Curriculum vitae
Alejandro Rodríguez García
05/03/25

Current Affiliation

Senior Researcher at the DMG of the University of Trieste

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Current research line

My research interest is at the border between physics and data analysis. In particular, I'm interested in how the analysis of data originated by simulations allows the inference of physical properties in an unsupervised way. This approach has proved useful in applications that range from fundamental physics and condensed matter problems to the understanding of complex biological systems. Additionally, these applications could not be carried out without the development of new tools of machine learning, that are of further interest in all fields of the science.

Research skills

- Data Mining, Machine Learning, Clustering, Density estimation.
- Critical behavior of physical systems.
- Large scale simulations of complex systems: Molecular Mechanics, Molecular Dynamics, Monte Carlo, Theoretical Chemistry, Computational Chemistry, QM/MM Enhanced Sampling techniques in molecular simulation, Metadynamics, Simulated Annealing, REMD, Umbrella Sampling.
- Bioinformatics: Protein sequence evolution, automatic classification of protein families, metagenomics.

Professional and Academy experience

- "Ludwig Boltzmann" Senior Postdoctoral Fellow at ICTP (International Centre for Theoretical Physics)
- AIRC (5xmille) Research Fellow at SISSA (International School for Advanced Studies
- FIRB Research Fellow at SISSA (International School for Advanced Studies)
- Research Assistant at the UPC (Universitat Politecnica de Catalunya)
- Phd in chemistry at the University of Barcelona with the thesis: "QM/MM investigation of the reaction mechanism of the NS3/NS4A hepatitis C protease with its main substrates" (April, 2012) under the supervision of Prof. Miguel Gonzalez.

Teaching experience

- Teacher at the Advanced School on Synchrotron Radiation Techniques and Nanotechnology: a Synergic Approach to Life Sciences and Medicine, Cape Town (2013).

- Lecturer at the Summer School on Machine Learning in the Molecular Sciences, Shanghai (2017).

- Teacher of Machine Learning at the MHPC - Master in High Performance Computing (courses from 2015-2016, 2016-2017, 2017-2018, 2018-2019 & 2019-2020).

- Teacher and co-organizer of the Workshop in statistical analysis of biomolecular simulations, Medellín 2018.

- Teacher at the School on Biophysical Approaches to Macromolecules and Cells: Integrated Tools for Life Sciences and Medicine. Arusha (Tanzania), Sept. 2019.

- Teacher and co-organizer at the "ICTP-SISSA-CECAM Workshop on Molecular Dynamics and its Applications to Biological Systems" (years 2020 & 2021).

- Teacher and Member of the Collegio Docenti at the phD program in Theoretical and Scientific Data Science, SISSA.

- Teacher of Numerical Methods at the ICTP Postgraduate Diploma (courses 2018-2019, 2019-2020, 2020-2021,2021-2022).

- Teacher of Introduzione al Machine Learning at the Artificial Intelligence and Data Analytics bachelor's degree (Course 2022-2023).

- Teacher of Unsupervised Machine Learning at the Data Science & Scientific Computing Master's degree (Course 2022-2023).

Scientific Publications

An updated list can be found at: https://scholar.google.com/citations?user=zUOi5sQAAAAJ&hl=es

Invited Talks

XXIII meeting of the *Xarxa de Química Teòrica i Computacional* Barcelona (Spain), Universitat Pompeu Fabra, July 2007

Proteins Physics: Structure, Dynamics and Function, Bressanone (Italy), February 2014

Internal talks at Intelligent Pharma, Barcelona (Spain), November 2014

Free-Energy Calculations. A Mathematical Perspective, Oaxaca (Mexico), July, 2015

Machine Learning in the Molecular Sciences, Shanghai (China), June, 2017

CECAM Workshop "Emerging Technologies in Scientific Data Visualisation", Pisa (Italy), April, 2018

Workshop in statistical analysis of biomolecular simulations, Medellín (Colombia), May, 2018

CECAM Workshop "Learning the Collective Variables of Biomolecular Processes", INRIA Paris, July, 2019

BAYES COMP, University of Florida (USA), Jan,2020
Summer School on Molecular Dynamics and Related Methods in Biological Applications, Arusha (Tanzania) November 2020.

The Biophysical Chemistry School (Tanzania) Sept. 2021.

Mentoring

Francesca Rizzato. Co-supervisor of the phD thesis with the title: Towards a deeper understanding of protein sequence evolution (2016).

Adu Offei-danso. Co-supervisor of the phD thesis with the title: Unsupervised Learning of the Structure and Dynamics of Liquid Water (2022).

Edward Donkor. Co-supervisor of the phD thesis with the title: Structural Characterization of Water in Different Thermodynamic Conditions Through Unsupervised Learning (2024).