

PERSONAL INFORMATION **Stefano Maestri**

## EDUCATION AND TRAINING

**2020 Double PhD in Computer Science and Theoretical Physics**

- Awarded by – International School of Advanced Studies, University of Camerino, Italy  
– Ecole Doctorale « Physique et Sciences de la Matière » (ED 352), Aix-Marseille Université, France
- Final grade Brilliant
- Thesis title Process-based Modelling of RNA and Protein Interactions: A Formal Approach (Modelling the effects of long-range forces in biological systems to better understand the global behaviour of molecular interactions)

**2019 Training course for teaching (PF24)**

- 24 CFU in anthropo-psycho-pedagogical disciplines and in teaching methodologies and technologies
- University of Camerino, Camerino, Italy

**2016 MSc degree in Computer Science (Curriculum: Systems Biology)**

- University of Camerino, Camerino, Italy
- Final grade 110/110 cum laude
- Subjects covered Advanced English, Cell Biology and Cellular Biotechnology, Chemistry, Complex System Design, Distributed Calculus and Coordination, E-health and Telemedicine, Genomics and Proteomics, Molecular Biology, Service-oriented Architecture, Theory of Complexity
- Thesis title A Formal Approach to the Study of Pathological Interactions in Protein Folding

**2009 Laurea di Primo Livello in Informatica**

- (Bachelor's degree in Computer Science)
- University of Camerino, Camerino, Italy
- Final grade 110/110 cum laude
- Thesis title Modellizzazione Funzionale della Membrana delle Cellule Cardiache (Functional Modelling of the Cardiac Cell Membrane)

**Seasonal Schools:**

- 2019** Algorithms in Structural Bioinformatics (AlgoSB) - Mathematical and computational methods for structured RiboNucleic Acids.  
CIRM - Centre International de Rencontres Mathématiques, Marseilles, France
- 2018** 5th International Synthetic & Systems Biology Summer School (SSBSS)  
Certosa di Pontignano, Siena, Italy

## RESEARCH AND TEACHING

## Summary of the research activity

My research activity focuses on modelling and simulating the behaviour of biological macromolecules, from the steps that lead them to reach their three-dimensional conformations to the way they interact with one another.

I exploited algebraic modelling approaches to formally define the local interactions performed by nucleotides in RNA molecules and by amino acids in the polypeptide sequence of proteins [1]. These methods allowed me to study the collective properties that characterise the expression of a fully functional macromolecule, bringing out congruences and dissimilarities, which I was consequently able to trace back to genetic pathologies (such as sickle cell anaemia) [2,3]. I also investigated, through agent-based models, the global behaviour of molecular long-distance electrodynamic interactions in metabolic pathways [4]. The resulting multiagent simulations gave me a new perspective on the effects of long-range forces on the efficiency of the glycolytic process. Furthermore, the generated agents' interaction matrix lent itself to be filtered through topological data analysis, allowing me to explore the role of three-body molecular interactions in biochemical reactions [5]. Based on these experiences, I contributed to develop a prototypical computational framework aimed at designing immunotherapy treatments for Renal Cell Carcinoma [6].

The core idea of my work is to show how algebraic and agent-based modelling approaches are highly suitable for uncovering complex phenomena in biological systems and supporting *in-silico* studies of tumours and genetic diseases.

## Publications

## Journal articles

- 1 Maestri, S., Merelli, E., 2019. Process calculi may reveal the equivalence lying at the heart of RNA and proteins. *Scientific Reports* 9, 559. <https://doi.org/10.1038/s41598-018-36965-1>
- 2 Maestri, S., Merelli, E., 2020. Algebraic Characterisation of Non-Coding RNA, in: Cazzaniga, P., Besozzi, D., Merelli, I., Manzoni, L. (Eds.), *Computational Intelligence Methods for Bioinformatics and Biostatistics*. Springer International Publishing, Cham, pp. 145–158. [https://doi.org/10.1007/978-3-030-63061-4\\_14](https://doi.org/10.1007/978-3-030-63061-4_14)
- 3 Maestri, S., Merelli, E., 2021. Algebraic lens for gene expression to shed light on protein misfolding. *BMC Bioinform.* (submitted).
- 4 Maestri, S., Merelli, E., Pettini, M., 2021. Agent-based Models for Detecting the Driving Forces of Biomolecular Interactions. *Scientific Reports* (under revision). PREPRINT (Version 1) available at Research Square: <https://doi.org/10.21203/rs.3.rs-911183/v1>
- 5 Piangerelli, M., Maestri, S., Merelli, E., 2020. Visualising 2-Simplex formation in metabolic reactions. *J. Mol. Graph. Model.* 97, 107576. <https://doi.org/10.1016/j.jmgm.2020.107576>
- 6 Belenchia, M., Rocchetti, G., Maestri, S., Cimadamore, A., Montironi, R., Santoni, M., Merelli, E., 2021. Agent-Based Learning Model for the Obesity Paradox in RCC. *Front. Bioeng. Biotechnol.* 9, 642760. <https://doi.org/10.3389/fbioe.2021.642760>
- 7 Maestri, S., Merelli, E., 2021. Automaton of molecular perceptions in biochemical reactions. *Theor. Comput. Sci.* (submitted). PREPRINT (Version 1) available at arXiv: <https://arxiv.org/abs/2111.11760v1>

## Proceedings

- 8 Maestri S., Merelli E., 2021. Environment perception in biochemical reactions. CIBB 2021: 17th International Conference on Computational Intelligence Methods for Bioinformatics and Biostatistics - Conference Proceedings. Online, 15-17 November 2021
- 9 Maestri S., Piangerelli M., Merelli E., 2020. 2-simplex modelling of interaction-as-perception in metabolic reactions. HSB 2020: 7th International Workshop on Hybrid Systems Biology - Conference Proceedings. Vienna, Austria, 4-5 September 2020
- 10 Maestri S., Merelli E., Pettini M., 2018. Multiagent Simulation of Long-Distance Electrodynamic Interactions among Biomolecules. NETTAB / BBCC 2019 Meeting, Fisciano Campus, University of Salerno, 11-13 November 2019
- 11 Maestri S., Merelli E., Pettini M., 2018. Process-based modelling towards the simulation of long-distance electrodynamic interactions of biomolecules. In: *Book of Abstracts of the 6th Scientific Day of School of Science and Technology*. p. 28, Università degli Studi di Camerino, Camerino, 28 September 2018

## Developed software

- OrionV2** Agent-based spatial simulator of metabolic pathways I developed in Java starting from a prototypical project. The software has the capability of reproducing the collective properties and behaviour of a system of biochemical reactions; it involves thousands of molecules, each represented as an agent. The simulations exploit agent perception to generate the effect of short- and long-range forces on local molecular interactions.
- OncoAgent** Multiagent simulator of the tumour microenvironment, designed to study kidney cancer. I contributed with my multidisciplinary background and my experience on multiagent systems to refine and validate the software.

## Research projects

- 2016 - 2020** EU FET Proactive *Topology Driven Methods for Complex Systems* (TOPDRIM) ([www.topdrim.eu](http://www.topdrim.eu)), number FP7-ICT- 318121

## Collaborations

- 2016 - 2021** Centre de Physique Théorique (CPT), Unité Mixte de Recherche (UMR 7332) multi-tutelles : CNRS, Aix-Marseille-Université et Université de Toulon
- modelling and simulating long-distances electrodynamic interactions among biomolecules
- 2018** School of Biosciences and Veterinary Medicine, University of Camerino; Department of Experimental and Clinical Medicine - Section Neuroscience and Cell Biology, Università Politecnica delle Marche
- construction of an *automaton* in which the miRNA concentration is used as a marker of the presence, in neurons, of alterations at the basis of sleep disorders
  - identification of some of the causes of sleep disorders in the relation between miRNA secondary and tertiary structures and in the way this molecule interacts with DNA and mRNA

## Organisational activities

- 2019** Co-organiser of the special session “Algebraic and Computational Methods for the Study of RNA Behaviour” at CIBB 2019, 16th International Conference on Computational Intelligence methods for Bioinformatics and Biostatistics, Bergamo, 4-6 September 2019
- 2018** Project drafting:
- LODE - The Language Of DrEams: relationship between sleep mentation, neurophysiology and clinical features of neurological disorders (PRIN - Progetti di Ricerca di Interesse Nazionale)
  - BELL - BiomolEcuLes computing Life (FAR - Fondo di Ateneo per la ricerca)

## Peer reviews

- 2021** Contribution to a peer review for CIBB 2021
- 2018** Contribution to a peer review for the NACO (Natural Computing) Journal  
Contribution to a peer review for the Bulletin of Mathematical Biology

## Teaching

- 2020** “Cultore della materia” for the disciplines of the S.S.D. INF/01

## Dissemination

- 2018 Process-based Modelling of RNA and Protein Folding: A Formal Approach, JSED - Journées Scientifiques de l'Ecole Doctorale 352, AMU (Aix-Marseille University), Marseilles (France), 28 - 29 May 2018

### WORK EXPERIENCE

#### Dec. 2011 – Dec. 2014 **Computer technician and staff trainer**

KTM STUDIO, Milan, Italy

- CMS (Content Management System) installation and administration
- network infrastructures installation and maintenance
- hw/sw assistance

#### Dec. 2008 – Sept. 2009 **Internship at the University of Camerino**

School of Science and Technology, Computer Science Division, Camerino, Italy

- collaboration on a systems biology project: studying a possible application of UML (Unified Modeling Language) in modelling the membrane of the cardiac muscle cells
- training for my bachelor's degree thesis

### PERSONAL SKILLS

Mother tongue Italian

#### Other languages

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	B2	B2	B2
	<ul style="list-style-type: none"> <li>– Trinity College London (B1)</li> <li>– Cambridge English: Preliminary (B1)</li> <li>– English Exam for the Level B2 - UNICAM</li> </ul>				
French	A2	A2	A1	A1	A1

Levels: A1 and A2: Basic user – B1 and B2: Independent user – C1 and C2: Proficient user  
[Common European Framework of Reference for Languages](#)

**Communication skills** Good written and verbal communication skills gained through my experience as a staff trainer and during my university studies

#### Digital competences

SELF-ASSESSMENT				
Information Processing	Communication	Content creation	Safety	Problem solving
Proficient user	Proficient user	Proficient user	Proficient user	Proficient user

[Digital competences - Self-assessment grid](#)

- Computer skills**
- strong modelling skills using UML (Unified Modeling Language) and process algebras
  - strong programming skills in Java
  - good command of LaTeX
  - competent with Microsoft Office, LibreOffice and Apple iWork suites
  - competent with WordPress
  - experience with HTML/CSS
  - basic skills in photo editing (Adobe Photoshop, GIMP) acquired as an amateur photographer

**Other skills** I studied piano and guitar and practiced martial arts (judo and jujutsu)