Salvatore M. Cosseddu

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EDUCATION

Doctor of Philosophy (PhD) Biophysics/Biophysical Chemistry — April 2010 to date
School of Engineering and Centre for Scientific Computing,
University of Warwick, Coventry, UK

Thesis:	*Structure and Dynamics of Protein in the Permeation and Gating of Potassium Ion Channels: Identifying Molecular Determinants and Developing Coarse-Grained Approaches*.
Research description:	The project has been developed under the supervision of Dr Igor Khovanov (School of Engineering), Prof Mike P Allen (Department of Physics) and Prof Mark Rodger (Department of Chemistry). The research aimed to investigate the inactivation process in potassium ion channel KcsA and its relation with the ions permeation using fine atomistic models such as Molecular Dynamics and free-energy methods (Metadynamics and Umbrella Sampling). The study was focused on the dynamics of the filter and the nearby network of residues able to regulate the conductivity. An additional goal was to further develop the outcomes into coarse-grained Brownian dynamics models.

Master of Science Physical Chemistry and Inorganic Chemistry (MSc, First-Class Honours) — March 2010
Università degli Studi di Sassari, Sassari, Italy

Thesis:	One year project on developing a Kinetic Monte Carlo model to describe diffusion and reactivity in MFI-type zeolites such as Silicalite-1 and ZSM-5, in particular xylene isomerization on HZSM-5.
Main subjects:	Physical chemistry, statistical mechanics, solid state chemistry, pharmaceutical chemistry, inorganic chemistry, asymmetric catalysis, aromatic compounds chemistry.

Bachelor of Science Chemistry (BSc, First-Class Honours) — March 2008
Università degli Studi di Sassari, Sassari, Italy

Thesis:	Six month project on developing a Cellular Lattice Gas Automaton to investigate the reactivity of molecules diffusing in zeolites.
Main subjects:	Physical chemistry, organic chemistry, analytical chemistry, inorganic chemistry, biochemistry, industrial chemistry and polymers, mathematics, physics and statistics.

PROFESSIONAL EXPERIENCE

Laboratory demonstrator
University of Warwick, Coventry, UK
Laboratory demonstrator for Material Microstructure Laboratory and Statistical Mechanics.

ADDITIONAL TRAINING AND CONFERENCES

Additional Training

- *CCP-BioSim workshop on Free energy methods for modelling of protein-ligand interactions*, 21 Nov 2012, University of Southampton, UK;
- *An Introduction to NAG Numerical Components*, 10 Jul 2012, University of Warwick, UK;
- *CECAM/TCBG Computational Biophysics Workshop in Bremen*, 17 - 21 Oct 2011, Jacobs University, Germany;
- *CCP5 DL_POLY Training Workshop*, 2 - 3 Feb 2011, Daresbury Laboratory, UK;
- *CSC / NAG Debugging, Profiling and Optimising*, 8 - 9 Nov 2011, University of Warwick, UK;
- *CSC / NAG Autumn School in Core Algorithms for High Performance Scientific Computing*, 26 - 30 Sep 2011, University of Warwick, UK;

- *High Performance Scientific Computing* module, 2010/2011, University of Warwick, UK;
- *Monte Carlo and molecular dynamics* module, 2010/2011, MPAGS, University of Warwick, UK;
- *CCP5 CECAM Methods in Molecular Simulation Summer School 2010*, 18 - 27 Jul 2010, Queens University Belfast, UK.

Conferences

- *CCP5/RSC workshop Advances in Theory and Simulation of non-Equilibrium Systems*, 26 - 27 Jun 2013, Imperial College, UK;
- *CCP5-MDNet Mathematical Challenges in Molecular Dynamics*, 2 - 5 Apr 2013, University of Warwick, UK;
- Poster presented to *2nd Annual CCP-BioSim Conference, Frontiers of Biomolecular Simulation*, 25 - 27 Mar 2013, University of Nottingham, UK;
- Poster presented to *Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations*, 26 - 29 Mar 2012, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany.
- *CCPB Collective Variable Methods in Biomolecular Simulation Principles and Applications*, 4 Nov 2011, University of Nottingham, UK
- *Mathematical Modelling of Ion Channels Workshop*, 5 - 6 Sep 2011, St Anne's College, Oxford, UK;
- *Trends in protein biophysics: from in silico molecules to in vivo and vitro proteins*, 17 - 19 May 2011, University of Warwick, UK;
- *MIRaW day on Monte Carlo Methods*, 7 Mar 2011, Mathematics Institute, University of Warwick, UK;
- *IOP Condensed Matter and Materials Physics CMMP10*, 14 -16 Dec 2010, University of Warwick, UK.

PRIZES

Awarded with the prize for the best talk at Centre for Scientific Computing's postgraduate day 2012.

COMPUTATIONAL SKILLS

Programming languages and tools

Excellent knowledge:
- FORTRAN,
- Tcl,
- Bash.

Good knowledge:
- Make,
- git.

Basic knowledge:
- C,
- Matlab,
- Python,
- profilers.

Tools for molecular simulations and statistical analysis:

- NAMD,
- VMD,
- R,
- gnuplot.

Office tools:

- LaTeX,
- Emacs,
- Microsoft Office,
- OpenOffice/LibreOffice.

System administrator:

- GNU/Linux (Debian and derived, Fedora, SUSE),
- Mac OS X,
- Windows OS.

Image manipulation programs and 2d and 3d graphics editor:

- Gimp,
- Inkscape,
- Blender.

PUBLICATIONS

- S. M. Cosseddu, I. A. Khovanov, M. P. Allen, P. M. Rodger, D. G. Luchinsky, P. V. E. McClintock, *Dynamics of Ions in the Selectivity Filter of the KcsA Channel: Towards a Coupled Brownian Particle Description*, EJP-ST, 2013, accepted.
- S. M. Cosseddu, M. P. Allen, P. M. Rodger, I. A. Khovanov, *Mechanism and Energetic of C-type Inactivation in K^+ Ion Channels*, in preparation.

MEMBERSHIPS

Associate member of the Institute of Physics.

LANGUAGES

- Italian - native language.
- English - speak fluently and read/write with high proficiency.