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Update on the Offline Framework for AugerPrime and production of reference simulation libraries using the VO Auger grid resources

Eva Santos[a,*] **for the Pierre Auger Collaboration**[b]

[a] *FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague, Czech Republic*
[b] *Observatorio Pierre Auger, Av. San Martín Norte 304, 5613 Malargüe, Argentina*
Full author list: https://www.auger.org/archive/authors_icrc_2023.html

E-mail: spokespersons@auger.org

Taking data stably since 2004, the Pierre Auger Observatory has published numerous results regarding the properties of ultra-high-energy cosmic rays with unprecedented statistics. However, questions about their origin and mass composition remain unanswered, motivating us to build AugerPrime, a major upgrade of our surface detector array with improved electronics and new detectors. The upgrade is swiftly approaching its completion. Phase II of the Pierre Auger Observatory has begun, which called for an update of the Offline software Framework and modules to handle the additional detectors and the new electronics. Thanks to its modular structure, Offline has proved flexible enough to accommodate all the changes required to handle AugerPrime data reconstruction and event simulation. Additionally, new reference libraries of shower and detector simulations, including dedicated libraries envisaging the searches for neutral particles, such as ultra-high-energy photons and neutrinos, profiting from the new AugerPrime detectors with the upgraded electronics, are in the pipeline. In this contribution, we report on the current status and prospects for the Auger Offline Framework and the production of reference Monte Carlo libraries for AugerPrime.

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*Speaker

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1. Introduction

As of the writing of these proceedings, the Pierre Auger Observatory [1] has entered its very first days of the Auger Phase II data taking with the surface particle detector array approaching its complete upgrade by the end of 2023. The systematic deployment of the new electronics known as Upgraded Unified Boards (UUB) [2] in the Surface Detector (SD) stations has just been finished. On top of most stations, a Surface Scintillator Detector (SSD) [3] and its respective SSD-PMT has been installed, and inside each station, a small PMT [4] was added. The installation of the Radio Detector (RD) [5], consisting of a Short Aperiodic Loaded Loop Antenna (SALLA) [6], which complements the AugerPrime SSD's sensitivity to the electromagnetic component of the shower for zenith angles above 55°, is swiftly progressing in the field. Finally, the deployment of a denser region of the SD array with Underground Muon Detectors (UMD) [7] will allow for direct measurement of the muon content of air showers in the energy range $10^{16.5} – 10^{19}$ eV. The photo of one of our AugerPrime [8] SD stations is shown in Figure 1.

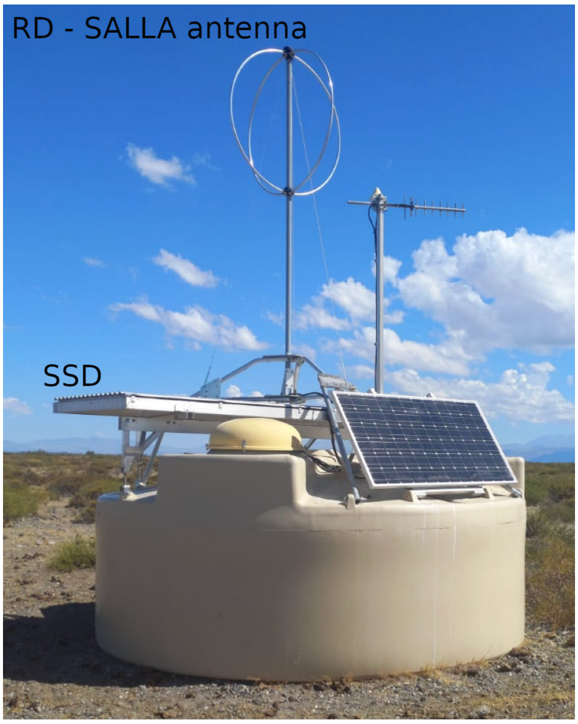

Figure 1: Photo of an AugerPrime SD station operating in the field. The visible AugerPrime enhancements are the RD - SALLA antenna and the aluminum case containing the SSD mounted on the station. Inside the station, an additional small PMT and the upgraded electronics board (UUB) are installed.

Given the installation of the AugerPrime detectors mentioned above, implementing these elements into the Offline Framework [9] was imperative. Also mandatory is the production of new reference simulation libraries contemplating the new multi-hybrid events and the AugerPrime increased detection potential of the first very-high and ultra-high-energy photons and neutrinos in the multi-messenger era.

Below, we give an update of [10, 11] regarding the improvements made to the Auger Offline Framework for AugerPrime and report on the production of the new reference shower and detector simulation libraries using grid computing via the Virtual Organization (VO) Auger and the simulation libraries layout.

2. The Auger Offline software Framework for the Pierre Auger Observatory

The Offline Framework was started in 2003 [9] to provide a universal event simulation and reconstruction framework [12]. Developed in C++, it was designed in a modular structure that would allow it to be flexible and robust enough to be used during the more than 20 years of expected operation of the Pierre Auger Observatory while ensuring the inclusion of a wide diversity of user applications and new detectors according to future needs, namely those of AugerPrime.

2.1 Structure

The modular structure of the Offline Framework consists of several packages for organizing the code. At the lowest level lies a set of useful general functions that do not require knowledge of the Observatory or cosmic-ray physics. Then, the framework layer provides the data structures for the detector description, the event, the sequencing of the execution of the analysis modules, and the overall configuration of the framework. Next, the event I/O fills, at the beginning of each loop, the data structures either with data from real events or simulations. It also handles the data streaming back to the disk. The main part of the physics code is split into individual modules, whose execution is sequenced by the `RunController`.

Data Structures The Offline Framework has two core data structures to the modules: the `Event` and `Detector`. Both data structures closely follow the hardware hierarchy of the Observatory.

The `Event` provides the accumulated knowledge for a single event, either recorded or simulated. Offline stores information about the detector calibration, raw and calibrated data, and the results from the different reconstruction stages for the events recorded by the Pierre Auger Observatory. In the case of air shower simulations, Offline stores additional information about the Monte Carlo event and the corresponding detector simulation.

The `Detector` structure provides slowly varying information, mostly unchanged for consecutive events. The atmosphere is considered part of the detector for the hybrid detection technique with the fluorescence detector, and data from atmospheric monitoring is also provided.

The managers provide access to different data sources, which could be XML or databases in MySQL or SQLite format.

Event I/O The Offline Framework can handle a large variety of I/O files for the main data stream. For recorded events, the Offline Framework can accept as input the raw data files from the Observatory and the internal Offline format. For simulations, it is possible to define as input CORSIKA [13], CONEX [14], AIRES [15], and also CoREAS [16], and ZHAireS [17], where the latter two contain the radio emission of air showers. The internal ROOT-based [18] data format allows users to save and restore the full information in the event data structure. It is also possible to save the result of simulations in the raw data format used for data acquisition.

At the higher level, most users prefer using the Advanced Data Summary Tree (ADST) files [19]. The ADST is a stand-alone package intended for high-level and fast data analysis. It includes a graphical display that allows us to view a subset of the event and a convenient mechanism for efficiently handling standard analysis cuts.

The raw data files, the internal Offline, and the ADST formats use the I/O component of the ROOT [18] Framework.

2.2 AugerPrime upgrade

The latest challenge, and one of the most significant changes to the Offline Framework, was the implementation of all the AugerPrime [8] components, namely:

- the addition of the Scintillator Surface Detector on top of each surface detector [3],
- the addition of the small PMT, which allows to extend the dynamic range of the SD stations [4],
- the UUB, the upgraded electronics board of the surface detector, which has a 3 times faster sampling rate with respect to the old electronics board [2, 20],
- the SALLA antennas of the RD [21] and their complete signal path consists of the low-noise amplifier, cables and digitizer. This was realized building on the functionality already implemented for the Auger Engineering Radio Array (AERA) antennas [6, 12], and
- the new electronics mounted on the buried modules and the new photo sensors for the UMD.

Given the large extent of the AugerPrime upgrade, the Offline developers decided to change the language standard from C++ version 98/03 to C++ 11/14, which had implications for the deprecation of old interfaces [10]. A detailed description of all the implications of the required changes can be found in [10]. Below, we highlight the most relevant changes to Offline since [10].

New electronics boards - UUB The most challenging change from the old electronic board to the upgraded one was the modification in the digitizer frequency from 40 MHz to 120 MHz since the previous signal bin of 1 ns implemented in Offline was not a natural least common multiple for the new time bin of 8.3 ns. The new natural timing unit also affected the calibration histograms of the vertical equivalent muon (VEM) charge. After properly implementing the 8.3 ns time bin in Offline, it was also necessary to adapt the fitting algorithm for the VEM peak. The new fitting procedure works for the new and old electronics, including the SSD. These changes are implemented in a new module that replaced the old algorithm in `SdCalibratorOG` after it was split into four modules. The new histogram fitting algorithm is robust enough to be applied to UB, UUB, and SSD data. Also, a new algorithm for the estimation of the baseline of the several channels of the UUB was developed and implemented in the `SdBaselineFinderKG` module, replacing the former algorithm.

Radio Detector stations The RD antennas of AugerPrime are co-located with the surface detector stations and share part of the local station electronics and data acquisition. Both detectors share the raw event I/O, as some channels carry information from the surface detector while others are used for the radio detector. In the calibration stage, data is split into independent parts of the event, loosely coupled by the station id and position. The analysis functionality required for the Auger RD largely overlaps with the one already existing for AERA [6]. Currently, the Offline Framework has analysis modules that can be used only for AERA or RD or in a mixed configuration. A newly developed reconstruction algorithm for radio emission from inclined air showers was also implemented [22].

Small PMT The installation of the small PMT inside the water-Cherenkov detectors required a break in the old paradigm, in which each station had three identical PMTs. Although its implementation inside the station was relatively straightforward, changes in signal for data calibration and signal simulation were required. For simulations, we apply the quantum efficiency of the PMT at the time of the emission of the photon to avoid tracking photons that will not produce a photo-electron. To avoid losing all the speedup gained by suppressing photons at production time, a hybrid scheme was developed, where the larger quantum efficiency was applied at the source and then re-applied according to the real quantum efficiency of the PMT hit. Also, unlike the large PMTs, the small PMT cannot be calibrated from the signal generated by atmospheric muons. Instead, the calibration is done using the signal from small showers detected by the small and the large PMTs. The calibration information has to be merged with the event stream at a later stage for the event reconstruction.

Time-dependent simulations for the water-Cherenkov detectors A true novelty in Offline concerning [10] was the development of a new module called `SdEvolution` that allows performing a more realistic time-dependent simulation of the SD array considering the aging effects of the water-Cherenkov detector observed in data. This temporal behavior is modeled by exploiting the light-time decay of muon pulses recorded in each station at different times. The optical properties of the simulated tanks are modified to match the data at the corresponding time of the simulated events accordingly. The calibration constants used in simulations are also modified accordingly to reproduce the time response of the tanks correctly.

3. Virtual Organization Auger

The VO Auger was created in 2006 in cooperation with the CESNET Metacentrum [23], which provides and maintains the central resources such as the registration portal and the VOMS (Virtual Organization Membership Service) server. Currently, the VO Auger comprises 13 grid sites in 8 countries. See [24] for the full list of the VO Auger computing resources and local computing clusters contributing to the Pierre Auger Collaboration.

All members of the Pierre Auger Collaboration can apply for membership by filling out a registration form which has to be approved by the VO manager. The membership is valid for one year and can be renewed upon request. Currently, about 30 individual members are registered in the VO Auger.

3.1 DIRAC interware

In 2014, the VO Auger adopted the DIRAC (Distributed Infrastructure with Remote Agent Control) interware for job submission, monitoring, and file catalog management [25]. The DIRAC server runs on the France Grilles Infrastructure. Its usage only requires having a running DIRAC client installed. A client version is provided in the DIRAC CVMFS - Cern Virtual Machine-File System repository `dirac.egi.eu`.

More than 7 million files are registered in the DIRAC File Catalog; these files are stored on 11 different sites and occupy around 1.5 PB of disk space. Given the unprecedented data volume produced in 2022, old files corresponding to outdated productions had to be deleted from the DIRAC File Catalog to give space to the updated shower libraries.

3.2 Grid computing in 2022

In 2022, according to the EGI - European Grid Infrastructure accounting portal, the VO Auger ran about 1 million single-core jobs, which used a normalized elapsed time HEPSCORE23 [26] of nearly 147 million CPU hours. The productions ran on 10 grid sites from 7 countries. When excluding the contributions of the LHCb, and Fermilab groups, which we consider to be incorrectly assigned as astrophysics experiments, the VO Auger appears as the second largest EGI user with a relative usage of 29.4%, slightly behind VIRGO, with 30.6%, as shown in Figure 2.

Still, according to the HEPSCORE23, including all members of the Astrophysics VOs, LHCb has a relative normalized elapsed time of 94.14%, followed by Fermilab with 2.14%. VIRGO and Auger appear in the third and fourth positions with 1.14% and 1.09%, respectively.

The used CPU time corresponds to the new CORSIKA [13] reference shower libraries for hadron cosmic-ray primaries and neutral primaries, namely, photons and electron neutrinos, described in section 4.

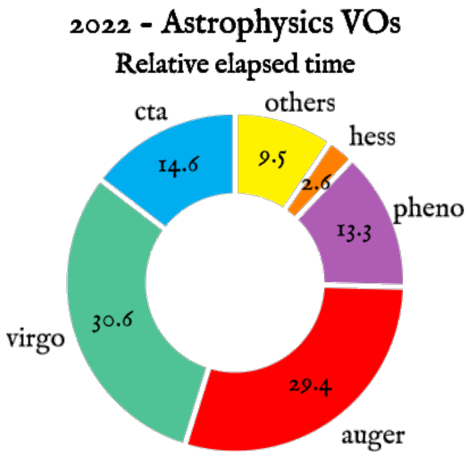

Figure 2: Relative elapsed time of the Astrophysics VOs in 2022, according to the EGI accounting portal. The contributions of the LHCb, and Fermilab groups were excluded.

4. Reference shower libraries

The reference simulation libraries consist of CORSIKA [13] extensive air shower simulations later processed with the Offline Framework [9]. The libraries are continuously updated, and several CORSIKA and Offline versions have been used. The most recent productions use the latest versions of CORSIKA 7.7420 and 7.7500.

4.1 Cosmic-ray shower library

Per each CORSIKA version, three high-energy hadronic interaction models are simulated: EPOS-LHC [27, 28], QGSJetII-0.4 [29, 30], and Sibyll 2.3 [31–33] (currently Sibyll 2.3d) and four hadronic species, namely: Hydrogen, Helium, Oxygen, and Iron. FLUKA [34, 35] is used to treat elastic and inelastic hadronic interactions below 80 GeV in air. The library comprises air shower simulations ranging from $10^{15.0} - 10^{20.2}$ eV, with zenith angles below 65° uniformly distributed in $\sin^2\theta$, arranged in energy bins of width $\log_{10}(E/\text{eV}) = 0.5$, except for the highest energy bin, with a spectral index of -1. There are 5,000 showers per bin simulated with an optimal thinning [13] of 10^{-6}. Up to 4 different Malargüe atmospheres, one per season, can be found in the simulations.

We have extended the reference shower library for the zenith angle region $\theta = 50°$ to 89°, following a similar layout to the previous library. However, in addition to the compilation option `SLANT`, we further activated `CURVED` and `UPWARD`, since above 70°, the effect of the curvature of the Earth in the atmosphere can no longer be neglected. This library ranges from $10^{15} - 10^{20.2}$ eV, following an energy bin of $\log_{10}(E/\text{eV}) = 0.6$. Per energy bin, there are 10,000 showers.

One extra feature of the new cosmic-ray shower libraries is also the activation of the CORSIKA options `MUPROD` and `prEHISTORY` [36], which enables extended additional information for all the shower particles that includes the "grandmother" and "mother" of the particles at the ground. This feature came at the cost of enlarging CORSIKA ground particle files by about a factor of 3.

Photon shower library Together with the reference cosmic-ray shower library, we also produce photon-induced air showers, in which the pre-shower is activated for energies above 10^{19} eV. The standard photon simulations follow a similar structure as the one described above. In this case, there are 10,000 showers per energy bin.

4.2 Neutrino shower libraries

The reference neutrino shower libraries are produced using CORSIKA [13]. Neutrino-induced showers require option `NUPRIM`, which calls the `HERWIG` [37] code, to treat the first interaction of a primary neutrino in the Earth's atmosphere. Also, one particularity of the neutrino shower libraries is the change of the default transition energy from the high-energy hadronic interaction model to FLUKA from 80 GeV to 200 GeV, allowing for a more conservative description of hadronic interactions occurring in the shower development. Unlike our standard cosmic-ray and photon shower libraries, neutrino shower libraries have fixed primary energy, zenith angle, and a fixed interaction depth in the atmosphere.

Downward Going Low (DGL) channel The simulations range from $\theta = 60°$ to $75°$, with a zenith angle step of $3°$. The energies range from $E = 0.01$ to 100.0 EeV, and the interaction depths are defined in steps of $100\,\mathrm{g\,cm^{-2}}$ from a starting depth of around $100\,\mathrm{g\,cm^{-2}}$ down to the ground level.

Downward Going Low (DGL) channel The library ranges from $\theta = 75°$ to $89°$ and uses the same CORSIKA compilation options. However for the zenith angle range $\theta = 75°$ to $83°$, the zenith angle step is of $2°$, decreasing to $1°$ above $\theta = 84°$. The energy range of the DGH library spans from $E = 0.05$ to 30.0 EeV. As before, the interaction depth step is $100\ \mathrm{g\ cm^{-2}}$, starting at a slant depth height of $100\ \mathrm{g\ cm^{-2}}$, down to the ground.

In both cases, we consider the interaction of electron neutrinos in the atmosphere through charged and neutral current interactions. The number of showers produced per zenith angle and interaction depth varies as a function of energy: there are 300 showers for $E < 0.1$ EeV, 200 for $0.1 \leq E\ [\mathrm{EeV}] \leq 0.3\,\mathrm{EeV}$, 150 for $E = 3\,\mathrm{EeV}$, and 50 showers for $E > 3\,\mathrm{EeV}$. We will soon produce a CoREAS DGH library and plan to simulate a tau neutrino-induced shower library encompassing the DGH and the Earth-skimming channel. Finally, we plan to repeat the neutrino shower libraries using AIRES [15] and ZHAireS [17].

4.3 Accessing the simulations

All Auger data and a subset of the simulations produced are stored in the IN2P3 Computing Center in Lyon, France. iRODS - integrated Rule-Oriented Data System is the preferred system to download simulations from the Lyon Computing Center. All the task's simulations and many others produced by several Auger groups are shared with the whole Collaboration this way.

5. Conclusions and Outlook

In recent years, the Pierre Auger Collaboration has moved the bulk of its production of reference shower libraries to the grid via the VO Auger. In 2022, an unprecedented amount of single-core jobs, normalized CPU hours, and disk space were reached, with the production of the new reference cosmic-ray and neutrino shower DGL libraries. We are consolidating our position as one of the most significant EGI users within the Astrophysics VO group, and we expect to surpass last year's statistics by continuing to produce the DGH electron and tau neutrino shower libraries. We also plan to produce neutrino shower libraries in CoREAS, AIRES, and ZHAireS and deliver the first AugerPrime Offline simulations.

Over 20 years of the Offline Framework establishment, its modular structure written in C++ following good practices has proved its robustness to implement all the required changes, with AugerPrime being the most challenging feat. Hosted in GitLab, the Offline Framework is provided with automated tests for frameworks, either integrated or as third-party integrations. The external testing framework Jenkins is used for automated testing.

In 2009, the Pierre Auger collaboration developed and adopted the Ape tool as a platform-independent installation tool for the Offline Framework and its dependencies. Since then, Conan established itself as a package manager for C++ projects.

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The Pierre Auger Collaboration

PIERRE AUGER OBSERVATORY

A. Abdul Halim[13], P. Abreu[72], M. Aglietta[54,52], I. Allekotte[1], K. Almeida Cheminant[70], A. Almela[7,12], R. Aloisio[45,46], J. Alvarez-Muñiz[79], J. Ammerman Yebra[79], G.A. Anastasi[54,52], L. Anchordoqui[86], B. Andrada[7], S. Andringa[72], C. Aramo[50], P.R. Araújo Ferreira[42], E. Arnone[63,52], J. C. Arteaga Velázquez[67], H. Asorey[7], P. Assis[72], G. Avila[11], E. Avocone[57,46], A.M. Badescu[75], A. Bakalova[32], A. Balaceanu[73], F. Barbato[45,46], A. Bartz Mocellin[85], J.A. Bellido[13,69], C. Berat[36], M.E. Bertaina[63,52], G. Bhatta[70], M. Bianciotto[63,52], P.L. Biermann[h], V. Binet[5], K. Bismark[39,7], T. Bister[80,81], J. Biteau[37], J. Blazek[32], C. Bleve[36], J. Blümer[41], M. Boháčová[32], D. Boncioli[57,46], C. Bonifazi[8,26], L. Bonneau Arbeletche[21], N. Borodai[70], J. Brack[j], P.G. Brichetto Orchera[7], F.L. Briechle[42], A. Bueno[78], S. Buitink[15], M. Buscemi[47,61], M. Büsken[39,7], A. Bwembya[80,81], K.S. Caballero-Mora[66], S. Cabana-Freire[79], L. Caccianiga[59,49], I. Caracas[38], R. Caruso[58,47], A. Castellina[54,52], F. Catalani[18], G. Cataldi[48], L. Cazon[79], M. Cerda[10], A. Cermenati[45,46], J.A. Chinellato[21], J. Chudoba[32], L. Chytka[33], R.W. Clay[13], A.C. Cobos Cerutti[6], R. Colalillo[60,50], A. Coleman[90], M.R. Coluccia[48], R. Conceição[72], A. Condorelli[37], G. Consolati[49,55], M. Conte[56,48], F. Convenga[41], D. Correia dos Santos[28], P.J. Costa[72], C.E. Covault[84], M. Cristinziani[44], C.S. Cruz Sanchez[3], S. Dasso[4,2], K. Daumiller[41], B.R. Dawson[13], R.M. de Almeida[28], J. de Jesús[7,41], S.J. de Jong[80,81], J.R.T. de Mello Neto[26,27], I. De Mitri[45,46], J. de Oliveira[17], D. de Oliveira Franco[21], F. de Palma[56,48], V. de Souza[19], E. De Vito[56,48], A. Del Popolo[58,47], O. Deligny[34], N. Denner[32], L. Deval[41,7], A. di Matteo[52], M. Dobre[73], C. Dobrigkeit[21], J.C. D'Olivo[68], L.M. Domingues Mendes[72], J.C. dos Anjos, R.C. dos Anjos[25], J. Ebr[32], F. Ellwanger[41], M. Emam[80,81], R. Engel[39,41], I. Epicoco[56,48], M. Erdmann[42], A. Etchegoyen[7,12], C. Evoli[45,46], H. Falcke[80,82,81], J. Farmer[89], G. Farrar[88], A.C. Fauth[21], N. Fazzini[e], F. Feldbusch[40], F. Fenu[41,d], A. Fernandes[72], B. Fick[87], J.M. Figueira[7], A. Filipčič[77,76], T. Fitoussi[41], B. Flaggs[90], T. Fodran[80], T. Fujii[89,f], A. Fuster[7,12], C. Galea[80], C. Galelli[59,49], B. García[6], C. Gaudu[38], H. Gemmeke[40], F. Gesualdi[7,41], A. Gherghel-Lascu[73], P.L. Ghia[34], U. Giaccari[48], M. Giammarchi[49], J. Glombitza[42,g], F. Gobbi[10], F. Gollan[7], G. Golup[1], M. Gómez Berisso[1], P.F. Gómez Vitale[11], J.P. Gongora[11], J.M. González[1], N. González[7], I. Goos[1], D. Góra[70], A. Gorgi[54,52], M. Gottowik[79], T.D. Grubb[13], F. Guarino[60,50], G.P. Guedes[22], E. Guido[44], S. Hahn[39], P. Hamal[32], M.R. Hampel[7], P. Hansen[3], D. Harari[1], V.M. Harvey[13], A. Haungs[41], T. Hebbeker[42], C. Hojvat[e], J.R. Hörandel[80,81], P. Horvath[33], M. Hrabovský[33], T. Huege[41,15], A. Insolia[58,47], P.G. Isar[74], P. Janecek[32], J.A. Johnsen[85], J. Jurysek[32], A. Kääpä[38], K.H. Kampert[38], B. Keilhauer[41], A. Khakurdikar[80], V.V. Kizakke Covilakam[7,41], H.O. Klages[41], M. Kleifges[40], F. Knapp[39], N. Kunka[40], B.L. Lago[16], N. Langner[42], M.A. Leigui de Oliveira[24], Y Lema-Capeans[79], V. Lenok[39], A. Letessier-Selvon[35], I. Lhenry-Yvon[34], D. Lo Presti[58,47], L. Lopes[72], L. Lu[91], Q. Luce[39], J.P. Lundquist[76], A. Machado Payeras[21], M. Majercakova[32], D. Mandat[32], B.C. Manning[13], P. Mantsch[e], S. Marafico[34], F.M. Mariani[59,49], A.G. Mariazzi[3], I.C. Mariş[14], G. Marsella[61,47], D. Martello[56,48], S. Martinelli[41,7], O. Martínez Bravo[64], M.A. Martins[79], M. Mastrodicasa[57,46], H.J. Mathes[41], J. Matthews[a], G. Matthiae[62,51], E. Mayotte[85,38], S. Mayotte[85], P.O. Mazur[e], G. Medina-Tanco[68], J. Meinert[38], D. Melo[7], A. Menshikov[40], C. Merx[41], S. Michal[33], M.I. Micheletti[5], L. Miramonti[59,49], S. Mollerach[1], F. Montanet[36], L. Morejon[38], C. Morello[54,52], A.L. Müller[32], K. Mulrey[80,81], R. Mussa[52], M. Muzio[88], W.M. Namasaka[38], S. Negi[32], L. Nellen[68], K. Nguyen[87], G. Nicora[9], M. Niculescu-Oglinzanu[73], M. Niechciol[44], D. Nitz[87], D. Nosek[31], V. Novotny[31], L. Nožka[33], A Nucita[56,48], L.A. Núñez[30], C. Oliveira[19], M. Palatka[32], J. Pallotta[9], S. Panja[32], G. Parente[79], T. Paulsen[38], J. Pawlowsky[38], M. Pech[32], J. Pękala[70], R. Pelayo[65], L.A.S. Pereira[23], E.E. Pereira Martins[39,7], J. Perez Armand[20], C. Pérez Bertolli[7,41], L. Perrone[56,48], S. Petrera[45,46], C. Petrucci[57,46], T. Pierog[41], M. Pimenta[72], M. Platino[7], B. Pont[80], M. Pothast[81,80], M. Pourmohammad Shahvar[61,47], P. Privitera[89], M. Prouza[32], A. Puyleart[87], S. Querchfeld[38], J. Rautenberg[38], D. Ravignani[7], M. Reininghaus[39], J. Ridky[32], F. Riehn[79], M. Risse[44], V. Rizi[57,46], W. Rodrigues de Carvalho[80], E. Rodriguez[7,41], J. Rodriguez Rojo[11], M.J. Roncoroni[7], S. Rossoni[43], M. Roth[41], E. Roulet[1], A.C. Rovero[4], P. Ruehl[44], A. Saftoiu[73], M. Saharan[80], F. Salamida[57,46], H. Salazar[64], G. Salina[51], J.D. Sanabria Gomez[30], F. Sánchez[7], E.M. Santos[20], E. Santos[32],

F. Sarazin[85], R. Sarmento[72], R. Sato[11], P. Savina[91], C.M. Schäfer[41], V. Scherini[56,48], H. Schieler[41], M. Schimassek[34], M. Schimp[38], F. Schlüter[41], D. Schmidt[39], O. Scholten[15,i], H. Schoorlemmer[80,81], P. Schovánek[32], F.G. Schröder[90,41], J. Schulte[42], T. Schulz[41], S.J. Sciutto[3], M. Scornavacche[7,41], A. Segreto[53,47], S. Sehgal[38], S.U. Shivashankara[76], G. Sigl[43], G. Silli[7], O. Sima[73,b], F. Simon[40], R. Smau[73], R. Šmída[89], P. Sommers[k], J.F. Soriano[86], R. Squartini[10], M. Stadelmaier[32], D. Stanca[73], S. Stanič[76], J. Stasielak[70], P. Stassi[36], S. Strähnz[39], M. Straub[42], M. Suárez-Durán[14], T. Suomijärvi[37], A.D. Supanitsky[7], Z. Svozilikova[32], Z. Szadkowski[71], A. Tapia[29], C. Taricco[63,52], C. Timmermans[81,80], O. Tkachenko[41], P. Tobiska[32], C.J. Todero Peixoto[18], B. Tomé[72], Z. Torrès[36], A. Travaini[10], P. Travnicek[32], C. Trimarelli[57,46], M. Tueros[3], M. Unger[41], L. Vaclavek[33], M. Vacula[33], J.F. Valdés Galicia[68], L. Valore[60,50], E. Varela[64], A. Vásquez-Ramírez[30], D. Veberič[41], C. Ventura[27], I.D. Vergara Quispe[3], V. Verzi[51], J. Vicha[32], J. Vink[83], J. Vlastimil[32], S. Vorobiov[76], C. Watanabe[26], A.A. Watson[c], A. Weindl[41], L. Wiencke[85], H. Wilczyński[70], D. Wittkowski[38], B. Wundheiler[7], B. Yue[38], A. Yushkov[32], O. Zapparrata[14], E. Zas[79], D. Zavrtanik[76,77], M. Zavrtanik[77,76]

———— • ————

[1] Centro Atómico Bariloche and Instituto Balseiro (CNEA-UNCuyo-CONICET), San Carlos de Bariloche, Argentina
[2] Departamento de Física and Departamento de Ciencias de la Atmósfera y los Océanos, FCEyN, Universidad de Buenos Aires and CONICET, Buenos Aires, Argentina
[3] IFLP, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
[4] Instituto de Astronomía y Física del Espacio (IAFE, CONICET-UBA), Buenos Aires, Argentina
[5] Instituto de Física de Rosario (IFIR) – CONICET/U.N.R. and Facultad de Ciencias Bioquímicas y Farmacéuticas U.N.R., Rosario, Argentina
[6] Instituto de Tecnologías en Detección y Astropartículas (CNEA, CONICET, UNSAM), and Universidad Tecnológica Nacional – Facultad Regional Mendoza (CONICET/CNEA), Mendoza, Argentina
[7] Instituto de Tecnologías en Detección y Astropartículas (CNEA, CONICET, UNSAM), Buenos Aires, Argentina
[8] International Center of Advanced Studies and Instituto de Ciencias Físicas, ECyT-UNSAM and CONICET, Campus Miguelete – San Martín, Buenos Aires, Argentina
[9] Laboratorio Atmósfera – Departamento de Investigaciones en Láseres y sus Aplicaciones – UNIDEF (CITEDEF-CONICET), Argentina
[10] Observatorio Pierre Auger, Malargüe, Argentina
[11] Observatorio Pierre Auger and Comisión Nacional de Energía Atómica, Malargüe, Argentina
[12] Universidad Tecnológica Nacional – Facultad Regional Buenos Aires, Buenos Aires, Argentina
[13] University of Adelaide, Adelaide, S.A., Australia
[14] Université Libre de Bruxelles (ULB), Brussels, Belgium
[15] Vrije Universiteit Brussels, Brussels, Belgium
[16] Centro Federal de Educação Tecnológica Celso Suckow da Fonseca, Petropolis, Brazil
[17] Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro (IFRJ), Brazil
[18] Universidade de São Paulo, Escola de Engenharia de Lorena, Lorena, SP, Brazil
[19] Universidade de São Paulo, Instituto de Física de São Carlos, São Carlos, SP, Brazil
[20] Universidade de São Paulo, Instituto de Física, São Paulo, SP, Brazil
[21] Universidade Estadual de Campinas, IFGW, Campinas, SP, Brazil
[22] Universidade Estadual de Feira de Santana, Feira de Santana, Brazil
[23] Universidade Federal de Campina Grande, Centro de Ciencias e Tecnologia, Campina Grande, Brazil
[24] Universidade Federal do ABC, Santo André, SP, Brazil
[25] Universidade Federal do Paraná, Setor Palotina, Palotina, Brazil
[26] Universidade Federal do Rio de Janeiro, Instituto de Física, Rio de Janeiro, RJ, Brazil
[27] Universidade Federal do Rio de Janeiro (UFRJ), Observatório do Valongo, Rio de Janeiro, RJ, Brazil
[28] Universidade Federal Fluminense, EEIMVR, Volta Redonda, RJ, Brazil
[29] Universidad de Medellín, Medellín, Colombia
[30] Universidad Industrial de Santander, Bucaramanga, Colombia

[31] Charles University, Faculty of Mathematics and Physics, Institute of Particle and Nuclear Physics, Prague, Czech Republic
[32] Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic
[33] Palacky University, Olomouc, Czech Republic
[34] CNRS/IN2P3, IJCLab, Université Paris-Saclay, Orsay, France
[35] Laboratoire de Physique Nucléaire et de Hautes Energies (LPNHE), Sorbonne Université, Université de Paris, CNRS-IN2P3, Paris, France
[36] Univ. Grenoble Alpes, CNRS, Grenoble Institute of Engineering Univ. Grenoble Alpes, LPSC-IN2P3, 38000 Grenoble, France
[37] Université Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, France
[38] Bergische Universität Wuppertal, Department of Physics, Wuppertal, Germany
[39] Karlsruhe Institute of Technology (KIT), Institute for Experimental Particle Physics, Karlsruhe, Germany
[40] Karlsruhe Institute of Technology (KIT), Institut für Prozessdatenverarbeitung und Elektronik, Karlsruhe, Germany
[41] Karlsruhe Institute of Technology (KIT), Institute for Astroparticle Physics, Karlsruhe, Germany
[42] RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany
[43] Universität Hamburg, II. Institut für Theoretische Physik, Hamburg, Germany
[44] Universität Siegen, Department Physik – Experimentelle Teilchenphysik, Siegen, Germany
[45] Gran Sasso Science Institute, L'Aquila, Italy
[46] INFN Laboratori Nazionali del Gran Sasso, Assergi (L'Aquila), Italy
[47] INFN, Sezione di Catania, Catania, Italy
[48] INFN, Sezione di Lecce, Lecce, Italy
[49] INFN, Sezione di Milano, Milano, Italy
[50] INFN, Sezione di Napoli, Napoli, Italy
[51] INFN, Sezione di Roma "Tor Vergata", Roma, Italy
[52] INFN, Sezione di Torino, Torino, Italy
[53] Istituto di Astrofisica Spaziale e Fisica Cosmica di Palermo (INAF), Palermo, Italy
[54] Osservatorio Astrofisico di Torino (INAF), Torino, Italy
[55] Politecnico di Milano, Dipartimento di Scienze e Tecnologie Aerospaziali , Milano, Italy
[56] Università del Salento, Dipartimento di Matematica e Fisica "E. De Giorgi", Lecce, Italy
[57] Università dell'Aquila, Dipartimento di Scienze Fisiche e Chimiche, L'Aquila, Italy
[58] Università di Catania, Dipartimento di Fisica e Astronomia "Ettore Majorana", Catania, Italy
[59] Università di Milano, Dipartimento di Fisica, Milano, Italy
[60] Università di Napoli "Federico II", Dipartimento di Fisica "Ettore Pancini", Napoli, Italy
[61] Università di Palermo, Dipartimento di Fisica e Chimica "E. Segrè", Palermo, Italy
[62] Università di Roma "Tor Vergata", Dipartimento di Fisica, Roma, Italy
[63] Università Torino, Dipartimento di Fisica, Torino, Italy
[64] Benemérita Universidad Autónoma de Puebla, Puebla, México
[65] Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas del Instituto Politécnico Nacional (UPIITA-IPN), México, D.F., México
[66] Universidad Autónoma de Chiapas, Tuxtla Gutiérrez, Chiapas, México
[67] Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán, México
[68] Universidad Nacional Autónoma de México, México, D.F., México
[69] Universidad Nacional de San Agustin de Arequipa, Facultad de Ciencias Naturales y Formales, Arequipa, Peru
[70] Institute of Nuclear Physics PAN, Krakow, Poland
[71] University of Łódź, Faculty of High-Energy Astrophysics,Łódź, Poland
[72] Laboratório de Instrumentação e Física Experimental de Partículas – LIP and Instituto Superior Técnico – IST, Universidade de Lisboa – UL, Lisboa, Portugal
[73] "Horia Hulubei" National Institute for Physics and Nuclear Engineering, Bucharest-Magurele, Romania
[74] Institute of Space Science, Bucharest-Magurele, Romania
[75] University Politehnica of Bucharest, Bucharest, Romania
[76] Center for Astrophysics and Cosmology (CAC), University of Nova Gorica, Nova Gorica, Slovenia
[77] Experimental Particle Physics Department, J. Stefan Institute, Ljubljana, Slovenia

[78] Universidad de Granada and C.A.F.P.E., Granada, Spain
[79] Instituto Galego de Física de Altas Enerxías (IGFAE), Universidade de Santiago de Compostela, Santiago de Compostela, Spain
[80] IMAPP, Radboud University Nijmegen, Nijmegen, The Netherlands
[81] Nationaal Instituut voor Kernfysica en Hoge Energie Fysica (NIKHEF), Science Park, Amsterdam, The Netherlands
[82] Stichting Astronomisch Onderzoek in Nederland (ASTRON), Dwingeloo, The Netherlands
[83] Universiteit van Amsterdam, Faculty of Science, Amsterdam, The Netherlands
[84] Case Western Reserve University, Cleveland, OH, USA
[85] Colorado School of Mines, Golden, CO, USA
[86] Department of Physics and Astronomy, Lehman College, City University of New York, Bronx, NY, USA
[87] Michigan Technological University, Houghton, MI, USA
[88] New York University, New York, NY, USA
[89] University of Chicago, Enrico Fermi Institute, Chicago, IL, USA
[90] University of Delaware, Department of Physics and Astronomy, Bartol Research Institute, Newark, DE, USA
[91] University of Wisconsin-Madison, Department of Physics and WIPAC, Madison, WI, USA

—–

[a] Louisiana State University, Baton Rouge, LA, USA
[b] also at University of Bucharest, Physics Department, Bucharest, Romania
[c] School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom
[d] now at Agenzia Spaziale Italiana (ASI). Via del Politecnico 00133, Roma, Italy
[e] Fermi National Accelerator Laboratory, Fermilab, Batavia, IL, USA
[f] now at Graduate School of Science, Osaka Metropolitan University, Osaka, Japan
[g] now at ECAP, Erlangen, Germany
[h] Max-Planck-Institut für Radioastronomie, Bonn, Germany
[i] also at Kapteyn Institute, University of Groningen, Groningen, The Netherlands
[j] Colorado State University, Fort Collins, CO, USA
[k] Pennsylvania State University, University Park, PA, USA

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