Europass
Curriculum Vitae

Personal information

Name / Surname	**Carlo Guardiani**

Current Research Organization Sapienza University, Rome, Department of Mechanical and Aerospace Engineering

Work experience

Date	From 01-02-2021 to present
Position held	Research Associate (Ricercatore a tempo determinato di tipo A)
Project name	ERC Project: *Atomistic simulations of hydrophobic gating in biological ion channels*
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
	From 01-06-2019 to 31-01-2021

Date	
Position held	Research Fellow (Assegnista di Ricerca)
Project name	ERC Project: *Molecular dynamics simulation of hydrophobic gating in biological ion channels*
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
	From 01-03-2018 to 31-05-2019

Date	
Position held	Senior Research Associate in Ion Channel Physics
Project name	Liverhulme Project: *Stochastic Dynamics of the KcsA channel*
Employer	Department of Physics, Lancaster University, Lancaster, U.K.
Main Activities	Molecular Dynamics simulations of ion channels; outreach activities
	From 01-09-2015 to 28-02-2018

Date	
Position held	Post-Doctoral position
Project name	EPSRC Project: *Ionic Coulomb blockade oscillations and the physical origins of permeation, selectivity, and their mutation transformations in biological ion channels.*
Employer	School of Engineering, Warwick University, Coventry, U.K.
Main Activities	Molecular Dynamics simulations of ion channels
	From 01-01-2014 to 31-08-2015

Date	
Position held	Post-Doctoral position
Project name	*Rational in-silico design of new antibiotics to contrast multi-resistance.*
Employer	Italian National Research Council (CNR-IOM), Cagliari, Italy
Main Activities	Molecular Dynamics simulations of ion channels

	From 01-01-2013 to 31-12-2013
Date	
Position held	Post-Doctoral position
Project name	*Chaotic and statistical properties of classical systems.*
Employer	Department of Physics, Sapienza University, Rome, Italy
Main Activities	Molecular Dynamics simulations of DNA/transcription factor interaction
	From 01-01-2013 to 31-12-2012
Date	
Position held	Research associate (Ricercatore a Tempo Determinato)
Project name	*In silico assessment of peptides with potential pharmaceutical properties for Multiple Sclerosis*
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
	From 01-05-2010 to 31-12-2010
Date	
Position held	Research Scholar
Employer	Department of Chemistry, Georgia State University, Atlanta, U.S.A.
Main Activities	Molecular Dynamics simulations of sliding clamp proteins
	From 01-11-2009 to 31-12-2009
Date	
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
	From 01-09-2006 to 31-08-2009
Date	
Position held	Post-doctoral position
Project name	*Study of the role of sugars in the etiology of multiple sclerosis*
Employer	Interdepartmental Center for the Study of Complex Dynamics (CSDC), University of Florence, Italy
Main Activities	Molecular Dynamics simulations of antigen/antiboby interactions in Multiple Sclerosis
	From 01-11-2004 to 31-07-2006
Date	
Position held	Post-doctoral position
Project name	*Mesoscopic Description of Protein Folding*
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
	From 01-03-2004 to 31-10-2004
Date	
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 awardes the habilitation as *Maitre de Conferences* in the following scientific sectors: **64 - Biochimie et biologie moleculaire** (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 ingenierie appliquee a la sante (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"
	9-3-2000
Date	
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), Rheumathoid 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[(*)]

	Understanding			Speaking				Writing	
	Listening		Reading	Spoken interaction		Spoken production			
English (**)	C1 Proficient user	C2	Proficient user	C2 Proficient user	C2	Proficient user		C2	Proficient user
French (***)	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, MSMBuilder, 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 Felloship 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 ofthe 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, 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

[2]   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

[3]   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

[4]   C. Guardiani, F. Cecconi, L. Chiodo, G. Cottone, P. Malgaretti, 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

[5]   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

[6]   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

[7]   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

[8]   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.jpcb.1c03255

[9]   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

[10] 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

[11] 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

[12] 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

Entropy 2020, 22, 1390, doi:10.3390/e22121390

[13] 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

[14] 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)

[15] M.L. Barabash, W.A.T. Gibby, C. Guardiani, D.G. Luchinsky, P.V.E. McClintock

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)

[16] C. Guardiani, O.A. Fedorenko, I. Khovanov, S.K. Roberts

Different roles for aspartates and glutamates for cation permeation in bacterial sodium channels

Biochimica et Biophysica Acta - Biomembranes, 2019, 1861, 495-503

[17] 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

[18] C. Guardiani, O.A. Fedorenko, S.K. Roberts, I.A. Khovanov

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

[19]   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

[20]   C. Guardiani, L. Leggio, M.A. Scorciapino, V. De Pinto, M. Ceccarelli

A computational study of ion current modulation in hVDAC3 induced by disulfide bonds

Biochimica et Biophysica Acta, 2016, 1858, 813-823.

[21]   S. Reina, V. Checchetto, R. Saletti, A. Gupta, D. Chaturvedi, C. Guardiani, F. Guarino, M. Scorciapino, A. Magrì, S. Foti, M. Ceccarelli, A. Messina, R. Mahalakshmi, I. Szabo, V De Pinto

VDAC3 as a sensor of oxidative state of the intermembrane space of mitochondria: the putative role of cysteine residue modifications

Oncotarget, 2016, 7(3), 2249-2268

[22]   C. Guardiani, M.A. Scorciapino, G.F. Amodeo, J. Grdadolnik, G. Pappalardo, V. De Pinto, M. Ceccarelli, M. Casu

The N-Terminal Peptides of the Three Human Isoforms of the Mitochondrial Voltage-Dependent Anion Channel Have Different Helical Propensities

Biochemistry, 2015, 54, 5646-5656

[23]   M. Banchelli, C. Guardiani, R. Sandberg, S. Menichetti, P. Procacci, G. Caminati

Media effects in modulating the conformational equilibrium of a model compound for tumor necrosis factor converting enzyme inhibition

Journal of Molecular Structure, 2015, 1091, 65-73

[24]   R.B. Sandberg, M. Banchelli, C. Guardiani, S. Menichetti, G. Caminati, P. Procacci

Efficient Nonequilibrium Method for Binding Free Energy Calculations in Molecular Dynamics Simulations

J. Chem. Theory Comput., 2015, 11 (2), pp 423-435

[25]   C. Guardiani, D. Di Marino, A. Tramontano, M. Chinappi, F. Cecconi

Exploring the unfolding pathway of Maltose Binding Proteins: an integrated computational approach

J. Chem. Theory Comput. 2014, 10, 3589-3597

[26]   C. Guardiani, M. Cencini, F. Cecconi

Coarse-grained modeling of protein unspecifically bound to DNA

Phys. Biol. 2014, 11, 026003 (11pp)

[27]   X. Xu, C. Guardiani, C. Yan, I. Ivanov

Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1

Nucleic Acids Res. 2013, 41(22), 10020-10031

[28]   M. Banchelli, C. Guardiani, E. Tenori, S. Menichetti, G. Caminati, P. Procacci

Chemical-physical analysis of a tartrate model compound for TACE inhibition

Phys. Chem. Chem. Phys. 2013, 15, 18881-18893

[29]   C. Guardiani and P. Procacci

The conformational landscape of Tartrate-based inhibitors of the TACE enzyme as revealed by Hamiltonian Replica Exchange Simulation

Phys. Chem. Chem. Phys. 2013, 15, 9186-9196

[30]   C. Guardiani, G.F. Signorini, R. Livi, A.M. Papini, P. Procacci

Conformational Landscape of N-Glycosylated Peptides Detecting Autoantibodies in Multiple Sclerosis, Revealed by Hamiltonian Replica Exchange

J. Phys. Chem. B. 2012, 116, 5458-5467

[31]   Y. Feng, J. Wang, S. Asher, L. Hoang, C. Guardiani, I. Ivanov, Y.G. Zheng

Histone H4 acetylation differentially modulates arginine methylation by an in cis mechanism

J. Biol. Chem. 2011, 286(23), 20323-20334.

[32]   C. Guardiani, S. Marsili, S. Marchetti, C. Gambi, P. Procacci, R. Livi

Conformational structure of the MOG-derived peptide 101-108 in solution

Pept. Science 2010, 96(3), 245-251

[33] C. Guardiani, S. Marsili, P. Procacci, R. Livi

Fragment 101-108 of Myelin Oligodendrocyte Glycoprotein: a possible lead compound for Multiple Sclerosis

J. Am. Chem. Soc., 2009, 131, 17176-17184

[34] C. Guardiani, R. Livi, F. Cecconi

Coarse grained modelling and approaches to protein folding

Curr. Bioinformatics 2010, 5, 217-240

[35] F. Cecconi, C. Guardiani, R. Livi

Analyzing pathogenic mutations of C5 domain from cardiac myosin binding protein C through MD simulations

Eur. Biophys. J., 2008, 37, 683-691.

[36] 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.

[37] C. Guardiani, F. Cecconi and R. Livi

Computational analysis of folding and mutation properties of C5 domain of Myosin binding protein C

Proteins: Struct. Func. Bioinf., 2008, 70, 1313-1322.

[38] C. Guardiani and F. Bagnoli

A toy model of polymer stretching

J. Chem. Phys. 2006, 125, 084908.

[39] F. Cecconi, C. Guardiani and R. Livi

Testing simplified protein models of the hPin1 WW domain

Biophys. J., 2006, 91, 694-704.

[40] F. Bagnoli and C. Guardiani

A model of sympatric speciation through assortative mating

Physica A 347 (2005) 534-574.

[41] F. Bagnoli and C. Guardiani

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, Saabrucken, 2010. ISBN: 978-3-8383-7425-3**

[4] C.Guardiani and F. Cecconi

Coarse-grained protein modeling

in **Nova Publishers, 2011, pp 531-578. ISBN: 978-61728-990-3**

[5] C. Guardiani, F. Cecconi and R. Livi

Computational characterization of the mutation impact on domain C5 of Myosin Binding protein C

in **Proc. SPIE, 2007, 6602, 660209**

[6] C. Guardiani, F. Cecconi and R. Livi

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.**

[7]   F. Cecconi, C. Guardiani and R. Livi

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.

Editors: Charles A. Long, Siavash H. Sohrab, Haris Catrakis, Andrei G. Fedorov, Fotis Sotiropoulos, A.C. Benim, Guanyu Wang, Tuan Pham.

[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

A microscopic model of evolution of recombination

in Proceedings of the **5th WSEAS Conference on Mathemathics and Computers in Biology and Chemistry** (MCBC 2004), Venice, November 15-17, 2004.

ISBN: 960-8457-05-X

Editors: C. Manikopoulos, B. Tafaghodinia, L. Simoni, D. Politis, V. Kluev, A. Genco, J.C. Quadrado, C. D'Attelis, N. Mastorakis. Associated Editors: Y. HaCohen-Kerner, N. Moussa, L. Tortosa, E. Venturino.

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 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*
[2]	Participation to congress: **14-th EBSA Congress**
	July 31th- August 4th 2023, Stockholm, Sweden
	Poster Title: *Decipering CRAC gating through MD simulations*
[3]	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*
[4]	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.*
[5]	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*
[6]	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*
[7]	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*
[8]	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*
[9]	Participation to: **APS March meeting 2021**
	March 15th-19th 2021, online.
	Talk title: *A computational approach to characterize gating in ion channels*
[10]	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*

[11]	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*
[12]	Participation to workshop: **Multiscale simulations and biological channels**
	September 14th-16th 2020, Rome, Italy.
	Title of flash presentation: *CRAC channel: a preliminary computational study*
[13]	Congress participation: **ICNF 2019: 25-th International Conference on noise and fluctuations**
	June 18th-21st Microcity-Neuchatêl, Switzerland.
	Talk title: *Prehistory probability distribution of ion transition through graphene nanopore*
[14]	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*
[15]	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*
[16]	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$^+$/Ca^{2+} selectivity mechanism of NaChBac channel: a computational study*
[17]	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.*
[18]	Congress participation: **19th IUPAB congress and 11th EBSA congress**
	16-20 July 2017, Edinburgh International Congress Centre, Edinburgh, UK.
	Poster presentation: *Exploring the Ca^{2+}/Na$^+$ selectivity of NaChBac channel through Molecular Dynamics simulations*
[19]	Congress participation: **Physics Meets Biology**
	12-14 September 2016, Clare College, Cambridge, UK.
	Poster presentation: *Characterizing the NaChBac channel through MD simulations*
[20]	**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*
[21]	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: Talk title: *Structural modeling of voltage gated sodium channels*
[22]	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*
[23]	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*
[24]	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*
[25]	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*
[26]	International Summer School, **"Fundamental Problems in statistical Physics XIII"**
	June 16-29, 2013, Leuven, Belgium.
	Poster presentation: *A computational study of facilitated diffusion*
[27]	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*
[28]	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*
[29]	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*
[30]	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*
[31]	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*
[32]	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*
[33]	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*
[34]	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*
[35]	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)