Constraining anomalous Higgs boson couplings to the heavy flavor fermions using matrix element techniques

Andrei V. Gritsan, 1 Raoul Röntsch, 2 Markus Schulze, 3 and Meng Xiao 1

1 Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, USA
2 Karlsruhe Institute of Technology, Karlsruhe, Germany
3 CERN, European Organization for Nuclear Research, Geneva, Switzerland

(Dated: June 9, 2016)

In this paper we investigate anomalous interactions of the Higgs boson with heavy fermions, employing shapes of kinematic distributions. We study the processes $pp \rightarrow t\bar{t} + H$, $b\bar{b} + H$, $tq + H$, and $pp \rightarrow H \rightarrow \tau^+\tau^-$, and present applications of event generation, re-weighting techniques for fast simulation of anomalous couplings, as well as matrix element techniques for optimal sensitivity. We extend the MELA technique, which proved to be a powerful matrix element tool for Higgs boson discovery and characterisation during Run I of the LHC, and implement all analysis tools in the JHU generator framework. A next-to-leading order QCD description of the $pp \rightarrow t\bar{t} + H$ process allows us to investigate the performance of MELA in the presence of extra radiation. Finally, projections for LHC measurements through the end of Run III are presented.

PACS numbers: 12.60.-i, 13.88.+e, 14.80.Bn

I. INTRODUCTION

The discovery 1 [1, 2] of the $H$ boson by the ATLAS and CMS experiments during Run I of the LHC marked an important milestone in the evolution of our understanding of fundamental particle physics. One of the most important goals now is a precise understanding of the newly discovered state, including its couplings to other particles as well as its $CP$ nature. Any significant deviation from Standard Model (SM) predictions would reveal the existence of new physics in the Higgs sector and should be classified according to its anomalous coupling structures. Likewise, in the case of a discovery of a new resonance at the LHC, a similar program of investigating properties and couplings is required.

Since experimental efforts during Run I mostly focused on the $H$ boson decaying to a pair of vector bosons 1, extensive studies of the $HVV$ couplings and corresponding $CP$ properties were performed 3–6, leading to results consistent with the Standard Model nature of the $H$ boson with quantum numbers $J^{PC} = 0^{++}$. However, many generic models of new physics predict deviations which are beyond the current experimental precision 7. This leaves ample room for anomalous interactions to hide as small modifications of the SM structure. Moreover, a complete knowledge of the SM Higgs mechanism requires the study of the $H$ boson interactions with fermions. While the observation of $Hgg$ and $H\gamma\gamma$ interactions established the $Ht\bar{t}$ coupling through a closed loop, a detailed understanding only arises from the observation of various mass hierarchies, as well as the minimal flavor-universal Yukawa interaction as predicted by the SM. Hence, it is of paramount importance to investigate possible anomalous coupling patterns with which different quarks and leptons may interact with the Higgs field. The most promising approach is the study of differential distributions in processes with direct sensitivity through the associated production of the $H$ boson with on-shell fermions, $j\bar{j} + H$, or through the decay $H \rightarrow j\bar{j}$.

There has been considerable effort in modeling the $Hjj$ couplings and developing tools for their analysis in associated production 8–31 and in the $H \rightarrow \tau^+\tau^-$ decay 32–35. Current experimental analyses have measured the coupling strength of $Hbb$ and $Htt$ only through closed loops 1–6. There have been experimental searches for the $H$ boson production in association with a single top quark 32–35, and with $t\bar{t}$ 40–43, with strong evidence for the latter in Run I of the LHC. The process $b\bar{b}H$ has not been studied with a dedicated analysis so far but there is evidence for the $H$ boson decay into $b\bar{b}$ pairs 44–46. The decay of $H \rightarrow \tau^+\tau^-$ is observed when results of CMS 47 and ATLAS 48

1 In this paper, $HVV$ couplings induced by closed fermionic loops are still considered to be couplings to vector bosons.
are combined, and searches in this decay channel have been performed for specific scenarios beyond the SM [39–51]. However, an interpretation in terms of generic anomalous couplings has not yet been undertaken.

All these measurements require sophisticated tools for the optimal extraction of statistical information, as data remain limited for detailed analyses of the fermion couplings. The matrix element approach is one such technique, which has been proven successful in setting constraints on $HVV$ couplings using Run I data from CMS [2, 3, 19] and ATLAS [3, 59, 60]. In this paper, we focus on applications to Run II of the LHC and extend our earlier developed techniques for $HVV$ coupling measurements [61] to $Hff$ couplings in $ttH$, $bbH$, and $tgH$ production, as well as to $H \rightarrow \tau^+ \tau^-$ decays. These matrix element techniques allow the optimal analysis of the dynamics in the production and decay processes. Such techniques have been proposed to enhance signal over background in application to $ttH$ production [61] and $Hff$ couplings for the first time. We define the complete set of kinematic observables and the minimal set of matrix-element-based observables necessary to perform the measurements. Moreover, using a NLO QCD simulation of $ttH$ process that includes a fully consistent treatment of production and decays at higher orders, we demonstrate the robustness of the matrix element approach with respect to additional radiation and loop corrections.

This paper expands our efforts within the broader framework of the JHUGen (JHU generator) and MELA (Matrix Element Likelihood Approach) frameworks [61–63]. The rest of the paper is organized as follows. In Section II the formalism of anomalous $H$ boson couplings is discussed. Monte Carlo simulation with the JHU generator is introduced in Section III. The matrix elements technique and the MELA framework are discussed in Section IV. A study of NLO QCD effects is presented in Section V. In Section VI we discuss the application of these techniques to LHC measurements and make projections to the end of Run III of LHC. Results are summarized in Section VII.

II. PARAMETERIZATION OF HIGGS BOSON COUPLINGS

We describe the interactions between a spin-zero particle $H$ and two fermions through the amplitude

$$A(Hff) = -\frac{m_f}{v} \bar{\psi}_f (\kappa_f + i \tilde{\kappa}_f \gamma_5) \psi_f,$$

(1)

where $\bar{\psi}_f$ and $\psi_f$ are the Dirac spinors, $m_f$ is the fermion mass, and $v$ is the SM Higgs field vacuum expectation value. In the SM, the couplings$^3$ have the values $\kappa_f = 1$ and $\tilde{\kappa}_f = 0$. Any deviation from these values indicates the presence of physics beyond the SM, which may for example arise through heavy loop-induced fields. In particular, the $\tilde{\kappa}_f$ coupling parameterizes the contribution of a CP-odd pseudoscalar boson, and CP violation occurs when both $\kappa_f$ and $\tilde{\kappa}_f$ are nonzero.

One may equivalently choose to express the couplings through a Lagrangian (up to an unphysical global phase)

$$\mathcal{L}(Hff) = -\frac{m_f}{v} \bar{\psi}_f (\kappa_f + i \tilde{\kappa}_f \gamma_5) \psi_f H,$$

(2)

which allows a connection to be made between the couplings $\kappa_f$ and $\tilde{\kappa}_f$ and anomalous operators in an effective field theory. We assume the couplings to be independent of kinematics, which corresponds to dimension-six operators in the effective field theory. Higher-dimension operators could easily be considered through $q^2$-dependent couplings in our framework, where $q$ is the momentum transfer. However, in our study we neglect these higher-dimension contributions because they are expected to be small. The hermiticity of the Lagrangian requires $\kappa_f$ and $\tilde{\kappa}_f$ to be real. Nevertheless, in order to consider the broadest range of scenarios, we allow $\kappa_f$ and $\tilde{\kappa}_f$ to be complex, and trust that, should the unitarity of scattering amplitudes be violated as a result, it will be restored in the full theory. It is convenient to parameterize anomalous couplings through a mixing angle, with $\kappa_f \propto \cos \alpha$ and $\tilde{\kappa}_f \propto \sin \alpha$. Equivalently, we introduce the fractions

$$f_{CP} = \frac{|\tilde{\kappa}_f|^2}{|\kappa_f|^2 + |\tilde{\kappa}_f|^2}, \quad \phi_{CP} = \text{arg}(\tilde{\kappa}_f/\kappa_f),$$

(3)

where the $f_{CP}$ parameter is conveniently bounded between 0 and 1, is uniquely defined, and can be interpreted as the cross section fraction corresponding to the pseudoscalar coupling, and therefore is directly related to experimentally observable effects. It is a convenient counterpart of the $f_{a3}$ parameter defined for the $HVV$ couplings [3, 5, 63]. While

\[ ^2 \text{Unless otherwise noted, } tqH \text{ refers to all combinations of } t\bar{q}H, t\bar{q}H, tqH, \text{ and } t\bar{q}H \text{ with a quark } q \neq t. \]

\[ ^3 \text{The coupling convention of Ref. } [61] \text{ corresponds to } \kappa_f = -\rho_1 \text{ and } \tilde{\kappa}_f = i\rho_2. \]
the phase $\phi_{CP}$ can in general take any value between 0 and $2\pi$, it is reasonable to assume that the ratio $\kappa_f/\kappa_f$ is real, that is $\phi_{CP} = 0$ or $\pi$. However, we do not need to impose this restriction and will also consider other values of $\phi_{CP}$. The parameters $f_{CP}$ and $\phi_{CP}$ in principle depend on the fermion couplings under consideration and should be denoted $f^{H\ell\ell}_{CP}$ and $\phi^{H\ell\ell}_{CP}$, but in most cases this will be clear from the context.

The $tqH$ production also involves the $HWW$ coupling. We therefore recall the coupling of the $H$ to two vector bosons \cite{63}.

\begin{equation}
A(HVV) = \frac{1}{v} \left( a_1 m_V^2 \epsilon_1^\ast \epsilon_2^\ast + a_2 f^{i(1)}_{\mu\nu} f^{i(2),\mu\nu} + a_3 f^{i(1)}_{\mu\nu} f^{i(2),\mu\nu} \right),
\end{equation}

where $\epsilon_i$ is the polarization of the vector boson of mass $m_V$ and momentum $q_i$, the field strength tensor is $f^{i,\mu\nu} = \epsilon_i^{\mu} q_i^\nu - \epsilon_i^{\nu} q_i^\mu$ and its dual $f^{i,\mu\nu} = 1/2 \epsilon^{\rho\sigma\mu\nu} f_{\rho\sigma}^{i}$. 

### III. MONTE CARLO SIMULATION

The JHU generator framework \cite{61,63} involves both the Monte Carlo generation of unweighted events and the MELA package used in the analysis of the $H$ boson couplings. For top quark pair production in association with a spin-zero boson $H$ we compute the leading-order processes $gg \to t\bar{t} + H$ and $gq \to t\bar{t} + H$, followed by spin-correlated top quark decays $t \to bW(\to f\bar{f})$ in the narrow-width approximation. Any leptonic or hadronic decay mode of the top quarks can be described. Representative Feynman diagrams are shown in Fig. 1 where we allow for the anomalous $Htt$ couplings shown in Eq. (1). The $H$ boson is considered stable in the respective matrix elements describing production, and its decay into any possible channel can be introduced subsequently through processing the generated events using the JHU generator framework.

Since hadronic production of $t\bar{t} + H$ final states involves color flow in initial and final states, additional jet radiation plays an important role in the description of this process. In fact, almost 40\% of all $t\bar{t}$ events are accompanied by jets with transverse momentum harder than 40 GeV \cite{66}. It is therefore important to study the impact of radiative corrections on event kinematics and the matrix element observables. To this end, we also calculate the next-to-leading order QCD correction to the $pp \to t\bar{t} + H$ process.

The framework for NLO QCD computations is an extension of the TOPAZ code which two of us developed for anomalous coupling studies of $t\bar{t} + Z$ final states \cite{67,68}. We calculate the virtual correction to the $gg$ and $gq$ initial states using the numerical implementation of $D$-dimensional generalized unitarity techniques \cite{69,72}. The real emission corrections involve the partonic processes $gg \to t\bar{t}g$, $gq \to t\bar{t}g$, $gg \to t\bar{t}q$ and $qg \to t\bar{t}q$, which we regularize using the massive dipole subtraction techniques of Refs. \cite{73,74}. A consistent expansion in the strong coupling constant also requires the computation of the NLO corrections to the top quark decay $t \to bW$ and the subsequent $W \to jj$ decay. We account for these contributions in the narrow-width approximation using the implementation developed in Ref. \cite{75}. Non-resonant and off-shell effects are expected to scale parametrically as $\Gamma_t/m_t \approx 1\%$ and hence can be safely neglected provided that phase space cuts do not severely constrain the top quark invariant mass. This has been explicitly confirmed in studies for $t\bar{t} + H$ production at LO \cite{76} and NLO QCD \cite{77}.

We obtain the $pp \to bb + H$ process from $pp \to t\bar{t} + H$ by replacing $m_t \to m_b$ in the matrix elements and phase space (and removing the top quark decay), while preserving the five flavor scheme with massless initial state quarks. Hence, we neglect the newly appearing $t$-channel diagram in $bb \to bb$ reactions which is, however, doubly-suppressed by the small $b$ quark parton luminosity. In this way the $H$ boson is always emitted from the massive final state quarks only. We believe these approximations are sufficient for studying anomalous interactions in our analysis.

---

4 The coupling convention of Ref. \cite{63} corresponds to $a_4 = g_4$, $a_3 = g_2$, and $a_3 = g_4$. 

---

FIG. 1: Representative Feynman diagrams for $t\bar{t}H$ production at leading order.
Simulation of the single top quark production process in association with a spin-zero boson relies on the partonic processes $q b \rightarrow q' t + H$ (t-channel process) and $q q' \rightarrow t b + H$ (s-channel process). The former topology is shown in Fig. 2 (a) and (b), and the latter topology is shown in Fig. 2 (c) and (d). We make use of analytic expressions for the leading-order SM matrix elements [78] and extend them to include anomalous couplings, keeping the five flavor scheme so that the $H$ boson is never radiated off the initial state $b$-quark. An extensive comparison of the four and five flavor schemes for this process was performed in Ref. [26]. Here, we only note that differences between the two schemes are due to missing higher orders in the truncated perturbative series. Since the perturbative convergence for this process is good, these ambiguities are adequately captured by the scale uncertainty. Interestingly, in contrast to $t t H$ and $b b H$ production, $t q H$ production includes not only $H f f$ coupling but also $H W W$ coupling (depicted in Fig. 2 (b) and (d)). The interference between these diagrams is destructive and leads to a strongly suppressed production rate in the SM [79]. Therefore any new physics modification of either the $H f f$ or $H W W$ coupling may spoil this suppression and lead to a substantially enhanced production rate and altered kinematics. We therefore include anomalous $H W W$ couplings, following Eq. (4).

The study of spin-zero $H$ boson anomalous couplings to tau leptons relies on the matrix element $H \rightarrow \tau^+ \tau^-$ with subsequent spin-correlated decays $\tau \rightarrow \mu \nu_{\tau} \nu_{\mu}$ or $\tau \rightarrow q' \bar{q}' \nu_{\tau}$. These decay chains are illustrated in Fig. 3. This decay mode supplements the existing $H \rightarrow V V$ decays ($V = W, Z, \gamma, g$) within the JHU generator framework such that any $H$ boson production process can be interfaced with this decay. An option for stable $\tau$ leptons allows one to study $H \rightarrow \mu^+ \mu^-$ or $H \rightarrow e^+ e^-$ decays as well. Moreover, the tau decay chain encompasses the same structure as the top quark decay, enabling the future study of fully spin-correlated decay $p p \rightarrow X \rightarrow t\bar{t} \rightarrow b\bar{b} W(\rightarrow f \bar{f}) W(\rightarrow f' \bar{f}')$, where $X$ is any massive spin-zero state. In this work, we will only focus on anomalous coupling studies in $p p \rightarrow H \rightarrow \tau^+ \tau^-$. In the current implementation, the form factors for hadronic tau decay are not implemented in the generator and instead the inclusive tau decay is simulated. Below we illustrate the re-weighting technique to obtain the $H \rightarrow \tau^+ \tau^-$ process with anomalous couplings using SM simulation of hadronic $\tau$ decays with hadronic form factors by the TAUOLA package [80].

The generation of unweighted events for $H$ boson production in association with heavy-flavor quarks is performed at leading order (LO), complemented with parton shower generated by PYTHIA8 [81, 82]. The $H$ boson decay is simulated independently from its production. In all cases, the Les Houches Event (LHE) file format [83] is used to interface the JHU generator program. We also generate weighted events at NLO in QCD for $t \bar{t} H$ production to investigate the impact of radiative corrections, as discussed above. The simulation of the SM processes $t \bar{t} H$ and $b b H$ has been checked against the NLO QCD production simulation by POWHEG [64, 86], pseudoscalar $t \bar{t} H$ production at NLO QCD has been checked against Ref. [77], while the $H \rightarrow \tau^+ \tau^-$ decay is validated with TAUOLA. The background $t \bar{t} V V$ samples in this study are generated with MadGraph [85].

In the following, we focus on the LHC energy of $\sqrt{s} = 13$ TeV and use the following input parameters throughout

$$m_H = 125.0 \text{GeV}, \quad m_t = 173.2 \text{GeV},$$
$$m_Z = 91.19 \text{GeV}, \quad m_W = 80.39 \text{GeV},$$
$$m_b = 4.2 \text{GeV}, \quad m_\tau = 1.8 \text{GeV},$$
$$G_F = 1.16639 \times 10^{-5} \text{GeV}^{-2},$$

(5)
TABLE I: Summary of MC processes with anomalous $Hff$ couplings in the production and decay implemented in the JHU generator and the MELA package. The cross sections are listed without systematic uncertainties at the $\sqrt{s} = 13$ TeV LHC for a SM Higgs boson mass of 125 GeV [26, 90].

| Process | SM cross section | Simulation          |
|---------|-----------------|---------------------|
| $ttH$   | 509 fb          | LO + parton shower  |
| $bbH$   | 512 fb          | NLO QCD weighted    |
| $tqH$ (t-channel) | 73 fb | LO + parton shower  |
| $tbH$ (s-channel) | 3 fb  | LO + parton shower  |
| $H \rightarrow \tau^+\tau^-$ | 6.3% | LO + parton shower  |

as well as the NNPDF3.0 parton distribution functions [89]. We summarize the processes relevant to our study of $H$ boson $CP$ properties in heavy flavor fermion interactions, discussed above, in Table I. We also show their SM production cross sections and the order in perturbative QCD to which they are simulated. For each process shown, we provide the matrix elements through the MELA library. One direct application of MELA is kinematic discriminants for the optimal analysis, as discussed in Section IV. This technique also allows one to re-weight an existing Monte Carlo sample to any model with anomalous couplings without the need for additional CPU-consuming simulation. This is particularly important for the LHC experiments where modeling ATLAS and CMS detector response sometimes requires months of wall-clock time. A successful application of this procedure has been presented in Ref. [3].

IV. MATRIX ELEMENT TECHNIQUE

The matrix elements, or multivariate per-event likelihoods, maximize the amount of information that can be extracted from a given event. These techniques were used for example in top and bottom quark, as well as electroweak boson measurements, and proved to be powerful tools for the $H$ boson discovery and characterization during Run I of the LHC on both CMS [21, 41, 52, 53, 55, 57, 91] and ATLAS [3, 59, 60] experiments. As part of the latter development, we investigated application of these techniques to the production and decay processes involving $H$ boson coupling to vector bosons in Refs. [61–63]. Here we extend the MELA technique to the processes involving $H$ boson coupling to heavy flavor fermions.

We take the $gg(q\bar{q} \rightarrow t\bar{t}H$ processes as an example to define a complete set of kinematic observables following the full sequence of the process, similar to the $HVV$ production and decay kinematics discussed in Refs. [61, 63]. These observables are equivalent to the more familiar observables defined in the laboratory frame, as shown in Appendix A, but provide a more intuitive insight into the production and decay dynamics. We then define the complete set of matrix element discriminants, following Refs. [62, 63], in application to the processes involving heavy fermion couplings to the $H$ boson.

A. Kinematics in the $H$ boson production and decay

The processes $gg(q\bar{q} \rightarrow t\bar{t}H$, $tqH$, or $bbH$ with subsequent decay of the top quarks and the $H$ boson can be characterized by the four-momenta of the decay products, such as leptons and quark jets. In the case of one final state neutrino, its momentum can be deduced from a kinematic fit using mass constraints and utilizing the missing transverse energy information. In the following description we consider the $ttH$ production in its center-of-mass frame. Both longitudinal and transverse momenta of the $ttH$ system can be parameterized separately. They are driven by QCD effects, either parton distribution functions of the proton for rapidity or additional jet radiation for transverse momentum.

Similar to the description of the $H$ boson production and decay with couplings to vector bosons [61, 63], it is convenient to describe the complete kinematics of the process by a set of angles and invariant masses, which we generically denote as $\Omega$, following the sequential processes. The definition of observables in the process $gg(q\bar{q} \rightarrow t\bar{t}H \rightarrow (W^+b)(W^-\bar{b})H \rightarrow (f_1^1\bar{f}_1^1)(f_2^2\bar{f}_2^2)(VV)$ is shown in Fig. 4. The following set of angles and invariant masses is
The decay of the $H$ boson with angles $\theta_V^t$ and $\Phi_V^t$ is shown only for illustration, their distribution is flat for a spin-zero $H$ boson production due to the lack of spin correlations between the production and decay processes. Their complete description is discussed in Ref. [61] in terms of the two equivalent angles $\theta^*$ and $\Phi_1$. The grouping of the $W^+W^-$ and $b\bar{b}$ systems, as opposed to $W^+b$ and $W^-\bar{b}$, is motivated by enhanced spin-correlation effects visible with the corresponding observables. The complete multidimensional distribution retains full information with either approach.

Figure 5 shows the non-trivial angular distributions in the process $pp \to t\bar{t}H$ corresponding to four scenarios of anomalous $t\bar{t}H$ couplings: pure scalar, pseudoscalar, and two mixed scenarios with $f_{CP} = 0.28$ (corresponding to the equal cross-section of scalar and pseudoscalar processes) and different phases. Most angular observables exhibit a clear difference between the scalar and pseudoscalar processes. Only observables appearing in sequential decay of the top quarks are sensitive to $\phi_{CP}$. As noted earlier, these observables together with the boost of the $t\bar{t}H$ system are equivalent to other observables defined in the laboratory frame, as shown in Appendix A, but provide complete kinematics required as input to the matrix element tools and emphasize particular features in the process.

The description of observables $\Omega$ in the other processes $pp \to tqH$ and $bbH$ follows by analogy, with only a subset of observables available due to lack of sequential decay of at least one associated quark.
FIG. 5: The normalized angular and mass distributions in the process \( pp \rightarrow t\bar{t}H \) corresponding to four scenarios of anomalous \( t\bar{t}H \) couplings: \( f_{CP} = 0 \) (SM \( 0^+ \), black circles), \( f_{CP} = 1 \) (pseudoscalar \( 0^- \), red crosses), \( f_{CP} = 0.28 \) with \( \phi_{CP} = 0 \) (blue triangles) and \( \phi_{CP} = \pi/2 \) (green diamonds). The LHC \( pp \) energy of 13 TeV and \( H \) boson mass of 125 GeV are used in simulation. See text for definition of all observables.
B. Matrix element likelihood approach

With the kinematics of a process reflected in the complete set of observables \( \vec{\Omega} \), one could in principle analyze the data in this multi-dimensional space. However, this often becomes impractical with a large number of observables, as illustrated in Section IV.A when parameterization of probabilities and detector effects in such a multi-dimensional space becomes difficult. Reducing the number of observables is a possible approach, but essential information may be lost. Machine learning techniques can approximate optimal functions that can depend on a large number of inputs, but those also require training and therefore perform only as well as training goes. These techniques are typically targeted to discriminate between certain categories of events and are not optimal for dealing with quantum mechanical interference effects which become essential in physics processes, though for possible solutions see Ref. [32].

The matrix element techniques are the methods based on multivariate per-event likelihoods prepared using a phenomenological calculation for the process of interest. They may employ the same calculation as used in the Monte Carlo event generators or may be reformulated to represent analytical distributions of observables of interest, such as \( \vec{\Omega} \). Such matrix elements, if used properly, are guaranteed to retain full information about the event. The difficulty in using matrix element methods often comes from non-trivial detector effects which alter multivariate likelihoods. This issue is greatly simplified by utilizing ratios of the matrix elements in which certain detector effects cancel, most importantly variation of reconstruction efficiency as a function of observables. Resolution effects may be introduced with transfer functions, or neglected when their effect on performance is small. Missing degrees of freedom, such as neutrinos, may be either constrained from the global event information, as we illustrate below, or integrated out in the matrix element calculation. In the end, either machine learning or matrix element techniques could be used in the analysis of the data, but in either approach, it is ultimately the matrix elements which guide us in maximizing the amount of information, as they are also used in machine training through Monte Carlo.

The basic idea of the MELA technique is to project kinematics on the minimal set of discriminants calculated as ratios of the matrix elements. It has already proved to be a powerful tool for the \( H \) boson discovery and characterization during Run I of the LHC as applied primarily to the \( H \) boson coupling to the vector bosons. For a simple discrimination of two hypotheses, the Neyman-Pearson lemma [33] guarantees that the ratio of probabilities \( P \) for the two hypotheses provides an optimal discrimination power. However, for a continuous set of hypotheses with an arbitrary quantum-mechanical mixture several discriminants are required for an optimal measurement of their relative contributions. For example, probability for interference of two contributions could be presented as

\[
\mathcal{P}_{\text{sq}}(\vec{x}; f_{\text{CP}}, \phi_{\text{CP}}) = (1 - f_{\text{CP}}) \mathcal{P}_{0^+} (\vec{x}) + f_{\text{CP}} \mathcal{P}_{0^-} (\vec{x}) + \sqrt{f_{\text{CP}}(1 - f_{\text{CP}})} \left( \mathcal{P}_{\text{int}} (\vec{x}) \cos \phi_{\text{CP}} + \mathcal{P}_{\text{int}}^\perp (\vec{x}) \sin \phi_{\text{CP}} \right),
\]

where \( \mathcal{P}_{\text{int}} \) and \( \mathcal{P}_{\text{int}}^\perp \) describe quantum mechanical interference of \( J^P = 0^+ \) and \( 0^- \) terms. One could apply the Neyman-Pearson lemma to each pair of points in the parameter space of \((f_{\text{CP}}, \phi_{\text{CP}})\), but this would require continuous, and therefore infinite, set of probability ratios. However, an equivalent information is contained in a linear combination of only three probability ratios, which can be treated as three independent observables. For \( H \) boson physics at proton or lepton colliders, such discriminants are introduced in Ref. [63] as

\[
\mathcal{D}_{0^-} = \frac{\mathcal{P}_{0^+}(\vec{\Omega})}{\mathcal{P}_{0^+}(\vec{\Omega}) + \mathcal{P}_{0^-}(\vec{\Omega})},
\]

\[
\mathcal{D}_{\text{CP}} = \frac{\mathcal{P}_{\text{int}}(\vec{\Omega})}{\mathcal{P}_{0^+}(\vec{\Omega}) + \mathcal{P}_{0^-}(\vec{\Omega})},
\]

\[
\mathcal{D}_{\text{CP}}^\perp = \frac{\mathcal{P}_{\text{int}}^\perp(\vec{\Omega})}{\mathcal{P}_{0^+}(\vec{\Omega}) + \mathcal{P}_{0^-}(\vec{\Omega})},
\]

which become the optimal discriminants for the process with four contributions in Eq. (6).

In Eq. (6), \( \vec{x} \) is a set of observables describing the process, which may be \( \vec{\Omega} \) when calculating the discriminants, or may be discriminants themselves when performing the analysis later. The number of discriminants can also be reduced by dropping \( \mathcal{D}_{\text{CP}}^\perp \) assuming \( \sin \phi_{\text{CP}} = 0 \), which is the case for real \( \kappa_f \) and \( \tilde{\kappa}_f \) in Eq. (2). On the other hand, with additional contributing amplitudes the number of observables grows. For example in the presence of background the \( \mathcal{D}_{\text{bkg}} \) discriminant is introduced which can also be supplemented by the interference discriminant if there is quantum mechanical interference between the signal and background processes. The corresponding two discriminants are defined as

\[
\mathcal{D}_{\text{bkg}} = \frac{\mathcal{P}_{0^+}(\vec{\Omega})}{\mathcal{P}_{0^+}(\vec{\Omega}) + \mathcal{P}_{\text{bkg}}(\vec{\Omega})},
\]
They are computed at LO and do not include detector effects. However, as we illustrate in the following studies, they are obtained from numerical simulation of the processes accounting for parton showering and detector effects. In the treatment of Eqs. (7) and (10) carries the needed information. The number of discriminants grows with the number of free parameters. They are convoluted with the partonic cross sections that are proportional to the squared matrix elements. The set of optimal discriminants when the analysis is performed. These templates are obtained from numerical simulation of the processes accounting for parton showering and detector effects. In the following studies, they remain nearly optimal even after higher order or detector effects are introduced. The probabilities $P$ in Eqs. (6) may be treated as templates of the limited number of optimal discriminants when the analysis is performed. These templates are obtained from numerical simulation of the processes accounting for parton showering and detector effects. In the following analysis we limit the maximum number of discriminants to three, which we find to be both practical and close to optimal.

The complete set of optimal discriminants in Eqs. (7) was introduced earlier in experimental analysis of $HVV$ processes with LHC data by the CMS [2, 3, 8, 9, 55, 57, 91] and ATLAS [5] experiments, and phenomenological studies supporting this development [61, 62, 63]. For example, it was shown that the complete set $x = \{D_0-, D_{CP}, D_{bkg}\}$ was optimal for the measurement of $f_{3a}$, a parameter equivalent to $f_{CP}$, for the real $HVV$ couplings. A subset of equivalent observables was also introduced independently in earlier work on different topics [94–96]. Here we apply this formalism to the measurement of the $H$ boson anomalous couplings to the heavy flavor fermions for the first time.

### C. Application to the $t\bar{t}H$ process

The large number of observables $\vec{\Omega}$ defined in Section IV A for the $t\bar{t}H$ process can be compressed in a compact form with only three discriminants $x = \{D_0-, D_{CP}, D_{bkg}\}$ as defined in Eqs. (7), which is sensitive to the measurement of anomalous $t\bar{t}H$ couplings. The distributions for the discriminants are shown in Fig. 6 for $J^P = 0^+, 0^-$, and mixed...
The complete set of discriminants. The nominal studies presented here are based on LO in QCD calculations. Variations due to NLO matrix elements, PDFs, and QCD scale uncertainties are also shown in Fig. 6 and are discussed in more detail in Section V.

As one can see from both the discriminant definitions and distributions in Fig. 6, the $D_{0-}$ is sensitive to the relative size of $CP$ contributions, while $D_{CP}$ and $D_{\bar{CP}}$ are sensitive to $CP$ mixture leading to forward-backward asymmetry in the presence of both $CP$ amplitudes for the real and complex ratio of couplings $\kappa_f/\bar{\kappa}_f$, respectively. It is interesting to observe that the asymmetry is not strongly pronounced in the case of real couplings even when using the full top decay chain information. The asymmetry is more pronounced in the case of complex couplings, as seen in the $D_{\bar{CP}}$ distribution, which can be traced to the $\Phi_{f1}$ distribution in Fig. 5. The asymmetry in both $D_{CP}$ and $D_{\bar{CP}}$ disappears when top decay information is not used in the matrix element, which reflects the fact that spin correlations in the $t\bar{t}$ system decay are essential for observing effects sensitive to $CP$ mixture.

At the moment of discovery of the $ttH$ process, precision will be limited by statistics and the $D_{0-}$ discriminant will provide the most information about the $CP$ components in the process. As smaller anomalous contributions get tested, the importance of the interference discriminant will grow, but ultimately the full information is contained in the complete set of discriminants.

**D. Application to the $bbH$ process**

The $bbH$ and $ttH$ processes are very similar with the main difference being the heavy quark mass which, in fact, has a significant impact on the sensitivity of kinematic shapes to the $Hff$ couplings. This is because shape sensitivity arises from the mixing of left- and right-handed helicities at the matrix element level. Therefore, this effect becomes proportional to the mass of the associated quark and becomes essentially invisible in the $bbH$ process. In Fig. 6, we plot the angular distributions as well as the matrix element discriminant for the $bbH$ process, analogous to $ttH$ process distributions shown in Figs. 5 and 6. The different $CP$ states have almost identical distributions, as follows from the helicity flip suppression discussed above. Therefore, we conclude that it will be very challenging to probe the $CP$ nature of $Hb\bar{b}$ coupling through shape analyses in the $bbH$ production mode.

**E. Application to the $tqH$ process**

The $tqH$ production process features both fermion and vector boson couplings of the $H$ boson, as shown in Fig. 2. Interference between the $Hff$ and $HHV$-induced diagrams in Fig. 2 is destructive in the SM, but any deviation in either size or sign of either contribution could lead to a significant change in observations. Therefore, in this paper we illustrate the approach where two parameters of interest are determined: relative size of the $Hff$ and $HHV$ contributions, including their relative phase, and the relative size of the anomalous $Hff$ coupling. In this context, contributions from the $HHV$ process could be considered as background and we consider only SM-like $HHV$ coupling with $a_1 \neq 0$ in Eq. (4), while the signal process with the $Hff$ coupling is allowed to have an arbitrary anomalous contribution. Therefore, the three discriminants $D_{0-}$, $D_{\text{bkg}}$, and $D_{\text{bkg}}$ as defined in Eqs. (7), (10), (11) provide the most relevant information for this analysis. Their distributions are shown in Fig. 8.
There is a clear difference between distributions for the alternative hypotheses, such as between \( J^P = 0^+ \) and \( 0^- \)-\( Hff \)-induced signal in \( D_{0-} \), or between \( J^P = 0^+ \) signal and \( HVV \)-induced process in \( D_{\text{bkg}} \). It is important to stress that destructive interference between the \( J^P = 0^+ \) signal and \( HVV \)-induced processes with SM couplings leads to distributions which are very different from the direct sum of the two distributions, as shown in Fig. 8. In particular, the \( D^{\text{int}}_{\text{bkg}} \) discriminant shape is significantly distorted due to effect of interference, while the other two discriminants also exhibit sizable differences as well. This feature leads to strong separation power between different hypotheses even with small number of events in analysis, as we show below.

**F. Application to the \( H \rightarrow \tau^+ \tau^- \) process**

In the \( H \rightarrow \tau^+ \tau^- \) process, it is possible to define the full sequential decay kinematics and construct the matrix elements using information about all final state particles. This is illustrated for the process \( H \rightarrow \tau^+ \tau^- \rightarrow (\ell \nu \nu)(\ell \nu \nu) \) with the \( D_{0-} \) discriminant in Fig. 9. Even though there is a strong separation power between the \( J^P = 0^+ \) and \( 0^- \) models in this case, there is little practical application because reconstruction of the four neutrinos is not possible. Therefore, only limited information can be retained in reconstructed observables and we use the matrix elements for the purpose of MC re-weighting techniques below.

In the case of hadronic \( \tau \) decay, we provide the matrix element for the \( H \rightarrow \tau^+ \tau^- \rightarrow (X\nu)(X'\nu) \) process, where \( X \) could be any hadronic particle decayed from \( \tau \), e.g. \( \pi, \rho, a_1 \). Figure 10 shows the \( D_{0-} \) discriminant constructed using...
this matrix element, in a hadronic final state. The events are decayed through TAUOLA, including hadronic form-factors for particle hadronization, for the \( J^P = 0^+ \) and \( 0^- \) models. In addition, the \( J^P = 0^+ \) events are re-weighted to the \( 0^- \) model using the MELA weights, which allow us to create any model with arbitrary anomalous couplings. The \( D_{0-} \) discriminant can be compared to other observables proposed for analysis of the \( H \to \tau^+ \tau^- \) decay, for example \( \Phi_{\text{CP}} \) \cite{36}, defined as

\[
\Phi_{\text{CP}} = \cos(\vec{n}_X \cdot \vec{n}_{X'}) \ ; \ \text{where} \ \vec{n}_X = \frac{\vec{q}_X \times \vec{q}_{\tau^-}}{|\vec{q}_X \times \vec{q}_{\tau^-}|},
\]

\( \vec{q}_{\tau^-} \) and \( \vec{q}_{X,X'} \) are the 3-momentum of \( \tau^- \) and \( X \) or \( X' \) in the \( H \) boson rest frame. The two observables, \( D_{0-} \) and \( \Phi_{\text{CP}} \), carry similar information for analysis of anomalous couplings, but the \( D_{0-} \) discriminant is somewhat more powerful.

\[\text{FIG. 10: The distributions of } D_{0-} \text{ (left) and } \Phi_{\text{CP}} \text{ (right) for } H \to \tau\tau \to (X\nu)(X'\nu) \text{ simulation, where } X \text{ is a hadronic state. The } J^P = 0^+ \text{ (black circles) and } 0^- \text{ (red squares) distributions are generated with TAUOLA, including hadronic form-factors, and the } 0^- \text{ (blue triangles) distributions are obtained from the } 0^+ \text{ simulation using MELA re-weighting.}\]

V. NLO QCD STUDY OF KINEMATIC DISCRIMINANTS

Let us now discuss the effects of higher order QCD corrections on the modeling and performance of anomalous coupling discrimination. As described in Section \[\text{III}\], we compute the NLO QCD predictions for \( pp \to t\bar{t}H \) production followed by the spin-correlated top quark decays at NLO QCD in the narrow-width approximation. Neglecting QCD corrections in the description of the \( pp \to t\bar{t} + H \) process constitutes the dominant theoretical uncertainty on its cross section. We find that residual scale uncertainty on the total cross section is reduced from 21\% to 9\% when going from LO to NLO in QCD. The corrections on shapes of basic kinematic distributions are up to \( \pm 10\% \).

In the earlier work \cite{63}, we studied the impact of NLO in QCD effects in production on the anomalous coupling discrimination in decay \( H \to VV \). However, the production and decay processes carry no spin correlation and additional radiation from the production stage is largely decoupled from the color-neutral \( H \to VV \) decay dynamics. Hence, it is straightforward to use LO matrix elements to characterize \( HVV \) couplings, even in the presence of initial-state radiation. This is in contrast to the \( pp \to tt \to (b\bar{b}WW) + H \to (VV/ff) \) process where initial and final state particles radiate color charges and the top quarks exhibit spin correlations, all of which affect the studied dynamics.

A fully consistent extension of the matrix element method beyond the LO requires both event generation and matrix element discriminants at higher orders. The main complication stems from kineomatic configurations where hadronic activity is clustered by a jet algorithm. Commonly-used jet algorithms combine soft and collinear radiation in subsequent 2 \( \to \) 1 recombination steps. Hence, the resulting jet either acquires some invariant mass which does not correspond to the fundamental parton mass, or the jet violates global momentum conservation. This feature prohibits the use of jet momenta in a LO matrix element, which has on-shellness (of quarks and gluons) and momentum conservation built-in from first principles. A systematic solution to this issue at NLO QCD is part of active research and first elegant solutions have been presented in Refs. \cite{97,100}, where modified jet algorithms are proposed to map resolved and unresolved parton configurations onto their proper matrix elements. These approaches have promising prospects for future measurements, but they require the use of new jet algorithms that are currently not used in experimental analyses. Moreover, only solutions for either colorless final states or colorless initial states have been
presented in the literature. A fully developed application to e.g. top quark pair production at NLO QCD is not yet available. A variation away from the exact NLO treatment has also been presented in Ref. [101], where additional radiation is included through a parton shower approximation. This approach allows to include multiple emissions and has been applied to Higgs boson physics in Refs. [102, 103].

In this paper, we take a pragmatic and more simplistic approach. We retain leading order matrix elements in the discriminants of Eqs. (7) and probe them with events from leading and next-to-leading order simulation, and also compare those to variations due to PDFs, QCD scales, and parton showering. The mismatch between the LO discriminants and NLO simulation does not formally allow us to claim optimal discrimination power by virtue of the Neyman-Pearson lemma, where constructed likelihoods should be interpreted as fundamental probabilities. However, we demonstrate that NLO corrections to the shapes of kinematic distributions in the \( pp \rightarrow t\bar{t}H \) process are small and sometimes indistinguishable when compared to other associated uncertainties. Therefore, the LO discriminants \( D \) maintain their discriminating power beyond the well-defined leading-order, and we can continue to use them as robust and powerful tools for anomalous coupling studies.

In Fig. [6] we compare the impact of LO versus NLO events probing the LO discriminants \( D \). The solid histograms show the distribution for LO events, whereas the hashed bands indicate the shift due to NLO corrections. We note that the general shapes of the various distributions are maintained and only minimally distorted. The separation power between the extreme \( J^P = 0^+ \) and \( 0^- \) hypotheses is largely unaffected by the presence of higher order corrections. The most powerful discriminating observable \( D_9 \) receives very small corrections in range within the bulk of the distributions, as shown in the lower pane of Fig. [6]. Moreover, most of this correction appears already with the PDF variations before NLO corrections at the matrix element level. Hence, the bulk of corrections that we observe stems only from different input parameters and PDFs. The width of the bands in all lower panes of Fig. [6] corresponds to scale variations by a factor of two around the central scale \( \mu = m_H/2 \). Studies presented in Fig. [6] do not include parton showering. However, as we show in Section IV A and Fig. [11] inclusion of parton showering in LO simulation brings this simulation even closer to NLO modeling with parton showering.

We therefore conclude that discrimination power of the MELA approach is guaranteed even when higher-order corrections are considered in the \( pp \rightarrow t\bar{t}H \) process and additional jets are present in the event sample. Soft and collinear radiation, which generates massive jet momenta, can be handled in the matrix element approach and does not spoil the discrimination power. These higher-order effects are within the uncertainties of the PDF, scale choice, and parton showering.

VI. APPLICATION TO CP PARITY MEASUREMENTS IN \( t\bar{t}H, tqH, AND b\bar{b}H \)

In this section, we estimate the potential for \( CP \) measurements in the \( t\bar{t}H, tqH, \) and \( b\bar{b}H \) processes on LHC with 300 fb\(^{-1}\) of proton-proton collision data collected at 13 TeV center-of-mass energy. This is the integrated luminosity expected by the end of Run III of LHC in about seven years. Projections to other luminosity scenarios are usually trivial extensions as long as uncertainties remain limited by statistics. While there is a strong evidence for the \( t\bar{t}H \) production in Run I of LHC, none of these processes have been firmly established yet. However, we rely on experimental studies of these processes in Refs. [39, 43] for realistic event reconstruction projections.

As the first observation, following Section IV D, we conclude that it will not be possible to measure \( CP \) in the \( b\bar{b}H \) production process in the LHC program. For the \( t\bar{t}H \) and \( tqH \) processes, we consider the \( H \rightarrow \gamma \gamma \) decay mode to tag the \( H \) boson, as a clean signature with sizable branching fraction. We also consider the \( H \rightarrow ZZ \rightarrow 4\ell \) final state in the \( t\bar{t}H \) process for comparison, but its contribution is small due to the small branching fraction. We use the hadronic decay of one top quark final state so that the full kinematics can be reconstructed. In the \( t\bar{t}H \) case, the other top quark is reconstructed in the leptonic channel. Inclusion of other final states of either \( H \) boson or top would only enhance expected precision, but the decays we consider are representative of the typical analyses of these processes. In this study, the \( t\bar{t}H, b\bar{b}H, \) and \( tqH \) processes with SM or anomalous couplings are generated with the JHU generator. The only non-negligible background that we need to consider is \( SM tt\gamma \gamma \) production as a background to the \( t\bar{t}H \) production with the photon decay of the \( H \) boson, which is simulated with MadGraph. The MC samples are interfaced to PYTHIA8 for parton shower and hadronization. In order to model detector effects, lepton and photon \( p_T \) are smeared with 1% and 4% resolution. The jets are reconstructed in a cone of \( R = 0.5 \) using anti-\( k_T \) algorithm and their energy is smeared by 20%.

The event selection criteria follow those of the LHC analyses [40]. We require the leptons, photons, and jets to have \( p_T > 5, 10, \) and 30 GeV, and \( |\eta| < 2.4, 2.4, \) and 4.7, respectively. Jets within \( \Delta R < 0.2 \) of the leptons or photons are removed. In the \( t\bar{t}H \) analysis, an event should have at least four jets and a \( b \)-tagged jet. The \( b \)-tagging efficiency (62%) and fake rate for the light quark jets (6%) follow experimental study [30]. To fully reconstruct the semileptonic decay of the \( t\bar{t} \) system, we use the constraint fit from Ref. [104]. The four-momenta of four jets, MET, and one lepton are used in the kinematic fit with the masses of the top quarks and the \( W \) bosons as constraints. If more than four
jets are reconstructed, the combination that gives the best \( \chi^2 \) is selected. The four-momenta of all decay products of the \( tt \) system are obtained from this fit and are used in the further analysis. In the \( tqH \) analysis, exactly four jets and a \( b \)-tagged jet are required in order to remove hadronic \( tt\bar{H} \) events. The combination of three jets with the mass closest to the top is treated as the top decay product in this process. The required number of reconstructed leptons and photons depends on the studied final state. If required, the leading photon should have \( p_T > 33 \text{ GeV} \) and \( p_T/m_{\gamma\gamma} > 0.5 \). In the \( H \to 4\ell \) channel, two pairs of opposite sign and same flavor leptons should have invariant mass greater than 40 and 12 GeV. The invariant mass of the \( H \) boson candidate is required to be between 100 and 140 GeV.

In the case of the \( tqH \) process with \( H \to \gamma\gamma \), the main other contribution is cross-feed from the \( t\bar{t}H \) process with the same \( H \) boson decay. The \( tt\bar{H} \) process with the \( 4\ell \) decay of the \( H \) boson has negligible background, while with the \( \gamma\gamma \) decay the dominant background is the SM \( tt\gamma\gamma \) production. The expected number of events of signal and background events at 300 fb\(^{-1}\) is shown in Table II. We would like to note that these expected yields are quoted for the SM scenario where destructive interference between the \( Hff \) and \( HVV \)-induced \( tqH \) processes leads to a small number of expected events. However, this interference may become constructive with the non-SM couplings. The cross section for \( tt\gamma\gamma \) processes suggests background yield to be smaller than the signal. However, the LHC studies with data-driven methods suggest larger background. Therefore, we conservatively set the \( tt\gamma\gamma \) background yield to be twice the signal in the invariant mass window specified above.

### Table II: Number of events expected in the SM for signal and other contributions in the study of \( Hff \) couplings discussed in text with 300 fb\(^{-1}\) at 13 TeV.

| signal process | signal yield | other process | other yield |
|----------------|--------------|---------------|-------------|
| \( ttH, H \to \gamma\gamma \) | 50.3         | \( tt\gamma\gamma \) | 100.6       |
| \( ttH, H \to 4\ell \) | 4.3          | negligible    | 0           |
| \( tqH, H \to \gamma\gamma \) | 3.2          | \( t\bar{t}H, H \to \gamma\gamma \) | 10.2       |

#### A. Study of the \( ttH \) process

The analysis of the \( tt\bar{H} \) process uses the \( D_{0-} \) discriminant, where decay of the top quarks is not considered in the matrix element. Consideration of the top quark decays is important in the calculation of the \( D_{CP} \) or \( D_{CP}^b \) discriminants, but only when the up and down flavors of the quarks in the decay chain is known. The latter is difficult to determine with the jet reconstruction techniques and therefore the \( CP \) discriminants are not used in this analysis. In the \( H \to \gamma\gamma \) channel, we use the invariant mass \( m_{\gamma\gamma} \) to separate the signal and background. Figure 11 shows the \( D_{0-} \) distribution in the \( H \to \gamma\gamma \) channel, where the \( j^P = 0^+, 0^- \) and background distributions are shown.

In Fig. 11 simulation of the \( 0^+ \) process is also shown with the POWHEG generator at NLO in QCD. In all cases, parton showering is performed with PYTHIA\(8\). Similar to the study presented in Section V, the NLO QCD effects are found to have a small effect on accuracy of \( D_{0-} \) simulation, especially after parton showering is included in simulation. Any residual effects are consistent with systematics also arising from PDF and QCD scale variations.

The expected precision of the \( f_{CP} \) measurement in the \( tt\bar{H} \) process with both \( H \to \gamma\gamma \) and \( H \to 4\ell \) decays, and their combination, is shown in Fig. 11 for integrated luminosity of 300 fb\(^{-1}\). The maximum likelihood fit is based on the probability density functions following Eq. (6) parameterized with template distributions filled with generated events as discussed above. About 3\( \sigma \) exclusion of the pure pseudoscalar state is expected in such a scenario, which is comparable to the current precision with the \( HVV \) measurements, but provides a fundamentally different approach through fermion couplings. Scenarios with a sizable \( CP \) mixture, \( |f_{CP}\cos\phi_{CP}| \gtrsim 0.8 \), are excluded at 2\( \sigma \).

#### B. Study of the \( tq\bar{H} \) process

The analysis of the \( tq\bar{H} \) process uses the \( D_{0-}, D_{bkg}, D_{int/\text{bkg}}^{\text{int}} \) discriminants, shown in Fig. 12. In this study, the \( Hff \)-induced process is considered as signal and the \( HVV \)-induced process is considered as background. Similar to the \( tt\bar{H} \) study, the decay of the top quarks is not considered in the matrix element and the \( D_{CP} \) discriminants provide little information and therefore are not used. There is a sizable contribution of the \( tt\bar{H} \) events misreconstructed as \( tq\bar{H} \) and they carry information on \( f_{CP} \). The above observables provide sufficient information to differentiate between \( CP \) components of the \( tt\bar{H} \) process as well.
contributions and exclude both extreme scenarios of either pure $Hf$ (middle plot), or to the measurement of $Hf$ in the right plot of Fig. 13. More than 3 SM expectation.

This measurement can be reduced either to the measurement of induced processes and of the anomalous contribution in the Fig. 13 (left plot). This approach allows simultaneous measurement of both the relative fraction of $L^\kappa$ as it is for interference between the $Hf$ distributions are shown:

$\sigma_{ttH} = \sigma_{bkg}^t + \sigma_{ttH}^0 + \sigma_{tqH}^0 + \sigma_{ttH}^{a_1} + \sigma_{tqH}^{a_1} + \sigma_{ttH}^{\kappa} + \sigma_{tqH}^{\kappa} + \sigma_{ttH}^{\kappa a_1} + \sigma_{tqH}^{\kappa a_1},$

$\sigma_{tqH} = \sigma_{bkg}^t + \sigma_{ttH}^0 + \sigma_{tqH}^0 + \sigma_{ttH}^{a_1} + \sigma_{tqH}^{a_1} + \sigma_{ttH}^{\kappa} + \sigma_{tqH}^{\kappa} + \sigma_{ttH}^{\kappa a_1} + \sigma_{tqH}^{\kappa a_1},$

where $L$ is integrated luminosity and $\sigma$ is the product of cross section and reconstruction efficiency of a particular process corresponding to the unit value of the coupling ($\kappa, \tilde{\kappa}$, or $a_1$). The interference cross section can be negative, as it is for interference between the $\kappa$ and $a_1$ terms in the $tqH$ process. In the $tqH$ process, we express $\kappa$, $\tilde{\kappa}$, and $a_1$ in terms of two effective cross section fractions with phases and the overall normalization as follows

\begin{align}
  f_\kappa &= \frac{\kappa^2 \sigma_{tqH}^0}{(a_1^2 \sigma_{bkg}^t + \kappa^2 \sigma_{tqH}^0 + \tilde{\kappa}^2 \sigma_{tqH}^{a_1})}, \quad \phi_\kappa = \arg(\kappa/a_1) = 0 \text{ or } \pi, \\
  f_{\tilde{\kappa}} &= \frac{\tilde{\kappa}^2 \sigma_{tqH}^0}{(a_1^2 \sigma_{bkg}^t + \kappa^2 \sigma_{tqH}^0 + \tilde{\kappa}^2 \sigma_{tqH}^{a_1})}, \quad \phi_{\tilde{\kappa}} = \arg(\tilde{\kappa}/a_1) = 0 \text{ or } \pi.
\end{align}

In the SM, $f_\kappa = 0.46, f_{\tilde{\kappa}} = 0, \text{ and } \phi_\kappa = 0.$ The ratios of cross section is $\sigma_{0+}^{tqH}/\sigma_{bkg}^{tqH} = 0.86.$

The maximum likelihood fit, similar to the $tH$ analysis, uses a 3D template approach of three observables $D_{0-}, D_{bkg}, D_{int}$, and with $f_\kappa, f_{\tilde{\kappa}}, \text{ and total event yield as free parameters. The expected precision of the fit is shown in Fig. [13] (left plot). This approach allows simultaneous measurement of both the relative fraction of $HVV$ and $Hff$ induced processes and of the anomalous contribution in the $Hff$ coupling, with proper accounting for all interference effects. This measurement can be reduced either to the measurement of $f_\kappa$ with the constraint $f_{\tilde{\kappa}} = f_{CP} = 0$ (middle plot), or to the measurement of $f_{CP}$ (right plot). Precision on the $Hff$ couplings is driven by both $tqH$ and $ttH$ processes in this analysis, as illustrated with the likelihood scans separated for the two samples of events in the right plot of Fig. [13]. More than 3σ exclusion of the pure pseudoscalar state is expected in such a scenario, which is a measurement independent from that discussed in Section [VIA] since $ttH$ events have little overlap. It is important to note that in this scenario it will be possible to determine the relative sign of the $Hff$ and $HVV$-induced contributions and exclude both extreme scenarios of either pure $Hff$ or pure $HVV$ processes, assuming events follow SM expectation.
All distributions appear after simulation and reconstruction discussed in text. Also shown are distributions of mis-reconstructed $ttH$ signal with $J^P = 0^+$ (magenta diamonds) and $0^-$ signal (green squares). All distributions appear after simulation and reconstruction discussed in text.

**FIG. 12:** Distributions of $D_{0-}$ (left), $D_{bkg}$ (middle), and $D_{bkg}^{int}$ (right) discriminants in the $tqH$ study where the $Hff\bar{f}$-induced process is considered as signal and the $HVV$-induced process is considered as background. The following three contributions are considered: $J^P = 0^+$ signal (red crosses), $0^-$ signal (blue triangles), $HVV$-induced process as background (black circles). Also shown are distributions of mis-reconstructed $ttH$ signal with $J^P = 0^+$ (magenta diamonds) and $0^-$ signal (green squares).

**FIG. 13:** The likelihood scan of parameters of interest in the $tqH$ study expected with 300 fb$^{-1}$ at LHC. Left: $f_\kappa \cos(\phi_\kappa)$ vs. $f_\phi \cos(\phi_\phi)$, where the SM expectation is $f_\kappa = 0.46$ and $f_\phi = 0$, and where $\phi_\kappa$ or $\phi_\phi = 0$ or $\pi$. Middle: $f_\kappa \cos(\phi_\kappa)$ with the constraint of no anomalous couplings, $f_\kappa = 0$. Right: $f_{CP} \cos(\phi_{CP})$ corresponding to the curved line on the left plot going from $f_\kappa = 0$ ($f_{CP} = 1$) to $f_\kappa = 0$ ($f_{CP} = 0$) following the minimum of $-2\Delta \ln L$. The solid line shows expectation considering all contributions, while the red dotted line assumes that only $ttH$ mis-reconstructed events are present in the sample, and the blue dashed line assumes no contribution of $ttH$ events.

**VII. SUMMARY AND CONCLUSIONS**

We have developed the Monte Carlo simulation and matrix element analysis tools and investigated prospects for measurement of anomalous interactions in the $H$ boson production in association with top or bottom quarks at the LHC, as well as its decay in two tau leptons. The study is based on the JHU generator framework and the matrix element MELA analysis technique. We find that it is difficult to measure anomalous couplings in the $bbH$ process, while in both $ttH$ and $tqH$ analyses it is possible to have more than 3$\sigma$ separation of the pseudoscalar hypothesis from the scalar with 300 fb$^{-1}$ of integrated luminosity at LHC at 13 TeV. It is also possible to separate the $Hff$ and $HVV$ processes and determine their relative phase in the $tqH$ production, where in the SM the two processes interfere strongly and destructively. This feasibility study considers only representative decay channels of the top quark (hadronic decay of one top) and $H$ boson (diboson decay) and inclusion of other final states would only enhance expected precision. Systematic uncertainties from QCD effects, such as PDFs, scale, parton showering, and higher order corrections, are shown to be relatively small compared to expected statistical precision. The tools and techniques presented should facilitate measurements of SM and anomalous $Hff$ couplings.

**Acknowledgments:** We acknowledge contribution of CMS collaboration colleagues to the MELA project develop-
ment and thank Roberto Covarelli, Chris Martin, Candice You for help with the generator validation. We are grateful to our co-authors of the JHU generator project for valuable contributions, and in particular to Ulascan Sarica and Heshy Roskes for the generator package support and Fabrizio Caola for providing useful comments on the manuscript. This research is partially supported by U.S. NSF under grant PHY-1404302 and by the German Federal Ministry for Education and Research (BMBF) under grant 05H15V/KCCA. Calculations reported in this paper were performed on the Homewood High Performance Cluster (HHPC) of the Johns Hopkins University and the Maryland Advanced Research Computing Center (MARCC).

Appendix A: Supplemental information on kinematics

Figure 14 shows the kinematic observables defined in the laboratory frame in the SM process $gg \rightarrow \bar{t}qH$, corresponding to four scenarios of anomalous $\bar{t}qH$ couplings. These observables can be derived from those shown in Fig. 5 and defined in Section IV A.

[1] CMS Collaboration, “Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC”, Phys. Lett. B716 (2012) 1–29, doi:10.1016/j.physletb.2012.08.020, arXiv:1207.7214

[2] CMS Collaboration, “Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC”, Phys. Lett. B716 (2012) 30–61, doi:10.1016/j.physletb.2012.08.021, arXiv:1207.7235

[3] CMS Collaboration, “Constraints on the spin-parity and anomalous HVV couplings of the Higgs boson in proton collisions at 7 and 8 TeV”, Phys. Rev. D92 (2015), no. 1, 012004, doi:10.1103/PhysRevD.92.012004, arXiv:1411.3441

[4] CMS Collaboration, “Precise determination of the mass of the Higgs boson and tests of compatibility of its couplings with the standard model predictions using proton collisions at 7 and 8 TeV”, Eur. Phys. J. C75 (2015), no. 5, 212, doi:10.1140/epjc/s10052-015-3351-7, arXiv:1412.8662

[5] ATLAS Collaboration, “Study of the spin and parity of the Higgs boson in diboson decays with the ATLAS detector”, Eur. Phys. J. C75 (2015), no. 10, 476, doi:10.1140/epjc/s10052-015-3685-1, arXiv:1506.05669

[6] ATLAS Collaboration, “Measurements of the Higgs boson production and decay rates and coupling strengths using pp collision data at $\sqrt{s} = 7$ and 8 TeV in the ATLAS experiment”, Eur. Phys. J. C76 (2016), no. 1, 6, doi:10.1140/epjc/s10052-015-3769-y, arXiv:1507.04548

[7] S. Dawson et al., “Working Group Report: Higgs Boson”, in Community Summer Study 2013: Snowmass on the Mississippi (CSS2013) Minneapolis, MN, USA, July 29-August 6, 2013, arXiv:1310.8361

[8] P. S. Bhupal Dev et al., “Determining the CP properties of the Higgs boson”, Phys. Rev. Lett. 100 (2008) 051801, doi:10.1103/PhysRevLett.100.051801, arXiv:0707.2878

[9] P. Agrawal, S. Mitra, and A. Shivaraj, “Effect of Anomalous Couplings on the Associated Production of a Single Top Quark and a Higgs Boson at the LHC”, JHEP 12 (2013) 077, doi:10.1007/JHEP12(2013)077, arXiv:1211.4362

[10] M. Farina et al., “Lifting degeneracies in Higgs couplings using single top production in association with a Higgs boson”, JHEP 05 (2013) 022, doi:10.1007/JHEP05(2013)022, arXiv:1211.3736

[11] K. Nishiwaki, S. Niyogi, and A. Shivaraj, “itH Anomalous Coupling in Double Higgs Production”, JHEP 04 (2014) 011, doi:10.1007/JHEP04(2014)011, arXiv:1309.6907

[12] S. Biswas, E. Gabrielli, F. Margaroli, and B. Mele, “Direct constraints on the top-Higgs coupling from the 8 TeV LHC data”, JHEP 07 (2013) 073, doi:10.1007/JHEP07(2013)073, arXiv:1304.1822

[13] J. Ellis, D. S. Hwang, K. Sakurai, and M. Takeuchi, “Disentangling Higgs-Top Couplings in Associated Production”, JHEP 04 (2014) 004, doi:10.1007/JHEP04(2014)004, arXiv:1312.5736

[14] S. Khatibi and M. M. Najafabadi, “Effect of Anomalous Higgs-top Couplings”, Phys. Rev. D90 (2014), no. 7, 074014, doi:10.1103/PhysRevD.90.074014, arXiv:1409.6855

[15] L. Wu, “Enhancing $t\bar{q}$ Production from Top-Higgs FCNC Couplings”, JHEP 02 (2015) 061, doi:10.1007/JHEP02(2015)061, arXiv:1407.6113

[16] F. Demartin et al., “Higgs characterisation at NLO in QCD: CP properties of the top-quark Yukawa interaction”, Eur. Phys. J. C74 (2014), no. 9, 3065, doi:10.1140/epjc/s10052-014-3065-2, arXiv:1407.5089

[17] J. Bramante, A. Delgado, and A. Martin, “Cornering a hyper Higgs boson: Angular kinematics for boosted Higgs bosons with top pairs”, Phys. Rev. D89 (2014), no. 9, 093006, doi:10.1103/PhysRevD.89.093006, arXiv:1402.5985

[18] A. Kobakhidze, L. Wu, and J. Yue, “Anomalous Top-Higgs Couplings and Top Polarisation in Single Top and Higgs Associated Production at the LHC”, JHEP 10 (2014) 100, doi:10.1007/JHEP10(2014)100, arXiv:1406.1961

[19] C. Englert and E. Re, “Bounding the top Yukawa coupling with Higgs-associated single-top-production”, Phys. Rev. D89 (2014), no. 7, 073020, doi:10.1103/PhysRevD.89.073020, arXiv:1402.0445

[20] J. Chang, K. Cheung, J. S. Lee, and C.-T. Lu, “Probing the Top-Yukawa Coupling in Associated Higgs production with a Single Top Quark”, JHEP 05 (2014) 062, doi:10.1007/JHEP05(2014)062, arXiv:1403.2053
FIG. 14: The kinematic distributions in the process $gg$ and $q\bar{q} \rightarrow t\bar{t}H$ defined in the laboratory frame: top quark rapidity ($Y(t)$), transverse momentum of the top quark ($p_T(t)$), $H$ boson rapidity ($Y(H)$), transverse momentum of the $H$ boson ($p_H(t)$), $t\bar{t}H$ system rapidity ($Y(t\bar{t}H)$), pseudorapidity difference between the two down type fermions decayed from top and anti-top ($\Delta \eta_{ll}$) and between two bottom quarks ($\Delta \eta_{bb}$), $\cos \theta_{ll}$ between the two down type fermions, and $\cos \theta_{bb}$ between the two bottom quarks. Four scenarios of anomalous $t\bar{t}H$ couplings are shown: $f_{\text{CP}} = 0$ (SM $0^+$, black circles), $f_{\text{CP}} = 1$ (pseudoscalar $0^-$, red crosses), $f_{\text{CP}} = 0.28$ with $\phi_{\text{CP}} = 0$ (blue triangles) and $\phi_{\text{CP}} = \pi/2$ (green diamonds). The LHC pp energy of 13 TeV and $H$ boson mass of 125 GeV are used in simulation.

[21] J. Yue, “Enhanced $thj$ signal at the LHC with $h \rightarrow \gamma\gamma$ decay and $CP$-violating top-Higgs coupling”, Phys. Lett. B744 (2015) 131–136, doi:10.1016/j.physletb.2015.03.044, arXiv:1410.2701.

[22] X.-G. He, G.-N. Li, and Y.-J. Zheng, “Probing Higgs boson $CP$ Properties with $t\bar{t}H$ at the LHC and the 100 TeV $pp$ collider”, Int. J. Mod. Phys. A30 (2015), no. 25, 1550156, doi:10.1142/S0217751X15501560, arXiv:1501.00012.

[23] F. Boudjema, R. M. Godbole, D. Guadagnoli, and K. A. Mohan, “Lab-frame observables for probing the top-Higgs interaction”, Phys. Rev. D92 (2015), no. 1, 015019, doi:10.1103/PhysRevD.92.015019, arXiv:1501.03157.

[24] K. Kolodziej and A. Slapik, “Probing the top-Higgs coupling through the secondary lepton distributions in the associated production of the top-quark pair and Higgs boson at the LHC”, Eur. Phys. J. C75 (2015), no. 10, 475, doi:10.1140/epjc/s10052-015-3696-y, arXiv:1507.01572.
[25] Y. Chen, D. Stolarski, and R. Vega-Morales, “Golden probe of the top Yukawa coupling”, Phys. Rev. D92 (2015), no. 5, 053003, doi:10.1103/PhysRevD.92.053003, arXiv:1505.01168

[26] F. Demartin, F. Maltoni, K. Mawatari, and M. Zaro, “Higgs production in association with a single top quark at the LHC”, Eur. Phys. J. C75 (2015), no. 6, 267, doi:10.1140/epjc/s10052-015-3475-9, arXiv:1504.00611

[27] M. R. Buckley and D. Goncalves, “Boosting the Direct CP Measurement of the Higgs-Top Coupling”, arXiv:1507.09726

[28] N. Mileo et al., “Pseudoscalar top-Higgs coupling: Exploration of CP-odd observables to resolve the sign ambiguity”, arXiv:1603.03632

[29] S. D. Rindani, P. Sharma, and A. Shivaji, “Unraveling the CP phase of top-Higgs coupling in associated production at the LHC”, arXiv:1605.03806

[30] V. Cirigliano, W. Dekens, J. de Vries, and E. Mereghetti, “Constraining the top-Higgs sector of the Standard Model Effective Field Theory”, arXiv:1605.04311

[31] M. J. Dolan, M. Spannowsky, Q. Wang, and Z.-H. Yu, “Determining the Quantum Numbers of Simplified Models in tX production at the LHC”, arXiv:1606.00019

[32] K. Desch, A. Imhof, Z. Was, and M. Worek, “Probing the CP nature of the Higgs boson at linear colliders with tau spin correlations: The Case of mixed scalar - pseudoscalar couplings”, Phys. Lett. B579 (2004) 157–164, doi:10.1016/j.physletb.2003.10.074, arXiv:hep-ph/0307331

[33] S. Berge, W. Bernreuther, and M. Spiesberger, “Determining the CP parity of Higgs bosons in their tau decay channels at the ILC”, arXiv:1208.1507

[34] R. Harnik et al., “Measuring CP violation in h → τ⁺τ⁻ at colliders”, Phys. Rev. D88 (2013), no. 7, 076009, doi:10.1103/PhysRevD.88.076009, arXiv:1308.1094

[35] S. Berge, W. Bernreuther, and H. Spiesberger, “Higgs CP properties using the τ decay modes at the ILC”, Phys. Lett. B727 (2013) 488–495, doi:10.1016/j.physletb.2013.11.006, arXiv:1308.2674

[36] P. Ilten, “Electroweak and Higgs Measurements Using Tau Final States with the LHCb Detector”, arXiv:1401.4902

[37] S. Berge, W. Bernreuther, and S. Kirchner, “Prospects of constraining the Higgs bosons CP nature in the tau decay channel at the LHC”, Phys. Rev. D92 (2015) 096012, doi:10.1103/PhysRevD.92.096012, arXiv:1510.03850

[38] A. Askew et al., “Prospect for measuring the CP phase in the hττ coupling at the LHC”, Phys. Rev. D91 (2015), no. 7, 075014, doi:10.1103/PhysRevD.91.075014, arXiv:1501.03156

[39] CMS Collaboration, “Search for the Associated Production of a Higgs Boson with a Single Top Quark in Proton-Proton Collisions at √s = 8 TeV”, arXiv:1509.08159

[40] CMS Collaboration, “Search for the associated production of the Higgs boson with a top-quark pair”, JHEP 09 (2014) 087, doi:10.1007/JHEP09(2014)087, 10.1007/JHEP10(2014)106, arXiv:1408.1682 [Erratum: JHEP10,106(2014)].

[41] CMS Collaboration, “Measurement of Higgs boson production and properties in the WW decay channel with leptonic final states”, Phys. Rev. D89 (2014), no. 1, 012003, doi:10.1103/PhysRevD.89.012003, arXiv:1310.3687

[42] ATLAS Collaboration, “Prospect for measuring the CP phase in the hττ coupling at the LHC”, Phys. Rev. D92 (2015), no. 5, 053003, doi:10.1103/PhysRevD.92.053003, arXiv:1504.00611

[43] ATLAS Collaboration, “Evidence for the 125 GeV Higgs boson decaying to a pair of τ leptons”, JHEP 05 (2014) 104, doi:10.1007/JHEP05(2014)104, arXiv:1401.5041

[44] CMS Collaboration, “Evidence for the Higgs-boson Yukawa coupling to tau leptons with the ATLAS detector”, JHEP 01 (2015) 069, doi:10.1007/JHEP01(2015)069, arXiv:1409.6212

[45] CMS Collaboration, “Search for the standard model Higgs boson produced through vector boson fusion and decaying to bطور”, Phys. Rev. D92 (2015), no. 3, 032008, doi:10.1103/PhysRevD.92.032008, arXiv:1506.01010

[46] CMS Collaboration, “Evidence for the 125 GeV Higgs boson decaying to a pair of τ leptons”, JHEP 05 (2014) 104, doi:10.1007/JHEP05(2014)104, arXiv:1401.5041

[47] ATLAS Collaboration, “Prospect for measuring the CP phase in the hττ coupling at the LHC”, Phys. Rev. D92 (2015), no. 5, 053003, doi:10.1103/PhysRevD.92.053003, arXiv:1504.00611

[48] CMS Collaboration, “Search for a very light NMSSM Higgs boson produced in decays of the 125 GeV scalar boson and decaying into τ leptons in pp collisions at √s = 8 TeV”, JHEP 01 (2016) 079, doi:10.1007/JHEP01(2016)079, arXiv:1510.06534

[49] CMS Collaboration, “Search for a low-mass pseudoscalar Higgs boson produced in association with a b-bbar pair in pp collisions at sqrt(s) = 8 TeV”, arXiv:1511.03610

[50] CMS Collaboration, “Study of the Mass and Spin-Parity of the Higgs Boson Candidate Via Its Decays to Z Boson Pairs”, Phys. Rev. Lett. 110 (2013), no. 8, 081803, doi:10.1103/PhysRevLett.110.081803, arXiv:1212.6639

[51] CMS Collaboration, “Measurement of the properties of a Higgs boson in the four-lepton final state”, Phys. Rev. D89 (2014), no. 9, 092007, doi:10.1103/PhysRevD.89.092007, arXiv:1312.5353

[52] CMS Collaboration, “Measurement of Higgs boson production and properties in the WW decay channel with leptonic final states”, JHEP 01 (2014) 090, doi:10.1007/JHEP01(2014)090, arXiv:1312.1129
