EvtGen and Pythia developments

EvtGen

Fernando Abudinén, John Back, Michal Kreps, Thomas Latham

Pythia

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



SwiftHep workshop November 21, 2023



Recap on EvtGen

- <u>EvtGen</u>: 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
 - Known decay branching fractions do not add up to 100%; Remainder is filled up by generating quark configurations and passing those to <u>Pythia8</u> for fragmentation
 - Fraction of decays passed to Pythia8 depends on particle (*b*-baryons rely more on Pythia8 than others)
- τ decays simulated using <u>TAUOLA</u>
- Final-state radiation (FSR) simulated using <u>PHOTOS</u>

Example collision simulated by Pythia8



Status

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

Challenges for updates

- Various code styles across models (due to contributions from various authors)
- Several code duplications across models (often same kinematics but different form factors)
- Experiments (main users) need generators to be thread-safe as they are moving their simulation frameworks towards multithreading to exploit modern CPUs

Recent developments

- Work on modernisation and clean-up
- First adaptation of core code towards thread safety (with help of software engineers)
- Implemented global testing framework for validation
- Studies of alternatives for τ and FSR simulation New!

Heather Ratcliffe

Chris Brady

Plans

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)
 - Improve method to update decay table

- Continue work towards thread safety
 - On alternatives for external dependencies that are not yet thread safe (TAUOLA and PHOTOS)
 - Implementing full adaptation of internal code redesign

Testing framework

- Simulation needs testing and validation after structural changes due to code consolidation and implementation of thread safety
- Tests (in different formats) existed only for about 40% of the 130 decay models
- Migrated all tests and added new ones to a common testing framework
 - \Rightarrow With common testing module and configuration files
- Finalized first working version with tests for all models
- Some models support various configurations
- \Rightarrow More tests needed to cover all configurations
- \Rightarrow Will require to add new tests for each new model



Testing framework

Implemented automatic recognition of tests to be run depending on changes

- Identify files modified in a commit
- If files associated with a model changed ⇒ run respective tests
- If framework files changed ⇒ run all tests
- Issue: Gitlab BEFORE_SHA variable not always set (for example when new branch created)

- git diff --numstat \$CI_COMMIT_BEFORE_SHA \$CI_COMMIT_SHA | awk '{print \$NF}' | xargs ./runTests.py Models.json SrcDeps.json

- \Rightarrow Use as reference best common ancestor commit
- git diff --numstat origin/master...\$CI_COMMIT_SHA | awk '{print \$NF}' | xargs ./runTests.py Models.json SrcDeps.json
- \Rightarrow Output files for reference will be used as comparison
- ⇒ Still need to establish storage of reference files (plan to use a separate GitLab project for storage)

Fixing of broken modules

- Testing framework helped uncover issues in models
- Repairing broken models has taken large fraction of recent effort
- Needs understanding and familiarisation with underlying dynamics
- \Rightarrow Contacting authors when possible
- Some models turned out to be obsolete (plan to remove those)

Fix initialisation

- Lb2Baryon1nu has prob of -nan and forward density matrix full of -nan . Solved in D91
- EvtSSD_DirectCP has prob > probmax for B+ -> f_2 pi+ (always 18.581 instead of 10.0). Solved in D92.
- BToDiBaryonlnupQCD__Bu_Deltappbarmunu.out has prob > probmax.
- BC_VNPI=VLL__Bc_psi2Spipipi_mumu.out has prob > probmax.
- PROPSLPOLE=VSS_D+_Kst0enu_Kpi.out needs easy fix removing if statement

Fix treatment of pole and initialisation

- VTOSLL=PHSP__Dst0_D0ee_Kpi.out has prob > probmax for D*0 -> MyD0 e+ e- (various numbers). Solved in D97
- X38722-+_PSI_GAMMA=VSS=VLL__X3872_omegaJpsi_pipi,mumu.out Solved in D102
- X38722-+_PSI_GAMMA=VSS=VLL__X3872_rho0Jpsi_pipi,mumu.out Solved in **D102**.
- BTOXELNU=VSS__Bu_rho0munu_pipi.out

New!

| | a open monas Latian requested to merge tratnam_1200 to moster 2 weeks ago | |
|--------------|---|--|
| 0 | Overview 1 Commits 5 Pipelines 2 Changes 43 | |
| As d | As described in T200, there are various obsolete or broken models, which should be removed. | |
| Mod | els removed (along with relevant tests, documentation entries, etc.): | |
| \checkmark | EvtBHadronic | |
| \checkmark | EvtMultibody | |
| ~ | EvtLb2Lll | |
| ~ | EvtVPHOtoV | |
| \checkmark | EvtVPHOtoVISR | |
| \checkmark | EvtLambdaB2LambdaV | |
| | EvtKstarstargamma | |
| | EvtbsToLLLL | |
| | EvtbsToLLLLHyperCP | |
| | Evtbs2llGommaISRFSR - to be retained | |
| | EvtVubAC | |
| Othe | er classes in EvtGenBase that are not used at all: | |
| | Evt3Rank3C | |
| | EvtAbsBinning | |
| | | |
| | EvtAmpAmpPdf | |
| | EvtAmpAmpPdf EvtAmpIndex | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex EvtBreitWignerPdf | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex EvtBreitWignerPdf EvtDecayParm | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex EvtBreitWignerPdf EvtDecayParm EvtIntegPdf1D | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex EvtBreitWignerPdf EvtDecayParm EvtIntegPdf1D EvtPointPred | |
| | EvtAmpAmpPdf EvtAmpIndex EvtAmpSubIndex EvtBreitWignerPdf EvtDecayParm EvtIntegPdf1D EvtPointPred EvtPropGounarisSakurai | |

Challenges for multithreading in EvtGen

Internal: structural limitations for multithreading inside EvtGen

- Global instance of random number generator
- Global instance of particle properties and decay table

⇒ Needed structural changes identified and first combination of solutions found

- External: limitations from dependences
 - TAUOLA
 - PHOTOS

⇒ Overcoming limitations from dependences are more challenging as they are external

- TAUOLA and PHOTOS authors currently exploring ways to enable thread safety
- Exploring use of Pythia8 as alternative to TAUOLA
- Exploring use of Vincia QED (Pythia8) shower and Sherpa's PHOTONS++ as alternative to PHOTOS New!

Progress on thread-safety

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 multithreading (plan to continue working on it)
- ⇒ Current preliminary status reached thread-safety, passing tests for all decay models
- \Rightarrow But performance limited by external dependencies



Heather Ratcliffe Chris Brady

Vincia QED shower for FSR

New! $I/\psi \rightarrow e^+e^-$ With help from GeV ---- VINCIA FSR of events per 0.02 10^{-1} - PHOTOS 10^{-2} 10^{-3} 10^{-4} Frac. 10^{-5} 0.5 1.5 $\operatorname{Sum}(E_{\gamma_{mn}})$ [GeV] $\rho^0 \rightarrow \pi^+ \pi^-$ Frac. of events per 0.01 GeV ·····VINCIA FSR -PHOTOS 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5} 0.2 0.4 0.6 0.8 $\operatorname{Sum}(E_{\gamma_{\text{ESP}}})$ [GeV] 10

Giacomo

Morgante

- Recently started exploring <u>Vincia's multipole QED shower</u> for hadron decays
- Vincia is embedded in Pythia8
- Algorithm implementation enables thread safety
- Can simulate $\gamma \rightarrow e^+e^-$ splitting (if turned on)
- \Rightarrow Developed EvtGen \leftrightarrow Vincia Interface based on existing dependency with Pythia8
- Currently exploring as alternative to PHOTOS
- Matrix-element corrections (form factors, etc) not implemented yet
- \Rightarrow A lot of room for improvement and validation
- \Rightarrow However, preliminary results look promising

Sherpa's PHOTONS++ for FSR

New!

- <u>PHOTONS++</u> in <u>Sherpa</u> can simulate emission of soft photons (to higher orders of perturbation theory)
- If switched on, also hard photons (to first order)
- Algorithm implementation enables thread safety
- \Rightarrow Can be explored as alternative to PHOTOS
- Recently started work on EvtGen \leftrightarrow Sherpa interface
- \Rightarrow Skeleton for interface ready
- ⇒ Need to implement event translation and transfer (currently in contact with M. Schönherr and co.)
- \Rightarrow Requires tuning (for instance of cut-off energy)
- \Rightarrow And validation of physics output



Energy of radiated soft photon

Pythia 8 for τ decays

- In addition to multithreading limitations, spin-state information of \u03c6 not propagated between EvtGen and TAUOLA:
 - needed for analyses sensitive to \(\tau\) polarization
- Simulation of \(\tau\) decays with spin-state propagation possible with PYTHIA8 using HME (helicity-matrix element) amplitude model.
- Main EvtGen ↔ Pythia interface ready
- Generalization of conversion of helicity/spin basis (and initialization) not yet finalized (interesting also for interface with TAUOLA)



Pythia status and plans

- 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.

Currently working on different aspects aimed at making simulation of *b*-hadron faster:

- B enhancement
- Doubly-heavy hadrons in Pythia

Progress scarce due to person power, but plan to pick up next year

Plans for future developments:

- Forced hadronization
- Optimizing simulation for colour-reconnection modes

B enhancement

- Goal: make b-hadron production faster (in LHCb simulation)
- Particularly important for cases where generator consumes more CPU time than detector simulation
- Examples: production of B_s , B_c , Ξ_{cc} , Ω_{bb}
- Produced *b*-hadrons should still be kinematically unbiased
- Module made flexible for user to enhance $g \rightarrow c\bar{c}, b\bar{b}$ splitting
- About to be ready to tested within LHCb simulation framework GAUSS



Double-heavy hadrons in Pythia

- Pythia currently not employed for B_c or other double heavy hadrons at LHCb
- Exploring ways to increase efficiency by vetoing events without desired heavy-quark composition at early simulation stage
- Possible vetoes based on presence of correctly colour-connected heavy quarks
- Currently comparing geometrical B_c distributions with dedicated generators like BcVegPy which currently has a limited list of supported production mechanisms
- $\Delta \phi$ sensitive to production mechanism
 - ⇒More mechanisms available in Pythia 8 and thus more uniform distributions



Improving colour-reconnection models

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

CR junction: choose "shortest" string configuration

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



Future plans

Simulation with more than one heavy-quark pair

- Currently investigating ways to improve efficiency of simulation for events with more than one heavy-quark pair produced in multiparton interactions
- Aim to study production mechanisms of quarkonia and compare simulated kinematic distributions with data

Forced hadronization

- Implement forced hadronization rather than current repeated hadronization
- Will make a considerable impact for events with baryons with multiple s like $\Omega_b(ssb)$
- Less significant impact expected for B^{\pm}, B^{0}

Summary and outlook

EvtGen:

- Continue work towards thread safety
- ⇒ Finalized common testing framework for validation
- ⇒ Converged on preliminary set of solutions to enable thread-safety of generator (full exploitation of multi-threading will require further structural changes)
- \Rightarrow Performance limited by external dependencies
- \Rightarrow Started exploring Vincia QED and Sherpa's PHOTONS++ as alternatives for FSR
- $\Rightarrow au$ decays: plan to iron out basis conversion for Pythia8 (interesting also for TAUOLA)

Pythia:

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

⇒ Plan to study production mechanisms and improve implementation of colourreconnection models