1 An example workflow

To motivate the design goals of HEPTAPOD and to illustrate the challenges involved in coordinating multi-stage high-energy-physics workflows, we introduce a representative example that will serve as a running case study. Specifically, we consider the Monte Carlo simulation pipeline required to study new BSM models that are not available by default in general-purpose event generators. In this situation, model implementation, event generation, and downstream simulation must be manually composed across multiple software packages. The design and automation of this pipeline was the subject of a series of international workshops, Monte Carlo Tools for Beyond the Standard Model Physics (MC4BSM), which ran in the 2000's and 2010's [1]. The example considered here is very close to the test case study demonstrated in the MC4BSM tutorials [2].

For concreteness, we consider a scalar leptoquark [3]

$$S_1 \sim (\bar{\mathbf{3}}, \mathbf{1}, 1/3), \tag{1.1}$$

with a simplified interaction Lagrangian

$$\mathcal{L} \supset (D_\mu S_1)^\dagger (D^\mu S_1) + y_{ij}\, \overline{u^c_{Ri}}\, e_{Rj}\, S_1 + \text{h.c.} \tag{1.2}$$

Assuming diagonal Yukawa couplings, pair production proceeds dominantly through QCD,

$$pp \to S_1 S_1^\dagger \to (\ell^+ j)(\ell^- j), \tag{1.3}$$

yielding a characteristic $2\ell + 2j$ topology. The task is to perform MC signal generation over a scan of the leptoquark mass m_{S_1} and predict the distribution of the reconstructed leptoquark mass $m_{\rm LQ}^{\rm min}$, which for concreteness is taken as the smaller of the two reconstructed masses of the leptoquark candidates $m_{\rm LQ}^{(1)}$ and $m_{\rm LQ}^{(2)}$

$$m_{\rm LQ}^{\rm min} \;=\; \min\left\{ m_{\rm LQ}^{(1)}, m_{\rm LQ}^{(2)} \right\}, \tag{1.4}$$

where the lepton-jet assignments are selected to minimize the absolute difference $\left| m_{\rm LQ}^{(1)} - m_{\rm LQ}^{(2)} \right|$. A typical phenomenological study varies m_{S_1} over a set of benchmark values, e.g., $(1.0, 1.5, 2.0$ TeV), generating and analyzing events for each mass point. This requires coordinated propagation of model parameters, consistent run-card configuration across tools, and synchronized analysis logic across the scan. The scan is simple, yet has the essential structure of a multi-stage HEP workflow: configuration must propagate consistently across several tools, intermediate files must be handled carefully, and analysis logic must remain synchronized across scan points.

Although not included here, realistic validation pipelines must also include the dominant SM backgrounds to this signature. For the $(\ell j)(\ell j)$ final state, the most relevant backgrounds are

- Drell–Yan + jets: $pp \to Z/\gamma^* + \text{jets} \to \ell^+\ell^- + \text{jets}$,
- Top-quark pair production: $pp \to t\bar{t} \to (b\ell^+\nu)(\bar{b}\ell^-\bar{\nu})$,
- Diboson production: WW, WZ, or ZZ events with associated jets.

Each background requires its own run card, generation chain, and analysis flow, producing multiple parallel branches that must remain consistent. These branches are straightforward to implement within the orchestration framework because they reuse the same tool chain with different run-card inputs. Here we focus solely on the signal to illustrate the orchestration framework.

For this example, a complete HEP workflow can be instantiated in several ways. One representative realization is considered here (see **??**), though comparable pipelines using, for example, SHERPA [4] follow the same basic structure:

1. **Model generation:** convert the FEYNRULES [5] model file into a Universal FeynRules Output (UFO) directory.
2. **Parton-level event generation:** use MADGRAPH5_AMC@NLO [6] to generate events for each mass point specified in the run card via a user-defined parameter scan.
3. **Showering and hadronization:** use PYTHIA [7] to process the LHE events into particle-level final states.
4. **Jet reconstruction:** apply anti-k_T or Cambridge/Aachen clustering via FASTJET [8].
5. **Resonance reconstruction:** pair leptons and jets, compute $m_{\mathrm{LQ}}^{(1)}, m_{\mathrm{LQ}}^{(2)}$, and derive $m_{\mathrm{LQ}}^{\min}$.

Careful management of run cards, file paths, tool configurations, and intermediate data formats is necessary to execute this sequence reliably. Manual pipelines are time-intensive and error-prone. In later sections we return to this example and show how HEPTAPOD treats each phase as a schema-validated tool, propagates scan metadata through the workflow automatically, and uses run cards as explicit coordination boundaries. This allows an LLM to orchestrate the full analysis while preserving transparency, reproducibility, and human oversight.

References

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