

# SILVINA CAÍNO-LORES

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## Education

- 2015 – 2019 » **Ph.D. in Computer Science and Technology.** University Carlos III of Madrid, Spain.  
Thesis: *On the Convergence of Big Data Analytics and High-Performance Computing: A Novel Approach for Runtime Interoperability*. Cum laude. International PhD distinction.  
Advisor: Prof. Dr. Jesús Carretero Pérez
- 2014 – 2015 » **M.Sc. in Computer Science and Technology.** University Carlos III of Madrid, Spain.  
Thesis: *Enabling Data Locality in Multidimensional Scientific Applications with Many-Task Computing and MapReduce*.  
Advisor: Prof. Dr. Jesús Carretero Pérez
- 2012 – 2014 » **Bilingual B.Sc. in Computer Science and Engineering.** University Carlos III of Madrid, Spain.  
Thesis: *Adaptation, deployment and evaluation of a railway simulator in cloud environments*.  
Advisor: Dr. Alberto García Fernández
- 2009 – 2012 » **Joint B.Sc. in Computer Science and Mathematics.** Autonomous University of Madrid, Spain.
- 2007 – 2009 » **Science and Technology Baccalaureate.** Felipe Trigo High School, Spain.

## Academic Positions

- 10/2023 – ... » **Research Scientist.** French Institute for Research in Computer Science and Automation (INRIA), France. *Tenured position.*
- 01/2022 – 04/2023 » **Research Assistant Professor.** Department of Electrical Engineering and Computer Science, University of Tennessee-Knoxville, USA. *Fixed-term position.*
- 02/2020 – 12/2021 » **Postdoctoral Research Associate.** Department of Electrical Engineering and Computer Science, University of Tennessee-Knoxville, USA. *Fixed-term position.*
- 09/2015 – 07/2019 » **Graduate Research and Teaching Assistant.** Computer Science Department, University Carlos III of Madrid, Spain. *Fixed-term position.*
- 08/2017 – 12/2017 » **Visiting Graduate Research Aide.** Mathematics and Computer Science Division, Argonne National Laboratory, USA. *Fixed-term position.*
- 01/2016, 02/2017 » **Short-Term Visiting Scholar.** Université de Neuchâtel, Switzerland. *Fixed-term position.*
- 09/2014 – 08/2015 » **Graduate Research and Teaching Assistant.** Computer Science Department, University Carlos III of Madrid, Spain. *Part-time position.*
- 05/2013 – 08/2014 » **Undergraduate Research Assistant.** Computer Architecture and Technology Group (ARCOS), Computer Science Department, University Carlos III of Madrid, Spain. *Part-time position.*

## Merits and Achievements

- 2022 » Outstanding Early Career Contribution Award at *18th IEEE International Conference on e-Science*, Salt Lake City, USA.
- 2020 » Spanish Society for Computer Science (SCIE)–BBVA Foundation Young Researcher in Computer Science Award, Spain.
- 2017 » PPI-B-17 Research Stay Grant, Carlos III University of Madrid, Spain.  
» FPU15 Stay and Exchange Program, Spanish Ministry of Education, Spain.  
» Graduate Research Aide Appointment, Argonne National Laboratory, USA.  
» IC1305 NESUS COST Action Short-Term Scientific Mission Grant, European Cooperation in Science and Technology (COST), European Union.
- 2016 » International IBM PhD Fellowship Award.

- » FPU15 Research Training Program for Academic Staff Fellowship, Spanish Ministry of Education, Spain.
- » IC1305 NESUS COST Action Short-Term Scientific Mission Grant, European Cooperation in Science and Technology (COST), European Union.
- 2015 » PIF03-1516 Research Training Program Grant, Carlos III University of Madrid, Spain.
- 2014 » itSMF–Spain B.Sc. Thesis Award.
- » Departmental Scholarship for Graduate Studies, Department of Computer Science, Carlos III University of Madrid, Spain.
- 2013 » Collaboration Scholarship to Participate in Research Activities, Computer Architecture and Technology Group (ARCOS), Carlos III University of Madrid, Spain.
- 2009 » Excellence Grant for Outstanding Student Performance, Spanish Ministry of Education, Spain.

## Research Funding

### Current

- » *Data-Centric Workflow Interfaces for Hybrid Quantum and Classical Computing Environments (DaWinQCe)*  
 Source of support: National Research Agency (ANR), France.  
 Funding instrument: Junior Researcher Program (JCJC).  
 Role: **PI**.  
 Total amount: 294,192 EUR.  
 Period: 01 Oct 2025 - 28 Feb 2029.  
 Location: Inria Center at Rennes University, France.  
 Description: This project aims to research new data-centric approaches for workflow composition in hybrid quantum/classical infrastructures in the HPC context, addressing the need to combine different programming models in a single workflow in a domain-agnostic manner; and the challenging diversity of data representations, volumes, and processing rates that hinder interoperability in these hybrid workflows.
- » *Workflow Provenance and Its Application to Responsible and Trustworthy Artificial Intelligence*  
 Source of support: Region of Brittany, France.  
 Funding instrument: Doctoral Research Grants (ARED).  
 Role: **co-PI**, with Gabriel Antoniu (PI).  
 Total amount: 60,000 EUR.  
 Period: 01 Oct 2025 - 30 Sep 2027.  
 Location: Inria Center at Rennes University, France.  
 Description: This project aims to investigate methods to leverage workflow provenance metadata in support of responsible and trustworthy artificial intelligence. It will investigate mechanisms to formalize, capture, store, retrieve, inspect, analyse and visualise metadata in AI-powered workflows, and will explore the relationship between model provenance, metadata, and model and system behavior, aiming to decipher how architectural and algorithmic characteristics impact in the model's outcome and efficiency.
- » *Methods, Workflows, and Data Commons for Reducing Training Costs in Neural Architecture Search on High-Performance Computing Platforms (NSF #2223704)*.  
 Source of support: National Science Foundation (NSF), USA.  
 Funding instrument: Division of Computing and Communication Foundations Standard Grants.  
 Role: **Co-PI**, with Michela Taufer (PI) and Catherine Schumman (co-PI).  
 Total amount: 623,999 USD.  
 Period: 01 Oct 2022 - 30 Sep 2025.  
 Location: University of Tennessee-Knoxville, USA.  
 Description: This project addresses the urgent need to reduce the use of high-performance computing resources for the training of neural networks while ensuring explainable, reproducible, and nearly optimal neural networks. To this end, the team of researchers proposes a flexible fitness prediction method that uses parametric modeling to predict the future fitness of neural networks and allows the design of workflows supporting early termination of the training process.

### Completed

- » *Training Next-Generation Data Scientists in Non-Deterministic Scientific Data Generation*.  
 Source of support: South Big Data Hub, USA.  
 Funding instrument: Southern Engagement and Enrichment in Data Science.  
 Role: **PI**, with Sanjukta Bhowmick (co-PI).  
 Total amount: 49,998 USD.  
 Period: 01 Oct 2022 - 30 Sep 2023.  
 Location: University of Tennessee-Knoxville, USA.  
 Description: This project tackles the need to educate data scientists in the challenges of HPC scientific simulations with respect to data generation. In particular, this project develops and delivers training on how non-deterministic computations can affect the generation and analysis of scientific data.

» *Containerized Environments for Reproducibility and Traceability of Scientific Workflows.*

Source of support: Extreme Science and Engineering Discovery Environment (XSEDE CIS-200053), USA.

Funding instrument: Startup Allocation Award.

Role: **PI**, with Michela Taufer (co-PI).

Total amount: 49,075 USD.

Period: 21 Jan 2021 - 20 Jul 2023.

Location: University of Tennessee-Knoxville, USA.

Description: This project proposes a computational environment that automatically creates a workflow execution's record trail and invisibly attaches it to the workflow's output, enabling two crucial features for domain scientists: traceability of data and explainability of results. Our solution transforms existing container technology, includes tools for automatically annotating provenance metadata, and allows effective movement of data and metadata across the workflow execution.

## Research Publications

### Peer-Reviewed Journal Articles

- 1 Marquez, J., M. A. Cuendet, **S. Caino-Lores**, T. Estrada, E. Deelman, H. Weinstein and M. Taufer. 'Increasing the Efficiency of Ensemble Molecular Dynamics Simulations with Termination of Unproductive Trajectories Identified at Runtime'. In: *The Journal of Physical Chemistry A* 129.9 (2025), pp. 2317–2324. ISSN: 1089-5639. DOI: 10.1021/acs.jpca.4c05182.
- 2 Afle, C., P. R. Miles, **S. Caino-Lores**, C. D. Capano, I. Tews, K. Vahi, E. Deelman, M. Taufer and D. A. Brown. 'Reproducing the Results for Neutron Star Interior Composition Explorer Observation of PSR J0030 + 0451'. In: *Computing in Science & Engineering* 25.6 (2023), pp. 16–26. ISSN: 1558-366X. DOI: 10.1109/MCSE.2024.3381080.
- 3 Do, T. M. A., L. Pottier, R. Ferreira da Silva, **S. Caino-Lores**, M. Taufer and E. Deelman. 'Performance Assessment of Ensembles of in Situ Workflows under Resource Constraints'. In: *Concurrency and Computation: Practice and Experience* n/a.n/a (2022), e7111. ISSN: 1532-0634. DOI: 10.1002/cpe.7111.
- 4 Keller Rorabaugh, A., **S. Caino-Lores**, T. Johnston and M. Taufer. 'Building High-Throughput Neural Architecture Search Workflows via a Decoupled Fitness Prediction Engine'. In: *IEEE Transactions on Parallel and Distributed Systems* 33.11 (2022), pp. 2913–2926. ISSN: 1558-2183. DOI: 10.1109/TPDS.2022.3140681.
- 5 Patel, R., B. Roachell, **S. Caño-Lores**, R. Ketron, J. Leonard, N. Tan, K. Vahi, D. A. Brown, E. Deelman and M. Taufer. 'Reproducibility of the First Image of a Black Hole in the Galaxy M87 From the Event Horizon Telescope Collaboration'. In: *Computing in Science & Engineering* 24.5 (2022), pp. 42–52. ISSN: 1558-366X. DOI: 10.1109/MCSE.2023.3241105.
- 6 Herbein, S., T. Patki, D. H. Ahn, S. Mobo, C. Hathaway, **S. Caino-Lores**, J. Corbett, D. Domyancic, T. R. Scogland, B. R. de Supinski and M. Taufer. 'An Analytical Performance Model of Generalized Hierarchical Scheduling'. In: *The International Journal of High Performance Computing Applications* 36.3 (2022), pp. 289–306. ISSN: 1094-3420. DOI: 10.1177/10943420211051039.
- 7 Rorabaugh, A. K., **S. Caino-Lores**, T. Johnston and M. Taufer. 'High Frequency Accuracy and Loss Data of Random Neural Networks Trained on Image Datasets'. In: *Data in Brief* 40 (2022), p. 107780. ISSN: 2352-3409. DOI: 10.1016/j.dib.2021.107780.
- 8 Do, T. M. A., L. Pottier, **S. Caino-Lores**, R. Ferreira da Silva, M. A. Cuendet, H. Weinstein, T. Estrada, M. Taufer and E. Deelman. 'A Lightweight Method for Evaluating in Situ Workflow Efficiency'. In: *Journal of Computational Science* 48 (2021), p. 101259. ISSN: 1877-7503. DOI: 10.1016/j.jocs.2020.101259.
- 9 **Caino-Lores, S.**, A. Lapin, J. Carretero and P. Kropf. 'Applying Big Data Paradigms to a Large Scale Scientific Workflow: Lessons Learned and Future Directions'. In: *Future Generation Computer Systems* 110 (2020), pp. 440–452. ISSN: 0167-739X. DOI: 10.1016/j.future.2018.04.014.

- 10 **Caino-Lores, S.**, J. Carretero, B. Nicolae, O. Yildiz and T. Peterka. 'Toward High-Performance Computing and Big Data Analytics Convergence: The Case of Spark-DIY'. In: *IEEE Access* 7 (2019), pp. 156929–156955. issn: 2169-3536. doi: 10.1109/ACCESS.2019.2949836.
- 11 **Caíno-Lores, S.**, A. García, F. García-Carballeira and J. Carretero. 'Efficient Design Assessment in the Railway Electric Infrastructure Domain Using Cloud Computing'. In: *Integrated Computer-Aided Engineering* 24.1 (2017), pp. 57–72. issn: 1069-2509. doi: 10.3233/ICA-160532.
- 12 **Caino-Lores, S.** and J. Carretero. 'A Survey on Data-Centric and Data-Aware Techniques for Large Scale Infrastructures'. In: *International Journal of Computer and Information Engineering* (2016). doi: 10.5281/zenodo.1112258.
- 13 **Caino-Lores, S.**, A. G. Fernández, F. García-Carballeira and J. C. Pérez. 'A Cloudification Methodology for Multidimensional Analysis: Implementation and Application to a Railway Power Simulator'. In: *Simulation Modelling Practice and Theory* 55 (2015), pp. 46–62. issn: 1569-190X. doi: 10.1016/j.simpat.2015.04.002.

## Peer-Reviewed International Conference Proceedings

- 1 Souza, R., **S. Caino-Lores**, M. Coletti, T. J. Skluzacek, A. Costan, F. Suter, M. Mattoso and R. F. Da Silva. 'Workflow Provenance in the Computing Continuum for Responsible, Trustworthy, and Energy-Efficient AI'. In: *2024 IEEE 20th International Conference on E-Science (e-Science)*. 2024, pp. 1–7. doi: 10.1109/e-Science62913.2024.10678731.
- 2 Sahni, H., H. Carrillo-Cabada, E. Kots, **S. Caino-Lores**, J. Marquez, E. Deelman, M. Cuendet, H. Weinstein, M. Taufer and T. Estrada. 'Online Boosted Gaussian Learners for In-Situ Detection and Characterization of Protein Folding States in Molecular Dynamics Simulations'. In: *2023 IEEE 19th International Conference on E-Science (e-Science)*. 2023, pp. 1–10. doi: 10.1109/e-Science58273.2023.10254895.
- 3 Channing, G., R. Patel, P. Olaya, A. Rorabaugh, O. Miyashita, **S. Caino-Lores**, C. Schuman, F. Tama and M. Taufer. 'Composable Workflow for Accelerating Neural Architecture Search Using In Situ Analytics for Protein Classification'. In: *Proceedings of the 52nd International Conference on Parallel Processing*. ICPP '23. New York, NY, USA: Association for Computing Machinery, 2023, p. 1. isbn: 979-8-4007-0843-5. doi: 10.1145/3605573.3605636.
- 4 **Caino-Lores, S.**, M. Cuendet, J. Marquez, E. Kots, T. Estrada, E. Deelman, H. Weinstein and M. Taufer. 'Runtime Steering of Molecular Dynamics Simulations Through In Situ Analysis and Annotation of Collective Variables'. In: *Proceedings of the Platform for Advanced Scientific Computing Conference*. PASC '23. New York, NY, USA: Association for Computing Machinery, 2023, pp. 1–11. isbn: 979-8-4007-0190-0. doi: 10.1145/3592979.3593420.
- 5 Olaya, P., **S. Caino-Lores**, V. Lama, R. Patel, A. K. Rorabaugh, O. Miyashita, F. Tama and M. Taufer. 'Identifying Structural Properties of Proteins from X-ray Free Electron Laser Diffraction Patterns'. In: *2022 IEEE 18th International Conference on E-Science (e-Science)*. 2022, pp. 21–31. doi: 10.1109/eScience55777.2022.00017.
- 6 **Caino-Lores, S.**, J. Carretero, B. Nicolae, O. Yildiz and T. Peterka. 'Spark-DIY: A Framework for Interoperable Spark Operations with High Performance Block-Based Data Models'. In: *2018 IEEE/ACM 5th International Conference on Big Data Computing Applications and Technologies (BDCAT)*. 2018, pp. 1–10. doi: 10.1109/BDCAT.2018.00010.
- 7 **Caino-Lores, S.**, F. Isaila and J. Carretero. 'Data-Aware Support for Hybrid HPC and Big Data Applications'. In: *2017 17th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID)*. 2017, pp. 719–722. doi: 10.1109/CCGRID.2017.55.
- 8 **Caino-Lores, S.**, A. Lapin, P. Kropf and J. Carretero. 'Methodological Approach to Data-Centric Cloudification of Scientific Iterative Workflows'. In: *International Conference on Algorithms and Architectures for Parallel Processing*. Ed. by J. Carretero, J. Garcia-Blas, R. K. Ko, P. Mueller and K. Nakano. Lecture Notes in Computer

Science. Cham: Springer International Publishing, 2016, pp. 469–482. ISBN: 978-3-319-49583-5. DOI: 10.1007/978-3-319-49583-5\_36.

- 9 Carretero, J., **S. Caino-Lores**, F. Garcia-Carballeira and A. Garcia. ‘A Multi-Objective Simulator for Optimal Power Dimensioning on Electric Railways Using Cloud Computing’. In: *International Conference on Simulation and Modeling Methodologies, Technologies and Applications*. Vol. 2. SCITEPRESS, 2015, pp. 428–438. ISBN: 978-989-758-120-5. DOI: 10.5220/0005573404280438.

## Peer-Reviewed National Conference Proceedings

- 1 **Caino-Lores, S.**, A. Lapin, P. Kropf and J. Carretero. ‘Cloudification of a Legacy Hydrological Simulator Using Apache Spark’. In: *27th SARTECO Parallelism Meeting*. Salamanca, Spain, 2016.
- 2 **Caino-Lores, S.**, A. García, F. García-Carballeira and J. Carretero. ‘Breaking Data Dependences in Numerical Simulations Using Map-Reduce’. In: *25th SARTECO Parallelism Meeting*. Valladolid, Spain, 2014.

## Peer-Reviewed Workshop Papers

- 1 Wong, E., **S. Caino-Lores**, D. Chaves Claudino, E. Dumitrescu, T. Humble and S. Lopez Alarcon. ‘Rethinking Programming Paradigms in the QC-HPC Context’. In: Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States), 2024.
- 2 Bader, J., J. Belak, M. Bement, M. Berry, R. Carson, D. Cassol, S. Chan, J. Coleman, K. Day, A. Duque, K. Fagnan, J. Froula, S. Jha, D. S. Katz, P. Kica, V. Kindratenko, E. Kirton, R. Kothadia, D. Laney, F. Lehmann, U. Leser, S. Licholai, M. Malawski, M. Melara, E. Player, M. Rolchigo, S. Sarrafan, S.-J. Sul, A. Syed, L. Thamsen, M. Titov, M. Turilli, **S. Caino-Lores** and A. Mandal. ‘Novel Approaches Toward Scalable Composable Workflows in Hyper-Heterogeneous Computing Environments’. In: *Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*. SC-W '23. New York, NY, USA: Association for Computing Machinery, 2023, pp. 2097–2108. ISBN: 979-8-4007-0785-8. DOI: 10.1145/3624062.3626283.
- 3 Do, T. M. A., L. Pottier, R. F. da Silva, F. Suter, **S. Caíno-Lores**, M. Taufer and E. Deelman. ‘Co-Scheduling Ensembles of In Situ Workflows’. In: *2022 IEEE/ACM Workshop on Workflows in Support of Large-Scale Science (WORKS)*. 2022, pp. 43–51. DOI: 10.1109/WORKS56498.2022.00011.
- 4 Luettgau, J., **S. Caino-Lores**, K. Suarez, D. H. Ahn, S. Herbein and M. Taufer. ‘Reproducing and Extending Analytical Performance Models of Generalized Hierarchical Scheduling’. In: *2022 IEEE 18th International Conference on E-Science (e-Science)*. 2022, pp. 450–455. DOI: 10.1109/eScience55777.2022.00081.
- 5 Do, T. M. A., L. Pottier, R. Ferreira da Silva, **S. Caíno-Lores**, M. Taufer and E. Deelman. ‘Assessing Resource Provisioning and Allocation of Ensembles of In Situ Workflows’. In: *50th International Conference on Parallel Processing Workshop*. ICPP Workshops '21. New York, NY, USA: Association for Computing Machinery, 2021, pp. 1–10. ISBN: 978-1-4503-8441-4. DOI: 10.1145/3458744.3474051.
- 6 **Caino-Lores, S.**, A. Lapin, P. Kropf and J. Carretero. ‘Lessons Learned from Applying Big Data Paradigms to a Large Scale Scientific Workflow’. In: *11th Workshop on Workflows in Support of Large-Scale Science (WORKS 2016)*. Salt Lake City, Utah, USA, 2016.
- 7 **Caino-Lores, S.**, A. García, F. García-Carballeira and J. Carretero. ‘A Cloudification Methodology for Numerical Simulations’. In: *Euro-Par 2014: Parallel Processing Workshops*. Ed. by L. Lopes, J. Žilinskas, A. Costan, R. G. Cascella, G. Kecskemeti, E. Jeannot, M. Cannataro, L. Ricci, S. Benkner, S. Petit, V. Scarano, J. Gracia, S. Hunold, S. L. Scott, S. Lankes, C. Lengauer, J. Carretero, J. Breitbart and M. Alexander. Lecture Notes in Computer Science. Cham: Springer International Publishing, 2014, pp. 375–386. ISBN: 978-3-319-14313-2. DOI: 10.1007/978-3-319-14313-2\_32.

## Peer-Reviewed Posters and Short Papers



- 1 **Caino-Lores, S.**, M. Cuendet, T. Estrada, E. Deelman, H. Weinstein and M. Taufer. ‘High-Throughput in-Situ Workflows for Ensemble Molecular Dynamics’. In: *Proceedings of the 18th IEEE International Conference on E-Science (eScience)*. Salt Lake City, Utah, USA: IEEE Computer Society, 2022, pp. 1–1.
- 2 Patel, R., A. K. Rorabaugh, P. Olaya, **S. Caino-Lores**, G. Channing, C. Schuman, O. Miyashita, F. Tama and M. Taufer. ‘A Methodology to Generate Efficient Neural Networks for Classification of Scientific Datasets’. In: *2022 IEEE 18th International Conference on E-Science (e-Science)*. Salt Lake City, Utah, USA, 2022, pp. 389–390. DOI: 10.1109/eScience55777.2022.00052.
- 3 Yeom, J.-S., D. H. Ahn, I. Lumsden, J. Luettgau, **S. Caino-Lores** and M. Taufer. ‘Ubique: A New Model for Untangling Inter-task Data Dependence in Complex HPC Workflows’. In: *2022 IEEE 18th International Conference on E-Science (e-Science)*. Salt Lake City, Utah, USA, 2022, pp. 421–422. DOI: 10.1109/eScience55777.2022.00068.
- 4 Ketron, R., J. Leonard, B. Roachell, R. Patel, R. White, **S. Caíno-Lores**, N. Tan, P. Miles, K. Vahi, E. Deelman, D. Brown and M. Taufer. ‘A Case Study in Scientific Reproducibility from the Event Horizon Telescope (EHT)’. In: *2021 IEEE 17th International Conference on eScience (eScience)*. Innsbruck, Austria, 2021, pp. 249–250. DOI: 10.1109/eScience51609.2021.00045.
- 5 Olaya, P., M. R. Wyatt II, **S. Caino-Lores** and F. Tama. ‘XPSI: X-ray Free Electron Laser-based Protein Structure Identifier’. In: *Research Posters - International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*. 2020.

## Technical Reports

- 1 Ferreira da Silva, R. et al. *Workflows Community Summit 2024: Future Trends and Challenges in Scientific Workflows*. Tech. rep. Zenodo, 2024. DOI: 10.5281/zenodo.13844759.
- 2 Ferreira Da Silva, R. et al. *Workflows Community Summit 2022: A Roadmap Revolution*. Tech. rep. ORNL/TM-2023/2885. Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States), 2023. DOI: 10.2172/2006942.
- 3 da Silva, R. F., H. Casanova, K. Chard, T. Coleman, D. Laney, D. Ahn, S. Jha, D. Howell, S. Soiland-Reys, I. Altintas, D. Thain, R. Filgueira, Y. Babuji, R. M. Badia, B. Balis, **S. Caino-Lores**, S. Callaghan, F. Coppens, M. R. Crusoe, K. De, F. Di Natale, T. M. A. Do, B. Enders, T. Fahringer, A. Fouilloux, G. Fursin, A. Gaignard, A. Ganose, D. Garijo, S. Gesing, C. Goble, A. Hasan, S. Huber, D. S. Katz, U. Leser, D. Lowe, B. Ludaescher, K. Maheshwari, M. Malawski, R. Mayani, K. Mehta, A. Merzky, T. Munson, J. Ozik, L. Pottier, S. Ristov, M. Roozmeh, R. Souza, F. Suter, B. Tovar, M. Turilli, K. Vahi, A. Vidal-Torreira, W. Whitcup, M. Wilde, A. Williams, M. Wolf and J. Wozniak. *Workflows Community Summit: Advancing the State-of-the-art of Scientific Workflows Management Systems Research and Development*. Tech. rep. 2021. DOI: 10.5281/zenodo.4915801. arXiv: 2106.05177 [cs].
- 4 Carretero, J., F. Garcia-Carballeira, F. J. Garcia, F. Isaila, **S. Caino-Lores** and E. Serrano. *Report on Techniques for Data Management on Integrated HPC and Big Data Platforms*. Tech. rep. 2018.
- 5 **Caino-Lores, S.**, F. J. R. Duro, F. J. Garcia and J. Carretero. *Technical Report on Techniques to Expose and Exploit Data Locality*. Tech. rep. 2017.
- 6 **Caino-Lores, S.**, E. Serrano, A. Garcia, R. Sotomayor and L. M. Sanchez. *Report on Application Adaptation and Deployment*. Tech. rep. 2017.

## Preprints

- 1 Rorabaugh, A. K., **S. Caíno-Lores**, M. R. Wyatt II, T. Johnston and M. Taufer. *PEng4NN: An Accurate Performance Estimation Engine for Efficient Automated Neural Network Architecture Search*. 2021. DOI: 10.48550/arXiv.2101.04185. arXiv: 2101.04185 [cs].

## Invited Talks and Seminars

- 2025 » *Scientific Workflows-Foundations, Applications and Future Directions*; International Summer School on High-Performance Computing for Science, Industry, and Society; Naples, Italy. *Invited lecture*.
- » *Workflow Provenance Data Management and Analysis in the Computing Continuum*, Birds-of-a-Feather session "Provenance and Reproducibility for HPC and Distributed Environments" at the ISC High Performance Conference (ISC), Hamburg, Germany. *Invited talk*.
- 2024 » *Unified Data Abstractions for Scientific Workflow Composition in the Computing Continuum*, Minisymposium "Driving Scientific Workflows from the Data Plane" at the SIAM Conference on Parallel Processing for Scientific Computing (PP), Baltimore, USA. *Invited talk*.
- 2023 » *A Data-Centric Perspective on Scientific Workflows in the Computing Continuum*, Minisymposium "Data Management across the Computing Continuum" at the Platform for Advanced Scientific Computing (PASC), Davos, Switzerland. *Invited talk*.
- 2022 » *High performance Data Management and In-Situ Workflows*, 4th Workflows Community Summit, Virtual. *Invited lightning talk*.
- 2021 » *Convergence of High-Performance Computing and Big Data Analytics: Applications and Open Challenges*, Center for Operational Research at the Miguel Hernández University of Elche, Spain. *Invited talk*.
- 2020 » *Convergence of High-Performance Computing and Big Data Analytics: Applications and Open Challenges*, CyberColombia 3rd HPC Summer School: Bio & Data Science, Colombia. *Invited lecture*.
- 2017 » *An Architecture for Scaling Spark on HPC Systems*, Argonne National Laboratory, USA. *Seminar*.
- 2016 » *Foundations of Big Data in Official Statistics*, National Statistics Institute (INE), Spain. *Lecture series*.
- » *Data-Centric Cloudification of Scientific Applications with Many-Task Computing and Map-Reduce*, Université de Neuchâtel, Switzerland. *Seminar*.

## Projects

- 2023 – 2029 » *Data-oriented Software and Tools for the Exascale (ANR PEPR NumPEx Exa-DoST)*, National Research Agency (ANR), France. *Participant*.
- 2023 – 2030 » *Secure and efficient data storage and processing on cloud-based infrastructures (ANR PEPR CLOUD STEEL)*, National Research Agency (ANR), France. *Participant*.
- 2020 – 2023 » *In Situ Data Analytics for Next Generation Molecular Dynamics Workflows (NSF BIGDATA: IA: Collaborative Research: #1841758)*, National Science Foundation, USA. *Lead participant*.
- 2016 – 2019 » *Towards unification of HPC and Big Data paradigms (TIN2016-79637-P)*, Ministry of Economy and Competitiveness, Spain. *Participant*.
- 2016 – 2018 » *Multiple Access to eDelivery (MADE 2016-EU-IA-0063)*, European Commission, European Union. *Participant*.
- » *Integrating the e-Identification in European cloud platforms according to the eIDAS Regulation (eID@Cloud 2016-EU-IA-0064)*, European Commission, European Union. *Participant*.
- » *Refactoring Parallel Heterogeneous Resource-Aware Applications - a Software Engineering Approach (RePhrase)*, European Commission, European Union. *Participant*.
- 2014 – 2018 » *Network for Sustainable Ultrascale Computing (NESUS ICT COST Action IC1305)*, European Cooperation in Science and Technology (COST), European Union. *Participant*.
- 2013 – 2016 » *Reengineering and Enabling Performance And power of Applications (PPI-B REPARA)*. *Participant*.
- 2012 – 2016 » *Scalable data management techniques for high-performance computing (TIN2010-16497)*. *Participant*.
- 2010 – 2015 » *Application of IT to the innovation in power deployments in railway infrastructures (SIRTE-ADIF)*. *Participant*.

## Academic Services

### Panels in Funding Agencies

- 2020 – 2022 » Spanish State Agency for Research (AEI).

### Participation in Organization Committees

- 2023 – ... » *IEEE/ACM Workshop on Workflows in Support of Large-Scale Science (WORKS)*. *General co-chair*.
- 2026 » *International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)*. *Art of HPC chair*.
- 2025 » *ISC High Performance Conference (ISC)*. *Birds-of-a-Feather organizer: Scientific Computational Workflows in Hybrid Quantum-Classical Environments*.
- » *IEEE/ACM International Conference on Big Data Computing, Applications, and Technologies (BDCAT)*. *Workshops chair*.

- » IEEE/ACM International Conference on Utility and Cloud Computing (UCC). *Workshops chair.*
- » IEEE International Symposium on Cluster, Cloud, and Internet Computing (CCGRID). *Track chair: Software Systems and Platforms; Programming Models and Runtime Systems.*
- 2024 » International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). *Reproducibility Challenge co-chair.*
- » International European Conference on Parallel and Distributed Computing (EuroPar). *Workshops co-chair.*
- » Workflow Monitoring, Observability, and in situ Analytics (WOWMON). *Organizer.*
- 2023 » IEEE International Conference on e-Science (e-Science). *Tutorials chair.*
- 2022 » Workflows Community Summit. *Session co-chair.*
- 2019 – 2022 » International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). *Student Cluster Competition Reproducibility Challenge committee member.*
- 2021 » Workshop on Reproducible Workflows, Data Management, and Security (ReWorDS). *Organization committee member.*
- 2020 » Robust Science Virtual World Cafés Series. *Organization team member.*

## Journal Technical Review Board Memberships

- 2024 » IEEE Transactions on Services Computing.
- 2023 » ACM Computing Surveys.
- 2018 – 2023 » Concurrency and Computation: Practice and Experience.
- 2015 – 2022 » International Journal of High Performance Computing Applications.
- 2014 – 2022 » Journal of Supercomputing.
- 2019 – 2022 » SC Reproducibility Initiative Journal Special Issue in Transactions on Parallel and Distributed Systems.
- 2015 – 2018 » Scalable Computing: Practice and Experience.

## Technical Program Committee Memberships

- 2021 – ... » International Conference for High Performance Computing, Networking, Storage, and Analysis (SC).
- 2025 » Workshop on Workflows, Intelligent Scientific Data and Optimization for Automated Management (WISDOM).
- » Workshop on Research Infrastructures for Experimenting across the HPC-Cloud-Edge Continuum (ContinuumRI).
- » Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP).
- 2023, 2025 » IEEE International Parallel and Distributed Processing Symposium (IPDPS).
- 2024 » International Symposium on High-Performance Parallel and Distributed Computing (HPDC).
- » Latin America High Performance Computing Conference (CARLA).
- » Workshop on Workflows in Distributed Environments (WiDE).
- 2023 » International European Conference on Parallel and Distributed Computing (EuroPar).
- » International Workshop on Democratizing High-Performance Computing (D-HPC).
- 2021 – 2023 » IEEE International Conference on Cluster Computing (CLUSTER).
- » IEEE/ACM International Symposium on Cluster, Cloud and Internet Computing (CCGRID).
- 2020 – 2022 » Workshop on Workflows in Support of Large-Scale Science (WORKS).
- 2020 » International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD).
- 2016 – 2019 » International Workshop in Theoretical Approaches to Performance Evaluation, Modeling and Simulation (TAPEMS).
- 2016 – 2017 » IEEE International Conference on Cloud Computing Technology and Science (CLOUDCOM).
- 2016 » International Conference on Algorithms and Architectures for Parallel Processing (ICA3PP).
- 2015 – 2019 » Workshop on Clusters, Clouds and Grids for Life Sciences (CCGRID-Life).
- 2014 » Workshop on Techniques and Applications for Sustainable Ultrascale Computing Systems (TASUS).

## Teaching

- 2024 – ... » Processing Machine Learning Workloads at Scale (ISTIC University of Rennes, M.Sc. in Artificial Intelligence).
- 2023 – ... » Big Data Storage and Processing Infrastructures (ISTIC University of Rennes, M.Sc. in Cloud and Network Infrastructures).
- 2018 – 2019 » Operating Systems (UC3M, B.Sc. in Computer Engineering, 2nd year).
- 2015, 2018 » Computer Architecture (UC3M, B.Sc. in Computer Engineering, 3rd year).
- 2015 – 2017 » Distributed Systems (UC3M, B.Sc. in Computer Engineering, 3rd year).



- 2015, 2017 » Operating Systems Design (UC3M, B.Sc. in Computer Engineering, 3rd year).  
2015 – 2016 » Computer Structure (UC3M, B.Sc. in Computer Engineering, 2nd year).  
2014 » Software System Development (UC3M, B.Sc. in Computer Engineering, 4th year).

## Student Supervision and Evaluation

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- » Arthur Jacquard, PhD. candidate (Oct 2024 - present). *Thesis co-supervisor.*
- » Elias del Pozo, Visiting PhD candidate (Mar 2025 - present). *Supervisor.*
- » Vanessa Lama, MSc. candidate (Aug 2021 - Apr 2023). *Thesis committee member.*
- » Georgia Channing, Undergraduate Research Assistant (Oct 2021 - Apr 2023). *Co-supervisor.*
- » Ria Patel, Undergraduate Research Assistant (Jan 2021 - Apr 2023). *Co-supervisor.*
- » Brandon Roachell, Undergraduate Research Assistant (Jan 2021 - Sep 2022). *Co-supervisor.*
- » Lauren Proctor, Undergraduate Research Assistant (Aug 2022 - Jan 2023). *Co-supervisor.*
- » Maria Camila Roa, Graduate Research Assistant (Aug 2022 - Jan 2023). *Co-supervisor.*
- » Treece Burgess, Graduate Research Assistant (Aug 2021 - Dec 2021). *Co-supervisor.*
- » Jacob Leonard, Undergraduate Research Assistant (Jan 2021 - Dec 2021). *Co-supervisor.*
- » Ross Ketron, Undergraduate Research Assistant (Jan 2021 - Oct 2021). *Co-supervisor.*
- » Clark Hathaway, Undergraduate Research Assistant (Jun 2020 - Aug 2021). *Co-supervisor.*
- » Sebastian Mobo, Undergraduate Research Assistant (Jun 2020 - May 2021). *Co-supervisor.*
- » Maxwell Fleming, Visiting Undergraduate Research Assistant (May 2019 - Jul 2019). *Supervisor.*

## Student Awards and Distinctions

- 2020 » Clark Hathaway and Sebastian Mobo, 3rd place at the ACM Student Research Competition (UG) at SC20.  
» Clark Hathaway and Sebastian Mobo, finalists at the Smoky Mountain Data Challenge Competition.

## PhD Juries

- 2024 » Dante Sanchez-Gallegos, *New Techniques to Build and Manage Agnostic Workflows for the Processing of Digital Products*, University Carlos III of Madrid, Spain.

## Professional Affiliations

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- » ACM, Member
- » IEEE, Member