

PERSONAL INFORMATION

Family name, First name: Furini, Simone

Researcher ID: A-7532-2013

ORCID: 0000-0002-1099-8279

Date of birth: 19/04/1979

Nationality: Italian

Web site: <http://furini.dbm.unisi.it>



CURRENT POSITION

Since 2009 Assistant Professor at the Department of Medical Biotechnologies
University of Siena, Italy

EDUCATION

- 2008 PhD in Bioengineering (Doctor Europaeus)
Department of Electronics, Computer Science and Systems, University of Bologna, Italy
Supervisor: Prof. Silvio Cavalcanti
Title of the thesis: Computational analyses on the structure-function relation in ion channels
- 2003 Master degree in Electronic Engineering, with honours
Specialization: Biomedical Engineering
University of Bologna, Italy

GRANTS AND AWARDS

- 2016 IS CRA grant for High-Performance Computing resources in CINECA. Markov state models of K⁺ channels estimated from atomistic simulations. 3.000.000 CPU hours
- 2015 ERC-starting grant. Project: A multiscale strategy to include atomic details in simulations of excitable cells. The project was ranked in class A (fully meet the ERC's excellence criterion)
- 2014 Grant by the Tumour Institute of Tuscany. Project: Identification of genetic bases of individual predisposition to lung cancer in non-smokers. Amount: 118.000 euros. Role: Coordinator of the bioinformatics research unit
- 2014 IS CRA grant for High-Performance Computing resources in CINECA. Bias-exchange simulations of ion conduction in Na⁺-channels. 4.300.000 CPU hours
- 2012 IS CRA grant for High-Performance Computing resources in CINECA. Molecular Dynamics simulations of Na⁺ conduction in potassium channels. 620.000 CPU hours
- 2011 IS CRA grant for High-performance computing resources in CINECA. Metadynamics simulations of the protein-DNA recognition process. 150.000 CPU hours
- 2010 IS CRA grant for High-performance computing resources in CINECA. Molecular Dynamics simulations of repressor proteins scanning the DNA sequence. 140.000 CPU hours
- 2009 *Paolo Inghingolo* prize for best thesis in Bioengineering, awarded by the Italian National Bioengineering Group (GNB)
- 2009 HPC-Europa2, Transnational access programme to European facilities for High Performance Computing. Project: Diffusion coefficient for the LacI sliding movement along non-specific DNA
- 2008 Award "Best experimental measurement" to the Team of the University of Bologna.

- ”International Genetically Engineered Machine competition” iGEM 2008. Boston (USA). 8- 9/11/ 2008. Role: supervisor of the team composed of 11 master students
- 2008 HPC-Europa2, Transnational access programme to European facilities for High Performance Computing. Project: Steered Molecular Dynamics simulations of the LacI sliding movements along non-specific DNA
- 2007 Marco Polo Grant for stay abroad (internal competitive call of the University of Bologna). Project: Atomic structure and conduction characteristics of the alpha-Hemolysin ion channel

TEACHING ACTIVITIES

- 2009 - *Biological Databases and Scientific Writing*
48 hours course in the bachelor degree in Biotechnologies
- 2010 - 2016 *Principles of Bioengineering*
48 hours course in the Master degree in Engineering
- 2017 - *Modelling and Simulations for Biological Systems*
48 hours course in the Master degree in Engineering
- 2015 - *Bioinformatics and Systems biology*
18 hours course in the Master degree in Biotechnologies

SUPERVISION OF STUDENTS

- 2017 – Marco Valentini – PhD programme in Biotechnologies
- 2014 – 2017 Marilisa Cortesi - PhD programme in Bioengineering
Thesis: Computational Tools and in-silico models to identify transcriptional determinants of cell phenotype decision making
- 2013 - 2016 Lucia Bandiera - PhD programme in Bioengineering
Thesis: Noise impact on the behaviour of genetic circuits

INVITATED TALKS

- 2017 Particle based simulations of ion conduction. Workshop on mathematical modelling and simulation of electrolytes with application to molecular physiology. January 10-11, 2017. National Center for Theoretical Sciences, Taipei, Taiwan
- 2017 Algorithms to accelerate sampling in atomistic simulations of membrane proteins. 25th annual workshop on differential equations. January 7-8, 2017. National Chiao Tung University, Hsinchu, Taiwan
- 2016 Multiscale Modeling in Molecular Systems. December 6, 2016. Institute of Advanced Studies. Kőszeg, Hungary
- 2013 Unveiling the atomic mechanisms of Na⁺/K⁺ selectivity by Molecular Dynamics Simulations. 4th Italian-Hispano-Portoguese Workshop. October 17-19, 2013. Mallorca, Spain
- 2011 All-atom Molecular Dynamics Simulations of Specific and Nonspecific Binding of Repressor CECAM workshop. Dynamics of Protein-Nucleic Acid Interactions: Integrating Simulations with Experiments. September 14-16, 2011. Zürich, Switzerland
- 2010 Synthetic circuits for memories and oscillators
29th Annual School on Bioengineering, September 13-17, 2010. Brixen, Italy
- 2010 Molecular Dynamics simulations of biological molecules
9th International Summer School Biocomplexity from gene to system. July 1-7, 2010. Istanbul, Turkey

SCIENTIFIC BOARDS

- 2018 Organizing committee. CECAM meeting: Multiscale modelling in electrophysiology: from atoms to organs. Lugano, Switzerland. March 26-28, 2018.

- 2018 Sixth National Congress of Bioengineering
<http://www.gnb2018.polimi.it/about-gnb-2018/scientific-committee/>
- 2017 4th International Synthetic & Systems Biology Summer School. July 17-21, 2017
 Robinson College, University of Cambridge
- 2016 3th International Synthetic & Systems Biology Summer School. July 8 – 14, 2016,
 Volterra (Pisa) Tuscany, Italy

VISITING PERIODS

- 2016 iASK fellowship. Host: Dezső Boda. Department of Physical Chemistry, University of Pannonia, Veszprém
- 2013 Visiting fellow at the Department of Chemistry, King's College London (United Kingdom)
 Host: Dr. Carmen Domene
- 2008 Physical and theoretical Chemistry Laboratory, University of Oxford (United Kingdom)
 Host Dr. Carmen Domene
- 2007 Physical and theoretical Chemistry Laboratory, University of Oxford (United Kingdom)
 Host Dr. Carmen Domene
- 2005 Max Planck Institute for Experimental Medicine, Goettingen (Germany)
 Host Dr. Luis A. Pardo

SELECTED PUBLICATIONS

- Bandiera, L., Pasini, A., Pasotti, L., Zucca, S., Mazzini, G., Magni, P., Giordano, E. & Furini, S. (2016). Experimental measurements and mathematical modeling of biological noise arising from transcriptional and translational regulation of basic synthetic gene circuits. *Journal of Theoretical Biology* 395, 153-160.
- Domene, C., Barbini, P. & Furini, S. (2015). Bias-exchange metadynamics simulations: An efficient strategy for the analysis of conduction and selectivity in ion channels. *Journal of Chemical Theory and Computation* 11, 1896-1906.
- Berti, C., Furini, S., Gillespie, D., Boda, D., Eisenberg, R. S., Sangiorgi, E. & Fiegna, C. (2014). Three-Dimensional Brownian Dynamics Simulator for the Study of Ion Permeation through Membrane Pores. *Journal of Chemical Theory and Computation* 10, 2911-2926.
- Furini, S., Barbini, P. & Domene, C. (2013). DNA-recognition process described by MD simulations of the lactose repressor protein on a specific and a non-specific DNA sequence. *Nucleic acids research* 41, 3963-72.
- Furini, S. & Domene, C. (2012). On conduction in a bacterial sodium channel. *PLOS Computational Biology* 8, e1002476.
- Furini, S., Domene, C. & Cavalcanti, S. (2010). Insights into the sliding movement of the lac repressor nonspecifically bound to DNA. *The Journal of Physical Chemistry B* 114, 2238-45.
- Furini, S. & Domene, C. (2009). Atypical mechanism of conduction in potassium channels. *Proceedings of the National Academy of Sciences of the United States of America* 106, 16074-7.

REVIEWING DUTIES

Grant applications reviewed for the Ministry of Education, University and Research
 Journal article reviewed, among others, in: *Journal of the American Chemical Society*; *PLoS Computational Biology*; *Biophysical Journal*; *Journal of Chemical Theory and Computation*; *Journal of Biological Physics*; *Neurocomputing*; *Journal of Computational Chemistry*; *Biopolymers*;