Observation of the Doubly Charmed Baryon \( \Xi_{cc}^{++} \)

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(Received 6 July 2017; revised manuscript received 2 August 2017; published 11 September 2017)

A highly significant structure is observed in the \( \Lambda_c^+ K^- \pi^+ \pi^+ \) mass spectrum, where the \( \Lambda_c^+ \) baryon is reconstructed in the decay mode \( pK^- \pi^+ \). The structure is consistent with originating from a weakly decaying particle, identified as the doubly charmed baryon \( \Xi_{cc}^{++} \). The difference between the masses of the \( \Xi_{cc}^{++} \) and \( \Lambda_c^+ \) states is measured to be \( 1334.94 \pm 0.72 \text{(stat.)} \pm 0.27 \text{(syst.)} \) MeV/c\(^2\), and the \( \Xi_{cc}^{++} \) mass is then determined to be \( 3621.40 \pm 0.72 \text{(stat.)} \pm 0.27 \text{(syst.)} \pm 0.14 \text{(\( \Lambda_c^+ \)) MeV/c\(^2\)}, where the last uncertainty is due to the limited knowledge of the \( \Lambda_c^+ \) mass. The state is observed in a sample of proton-proton collision data collected by the LHCb experiment at a center-of-mass energy of 13 TeV, corresponding to an integrated luminosity of 1.7 fb\(^{-1}\), and confirmed in an additional sample of data collected at 8 TeV.

DOI: 10.1103/PhysRevLett.119.112001

The quark model [1–3] predicts the existence of multiplets of baryon and meson states. Those states composed of the lightest four quarks \( (u, d, s, c) \) form SU(4) multiplets [4]. Numerous states with charm quantum number \( C \) or \( q \) expected \( qqq \) decaying colliders [37–39].

States composed of a variety of theoretical models. In most cases, the masses of the \( \Xi_{cc}^{++} \) and \( \Lambda_c^+ \) states are expected to differ by only a few MeV/c\(^2\), due to approximate isospin symmetry [34–36]. Most predictions for the lifetime of the \( \Xi_{cc}^{++} \) baryon are in the range 50 to 250 fs, and the lifetime of the \( \Xi_{cc}^{++} \) baryon is expected to be three to four times longer at 200 to 700 fs [10,11,19,24,37–40]. While both are expected to be produced at hadron colliders [41–43], the longer lifetime of the \( \Xi_{cc}^{++} \) baryon should make it significantly easier to observe than the \( \Xi_{cc}^{++} \) baryon in such experiments, due to the use of real-time (online) event-selection requirements designed to reject backgrounds originating from the primary interaction point.

Experimentally, there is a long-standing puzzle in the \( \Xi_{cc}^{++} \) system. Observations of the \( \Xi_{cc}^{++} \) baryon at a mass of \( 3519 \pm 2 \) MeV/c\(^2\) with signal yields of 15.9 events over \( 6.1 \pm 0.5 \) background in the final state \( \Lambda_c^+ K^- \pi^+ \) (6.3\( \sigma \) significance), and 5.62 events over 1.38 \pm 0.13 background in the final state \( pD^+ K^- \) (4.8\( \sigma \) significance) were reported by the SELEX Collaboration [44,45]. Their results included a number of unexpected features, notably a short lifetime and a large production rate relative to that of the singly charmed \( \Lambda_c^+ \) baryon. The lifetime was stated to be shorter than 33 fs at the 90\% confidence level, and SELEX concluded that 20\% of all \( \Lambda_c^+ \) baryons observed by the experiment originated from \( \Xi_{cc}^{++} \) decays, implying a relative \( \Xi_{cc}^{++} \) production rate several orders of magnitude larger than theoretical expectations [11]. Searches from the FOCUS [46], BABAR [47], and Belle [48] experiments did not find evidence for a state with the properties reported by SELEX, and neither did a search at LHCb with data collected in 2011 corresponding to an integrated luminosity of 0.65 fb\(^{-1}\) [49]. However, because the production environments at these experiments differ from that of SELEX, which studied collisions of a hyperon beam on fixed nuclear targets, these null results do not exclude the original observations.

This Letter presents the observation of the \( \Xi_{cc}^{++} \) baryon [50] via the decay mode \( \Lambda_c^+ K^- \pi^+ \pi^+ \) (Fig. 1), which is expected to have a branching fraction of up to 10\% [51]. The \( \Lambda_c^+ \) baryon is reconstructed in the final state \( pK^- \pi^+ \).

![FIG. 1. Example Feynman diagram contributing to the decay \( \Xi_{cc}^{++} \rightarrow \Lambda_c^+ K^- \pi^+ \pi^+ \).](image-url)
The data consist of $pp$ collisions collected by the LHCb experiment at the Large Hadron Collider at CERN with a center-of-mass energy of 13 TeV taken in 2016, corresponding to an integrated luminosity of 1.7 fb$^{-1}$.

The LHCb detector is a single-arm forward spectrometer covering the pseudorapidity range $2 < \eta < 5$, designed for the study of particles containing $b$ or $c$ quarks, and is described in detail in Refs. [52,53]. The detector elements most relevant to this analysis are a silicon-strip vertex detector surrounding the $pp$ interaction region, a tracking system that provides a measurement of the momentum of charged particles, and two ring-imaging Cherenkov detectors [54] that are able to discriminate between different species of charged hadrons. The on-line event selection is performed by a trigger that consists of a hardware stage, which is based on information from the calorimeter and muon systems, followed by a software stage, which fully reconstructs the event [55]. The on-line reconstruction incorporates near-real-time alignment and calibration of the detector [56], which in turn allows the reconstruction of the $\Xi_{cc}^{+}$ decay to be performed entirely in the trigger software.

The reconstruction of $\Xi_{cc}^{++} \rightarrow \Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+}$ decays proceeds as follows. Candidate $\Lambda_{c}^{+} \rightarrow pK^{-}\pi^{+}$ decays are reconstructed from three charged particles that form a good-quality vertex and that are inconsistent with originating from any $pp$ collision primary vertex (PV). The PV of any single particle is defined to be the PV with respect to which the particle has the smallest impact parameter ($\chi_{IP}^{2}$), which is the difference in $\chi^{2}$ of the PV fit with and without the particle in question. The $\Lambda_{c}^{+}$ vertex is required to be displaced from its PV by a distance corresponding to a proper decay time greater than 150 fs. The $\Lambda_{c}^{+}$ candidate is then combined with three additional charged particles to form a $\Xi_{cc}^{++} \rightarrow \Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+}$ candidate. These additional particles must form a good-quality vertex with the $\Lambda_{c}^{+}$ candidate, and the $\Lambda_{c}^{+}$ decay vertex must be downstream of the $\Xi_{cc}^{++}$ vertex. Each of the six final-state particles is required to pass track-quality requirements, to have hadron-identification information consistent with the appropriate hypothesis ($p$, $K$, or $\pi$), and to have transverse momentum $p_{T} > 500$ MeV/c. To avoid duplicate tracks, the angle between each pair of final-state particles with the same charge is required to be larger than 0.5 mrad. The $\Xi_{cc}^{++}$ candidate must have $p_{T} > 4$ GeV/c and must be consistent with originating from its PV. The selection above includes criteria applied in the trigger software, plus additional requirements chosen based on simulated signal events and a control sample of data. Simulated signal events are produced with the standard LHCb simulation software [57–63] interfaced to a dedicated generator, GENXicc [64–66], for $\Xi_{cc}^{++}$ baryon production. In the simulation, the $\Xi_{cc}^{++}$ mass and lifetime are assumed to be 3600 MeV/$c^{2}$ and 333 fs. The background control sample consists of wrong-sign (WS) $\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{-}$ combinations.

The background level is further reduced with a multivariate selector based on the multilayer perceptron algorithm [67]. The selector is trained with simulated signal events and with the WS control sample of data to represent the background. For both signal and background training samples, candidates are required to pass the selection described above and to fall within a signal search region defined as $2270 < m_{\text{cand}}(\Lambda_{c}^{+}) < 2306$ MeV/$c^{2}$ and $3300 < m_{\text{cand}}(\Xi_{cc}^{++}) < 3800$ MeV/$c^{2}$, where $m_{\text{cand}}(\Lambda_{c}^{+})$ is the reconstructed mass of the $\Lambda_{c}^{+}$ candidate, $m_{\text{cand}}(\Xi_{cc}^{++}) = m(\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+}) - m(\Lambda_{c}^{+}) + m_{\text{PDG}}(\Lambda_{c}^{+})$, $m(\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+})$ is the reconstructed mass of the $\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+}$ combination, and $m_{\text{PDG}}(\Lambda_{c}^{+}) = 2286.46 \pm 0.14$ MeV/$c^{2}$ is the known value of the $\Lambda_{c}^{+}$ mass [5]. The $m_{\text{cand}}(\Lambda_{c}^{+})$ window corresponds to approximately $\pm 3$ times the $\Lambda_{c}^{+}$ mass resolution. The use of $m_{\text{cand}}(\Xi_{cc}^{++})$ rather than $m(\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+})$ cancels fluctuations in the reconstructed $\Lambda_{c}^{+}$ mass to first order, and thereby improves the $\Xi_{cc}^{++}$ mass resolution by approximately 40%.

Based on studies with simulated events and control samples of data, ten input variables that together provide good discrimination between signal and background candidates are used in the multivariate selector. They are as follows: the $\chi^{2}$ per degree of freedom of each of the $\Lambda_{c}^{+}$ vertex fit, the $\Xi_{cc}^{++}$ vertex fit, and a kinematic refit [68] of the $\Xi_{cc}^{++}$ decay chain requiring it to originate from its PV; the smallest $p_{T}$ of the three decay products of the $\Lambda_{c}^{+}$; the smallest $p_{T}$ of the four decay products of the $\Xi_{cc}^{++}$; the scalar sum of the $p_{T}$ of the four decay products of the $\Xi_{cc}^{++}$; the angle between the $\Xi_{cc}^{++}$ momentum vector and the direction from the PV to the $\Xi_{cc}^{++}$ decay vertex; the flight distance $\chi_{IP}^{2}$ between the PV and the $\Xi_{cc}^{++}$ decay vertex; the $\chi_{IP}^{2}$ of the $\Xi_{cc}^{++}$ with respect to its PV; and the smallest $\chi_{IP}^{2}$ of the decay products of the $\Xi_{cc}^{++}$ with respect to its PV. Here, the flight distance $\chi^{2}$ is defined as the $\chi^{2}$ of the hypothesis that the $\Xi_{cc}^{++}$ decay vertex coincides with its PV. Candidates are retained for analysis only if their multivariate selector output values exceed a threshold chosen by maximizing the expected value of the figure of merit $\varepsilon/(\sqrt{B} + \sqrt{\varepsilon})$ [69], where $\varepsilon$ is the estimated signal efficiency and $B$ is the estimated number of background candidates underneath the signal peak. The quantity $B$ is computed with the WS control sample and, purely for the purposes of this optimization, it is calculated in a window centered at a mass of 3600 MeV/$c^{2}$ and of half-width 12.5 MeV/$c^{2}$ (corresponding to approximately twice the expected resolution). Its evaluation takes into account the difference in background rates between the $\Lambda_{c}^{+} K^{-} \pi^{+} \pi^{+}$ signal mode and the WS sample, scaling the WS background by the ratio seen in data in the sideband regions $3200 < m_{\text{cand}}(\Xi_{cc}^{++}) < 3300$ MeV/$c^{2}$ and $3800 < m_{\text{cand}}(\Xi_{cc}^{++}) < 3900$ MeV/$c^{2}$. The performance of the multivariate selector is also tested for simulated signal events under other lifetime hypotheses; while the signal efficiency increases with the lifetime, it is
found that the training obtained for 333 fs is close to optimal (i.e., gives comparable performance to a training optimized for the new lifetime hypothesis) even for much shorter or longer lifetimes.

After the multivariate selection is applied, events may still contain more than one \( \Xi^{++} \) candidate in the signal search region. Based on studies of simulation and the control data sample, no peaking background arises due to multiple candidates except for the special case in which the candidates are formed from the same six decay products but two of the decay products are interchanged (e.g., the \( K^- \) particle from the \( \Xi^{++} \) decay and the \( K^- \) particle from the \( \Lambda^+ \) decay). In such instances, one of the candidates is chosen at random to be retained and all others are discarded. In the remaining events, the fraction

The selection described above is then applied to data in the search region. Figure 2 shows the \( \Lambda^+_c \) mass distribution, and the \( \Xi^{++} \) mass spectra for candidates in the mass range 2270 < \( m_{\text{cand}}(\Lambda^+_c) \) < 2360 MeV/c\(^2\). A structure is visible in the signal mode at a mass of approximately 3620 MeV/c\(^2\). No significant structure is visible in the WS control sample, or for events in the \( \Lambda^+ \) mass sidebands. To measure the properties of the structure, an unbinned extended maximum likelihood fit is performed to the invariant mass distribution in the restricted mass window of 3620 ± 150 MeV/c\(^2\) (Fig. 3). The peak structure is empirically described by a Gaussian function plus a modified Gaussian function with power-law tails on both sides [70]. All peak parameters are fixed to values obtained from simulation apart from the mass, yield, and an overall resolution parameter. The background is described by a second-order polynomial with parameters free to float in the fit. The signal yield is measured to be 313 ± 33, corresponding to a local statistical significance in excess of 12σ when evaluated with a likelihood ratio test. The fitted resolution parameter is 6.6 ± 0.8 MeV/c\(^2\), consistent with simulation. The same structure is also observed in the \( \Lambda^+_c K^- \pi^+ \pi^+ \) spectrum in a \( pp \) data sample collected by LHCb at \( \sqrt{s} = 8 \) TeV (see the Supplemental Material [71] for results from the 8 TeV cross-check sample). The local statistical significance of the peak in the 8 TeV sample is above 7σ, and its mass is consistent with that in the 13 TeV data sample.

Additional cross-checks are performed confirming the robustness of the observation. The significance of the structure in the \( \Lambda^+_c K^- \pi^+ \pi^+ \) final state remains above 12σ when fixing the resolution parameter in the invariant mass fit to the value obtained from simulation, changing the threshold value for the multivariate selector, removing events containing multiple candidates in the fitted mass

FIG. 2. Mass spectra of (upper) \( \Lambda^+_c \) and (lower) \( \Xi^{++} \) candidates. The full selection is applied, except for the \( \Lambda^+_c \) mass requirement in the case of the upper plot. For the \( \Lambda^+_c \) mass distribution the (cross-hatched) signal and (vertical line) sideband regions are indicated; to avoid duplication, the histogram is filled only once in events that contain more than one \( \Xi^{++} \) candidate. In the lower plot the right-sign (RS) signal sample \( \Xi^{++}_{\text{RS}} \rightarrow \Lambda^+_c K^- \pi^+ \pi^+ \) is shown, along with the control samples: \( \Lambda^+ \) sideband (SB) \( \Lambda^+_c K^- \pi^+ \pi^+ \) candidates and wrong-sign (WS) \( \Lambda^+_c K^- \pi^+ \pi^- \) candidates, normalized to have the same area as the RS sample in the \( m_{\text{cand}}(\Xi^{++}_{\text{cc}}) \) sidebands.

that has more than one \( \Xi^{++} \) candidate in the range 3300–3800 MeV/c\(^2\) is approximately 8%. The structure in the 13 TeV data sample. The local statistical significance of the peak in the \( \Lambda^+_c \) mass sidebands. To measure the properties of the structure, an unbinned extended maximum likelihood fit is performed to the invariant mass distribution in the restricted \( \Lambda^+_c K^- \pi^+ \pi^+ \) mass window of 3620 ± 150 MeV/c\(^2\) (Fig. 3). The peak structure is empirically described by a Gaussian function plus a modified Gaussian function with power-law tails on both sides [70]. All peak parameters are fixed to values obtained from simulation apart from the mass, yield, and an overall resolution parameter. The background is described by a second-order polynomial with parameters free to float in the fit. The signal yield is measured to be 313 ± 33, corresponding to a local statistical significance in excess of 12σ when evaluated with a likelihood ratio test. The fitted resolution parameter is 6.6 ± 0.8 MeV/c\(^2\), consistent with simulation. The same structure is also observed in the \( \Lambda^+_c K^- \pi^+ \pi^+ \) spectrum in a \( pp \) data sample collected by LHCb at \( \sqrt{s} = 8 \) TeV (see the Supplemental Material [71] for results from the 8 TeV cross-check sample). The local statistical significance of the peak in the 8 TeV sample is above 7σ, and its mass is consistent with that in the 13 TeV data sample.

Additional cross-checks are performed confirming the robustness of the observation. The significance of the structure in the \( \Lambda^+_c K^- \pi^+ \pi^+ \) final state remains above 12σ when fixing the resolution parameter in the invariant mass fit to the value obtained from simulation, changing the threshold value for the multivariate selector, removing events containing multiple candidates in the fitted mass
range, or using an alternative selection without a multivariate classifier. The significance also remains above 12σ in a subsample of candidates for which the reconstructed decay time exceeds five times its uncertainty. This is consistent with a weakly decaying state and inconsistent with the strong decay of a resonance. No fake peaking structures are observed in the control samples when requiring various intermediate resonances to be present ($\rho^0$, $K^{*0}$, $\Sigma_{cc}^{++}$, $\Lambda_{cc}^+$) nor are they observed when combining $\Xi_{cc}^+$ and $\Lambda_{cc}^+$ decay products. The contributions of misidentified $D_1^+ \to K^+ K^+\pi^+$ and $D^+ \to K^+\pi^+\pi^+$ decays are found to be negligible.

The sources of systematic uncertainty affecting the measurement of the $\Xi_{cc}^{++}$ mass (Table I) include the momentum-scale calibration, the event selection, the unknown $\Xi_{cc}^{++}$ lifetime, the invariant mass fit model, and the uncertainty on the $\Lambda_{cc}^+$ mass. The momentum scale is calibrated with samples of $J/\psi \to \mu^+\mu^-$ and $B^+ \to J/\psi K^+$ decays [72,73]. After calibration, an uncertainty of $\pm 0.03\%$ is assigned, which corresponds to a systematic uncertainty of $0.22$ MeV/$c^2$ on the reconstructed $\Xi_{cc}^{++}$ mass. The selection procedure is more efficient for vertices that are well separated from the PV, and therefore preferentially retains longer-lived $\Xi_{cc}^{++}$ candidates. Because of a correlation between the reconstructed decay time and the reconstructed mass, this induces a positive bias on the mass for both $\Xi_{cc}^{++}$ and $\Lambda_{cc}^+$ candidates. The effect is studied with simulation and the bias on the $\Xi_{cc}^{++}$ mass is determined to be $+0.45 \pm 0.14$ MeV/$c^2$ (assuming a lifetime of 333 fs), where the uncertainty is due to the limited size of the simulation sample. A corresponding correction is applied to the fitted value in data. To validate this procedure, the $\Lambda_{cc}^+$ mass in an inclusive sample is measured and corrected in the same way; after the correction, the $\Lambda_{cc}^+$ mass is found to agree with the known value [5]. The bias on the $\Xi_{cc}^{++}$ mass depends on the unknown $\Xi_{cc}^{++}$ lifetime, introducing a further source of uncertainty on the correction. This is estimated by repeating the procedure for other $\Xi_{cc}^{++}$ lifetime hypotheses between 200 and 700 fs. The largest deviation in the correction, $0.06$ MeV/$c^2$, is taken as an additional systematic uncertainty. Final-state photon radiation also causes a bias in the measured mass, which is determined to be $-0.05$ MeV/$c^2$ with simulation [61]. The uncertainty on this correction is approximately $0.01$ MeV/$c^2$ and is neglected. The dependence of the measurement on the fit model is estimated by varying the shape parameters that are fixed according to simulation, by using alternative signal and background models, and by repeating the fits in different mass ranges. The largest deviation seen in the mass, $0.07$ MeV/$c^2$, is assigned as a systematic uncertainty. Finally, since the $\Xi_{cc}^{++}$ mass is measured relative to the $\Lambda_{cc}^+$ mass, the uncertainty of $0.14$ MeV/$c^2$ on the world-average value of the latter is included. After taking these systematic effects into account and combining their uncertainties (except that on the $\Lambda_{cc}^+$ mass) in quadrature, the $\Xi_{cc}^{++}$ mass is measured to be $3621.40 \pm 0.72$(stat.) $\pm 0.27$(syst.) $\pm 0.14(\Lambda_{cc}^+)$ MeV/$c^2$. The mass difference between the $\Xi_{cc}^{++}$ and $\Lambda_{cc}^+$ states is $1334.94 \pm 0.72$(stat.) $\pm 0.27$(syst.) MeV/$c^2$.

In summary, a highly significant structure is observed in the final state $\Lambda_{cc}^+K^+\pi^+\pi^+$ in a $pp$ data sample collected by LHCb at $\sqrt{s} = 13$ TeV, with a signal yield of $313 \pm 33$. The mass of the structure is measured to be $3621.40 \pm 0.72$(stat.) $\pm 0.27$(syst.) $\pm 0.14(\Lambda_{cc}^+)$ MeV/$c^2$, where the last uncertainty is due to the limited knowledge of the $\Lambda_{cc}^+$ mass, and its width is consistent with experimental resolution. The structure is confirmed with consistent mass in a data set collected by LHCb at $\sqrt{s} = 8$ TeV. The signal candidates have significant decay lengths, and the signal remains highly significant after a minimum lifetime requirement of approximately five times the expected decay-time resolution is imposed. This state is therefore incompatible with a strongly decaying particle but is consistent with the expectations for the weakly decaying $\Xi_{cc}^{++}$ baryon. The mass of the observed $\Xi_{cc}^{++}$ state is greater than that of the $\Xi_{cc}^0$ peaks reported by the SELEX Collaboration [44,45] by $103 \pm 2$ MeV/$c^2$. This difference would imply an isospin splitting vastly larger than that seen in any other baryon system and is inconsistent with the expected size of a few MeV/$c^2$ [34–36]. Consequently, while the state reported here is consistent with most theoretical expectations for the $\Xi_{cc}^{++}$ baryon, it is inconsistent with being an isospin partner to the $\Xi_{cc}^0$ state reported previously by the SELEX Collaboration.

We thank Chao-Hsi Chang, Cai-Dian Lü, Xing-Gang Wu, and Fu-Sheng Yu for frequent and interesting discussions on the production and decays of double-heavy-flavor baryons. We express our gratitude to our colleagues in the CERN accelerator departments for the excellent performance of the LHC. We thank the technical and administrative staff at the LHCb institutes. We acknowledge support from CERN and from the national agencies: CAPES, CNPq, FAPERJ, and FINEP (Brazil); MOST and NSFC (China); CNRS/IN2P3 (France); BMBF, DFG, and MPG (Germany); INFN (Italy); NWO (The Netherlands); MNiSW and NCN (Poland); MEN/IFA (Romania); MinES and FASO (Russia); MinECo (Spain); SNSF and SER (Switzerland); NASU (Ukraine); STFC (United Kingdom).

### Table I. Systematic uncertainties on the $\Xi_{cc}^{++}$ mass measurement.

<table>
<thead>
<tr>
<th>Source</th>
<th>Value (MeV/$c^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum-scale calibration</td>
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</tr>
<tr>
<td>Selection bias correction</td>
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<tr>
<td>Unknown $\Xi_{cc}^{++}$ lifetime</td>
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</tr>
<tr>
<td>Mass fit model</td>
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<tr>
<td>Sum of above in quadrature</td>
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</tr>
<tr>
<td>$\Lambda_{cc}^+$ mass uncertainty</td>
<td>0.14</td>
</tr>
</tbody>
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NSF (USA). We acknowledge the computing resources that are provided by CERN, IN2P3 (France), KIT and DESY (Germany), INFN (Italy), SURF (The Netherlands), PIC (Spain), GridPP (United Kingdom), RRCKI and Yandex LLC (Russia), CSCS (Switzerland), IFIN-HH (Romania), CBPF (Brazil), PL-GRID (Poland) and OSC (USA). We are indebted to the communities behind the multiple open source software packages on which we depend. Individual groups or members have received support from AvH Foundation (Germany), EPLANET, Marie Skłodowska-Curie Actions, and ERC (European Union), Conseil Général de Haute-Savoie, Labex ENIGMASS, and OCEVU, Région Auvergne (France), RFBR and Yandex LLC (Russia), GVA, XuntaGal, and GENCAT (Spain), Herchel Smith Fund, The Royal Society, Royal Commission for the Exhibition of 1851, and the Leverhulme Trust (United Kingdom).

[50] Inclusion of charge-conjugate processes is implied throughout.

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