Antonio Iorio

Academic Curriculum Vitae

Education and Research Experience

2024- **Post-Doc,** *School of Life Sciences - University of Dundee*, Dundee (UK).
Supervisor: Prof. Tomoyuki Tanaka and Prof. Rastko Sknepnek.

2021-2023 **Post-Doc,** *Laboratoire de Biochimie Théorique (LBT IBPC - CNRS)*, Paris (FR).
Supervisor: Dr. Fabio Sterpone.

2019-2021 **Post-Doc,** *Laboratoire de Biochimie Théorique (LBT IBPC - CNRS)*, Paris (FR).
Supervisor: Dr. Fabio Sterpone.

2019 **Ph.D. in Physics,** *Università degli Studi Roma Tre*, Rome (IT).
Thesis: *Slow Dynamics in Supercooled Aqueous Solutions for Cryopreservation.*
Supervisor: Prof. Paola Gallo.

2015 **Master's Degree in Physics,** *Università "La Sapienza"*, Rome (IT).
Thesis: *Random walks in random environment in infinite volume and infinitely repeated volume.*
Supervisor: Prof. Enzo Marinari.

2012 **Bachelor's Degree in Physics,** *Università "Sapienza"*, Rome (IT).
Thesis: *Simulations of the Ising model with Monte Carlo methods.*
Supervisor: Prof. Federico Ricci-Tersenghi.

Experience

Participation at conferences

2025 **Opening Conference for Mathematical Challenges in Brain Mechanics**, Oslo (NO).
Invited talk.

2025 **Supa Annual Gathering**, Dundee (UK).
Poster contribution.

2025 **Physics of Life 2025**, Harrogate (UK).
Poster contribution.

2025 **Scottish Soft Matter Meeting**, Edinburgh (UK).

2023 **FédCUP Young researchers meeting**, Paris (FR).
Oral contribution - Prize for best talk.

2023 **5th Manchester Multiscale Conference**, Manchester (UK).
Poster contribution.

2022 **Molecular Simulation 2022: Present, Past and Future**, Erice (IT).
Poster contribution.

2019 **Roma Tre Congress on Water under Extreme Conditions 2019**, Rome (IT).
Oral contribution.

2018 **1st Course of the International School of Water and Water System**, Erice (IT).
Poster and oral contribution.

2017 **8th International Discussion Meeting on Relaxations in Complex Systems**, Wisła (PL).
Poster contribution.

2017 **Roma Tre Congress on Water under Extreme Conditions 2017**, Rome (IT).
Poster contribution.

2017 **Frontiers in Water Biophysics 2017**, Erice (IT).
Poster contribution.

Schools

2025 **CompSysBio2025 - Advanced Lecture Course on Computational Systems Biology**, Aussois (FR).

2023 **CFD parschool - Summer School on Computational Fluid Dynamics & SuperComputing 2023**, Gran Sasso Science Institute, L'Aquila (IT).

2018 **1st Course of the International School of Water and Water System**, Erice (IT).

2017 **25th Summer School on Parallel Computing**, CINECA-SCAI, Rome (IT).

2016 **CCP5 Methods in Molecular Simulation Summer School**, Lancaster University, Lancaster (UK).

Vocational and Mentoring

2025 **Teaching**
Lectures for the course "Advanced Statistical Physics", University of Dundee, Dundee (UK).

2025 **Teaching**
"Physics (Summer School)", University of Dundee, Dundee (UK).

2024 **Teaching**
Lectures on mathematical foundations for machine learning for the course "PH51001: Computational Physics II", University of Dundee, Dundee (UK).

2024 **Teaching**
Lecture on multi-scale simulations for the "Label de Chimie Théorique 2024", Paris (FR).

2021 **Mentoring of an Erasmus student**
Molecular Dynamics simulations and study of large prefibrillar amyloid aggregate.

2017-2019 **Teaching Assistant** *Università degli Studi Roma Tre*, Rome (IT).
Teaching Assistant for the course "Fisica della Materia Condensata" (Condensed Matter Physics).

2017-2018 **Academic Tutor** *Università degli Studi Roma Tre*, Rome (IT).
Academic Tutor for the course FISICA I - FS210 (Mechanics and Thermodynamics).

2017, 2019 **Local Organizing Committee**
Local Organizing Committee "Roma Tre Congress on Water under Extreme Conditions", Rome (IT).

Publications

Papers

1. B. Caviglia, **A. Iorio**, Š. Timr, S. Melchionna, P. Derreumaux, F. Sterpone, *Hydrodynamic impact on the dynamics and shear of crowded cytoplasmic proteins solutions*, In preparation.

2. **A. Iorio**, S. Melchionna, P. Derreumaux, F. Sterpone, *Fluid flow and amyloid transport and aggregation in the brain interstitial space*, PNAS Nexus **4**, 1 (2024).
3. **A. Iorio**, L. Perin, P. Gallo, *Structure and slow dynamics of protein hydration water with cryopreserving DMSO and trehalose upon cooling*, J. Chem. Phys. **160**, 24 (2024).
4. L. E. Coronas, V. Thong, **A. Iorio**, M. Feig, L. J. Lapidus, F. Sterpone, *Shear effects on the structure and stabilization of biomolecular condensates: coupling residue-based models with an external fluid field*, J. Chem. Phys., **160**, 21 (2024).
5. **A. Iorio**, S. Melchionna, P. Derreumaux, F. Sterpone, *Dynamics and Structures of Amyloid Aggregates Under Fluid Flows*, J. Phys. Chem. Lett. **15**, 7 (2024).
6. Q. Bertrand, S. Coquille, **A. Iorio**, F. Sterpone, D. Madern, *Biochemical, structural and dynamical characterizations of the lactate dehydrogenase from Selenomonas ruminantium provide information about an intermediate evolutionary step prior to complete allosteric regulation acquisition in the super family of lactate and malate dehydrogenases*, J. Struct. Biol. **215**, 4 (2023).
7. **A. Iorio**, Š. Timr, L. Chiodo, P. Derreumaux, F. Sterpone, *Evolution of Large $A\beta_{16-22}$ Aggregates at Atomic Details and Potential of Mean force Associated to Peptide Unbinding and Fragmentation Events*, Proteins **91**, 8 (2023).
8. **A. Iorio**, C. Brochier-Armanet, C. Mas, F. Sterpone, D. Madern, *Protein Conformational Space at the Edge of Allostery: Turning a Nonallosteric Malate Dehydrogenase into an "Allosterized" Enzyme Using Evolution-Guided Punctual Mutations*, Mol. Biol. Evol. **39**, 9 (2022).
9. **A. Iorio**, J. Roche, S. Engilberge, N. Coquelle, E. Girard, F. Sterpone, D. Madern, *Biochemical, structural and dynamical studies reveal strong differences in the thermal-dependent allosteric behaviour of two extremophilic lactate dehydrogenates*, J. Struct. Biol. **213**, 3 (2021).
10. **A. Iorio**, M. Minozzi, L. Lupi, G. Camisasca, P. Gallo, *Slow dynamics of supercooled trehalose hydration water in comparison with bulk water*, Atti Accad. Pelorit. Pericol. Cl. Sci. Fis. Mat. Nat. **98**, A8 (2020).
11. **A. Iorio**, M. Minozzi, G. Camisasca, M. Rovere and P. Gallo, *Slow dynamics of supercooled hydration water in contact with lysozyme: examining the cage effect at different length scales*, Phil. Mag. **100**, 20 (2020).
12. **A. Iorio**, G. Camisasca and P. Gallo, *Glassy dynamics of water at interface with biomolecules: a Mode Coupling Theory test*, Sci. China-Phys. Mech. Astron. **62**, 107011 (2019).
13. **A. Iorio**, G. Camisasca, M. Rovere and P. Gallo, *Characterization of hydration water in supercooled water-trehalose solutions: the role of the hydrogen bonds network*, J. Chem. Phys. **151**, 4 (2019).
14. **A. Iorio**, G. Camisasca and P. Gallo, *Slow dynamics of hydration water and the trehalose dynamical transition*, J. Mol. Liq., **282**, 617 (2019).
15. G. Camisasca, **A. Iorio**, M. De Marzio and P. Gallo, *Structure and slow dynamics of protein hydration water* , J. Mol. Liq. **268**, 903 (2018).
16. D. S. Dean, **A. Iorio**, E. Marinari and G. Oshanin, *Sample-to-sample fluctuations of power spectrum of a random motion in a periodic Sinai model*, Phys. Rev. E **94**, 032131 (2016).

Book chapters

1. G. Camisasca, **A. Iorio**, L. Tenuzzo, P. Gallo, *Slow Dynamics of Biological Water*, In: Bulavin, L., Lebovka, N. (eds) Soft Matter Systems for Biomedical Applications. Springer Proceedings in Physics, vol 266 (2022).

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