

Europass Curriculum Vitae



Personal information

Surname(s) / First name(s)

Carlo Guardiani

Current Research Organization

Sapienza University, Rome, Department of Mechanical and Aerospace Engineering

Work experience

Date	From 01-02-2024 to present
Position held	Research Fellow (Assegnista di Ricerca)
Project name	PRIN 2022 PNRR v-EV Prot. P2022EKHKL, CUP B53D23027530001: <i>Characterization of mesoscale properties of extracellular vesicles via molecular dynamics simulations</i>
Employer	Department of Mechanical and Aerospace Engineering, Sapienza University, Rome, Italy
Main Activities	Molecular Dynamics simulations of biological membranes; supervision of PhD and Master students; congress organization; design and co-management of Tier0 projects
Date	From 01-02-2021 to 31-01-2024
Position held	Research Associate (Ricercatore a tempo determinato di tipo A)
Project name	ERC Project: <i>Atomistic simulations of hydrophobic gating in biological ion channels</i>
Employer	Department of Mechanical and Aerospace Engineering, Sapienza University, Rome, Italy
Main Activities	Molecular Dynamics simulations of ion channels and curvature sensing peptides; supervision of PhD and Master students; congress organization; design and co-management of Tier0 projects
Date	From 01-06-2019 to 31-01-2021
Position held	Research Fellow (Assegnista di Ricerca)
Project name	ERC Project: <i>Molecular dynamics simulation of hydrophobic gating in biological ion channels</i>
Employer	Department of Mechanical and Aerospace Engineering, Sapienza University, Rome, Italy
Main Activities	Molecular Dynamics simulations of ion channels; supervision of PhD and Master students; congress organization; design and co-management of Tier0 projects
Date	From 01-03-2018 to 31-05-2019
Position held	Senior Research Associate in Ion Channel Physics
Project name	Liverhulme Project: <i>Stochastic Dynamics of the KcsA channel</i>
Employer	Department of Physics, Lancaster University, Lancaster, U.K.
Main Activities	Molecular Dynamics simulations of ion channels; outreach activities
Date	From 01-09-2015 to 28-02-2018
Position held	Post-Doctoral position

Project name	EPSRC Project: <i>Ionic Coulomb blockade oscillations and the physical origins of permeation, selectivity, and their mutation transformations in biological ion channels.</i>
Employer	School of Engineering, Warwick University, Coventry, U.K.
Main Activities	Molecular Dynamics simulations of ion channels
Date	From 01-01-2014 to 31-08-2015
Position held	Post-Doctoral position
Project name	<i>Rational in-silico design of new antibiotics to contrast multi-resistance.</i>
Employer	Italian National Research Council (CNR-IOM), Cagliari, Italy
Main Activities	Molecular Dynamics simulations of ion channels
Date	From 01-01-2013 to 31-12-2013
Position held	Post-Doctoral position
Project name	<i>Chaotic and statistical properties of classical systems.</i>
Employer	Department of Physics, Sapienza University, Rome, Italy
Main Activities	Molecular Dynamics simulations of DNA/transcription factor interaction
Date	From 01-01-2013 to 31-12-2012
Position held	Research associate (Ricercatore a Tempo Determinato)
Project name	<i>In silico assessment of peptides with potential pharmaceutical properties for Multiple Sclerosis</i>
Employer	Department of Chemistry, University of Florence, Florence, Italy
Main Activities	Molecular Dynamics simulations of peptides and small organic molecules with potential applications in treatment and diagnosis of auto-immune diseases
Date	From 01-05-2010 to 31-12-2010
Position held	Research Scholar
Employer	Department of Chemistry, Georgia State University, Atlanta, U.S.A.
Main Activities	Molecular Dynamics simulations of sliding clamp proteins
Date	From 01-11-2009 to 31-12-2009
Position held	Post-Doctoral position
Employer	Interdepartmental Center for the Study of Complex Dynamics (CSDC), University of Florence, Italy
Main Activities	Preparation of a review paper on coarse-grained protein models
Date	From 01-09-2006 to 31-08-2009
Position held	Post-doctoral position
Project name	<i>Study of the role of sugars in the etiology of multiple sclerosis</i>
Employer	Interdepartmental Center for the Study of Complex Dynamics (CSDC), University of Florence, Italy
Main Activities	Molecular Dynamics simulations of antigen/antibody interactions in Multiple Sclerosis
Date	From 01-11-2004 to 31-07-2006
Position held	Post-doctoral position
Project name	<i>Mesosopic Description of Protein Folding</i>

Employer Interdepartmental Center for the Study of Complex Dynamics (CSDC), University of Florence, Italy
Main Activities Molecular Dynamics simulations of protein folding using coarse-grained models

Date From 01-03-2004 to 31-10-2004
Position held Post-doctoral position
Employer Interdepartmental Center for the Study of Complex Dynamics (CSDC), University of Florence, Italy
Main Activities Monte Carlo simulations of polymer stretching using an Ising-like model

Habilitations

Habilitation 1 Scientific Habilitation as Associate Professor in Applied Physics (Abilitazione Scientifica Nazionale come Professore di seconda fascia nel Settore Concorsuale **02/D1 - Fisica applicata, didattica e storia della Fisica**). The habilitation is valid for 11 years, from 29/09/2023 to 29/09/2034.

Habilitation 2 In the 2009 recruitment campaign of the French Ministry of Higher Education and Research I was awarded the habilitation as *Maitre de Conférences* in the following scientific sectors: **64 - Biochimie et biologie moléculaire** (date of qualification 27/01/2009, qualification number: 09264196515); **65 - Biologie cellulaire** (date of qualification 29/01/2009, qualification number: 09265196515); **85 - Sc. physicochim. et ingénierie appliquée à la santé (ex 39è)** (date of qualification 28/01/2009, qualification number: 09285196515).

Training and Education

Date 25-7-2003
Title of qualification awarded Philosophy Doctor in *Non linear dynamics and complex systems*
Principal subjects Automatic control, System Theory, Mathematical Methods for Engineering, Statistical Mechanics, Biophysics, Computational Chemistry
Name and type of organization providing education and training Department of Systems and Computer Science, University of Florence, Italy
Thesis title *An adaptive evolution strategy for protein folding*
Level in national or international classification Final assessment: "Very Good"

Date 9-3-2000
Title of qualification awarded Master of Science in *Biological Sciences*
Principal subjects Biochemistry, Molecular Biology, Genetics, Microbiology, Physiology, Botany, Zoology
Name and type of organization providing education and training University of Florence, Italy
Thesis title *A theoretical model of evolution of quasi-species*
Level in national or international classification Final score: 110/110 *summa cum laude*

Research areas

Research interest Computational Biophysics, Molecular Dynamics simulation of biomolecules, Ion Channels, Peptides for treatment and diagnosis of autoimmune diseases, protein folding, coarse-grained protein models

scientific profile

The hallmark of my scientific profile is interdisciplinarity. Despite being a biologist by training, I got a PhD in Nonlinear Dynamics and Complex Systems and I always worked in close cooperation with theoretical physicists and computational chemists. In hindsight, my career proceeded through three different stages. In the first part of my career I worked on the protein folding problem using a wide range of coarse-grained models from Ising-like to single- and double bead. A special attention was devoted to the topological Gō-model whose merits I analysed in a comparative study with a sequence-based model introduced by Sorenson and Head-Gordon. Despite its simplicity, I was able to apply the Gō model to rationalize the different impact of pathological mutations of Myosin Binding Protein C. The second part of my career was focused on the characterization of small peptides and organic molecules with a potential application to the diagnosis and treatment of Multiple Sclerosis (MS), Rheumatoid Arthritis (RA) and other autoimmune diseases. From a methodological point of view I switched to atomistic simulations, possibly in combination with implicit solvent models, to reach biologically relevant time scales. For the same reason, I systematically used enhanced sampling methods like Replica Exchange Molecular Dynamics (REMD) both in the temperature- and Hamiltonian versions. Using this methodology I showed that CSF114(Glc), a synthetic glycopeptide already used in a diagnostic assay of MS, is also fit for an application as a drug. Similarly, I discovered a correlation between compactness and TACE enzyme inhibition potency of a small family of derivatives of tartaric acid, thus identifying a criterion for the rational design of potential drugs for RA. The third and last part of my career was devoted to the study of ion channels. After a study of the mesoscopic VDAC nanopores with a basic approach based on simulations with a constant electric field, I switched to the characterization of NaChBac, a voltage-gated sodium channel. Using a combination of Metadynamics and the Nudged Elastic Band algorithm and building a Markov State Model from the equilibrium trajectory, I could reconstruct the 2-3 ions knock-on permeation mechanism of sodium. I also clarified the mechanism of Sodium/Calcium selectivity and the differential roles of aspartate and glutamate residues in the selectivity filter. I am currently working on gating *i.e.* the ability of an ion channel to open and close in response of specific stimuli. My investigation of CRAC channel revealed a hydrophobic gating mechanism through the formation/breakdown of a vapour bubble and highlighted an allosteric process whereby the extension of peripheral TM4 helices is transduced long-range into the opening of the pore delimited by the innermost ring of helices. Conversely, the study of hERG channel with a combination of Molecular Dynamics and network theory methods revealed that the electro-mechanical coupling between Voltage Sensor Domain and Pore Domain is mediated by two dynamic communication pathways where several pathologic mutation sites are located. A new research line that I have just started concerns the study of curvature-sensing peptides that we hope to employ as baits to purify exosomes, vesicles with a huge potential for drug targeting applications.

Personal skills and competences

Mother Tongue

Italian

Other languages

Self-assessment
European level^()*

English ()**

French (*)**

Understanding				Speaking				Writing	
Listening		Reading		Spoken interaction		Spoken production			
C1	Proficient user	C2	Proficient user	C2	Proficient user	C2	Proficient user	C2	Proficient user
A1	Basic user	A2	Basic user	A1	Basic user	A1	Basic user	A2	Basic user

^(*)Common European Framework of Reference (CEF) level

(**) In 1999 I received the Certificate of proficiency in English of the University of Cambridge with final score B from the British Institute of Florence.

(***) In 2009 I was awarded the DELF A1 Certificate with a final score of 98/100 from the French Institute of Florence.

Computer skills and competences

Programming languages

Pascal, C, Fortran 77, Fortran 90/95

Operating Systems

Linux

Applicative software

Latex, Gnuplot, Xmgrace, awk, Xfig, Xdrawchem

Biomolecular Packages

Rasmol, VMD, Amber, NAMD, ORAC, ACEMD, PLUMED, GOLD, Haddock, MSMBuilders, Proflex

Projects

Tier0 projects

Project 1

From June 2023 to June 2024: PI of Iscra-C project *CurvRec - Investigating curvature sensing peptides through Molecular Dynamics simulations* (project code: HP10CXOZ26). The project was allocated 10000 GPU hours on the LEONARDO machine (CINECA, Italy).

Project 2

From April 2020 to April 2021: co-authoring and co-management of PRACE project *CRAC-Gate – Gating in calcium release-activated calcium channel*. The project was allocated 44.0M core hours on the Marconi100 machine (CINECA, Italy).

Research projects

Project 1

In 2015 I was awarded a one-year Research Fellowship from *Le Studium*, a French funding agency to implement my project *Exploring actin dynamics through molecular dynamics and breather analysis*. I declined the offer because I had received a better offer from Warwick University.

Project 2

In 2009 I was co-author of the Project *In silico assessment of peptides with potential pharmaceutical properties for Multiple Sclerosis*. The Project was financially supported by Regione Toscana within the framework of the "Regional Health Research Program 2009". The grant supported my position as Research Associate at the Department of Chemistry of the University of Florence in 2010-2012.

Project 3

In 2022 my Project *CRAC-String - Exploring the gating of CRAC channel through string method molecular dynamics simulations* (protocol number: RP1221813A0B5113) was financially supported by Sapienza University of Rome within the framework of the initiative "Bando di Ateneo per la Ricerca 2022" under the category "small research projects".

Congress Organization

Congress 1

Co-organizer of Workshop *Frontiers in ion channels and nanopores: where technology and biology meet* held in Rome, September 18-21 2023.

Congress 2

Co-organizer of Workshop *Frontiers in ion channels and nanopores: theory, experiments and simulation* held in Rome and online, February 2-5 2021.

Teaching

Courses

Course 1

Academic year 2020/2021: Teaching Assistant in the course of Laboratory of Numerical Aerodynamics (Laboratorio di calcolo aerodinamico), 3 CFU, 3-rd year course in the degree in Aerospace Engineering.

Student supervision

Student 1

From March to October 2023 I supervised Valerio Vagnoni in a research project of the *School for Advanced studies* (SSAS - Scuola Superiore di Studi Avanzati) of Sapienza University. Mr Vagnoni, student of the class of Science and Technology, implemented a project entitled *Analysis of activation pathways of ion channel Kv7.1* and passed his exam with top grades on 25/10/2023.

Student 2

March 2020 to July 2021: Master thesis co-supervisor of Delia Sun. Miss Sun graduated in Biomedical Biotechnology on July 22-nd, 2021 with final score 110/110 *cum laude*. Thesis title: *Exploring CRAC ion channel gating through Molecular Dynamics simulations*.

Student 3

Flavio Costa, from November 2019 to January 2023 (PhD Student in Theoretical and Applied Mechanics). Thesis title *Fluid behaviour in biological confinement: gating of the hERG potassium channel via Molecular Dynamics simulations and network analysis*

Student 4

Xiaojun Xu, May to December 2010, (PhD student in Chemistry). PhD awarded 05/2014, thesis title: *Modeling assemblies and interactions at the replication fork: Sliding clamps and clamp interacting enzymes*.

PUBLICATIONS

[1]

F. Costa, G. Giogini, C. Minelli, G. Mobbili, C. Guardiani, A. Giacomello, R. Galeazzi
Membrane composition allows the optimization of berberine encapsulation in liposomes.
Mol. Pharmaceutics 2024, 21, 5818-5826. doi: <https://doi.org/10.1021/acs.molpharmaceut.4c00830>

[2]

D. Caprini, F. Battista, P. Zajdel, G. Di Muccio, C. Guardiani, B. Trump, M. Carter, A.A. Yakovenko, E. Amayuelas, L. Bartolomé, S. Meloni, Y. Grosu, C.M. Casciola, A. Giacomello

- Bubbles enable volumetric negative compressibility in metastable elastocapillary systems.*
Nature Communications 2024, **15**, 5076. doi: <https://doi.org/10.1038/s41467-024-49136-w>
- [3] F. Costa, R. Ocello, C. Guardiani, A. Giacomello, M. Masetti
Integrated approach including docking, MD simulations, and network analysis highlights the action mechanism of the cardiac hERG activator RPR260243.
J. Chem. Inf. Model. 2023, **63**, 4888-4899. doi: <https://doi.org/10.1021/acs.jcim.3c00596>
- [4] F. Cecconi, G. Costantini, C. Guardiani, M. Baldovin, A. Vulpiani
Correlation, response and entropy approaches to allosteric behaviors: a critical comparison on the ubiquitin case
Phys. Biol. 2023, **056002**, doi: <https://doi.org/10.1088/1478-3975/ace1c5>
- [5] C.A.Z. Bassetto Jr, F. Costa, C. Guardiani, F. Bezanilla, A. Giacomello
Noncanonical electromechanical coupling paths in cardiac hERG potassium channel
Nature Communications 2023, **14**, 1110, doi: <https://doi.org/10.1038/s41467-023-36730-7>
- [6] C. Guardiani, F. Cecconi, L. Chiodo, G. Cottone, P. Margaretti, L. Maragliano, M.L. Barabash, G. Camisasca, M. Ceccarelli, B. Corry, R. Roth, A. Giacomello, B. Roux
Computational methods and theory for ion channel research
Advances in Physics: X 2022, **7(1)**, 2080587
- [7] F. Costa, C. Guardiani, A. Giacomello
Molecular dynamics simulations suggest possible activation and deactivation pathways in the hERG channel
Communications Biology 2022, **5**, 165., doi: <https://doi.org/10.1038/s42003-022-03074-9>
- [8] F. Costa, C. Guardiani, A. Giacomello
Exploring $K_v1.2$ Channel Inactivation Through MD Simulations and Network Analysis
Front. Mol. Biosci. 2021, **8**, 784276., doi: [10.3389/fmolb.2021.784276](https://doi.org/10.3389/fmolb.2021.784276)
- [9] C. Guardiani, D. Sun, A. Giacomello
Unveiling the Gating Mechanism of CRAC Channel: A Computational Study
Front. Mol. Biosci. 2021, **8**, 773388, doi: [10.3389/fmolb.2021.773388](https://doi.org/10.3389/fmolb.2021.773388)
- [10] M.L. Barabash, W.A.T. Gibby, C. Guardiani, D.G. Luchinsky, B. Luan, A. Smolyanitsky, P.V.E. McClintock
Field-dependent dehydration and optimal ionic escape paths for C_2N membranes
J. Phys. Chem. B 2021, **125**, 7044–7059, doi: [10.1021/acs.jpcc.1c03255](https://doi.org/10.1021/acs.jpcc.1c03255)
- [11] M.L. Barabash, W.A.T. Gibby, C. Guardiani, A. Smolyanitsky, D.G. Luchinsky, P.V.E. McClintock
Origin and control of ionic hydration patterns in nanopores
Commun. Mater. 2021, **2**, 65, doi: [10.1038/s43246-021-00162-x](https://doi.org/10.1038/s43246-021-00162-x)
- [12] W.A.T. Gibby, M.L. Barabash, C. Guardiani, M.L. Barabash, D.G. Luchinsky, P.V.E. McClintock
Physics of selective conduction and point mutation in biological ion channels
Phys. Rev. Lett. 2021, **126**, 218102
- [13] W.A.T. Gibby, O.A. Fedorenko, C. Guardiani, M.L. Barabash, T. Mumby, S.K. Roberts, D.G. Luchinsky, P.V.E. McClintock
Application of a statistical and linear response theory to multi-ion Na^+ conduction in NaChBac
Entropy 2021, **23**, 249, doi:[10.3390/e23020249](https://doi.org/10.3390/e23020249)
- [14] O.A. Fedorenko, I.A. Khovanov, S.K. Roberts, C. Guardiani
Changes in ion selectivity following the asymmetrical addition of charge to the selectivity filter of bacterial sodium channel

- [15] C. Guardiani, W.A.T. Gibby, M.L. Barabash, D.G. Luchinsky, P.V.E. McClintock
Exploring the pore charge dependence of K^+ and Cl^- permeation across a graphene monolayer: a Molecular Dynamics study
RSC Advances, 2019, 9, 20402
- [16] W.A.T. Gibby, M.L. Barabash, C. Guardiani, D.G. Luchinsky, O.A. Fedorenko, S.K. Roberts, P.V.E. McClintock
Theory and experiments on multi-ion permeation and selectivity in the NaChBac ion channel
Fluctuation and Noise Letters, 2019, 18(2), 1940007 (13 pages)
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From the Potential of Mean Force to a Quasiparticle's Effective Potential in Narrow Ion Channels
Fluctuation and Noise Letters, 2019, 18(2), 1940006 (13 pages)
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Different roles for aspartates and glutamates for cation permeation in bacterial sodium channels
Biochimica et Biophysica Acta - Biomembranes, 2019, 1861, 495-503
- [19] C. Guardiani, A. Magrì, A. Karachitos, M.C. Di Rosa, S. Reina, I. Bodrenko, A. Messina, H. Kmita, M. Ceccarelli, V. De Pinto
*yVDAC2, the second mitochondrial porin isoform of *Saccharomyces cerevisiae**
Biochimica et Biophysica Acta - Bioenergetics, 2018, 1859, 270-279
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On the selectivity of the NaChBac channel: an integrated computational and experimental analysis of sodium and calcium permeation
Physical Chemistry Chemical Physics, 2017, 19, 29840-29854
This paper was highlighted as PCCP HOT article of 2017
- [21] C. Guardiani, P.M. Rodger, O.A. Fedorenko, S.K. Roberts, I.A. Khovanov
Sodium Binding Sites and Permeation Mechanism in the NaChBac Channel: a Molecular Dynamics Study
J. Chem. Theory Comput., 2017, 13, 1389-1400
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Biochimica et Biophysica Acta, 2016, 1858, 813-823.
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J. Chem. Theory Comput., 2015, 11 (2), pp 423-435
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Exploring the unfolding pathway of Maltose Binding Proteins: an integrated computational approach
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Coarse-grained modeling of protein unspecifically bound to DNA
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Conformational Landscape of N-Glycosylated Peptides Detecting Autoantibodies in Multiple Sclerosis, Revealed by Hamiltonian Replica Exchange
J. Phys. Chem. B. 2012, 116, 5458-5467
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- [34] C. Guardiani, S. Marsili, S. Marchetti, C. Gambi, P. Procacci, R. Livi
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Fragment 101-108 of Myelin Oligodendrocyte Glycoprotein: a possible lead compound for Multiple Sclerosis
J. Am. Chem. Soc., 2009, 131, 17176-17184
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- [37] F. Cecconi, C. Guardiani, R. Livi
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- [38] C. Guardiani, F. Cecconi and R. Livi
Stability and kinetic properties of C5-domain of Myosin binding protein C and its mutants
Biophys. J. 2008, 94(4), 1403-1411.

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Computational analysis of folding and mutation properties of C5 domain of Myosin binding protein C
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J. Chem. Phys. 2006, **125**, 084908.
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Biophys. J., 2006, **91**, 694-704.
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A model of sympatric speciation through assortative mating
Physica A 347 (2005) 534-574.
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A microscopic model of evolution of recombination
Physica A 347 (2005) 489-533.

BOOKS, BOOK CHAPTERS AND PROCEEDINGS

- [1] W.A.T. Gibby, M. Barabash, C. Guardiani, D. G. Luchinsky, and P. V. E. McClintock
The role of noise in determining selective ionic conduction through nano-pores
in **Proceedings of 2018 IEEE 13th Nanotechnology Materials and Devices Conference (NMDC)**
ISBN: 978-1-5386-1016-9/18
- [2] C. Guardiani and P. Procacci
Computational characterization of tartrate-based TACE inhibitors
in **High performance computing on CRESCO infrastructure: research activities and results 2010-2011**
Progress report of CRESCO Project, ENEA, Italian National Agency for New technologies, Energy and Sustainable Economic Development. July 2012, ISBN: 978-88-8286-268-8.
- [3] C. Guardiani
BOOK: An adaptive evolution strategy for protein folding
in **Lambert Academic Publishing, Saarbrücken, 2010. ISBN: 978-3-8383-7425-3**
- [4] C. Guardiani and F. Cecconi
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Computational characterization of the mutation impact on domain C5 of Myosin Binding protein C
in **Proc. SPIE**, 2007, **6602**, 660209
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Identification of kinetic bottlenecks of hPin1 WW domain through molecular dynamics simulations using simplified protein models
in **WSEAS Transactions on Biology and Biomedicine**, ISSN 1109-9518, Issue 3, Volume 3, March 2006, pag 249-256.

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A molecular dynamics investigation of the kinetic bottlenecks of the hPin1 WW domain. I: simulations with the Sorenson/Head-Gordon model
 in Proceedings of the **2006 WSEAS International Conference on Mathematical Biology and Ecology**, Miami, Florida, USA, January 18-20, 2006.
 ISSN: 1790-5095, ISSN: 1790-5125, ISBN: 960-8457-40-8.
 Editors: Charles A. Long, Siavash H. Sohrab, Haris Catrakis, Andrei G. Fedorov, Fotis Sotiropoulos, A.C. Benim, Guanyu Wang, Tuan Pham.
- [8] F. Cecconi, C. Guardiani and R. Livi
A molecular dynamics investigation of the kinetic bottlenecks of the hPin1 WW domain. II: simulations with the Go model
 in Proceedings of the **2006 WSEAS International Conference on Mathematical Biology and Ecology**, Miami, Florida, USA, January 18-20, 2006.
 ISSN: 1790-5095, ISSN: 1790-5125, ISBN: 960-8457-40-8.
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- [9] F. Bagnoli and C. Guardiani
A microscopic model of evolution of recombination
 in **WSEAS Transactions on Biology and Biomedicine, Issue 4, Volume 1, pag 416, October 2004**
- [10] F. Bagnoli and C. Guardiani
Sympatric Speciation through Assortative Mating in a Long-Range Cellular Automaton
 in **Cellular Automata, Proceedings of the 6-th International Conference on Cellular Automata for Research and Industry, ACRI 2004 Amsterdam, LNCS 3305, The Netherlands, October 2004, editors Peter M.A. Sloot, Bastien Chopard, Alfons Hoekstra (Springer 2004); p. 405**
- [11] F. Bagnoli and C. Guardiani
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 in Proceedings of the **5th WSEAS Conference on Mathematics and Computers in Biology and Chemistry (MCBC 2004)**, Venice, November 15-17, 2004.
 ISBN: 960-8457-05-X
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INVITED TALKS

- [1] Congress: **International Experts Summit on Material Science, Semiconductors and Optoelectronics IESMSSO2023**, Nice (France) and online, 6-8 November 2023
 Invited Talk: *A Molecular Dynamics Investigation of the Charge Dependence of K^+ and Cl^- Permeation Through a Graphene Monolayer*
- [2] Mini-Workshop: **Theoretical models of ion channels activity**, Perugia (Italy), 9 September 2023, Department of Chemistry, Biology and Biotechnology
 Invited Talk: *A computational exploration of gating of CRAC channel*
- [3] Workshop: **Statistical mechanics of non-Hamiltonian systems**, Rome, 12-13 May 2015, Department of Physics, University "La Sapienza"
 Invited Talk: *An Integrated Computational Approach to characterize the unfolding pathway of Maltose Binding Proteins.*
- [4] Workshop: **Physics of protein folding and aggregation. 2nd Workshop**, Bressanone (Bolzano), Italy, February 16-18, 2012.
 Invited Talk: *An Computational studies of potential drugs of autoimmune diseases*

- [5] Two invited lectures at the **Computational Nanotechnology Intensive Programme CoNan 2011**, 31 July-14 August 2011, Gdansk, Poland.
Lectures: *Introduction to protein modelling (1) and (2)*
- [6] Invited Talk at **Les cycles thematiques de l'institut d'etudes avancees: Dynamiques des systemes complexes; axe: modelisation de macromolecules biologiques**, University of Cergy-Pontoise, March 22nd - April 1st 2011, France.
Invited Talks: *Application of REM method in the simulation of glycopeptides (I) and (II)*
- [7] **BIT's 3-rd Annual Protein and Peptide Conference (PepCon-2010)** Theme: After a Solution for the Machines of Life. Beijing, China, March 21-23, 2010.
Invited Talk: *Computational Study of a Potentially Bioactive Peptide for the Treatment and Diagnosis of Multiple Sclerosis.*
- [8] Workshop: **Physics of protein folding and aggregation** Bressanone (Bolzano), Italy, February 11-12, 2010.
Invited Talk: *A possible lead compound for Multiple Sclerosis*
- [9] Invited Talk at the **XXIV Meeting on "Theoretical Physics and Structure of Matter"**, Levico Terme (Trento), Italy, September 17-20, 2006.
Talk Title: *Folding and unfolding simulations of hPin1 WW domain and MyBPC C5 domain through simplified models*

CONGRESSES, WORKSHOPS AND SCHOOLS

- [1] Participation to Congress: **37-th European Peptide Symposium, 14-th International Peptide Symposium and Satellite Workshops**
August 25th-31st 2024, Florence, Italy
Poster Title: *Characterizing bradykinin-derived membrane-sensing peptides through Molecular Dynamics*
- [2] Participation to Conference: **Gordon Research Conference on Calcium Signaling**
June 30th-July 5th 2024, Renaissance Tuscany Il Ciocco, Barga, Lucca, Italy
Poster Title: *Computational Investigations of ion channel gating*
- [3] Participation to: **SNAFU proto-kick-off meeting**
June 3rd 2024, Brescia, Italy
Talk Title: *Characterizing the mechanical properties of EV membranes: preliminary MD simulations*
- [4] Participation to Workshop: **Frontiers in ion channels and nanopores: where technology and biology meet (FICN2023)**
September 18th-21st 2023, Rome, Italy
Talk Title: *Unraveling ion channel gating mechanism through computational approaches*
Poster Title: *Calmodulin modulation of Kv7.1 inactivation: a preliminary study*
- [5] Participation to congress: **14-th EBSA Congress**
July 31th- August 4th 2023, Stockholm, Sweden
Poster Title: *Deciphering CRAC gating through MD simulations*
- [6] Participation to congress: **Biophysics at Rome - Research on the path to sustainability**
April 19th-20th 2023, Rome, Italy
Talk Title: *CRACKing the allosteric gating of CRAC channel: a MD study*
- [7] Participation to congress: **Ions, membrane and channels: multiscale simulations from quantum to coarse-grain.**

- October 27th-29th 2022, Rome, Italy
Poster title: *Exploring ion channel gating through computational approaches.*
- [8] Participation to congress: **The 2-nd DISVA-MASBIC annual symposium - Protein structure and function in biology, medicine and nanotechnology**
October 13th-14th 2022, Ancona, Italy
Talk title: *Exploring the gating mechanism of CRAC channel through Molecular Dynamics simulations*
- [9] Participation to congress: **Molecular Simulation 2022: Past, Present and Future** Celebrating Michael L. Klein's career
June 25th-29th 2022, Erice, Italy
Poster title: *Cracking the gating mechanism of a ion channel: a MD study of CRAC channel*
- [10] Participation to summer workshop: **From biology to bioinspiration: theory, simulation and experiments for biophysical systems**
June 20th-23rd 2022, Le Terre di Poreta, Poreta, Italy
Talk title: *Characterizing ion channels and membrane-sensing peptides through Molecular Dynamics*
- [11] Participation to summer workshop: **Phase transitions at the nanoscale: wetting of nanoporous materials, cluster formation and nanofriction**
June 23rd-26th 2021, S. Anna in Camprena, Italy
Talk title: *Unveiling the gating of CRAC channel through Targeted MD simulations*
- [12] Participation to: **APS March meeting 2021**
March 15th-19th 2021, online.
Talk title: *A computational approach to characterize gating in ion channels*
- [13] Participation to: **65-th Biophysical Society Annual Meeting**
February 22nd-26th 2021, online.
Poster title: *Hydrophobic gating in CRAC channel: a Molecular Dynamics simulation study*
- [14] Participation to workshop: **Frontiers in ion channels and nanopores: theory, experiments and simulation**
February 2nd-5th 2021, online.
Talk title: *Characterizing gating in ion channels through MD simulations: hERG and CRAC channels*
- [15] Participation to workshop: **Multiscale simulations and biological channels**
September 14th-16th 2020, Rome, Italy.
Title of flash presentation: *CRAC channel: a preliminary computational study*
- [16] Congress participation: **ICNF 2019: 25-th International Conference on noise and fluctuations**
June 18th-21st Microcity-Neuchâtel, Switzerland.
Talk title: *Prehistory probability distribution of ion transition through graphene nanopore*
- [17] Congress participation: **4-th N8 Biophysical and Biochemical Symposium, Computational and experimental Methods in Biology**
18-th January 2019, University of Sheffield, UK.
Poster title: *An integrated analysis of Na^+/Ca^{2+} selectivity of a voltage-gated Na^+ channel*
- [18] Congress participation: **Physics of Biological Oscillators. New Insights into Non-Equilibrium and Non-Autonomous Systems**
November 27-30, 2018, Chicheley Hall, Buckinghamshire, United Kingdom.
Poster Title: *Modelling graphene to understand biological ion channels*
- [19] Congress participation: **Biophysical Society Thematic Meeting: Emerging Concepts in Ion Channel Biophysics**

October 10-13, 2017, Mexico City, Mexico

Poster Title: *Characterizing the permeation and Na⁺/Ca²⁺ selectivity mechanism of NaChBac channel: a computational study*

- [20] Congress participation: **5-th Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation**
13th-15th September 2017, University of Southampton.
Talk title: *Permeation and selectivity mechanism in NaChBac channel and its mutants.*
- [21] Congress participation: **19th IUPAB congress and 11th EBSA congress**
16-20 July 2017, Edinburgh International Congress Centre, Edinburgh, UK.
Poster presentation: *Exploring the Ca²⁺/Na⁺ selectivity of NaChBac channel through Molecular Dynamics simulations*
- [22] Congress participation: **Physics Meets Biology**
12-14 September 2016, Clare College, Cambridge, UK.
Poster presentation: *Characterizing the NaChBac channel through MD simulations*
- [23] **International Conference on Biological Oscillations** (9th meeting of European Study Group on Cardiovascular Oscillations)
April 10th-14th 2016, Lancaster, UK.
Talk title: *A simulation study of the NaChBac channel: Stability, Na⁺ binding sites and hydration*
- [24] Kick-off meeting of EPSRC Project (EPSRC reference: EP/M015831/1) **Ionic Coulomb blockade oscillations and the physical origins of permeation, selectivity, and their mutation transformations in biological ion channels**
Lancaster, UK, 27 October 2015.
Talk title: *Structural modeling of voltage gated sodium channels*
- [25] Final meeting of the Project of Relevant National Interest PRIN 2010-11 2010CSJX4F **Intracellular channels and pores: structural and functional studies provide new rules for engineering artificial channels**
Catania, 5/10/2015
Talk title: *Characterizing VDAC channels through MD simulations*
- [26] Annual meeting of the Project of Relevant National Interest PRIN 2010-11 CSJX4F **Intracellular channels and pores: structural and functional studies provide new rules for engineering artificial channels**
Pisa, 27/09/2014
Talk title: *Computational studies of VDAC channels*
- [27] International Focus Workshop **From Dynamics to Statistical Physics and Back**,
Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany, October 21-23, 2013.
Poster presentation: *A coarse-grained simulation study of facilitated diffusion*
- [28] Congress participation: **6-th Giovanni Paladin Memorial, Large deviations and rare events in physics and biology**
Department of Physics, University of Rome La Sapienza, September 23-25, 2013.
Poster presentation: *A coarse-grained model of facilitated diffusion*
- [29] International Summer School, "**Fundamental Problems in statistical Physics XIII**"
June 16-29, 2013, Leuven, Belgium.
Poster presentation: *A computational study of facilitated diffusion*
- [30] Congress participation: **Biophys 11, Biology and Beyond**
September 7-9, 2011 Arcidosso (GR), Italy.

Talk title: *Computational exploration of the conformational landscape of a peptide with a potential for the diagnosis and treatment of Multiple Sclerosis*

- [31] Poster presentation at the **7th EBSA European Biophysics Congress**, July 11-15 2009, Genova, Italy.
Talk title: Poster title: *A simulation approach to Multiple Sclerosis: study of a peptide with a pharmaceutical potential*
- [32] Poster presentation at the Workshop **BioStruct09 Unraveling the structure of biomolecules: from nonequilibrium statistical mechanics to mechanical manipulation** February 16-18 2009, Area CNR Sesto Fiorentino (Firenze), Italy.
Workshop sponsored by the Sim.Bio.Ma. program (Simulations of Biosystems and Material Science) of the European Science Foundation.
Poster title: *A computational study of a peptide related to Multiple Sclerosis*
- [33] Poster presentation at the **6th European Biophysics Congress** Imperial College, London, July 14-18 2007.
Poster title: *A computational study of pathogenic mutations in domain C5 of MyBPC*
- [34] Poster presentation at the **6th European Biophysics Congress** Imperial College, London, July 14-18 2007.
Poster title: *A computational study of pathogenic mutations in domain C5 of MyBPC*
- [35] Poster presentation at the Workshop **Progress in ab-initio modelling of biomolecules: towards computational spectroscopy** April 02 2007–April 04 2007, Physics Department, Sapienza University of Rome, Italy
Workshop organized by the Sim.Bio.Ma. program (Simulations of Biosystems and Material Science) of the European Science Foundation.
Poster title: *Mutations in domain C5 of MyBPC: a MD study*
- [36] International School of Physics "Enrico Fermi", course CLXV, "**Protein folding and drug design**" Villa Monastero, Varenna, Italy, July 4th-14th 2006.
Poster and talk: *A study of folding of hPin1 WW domain through simplified protein models*
- [37] Poster presentation, 15th **IUPAB**, 5th **EBSA International Biophysics Congress** Montpellier, France, August 27th-September 1st, 2005.
Poster title: *Kinetic bottlenecks identification in different folding models*
- [38] Poster presentation at **Lectures in Complex Systems** 6-8 October 2004, Centro per lo Studio delle Dinamiche Complesse (CSDC), Firenze, Italy.
Poster 1: *A microscopic model of evolution of recombination and sympatric speciation*
Poster 2: *Polymer stretching: experimental setup and simple Monte Carlo simulations*

Trattamento dei dati personali

Autorizzo il trattamento dei dati personali ai sensi dell'attuale Decreto Legislativo (art. 4 D.Lgs. 196/03)