CP Properties of Higgs Boson Interactions with Top Quarks in the $t\bar{t}H$ and tH Processes Using $H \to \gamma\gamma$ with the ATLAS Detector

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(Received 10 April 2020; accepted 15 June 2020; published 5 August 2020)

A study of the charge conjugation and parity (CP) properties of the interaction between the Higgs boson and top quarks is presented. Higgs bosons are identified via the diphoton decay channel ($H \to \gamma\gamma$), and their production in association with a top quark pair ($t\bar{t}H$) or single top quark (tH) is studied. The analysis uses 139 fb^{-1} of proton–proton collision data recorded at a center-of-mass energy of $\sqrt{s} = 13$ TeV with the ATLAS detector at the Large Hadron Collider. Assuming a CP-even coupling, the $t\bar{t}H$ process is observed with a significance of 5.2 standard deviations. The measured cross section times $H \to \gamma\gamma$ branching ratio is $1.64^{+0.38}_{-0.36}(\mathrm{stat})^{+0.17}_{-0.14}(\mathrm{sys})$ fb, and the measured rate for $t\bar{t}H$ is $1.43^{+0.33}_{-0.31}(\mathrm{stat})^{+0.21}_{-0.15}(\mathrm{sys})$ times the Standard Model expectation. The tH production process is not observed and an upper limit on its rate of 12 times the Standard Model expectation is set. A CP-mixing angle greater (less) than 43 $(-43)°$ is excluded at 95% confidence level.

DOI: 10.1103/PhysRevLett.125.061802

The observation of Higgs boson production in association with top quarks at the LHC [1,2] provides an opportunity to probe the charge conjugation and parity (CP) properties of the Yukawa coupling of the Higgs boson to the top quark. The Standard Model (SM) of particle physics predicts the Higgs boson to be a scalar particle ($J^{CP} = 0^{++}$) with a prescribed coupling to the top quark. However, the presence of a $J^{CP} = 0^{+-}$ pseudoscalar admixture, which introduces a second coupling to the top quark, has not yet been excluded. Any measured CP-odd contribution would be a sign of physics beyond the SM and could account for the explanation of the observed baryon asymmetry of the universe. This Letter presents a search for CP violation in this coupling and measurements of the production rate of the Higgs boson, via its decay into two photons, in association with top quarks. Recently, the CMS Collaboration performed a similar study [3].

Studies of CP properties of the Higgs boson interactions with gauge bosons have been performed by the ATLAS and CMS experiments [4–9]; the results show no deviations from the SM predictions. However, these measurements probe the bosonic couplings in which CP-odd contributions enter only via higher-order operators that are suppressed by powers of $1/\Lambda^2$ [10], where Λ is the scale of the new physics in an effective field theory (EFT). In the case of the Yukawa couplings, the CP-odd contributions are not suppressed by powers of $1/\Lambda^2$.

The CP properties of the top Yukawa coupling can be probed directly using Higgs boson production in association with top quarks: $t\bar{t}H$ and tH processes. The couplings impact the production rates [11–14] and some kinematic distributions. The tH rate is particularly sensitive to deviations from SM couplings due to destructive interference in the SM between diagrams where the Higgs boson radiates from a top quark and from a W boson. The presence of CP-mixing in the top Yukawa coupling also modifies the gluon–gluon fusion (ggF) production rate and the $H \to \gamma\gamma$ decay rate.

This analysis is performed using 139 fb^{-1} of $\sqrt{s} = 13$ TeV proton–proton (pp) collision data recorded from 2015 to 2018 with the ATLAS detector. The ATLAS detector [15–17] is a multipurpose particle detector with a forward-backward symmetric cylindrical geometry and near 4π coverage in solid angle [18]. The trigger system consists of a hardware-based first-level trigger and a software-based high-level trigger [19]. Events used in this analysis were triggered by requiring two photons with a *loose* identification requirement [20] in the 2015–2016 data-taking period and transverse energies of at least 25 GeV and 35 GeV for the subleading and leading photons, respectively. Due to the greater instantaneous luminosity, the photon trigger identification requirement was tightened in the 2017–2018 data-taking period. The average trigger efficiency is over 98% for events passing the full diphoton event selection for this analysis.

The EFT definition used in this Letter is provided by the Higgs characterization model [21], which is implemented in the MadGraph5_aMC@NLO generator [22]. Within

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this model, the term in the effective Lagrangian that describes the top Yukawa coupling is

$$\mathcal{L} = -\frac{m_t}{v}\{\bar{\psi}_t\kappa_t[\cos(\alpha) + \mathrm{i}\sin(\alpha)\gamma_5]\psi_t\}H$$

where m_t is the top quark mass, v is the Higgs vacuum expectation value, κ_t (> 0) is the top Yukawa coupling parameter, and α is the CP-mixing angle. The SM corresponds to a CP-even coupling with $\alpha = 0$ and $\kappa_t = 1$, while a CP-odd coupling is realized when $\alpha = 90°$.

Simulated $t\bar{t}H$ and tH samples were generated using MadGraph5_aMC@NLO 2.6.2 at next-to-leading order in QCD for different α and κ_t (for tH) values, with the NNPDF30NLO [23] parton distribution function (PDF) set used for the matrix element (ME) evaluation, and interfaced to PYTHIA 8 [24] using the NNPDF23LO [25] PDF set for parton showering (PS). The A14 parameter set [26], tuned to data, was used for both PS and underlying event (UE). From these samples, the yields for $t\bar{t}H$ and tH are parameterized as functions of α and κ_t, which are used in the statistical interpretations. Samples for other Higgs boson production processes, ggF [27], vector-boson fusion (VBF) [28], and vector-boson associated production (VH) [29,30] were produced with POWHEG-BOX v2 generator [31] using the PDF4LHC15 PDF set [32] for ME, with the AZNLO set of tuned parameters [33] and PYTHIA 8 for PS using the CTEQ6L1 [34] PDF set. Samples generated with Herwig 7 [35] are used for systematic uncertainty studies that involve modeling of the PS, hadronization and UE. The simulated Higgs boson samples are normalized to the SM cross sections (Refs. [36–54]) times the SM branching ratio (BR) to diphotons (Refs. [36,55–58]) with a Higgs boson mass of 125.09 GeV [59], and specifically for $t\bar{t}H$, the SM predicted cross section times the $H \to \gamma\gamma$ BR is $\sigma_{t\bar{t}H} \times B_{\gamma\gamma} = 1.15^{+0.09}_{-0.12}$ fb.

Although this analysis relies on a data-driven approach for background estimations, a simulated background sample for the $t\bar{t}\gamma\gamma$ process was generated to optimize the event selection and develop the background model. This sample was generated using the MadGraph5_aMC@NLO generator, with the NNPDF23LO PDF set and showered with PYTHIA 8.

All generated Higgs boson events were passed through a full simulation of the ATLAS detector response [60] using GEANT 4 [61]. The $t\bar{t}\gamma\gamma$ events were processed with a fast simulation in which the full simulation of the calorimeter is replaced with a parameterization of the calorimeter response [62]. The effects of multiple pp interactions in the same or neighboring bunch crossings are included using events generated with PYTHIA 8. Events are weighted such that the distribution of the average number of interactions per bunch crossing matches that observed in data, which is typically around 30 to 40.

Events are selected by requiring two isolated photon candidates with transverse momenta p_{T} greater than 35 GeV and 25 GeV. Both photons must satisfy the *tight* identification requirement [20]. The identification is constructed from a cut-based selection using the electromagnetic shower shape variables. The leading (subleading) photon must have $p_{\mathrm{T}}/m_{\gamma\gamma} > 0.35$ (0.25), and the diphoton invariant mass $m_{\gamma\gamma}$ is required to be in the range $m_{\gamma\gamma} \in [105, 160]$ GeV. Jets are reconstructed using the anti-k_t algorithm [63] with a radius parameter of $R = 0.4$. Events are required to have at least one jet with $p_{\mathrm{T}} > 25$ GeV containing a b-hadron (b-jet), identified using a b-tagging algorithm with an efficiency of 77% and a mistagging rate of 0.9% for light-flavor jets [64].

Selected events are sorted into two $t\bar{t}H$-enriched regions. The "Lep" region, targeting top quark decays in which at least one of the resulting W bosons decays leptonically, requires events to have at least one isolated lepton (muon or electron) candidate with $p_{\mathrm{T}} > 15$ GeV passing *medium* identification requirements (Refs. [20,65]). The "Had" region targets hadronic top quark decays (as well as top quark decays to both hadronically decaying τ leptons and unreconstructed leptons) and requires events to have at least two additional jets with $p_{\mathrm{T}} > 25$ GeV and no selected lepton.

A boosted decision tree (BDT) used for the top quark reconstruction, denoted by "Top Reco BDT," is trained with the $t\bar{t}H$ sample by using the XGBOOST package [66] to extract the three-jet (triplet) combination best matching the hadronic decay products of a top quark. This BDT uses p_{T}, η, ϕ, and the energy E of W boson and b jet (where the W boson candidate is formed by a pair of jets). Furthermore, this BDT uses the angular distance ΔR_{Wb} between the W boson and b jet, ΔR_{jj} between the two jets composing the W boson candidate, and b-tagging information about all three jets in the triplet and the invariant mass of the triplet. For events in the Had region, the triplet with the highest Top Reco BDT score is taken as the primary top quark candidate (t_1). In the Lep region, for events containing only one lepton, a W boson candidate is first constructed from the lepton and missing transverse momentum $E_{\mathrm{T}}^{\mathrm{miss}}$. Then t_1 is reconstructed from this leptonic W boson candidate and the jet giving the highest Top Reco BDT score. No top quark candidate is reconstructed for events containing more than one lepton. After t_1 is selected, if there are at least three additional jets, a second top quark candidate (t_2) is reconstructed by selecting the triplet with the highest BDT score from the remaining jets; if there is only one or two additional jets, then t_2 is taken as the sum of the remaining jets; otherwise no t_2 is reconstructed.

To improve the analysis sensitivity, selected events are categorized using partitions of a two-dimensional BDT space. Two independent BDTs are trained using the XGBOOST algorithm: "Background Rejection BDT" and "CP BDT," and each of them is trained separately in the Had and Lep regions. The Background Rejection BDT is trained to separate $t\bar{t}H$-like events from background that are mainly nonresonant diphoton production processes, including $\gamma\gamma$ + jets and $t\bar{t}\gamma\gamma$. A detailed discussion of this methodology is given in Ref. [1]. The *CP* BDT is trained to separate *CP*-even from *CP*-odd couplings using $t\bar{t}H$ and tH processes. The *CP* BDT uses p_{T} and η of the diphoton system, p_{T} and η of t_1 and t_2, their azimuthal angles calculated relative to the diphoton system $\phi_{\gamma\gamma,t_1}$, $\phi_{\gamma\gamma,t_2}$, as well as their Top Reco BDT scores. It also uses differences in pseudorapidity and azimuthal angle $\Delta\eta_{t_1t_2}$ and $\Delta\phi_{t_1t_2}$ between the two top quark candidates, the invariant mass of the diphoton and primary top quark system $m_{\gamma\gamma,t_1}$, the invariant mass of the two top quark candidates $m_{t_1t_2}$, the scalar p_{T} sum of jets H_{T}, the $E_{\mathrm{T}}^{\mathrm{miss}}$ divided by $\sqrt{H_{\mathrm{T}}}$, the number of jets and b-tagged jets, and the minimum and second smallest angular differences $\Delta R_{\gamma j}$ between a photon and a jet.

Figure 1 shows the BDT discriminant distributions in the data as well as those expected from *CP*-even and *CP*-odd Higgs boson signals in the Had region. The discriminating power can be seen by comparing the *CP*-even, *CP*-odd, and data shapes. Events with low values of the Background Rejection BDT response are removed, and the remaining events are categorized. The number of categories and the boundary locations are chosen to optimize the $t\bar{t}H$ significance and the discriminating power between the *CP*-even and *CP*-odd cases. There are 20 categories in total: 12 in the Had region and 8 in the Lep region.

The results are impacted by three distinct types of uncertainties: the statistical uncertainty associated with the data, theoretical modeling systematic uncertainties, and experimental systematic uncertainties. The first dominates. Theoretical uncertainties for $t\bar{t}H$ and tH rates in the various categories are assessed. The following effects are considered: the value of the strong coupling constant; alternative generator for the PS, hadronization, and UE; and PDF uncertainty. In the three (two) most *CP*-even sensitive Had (Lep) categories, each of these uncertainties is less than 10%. The background from ggF is less than 0.25 events in each of the most sensitive categories; conservative uncertainties, including a 100% theoretical uncertainty in the modeling of the radiation of additional heavy-flavor jets, are assigned to it in the Had region. The same heavy-flavor uncertainty is also assigned to the VBF and VH processes.

Experimental uncertainties arise from identification and isolation criteria for photons, electrons, and muons and from their energy scale and resolution [20,65]. Jets have uncertainties from b tagging [64] and vertex identification [67] in addition to the energy scale and resolution [68]. Uncertainties in the measurement of $E_{\mathrm{T}}^{\mathrm{miss}}$ [69], which is used in the leptonic categories, are also included. These experimental effects impact the expected event yield in each category and can cause events to migrate between the categories. The overall uncertainty is less than 20% in each category. In addition, uncertainties in the luminosity [70] obtained using the LUCID-2 detector [71] and trigger efficiency [19] are responsible for uncertainties in the overall event yield of 1.7% and 0.4%, respectively.

A simultaneous maximum-likelihood fit is performed to the $m_{\gamma\gamma}$ spectra in all the categories. Signal and background shapes are modeled by analytic functions using the strategy discussed in Ref. [6]. The chosen background function is

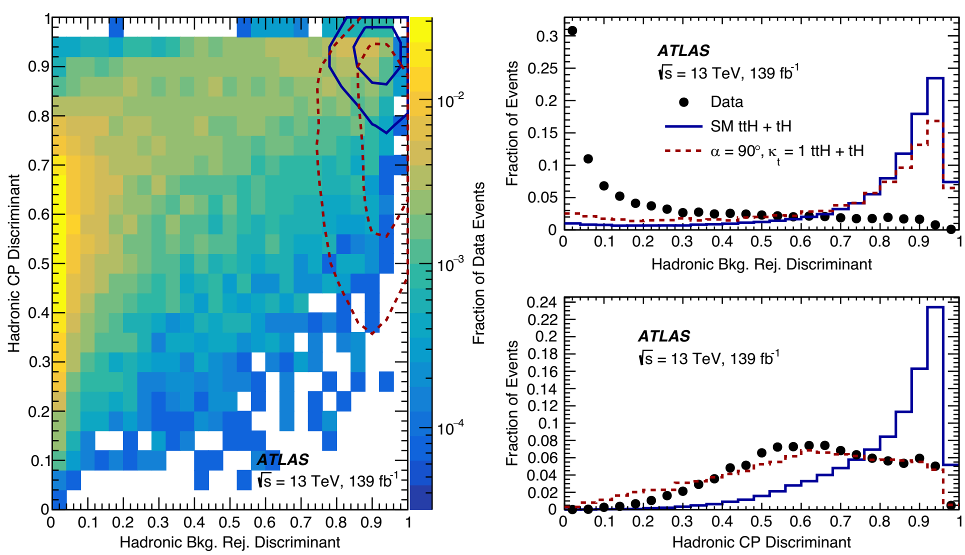

FIG. 1. Left: two-dimensional BDT distribution in the selected data events ($m_{\gamma\gamma} \in [105, 160]$ GeV) from the Had region showing the Background Rejection BDT and *CP* BDT. The inner (outer) contours capture 25% (50%) of the $t\bar{t}H$ and tH signal events for *CP*-even (blue) and *CP*-odd (red) hypotheses. Right: projections onto the background rejection and *CP* BDT axes. Contributions from *CP*-even (blue) and *CP*-odd (red) $t\bar{t}H/tH$ processes and the data (black) are shown and normalized to unit area. The error bars on data are statistical.

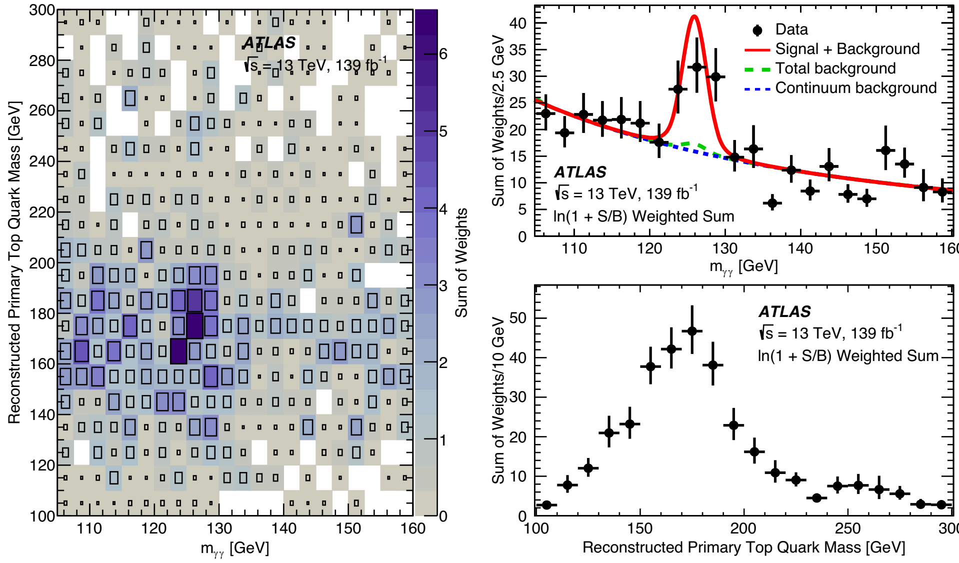

FIG. 2. Distribution of reconstructed primary top quark mass versus reconstructed Higgs boson mass in the data events. The right panels show the projections onto the Higgs boson mass and primary top quark mass axes. In the upper panel, the fitted continuum background (blue), the total background including non-$t\bar{t}H/tH$ Higgs boson production (green), and the total fitted signal plus background (red) are shown. The error bars on data are statistical.

based on the simulated $t\bar{t}\gamma\gamma$ events following the procedure in Ref. [1], which imposes stringent conditions on potential biases in the extracted signal yield to avoid losses in sensitivity. The parameters of the background model and background normalization in each category are left free in the fit. The profile likelihood ratio is used as the test statistic, and the asymptotic approximation [72] is used for statistical interpretations. Yields from $t\bar{t}H$ and tH are extracted after subtracting the very small contribution from other Higgs boson production modes using their SM expected values. Figure 2 shows the distributions of the reconstructed masses for the diphoton system and primary top quark. The events are weighted by $\ln(1 + S/B)$ with S and B being the fitted signal and background yields in the smallest $m_{\gamma\gamma}$ interval containing 90% of the signal in each category. The p value associated with the compatibility between the observed spectra and the fit model using the goodness-of-fit test method described in Ref. [73] is 35%. Assuming a CP-even coupling, the $\sigma_{t\bar{t}H} \times B_{\gamma\gamma}$ is derived by constraining all the non-$t\bar{t}H$ Higgs boson processes to their SM predictions and measured to be $1.64^{+0.38}_{-0.36}(\text{stat})^{+0.17}_{-0.14}(\text{sys})$ fb. The measured rate for $t\bar{t}H$ is $1.43^{+0.33}_{-0.31}(\text{stat})^{+0.21}_{-0.15}(\text{sys})$ times the SM expectation. The background-only hypothesis is rejected with an observed (expected) significance of 5.2σ (4.4σ). The rate for tH is derived by constraining all the non-$t\bar{t}H/tH$ Higgs boson processes to their SM prediction without prior constraint on the rate of $t\bar{t}H$. Using the CLs method [74], this yields a 95% confidence level (CL) upper limit of 12 times the SM prediction, the same as expected assuming the presence of SM tH signal. This is stricter than the previous best limit of 25 times the SM prediction on tH from the CMS analysis performed using 35.9 fb^{-1} of data at $\sqrt{s} = 13$ TeV [75] with the $t\bar{t}H$ process constrained to the SM prediction.

Extraction of values for the top Yukawa coupling requires additional information. In particular, the BR of $H \to \gamma\gamma$ is needed to recover the total Higgs boson production rate, and the Higgs boson coupling to gluons is needed to account for the small ggF background. The corresponding Higgs boson coupling modifiers κ_γ and κ_g are measured in the Run 2 Higgs boson coupling combination [76]. This combination includes the first 80 fb^{-1} of data used in this paper, and $t\bar{t}H$ and tH analyses from other decay channels. The combination analysis is repeated without the $t\bar{t}H$ and tH inputs, and this result is used to constrain κ_g and κ_γ. The impact on κ_g and κ_γ of removing input $t\bar{t}H$ and tH analyses from the combination is small. The correlation of the systematic uncertainties between the Higgs boson coupling combination and this analysis is neglected. The correlation has a small impact on α, and a similar effect on κ_t as on signal strength reported in Ref. [76]. This analysis is insensitive to the potential modifications of ggF kinematics due to CP mixing, which is therefore neglected. The results of the fit for $\kappa_t \cos(\alpha)$ and $\kappa_t \sin(\alpha)$ are shown as contours in Fig. 3. A limit on α is set without prior constraint on κ_t in the fit: $|\alpha| > 43°$ is excluded at 95% CL. The expected exclusion is $|\alpha| > 63°$ under the CP-even hypothesis. A value of $\alpha = 90\,(180)°$ is excluded at 3.9σ (2.5σ). A comparable study from the CMS experiment excluded $\alpha = 90°$ at 3.2σ [3]. If κ_γ and κ_g are parameterized using α and κ_t [11], the observed (expected) exclusion is $|\alpha| > 43\,(56)°$ without prior constraint on κ_t in the fit. The impact of the systematic uncertainties is negligible.

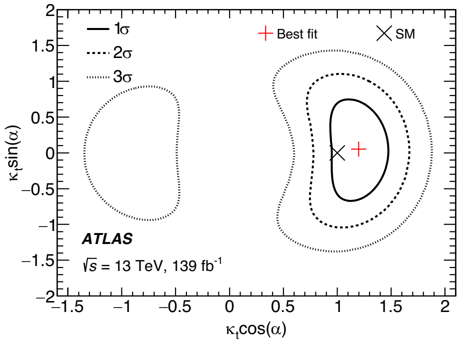

FIG. 3. Two-dimensional likelihood contours for $\kappa_t \cos(\alpha)$ and $\kappa_t \sin(\alpha)$ with ggF and $H \to \gamma\gamma$ constrained by the Higgs boson coupling combination.

In summary, the production rate of the Higgs boson in association with top quarks is measured, and the *CP* property of the top Yukawa coupling is studied. The no-$t\bar{t}H$ hypothesis is rejected with a significance of 5.2σ, and the measured $\sigma_{t\bar{t}H} \times B_{\gamma\gamma}$ is $1.64^{+0.38}_{-0.36}(\text{stat})^{+0.17}_{-0.14}(\text{sys})$ fb. The measured rate for $t\bar{t}H$ is $1.43^{+0.33}_{-0.31}(\text{stat})^{+0.21}_{-0.15}(\text{sys})$ times the SM expectation. The tH process is not observed, and an upper limit of 12 times the SM expectation is set on its rate at 95% CL. All measurements are consistent with the SM expectations, and the possibility of *CP*-odd couplings between the Higgs boson and top quark is severely constrained. A pure *CP*-odd coupling is excluded at 3.9σ, and $|\alpha| > 43°$ is excluded at 95% CL.

We thank CERN for the very successful operation of the LHC, as well as the support staff from our institutions without whom ATLAS could not be operated efficiently. We acknowledge the support of ANPCyT, Argentina; YerPhI, Armenia; ARC, Australia; BMWFW and FWF, Austria; ANAS, Azerbaijan; SSTC, Belarus; CNPq and FAPESP, Brazil; NSERC, NRC, and CFI, Canada; CERN; CONICYT, Chile; CAS, MOST, and NSFC, China; COLCIENCIAS, Colombia; MSMT CR, MPO CR, and VSC CR, Czech Republic; DNRF and DNSRC, Denmark; IN2P3-CNRS and CEA-DRF/IRFU, France; SRNSFG, Georgia; BMBF, HGF, and MPG, Germany; GSRT, Greece; RGC and Hong Kong SAR, China; ISF and Benoziyo Center, Israel; INFN, Italy; MEXT and JSPS, Japan; CNRST, Morocco; NWO, Netherlands; RCN, Norway; MNiSW and NCN, Poland; FCT, Portugal; MNE/IFA, Romania; MES of Russia and NRC KI, Russia Federation; JINR; MESTD, Serbia; MSSR, Slovakia; ARRS and MIZŠ, Slovenia; DST/NRF, South Africa; MINECO, Spain; SRC and Wallenberg Foundation, Sweden; SERI, SNSF, and Cantons of Bern and Geneva, Switzerland; MOST, Taiwan; TAEK, Turkey; STFC, United Kingdom; and DOE and NSF, USA. In addition, individual groups and members have received support from BCKDF, CANARIE, Compute Canada, and CRC, Canada; ERC, ERDF, Horizon 2020, Marie Skłodowska-Curie Actions, and COST, European Union; Investissements d'Avenir Labex, Investissements d'Avenir Idex, and ANR, France; DFG and AvH Foundation, Germany; Herakleitos, Thales, and Aristeia programs cofinanced by EU-ESF and the Greek NSRF, Greece; BSF-NSF and GIF, Israel; CERCA Programme Generalitat de Catalunya and PROMETEO Programme Generalitat Valenciana, Spain; Göran Gustafssons Stiftelse, Sweden; The Royal Society and Leverhulme Trust, United Kingdom. The crucial computing support from all WLCG partners is acknowledged gratefully, in particular from CERN, the ATLAS Tier-1 facilities at TRIUMF (Canada), NDGF (Denmark, Norway, Sweden), CC-IN2P3 (France), KIT/GridKA (Germany), INFN-CNAF (Italy), NL-T1 (Netherlands), PIC (Spain), ASGC (Taiwan), RAL (UK), and BNL (USA), the Tier-2 facilities worldwide, and large non-WLCG resource providers. Major contributors of computing resources are listed in Ref. [77].

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