# Interfacing to specialized tools

Fernando Abudinén, John Back, Michal Kreps, Thomas Latham



MC support tools workshop

IPPP Durham April 03, 2025



## Outline

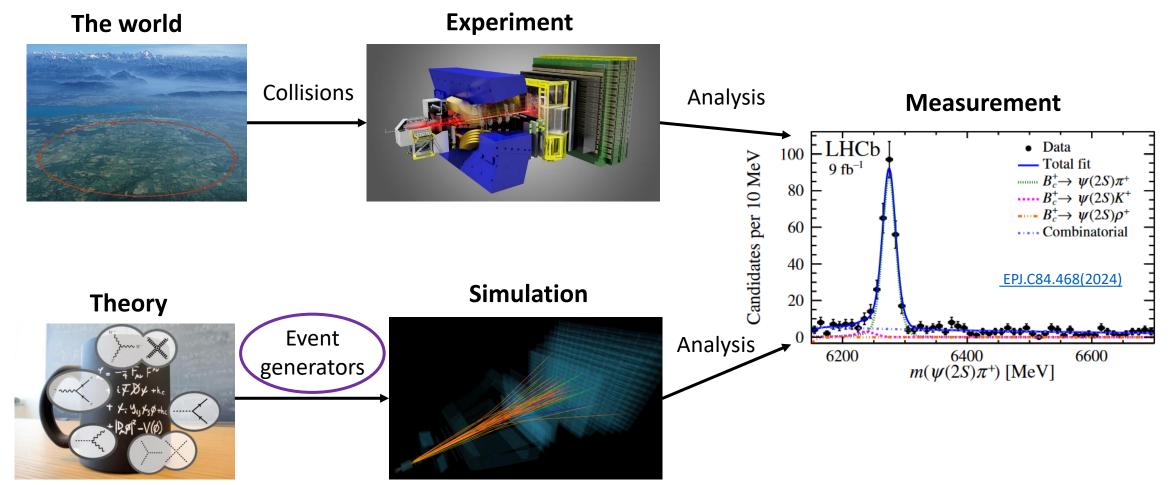
Introduction

Discussion from EvtGen's perspective on
 Decay weighting to study effect of alternative configurations
 Plugins for final-state radiation
 Propagating spin-information

## Introduction

# Simulation in high-energy physics

Essential since we interpret measurements by comparing simulation with collision data  $\Rightarrow$  Ideally, simulation should mirror data differing only by the knowledge of the "truth"

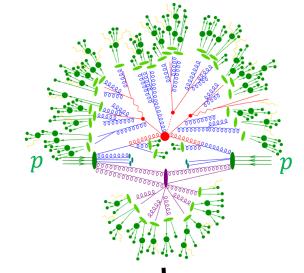


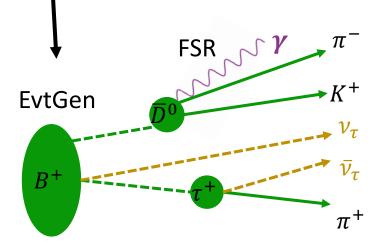
## The EvtGen generator

Simulation generator package specialised for decays of heavy particles containing b and c quarks.

- Implements detailed decay dynamics based on theoretical models
- Originally developed for BaBar and CLEO by Anders Ryd and David Lange
- Used in multiple high-energy physics experiments: ATLAS, Belle II, BES III, CMS, LHCb, ...

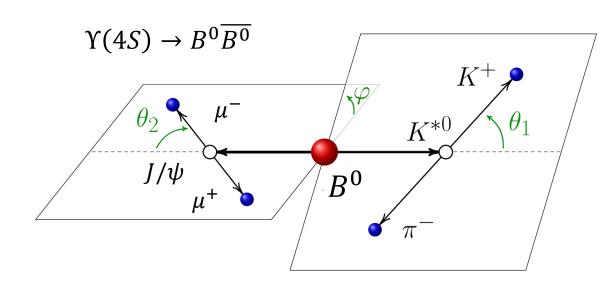
Example collision simulated by PYTHIA8



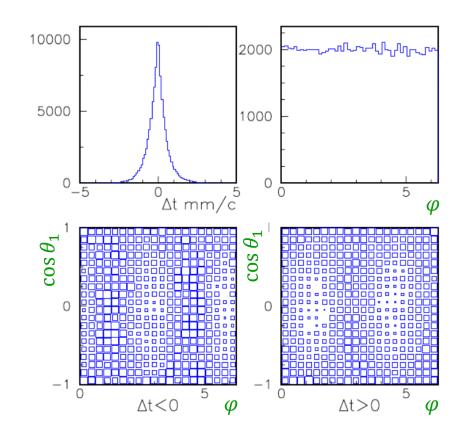


### Physics motivation

- Designed to handle complicated decay chains
- Account for dependencies between different observables

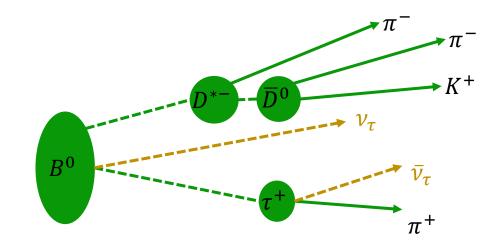


Example decay with *CP* violation and dependencies between decay time and angular observables.



# Decay Chains

Decays of heavy-flavour particles often involve many sequential decays

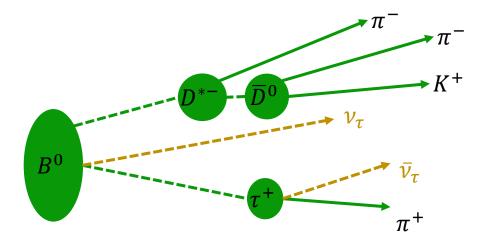


#### **Concept for a reusable generic tool**

- Simulate correctly the full decay chain implementing only individual nodes
- $\Rightarrow$  Use **decay amplitudes** instead of probabilities
- $\Rightarrow$  Make use of **modular design** in C++ implementation

## Decay amplitudes

- Use decay amplitudes to simulate sequences of decays
- Each node in the chain generated separately
  - $\Rightarrow$  Must be associated with a **decay model**
- Decay models provide the amplitudes
- Framework handles bookkeeping to generate full decay chain



#### Workflow

Generate kinematics of  $B^0$  according to phase space

Perform accept/reject based on  $P_B = \sum_{\lambda_D^* \lambda_\tau} \left| A_{\lambda_D^* \lambda_\tau}^{B \to D^* \tau \nu} \right|^2$  Propagate the spin-state information to subsequent decays through spin-density matrix

# Decay models

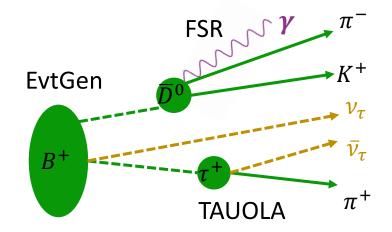
EvtGen contains about 130 decay models

- General purpose models
  - Based on particle spin properties
  - Or specified helicity/partial wave amplitudes
- Semileptonic models with form-factors
- Dalitz plot decays (generic and specific Dalitz models)
- Specific models for electroweak penguins / radiative decays
  - For example  $b \to s\ell\ell$ ,  $b \to s\gamma$
- Many models have versions including CP violation

## External dependencies

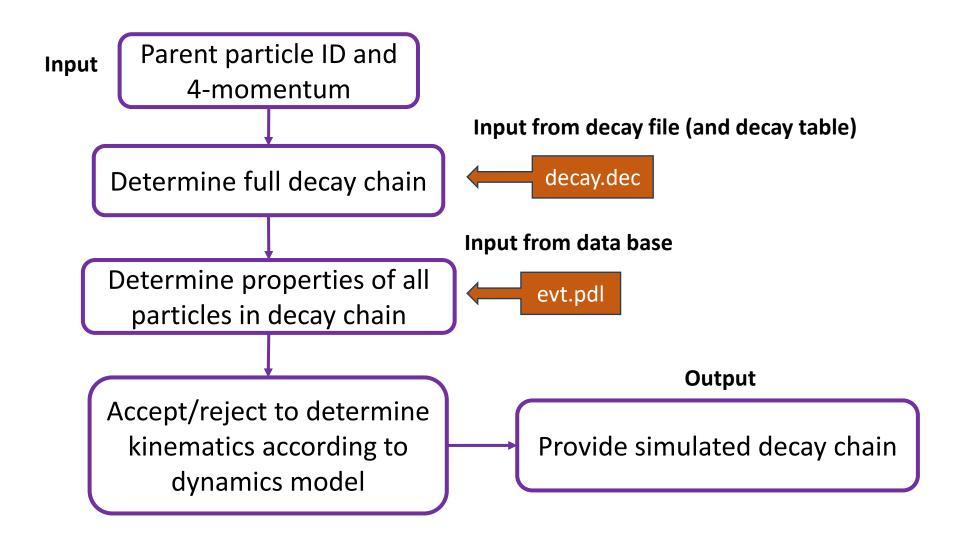
Interface with external packages for additional features

- HepMC for writing events in HepMC format (mandatory)
- Pythia8 for decays of generic quark configurations (optional)
- TAUOLA for decays of \(\tau\) particles (optional)
- PHOTOS for final-state photon radiation (FSR) (optional)
- PHOTONS++ for final-state photon radiation (FSR) (optional)



Inconsistencies can result from mixing other (typically Pythia) hadron models into another generator's decay chains (and unresponsive to tunes)

## EvtGen decay algorithm



## Decay files and decay table

**Decay files** determine the decay chain

- Specify decay modes and their branching fractions
- Specify decay models and their input parameters
- Can be provided as text (.dec) or XML file

Decay B0sig					
0.90 J/psi K*0	SVV_HELAMP Hp pHp Hz pHz Hm pHm;				
0.10 Jpsi K+ p	i- PHSP;				
Enddecay					

EvtGen maintains a generic decay table (DECAY.dec) with properties of  $\sim 10^4$  explicit decays

- Updated from PDG at intervals (nontrivial effort)
- When known branching fractions do not add up to 100%
  - $\Rightarrow$  Fill up remainder with generic quark configurations and pass to <u>Pythia8</u>
  - $\Rightarrow$  *b*-baryons rely more on Pythia8 than other particles

## Decay table and custom IDs

- General Decay table does not consider uncertainties in branching fractions
- Each user can have custom general Decay table
- Currently no possibility to provide uncertainty or weighting variation for decays
- Challenges: Inconsistencies, PDG BFs not adding up to 1, theory uncertainties (form factors, etc)
- Particle ID standards: some particle IDs used in EvtGen are outside the standard range
- First step would be to support alternative BFs

#### Example from general Decay table

Decay B0				
# # b -> s gamma #				
0.0003118 Xsd g #	gamma	BTOXSGAMMA	2	;
Decay Xsd 1.00000 d anti-s PYTHIA 42; Enddecay				

#### Interface between EvtGen and Pythia

- EvtGen calls Pythia to decay and hadronise quark configurations in some cases
- Nothing to be put into the event record before Pythia simulation
- Direct translation of EvtGen objects into Pythia event (and back)
- Needs interplay between generators (making sure to avoid double counting)
- Needs matching of particle properties and decay table.

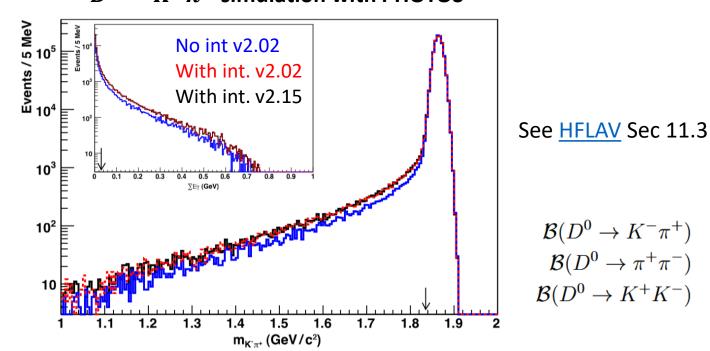
#### **Example from general Decay table**

Decay Omega\_b-SemiLeptonic Decays # 0.05460 Omega\_c0 anti-nu\_e PHSP; e -0.05460 Omega\_c0 anti-nu\_mu PHSP; mu-0.02000 Omega\_c0 anti-nu\_tau PHSP; tau-# Hadronic Decays with Xi\_c+ 0.00600 PHSP: Omega\_c0 pi-0.02200 Omega\_c0 PHSP; pipi+ pi-PHSP; 0.00055 Omega\_c0 К-0.02200 Omega\_c0 D\_s-PHSP; 0.0011 DO Xi-PHSP; # 0.00047 Omega-J/psi PHSP; psi(2S) 0.00038 Omega-PHSP; filling out with inclusives # 0.68192 d anti-u s cs\_0 PYTHIA 43; 0.10910 d anti-u d cs\_0 PYTHIA 43; 0.02728 d anti-u s su\_0 PYTHIA 43; Enddecay

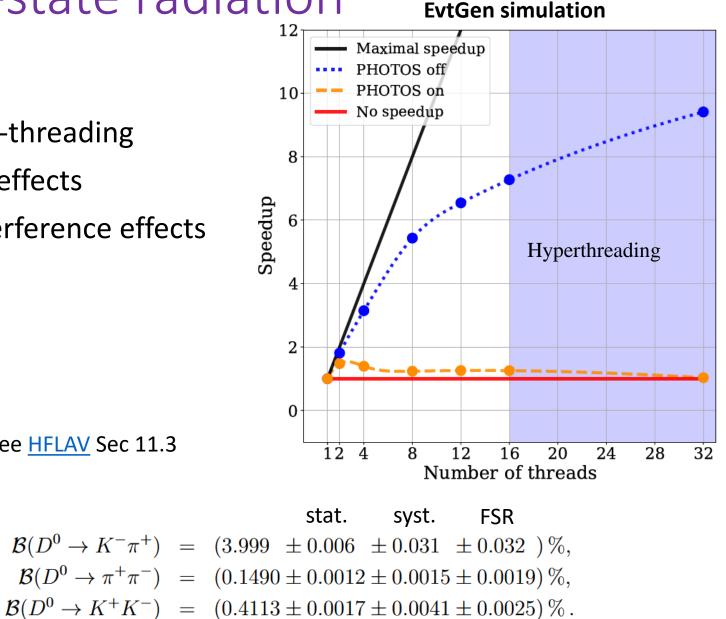
### Studies of final-state radiation

### Alternatives for final-state radiation

- FSR is main limitation to exploit multi-threading
- Find alternatives to study systematic effects
- $\Rightarrow$  Especially those associated with interference effects



#### $D^0 \rightarrow K^+ \pi^-$ simulation with PHOTOS



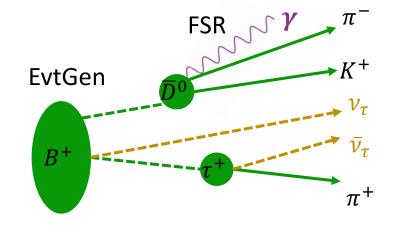
## Final-state radiation in EvtGen

- EvtGen relies on external specialised generators to add QED FSR corrections
- Generators generally treat the effect of FSR as a multiplicative correction to the decay rate

 $d\Gamma^{\text{radiative}} = d\Gamma^{\text{Born}} f(\Phi) d\Phi$ 

 $\Phi$ : Phase-space of photons

- Generators add photons (accept/reject) based on  $f(\Phi)$
- Default generator is <u>PHOTOS</u>
- Recently included Sherpa's <u>PHOTONS++</u> as alternative
- Currently developing <u>Vincia</u> (inside Pythia8) as alternative



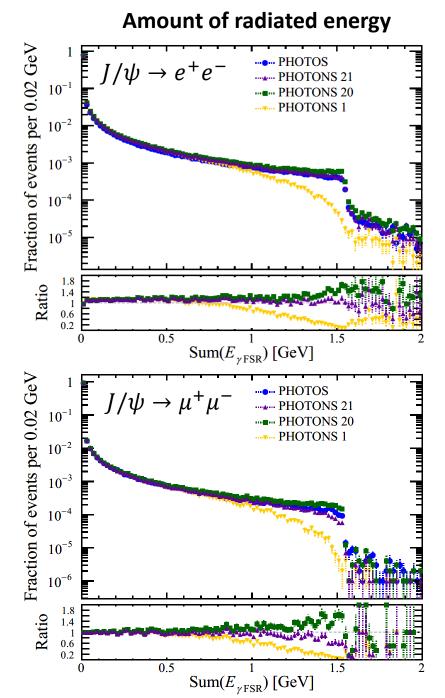
Decay D0sig	
0.0390 K- pi+	PHOTOS PHSP;
Enddecay	
CDecay anti-D0sig	

PHOTOS flag deprecated with FSR flag in EvtGen r3.X.X

# Sherpa's PHOTONS++ for FSR

- <u>PHOTONS++</u> in <u>Sherpa</u> can simulate emission of soft photons based on YFS approximation (mode 1)
- If switched on also hard photons based on collinear approximation (mode 2)
  - Approx. matrix-element corrections (mode 20) or
  - Exact matrix-element corrections (mode 21)
- With mode 1: fewer hard photons compared to PHOTOS (PHOTOS has matrix-element corrections implemented)
- With mode 2: generally good agreement with PHOTOS
- $\Rightarrow$  Implemented switches for systematic studies

New in EvtGen <u>R03-00-00-beta1</u>!



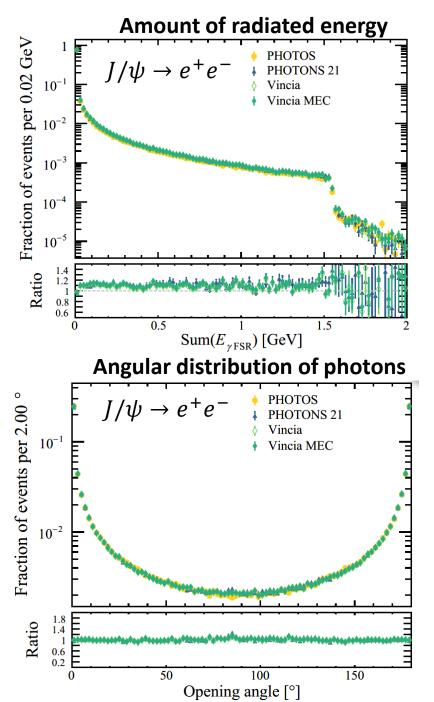
## Vincia QED shower for FSR

With Giacomo Morgante and Peter Skands @ Monash

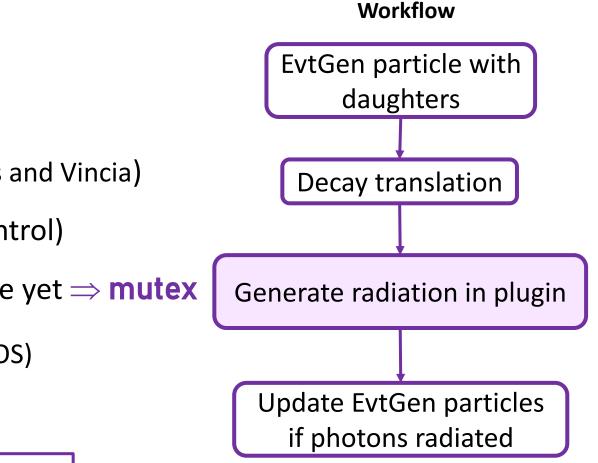
- <u>Vincia</u> parton shower evolution based on Antenna approximation (can be interleaved)
- Recently adapted to radiate off hadrons (previously supporting only leptons)
- Matrix-element corrections (MECs) in progress
- $\Rightarrow$  Currently implementing and validating
- ⇒ Preliminary results look promising

#### Technical aspects

- Vincia is embedded in Pythia8
- Algorithm implementation enables thread safety
- Developed EvtGen ↔ Vincia interface based on existing dependency with Pythia8
- $\Rightarrow$  To be added to release (once in Pythia8 release)



## Interfaces between EvtGen and Plugins



- Each decay-chain node translated
  - Into intermediate HepMC events (for PHOTOS)
  - Directly into Sherpa or Pythia objects (for Photons and Vincia)
- EvtGen random number propagated (full seed control)
- PHOTOS and Sherpa's PHOTONS++ not thread-safe yet => mutex
  - Need to mutex also HepMC translation (for PHOTOS)

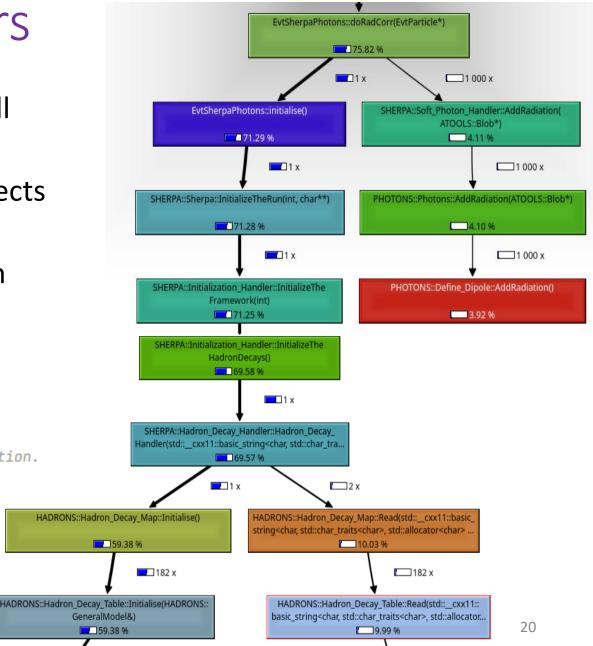
Review (for Sherpa) by Marek Schönherr and Frank Krauss

# Initialisation of afterburners

- For external dependencies EvtGen creates full Pythia/Sherpa objects
- Would be useful to initialise only needed objects (shower/soft-photon handler)
- Example: Sherpa's initialisation takes as much time as  $\sim 10^4$  decay events
- Several initialised objects are not used

// Vector containing the configuration strings for Sherpa
// INIT\_ONLY=6 intialises the Sherpa objects without launching simulation.
std::vector<std::string> m\_configs{ "Sherpa", "INIT\_ONLY=6" };

// Create instance and initialise Sherpa.
m\_sherpaGen = std::make\_unique<SHERPA::Sherpa>();
m\_sherpaGen->InitializeTheRun( argv.size(), &argv[0] );
m\_sherpaGen->InitializeTheEventHandler();



### Static destructor fiasco

When generators have static instances the destruction order is undefined (C++ issue)

#### #ifdef EVTGEN SHERPA

#### **Our current solution**

// The Sherpa and PHOTONS++ instances are static global instances inside EvtGen // as they are not thread safe (they are mutexed). From Sherpa 3.0.0 on, // the internal Sherpa settings are also a static global instance. // Because of the static destruction order fiasco, // we need to control the order in which the static instances are destroyed. // This is done by hand inside the function below. If the function below is not called, // a SegFault occurs at the end of the program execution when using Sherpa for FSR. EvtSherpaPhotons::finalise(); #endif

#### void EvtSherpaPhotons::finalise()

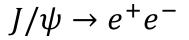
```
// Mutex this since Sherpa instances are static
const std::lock_guard<std::mutex> lock( m_sherpa_mutex );
if ( !m_initialised ) {
    return;
}
// We explicitly destroy the static instances to make sure that this essure is
// We explicitly destroy the static instances to make sure that this essure is
// We explicitly destroy the static instances to make sure that this essure is
// We explicitly destroy the static instances to make sure that this essure is
// we explicitly destroy the static instances to make sure that this essure is
// we explicitly destroy the static instances to make sure that this essure is
// we explicitly destroy the static instances to make sure that the static is of the static is a static
```

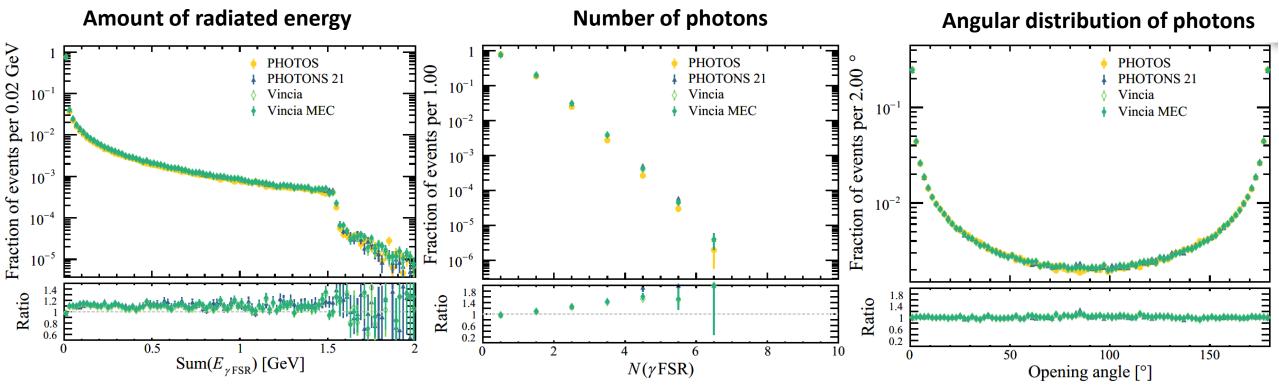
// We explicitly destroy the static instances to make sure that this occurs in the right order.
// This is needed due to the static destruction order fiasco.

```
m_photonsGen.reset();
m sherpaGen.reset();
```

```
m_initialised = false;
```

### Comparisons between generators





- Good agreement (within  $\sim 10\%$ ) for energy and angular distributions
- All generators radiate more photons that PHOTOS

### Comparisons between generators

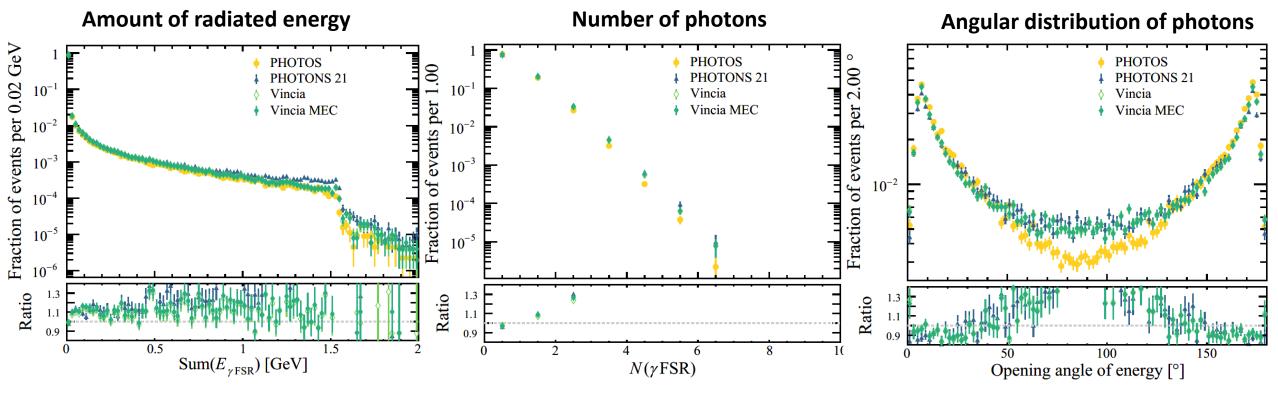
 $J/\psi \rightarrow e^+e^-$ 

#### Amount of radiated energy $N(\gamma_{\rm FSR}) = 3$ $N(\gamma_{\rm FSR}) = 1$ $N(\gamma_{\rm FSR}) = 2$ Fraction of events per 0.02 GeV GeV events per 0.02 GeV PHOTOS PHOTOS PHOTOS $10^{-1}$ PHOTONS 21 PHOTONS 21 PHOTONS 21 $10^{-1}$ of events per 0.02 Vincia Vincia Vincia $10^{-1}$ Vincia MEC Vincia MEC Vincia MEC $10^{-2}$ $10^{-2}$ $10^{-}$ $10^{-3}$ of $10^{-3}$ Fraction Fraction 10 $10^{-4}$ $10^{-1}$ 1.4 1.2 Ratio Ratio Ratio 12 0.8 0.5 1.5 0.5 1.5 0.5 $Sum(E_{\gamma FSR})$ [GeV] $Sum(E_{\gamma FSR})$ [GeV] $Sum(E_{\gamma FSR})$ [GeV]

• Energy range above  $M_{J\psi}/2$  kinematically accessible for events with more than one photon

## Comparisons between generators

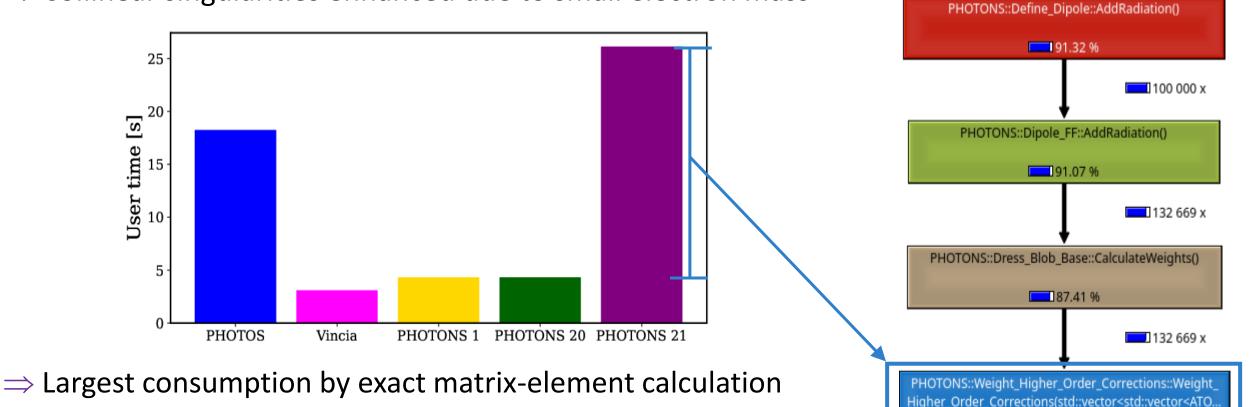
Reject photons with 
$$\Delta R = \sqrt{\Delta \eta^2 + \Delta \varphi^2} < 0.1$$
 and  $E_{\gamma} < 0.1$  MeV  $J/\psi \rightarrow e^+e^-$ 



- Good agreement (within  $\sim 10\%$ ) for energy and angular distributions
- All generators radiate more photons that PHOTOS

# A word on timing

- Compare simulation time using  $J/\psi \rightarrow e^+e^-$  decay as benchmark
- $\Rightarrow$  Collinear singularities enhanced due to small electron mass



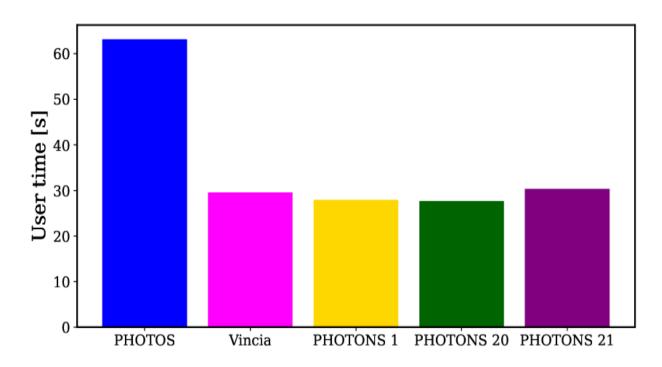
- $\Rightarrow$  Good precision/time trade-off for option 20 (will use as default)
- $\Rightarrow$  Potential speedup using Vincia or PHOTONS by about factor 4

86.48 %

## Another word on timing

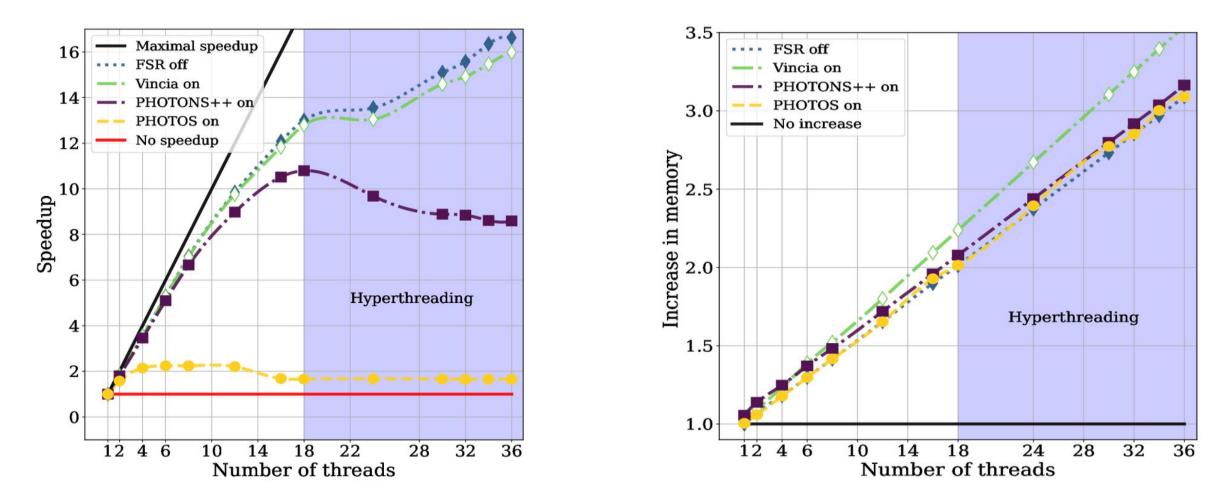
• Compare simulation time when simulating generic  $\Upsilon(4S) \rightarrow B\overline{B}$ 

 $\Rightarrow$  Benchmark for general use



 $\Rightarrow$  No large difference between PHOTONS options in generic case  $\Rightarrow$  Potential speedup using Vincia or PHOTONS by about factor 2

# Performance with multithreading

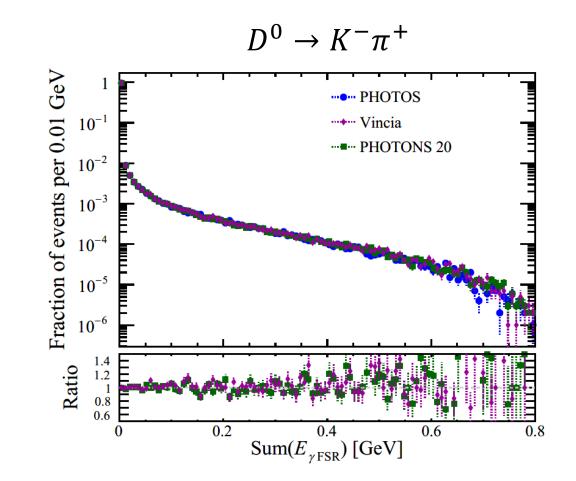


 $\Rightarrow$  Better performance with new FSR alternatives

⇒ Deeper structural changes needed to fully exploit multithreading with increased memory sharing

## Ideas for future FSR generation

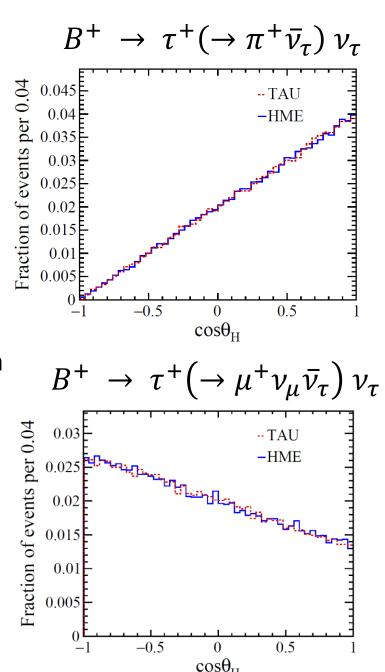
- FSR added by passing decay tree step-by-step (node-by-node) to the FSR generators
- Prototyped EvtGen ↔ Vincia interface using existing Pythia dependency (step-by-step)
- Aim to propagate full decay chain to Vincia to simulate radiation standalone
- Could simulate interference and resonance interleaving effects



### Spin-info propagation for au decays

## Plugins for au decays

- EvtGen ↔ TAUOLA interface based on HEPMC
- Spin-state information of  $\tau$  not propagated
  - TAUOLA reconstructs spin info from ancestors
  - Needed for analyses sensitive to \(\tau\) polarization
- Simulation of  $\tau$  decays with spin-state propagation possible with PYTHIA8 using HME (helicity-matrix element) model
  - $\Rightarrow$  Prototyped EvtGen  $\leftrightarrow$  Pythia interface with spin-density matrix propagation
- Generalisation of helicity/spin basis conversion has turned out challenging (but wish to continue work)



# Snippet from Herwig

EvtGenInterface.cc

Custom interfaces are efficient but need to align details about frame/conventions

```
else if ( thisSpin == EvtSpinType::DIRAC ) {
  EvtDiracParticle *myPart =new EvtDiracParticle;
 // get the spin info
  tcFermionSpinPtr sp(dynamic_ptr_cast<tcFermionSpinPtr>(spin));
 // has spin info transfer
  if(sp) {
    vector<EvtDiracSpinor> prod,decay;
    // transfer spinors
    for(unsigned int ix=0;ix<2;++ix) {</pre>
      prod .push_back(EvtGenSpinor(sp->getProductionBasisState(ix)));
      decay.push_back(EvtGenSpinor(sp->getDecayBasisState
                                                               (ix)));
    myPart->init(id, p4,prod[0],prod[1],decay[0],decay[1]);
    // set the density matrix
   myPart->setSpinDensityForward(EvtGenSpinDensity(sp->rhoMatrix()));
  }
```

## Snippet from Herwig

```
/**
 * Convert our tensor to the EvtGen one.
 * Oparam ten Our tensor
 */
EvtTensor4C EvtGenTensor(const LorentzTensor<double> & ten) const {
  EvtTensor4C output;
 unsigned int ix, iy;
 for(ix=0;ix<4;++ix){</pre>
    for(iy=0;iy<4;++iy) output.set(ix,iy,EvtGenComplex(ten(ix,iy)));</pre>
  }
  return output;
/**
 * Convert a spin density matrix to an EvtGen spin density matrix.
 * Oparam rho The spin density matrix to be converted.
 */
EvtSpinDensity EvtGenSpinDensity(const RhoDMatrix & rho) const {
  EvtSpinDensity rhoout;
  unsigned int ix,iy,ispin(rho.iSpin());
  rhoout.setDim(ispin);
  for(ix=0;ix<ispin;++ix) {</pre>
    for(iy=0;iy<ispin;++iy)</pre>
      rhoout.set(ix,iy,EvtGenComplex(rho(ix,iy)));
  return rhoout;
```

## Snippet from Herwig

#### EvtGenInterface.h

/\*\*

- \* Convert a LorentzSpinor to an EvtGen one. The spinor is converted to the
- \* EvtGen Dirac representation/
- \* @param sp The LorentzSpinor

\*/

```
EvtDiracSpinor EvtGenSpinor(const LorentzSpinor<SqrtEnergy> & sp) const {
    InvSqrtEnergy norm(sqrt(0.5)/sqrt(GeV));
    EvtDiracSpinor output;
    output.set(EvtGenComplex(-norm*( sp.s1()+sp.s3())),
        EvtGenComplex(-norm*( sp.s2()+sp.s4())),
        EvtGenComplex(-norm*(-sp.s1()+sp.s3())),
        EvtGenComplex(-norm*(-sp.s2()+sp.s4())));
    return output;
}
```

## Summary and discussion

#### EvtGen

- Decay weighting: feasible based on alternative BFs, different models/params challenging
- FSR: introduced new alternative using Sherpa's PHOTONS++
- FSR: Vincia under development (envisaged plans for full decay-chain propagation)
- $\tau$  decays: check interface between HERWIG EvtGen

#### General

- We can revisit particle ID definitions, but must coordinate with experiments
- Possibility of a "bidirectional" API between main generator and specialist afterburners?