Marco Pasi

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Qualification CNU **sections 31** & **64**.

Research Experience and Education

2014 –	**Researcher** BMSSI Lyon, with R. Lavery: **structure, mechanics, electrostatics and interactions of DNA** based on microsecond MD simulations.
2012 – 2014	**Postdoctoral Researcher** at LCVMM EPFL Lausanne, with J. H. Maddocks: efficient **coarse-grain modelling of DNA** mechanics based on long MD simulations.
2010 – 2012	**Postdoctoral Researcher** at IBCP Lyon with K. Zakrzewska, R. Lavery: develop and parameterize a coarse-grain model of **protein mechanics** and its associated simulation & analysis **software package** in (C)Python; study the molecular basis of **lipase enantioselectivity** using MD and metadynamics.
2006 – 2010	**Ph.D. Industrial Biotechnology** at LMM University of Milano-Bicocca. Advisors: Prof. P. Fantucci, Prof. L. De Gioia and Dr. E. Papaleo: studying the molecular basis of **enzyme cold adaptation** with MD simulations and **phylogenetic analysis**.
1999 – 2006	**B.Sc. and M.Sc. Industrial Biotechnology** with full marks at University of Milano-Bicocca: specialising in bioinformatics and biomolecular simulations.

Research interests

▶ Mechanical properties of proteins and DNA; relationship between mechanics, weak interactions, electrostatics and biological function;

▶ **DNA-protein** and DNA-drug **interactions**: mechanics and thermodynamics of specific binding; role of the solvent and ions;

▶ Development of efficient **physical models of proteins and DNA**, and of tools for the **analysis and prediction of DNA-protein interactions**.

Teaching experience

2014	**Assistant lecturer** *Mathematics II* (14h) Architecture, EPFL;
2013	**Assistant lecturer** *Advanced Analysis I* (56h) Physics, EPFL;
2012 – 2013	**Assistant lecturer** *Linear Algebra I & II* (56h) Chemical Engineering, EPFL;
2008 – 2009	**Assistant lecturer** *Theory of Biological Systems* (20h) Master in Bioinformatics, University of Milano-Bicocca;

Publications

12 articles published in international, peer-reviewed journals (180 citations, h-index: 8); **12** talks and **8** posters at international conferences.

Skills

Chemistry and biomolecular modelling	▶ Computational physical chemistry of **proteins** and **DNA**; ▶ **Molecular dynamics simulation** of biological systems; ▶ **Free energy** methods (Metadynamics), continuum **electrostatics** (APBS); ▶ **Collective motions** analysis, **Markov state models**; ▶ **Force field** development, DFT (Gaussian); ▶ **Coarse-grain** modelling of proteins and DNA; ▶ **Sequence analysis** (BLAST, FASTA), **HMM**s, **phylogenesis** (Phylip), biological DBs (Uniprot, PDB, SCOP, ENCODE); ▶ Molecular simulation, analysis and visualisation: GROMACS, Amber, NAMD, MMTK, Chimera, PyMOL & VMD.
Programming and data analysis	▶ 10+ years experience **scientific programming**: molecular simulation and visualisation, mathematical modelling and algorithm development, biological data mining, statistical analysis and quantitative graphical display. ; ▶ Fluent in **Python** (numpy, pandas, scipy, CPython), **C, Fortran, C++**; ▶ **MPI** / **OpenMP**: scalable programming on hybrid HPC architectures; ▶ Data analysis and visualisation: **Matlab**, **R**, **PyLab** & **Gnuplot**; ▶ **PHP, HTML5, CSS3, JavaScript**: experience in web development;
Languages	**Italian**: native; **English**: native; **French**: excellent, written and spoken; **Spanish, German**: beginner.

Grants and Fellowships

2014 –	Post-doctoral fellowship on ANR project “Chrome”;
2010 – 2011	Awarded 150k hours of simulation time on the resources of CINES;
2009 – 2010	Post-doctoral fellowship on ANR project “Expenantio”;
2009	Fellowship from the MIUR to perform 6 months research abroad (IBCP, Lyon);
2008 – 2009	Awarded 100k hours of simulation time on the resources of Cineca;
2006 – 2009	Fellowship from the MIUR for Ph.D. studies.

Publications

1. Pasi M., Maddocks J.H., Lavery R. Analyzing ion distributions around DNA: sequence dependent potassium ion distributions from microsecond MD simulations. *Nucl. Acids Res.* **43** 2412–23 (2015)
2. Pasi M., Maddocks J.H., *et al.*, Lavery R. μABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucl. Acids Res.*, **42** 12272–83 (2014)
3. Petkevičiūtė D., Pasi M., Gonzalez O. and Maddocks J.H. cgDNA: a software package for the prediction of sequence-dependent coarse-grain free energies of B-form DNA. *Nucl. Acids Res.* **42** e153 (2014)
4. Lavery R., Maddocks J.H., Pasi M. and Zakrzewska K. Analyzing ion distributions around DNA. *Nucl. Acids Res.* **42**, 8138–8149 (2014)
5. Pasi M., Lavery R. and Ceres N. PaLaCe: a coarse-grain model to study mechanical properties of proteins. *J. Chem. Theory. Comput.* **9**, 785–793 (2013)

6. Ceres N., Pasi M. and Lavery R. Protein solvation energies based on residue burial. *J. Chem. Theory Comput.* **8**, 2141–2144 (2012)
7. Pasi M., Tiberti M., Arrigoni A. and Papaleo E. Xpyder: a PyMOL plugin to map correlated motions and their networks on the three-dimensional structure. *J. Chem. Inf. Model.* **52** 1865–1874 (2012)
8. Papaleo E., Pasi M., Tiberti M. and De Gioia L. Molecular dynamics of mesophilic-like mutants of a cold-adapted enzyme: insights into distal effects induced by the mutations. *PLOS ONE*, **6** e24214 (2011)
9. Papaleo E., Tiberti M., Invernizzi G., Pasi M., and Ranzani V. Molecular determinants of enzyme cold adaptation: comparative structural and computational studies of cold- and warm-adapted enzymes. *Curr. Prot. Pept. Sci.*, **12** 657–683 (2011)
10. Blanchet C., Pasi M., Zakrzewska K. and Lavery R. CURVES+ web server for analyzing and visualizing the helical, backbone and groove parameters of nucleic acid structures. *Nucl. Acids Res.*, **39 suppl 3** W68–W73 (2011)
11. Pasi M., Riccardi L., Fantucci P., De Gioia L. and Papaleo E. Dynamic properties of a psychrophilic α-amylase in comparison with a mesophilic homologue. *J. Phys. Chem. B*, **113** 13585–13595 (2009)
12. Papaleo E., Pasi M., Riccardi L., Sambi I., Fantucci P. and De Gioia L. Protein flexibility in psychrophilic and mesophilic trypsins. Evidence of evolutionary conservation of protein dynamics in trypsin-like serine-proteases. *FEBS Letters*, **582** 1008–1018 (2008)

Talks (selection)

1. Pasi M*, Maddocks J. H. and Lavery R. Sequence determines the structure and microsecond-scale dynamics of B-DNA and its bound cations. *Journées Ouvertes en Biologie, Informatique & Mathématiques*, Clermont-Ferrand (2015)
2. Pasi M*, Maddocks J. H. and Lavery R. Systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Fluctuations in Structured Coulomb Fluids*, ENS Lyon (2015)
3. Lavery R.*, Pasi M. and Ceres N. Coarse-grain and all-atom approaches to macromolecular recognition. *Modeling cellular life: From single molecules to cellular function*, CECAM EPFL Lausanne (2014)
4. Pasi M*, Maddocks J. H. and Lavery R. Systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *ABC general meeting*, Barcelona (2014)
5. Lavery R.*, Ceres N. and Pasi M. Atomistic and coarse-grain studies of biomacromolecules and their interactions. *Frontiers in dynamics simulations of biological molecules*, Barcelona (2013)
6. Lavery R.*, Ceres N. and Pasi M. Steps towards predicting protein-protein interactions. *Exploring protein interactions through theory and experiment* CECAM EPFL Lausanne (2012)
7. Pasi M.*, Ceres N. and Lavery R. PaLaCe: a coarse-grain model to study mechanical properties of proteins. *Nordita Scientific Program: Dynamics of Biomolecular Processes* Nordita Stockholm (2012)
8. Pasi M.* and Zakrzewska K. Thermodynamics and kinetics of substrate recognition by CALB. *Expenantio general meeting* IBCP Lyon (2012)

9. Lavery R.*, Sacquin-Mora S., Ceres N. and Pasi M. From molecular mechanics to function. *CBSB11: From Computational Biophysics to Systems Biology* Forschungszentrum Jülich (2011)
10. Pasi M.*, Ceres N. and Lavery R. PaLaCe: a coarse-grain model to study mechanical properties of proteins. *Journées du Centre Blaise Pascal* ENS Lyon (2011)
11. Pasi M.* and Zakrzewska K. The role of substrate recognition in the enantioselectivity of CALB. *BMSSI Seminar* Aussois (2011)

Posters (selection)

1. Pasi M.*, Maddocks J.H. and Lavery R. *Joint FEBS-EMBO conference*, Paris (2014)
2. Tiberti M.*, Arrigoni A., Invernizzi G., Lambrughi M., Pasi M. and Papaleo E. *Frontiers in dynamics simulations of biological molecules*, Barcelona (2013)
3. Pasi M.*, Ceres N. and Lavery R. *Topological Aspects of DNA Function and Protein Folding* Isaac Newton Institute, Cambridge (2012)
4. Ceres N.*, Pasi M. and Lavery R. *CBSB11: From Computational Biophysics to Systems Biology* Forschungszentrum Jülich (2011)
5. Papaleo E.*, Tiberti M., Pasi M., Riccardi L., Mereghetti P., Fantucci P. and De Gioia L. *Free-energy calculations with PLUMED* CECAM EPFL Lausanne (2010)
6. Pasi M.*, Tiberti M., Riccardi L., Fantucci P., De Gioia L. and Papaleo E. *Computational Systems Biology* CECAM EPFL Lausanne (2009)
7. Papaleo E.*, Pasi M., Riccardi L., Mereghetti P., Fantucci P. and De Gioia L. *Biomolecular Simulation EMBO Pratical Course, 2008* Institut Pasteur Paris (2008)
8. Papaleo E.*, Pasi M., Riccardi L., Fantucci P., and De Gioia L. *PNRA Meeting on Antarctic Biology* Follonica (2007)