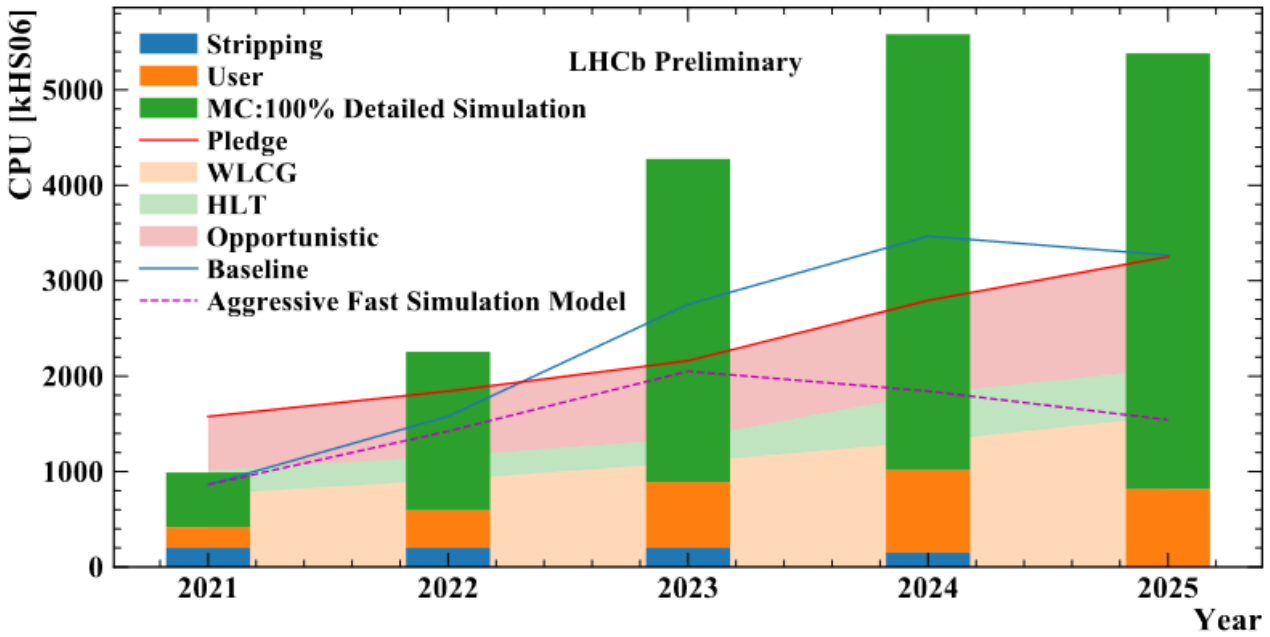
Gauss

Monte Carlo

Simulation is produced by a collection of specialized packages performing various assumptions and approximations depending on specifications

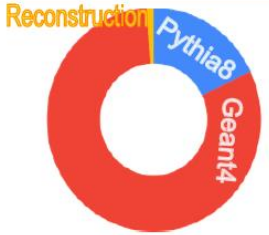
How much CPU does simulation consume?

LHCb-FIGURE-2019-018



Today

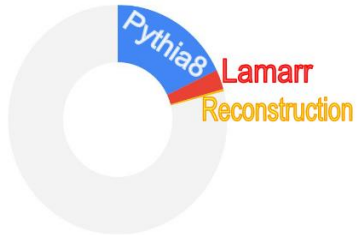
Detailed simulation: Pythia8 + Geant4
1M events @ 2.5 kHS06.s/event ≈ 80 HS06.y



Geant4: detailed simulation of interaction with detector material

Eventually in the future

Ultra-fast simulation: Pythia8 + Lamarr
1 M events @ 0.5 kHS06.s/event ≈ 15 HS06.y



Lamarr: simulation of detector response based on neural networks

- CPU consumption of generators (and analysis tools) not yet critical in general
- But developments in full sim (e.g. use of parametric sim) could soon change the picture
- Hardware developments (hyperthreading, GPUs, etc) call for modernization

Pythia

Ulrik Egede, Tom Hadavizadeh, Philip Ilten,
Minni Singla, Peter Skands

- General purpose generator for simulation of collision events of particles (electrons, protons, photons, heavy nuclei) at high-energies.
- Contains models for several aspects: hard/soft interactions, parton distributions, initial/final-state parton showers, multiparton interactions, fragmentation and decay.

Heavy (double heavy) hadron production occurs in only a (small) fraction of pp collisions
Simulation in Pythia is very inefficient (just keep trying until one is produced)
$\Rightarrow$ Currently working on different aspects aimed at making simulation of b-hadrons faster:

- B enhancement
- Forced hadronization/Doubly-heavy hadrons
- Optimize simulation for color-reconnection modes

MWAPP meeting
Tuesday 25 Oct 2022, 08:00 → 10:10 Europe/London

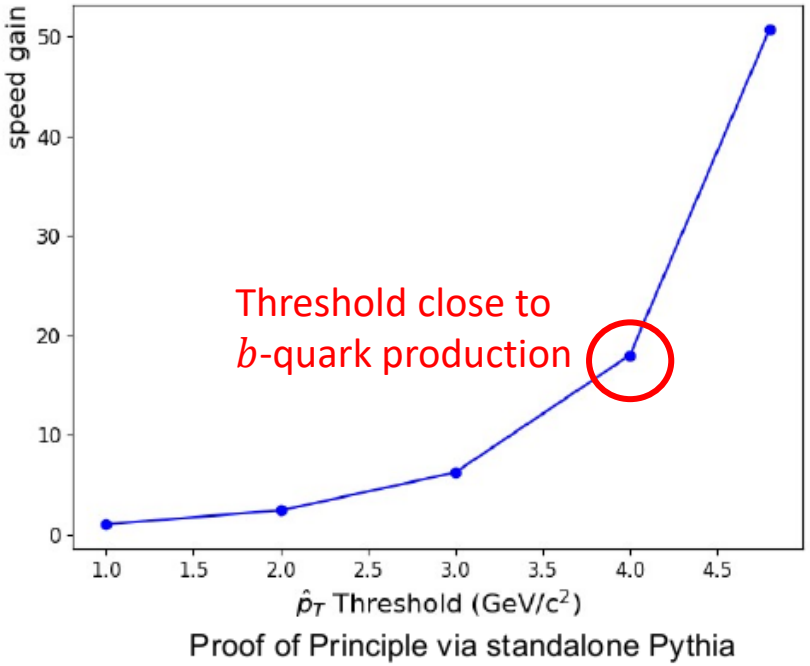
Fields with potential active collaboration with Monash

B enhancement

- Particularly when current generator exceeds CPU use wrt. detector simulation

$\Rightarrow$ Veto partons below p_{T} threshold

- Module made flexible for user to enhance $g \to c\bar{c}, b\bar{b}$ splitting
- Should be kinematically unbiased



Proof of Principle via standalone Pythia

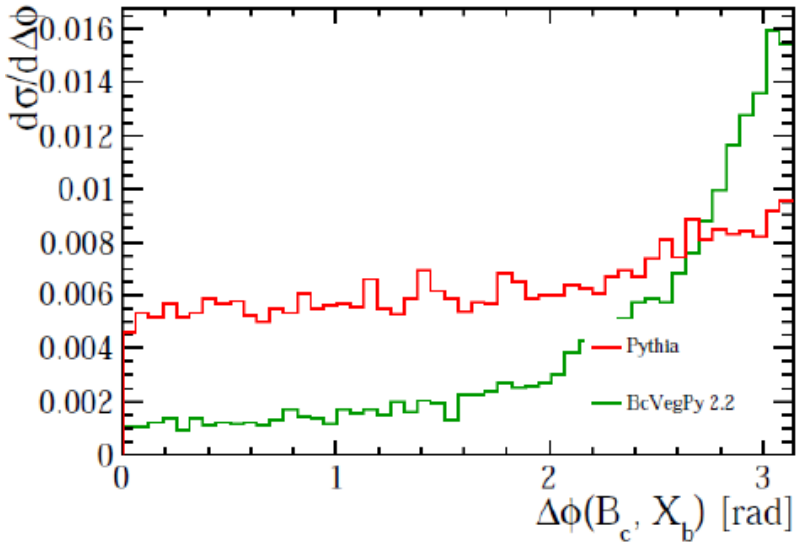
Double-heavy hadrons

- Production currently very inefficient in Pythia

$\Rightarrow$ Study vetoes based on presence of correctly colour-connected heavy quarks at early stages

- Currently comparing geometrical B_c distributions with dedicated generators like BcVegPy with limited list of supported production mechanisms

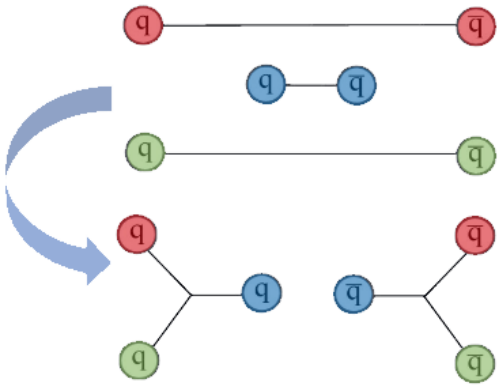
$\Delta\phi$: angle between B_c and $X_{b(c)}$ hadron on transverse plane



Improving color-reconnection models

- QCD-based color-reconnection models with junction agree well with collision data (without particular tuning)

CR junction: choose "shortest" string configuration



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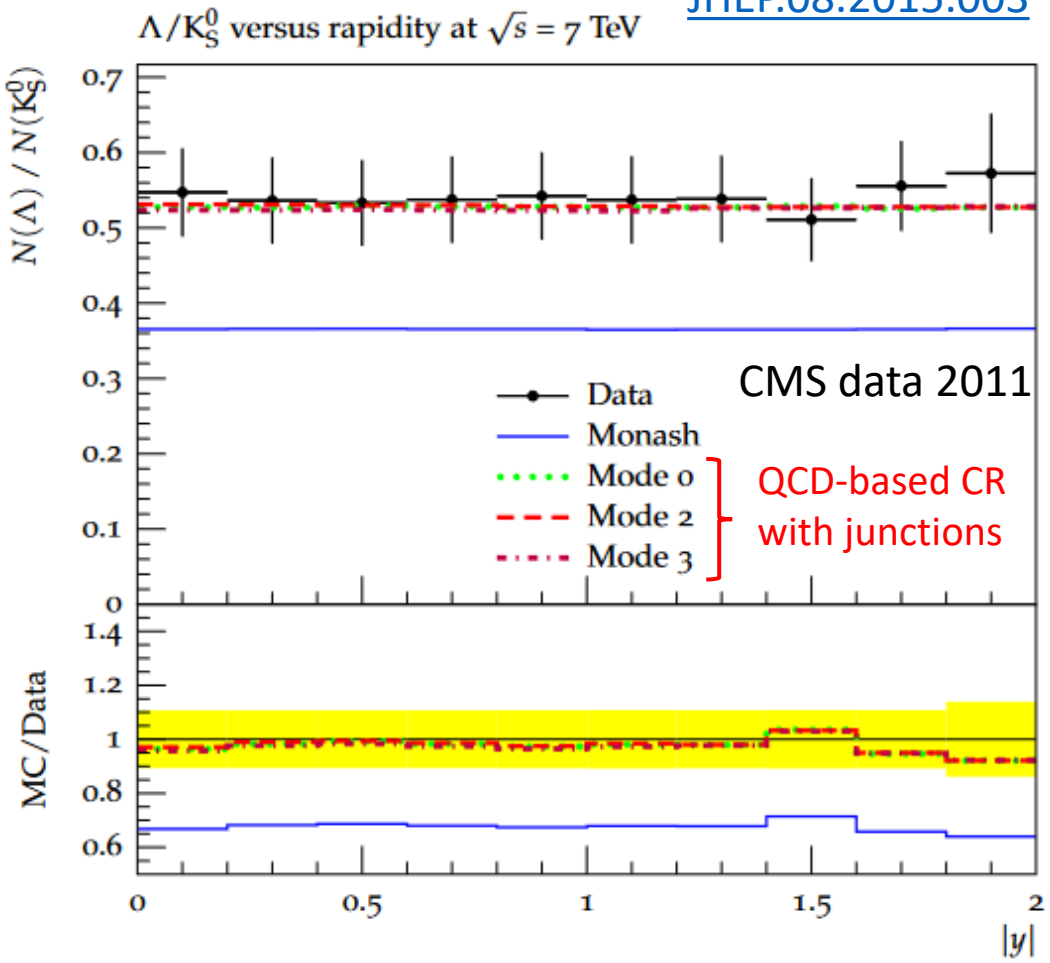


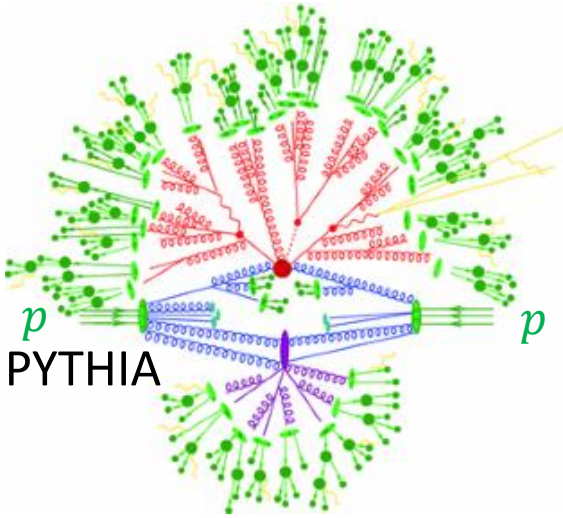
- However inefficient and CPU expensive
- Structural changes and efficient alternative (Hungarian algorithm) for minimization identified
- Need to be implemented and tested, but promising for enhancement of baryon production

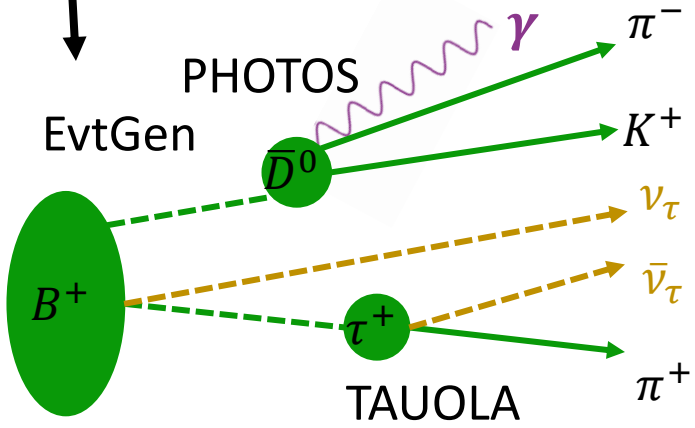
EvtGen

- Generator package specialised for heavy-flavour hadron decays
  - Used as well inside simulation of b jets
- Contains about 130 decay models implementing specific dynamics of various decays
- Maintains detailed decay table with large number of explicit decays
- τ decays simulated using TAUOLA
- PHOTOS used for simulation of final-state radiation

External

- Developed in the 90's, stable over past 10 years (changes mostly additions of new models)





Plans for EvtGen

- Physics wise no plan for changes in near future
- Currently working on code consolidation
  - Unify coding style, C++ modernisation
  - Plan to decrease code duplication within decay models
  - Improve/Update documentation (Doxygen and paper/guide)
  - Implemented common testing framework for validation
- Currently making EvtGen thread safe
  - Event ≙ particle whose decay is simulated (through full decay chain)
  - Main blockers are TAUOLA and PHOTOS, which are not yet thread safe
  - Work on source-code redesign currently ongoing with help of RSE engineers
  - Full adaptation is challenging (first core code adaptation almost finalized)

Heather Ratcliffe
Chris Brady

Progress on thread-safety

- Internal challenges: global instances (random number generator, particle properties and decay table)
- External challenges: limitations from dependences (TAUOLA, PHOTOS)

Set of solutions to reach thread-safety (preliminary):

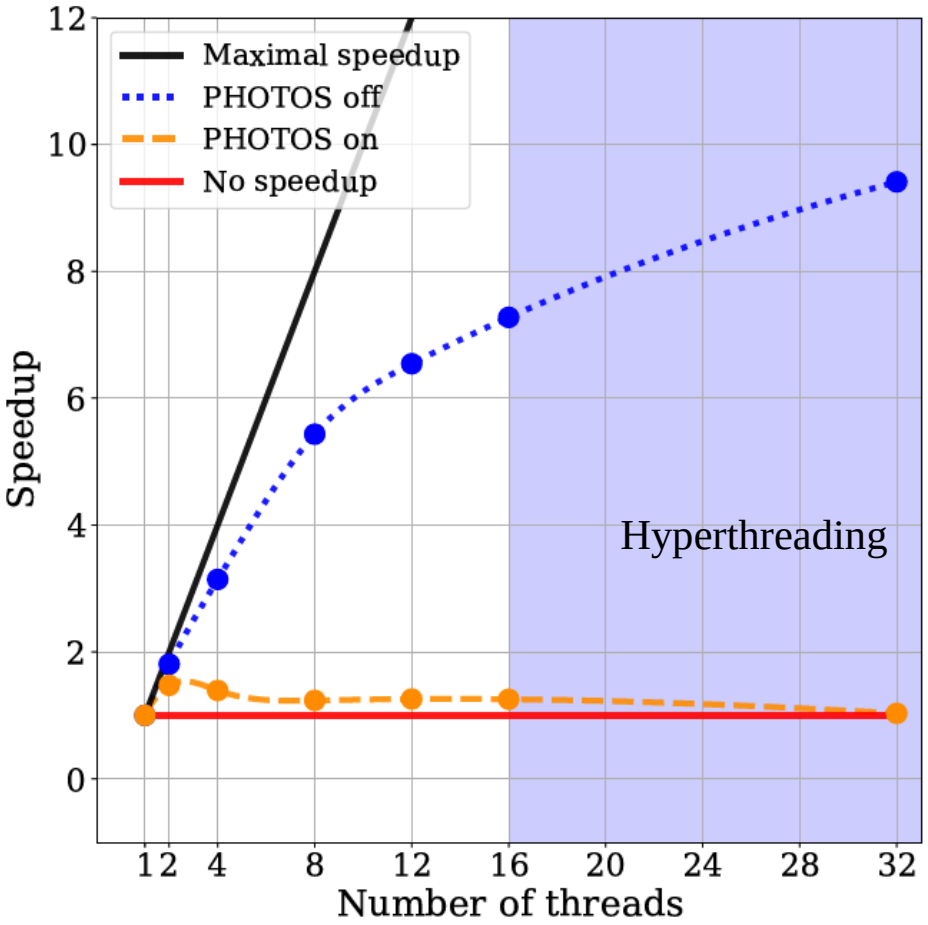
- Converted **static** objects to **static const** where possible
- Global singleton objects made thread-local
- Serialized (mutexed) calls to PHOTOS and TAUOLA

⇒ Deeper structural changes needed to fully exploit multi-threading (plan to continue working on it)

⇒ Current preliminary status reached thread-safety, passing physics tests for all decay models

⇒ But performance limited by external dependencies

⇒ Overcoming limitations from dependencies are more challenging as they are external (exploring alternatives)



Summary and outlook

Pythia:

- Working on enhancement of b-hadron production to make simulation faster
- Exploring how to improve efficiency for events with multiple heavy quarks

EvtGen:

- Currently making EvtGen threadsafe

$\Rightarrow$ Finalized common testing framework for validation

$\Rightarrow$ Converged on preliminary set of solutions to enable thread-safety of generator (exploitation of multi-threading will require further structural changes)

$\Rightarrow$ Performance limited by external dependencies (exploring alternatives)