Raffaello Potestio, Ph.D.
Curriculum Vitæ et Studiorum
August 2017

Personal Data

Name:	Raffaello Potestio
Date of birth:	November 26, 1982
Place of birth:	Rome, Italy
Citizenship:	Italian
Family status:	married, one daughter
Current Address:	Kiedricher Straße 7 - 65197 Wiesbaden, Germany
Current position:	Project Leader, *Statistical Mechanics of Biomacromolecules* group (Theory group)
Institute:	Max Planck Institute for Polymer Research
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Languages

Italian:	native language
English:	proficient level in speaking, listening and writing
German:	proficient level in speaking, listening and writing
French:	basic level in speaking, listening and writing

EDUCATION

11/2006-10/2010: Ph.D. in Physics at SISSA

- Curriculum: *Physics and Chemistry of Biological Systems*
- Thesis title: *Coarse-grained modelling of protein structure and internal dynamics: comparative methods and applications*
- Supervisor: Prof. Cristian Micheletti
- External examiners: Prof. Alejandro Giorgetti, Prof. Jens Kleinjung

10/2004-10/2006: Laurea specialistica (master) in Theoretical Physics at the *Sapienza* University of Rome

- Grade: 110/110 cum laude
- Thesis title: *Rinormalizzazione non perturbativa nello spazio delle X e gruppo di rinormalizzazione* (Non perturbative renormalization in X-space and renormalization group)
- Supervisor: Prof. Guido Martinelli
- External examiner: Prof. Massimo Testa

10/2001-10/2004: Laurea trienniale (bachelor) in Theoretical Physics at the *Sapienza* University of Rome

- Grade: 110/110 cum laude
- Dissertation title: *Gli integrali di cammino di Feynman - sviluppo e applicazioni* (Feynman's path integrals - development and applications)
- Supervisor: Prof. Massimo Testa
- External examiner: Prof. Guido Martinelli

REFERENCES

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PUBLICATION HIGHLIGHTS

- K. Kreis, M. E. Tuckerman, D. Donadio, K. Kremer and R. Potestio, From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations, J. Chem. Theory Comput. 12 (7), 3030-3039 (2016)
- A. C. Fogarty, R. Potestio and K. Kremer, A multi-resolution model to capture both global fluctuations of an enzyme and molecular recognition in the ligand-binding site, Proteins: Structure, Function, and Bioinformatics, 10.1002/prot.25173 (2016)
- S. Najafi and R. Potestio, Folding of small knotted proteins: insights from a mean field coarse-grained model, J. Chem. Phys. 143, 243121 (2015)
- R. Potestio, S. Fritsch, P. Español, R. Delgado-Buscalioni, K. Kremer, R. Everaers, and D. Donadio, Hamiltonian Adaptive Resolution Simulation for Molecular Liquids, Phys. Rev. Lett. 110, 108301 (2013)
- R. Potestio, F. Pontiggia and C. Micheletti, Coarse-grained description of proteins' internal dynamics: an optimal strategy for decomposing proteins in rigid subunits, Biophys. J. 96, 4993–5002 (2009)

PUBLICATION SUMMARY (DATA AS OF FEB. 9, 2017)

- Number of publications: 30 articles in peer reviewed journals; 1 book chapter; 2 review articles
- Number of peer-reviewed publications without PhD supervisor: 22
- Citations: 374 (ResearcherID) | 472 (Google Scholar)
- H-index: 13 (ResearcherID) | 13 (Google Scholar)

PUBLICATIONS | PEER-REVIEWED JOURNALS

[OA]: open access journals

31. R. Fiorentini, K. Kremer, R. Potestio, A. C. Fogarty, Using force-based adaptive resolution simulations to calculate solvation free energies of amino acid sidechain analogues, J. Chem. Phys. 146, 244113 (2017)
30. P. A. Netz, R. Potestio and K. Kremer, Adaptive resolution simulation of oligonucleotides, J. Chem. Phys. 145, 234101 (2016)
29. R. Cortes Huerto, K. Kremer and R. Potestio, Kirkwood-Buff integrals in the thermodynamic limit from small-sized molecular dynamics simulations, J. Chem. Phys. 145, 141103 (2016)
28. A. C. Fogarty, R. Potestio and K. Kremer, A multi-resolution model to capture both global fluctuations of an enzyme and molecular recognition in the ligand-binding site, Proteins: Structure, Function, and Bioinformatics, 10.1002/prot.25173 (2016)
27. S. Najafi, R. Podgornik, R. Potestio and L. Tubiana, Role of Bending Energy and Knot Chirality in Knot Distribution and Their Effective Interaction along Stretched Semiflexible Polymers, Polymers, 8(10), 347 (2016)
26. K. Kreis and R. Potestio, The relative entropy is fundamental to adaptive resolution simulations, J. Chem. Phys. 145, 044104 (2016)

25. S. Najafi, R. Podgornik, L. Tubiana and R. Potestio, Chirality modifies the interaction between knots, EuroPhys. Lett. 114(5), 50007 (2016)

24. K. Kreis, M. E. Tuckerman, D. Donadio, K. Kremer and R. Potestio, From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations, J. Chem. Theory Comput. 12 (7), 3030-3039 (2016)

23. M. Heidari, R. Cortes-Huerto, D. Donadio and R. Potestio, Accurate and general treatment of electrostatic interaction in Hamiltonian adaptive resolution simulations, Eur. Phys. J. Special Topics 225, 1505-1526 (2016)

22. J. M. Boereboom, R. Potestio, D. Donadio and R. E. Bulo, Toward Hamiltonian Adaptive QM/MM: Accurate Solvent Structures using Many-body Potentials, J. Chem. Theory Comput. 12 (8), 3441-3448 (2016)

21. K. Kreis, R. Potestio, K. Kremer and A. C. Fogarty, Adaptive Resolution Simulations with Self-Adjusting High-Resolution Regions, J. Chem. Theory Comput. 12 (8), 4067-4081 (2016)

20. R. Potestio and L. Tubiana, Discretized knot motion on a tensioned fiber induced by transverse waves, Soft Matter, doi: 10.1039/C5SM01766A (2016)

19. S. Najafi and R. Potestio, Folding of small knotted proteins: insights from a mean field coarse-grained model, invited contribution to *Coarse Graining of Macromolecules, Biopolymers, and Membranes*, J. Chem. Phys. 143, 243121 (2015)

18. **[OA]** S. Najafi and R. Potestio, Two Adhesive Sites Can Enhance the Knotting Probability of DNA, PLoS ONE 10(7): e0132132. doi: 10.1371/journal.pone.0132132 (2015)

17. A. C. Fogarty, R. Potestio and K. Kremer, Adaptive resolution simulation of a biomolecule and its hydration shell: Structural and dynamical properties, J. Chem. Phys. 142, 195101 (2015)

16. K. Kreis, A. C. Fogarty, K. Kremer and R. Potestio, Reply to comments by R. Klein on Advantages and challenges in coupling an ideal gas to atomistic models in adaptive resolution simulations, follow-up in *Discussion and Debate: Recurrent Problems in Scale Bridging Techniques in Molecular Simulation – What are the Current Options?*, Eur. Phys. J. Special Topics, 224, 2505-2506 (2015)

15. K. Kreis, A. C. Fogarty, K. Kremer and R. Potestio, Advantages and challenges in coupling an ideal gas to atomistic models in adaptive resolution simulations, regular article in *Discussion and Debate: Recurrent Problems in Scale Bridging Techniques in Molecular Simulation – What are the Current Options?*, Eur. Phys. J. Special Topics, 224, 2289-2304 (2015)

14. P. Español, R. Delgado-Buscalioni, R. Everaers, R. Potestio, D. Donadio and K. Kremer, Statistical mechanics of Hamiltonian adaptive resolution simulations, J. Chem. Phys. 142, 064115 (2015)

13. K. Kreis, D. Donadio, K. Kremer and R. Potestio, A unified framework for force-based and energy-based adaptive resolution simulations, Europhys. Lett. 108, 30007 (2014)

12. R. Potestio, Computer simulation of particles with position-dependent mass, Eur. Phys. J. B, 87, 245 (2014)

11. S. Fritsch, R. Potestio, D. Donadio, and K. Kremer, Nuclear Quantum Effects in Water: A Multiscale Study, J. Chem. Theory Comput., 10 (2), 816–824 (2014)

10. **[OA]** G. Polles, G. Indelicato, R. Potestio, P. Cermelli, R. Twarock, C. Micheletti, Mechanical and Assembly Units of Viral Capsids Identified via Quasi-Rigid Domain Decomposition, PLoS Comput. Biol. 9(11): e1003331. doi: 10.1371/journal.pcbi. (2013)

9. R. Potestio, P. Español, R. Delgado-Buscalioni, R. Everaers, K. Kremer, and D. Donadio, Monte Carlo Adaptive Resolution Simulation of Multicomponent Molecular Liquids, Phys. Rev. Lett. 111, 060601 (2013)

8. R. Potestio, S. Fritsch, P. Español, R. Delgado-Buscalioni, K. Kremer, R. Everaers, and D. Donadio, Hamiltonian Adaptive Resolution Simulation for Molecular Liquids, Phys. Rev. Lett. 110, 108301 (2013)
7. **[OA]** G. Morra, R. Potestio, C. Micheletti and Giorgio Colombo, Corresponding functional dynamics across the Hsp90 chaperone family: insights from a multiscale analysis of MD simulations, PLoS Comput. Biol. 8(3): e1002433. doi:10.1371/journal.pcbi.1002433 (2012)
6. R. Potestio and L. Delle Site, Quantum locality and equilibrium properties in low-temperature parahydrogen: a multiscale simulation study, J. Chem. Phys. 136(5), pp. 054101 (2012)
5. **[OA]** R. Potestio, C. Micheletti and H. Orland, Knotted vs. Unknotted Proteins: Evidence of Knot-Promoting Loops, PLoS Comput. Biol., 6(7): e1000864 (2010)
4. **[OA]** R. Potestio, T. Aleksiev, F. Pontiggia, S. Cozzini and C. Micheletti, ALADYN: a web server for dynamics-based alignment of proteins, Nucleic Acids Res. web-server issue (2010)
3. R. Potestio, F. Caccioli and P. Vivo, Random matrix approach to collective behavior and bulk universality in protein dynamics, Phys. Rev. Lett. 103, 268101 (2009)
2. **[OA]** T. Aleksiev, R. Potestio, F. Pontiggia, S. Cozzini and C. Micheletti, PiSQRD: a web server for decomposing proteins into quasi-rigid dynamical domains, Bioinformatics 25(20), 2743-4 (2009)
1. **[OA]** R. Potestio, F. Pontiggia and C. Micheletti, Coarse-grained description of proteins' internal dynamics: an optimal strategy for decomposing proteins in rigid subunits, Biophys. J. 96, 4993–5002 (2009)

PUBLICATIONS | REVIEWS AND BOOK CHAPTERS

- **[OA]** R. Potestio, C. Peter, and K. Kremer, Computer Simulations of Soft Matter: Linking the Scales, Entropy, 16(8), pp 4199–4245 (2014)
- **[OA]** R. Potestio and K. Kremer, Theory and practice of adaptive resolution simulations, Proceedings of the HYBRID2013 workshop of the John von Neumann Institute for Computing, vol. 46 (2013)
- R. Potestio, F. Pontiggia, V. Carnevale and C. Micheletti, Bridging the atomic and coarse-grained descriptions of collective motions in proteins, invited contribution for the book *Multiscale approaches to protein modeling: structure prediction, dynamics, thermodynamics and macromolecular assemblies*, edited by A. Kolinski, Springer (2010)

APPOINTMENTS, GRANTS AND AWARDS

February 2016	Project contributor of a project proposal for HPC Access to the JURECA supercomputer at the Forschungszentrum Jülich (assigned)
May 2014	Co-PI of a Project (B4) of the Collaborative Research Center / Transregio TRR 146 (funded, 4 years time window, 165,400 euro assigned to the B4 project)
August 2013	Project Leader in the Max Planck Institute for Polymer Research
April-June 2012	Participant at the KITP program *Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter*, Santa Barbara (USA)
December 2011	Awarded the prize for the best PhD thesis in Physics at SISSA in the year 2010
November 2010	PostDoc position and fellowship at Max Planck Institute for Polymer Research
November 2006	PhD position and fellowship at SISSA

Supervision of graduate students and postdocs

2013 - 2017	Supervision of 4 PhD students, supervision of 3 Postdocs

Reviewing Activity

I have reviewed articles for several international journals relevant for my field, among which the Journal of Chemical Physics, PLoS One, and Nature Scientific Reports.

Workshop organization

March 2017	I have promoted and co-organized the Focus Session (*Topological problems in the Physics of polymers, biopolymers, and fibers*) of the German Physical Society (DPG) Spring Meeting 2017 in Dresden
April 2016	I have co-organized the MPIP Theory Group Retreat in Berlin
June 2015	I have co-organized the 6th Mainz Materials Simulation Days (MMSD) workshop, focussing on *Non-equilibium Processes in Soft Matter*

Teaching Activity

Jan.-Feb. 2016	Part (10 lectures) of the course *From particles to continuum I* of the RWTH Aachen, Aachen (Germany)
WS 2015-2016	Special Course (Spezialvorlesung) on *Theoretical and Computational Methods in Soft Matter Physics*, Physics dept., Goethe University, Frankfurt (Germany)
October 2015	IRTG School (1 lecture), Mainz (Germany)
October 2015	ESPResSo Summer School (1 lecture), Stuttgart (Germany)
July 2015	Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics (4 lectures), SISSA, Trieste (Italy)
October 2013	ESPResSo Summer School (1 lecture), Stuttgart (Germany)
July 2013	Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics (4 lectures), SISSA, Trieste (Italy)

Invited talks

November 2016	*Adaptive dual-resolution methods for soft matter - Where from, where to?* - invited talk at the joint CASA/EMI colloquium, Technische Universiteit Eindhoven, Eindhoven (The Netherlands)
May 2016	*Adaptive dual-resolution methods for soft matter - Where from, where to?* - invited talk at the conference *Mathematical aspects of material science*, Philadelphia (USA)
April 2016	*Adaptive dual-resolution methods for soft matter - Where from, where to?* - invited talk at the Vrije Universiteit of Amsterdam (The Netherlands)

March 2016	*Up and down the ladder - A personal account of multi-scale modeling of biophysical systems* - invited talk at the University of Potsdam (Germany)
January 2016	*Building bridges: multi-scale computational methods in biophysics* - invited talk at the Max Planck Institute of Colloids and Interfaces, Golm-Potsdam (Germany)
December 2015	*Building bridges: multi-scale computational methods in biophysics* - invited talk at the Max Planck Institute for Biochemistry, Göttingen (Germany)
October 2015	*Building bridges: multi-scale computational methods in biophysics* - Symposium in the occasion of the Theodore von Kármán Fellowship awarded to Prof. R. Nussinov, Forschungszentrum Jülich, Jülich (Germany)
July 2015	*Computer simulations of soft matter: bridging the scales* - CECAM school topic seminar, SISSA, Trieste (Italy)
June 2015	*Computer simulations of soft matter: bridging the scales* - Scientific Workshop on Multiscale modeling, experimental characterization and simulations of nanocomposite, Université Paris-Est Marne-la-Vallée, Paris (France)
April 2015	*Computer simulations of soft matter: bridging the scales* - invited talk, University of Vienna (Computational Physics dept.), Vienna (Austria)
April 2015	*Hamiltonian Adaptive Resolution Simulations of Soft Matter* - invited talk, Università della Svizzera Italiana (Faculty of Informatics), Lugano (Switzerland)
March 2015	*Computer simulations of soft matter: bridging the scales* - Theoretical Physics Seminar, Goethe University, Frankfurt (Germany)
January 2015	*Nuclear quantum effects in water: a multiscale study* - Theoretical Chemistry Seminar, Goethe University, Frankfurt (Germany)
September 2014	*Nuclear quantum effects in water: a multiscale study* - Theoretical Physics Seminar, Universidad Autonoma de Madrid, Madrid (Spain)
September 2014	*Nuclear quantum effects in water: a multiscale study* - Theoretical Physics Seminar, Jozef Stefan Institute, Ljubljana (Slovenia)
March 2013	*Theory and practice of adaptive resolution simulations* - HYBRID2013 workshop, John von Neumann Institute for Computing, Jülich (Germany)
August 2012	*Adaptive coupling of classical and quantum description of molecular fluids* - Modeling the Dynamics of Complex Molecular Systems, Leiden (The Netherlands)
August 2012	*Coupling Classical and Quantum Mechanics in Adaptive Resolution Molecular Dynamics Simulations* - Bridging Scales in Computational Polymer Chemistry, ICERM, Providence (USA)
April 2012	*Multiscale simulations of quantum fluids* - informal talk, Kavli Institute for Theoretical Physics, Multiscale12 program, Santa Barbara (USA)
September 2011	*Quantum Locality in Low-temperature Para-Hydrogen: a multiscale study of equilibrium properties* - Statistical and Biological Physics group seminar, International School for Advanced Studies, Trieste (Italy)
February 2011	*Similarities and differences in knotted-unknotted protein pairs - evidence for knot-promoting loops* - Physics Department of Gutenberg University, Mainz (Germany)