

2 Highly-parallelized simulation of a pixelated LArTPC on a 3 GPU

4 The DUNE Collaboration

5 A. Abed Abud,³⁴ B. Abi,¹⁶³ R. Acciarri,⁶⁷ M. A. Acero,¹⁰ M. R. Adames,²⁰⁰ G. Adamov,⁷³
6 M. Adamowski,⁶⁷ D. Adams,¹⁹ M. Adinolfi,¹⁸ C. Adriano,²⁹ A. Aduszkiewicz,⁸² J. Aguilar,¹³¹
7 Z. Ahmad,²¹² J. Ahmed,²¹⁵ B. Aimard,⁵² F. Akbar,¹⁸¹ K. Allison,⁴² S. Alonso Monsalve,³⁴
8 M. Alrashed,¹²³ C. Alt,⁶¹ A. Alton,¹¹ R. Alvarez,³⁸ P. Amedo,^{87,86} J. Anderson,⁶ D. A.
9 Andrade,⁸⁸ C. Andreopoulos,^{184,133} M. Andreotti,^{95,68} M. P. Andrews,⁶⁷ F. Andrianala,⁴
10 S. Andringa,¹³² N. Anfimov,¹²¹ W. L. Anicézio Campanelli,⁶³ A. Ankowski,¹⁹⁰
11 M. Antoniassi,²⁰⁰ M. Antonova,⁸⁶ A. Antoshkin,¹²¹ S. Antusch,¹² A. Aranda-Fernandez,⁴¹
12 L. Arellano,¹³⁹ L. O. Arnold,⁴⁴ M. A. Arroyave,⁵⁹ J. Asaadi,²⁰⁴ A. Ashkenazi,²⁰¹ L. Asquith,¹⁹⁸
13 A. Aurisano,³⁹ V. Aushev,¹²⁹ D. Autiero,¹¹² M. Ayala-Torres,⁴⁰ F. Azfar,¹⁶³ A. Back,⁹²
14 H. Back,¹⁶⁴ J. J. Back,²¹⁵ I. Bagaturia,⁷³ L. Bagby,⁶⁷ N. Balashov,¹²¹ S. Balasubramanian,⁶⁷
15 P. Baldi,²³ W. Baldini,⁹⁵ B. Baller,⁶⁷ B. Bambah,⁸³ F. Barao,^{132,114} G. Barenboim,⁸⁶ P.
16 Barham Alzás,³⁴ G. J. Barker,²¹⁵ W. Barkhouse,¹⁵⁵ C. Barnes,¹⁴³ G. Barr,¹⁶³ J. Barranco
17 Monarca,⁷⁸ A. Barros,²⁰⁰ N. Barros,^{132,62} J. L. Barrow,¹⁴⁰ A. Basharina-Freshville,²¹⁰
18 A. Bashyal,⁶ V. Basque,⁶⁷ C. Batchelor,⁵⁸ J.B.R. Battat,²¹⁶ F. Battisti,¹⁶³ F. Bay,³
19 M. C. Q. Bazetto,²⁹ J. L. L. Bazo Alba,¹⁷⁶ J. F. Beacom,¹⁶¹ E. Bechetoille,¹¹² B. Behera,⁴³
20 E. Belchior,²⁹ L. Bellantoni,⁶⁷ G. Bellettini,^{104,174} V. Bellini,^{94,30} O. Beltramello,³⁴
21 N. Benekos,³⁴ C. Benitez Montiel,⁸ D. Benjamin,¹⁹ F. Bento Neves,¹³² J. Berger,⁴³
22 S. Berkman,⁶⁷ P. Bernardini,^{98,185} R. M. Berner,¹³ A. Bersani,⁹⁷ S. Bertolucci,^{93,16}
23 M. Betancourt,⁶⁷ A. Betancur Rodríguez,⁵⁹ A. Bevan,¹⁷⁹ Y. Bezawada,²² A. T. Bezerra,⁶³
24 T. J. Bezerra,¹⁹⁸ J. Bhambure,¹⁹⁵ A. Bhardwaj,¹³⁵ V. Bhatnagar,¹⁶⁶ M. Bhattacharjee,⁹⁰
25 M. Bhattacharya,⁶⁷ D. Bhattarai,¹⁴⁹ S. Bhuller,¹⁸ B. Bhuyan,⁹⁰ S. Biagi,¹⁰⁶ J. Bian,²³
26 M. Biassoni,⁹⁹ K. Biery,⁶⁷ B. Bilki,^{14,110} M. Bishai,¹⁹ V. Bisignani,¹⁰¹ A. Bitadze,¹³⁹ A. Blake,¹³⁰
27 F. D. Blaszczyk,⁶⁷ G. C. Blazey,¹⁵⁶ D. Blend,¹¹⁰ E. Blucher,³⁶ J. Boissevain,¹³⁴ S. Bolognesi,³³
28 T. Bolton,¹²³ L. Bomben,^{99,109} M. Bonesini,^{99,145} C. Bonilla-Diaz,³¹ F. Bonini,¹⁹ A. Booth,¹⁷⁹
29 F. Boran,¹⁴ S. Bordoni,³⁴ A. Borkum,¹⁹⁸ N. Bostan,¹¹⁰ P. Bour,⁴⁹ D. Boyden,¹⁵⁶ J. Bracinik,¹⁵
30 D. Braga,⁶⁷ D. Brailsford,¹³⁰ A. Branca,⁹⁹ A. Brandt,²⁰⁴ M. Bravo-Moreno,⁷⁴ J. Bremer,³⁴
31 C. Brew,¹⁸⁴ S. J. Brice,⁶⁷ C. Brizzolari,^{99,145} C. Bromberg,¹⁴⁴ J. Brooke,¹⁸ A. Bross,⁶⁷
32 G. Brunetti,^{99,145} M. Brunetti,²¹⁵ N. Buchanan,⁴³ H. Budd,¹⁸¹ J. Buergi,¹³ G. Caceres V.,²²
33 I. Cagnoli,^{93,16} T. Cai,²²² D. Caiulo,¹¹² R. Calabrese,^{95,68} P. Calafiura,¹³¹ J. Calcutt,¹⁶²
34 M. Calin,²⁰ L. Calivers,¹³ S. Calvez,⁴³ E. Calvo,³⁸ A. Caminata,⁹⁷ D. Caratelli,²⁶ D. Carber,⁴³
35 J. C. Carceller,²¹⁰ G. Carini,¹⁹ B. Carlus,¹¹² M. F. Carneiro,¹⁹ P. Carniti,⁹⁹ I. Caro Terrazas,⁴³
36 H. Carranza,²⁰⁴ N. Carrara,²² L. Carroll,¹²³ T. Carroll,²¹⁹ A. Carter,¹⁸² J. F. Castaño Forero,⁵
37 A. Castillo,¹⁸⁸ E. Catano-Mur,²¹⁸ C. Cattadori,⁹⁹ F. Cavalier,¹⁶⁷ G. Cavallaro,⁹⁹ F. Cavanna,⁶⁷

38 S. Centro,¹⁶⁵ G. Cerati,⁶⁷ A. Cervelli,⁹³ A. Cervera Villanueva,⁸⁶ K. Chakraborty,¹⁷³
 39 M. Chalifour,³⁴ A. Chappell,²¹⁵ E. Chardonnet,¹⁶⁸ N. Charitonidis,³⁴ A. Chatterjee,¹⁷⁵
 40 S. Chattopadhyay,²¹² H. Chen,¹⁹ M. Chen,²³ Y. Chen,^{13,190} Z. Chen,¹⁹⁵ Z. Chen-Wishart,¹⁸²
 41 Y. Cheon,²⁰⁹ D. Cherdack,⁸² C. Chi,⁴⁴ S. Childress,⁶⁷ R. Chirco,⁸⁸ A. Chiriacescu,²⁰
 42 N. Chitirasreemadam,^{104,174} K. Cho,¹²⁶ S. Choate,¹⁵⁶ D. Chokheli,⁷³ P. S. Chong,¹⁷¹
 43 B. Chowdhury,⁶ A. Christensen,⁴³ D. Christian,⁶⁷ G. Christodoulou,³⁴ A. Chukanov,¹²¹
 44 M. Chung,²⁰⁹ E. Church,¹⁶⁴ V. Cicero,^{93,16} D. Clapa,²¹⁴ P. Clarke,⁵⁸ G. Cline,¹³¹ T. E. Coan,¹⁹⁴
 45 A. G. Cocco,¹⁰¹ J. A. B. Coelho,¹⁶⁸ A. Cohen,¹⁶⁸ J. Collot,⁷⁷ E. Conley,⁵⁶ J. M. Conrad,¹⁴⁰
 46 M. Convery,¹⁹⁰ S. Copello,⁹⁷ P. Cova,^{100,169} C. Cox,¹⁸² L. Cremaldi,¹⁴⁹ L. Cremonesi,¹⁷⁹
 47 J. I. Crespo-Anadón,³⁸ M. Crisler,⁶⁷ E. Cristaldo,^{100,8} J. Crnkovic,⁶⁷ G. Crone,²¹⁰ R. Cross,¹³⁰
 48 A. Cudd,⁴² C. Cuesta,³⁸ Y. Cui,²⁵ D. Cussans,¹⁸ J. Dai,⁷⁷ O. Dalager,²³ R. Dallavalle,¹⁶⁸ H. da
 49 Motta,³² Z. A. Dar,²¹⁸ R. Darby,¹⁹⁸ L. Da Silva Peres,⁶⁶ C. David,^{222,67} Q. David,¹¹²
 50 G. S. Davies,¹⁴⁹ S. Davini,⁹⁷ J. Dawson,¹⁶⁸ K. De,²⁰⁴ S. De,¹ R. De Aguiar,²⁹ P. De Almeida,²⁹
 51 P. Debbins,¹¹⁰ I. De Bonis,⁵² M. P. Decowski,^{153,2} A. de Gouvêa,¹⁵⁷ P. C. De Holanda,²⁹ I. L. De
 52 Icaza Astiz,¹⁹⁸ A. Deisting,¹³⁸ P. De Jong,^{153,2} A. De la Torre,³⁸ A. Delbart,³³ V. De Leo,^{187,105}
 53 D. Delepine,⁷⁸ M. Delgado,^{99,145} A. Dell'Acqua,³⁴ N. Delmonte,^{100,169} P. De Lurgio,⁶ J. R. T. de
 54 Mello Neto,⁶⁶ D. M. DeMuth,²¹¹ S. Dennis,²⁸ C. Densham,¹⁸⁴ P. Denton,¹⁹ G. W. Deptuch,¹⁹
 55 A. De Roeck,³⁴ V. De Romeri,⁸⁶ G. De Souza,²⁹ J. P. Detje,²⁸ R. Devi,¹¹⁸ R. Dharmapalan,⁸¹
 56 M. Dias,²⁰⁸ J. S. Díaz,⁹² F. Díaz,¹⁷⁶ F. Di Capua,^{101,150} A. Di Domenico,^{187,105} S. Di
 57 Domizio,^{97,72} S. Di Falco,¹⁰⁴ L. Di Giulio,³⁴ P. Ding,⁶⁷ L. Di Noto,^{97,72} E. Diociaiuti,⁹⁶
 58 C. Distefano,¹⁰⁶ R. Diurba,¹³ M. Diwan,¹⁹ Z. Djurcic,⁶ D. Doering,¹⁹⁰ S. Dolan,³⁴ F. Dolek,¹⁴
 59 M. J. Dolinski,⁵⁵ D. Domenici,⁹⁶ L. Domine,¹⁹⁰ S. Donati,^{104,174} Y. Donon,³⁴ S. Doran,¹¹¹
 60 D. Douglas,¹⁴⁴ A. Dragone,¹⁹⁰ F. Drielsma,¹⁹⁰ L. Duarte,²⁰⁸ D. Duchesneau,⁵² K. Duffy,^{163,67}
 61 K. Dugas,²³ P. Dunne,⁸⁹ B. Dutta,²⁰² H. Duyang,¹⁹¹ O. Dvornikov,⁸¹ D. A. Dwyer,¹³¹
 62 A. S. Dyshkant,¹⁵⁶ M. Eads,¹⁵⁶ A. Earle,¹⁹⁸ D. Edmunds,¹⁴⁴ J. Eisch,⁶⁷ L. Emberger,^{139,141}
 63 P. Englezos,¹⁸³ A. Ereditato,²²⁰ T. Erjavec,²² C. O. Escobar,⁶⁷ J. J. Evans,¹³⁹ E. Ewart,⁹²
 64 A. C. Ezeribe,¹⁸⁹ K. Fahey,⁶⁷ L. Fajt,³⁴ A. Falcone,^{99,145} M. Fani,¹³⁴ C. Farnese,¹⁰²
 65 Y. Farzan,¹¹³ D. Fedoseev,¹²¹ J. Felix,⁷⁸ Y. Feng,¹¹¹ E. Fernandez-Martinez,¹³⁷ F. Ferraro,^{97,72}
 66 L. Fields,¹⁵⁸ P. Filip,⁴⁸ A. Filkins,¹⁹⁹ F. Filthaut,^{153,180} R. Fine,¹³⁴ G. Fiorillo,^{101,150}
 67 M. Fiorini,^{95,68} V. Fischer,¹¹¹ R. S. Fitzpatrick,¹⁴³ W. Flanagan,⁵¹ B. Fleming,^{36,220} R. Flight,¹⁸¹
 68 S. Fogarty,⁴³ W. Foreman,⁸⁸ J. Fowler,⁵⁶ J. Franc,⁴⁹ D. Franco,²²⁰ J. Freeman,⁶⁷ J. Fried,¹⁹
 69 A. Friedland,¹⁹⁰ S. Fuess,⁶⁷ I. K. Furic,⁶⁹ K. Furman,¹⁷⁹ A. P. Furmanski,¹⁴⁸ A. Gabrielli,^{93,16}
 70 A. Gago,¹⁷⁶ H. Gallagher,²⁰⁷ A. Gallas,¹⁶⁷ A. Gallego-Ros,³⁸ N. Gallice,^{100,146} V. Galymov,¹¹²
 71 E. Gamberini,³⁴ T. Gamble,¹⁸⁹ F. Ganacim,²⁰⁰ R. Gandhi,⁷⁹ S. Ganguly,⁶⁷ F. Gao,¹⁷⁵ S. Gao,¹⁹
 72 D. Garcia-Gamez,⁷⁴ M. Á. García-Peris,⁸⁶ S. Gardiner,⁶⁷ D. Gastler,¹⁷ A. Gauch,¹³
 73 J. Gauvreau,¹⁶⁰ P. Gauzzi,^{187,105} G. Ge,⁴⁴ N. Geffroy,⁵² B. Gelli,²⁹ A. Gendotti,⁶¹ S. Gent,¹⁹³
 74 L. Gerlach,¹⁹ Z. Ghorbani-Moghaddam,⁹⁷ P. Giammaria,²⁹ T. Giammaria,^{95,68}
 75 N. Giangiacomi,²⁰⁶ D. Gibin,^{165,102} I. Gil-Botella,³⁸ S. Gilligan,¹⁶² A. Gioiosa,¹⁰⁴
 76 S. Giovannella,⁹⁶ C. Girerd,¹¹² A. K. Giri,⁹¹ D. Gnani,¹³¹ O. Gogota,¹²⁹ M. Gold,¹⁵¹
 77 S. Gollapinni,¹³⁴ K. Gollwitzer,⁶⁷ R. A. Gomes,⁶⁴ L. V. Gomez Bermeo,¹⁸⁸ L. S. Gomez
 78 Fajardo,¹⁸⁸ F. Gonnella,¹⁵ D. Gonzalez-Diaz,⁸⁷ M. Gonzalez-Lopez,¹³⁷ M. C. Goodman,⁶
 79 O. Goodwin,¹³⁹ S. Goswami,¹⁷³ C. Gotti,⁹⁹ J. Goudeau,¹³⁵ E. Goudzovski,¹⁵ C. Grace,¹³¹
 80 R. Gran,¹⁴⁷ E. Granados,⁷⁸ P. Granger,¹⁶⁸ C. Grant,¹⁷ D. Gratieri,⁷¹ P. Green,¹⁶³

81 S. Greenberg,^{21,131} L. Greenler,²¹⁹ J. Greer,¹⁸ J. Grenard,³⁴ W. C. Griffith,¹⁹⁸
82 F. T. Groetschla,³⁴ M. Groh,⁴³ K. Grzelak,²¹⁴ W. Gu,¹⁹ V. Guarino,⁶ M. Guarise,^{95,68}
83 R. Guenette,¹³⁹ E. Guerard,¹⁶⁷ M. Guerzoni,⁹³ D. Guffanti,⁹⁹ A. Guglielmi,¹⁰² B. Guo,¹⁹¹
84 A. Gupta,¹⁹⁰ V. Gupta,^{153,2} K. K. Guthikonda,¹²⁷ P. Guzowski,¹³⁹ M. M. Guzzo,²⁹ S. Gwon,³⁷
85 C. Ha,³⁷ K. Haaf,⁶⁷ A. Habig,¹⁴⁷ H. Hadavand,²⁰⁴ A. Hadeif,¹³⁸ R. Haenni,¹³ L. Hagaman,²²⁰
86 A. Hahn,⁶⁷ J. Haiston,¹⁹² P. Hamacher-Baumann,¹⁶³ T. Hamernik,⁶⁷ P. Hamilton,⁸⁹ J. Han,¹⁷⁵
87 J. Hancock,¹⁵ F. Happacher,⁹⁶ D. A. Harris,^{222,67} J. Hartnell,¹⁹⁸ T. Hartnett,¹⁸⁴ J. Harton,⁴³
88 T. Hasegawa,¹²⁵ C. Hasnip,¹⁶³ R. Hatcher,⁶⁷ K. W. Hatfield,²³ A. Hatzikoutelis,¹⁸⁶ C. Hayes,⁹²
89 K. Hayrapetyan,¹⁷⁹ J. Hays,¹⁷⁹ E. Hazen,¹⁷ M. He,⁸² A. Heavey,⁶⁷ K. M. Heeger,²²⁰ J. Heise,¹⁹⁷
90 S. Henry,¹⁸¹ M. A. Hernandez Morquecho,⁸⁸ K. Herner,⁶⁷ V. Hewes,³⁹ C. Hilgenberg,¹⁴⁸
91 T. Hill,⁸⁴ S. J. Hillier,¹⁵ A. Himmel,⁶⁷ E. Hinkle,³⁶ L.R. Hirsch,²⁰⁰ J. Ho,⁵⁴ J. Hoff,⁶⁷ A. Holin,¹⁸⁴
92 T. Holvey,¹⁶³ E. Hoppe,¹⁶⁴ G. A. Horton-Smith,¹²³ M. Hostert,¹⁴⁸ T. Houdy,¹⁶⁷ A. Hourlier,¹⁴⁰
93 B. Howard,⁶⁷ R. Howell,¹⁸¹ J. Hoyos Barrios,¹⁴² I. Hristova,¹⁸⁴ M. S. Hronek,⁶⁷ J. Huang,²²
94 R.G. Huang,¹³¹ Z. Hulcher,¹⁹⁰ G. Iles,⁸⁹ N. Ilic,²⁰⁶ A. M. Iliescu,⁹³ R. Illingworth,⁶⁷
95 G. Ingrassia,^{93,16} A. Ioannian,²²¹ B. Irwin,¹⁴⁸ L. Isenhour,⁰ M. Ismerio Oliveira,⁶⁶ R. Itay,¹⁹⁰
96 C.M. Jackson,¹⁶⁴ V. Jain,¹ E. James,⁶⁷ W. Jang,²⁰⁴ B. Jargowsky,²³ F. Jediny,⁴⁹ D. Jena,⁶⁷
97 Y. S. Jeong,³⁷ C. Jesús-Valls,⁸⁵ X. Ji,¹⁹ J. Jiang,¹⁹⁵ L. Jiang,²¹³ A. Jipa,²⁰ J. H. Jo,²²⁰
98 F. R. Joaquim,^{132,114} W. Johnson,¹⁹² B. Jones,²⁰⁴ R. Jones,¹⁸⁹ N. Jovancevic,¹⁵⁹ M. Judah,¹⁷⁵
99 C. K. Jung,¹⁹⁵ T. Junk,⁶⁷ Y. Jwa,⁴⁴ M. Kabirnezhad,⁸⁹ A. Kaboth,^{182,184} I. Kadenko,¹²⁹
100 I. Kakorin,¹²¹ A. Kalitkina,¹²¹ D. Kalra,⁴⁴ O. Kamer Koseyan,¹¹⁰ F. Kamiya,⁶⁵ D. M. Kaplan,⁸⁸
101 G. Karagiorgi,⁴⁴ G. Karaman,¹¹⁰ A. Karcher,¹³¹ Y. Karyotakis,⁵² S. Kasai,¹²⁸ S. P. Kasetti,¹³⁵
102 L. Kashur,⁴³ I. Katsioulas,¹⁵ N. Kazaryan,²²¹ E. Kearns,¹⁷ P. Keener,¹⁷¹ K.J. Kelly,³⁴
103 E. Kemp,²⁹ O. Kemularia,⁷³ Y. Kermaidic,¹⁶⁷ W. Ketchum,⁶⁷ S. H. Kettell,¹⁹ M. Khabibullin,¹⁰⁸
104 A. Khotjantsev,¹⁰⁸ A. Khvedelidze,⁷³ D. Kim,²⁰² B. King,⁶⁷ B. Kirby,⁴⁴ M. Kirby,⁶⁷ J. Klein,¹⁷¹
105 J. Kleykamp,¹⁴⁹ A. Klustova,⁸⁹ T. Kobilarcik,⁶⁷ K. Koehler,²¹⁹ L. W. Koerner,⁸² D. H. Koh,¹⁹⁰
106 S. Kohn,^{21,131} P. P. Koller,¹³ L. Kolupaeva,¹²¹ D. Korablev,¹²¹ M. Kordosky,²¹⁸ T. Kosc,⁷⁷
107 U. Kose,³⁴ V. A. Kostelecký,⁹² K. Kotheke,¹⁸ I. Kotler,⁵⁵ V. Kozhukalov,¹²¹ R. Kralik,¹⁹⁸
108 L. Kreczko,¹⁸ F. Krennrich,¹¹¹ I. Kreslo,¹³ W. Kropp,²³ T. Kroupova,¹⁷¹ M. Kubu,³⁴
109 Y. Kudenko,¹⁰⁸ V. A. Kudryavtsev,¹⁸⁹ S. Kuhlmann,⁶ S. Kulagin,¹⁰⁸ J. Kumar,⁸¹ P. Kumar,¹⁸⁹
110 P. Kunze,⁵² R. Kuravi,¹³¹ N. Kurita,¹⁹⁰ C. Kuruppu,¹⁹¹ V. Kus,⁴⁹ T. Kutter,¹³⁵ J. Kvasnicka,⁴⁸
111 D. Kwak,²⁰⁹ A. Lambert,¹³¹ B. J. Land,¹⁷¹ C. E. Lane,⁵⁵ K. Lang,²⁰⁵ T. Langford,²²⁰
112 M. Langstaff,¹³⁹ F. Lanni,³⁴ O. Lantwin,⁵² J. Larkin,¹⁹ P. Lasorak,⁸⁹ D. Last,¹⁷¹ A. Landrie,²¹⁹
113 G. Laurenti,⁹³ A. Lawrence,¹³¹ P. Laycock,¹⁹ I. Lazanu,²⁰ M. Lazzaroni,^{100,146} T. Le,²⁰⁷
114 S. Leardini,⁸⁷ J. Learned,⁸¹ P. LeBrun,¹¹² T. LeCompte,¹⁹⁰ C. Lee,⁶⁷ V. Legin,¹²⁹ G. Lehmann
115 Miotto,³⁴ R. Lehnert,⁹² M. A. Leigui de Oliveira,⁶⁵ M. Leitner,¹³¹ L. M. Lepin,¹³⁹ S. W. Li,¹⁹⁰
116 Y. Li,¹⁹ H. Liao,¹²³ C. S. Lin,¹³¹ S. Lin,¹³⁵ D. Lindebaum,¹⁸ R. A. Lineros,³¹ J. Ling,¹⁹⁶
117 A. Lister,²¹⁹ B. R. Littlejohn,⁸⁸ J. Liu,²³ Y. Liu,³⁶ S. Lockwitz,⁶⁷ T. Loew,¹³¹ M. Lokajicek,⁴⁸
118 I. Lomidze,⁷³ K. Long,⁸⁹ T. Lord,²¹⁵ J. M. LoSecco,¹⁵⁸ W. C. Louis,¹³⁴ X.-G. Lu,²¹⁵
119 K.B. Luk,^{21,131} B. Lunday,¹⁷¹ X. Luo,²⁶ E. Luppi,^{95,68} T. Lux,⁸⁵ V. P. Luzio,⁶⁵ J. Maalmi,¹⁶⁷
120 D. MacFarlane,¹⁹⁰ A. A. Machado,²⁹ P. Machado,⁶⁷ C. T. Macias,⁹² J. R. Macier,⁶⁷
121 M. MacMahon,²¹⁰ A. Maddalena,⁷⁶ A. Madera,³⁴ P. Madigan,^{21,131} S. Magill,⁶ K. Mahn,¹⁴⁴
122 A. Maio,^{132,62} A. Major,⁵⁶ K. Majumdar,¹³³ J. A. Maloney,⁵⁰ M. Man,²⁰⁶ G. Mandrioli,⁹³
123 R. C. Mandujano,²³ J. Maneira,^{132,62} L. Manenti,²¹⁰ S. Manly,¹⁸¹ A. Mann,²⁰⁷

124 K. Manolopoulos,¹⁸⁴ M. Manrique Plata,⁹² V. N. Manyam,¹⁹ M. Marchan,⁶⁷ A. Marchionni,⁶⁷
125 W. Marciano,¹⁹ D. Marfatia,⁸¹ C. Mariani,²¹³ J. Maricic,⁸¹ F. Marinho,¹¹⁵ A. D. Marino,⁴²
126 T. Markiewicz,¹⁹⁰ D. Marsden,¹³⁹ M. Marshak,¹⁴⁸ C. M. Marshall,¹⁸¹ J. Marshall,²¹⁵
127 J. Marteau,¹¹² J. Martín-Albo,⁸⁶ N. Martinez,¹²³ D.A. Martinez Caicedo,¹⁹² F. Martínez
128 López,¹⁷⁹ P. Martínez Miravé,⁸⁶ S. Martynenko,¹⁹ V. Mascagna,^{99,109} K. Mason,²⁰⁷
129 A. Mastbaum,¹⁸³ F. Matichard,¹³¹ S. Matsuno,⁸¹ J. Matthews,¹³⁵ C. Mauger,¹⁷¹ N. Mauri,^{93,16}
130 K. Mavrokoridis,¹³³ I. Mawby,²¹⁵ R. Mazza,⁹⁹ A. Mazzacane,⁶⁷ T. McAskill,²¹⁶ E. McCluskey,⁶⁷
131 N. McConkey,²¹⁰ K. S. McFarland,¹⁸¹ C. McGrew,¹⁹⁵ A. McNab,¹³⁹ A. Mefodiev,¹⁰⁸ P. Mehta,¹¹⁹
132 P. Melas,⁹ O. Mena,⁸⁶ H. Mendez,¹⁷⁷ P. Mendez,³⁴ D. P. Méndez,¹⁹ A. Menegolli,^{103,170}
133 G. Meng,¹⁰² M. D. Messier,⁹² W. Metcalf,¹³⁵ M. Mewes,⁹² H. Meyer,²¹⁷ T. Miao,⁶⁷ G. Michna,¹⁹³
134 V. Mikola,²¹⁰ R. Milincic,⁸¹ G. Miller,¹³⁹ W. Miller,¹⁴⁸ J. Mills,²⁰⁷ O. Mineev,¹⁰⁸ A. Minotti,^{99,145}
135 O. G. Miranda,⁴⁰ S. Miryala,¹⁹ S. Miscetti,⁹⁶ C. S. Mishra,⁶⁷ S. R. Mishra,¹⁹¹ A. Mislivec,¹⁴⁸
136 M. Mitchell,¹³⁵ D. Mladenov,³⁴ I. Mocioiu,¹⁷² K. Moffat,⁵⁷ A. Mogan,⁴³ N. Moggi,^{93,16}
137 R. Mohanta,⁸³ T. A. Mohayai,⁶⁷ N. Mokhov,⁶⁷ J. Molina,⁸ L. Molina Bueno,⁸⁶ E. Montagna,^{93,16}
138 A. Montanari,⁹³ C. Montanari,^{103,67,170} D. Montanari,⁶⁷ D. Montanino,^{98,185} L. M. Montaña
139 Zetina,⁴⁰ S. H. Moon,²⁰⁹ M. Mooney,⁴³ A. F. Moor,²⁸ D. Moreno,⁵ L. Morescalchi,¹⁰⁴
140 D. Moretti,⁹⁹ C. Morris,⁸² C. Mossey,⁶⁷ M. Mote,¹³⁵ E. Motuk,²¹⁰ C. A. Moura,⁶⁵
141 J. Mousseau,¹⁴³ G. Moustier,¹³⁰ W. Mu,⁶⁷ L. Mualem,²⁷ J. Mueller,⁴³ M. Muether,²¹⁷
142 F. Muheim,⁵⁸ A. Muir,⁵³ M. Mulhearn,²² D. Munford,⁸² L. J. Munteanu,³⁴ H. Muramatsu,¹⁴⁸
143 J. Muraz,⁵² M. Murphy,²¹³ S. Murphy,⁶¹ J. Musser,⁹² J. Nachtman,¹¹⁰ Y. Nagai,⁶⁰ S. Nagu,¹³⁶
144 M. Nalbandyan,²²¹ R. Nandakumar,¹⁸⁴ D. Naples,¹⁷⁵ S. Narita,¹¹⁶ A. Nath,⁹⁰
145 A. Navrer-Agasson,¹³⁹ N. Nayak,¹⁹ M. Nebot-Guinot,⁵⁸ K. Negishi,¹¹⁶ J. K. Nelson,²¹⁸
146 M. Nelson,¹¹⁰ J. Nesbit,²¹⁹ M. Nessi,^{67,34} D. Newbold,¹⁸⁴ M. Newcomer,¹⁷¹ H. Newton,⁵³
147 R. Nichol,²¹⁰ F. Nicolas-Arnaldos,⁷⁴ A. Nikolica,¹⁷¹ J. Nikolov,¹⁵⁹ E. Niner,⁶⁷ K. Nishimura,⁸¹
148 A. Norman,⁶⁷ A. Norrick,⁶⁷ P. Novella,⁸⁶ J. A. Nowak,¹³⁰ M. Oberling,⁶ J. P. Ochoa-Ricoux,²³
149 A. Olivier,¹⁸¹ A. Olshevskiy,¹²¹ Y. Onel,¹¹⁰ Y. Onishchuk,¹²⁹ J. Ott,²³ L. Pagani,²² G. Palacio,⁵⁹
150 O. Palamara,⁶⁷ S. Palestini,³⁴ J. M. Paley,⁶⁷ M. Pallavicini,^{97,72} C. Palomares,³⁸ S. Pan,¹⁷³
151 W. Panduro Vazquez,¹⁸² E. Pantic,²² V. Paolone,¹⁷⁵ V. Papadimitriou,⁶⁷ R. Papaleo,¹⁰⁶
152 A. Papanestis,¹⁸⁴ S. Paramesvaran,¹⁸ S. Parke,⁶⁷ E. Parozzi,^{99,145} S. Parsa,¹³ Z. Parsa,¹⁹
153 S. Parveen,¹¹⁹ M. Parvu,²⁰ D. Pasciuto,¹⁰⁴ S. Pascoli,^{57,16} L. Pasqualini,^{93,16} J. Pasternak,⁸⁹
154 J. Pater,¹³⁹ C. Patrick,^{58,210} L. Patrizii,⁹³ R. B. Patterson,²⁷ S. J. Patton,¹³¹ T. Patzak,¹⁶⁸
155 A. Paudel,⁶⁷ L. Paulucci,⁶⁵ Z. Pavlovic,⁶⁷ G. Pawloski,¹⁴⁸ D. Payne,¹³³ V. Pec,⁴⁸
156 S. J. M. Peeters,¹⁹⁸ A. Pena Perez,¹⁹⁰ E. Pennacchio,¹¹² A. Penzo,¹¹⁰ O. L. G. Peres,²⁹
157 Y. F. Perez Gonzalez,⁵⁷ L. Pérez-Molina,³⁸ C. Pernas,²¹⁸ J. Perry,⁵⁸ D. Pershey,⁵⁶
158 G. Pessina,⁹⁹ G. Petrillo,¹⁹⁰ C. Petta,^{94,30} R. Petti,¹⁹¹ V. Pia,^{93,16} F. Piastra,¹³ L. Pickering,¹⁸²
159 F. Pietropaolo,^{34,102} V. L. Pimentel,^{46,29} G. Pinaroli,¹⁹ K. Plows,¹⁶³ R. Plunkett,⁶⁷
160 T. Pollman,^{153,2} F. Pompa,⁸⁶ X. Pons,³⁴ N. Poonthottathil,¹¹¹ F. Poppi,^{93,16} S. Pordes,⁶⁷
161 J. Porter,¹⁹⁸ M. Potekhin,¹⁹ R. Potenza,^{94,30} B. V. K. S. Potukuchi,¹¹⁸ J. Pozimski,⁸⁹
162 M. Pozzato,^{93,16} S. Prakash,²⁹ T. Prakash,¹³¹ C. Pratt,²² M. Prest,⁹⁹ F. Psihas,⁶⁷
163 D. Pugnere,¹¹² X. Qian,¹⁹ J. L. Raaf,⁶⁷ V. Radeka,¹⁹ J. Rademacker,¹⁸ R. Radev,³⁴
164 B. Radics,²²² A. Rafique,⁶ E. Raguzin,¹⁹ M. Rai,²¹⁵ M. Rajaoalisoa,³⁹ I. Rakhno,⁶⁷
165 A. Rakotonandrasana,⁴ L. Rakotondravohitra,⁴ R. Rameika,⁶⁷ M. A. Ramirez Delgado,¹⁷¹
166 B. Ramson,⁶⁷ A. Rappoldi,^{103,170} G. Raselli,^{103,170} P. Ratoff,¹³⁰ S. Raut,¹⁹⁵ H. Razafinime,³⁹

167 R. F. Razakamiandra,⁴ E. M. Rea,¹⁴⁸ J. S. Real,⁷⁷ B. Rebel,^{219,67} R. Rechenmacher,⁶⁷
 168 M. Reggiani-Guzzo,¹³⁹ J. Reichenbacher,¹⁹² S. D. Reitzner,⁶⁷ H. Rejeb Sfar,³⁴ A. Renshaw,⁸²
 169 S. Rescia,¹⁹ F. Resnati,³⁴ M. Ribas,²⁰⁰ S. Riboldi,¹⁰⁰ C. Riccio,¹⁹⁵ G. Riccobene,¹⁰⁶
 170 L. C. J. Rice,¹⁷⁵ J. S. Ricol,⁷⁷ A. Rigamonti,³⁴ Y. Rigaut,⁶¹ E. V. Rincón,⁵⁹ A. Ritchie-Yates,¹⁸²
 171 D. Rivera,¹³⁴ R. Rivera,⁶⁷ A. Robert,⁷⁷ J. L. Rocabado Rocha,⁸⁶ L. Rochester,¹⁹⁰ M. Roda,¹³³
 172 P. Rodrigues,¹⁶³ M. J. Rodriguez Alonso,³⁴ J. Rodriguez Rondon,¹⁹² E. Romeo,¹⁰¹
 173 S. Rosauero-Alcaraz,¹⁶⁷ P. Rosier,¹⁶⁷ M. Rossella,^{103,170} M. Rossi,³⁴ M. Ross-Lonergan,¹³⁴
 174 J. Rout,¹¹⁹ P. Roy,²¹⁷ A. Rubbia,⁶¹ C. Rubbia,⁷⁵ G. Ruiz Ferreira,¹³⁹ B. Russell,¹³¹
 175 D. Ruterbories,¹⁸¹ A. Rybnikov,¹²¹ A. Saa-Hernandez,⁸⁷ R. Saakyan,²¹⁰ S. Sacerdoti,¹⁶⁸
 176 N. Sahu,⁹¹ P. Sala,^{100,34} N. Samios,¹⁹ O. Samoylov,¹²¹ M. C. Sanchez,⁷⁰ V. Sandberg,¹³⁴
 177 D. A. Sanders,¹⁴⁹ D. Sankey,¹⁸⁴ D. Santoro,¹⁰⁰ N. Saoulidou,⁹ P. Sapienza,¹⁰⁶ C. Sarasty,³⁹
 178 I. Sarcevic,⁷ I. Sarra,⁹⁶ G. Savage,⁶⁷ V. Savinov,¹⁷⁵ G. Scanavini,²²⁰ A. Scaramelli,¹⁰³
 179 A. Scarff,¹⁸⁹ A. Scarpelli,¹⁹ T. Schefke,¹³⁵ H. Schellman,^{162,67} S. Schifano,^{95,68}
 180 P. Schlabach,⁶⁷ D. Schmitz,³⁶ A. W. Schneider,¹⁴⁰ K. Scholberg,⁵⁶ A. Schukraft,⁶⁷
 181 E. Segreto,²⁹ A. Selyunin,¹²¹ C. R. Senise,²⁰⁸ J. Sensenig,¹⁷¹ D. Sgalaberna,⁶¹
 182 M. H. Shaevitz,⁴⁴ S. Shafaq,¹¹⁹ F. Shaker,²²² M. Shamma,²⁵ P. Shanahan,⁶⁷ R. Sharankova,²⁰⁷
 183 H. R. Sharma,¹¹⁸ R. Sharma,¹⁹ R. Kumar,¹⁷⁸ K. Shaw,¹⁹⁸ T. Shaw,⁶⁷ K. Shchablo,¹¹²
 184 C. Shepherd-Themistocleous,¹⁸⁴ A. Sheshukov,¹²¹ W. Shi,¹⁹⁵ S. Shin,¹²⁰ I. Shoemaker,²¹³
 185 D. Shooltz,¹⁴⁴ R. Shrock,¹⁹⁵ J. Silber,¹³¹ L. Simard,¹⁶⁷ J. Sinclair,¹⁹⁰ G. Sinev,¹⁹² Jaydip
 186 Singh,¹³⁶ J. Singh,¹³⁶ L. Singh,⁴⁷ P. Singh,¹⁷⁹ V. Singh,⁴⁷ S. Singh Chauhan,¹⁶⁶ R. Sipos,³⁴
 187 G. Sirri,⁹³ A. Sitraka,¹⁹² K. Siyeon,³⁷ K. Skarpaas,¹⁹⁰ E. Smith,⁹² P. Smith,⁹² J. Smolik,⁴⁹
 188 M. Smy,²³ E.L. Snider,⁶⁷ P. Snopok,⁸⁸ D. Snowden-Ifft,¹⁶⁰ M. Soares Nunes,¹⁹⁹ H. Sobel,²³
 189 M. Soderberg,¹⁹⁹ S. Sokolov,¹²¹ C. J. Solano Salinas,¹⁰⁷ S. Söldner-Rembold,¹³⁹
 190 S.R. Soleti*,¹³¹ N. Solomey,²¹⁷ V. Solovov,¹³² W. E. Sondheim,¹³⁴ M. Sorel,⁸⁶ A. Sotnikov,¹²¹
 191 J. Soto-Oton,³⁸ A. Sousa,³⁹ K. Soustruznik,³⁵ F. Spagliardi,¹⁶³ M. Spanu,^{99,145} J. Spitz,¹⁴³
 192 N. J. C. Spooner,¹⁸⁹ K. Spurgeon,¹⁹⁹ D. Stalder,⁸ M. Stancari,⁶⁷ L. Stanco,^{102,165} J. Steenis,²²
 193 R. Stein,¹⁸ H. M. Steiner,¹³¹ A. F. Steklain Lisboa,²⁰⁰ A. Stepanova,¹²¹ J. Stewart,¹⁹
 194 B. Stillwell,³⁶ J. Stock,¹⁹² F. Stocker,³⁴ T. Stokes,¹³⁵ M. Strait,¹⁴⁸ T. Strauss,⁶⁷ L. Strigari,²⁰²
 195 A. Stuart,⁴¹ J. G. Suarez,⁵⁹ J. Subash,¹⁵ A. Surdo,⁹⁸ V. Susic,¹² L. Suter,⁶⁷ C. M. Suter,^{94,30}
 196 K. Sutton,²⁷ Y. Suvorov,^{101,150} R. Svoboda,²² S. K. Swain,¹⁵⁴ B. Szczerbinska,²⁰³
 197 A. M. Szelc,⁵⁸ A. Taffara,¹⁰⁴ N. Talukdar,¹⁹¹ J. Tamara,⁵ H. A. Tanaka,¹⁹⁰ S. Tang,¹⁹
 198 N. Taniuchi,²⁸ B. Tapia Oregui,²⁰⁵ A. Tapper,⁸⁹ S. Tariq,⁶⁷ E. Tarpara,¹⁹ N. Tata,⁸⁰ E. Tatar,⁸⁴
 199 R. Tayloe,⁹² A. M. Teklu,¹⁹⁵ P. Tennessen,^{131,3} M. Tenti,⁹³ K. Terao,¹⁹⁰ F. Terranova,^{99,145}
 200 G. Testera,⁹⁷ T. Thakore,³⁹ A. Thea,¹⁸⁴ A. Thompson,²⁰² C. Thorn,¹⁹ S. C. Timm,⁶⁷
 201 V. Tishchenko,¹⁹ N. Todorović,¹⁵⁹ L. Tomassetti,^{95,68} A. Tonazzo,¹⁶⁸ D. Torbunov,¹⁹
 202 M. Torti,^{99,145} M. Tortola,⁸⁶ F. Tortorici,^{94,30} N. Tosi,⁹³ D. Totani,²⁶ M. Touns,⁶⁷
 203 C. Touramanis,¹³³ R. Travaglini,⁹³ J. Trevor,²⁷ S. Trilov,¹⁸ W. H. Trzaska,¹²² Y. Tsai,²³
 204 Y.-T. Tsai,¹⁹⁰ Z. Tsamalaidze,⁷³ K. V. Tsang,¹⁹⁰ N. Tsverava,⁷³ S. Z. Tu,¹¹⁷ S. Tufanli,³⁴
 205 C. Tull,¹³¹ J. Turner,⁵⁷ M. Tuzi,⁸⁶ J. Tyler,¹²³ E. Tyley,¹⁸⁹ M. Tzanov,¹³⁵ L. Uboldi,³⁴
 206 M. A. Uchida,²⁸ J. Urheim,⁹² T. Usher,¹⁹⁰ H. Utaegbulam,¹⁹⁹ S. Uzunyan,¹⁵⁶ M. R. Vagins,^{124,23}
 207 P. Vahle,²¹⁸ S. Valder,¹⁹⁸ G. A. Valdivieso,⁶³ E. Valencia,⁷⁸ R. Valentim,²⁰⁸ Z. Vallari,²⁷

*Corresponding author.

208 E. Vallazza,⁹⁹ J. W. F. Valle,⁸⁶ S. Vallecorsa,³⁴ R. Van Berg,¹⁷¹ R. G. Van de Water,¹³⁴
209 D. Vanegas Forero,¹⁴² D. Vannerom,¹⁴⁰ F. Varanini,¹⁰² D. Vargas Oliva,²⁰⁶ G. Varner,⁸¹
210 S. Vasina,¹²¹ N. Vaughan,¹⁶² K. Vaziri,⁶⁷ J. Vega,⁴⁵ S. Ventura,¹⁰² A. Verdugo,³⁸ S. Vergani,²⁸
211 M. A. Vermeulen,¹⁵³ M. Verzocchi,⁶⁷ M. Vicenzi,^{97,72} H. Vieira de Souza,¹⁶⁸ C. Vignoli,⁷⁶
212 C. Vilela,³⁴ B. Viren,¹⁹ A. Vizcaya-Hernandez,⁴³ T. Vrba,⁴⁹ Q. Vuong,¹⁸¹ T. Wachala,¹⁵²
213 A. V. Waldron,¹⁷⁹ M. Wallbank,³⁹ T. Walton,⁶⁷ H. Wang,²⁴ J. Wang,¹⁹² L. Wang,¹³¹
214 M.H.L.S. Wang,⁶⁷ X. Wang,⁶⁷ Y. Wang,²⁴ Y. Wang,¹⁹⁵ K. Warburton,¹¹¹ D. Warner,⁴³
215 M.O. Wascko,⁸⁹ D. Waters,²¹⁰ A. Watson,¹⁵ K. Wawrowska,^{184,198} P. Weatherly,⁵⁵
216 A. Weber,^{138,67} M. Weber,¹³ H. Wei,¹³⁵ A. Weinstein,¹¹¹ D. Wenman,²¹⁹ M. Wetstein,¹¹¹
217 J. Whilhelmi,²²⁰ A. White,²⁰⁴ A. White,²²⁰ L. H. Whitehead,²⁸ D. Whittington,¹⁹⁹
218 M. J. Wilking,¹⁹⁵ A. Wilkinson,²¹⁰ C. Wilkinson,¹³¹ Z. Williams,²⁰⁴ F. Wilson,¹⁸⁴ R. J. Wilson,⁴³
219 W. Wisniewski,¹⁹⁰ J. Wolcott,²⁰⁷ J. Wolfs,¹⁸¹ T. Wongjirad,²⁰⁷ A. Wood,⁸² K. Wood,¹³¹
220 E. Worcester,¹⁹ M. Worcester,¹⁹ M. Wospakrik,⁶⁷ K. Wresilo,²⁸ C. Wret,¹⁸¹ S. Wu,¹⁴⁸ W. Wu,⁶⁷
221 W. Wu,²³ M. Wurm,¹³⁸ J. Wyenberg,⁵⁴ Y. Xiao,²³ I. Xiotidis,⁸⁹ B. Yaeggy,³⁹ N. Yahlali,⁸⁶
222 E. Yandel,²⁶ G. Yang,¹⁹⁵ K. Yang,¹⁶³ T. Yang,⁶⁷ A. Yankelevich,²³ N. Yershov,¹⁰⁸
223 K. Yonehara,⁶⁷ Y. S. Yoon,³⁷ T. Young,¹⁵⁵ B. Yu,¹⁹ H. Yu,¹⁹ H. Yu,¹⁹⁶ J. Yu,²⁰⁴ Y. Yu,⁸⁸
224 W. Yuan,⁵⁸ R. Zaki,²²² J. Zalesak,⁴⁸ L. Zambelli,⁵² B. Zamorano,⁷⁴ A. Zani,¹⁰⁰ L. Zazueta,²¹⁸
225 G. P. Zeller,⁶⁷ J. Zennamo,⁶⁷ K. Zeug,²¹⁹ C. Zhang,¹⁹ S. Zhang,⁹² Y. Zhang,¹⁷⁵ M. Zhao,¹⁹
226 E. Zhivun,¹⁹ E. D. Zimmerman,⁴² S. Zucchelli,^{93,16} J. Zuklin,⁴⁸ V. Zutshi,¹⁵⁶ and R. Zwaska⁶⁷

227 ⁰Abilene Christian University, Abilene, TX 79601, USA

228 ¹University of Albany, SUNY, Albany, NY 12222, USA

229 ²University of Amsterdam, NL-1098 XG Amsterdam, The Netherlands

230 ³Antalya Bilim University, 07190 Döşemealtı/Antalya, Turkey

231 ⁴University of Antananarivo, Antananarivo 101, Madagascar

232 ⁵Universidad Antonio Nariño, Bogotá, Colombia

233 ⁶Argonne National Laboratory, Argonne, IL 60439, USA

234 ⁷University of Arizona, Tucson, AZ 85721, USA

235 ⁸Universidad Nacional de Asunción, San Lorenzo, Paraguay

236 ⁹University of Athens, Zografou GR 157 84, Greece

237 ¹⁰Universidad del Atlántico, Barranquilla, Atlántico, Colombia

238 ¹¹Augustana University, Sioux Falls, SD 57197, USA

239 ¹²University of Basel, CH-4056 Basel, Switzerland

240 ¹³University of Bern, CH-3012 Bern, Switzerland

241 ¹⁴Beykent University, Istanbul, Turkey

242 ¹⁵University of Birmingham, Birmingham B15 2TT, United Kingdom

243 ¹⁶Università del Bologna, 40127 Bologna, Italy

244 ¹⁷Boston University, Boston, MA 02215, USA

245 ¹⁸University of Bristol, Bristol BS8 1TL, United Kingdom

246 ¹⁹Brookhaven National Laboratory, Upton, NY 11973, USA

247 ²⁰University of Bucharest, Bucharest, Romania

248 ²¹University of California Berkeley, Berkeley, CA 94720, USA

249 ²²University of California Davis, Davis, CA 95616, USA

250 ²³University of California Irvine, Irvine, CA 92697, USA

251 ²⁴ *University of California Los Angeles, Los Angeles, CA 90095, USA*
252 ²⁵ *University of California Riverside, Riverside CA 92521, USA*
253 ²⁶ *University of California Santa Barbara, Santa Barbara, California 93106 USA*
254 ²⁷ *California Institute of Technology, Pasadena, CA 91125, USA*
255 ²⁸ *University of Cambridge, Cambridge CB3 0HE, United Kingdom*
256 ²⁹ *Universidade Estadual de Campinas, Campinas - SP, 13083-970, Brazil*
257 ³⁰ *Università di Catania, 2 - 95131 Catania, Italy*
258 ³¹ *Universidad Católica del Norte, Antofagasta, Chile*
259 ³² *Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, RJ 22290-180, Brazil*
260 ³³ *IRFU, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France*
261 ³⁴ *CERN, The European Organization for Nuclear Research, 1211 Meyrin, Switzerland*
262 ³⁵ *Institute of Particle and Nuclear Physics of the Faculty of Mathematics and Physics of the Charles University,*
263 *180 00 Prague 8, Czech Republic*
264 ³⁶ *University of Chicago, Chicago, IL 60637, USA*
265 ³⁷ *Chung-Ang University, Seoul 06974, South Korea*
266 ³⁸ *CIEMAT, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, E-28040 Madrid,*
267 *Spain*
268 ³⁹ *University of Cincinnati, Cincinnati, OH 45221, USA*
269 ⁴⁰ *Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional (Cinvestav), Mexico*
270 *City, Mexico*
271 ⁴¹ *Universidad de Colima, Colima, Mexico*
272 ⁴² *University of Colorado Boulder, Boulder, CO 80309, USA*
273 ⁴³ *Colorado State University, Fort Collins, CO 80523, USA*
274 ⁴⁴ *Columbia University, New York, NY 10027, USA*
275 ⁴⁵ *Comisión Nacional de Investigación y Desarrollo Aeroespacial, Lima, Peru*
276 ⁴⁶ *Centro de Tecnologia da Informacao Renato Archer, Amarais - Campinas, SP - CEP 13069-901*
277 ⁴⁷ *Central University of South Bihar, Gaya, 824236, India*
278 ⁴⁸ *Institute of Physics, Czech Academy of Sciences, 182 00 Prague 8, Czech Republic*
279 ⁴⁹ *Czech Technical University, 115 19 Prague 1, Czech Republic*
280 ⁵⁰ *Dakota State University, Madison, SD 57042, USA*
281 ⁵¹ *University of Dallas, Irving, TX 75062-4736, USA*
282 ⁵² *Laboratoire d'Annecy de Physique des Particules, Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS,*
283 *LAPP-IN2P3, 74000 Annecy, France*
284 ⁵³ *Daresbury Laboratory, Cheshire WA4 4AD, United Kingdom*
285 ⁵⁴ *Dordt University, 700 7th St NE, Sioux Center, IA 51250, USA*
286 ⁵⁵ *Drexel University, Philadelphia, PA 19104, USA*
287 ⁵⁶ *Duke University, Durham, NC 27708, USA*
288 ⁵⁷ *Durham University, Durham DH1 3LE, United Kingdom*
289 ⁵⁸ *University of Edinburgh, Edinburgh EH8 9YL, United Kingdom*
290 ⁵⁹ *Universidad EIA, Envigado, Antioquia, Colombia*
291 ⁶⁰ *Eötvös Loránd University, 1053 Budapest, Hungary*
292 ⁶¹ *ETH Zurich, Zurich, Switzerland*
293 ⁶² *Faculdade de Ciências da Universidade de Lisboa - FCUL, 1749-016 Lisboa, Portugal*
294 ⁶³ *Universidade Federal de Alfenas, Poços de Caldas - MG, 37715-400, Brazil*

295 ⁶⁴*Universidade Federal de Goiás, Goiania, GO 74690-900, Brazil*
296 ⁶⁵*Universidade Federal do ABC, Santo André - SP, 09210-580, Brazil*
297 ⁶⁶*Universidade Federal do Rio de Janeiro, Rio de Janeiro - RJ, 21941-901, Brazil*
298 ⁶⁷*Fermi National Accelerator Laboratory, Batavia, IL 60510, USA*
299 ⁶⁸*University of Ferrara, Ferrara, Italy*
300 ⁶⁹*University of Florida, Gainesville, FL 32611-8440, USA*
301 ⁷⁰*Florida State University, Tallahassee, FL, USA*
302 ⁷¹*Fluminense Federal University, 9 Icaraí Niterói - RJ, 24220-900, Brazil*
303 ⁷²*Università degli Studi di Genova, Genova, Italy*
304 ⁷³*Georgian Technical University, Tbilisi, Georgia*
305 ⁷⁴*University of Granada & CAFPE, 18002 Granada, Spain*
306 ⁷⁵*Gran Sasso Science Institute, L'Aquila, Italy*
307 ⁷⁶*Laboratori Nazionali del Gran Sasso, L'Aquila AQ, Italy*
308 ⁷⁷*University Grenoble Alpes, CNRS, Grenoble INP, LPSC-IN2P3, 38000 Grenoble, France*
309 ⁷⁸*Universidad de Guanajuato, Guanajuato, C.P. 37000, Mexico*
310 ⁷⁹*Harish-Chandra Research Institute, Jhansi, Allahabad 211 019, India*
311 ⁸⁰*Harvard University, Cambridge, MA 02138, USA*
312 ⁸¹*University of Hawaii, Honolulu, HI 96822, USA*
313 ⁸²*University of Houston, Houston, TX 77204, USA*
314 ⁸³*University of Hyderabad, Gachibowli, Hyderabad - 500 046, India*
315 ⁸⁴*Idaho State University, Pocatello, ID 83209, USA*
316 ⁸⁵*Institut de Física d'Altes Energies (IFAE)—Barcelona Institute of Science and Technology (BIST), Barcelona,*
317 *Spain*
318 ⁸⁶*Instituto de Física Corpuscular, CSIC and Universitat de València, 46980 Paterna, Valencia, Spain*
319 ⁸⁷*Instituto Galego de Física de Altas Enerxías, University of Santiago de Compostela, 15782 Santiago de*
320 *Compostela, Spain*
321 ⁸⁸*Illinois Institute of Technology, Chicago, IL 60616, USA*
322 ⁸⁹*Imperial College of Science Technology and Medicine, London SW7 2BZ, United Kingdom*
323 ⁹⁰*Indian Institute of Technology Guwahati, Guwahati, 781 039, India*
324 ⁹¹*Indian Institute of Technology Hyderabad, Hyderabad, 502285, India*
325 ⁹²*Indiana University, Bloomington, IN 47405, USA*
326 ⁹³*Istituto Nazionale di Fisica Nucleare Sezione di Bologna, 40127 Bologna BO, Italy*
327 ⁹⁴*Istituto Nazionale di Fisica Nucleare Sezione di Catania, I-95123 Catania, Italy*
328 ⁹⁵*Istituto Nazionale di Fisica Nucleare Sezione di Ferrara, I-44122 Ferrara, Italy*
329 ⁹⁶*Istituto Nazionale di Fisica Nucleare Laboratori Nazionali di Frascati, Frascati, Roma, Italy*
330 ⁹⁷*Istituto Nazionale di Fisica Nucleare Sezione di Genova, 16146 Genova GE, Italy*
331 ⁹⁸*Istituto Nazionale di Fisica Nucleare Sezione di Lecce, 73100 - Lecce, Italy*
332 ⁹⁹*Istituto Nazionale di Fisica Nucleare Sezione di Milano Bicocca, 3 - I-20126 Milano, Italy*
333 ¹⁰⁰*Istituto Nazionale di Fisica Nucleare Sezione di Milano, 20133 Milano, Italy*
334 ¹⁰¹*Istituto Nazionale di Fisica Nucleare Sezione di Napoli, I-80126 Napoli, Italy*
335 ¹⁰²*Istituto Nazionale di Fisica Nucleare Sezione di Padova, 35131 Padova, Italy*
336 ¹⁰³*Istituto Nazionale di Fisica Nucleare Sezione di Pavia, I-27100 Pavia, Italy*
337 ¹⁰⁴*Istituto Nazionale di Fisica Nucleare Laboratori Nazionali di Pisa, Pisa PI, Italy*
338 ¹⁰⁵*Istituto Nazionale di Fisica Nucleare Sezione di Roma, 00185 Roma RM, Italy*

339 ¹⁰⁶*Istituto Nazionale di Fisica Nucleare Laboratori Nazionali del Sud, 95123 Catania, Italy*
340 ¹⁰⁷*Universidad Nacional de Ingeniería, Lima 25, Perú*
341 ¹⁰⁸*Institute for Nuclear Research of the Russian Academy of Sciences, Moscow 117312, Russia*
342 ¹⁰⁹*University of Insubria, Via Ravasi, 2, 21100 Varese VA, Italy*
343 ¹¹⁰*University of Iowa, Iowa City, IA 52242, USA*
344 ¹¹¹*Iowa State University, Ames, Iowa 50011, USA*
345 ¹¹²*Institut de Physique des 2 Infinis de Lyon, 69622 Villeurbanne, France*
346 ¹¹³*Institute for Research in Fundamental Sciences, Tehran, Iran*
347 ¹¹⁴*Instituto Superior Técnico - IST, Universidade de Lisboa, Portugal*
348 ¹¹⁵*Instituto Tecnológico de Aeronáutica, Sao Jose dos Campos, Brazil*
349 ¹¹⁶*Iwate University, Morioka, Iwate 020-8551, Japan*
350 ¹¹⁷*Jackson State University, Jackson, MS 39217, USA*
351 ¹¹⁸*University of Jammu, Jammu-180006, India*
352 ¹¹⁹*Jawaharlal Nehru University, New Delhi 110067, India*
353 ¹²⁰*Jeonbuk National University, Jeonrabuk-do 54896, South Korea*
354 ¹²¹*Joint Institute for Nuclear Research, Dzhelapov Laboratory of Nuclear Problems 6 Joliot-Curie, Dubna,*
355 *Moscow Region, 141980 RU*
356 ¹²²*University of Jyväskylä, FI-40014, Finland*
357 ¹²³*Kansas State University, Manhattan, KS 66506, USA*
358 ¹²⁴*Kavli Institute for the Physics and Mathematics of the Universe, Kashiwa, Chiba 277-8583, Japan*
359 ¹²⁵*High Energy Accelerator Research Organization (KEK), Ibaraki, 305-0801, Japan*
360 ¹²⁶*Korea Institute of Science and Technology Information, Daejeon, 34141, South Korea*
361 ¹²⁷*K L University, Vaddeswaram, Andhra Pradesh 522502, India*
362 ¹²⁸*National Institute of Technology, Kure College, Hiroshima, 737-8506, Japan*
363 ¹²⁹*Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine*
364 ¹³⁰*Lancaster University, Lancaster LA1 4YB, United Kingdom*
365 ¹³¹*Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*
366 ¹³²*Laboratório de Instrumentação e Física Experimental de Partículas, 1649-003 Lisboa and 3004-516*
367 *Coimbra, Portugal*
368 ¹³³*University of Liverpool, L69 7ZE, Liverpool, United Kingdom*
369 ¹³⁴*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
370 ¹³⁵*Louisiana State University, Baton Rouge, LA 70803, USA*
371 ¹³⁶*University of Lucknow, Uttar Pradesh 226007, India*
372 ¹³⁷*Madrid Autonoma University and IFT UAM/CSIC, 28049 Madrid, Spain*
373 ¹³⁸*Johannes Gutenberg-Universität Mainz, 55122 Mainz, Germany*
374 ¹³⁹*University of Manchester, Manchester M13 9PL, United Kingdom*
375 ¹⁴⁰*Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
376 ¹⁴¹*Max-Planck-Institut, Munich, 80805, Germany*
377 ¹⁴²*University of Medellín, Medellín, 050026 Colombia*
378 ¹⁴³*University of Michigan, Ann Arbor, MI 48109, USA*
379 ¹⁴⁴*Michigan State University, East Lansing, MI 48824, USA*
380 ¹⁴⁵*Università del Milano-Bicocca, 20126 Milano, Italy*
381 ¹⁴⁶*Università degli Studi di Milano, I-20133 Milano, Italy*
382 ¹⁴⁷*University of Minnesota Duluth, Duluth, MN 55812, USA*

383 ¹⁴⁸*University of Minnesota Twin Cities, Minneapolis, MN 55455, USA*
384 ¹⁴⁹*University of Mississippi, University, MS 38677 USA*
385 ¹⁵⁰*Università degli Studi di Napoli Federico II , 80138 Napoli NA, Italy*
386 ¹⁵¹*University of New Mexico, Albuquerque, NM 87131, USA*
387 ¹⁵²*H. Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland*
388 ¹⁵³*Nikhef National Institute of Subatomic Physics, 1098 XG Amsterdam, Netherlands*
389 ¹⁵⁴*National Institute of Science Education and Research (NISER), Odisha 752050, India*
390 ¹⁵⁵*University of North Dakota, Grand Forks, ND 58202-8357, USA*
391 ¹⁵⁶*Northern Illinois University, DeKalb, IL 60115, USA*
392 ¹⁵⁷*Northwestern University, Evanston, IL 60208, USA*
393 ¹⁵⁸*University of Notre Dame, Notre Dame, IN 46556, USA*
394 ¹⁵⁹*University of Novi Sad, 21102 Novi Sad, Serbia*
395 ¹⁶⁰*Occidental College, Los Angeles, CA 90041*
396 ¹⁶¹*Ohio State University, Columbus, OH 43210, USA*
397 ¹⁶²*Oregon State University, Corvallis, OR 97331, USA*
398 ¹⁶³*University of Oxford, Oxford, OX1 3RH, United Kingdom*
399 ¹⁶⁴*Pacific Northwest National Laboratory, Richland, WA 99352, USA*
400 ¹⁶⁵*Universtà degli Studi di Padova, I-35131 Padova, Italy*
401 ¹⁶⁶*Panjab University, Chandigarh, 160014 U.T., India*
402 ¹⁶⁷*Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*
403 ¹⁶⁸*Université Paris Cité, CNRS, Astroparticule et Cosmologie, Paris, France*
404 ¹⁶⁹*University of Parma, 43121 Parma PR, Italy*
405 ¹⁷⁰*Università degli Studi di Pavia, 27100 Pavia PV, Italy*
406 ¹⁷¹*University of Pennsylvania, Philadelphia, PA 19104, USA*
407 ¹⁷²*Pennsylvania State University, University Park, PA 16802, USA*
408 ¹⁷³*Physical Research Laboratory, Ahmedabad 380 009, India*
409 ¹⁷⁴*Università di Pisa, I-56127 Pisa, Italy*
410 ¹⁷⁵*University of Pittsburgh, Pittsburgh, PA 15260, USA*
411 ¹⁷⁶*Pontificia Universidad Católica del Perú, Lima, Perú*
412 ¹⁷⁷*University of Puerto Rico, Mayaguez 00681, Puerto Rico, USA*
413 ¹⁷⁸*Punjab Agricultural University, Ludhiana 141004, India*
414 ¹⁷⁹*Queen Mary University of London, London E1 4NS, United Kingdom*
415 ¹⁸⁰*Radboud University, NL-6525 AJ Nijmegen, Netherlands*
416 ¹⁸¹*University of Rochester, Rochester, NY 14627, USA*
417 ¹⁸²*Royal Holloway College London, TW20 0EX, United Kingdom*
418 ¹⁸³*Rutgers University, Piscataway, NJ, 08854, USA*
419 ¹⁸⁴*STFC Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom*
420 ¹⁸⁵*Università del Salento, 73100 Lecce, Italy*
421 ¹⁸⁶*San Jose State University, San José, CA 95192-0106, USA*
422 ¹⁸⁷*Sapienza University of Rome, 00185 Roma RM, Italy*
423 ¹⁸⁸*Universidad Sergio Arboleda, 11022 Bogotá, Colombia*
424 ¹⁸⁹*University of Sheffield, Sheffield S3 7RH, United Kingdom*
425 ¹⁹⁰*SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA*
426 ¹⁹¹*University of South Carolina, Columbia, SC 29208, USA*

- 427 ¹⁹²*South Dakota School of Mines and Technology, Rapid City, SD 57701, USA*
- 428 ¹⁹³*South Dakota State University, Brookings, SD 57007, USA*
- 429 ¹⁹⁴*Southern Methodist University, Dallas, TX 75275, USA*
- 430 ¹⁹⁵*Stony Brook University, SUNY, Stony Brook, NY 11794, USA*
- 431 ¹⁹⁶*Sun Yat-Sen University, Guangzhou, 510275*
- 432 ¹⁹⁷*Sanford Underground Research Facility, Lead, SD, 57754, USA*
- 433 ¹⁹⁸*University of Sussex, Brighton, BN1 9RH, United Kingdom*
- 434 ¹⁹⁹*Syracuse University, Syracuse, NY 13244, USA*
- 435 ²⁰⁰*Universidade Tecnológica Federal do Paraná, Curitiba, Brazil*
- 436 ²⁰¹*Tel Aviv University, Tel Aviv-Yafo, Israel*
- 437 ²⁰²*Texas A&M University, College Station, Texas 77840*
- 438 ²⁰³*Texas A&M University - Corpus Christi, Corpus Christi, TX 78412, USA*
- 439 ²⁰⁴*University of Texas at Arlington, Arlington, TX 76019, USA*
- 440 ²⁰⁵*University of Texas at Austin, Austin, TX 78712, USA*
- 441 ²⁰⁶*University of Toronto, Toronto, Ontario M5S 1A1, Canada*
- 442 ²⁰⁷*Tufts University, Medford, MA 02155, USA*
- 443 ²⁰⁸*Universidade Federal de São Paulo, 09913-030, São Paulo, Brazil*
- 444 ²⁰⁹*Ulsan National Institute of Science and Technology, Ulsan 689-798, South Korea*
- 445 ²¹⁰*University College London, London, WC1E 6BT, United Kingdom*
- 446 ²¹¹*Valley City State University, Valley City, ND 58072, USA*
- 447 ²¹²*Variable Energy Cyclotron Centre, 700 064 West Bengal, India*
- 448 ²¹³*Virginia Tech, Blacksburg, VA 24060, USA*
- 449 ²¹⁴*University of Warsaw, 02-093 Warsaw, Poland*
- 450 ²¹⁵*University of Warwick, Coventry CV4 7AL, United Kingdom*
- 451 ²¹⁶*Wellesley College, Wellesley, MA 02481, USA*
- 452 ²¹⁷*Wichita State University, Wichita, KS 67260, USA*
- 453 ²¹⁸*William and Mary, Williamsburg, VA 23187, USA*
- 454 ²¹⁹*University of Wisconsin Madison, Madison, WI 53706, USA*
- 455 ²²⁰*Yale University, New Haven, CT 06520, USA*
- 456 ²²¹*Yerevan Institute for Theoretical Physics and Modeling, Yerevan 0036, Armenia*
- 457 ²²²*York University, Toronto M3J 1P3, Canada*
- 458 E-mail: roberto@lbl.gov

459 ABSTRACT: The rapid development of general-purpose computing on graphics processing units
460 (GPGPU) is allowing the implementation of highly-parallelized Monte Carlo simulation chains for
461 particle physics experiments. This technique is particularly suitable for the simulation of a pixelated
462 charge readout for time projection chambers, given the large number of channels that this technology
463 employs. Here we present the first implementation of a full microphysical simulator of a liquid
464 argon time **projection** chamber (LArTPC) equipped with light readout and pixelated charge readout,
465 developed for the DUNE Near Detector. The software is implemented with an end-to-end set of
466 GPU-optimized algorithms. The algorithms have been written in Python and translated into CUDA
467 kernels using Numba, a just-in-time compiler for a subset of Python and NumPy instructions. The
468 GPU implementation achieves a speed up of four orders of magnitude compared with the equivalent
469 CPU version. The simulation of the current induced on 10^3 pixels takes around 1 ms on the GPU,
470 compared with approximately 10 s on the CPU. The results of the simulation are compared against
471 data from a pixel-readout LArTPC prototype.

472 KEYWORDS: Computing, Time projection chambers, Simulation methods and programs

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492 1 Introduction

493 The idea of using a liquid argon time projection chambers (LArTPC) for the detection of neutrino
494 interactions was first proposed in 1977 [1]. The detection mechanism is the following: charged
495 particles produced by neutrino interactions ionize the argon, leaving a trail of ionization electrons.
496 In addition, liquid argon also produces scintillation light, which provides calorimetric information
497 and a fast timing signal ($O(10\text{ ns})$ [2]). A fraction of the ionized electrons recombine immediately
498 with the positive argon ions, while the remaining ones drift towards the anode side of the detector
499 in a homogeneous electric field applied to the argon volume, which is usually $O(100\text{ V/cm})$.
500 Impurities present in the LAr (e.g. O_2 , H_2O , N_2) can attach a portion of the drifting electrons.
501 The amount of drifting electrons declines as a function of the distance from the anode, since the
502 electrons need to travel a longer path.

503 Typically, two or more arrays of sense wires are placed at the anode and assembled into planes.
504 The drifting of negative charges in a constant electric field induces a signal on the wires. Each
505 plane provides a two-dimensional image of the ionization: the position of the wire provides one

506 dimension, and the time of the arrival provides the second one, since the drift velocity of the
507 electrons in the LAr is known and is typically $O(1 \text{ m/ms})$. Using multiple wire planes can help
508 estimate the position of the ionization in three dimensions. However, ambiguities arise when drifting
509 electrons are isochronous or parallel to a wire orientation. Unambiguous 3D imaging of LArTPC
510 charge signals is possible using a readout system based on a pixelated array of charged-sensitive
511 pads, which has been demonstrated in ref. [3]. Both the typical distance between adjacent wires
512 and the typical pixel pitch are in the order of few millimeters. The position on the anode plane of
513 the involved pads provides two spatial dimensions, and the time of the induced signal provides the
514 third one. This truly three-dimensional readout provides better reconstruction efficiency and purity
515 than the 2D combined wire readout, as demonstrated in ref. [4].

516 Pixel readout requires the channel count used to be increased by a factor of 10 to 100 with
517 respect to wire planes. Thus, with this increased channel count and granularity simulation burden,
518 the transport of electrons in LAr and the signal induction on the pixel pads represent an ideal use
519 case for highly-parallelized, concurrent simulation algorithms. The development of general-purpose
520 computing on graphics processing units (GPGPU), which went hand in hand with the advances
521 in the machine learning and deep learning fields, has driven the design of the current generation
522 of supercomputers, such as Perlmutter at NERSC [5], which is a heterogeneous system with both
523 GPU-accelerated and CPU-only nodes. Implementing highly-parallelized simulation chains allows
524 full advantage of these new systems to be taken and enables the simulation of future pixelated
525 LArTPCs, which would otherwise not be viable with current resources.

526 The US-based neutrino physics program relies on present and future experiments using LArTPC
527 technology. The flagship experiment is the Deep Underground Neutrino Experiment (DUNE),
528 which will consist of a high-intensity accelerator neutrino beam, measured by near and far detectors
529 [6]. The Far Detector will consist of four 17-kiloton LArTPC modules located deep underground
530 at the Sanford Underground Research Facility in Lead, South Dakota, located 1285 km from the
531 beam source [7]. The Near Detector will be located at Fermilab, 574 m from the beam source, and
532 will contain a 67 t modular LArTPC called ND-LAr [8].

533 There are already some software toolkits for LArTPCs [9, 10] and there has been some effort
534 towards parallelizing the reconstruction stage [11]. However, the simulation stages have remained
535 mostly sequential and their speed up has been recognized as a priority by the community [12].

536 In this document we will describe the implementation of a set of highly-parallelized algorithms,
537 organized in a module called `larnd-sim` [13], that run on GPUs. They simulate the ionized
538 electrons recombination and drifting towards the anode, the generation of electronics signals on the
539 pixelated readout, and the processing of the signal by the front-end electronics.

540 **2 Technical implementation**

541 Recent rapid developments in the field of machine learning have stimulated the creation of several
542 tool-kits for GPU-accelerated applications. In particular, the NVIDIA® CUDA platform [14] allows
543 to use GPUs for general purpose computing via different programming languages. We opted for
544 Numba [15], which generates CUDA computing kernels using a subset of native Python and NumPy
545 code [16].

546 A CUDA kernel is a function that is executed N times in parallel by N CUDA threads. The
 547 threads can be organized in one-dimensional, two-dimensional, or three-dimensional *blocks*, which
 548 in turn can be organized in one-dimensional, two-dimensional, or three-dimensional *grids*. Blocks
 549 in the same grid contain the same number of threads, can run independently, and can be executed in
 550 any order, while threads in the same block can co-operate through shared memory. CUDA kernels
 551 typically store the result of the computation in a pre-allocated array passed to the kernel function.
 552 The CUDA programming model requires a careful design of the algorithm: the shape and size
 553 of the array where the result is stored must be known in advance and the threads must avoid race
 554 conditions during execution*, thus the result of the algorithm must not depend on the order of
 555 execution of the threads.

556 The software described in this document contains several CUDA kernel functions, separated
 557 into two logical categories: one for the charge simulation, described in section 3, and one for the
 558 light simulation, described in section 4. The functions simulate the detector response, including:
 559 (1) the recombination of the electrons with the argon ions, (2) the drifting of the electrons towards
 560 the anode, (3) the induction of electronic signals on the pixel pads and optical detectors, and (4) the
 561 electronics response of the charge and light readout systems.

562 The simulation of the passage of the initial particles through matter is performed using
 563 `edep-sim` [17], a wrapper around `GEANT4` [18], which is independent from the `larnd-sim` pack-
 564 age described here. The output consists of a set of short particle track segments, in the order of few
 565 millimeters, which describe the energy deposition trail of each particle. The length of the segments
 566 depends on the derivative of the stopping power dE/dx : the portion of a particle trail where the
 567 dE/dx changes abruptly will be divided in finer segments than the portion where the dE/dx is
 568 mostly constant. Thus, in a single segment, the energy deposition per unit length is assumed to be
 569 constant. **This approximation is valid when the segment length is of the same order as the detector
 570 resolution – at much shorter lengths, fluctuations from the long tail of the dE/dx distribution fall
 571 outside of the applicable region of recombination models, and at much longer lengths, correlations
 572 in the dE/dx fluctuations become significant and the dE/dx width will be under-simulated. Within
 573 these broad considerations, reducing the minimum size of the segments has not shown a significant
 574 impact on the result of the charge simulation.** This set S_i is stored in a bi-dimensional NumPy array
 575 containing the energy deposition and the spatial distribution of the segments:

$$S_i = (\vec{r}_s, \vec{r}_e, E)_i, \quad (2.1)$$

576 where \vec{r}_s and \vec{r}_e are four-dimensional vectors containing the spatial and timing coordinates of the
 577 segment start and end points, and E is the deposited energy. This array is used as input for our
 578 module. In order to minimize the memory transfer between the host and the device (in our case the
 579 GPU), we allocate the NumPy array directly on the device memory using CuPy [19], a GPU array
 580 backend that implements a subset of the NumPy interface. The output of the `larnd-sim` simulation
 581 is then saved in a HDF5 file [20]. The entire simulation workflow is shown in figure 1.

*In software, a race condition can happen when the behavior of the program depends on the relative timing of multiple threads or processes.

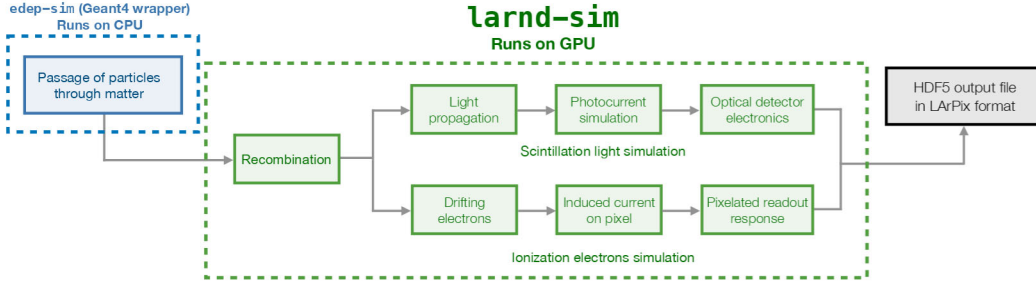


Figure 1: Diagram showing the full simulation workflow. The passage of the particle through matter is simulated by `edep-sim` on the CPU. The output is fed to `larnd-sim`, which runs entirely on GPU. Its output is finally saved in a HDF5 file.

3 Charge simulation

3.1 Electron recombination

The first step of our simulation is to calculate the number of electrons that remain after the recombination and start drifting towards the anode. We denote the initial charge ionized by the particle as Q_0 , while the charge remaining after the recombination is given by $Q_R = \mathcal{R} \cdot Q_0$, where \mathcal{R} is our recombination factor.

Two different models are commonly used to describe this phenomenon: the Birks model [21], which gives spurious values when applied to high-ionization particles [22], and the modified Box model [22], which doesn't suffer from these issues but is inadequate to describe particles at low stopping power (low dE/dx).

The recombination factor for the Birks model $\mathcal{R}_{\text{Birks}}$ can be parametrized as:

$$\mathcal{R}_{\text{Birks}} = \frac{A_b}{1 + k_b/\epsilon \cdot dE/dx}, \quad (3.1)$$

where A_b and k_b are free parameters that usually depend on the detector and ϵ is the product of the electric field with the liquid argon density. The ICARUS collaboration obtained $A_b = 0.800$ and $k_b = 0.0486$ (kV/MeV) (g/cm³) [23], which are the values used in our simulation.

The recombination factor the modified Box model \mathcal{R}_{Box} is defined as:

$$\mathcal{R}_{\text{Box}} = \frac{\log(\alpha + \beta/\epsilon \cdot dE/dx)}{\beta/\epsilon \cdot dE/dx}, \quad (3.2)$$

where α and β are free parameters which were measured by the ArgoNeuT collaboration to be $\alpha = 0.93$ and $\beta = 0.207$ (kV/MeV)(g/cm³) [22]. In both cases, the typical recombination factor for a minimum ionizing particle (MIP) is around 0.7. Our simulation assumes the Birks model by default.

The implementation of the calculation of the recombination factors $\mathcal{R}_{\text{Birks}}$ or \mathcal{R}_{Box} on the GPU is trivial: the i -th thread of the $K_{\text{recomb}}(S_i, \mathcal{R})$ CUDA kernel takes as input the i -th row of the NumPy array containing the segments S and applies the recombination formula, so eq. (3.1) or eq. (3.2). The result is stored in an appropriate column of the NumPy array. **Currently, the simulation**

605 treats the recombination factor as a fixed number: although this is an approximation, the level of
 606 fluctuations associated with it is significantly lower than the expected intrinsic noise of the detector,
 607 which was measured with the prototype described in section 6.

608 Even if this operation is computationally inexpensive, it’s instructive to take a look at the perfor-
 609 mance comparison between a sequential, interpreted Python `for` loop, a loop compiled on the CPU
 610 using Numba, and the GPU implementation using a CUDA kernel. Figure 2 shows the processing
 611 time needed to calculate $\mathcal{R}_{\text{Birks}}$ of eq. (3.1) as a function of the number of GEANT4 segments
 612 given as input. The CPU-compiled version is obviously faster than the sequential interpreted loop
 613 since the function is now translated into machine code. While the CUDA kernel processing time is
 614 initially the largest, it doesn’t immediately scale with the number of input segments, so it starts being
 615 the exponentially faster implementation with more than $\mathcal{O}(10^4)$ segments, where it starts taking
 616 advantage of the massive parallelization achievable by the GPU. The NVIDIA® Tesla® V100 GPU
 617 used for this study can run more than 10^5 parallel threads. To give a figure of merit, a typical
 618 neutrino beam spill in the ND-LAr corresponds on average to $\mathcal{O}(10^5)$ segments.

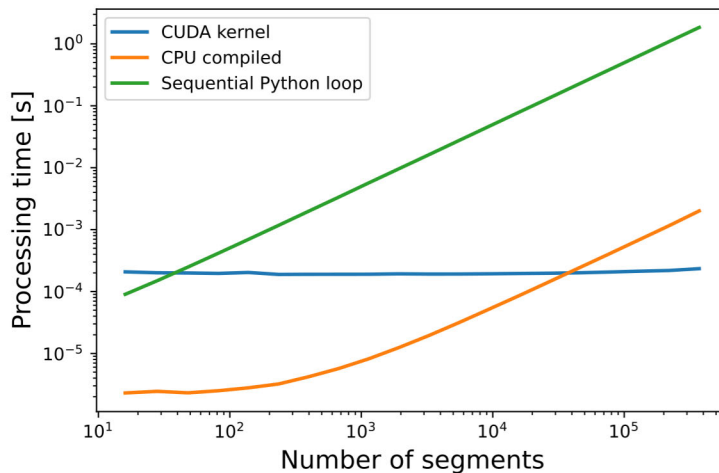


Figure 2: Processing time for the calculation of the recombination factor $\mathcal{R}_{\text{Birks}}$ of eq. (3.1) with the GPU implementation using a CUDA kernel (blue), the CPU implementation using Numba (orange), and a sequential Python `for` loop (green). For reference, a neutrino beam spill corresponds on average to $\mathcal{O}(10^5)$ energy deposition segments in the ND-LAr. This computation was performed on a node of the NERSC Cori supercomputer, which contains two sockets of 20-core Intel Xeon Gold 6148 (Skylake) at 2.40 GHz and 8 NVIDIA® Tesla® V100 (Volta) GPUs.

619 3.2 Electron transport in liquid argon

620 The electrons remaining after the recombination travel towards the anode at a constant velocity v_{drift}
 621 (assuming perfect uniformity of the electric field), which is typically $\mathcal{O}(1 \text{ mm}/\mu\text{s})$. The time they
 622 take to reach the anode is given by:

$$t_{\text{drift}} = (z - z_{\text{anode}})/v_{\text{drift}}, \quad (3.3)$$

623 where the electron drift direction is assumed to be along the z axis and where z_{anode} is the z
 624 coordinate of the anode.

625 The impurities in the liquid argon, such as O_2 , N_2 and H_2O , can attach a portion of the drifting
 626 electrons, so electrons farther from the anode will have a higher chance to be attached. This effect is
 627 usually parametrized by a negative exponential, so the charge Q_a that effectively reaches the anode,
 628 assuming uniform impurities and a perfect electronics response, is:

$$Q_a = Q_R \cdot \exp(-t_{\text{drift}}/\tau), \quad (3.4)$$

629 where t_{drift} is the time the charge takes to reach the anode and τ is a parameter that depends on
 630 the concentration of impurities and it is usually called *electron lifetime*, which is in the order of
 631 milliseconds for concentrations of O_2 at tens of parts per trillion.

632 Electrons drifting in strong electric fields do not diffuse isotropically, so it is necessary to
 633 estimate both the longitudinal and transverse components with respect to the drift direction [24].
 634 The diffusion length is given by:

$$\sigma = \sqrt{2Dt_{\text{drift}}}, \quad (3.5)$$

635 where D is the longitudinal or transverse diffusion coefficient, which depends on the electric field
 636 and liquid argon temperature. In our simulation we set the longitudinal and transverse diffusion
 637 coefficients to $D_l = 4 \text{ cm}^2/\text{s}$ and $D_t = 8.8 \text{ cm}^2/\text{s}$, respectively. These values were obtained by a
 638 preliminary ProtoDUNE-SP [25] analysis.

639 This information is calculated and stored in appropriate columns of the NumPy array in a
 640 way analogous to the one described in section 3.1, where each thread processes a single segment
 641 independently.

642 3.3 Electronic signal induction on a pixel

643 3.3.1 Field response

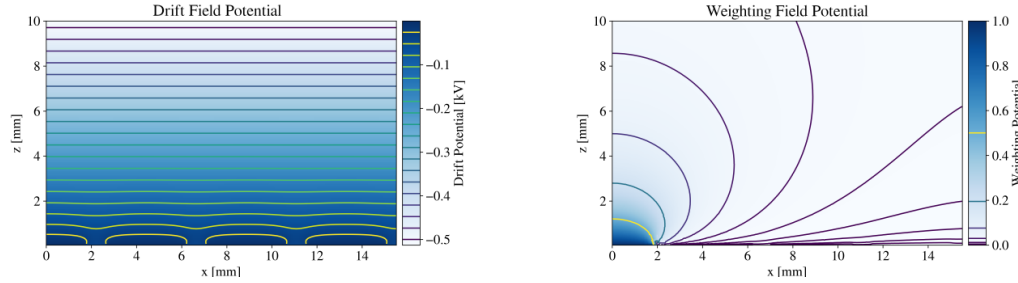
644 The current induced by a point charge on a given pixel within the anode is calculated using the
 645 Shockley-Ramo theorem [26]:

$$I_{\text{pixel}} = q \vec{v} \cdot \nabla W, \quad (3.6)$$

646 where W is the *weighting field potential*, the normalized contribution of a single electrode to the
 647 overall field, q is the particle charge, and \vec{v} is the velocity of the particle. Within `larnd-sim`, the
 648 induced current is pre-calculated for a point-like charge and referenced as a $I_{\text{pixel}}[t, x, y]$ look-up
 649 table (LUT). The table contains the current induced by an electron placed at discrete (x, y) locations
 650 on the anode plane at a discrete time t , where $t = 0$ is the time when the electron is at $z = 0.5 \text{ cm}$.
 651 This value is chosen because of the observed flatness of the electric and weighting fields at this
 652 distance.

653 The $I_{\text{pixel}}[t, x, y]$ values are calculated as follows. In the region very close to the anode, the
 654 electric field and the weighting field are calculated numerically. The geometry of a small volume,
 655 including a central pixel with a pitch of 4.4 mm and its 8 nearest neighbor pixels, is modeled using
 656 CAD software and converted into a 3-dimensional mesh using the Gmsh package [27]. The fields
 657 are then calculated using the successive over-relaxation method as implemented in the Elmer FEM
 658 [28] software package. The electric and weighting fields share the same geometry, but differ in

659 the boundary conditions imposed on the problem. In the electric field calculation, the pixels are
 660 grounded, with the backing plane at a small offset voltage, and the field on the cathode-facing side
 661 of the volume is set to the nominal field of 500 V/cm. In the calculation of the weighting field, all
 662 electrodes other than the central pixel are grounded, the central pixel is set to unit voltage, and the
 663 voltage on the remaining conductors is set to zero. The results of these two field calculations are
 664 shown in figure 3.



(a) Drift electric potential field in the region near the pixel plane. Shown is a slice in y along on a pixel center. The pixel surfaces are set to 0 kV, while the gradient of the far field at the surface of $z = 10$ mm is set to 0.5 kV/cm. The color scale corresponds to the value of the drift potential.

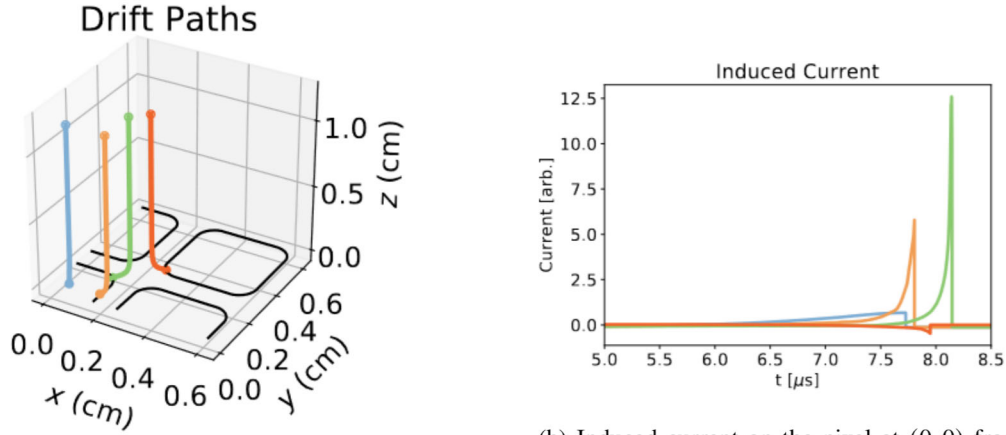
(b) Weighting potential field in the region near a "pixel of interest". The central ($x = y = 0$) pixel is set to a unit potential, while all other surfaces are set to 0 potential. The resulting unitless field defines the susceptibility to current induction by charges moving nearby.

Figure 3: The drift (left) and weighting (right) **field potentials** obtained by finite-element analysis in the region near a generic pixel. Shown are slices of the potential fields along an $x - z$ plane which crosses through the centerline of a pixel.

665 Next, the idealized drift paths (ignoring diffusion and attenuation effects) are integrated using
 666 the ICARUS and Walkowiak [29, 30] electron transport models evaluated within the calculated
 667 electric field. This model allows for the drift velocity to change as a function of the local electric
 668 field, as the assumption of a perfectly uniform field is not necessarily true very close to the anode.
 669 The drift paths are calculated for a grid of four hundred (x, y) positions, 0.5 cm from the anode
 670 on the z axis. The resulting granularity on the x and y axes is 0.33 mm. Finally, we compute the
 671 time-derivative of the weighting field **potential** along each path, which yields a charge-normalized
 672 current series for a given initial charge position. The sampling in time is $0.1 \mu\text{s}$. A select few drift
 673 paths are shown in figure 4a, with their corresponding current series in figure 4b.

674 Farther from the pixel at $z > 0.5$ cm, the weighting potential is solved by treating the pixel as
 675 point-like and using a method-of-image-charges approximation to fix the boundary conditions at
 676 the anode and the cathode. The drift velocity is assumed to be uniform. The relative normalization
 677 to the near-field calculation is then fixed by enforcing continuity in the current series at the time
 678 boundary. Some re-scaling is performed on these current series to ensure they integrate to one
 679 electron charge, as error is introduced in the drift path integration, as well as numerical error
 680 present in the FEM solutions and their interpolated values. Figure 5 shows the tabulated induced
 681 current on a pixel up to $30 \mu\text{s}$ from the time of arrival of the drift electron. The agreement of the
 682 near-field FEM model and the dipole far-field approximation across this surface seen in figure 5

683 demonstrates that the transition surface at 0.5 cm is sufficiently far from the pixel plane.



(a) Example drift paths for electrons starting at a short distance from a pixel centered at (0, 0).

(b) Induced current on the pixel at (0, 0) from example drift paths

Figure 4: To determine the near-field pixel response, we simulate the paths and velocities of drift electron within a 3D FEM field model. Here we show the simulated electron drift paths (left), and the corresponding induced current on the pixel (right) for a subset of the starting points used. The color of the trajectory on the left corresponds to the color of the current induced curve on the right.

684 3.3.2 Induced current calculation

The electrons drifting towards the anode are diffused in the longitudinal and transverse directions, as described in section 3.2. The ionization electrons corresponding to a GEANT4 segment will then form a three-dimensional charge cloud. The induced current on a given pixel from this can be calculated by taking the convolution of the pre-calculated pixel response model (see section 3.3.1) and the charge density of the track segment:

$$I(t) = \int I_{\text{pixel}}(t - z/v_d, x, y) \rho(x, y, z) dx dy dz \quad (3.7)$$

685 where $\rho(x, y, z)$ is the 3-dimensional charge density including diffusion and $I_{\text{pixel}}(t - z/v_d, x, y)$ is
 686 the current response model at the given position and time tick, which is stored in the LUT described
 687 in section 3.3.1. The positively charged ions also produce a current on the pixel, however the
 688 magnitude of this current is more than 7 orders of magnitude smaller than the signal from the drift
 689 electrons due to the small drift velocity of the ions, and so it is neglected in the detector simulation.

The calculation of $I(t)$ is the most computational-intensive step of the detector simulation. In order to reduce its complexity, we apply two approximations to the charge density: first, we discretize the track segment along the track length into N points; and second, we approximate the effect of diffusion summing the contribution from M random 3D perturbations of the sample point.