Savíns Puertas Martín, Ph.D.

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Employment History

01.02.2021 – now
Post-doctoral Researcher working on the project *High Performance Computing for Optimizing Intensity Modulated Radiation Therapy Schedules*. Dept. of Informatics, University of Almería.

01.10.2016 – 30.09.2020
Pre-doctoral Researcher. National Competitive Scholarship FPU (Formación de Profesorado Universitario (University Teacher Training)). Dept. of Informatics, University of Almería.

01.06.2016 – 30.09.2016
Research Labor Staff. Supercomputing-Algorithm Research Group, Dept of Informatics, University of Almería.

Education

2016 – 2020
PhD in Informatics, University of Almería, Spain.
Score: Cum laude (maximum score). International Mention.
Thesis title: *High Performance Computing for Optimization Problem Solving in Bioinformatics.*

2015 – 2017
Master in Informatics, University of Almería, Spain.
Average score: 9.79 out 10.
Final master project title: *Solving optimization problems in the pharmaceutical industry through evolutionary algorithms.*

2011 – 2015
Degree in Informatics, University of Almería, Spain.
Average score: 9.55 out 10.
Final degree project title: *a voice interaction system for handling mashup interfaces.*

Research Publications

Journal Articles

[1] **S. Puertas-Martín**, J. L. Redondo, M. R. Ferrández, H. Pérez-Sánchez, and P. M. Ortigosa, "MultiPharmDT: A Multi-Objective Decision Tool for Ligand-Based Virtual Screening Problems," *Informatica*, pp. 1–26, Dec. 2021, ISSN: 0868-4952. DOI: 10.15388/21-INFOR469. [Online]. Available: https://informatica.vu.lt/doi/10.15388/21-INFOR469.

[2] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Optimizing Electrostatic Similarity for Virtual Screening: A New Methodology," *Informatica*, pp. 1–19, Jul. 2020, ISSN: 0868-4952. DOI: 10.15388/20-INFOR424. [Online]. Available: https://informatica.vu.lt/doi/10.15388/20-INFOR424.

[3] **S. Puertas-Martín**, A. J. Banegas-Luna, M. Paredes-Ramos, J. L. Redondo, P. M. Ortigosa, O. O. Brovarets', and H. Pérez-Sánchez, "Is high performance computing a requirement for novel drug discovery and how will this impact academic efforts?" *Expert Opinion on Drug Discovery*, vol. 15, no. 9, pp. 981–986, 2020, ISSN: 1746045X. DOI: 10.1080/17460441.2020.1758664. [Online]. Available: https://doi.org/10.1080/17460441.2020.1758664.

[4] **S. Puertas-Martín**, J. L. Redondo, P. M. Ortigosa, and H. Pérez-Sánchez, "OptiPharm: An evolutionary algorithm to compare shape similarity," *Scientific Reports*, vol. 9, no. 1, p. 1398, Dec. 2019, ISSN: 2045-2322. DOI: 10.1038/s41598-018-37908-6. [Online]. Available: https://doi.org/10.1038/s41598-018-37908-6%20http://www.nature.com/articles/s41598-018-37908-6.

[5] A. J. Banegas-Luna, J. P. Cerón-Carrasco, **S. Puertas-Martín**, and H. Pérez-Sánchez, "BRUSELAS: HPC Generic and Customizable Software Architecture for 3D Ligand-Based Virtual Screening of Large Molecular Databases," *Journal of Chemical Information and Modeling*, vol. 59, no. 6, pp. 2805–2817, Jun. 2019, ISSN: 1549-9596. DOI: 10.1021/acs.jcim.9b00279. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.jcim.9b00279.

[6] M. R. Ferrández, **S. Puertas-Martín**, J. L. Redondo, B. Ivorra, A. M. Ramos, and P. M. Ortigosa, "High-performance computing for the optimization of high-pressure thermal treatments in food industry," *The Journal of Supercomputing*, vol. 75, no. 3, pp. 1187–1202, Mar. 2019, ISSN: 0920-8542. DOI: 10.1007/s11227-018-2351-4. [Online]. Available: http://link.springer.com/10.1007/s11227-018-2351-4.

International Conferences

[7] **S. Puertas-Martín**, J. J. Moreno, J. L. Redondo, P. M. Ortigosa, and E. M. Garzón, "Optimizing eud model parameters in radiotherapy planning," in *The 7th Int'l Conf on Health Informatics and Medical Systems*, American Council on Science and Education, Las Vegas, USA, Jul. 2021.

[8] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Optimization of molecular descriptors using memetic algorithms," in *18th Workshop on Advances in Continuous Optimization, EurOpt2021*, Ecole Nationale de l'Aviation Civile, Toulouse, France, Jul. 2021.

[9] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Maximizing the electrostatic similarity in drug discovery through evolutionary algorithms," in *8th International Work-Conference on Bioinformatics and Biomedical Engineering*, University of Granada, Granada, Spain, Sep. 2020.

[10] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Virtual screening in electrostatic potential using an evolutionary algorithm," in *Proceedings of META18: 7th International Conference on Metaheuristics and Nature Inspired Computing*, Université de Lille, Marrakech, Morocco, Oct. 2018, pp. 207–209.

[11] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Multi-objective evolutionary algorithm for evaluation of shape and electrostatic similarity," in *Proceedings of LeGO 2018 - Int. Workshop on Global Optimization. AIP Conference Proceedings*, Leiden University, vol. 1, Sep. 2018, pp. 1–4, ISBN: 9780735417984. DOI: 10.1063/1.5089986. [Online]. Available: http://aip.scitation.org/doi/abs/10.1063/1.5089986.

[12] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Optimizing electrostatic similarity using a global evolutionary algorithm," in *Proceedings of 6th EUROPT Workshop on Advances in Continuous Optimization*, University of Almería, Almería, Spain, Jul. 2018.

[13] **S. Puertas-Martín**, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Virtual screening in molecular shape by using an evolutionary algorithm," in *Proceedings OLA'2018 International Workshop on Optimization and Learning: Challenges and Applications*, Université de Lille, Alicante, Spain, Feb. 2018, pp. 63–64.

[14] M. R. Ferrández, **S. Puertas-Martín**, J. L. Redondo, B. Ivorra, R. A. M, and O. P. M, "High-performance computing for optimizing high-pressure thermal treatments in food processing," in *Proceedings of the 17th International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE 2017*, University of Cadiz, Alicante, Spain, Jul. 2017, pp. 862–869, ISBN: 978-84-617-8694-7.

[15] **S. Puertas-Martín**, M. R. Ferrández, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Enhancing molecular shape comparison by a parallel global evolutionary algorithm," in *Proceedings of the 17th International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE 2017*, University of Cadiz, Rota, Spain, Jul. 2017, pp. 1722–1728, ISBN: 978-84-617-8694-7.

[16] **S. Puertas-Martín**, H. den-Haan, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Enhancing molecular shape comparison by a global evolutionary algorithm," in *4th International Work-Conference on Bioinformatics and Biomedical Engineering*, University of Granada, Granada, Spain, 2016.

[17] **S. Puertas-Martín**, J. L. Redondo, H. den-Haan, H. Pérez-Sánchez, and P. M. Ortigosa, "Multi-objective based scoring function for ligand based virtual screening," in *Proceedings of the XIII Global Optimization Workshop*, University of Minho, Braga, Portugal, 2016, ISBN: 978-989-20-6764-3.

Education Conferences

[18] J. J. Moreno, **S. Puertas-Martín**, F. Orts, N. C. Cruz, J. L. Redondo, E. Garzón, and O. P. M., "On simulating an arm processor for teaching computer structure," in *12th annual International Conference of Education, Research and Innovation (ICERI 2019)*, Seville, Spain, Dec. 2019.

[19] F. Orts, N. C. Cruz, **S. Puertas-Martín**, M. Ruiz-Ferrández, J. J. Moreno, C. Medina-López, P. M. Ortigosa, V. Ruíz, L. Casado, J. M. Salmerón, J. L. Redondo, G. E. Garzón, G. Ortega, and R. Villegas, "Learning quantum computation through simple examples," in *11th International Conference of Education, Research and Innovation (ICERI 2019)*, Seville, Spain, Dec. 2019.

[20] N. C. Cruz, M. R. Ferrández, E. M. Garzón, J. M. García Salmerón, L. González Casado, V. González Ruiz, C. Medina-López, J. J. Moreno, G. Ortega López, P. M. Ortigosa, F. J. Orts, **S. Puertas-Martín**, J. L. Redondo, J. F. Sanjuan Estrada, and T. Santamaría López, "Simulación de un procesador arm para la enseñanza de estructura de computadores. poster," in *Jornadas de Innovación Docente y Experiencias Profesionales en la Universidad de Almería. Curso 2019-20*, Vicerrectorado de Enseñanzas Oficiales y Formación Continua y por la Coordinación de Gobierno e Interacción con la Sociedad y las Empresas de la Universidad de Almería, Almería, Spain, Sep. 2019.

[21] **S. Puertas-Martín**, J. J. Moreno, F. J. Orts, N. C. Cruz, J. L. Redondo, E. M. Garzón, and P. M. Ortigosa, "Simulación de un procesador arm para la enseñanza de estructura de computadores," in *Actas de las Jornadas SARTECO 2019*, Cáceres, Spain, Sep. 2019, pp. 235–240, ISBN: 978-84-09-12127-4.

[22] V. González-Ruiz, G. Ortega, E. Garzón, N. Calvo-Cruz, R. J. L., J. Salmerón, L. Casado, P. M. Ortigosa, C. Medina-López, J. J. Moreno, M. R. Ferrández, F. Orts, **S. Puertas-Martín**, and T. Santamaría-López, "Project-based learning: An experience," in *11th International Conference on Education and New Learning Technologies (EDULEARN 2019)*, Palma, Spain, Jul. 2019.

[23] N. C. Cruz, M. R. Ferrández, E. M. Garzón, J. M. García Salmerón, L. González Casado, V. González Ruiz, C. Medina-López, J. J. Moreno, G. Ortega López, P. M. Ortigosa, F. J. Orts, **S. Puertas-Martín**, J. L. Redondo, J. F. Sanjuan Estrada, T. Santamaría López, and R. Villegas, "Recursos para el aprendizaje de computación cuántica en el grado de ingeniería informática. poster," in *Jornadas de Innovación Docente y Experiencias Profesionales en la Universidad de Almería. Curso 2018-19*, Vicerrectorado de Enseñanzas Oficiales y Formación Continua y por la Coordinación de Gobierno e Interacción con la Sociedad y las Empresas de la Universidad de Almería, Almería, Spain, Sep. 2018.

National Conferences

[24] M. R. Ferrández, **S. Puertas-Martín**, J. L. Redondo, B. Ivorra, A. M. Ramos, and P. M. Ortigosa, "Computación de alto rendimiento para optimizar tratamientos térmicos de alta presión en la industria alimenticia," in *Avances en arquitectura y tecnología de computadores. Actas de las Jornadas SARTECO 2017*, Málaga, Spain, Sep. 2017, pp. 119–122, ISBN: 978-84-697-4835-0.

[25] **S. Puertas-Martín**, M. R. Ferrández, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Cribado virtual mediante un algoritmo evolutivo global paralelo," in *Actas de las Jornadas SARTECO 2017*, Cácares, Spain, Sep. 2017, pp. 177–179, ISBN: 978-84-697-4835-0.

[26] **S. Puertas-Martín**, M. R. Ferrández, J. L. Redondo, H. Pérez-Sánchez, and P. M. Ortigosa, "Algoritmo evolutivo global como herramienta de cribado virtual utilizando la forma molecular," in *III Jornadas Doctorales de la Universidad de Murcia*, Murcia, Spain, May 2017, pp. 236–240, ISBN: 978-84-608-9779-8.

Patents and Intellectual Properties

2018 **OPTIPHARM: an innovative evolutionary algorithm for virtual screening**, P. M. Ortigosa, J. L. Redondo, **S. Puertas-Martín** and H. Pérez-Sánchez.
University of Almería and Universidad Católica San Antonio de Murcia.
Application Number: 201899900606752. Register number: RTA-94-18.
Registration Date: 16/02/2018. Concession date: 09/08/2018.

Research Stays

Sep. 2018 – Dec. 2018 **Predoctoral Stay**, Centre for Logistics and Heuristic Optimization (CLHO), Kent Business School, University of Kent.
Canterbury, CT2 7NZ, United Kingdom.

Projects

01.01.2019 – 31.12.2021 **Soluciones de Alto Rendimiento para retos actuales de la computación científica (HPC4Sci) (High Performance Solutions for Today's Scientific Computing Challenges (HPC4Sci))**.
National project.
Principal Research: Pilar Martínez Ortigosa and Gracia Ester Martín Garzón.
Number of researchers: 31.
Code: RTI2018-095993-B-100.
Funding: Spanish Ministry of Science and Innovation. National Program for Scientific Research, Development and Technological Innovation.
Total amount: 186.461,00 Euros.

15.10.2019 – 14.10.2021 **Computación de Altas Prestaciones para Optimizar Planificaciones de Radioterapia de Intensidad Modulada (High Performance Computing to Optimize Intensity Modulated Radiation Therapy Planning)**.
Regional project.
Principal Research: Ester Martín Garzón and Juana López Redondo.
Number of researchers: 14.
Code: UAL18-TIC-A020-B.
Funding: Junta de Andalucia, Fondos Feder UAL.
Total amount: 76.800,00 Euros.

01.01.2019 – 31.12.2019 **Descubrimiento y optimización de compuestos bioactivos mediante técnicas avanzadas de química computacional (Discovery and optimization of bioactive compounds through advanced computational chemistry techniques)**.
Principal Research: Horacio Emilio Pérez Sánchez.
Number of researchers: 12.
Code: 20988/PI/18.
Funding: Fundación Séneca.
Total amount: 62.000 Euros.

Projects (continued)

01.01.2016 – 31.12.2019 **Metodologías computacionales para desafíos de la sociedad (Computational methodologies for societal challenges)**.
National project.
Principal Research: Leocadio González Casado and Pilar Martínez Ortigosa.
Number of researchers: 21.
Code: TIN2015-66680-C2-1-R.
Funding: Spanish Ministry of Economy and Competitiveness.
Total amount: 147.620 Euros.

Teaching Innovation Projects

2019 **Desarrollo de Recursos para motivar el estudio de la Ingeniería de Computadores (Development of Resources to motivate the study of Computer Engineering)**.
Convocatoria de Grupos Docentes para la Creación de Materiales Didácticos en la Universidad de Almería. Bienio 2018 y 2019 (Call for Teaching Groups for the Creation of Didactic Materials at the University of Almeria. Biennial 2018 and 2019).
Funding: University of Almería.
Total amount: 800 Euros.

2018 **Desarrollo de Recursos para motivar el estudio de la Ingeniería de Computadores (Development of Resources to motivate the study of Computer Engineering)**.
Convocatoria de Grupos Docentes para la Creación de Materiales Didácticos en la Universidad de Almería. Bienio 2018 y 2019 (Call for Teaching Groups for the Creation of Didactic Materials at the University of Almeria. Biennial 2018 and 2019).
Funding: University of Almería.
Total amount: 800 Euros.

Teaching

2019 – 2020 **Degree in Informatics**, University of Almería, Spain.
Network access technologies. Third year. 41 hours.
Peripherals and interfaces. Third year. 19 hours.
Quality Assurance System of the University of Almeria. Academic quality 4.72 out of 5.

2018 – 2019 **Degree in Informatics**, University of Almería, Spain.
Structure and computer technology. First year. 38 hours.
Network access technologies. Third year. 19 hours.
Quality Assurance System of the University of Almeria. Academic quality 4.65 out of 5.

2017 – 2018 **Degree in Informatics**, University of Almería, Spain.
Peripherals and interfaces. Third year. 19 hours.
Network access technologies. Third year. 19 hours.
Multi-processorss. Third year. 18 hours.
Structure and computer technology. First year. 2 hours.
Quality Assurance System of the University of Almeria. Academic quality 4.82 out of 5.

Final Project Supervisor

2020 – 2021 — **Degree in Informatics**, University of Almería, Spain.
Co-supervisor in a Final Degree Project: Artificial vision-based fall recognition (Reconocimiento de caídas con Visión Artificial)
Co-supervisor in a Final Degree Project: Gesture control monitoring (Monitorización mediante control gestual)

2019 – 2020 — **Degree in Informatics**, University of Almería, Spain.
Co-supervisor in a Final Degree Project: SMARTFRIDGE: Recognition of Actions in a Refrigerator and Decision Making in a Smart Enviroment.
Prize: Best final degree project.

Awards and Achievements

2021 — **Third prize in *Your PhD Thesis in Three Minutes* competition**.
Jornadas Sarteco 22-24 September.
`https://www.youtube.com/watch?v=ue9mnW8DX4k`

National Agency for Quality Assessment and Accreditation.
Accreditation of:

- Assistant Doctor Professor
- Professor Private University
- Hired Doctor Professor

2016 - 2020 — **FPU Scholarship**, Spanish Ministry of Education, Culture and Sport. The FPU scholarship provides financial support for awardees to complete an official PhD program and to carry out research and teaching activities, in any discipline, by signing a predoctoral contract. Code: FPU15/02912.

2018 — **Best final project award in Informatics Master**. EPS-FCCEE - University of Almería.

Best academic record award in Informatics Master. University of Almeria. Informatics Master.

2016 — **Collaboration grant with the Department of Informatics of the University of Almeria**, Spanish Ministry of Education, Culture and Sport.
Project Title: *Optimization of protein folding using HPC techniques.*

2015 — **Best final project award in Informatics Degree**. EPS-FCCEE - University of Almería.

Best academic record award in Informatics Degree. University of Almeria. Informatics Degree.

Skills

Languages — C, C++, JAVA, Python, LaTeX.

Parallel Programming Paradigms — MPI, PThreads.

Software applied to drug discovery — OpenEye's Software (ROCS, EON, VIDA, OMEGA), OpenEye's Toolkit, Pymol, Reflex3D, WEGA, OptiPharm.