Raffaello Potestio, Ph.D.
Curriculum Vitæ et Studiorum
September 2021

Personal Data

Name:	Raffaello Potestio, I
Date of birth:	
Place of birth:	
Citizenship:	
Current position:	Associate professor
Institute:	Physics Department - University of Trento
Email address:	raffaello.potestio@unitn.it
Personal homepage:	http://variamols.physics.unitn.eu
ORCID:	0000-0001-6408-9380

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 (PREVIOUS SUPERVISORS)

Prof. Kurt Kremer
Max Planck Institute for Polymer Research
Ackermannweg 10, 55128 Mainz (Germany)
Office: +49-(0)6131-379-141
e-mail: kremer@mpip-mainz.mpg.de

Prof. Cristian Micheletti
SISSA - International School for Advanced Studies
Via Beirut 2-4 - 34151 Trieste - Italy
Office: +39-(0)40-3787-300
e-mail: michelet@sissa.it

APPOINTMENTS

2021–present	Associate professor at the University of Trento, Physics Dept.
2018–2020	Tenure track assistant professor (RTDB) at the University of Trento, Physics Dept.
2013–2017	Project Leader at Max Planck Institute for Polymer Research
2010–2013	PostDoc position and fellowship at Max Planck Institute for Polymer Research
2006–2010	PhD position and fellowship at SISSA

ADMINISTRATIVE ROLES IN SCIENTIFIC ORGANISATIONS

October 2018–present Co-responsible for the University of Trento's Joint Degree in Physics programme with SISSA and the Double Master Degree programme with the University of Tübingen

October 2018–present Scientific Representative of the COST Action EUTOPIA - European Topology Interdisciplinary Action

October 2018–November 2019 Chair of the COST Action EUTOPIA - European Topology Interdisciplinary Action

PUBLICATION HIGHLIGHTS

- M. Giulini, R. Menichetti, M. S. Shell, and R. Potestio, An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules, J. Chem. Theor. Comput. (2020)
- P. Diggins, C. Liu, M. Deserno, R. Potestio, Optimal coarse-grained site selection in elastic network models of biomolecules, J. Chem. Theor. Comput. (2018)
- M. Heidari, K. Kremer, R. Cortes-Huerto, R. Potestio, Spatially Resolved Thermodynamic Integration: An Efficient Method To Compute Chemical Potentials of Dense Fluids, J. Chem. Theor. Comput. (2018)
- 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)
- 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 SEPTEMBER 17, 2021)

- Number of publications: 52 articles in peer reviewed journals; 2 book chapter; 4 review articles
- Number of peer-reviewed publications without PhD supervisor: 51
- Citations: 1043 (Publons) | 1464 (Google Scholar)
- H-index: 20 (Publons) | 22 (Google Scholar)

PUBLICATIONS | PEER-REVIEWED JOURNALS

[OA]: open access journals | **[ERC]**: ERC-supported publications (implicitly open access)

53. **[OA]** L. F. Signorini, C. Perego, and R. PotestioProtein self-entanglement modulates successful folding to the native state: A multi-scale modeling study, J. Chem. Phys. (2021)
52. **[OA]** L. Tubiana, H. Kobayashi, R. Potestio, B. Duenweg, K. Kremer, P. Virnau, and K. Daoulas, Comparing equilibration schemes of high-molecular-weight polymer melts with topological indicators, Journal of Physics: Condensed Matter (2021)
51. **[ERC]** F. Errica, M. Giulini, D. Bacciu, R. Menichetti, A. Micheli, and R. Potestio, A deep graph network-enhanced sampling approach to efficiently explore the space of reduced representations of proteins, Front. Mol. Biosci. (2021)
50. **[ERC]** A. Baptista, R. Chandra Dutta, M. Sevilla, M. Heidari, K. Kremer, R. Potestio, and R. Cortes-Huerto, Density-Functional-Theory Approach to the Hamiltonian Adaptive Resolution Simulation Method, Journal of Physics: Condensed Matter (2021)
49. **[ERC]** M. Giulini, R. Menichetti, M. S. Shell, and R. Potestio, An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules, J. Chem. Theor. Comput. (2020)
48. **[ERC]** R. Fiorentini, K. Kremer, and R. Potestio, Ligand-protein interactions in lysozyme investigated through a dual-resolution model, Proteins (2020)
47. **[ERC]** M. Heidari, K. Kremer, R. Golestanian, R. Potestio, and R. Cortes-Huerto, Open-Boundary Hamiltonian adaptive resolution. From grand canonical to non-equilibrium molecular dynamics simulations, J. Chem. Phys. (2020)
46. I. Tabujew, M. Heidari, C. Freidel, M. Helm, L. Tebbe, U. Wolfrum, K. Nagel-Wolfrum, K. Koynov, P. Biehl, F. H. Schacher, R. Potestio, and K. Peneva, Tackling the Limitations of Copolymeric Small Interfering RNA Delivery Agents by a Combined Experimental-Computational Approach, Biomacromolecules (2019)
45. **[OA]** M. Heidari, R. Cortes-Huerto, R. Potestio, and K. Kremer, Steering a solute between coexisting solvation states: Revisiting nonequilibrium work relations and the calculation of free energy differences, J. Chem. Phys. (2019)
44. **[OA]** C. Perego and R. Potestio, Searching the Optimal Folding Routes of a Complex Lasso Protein, Biophysical Journal (2019)
43. **[ERC]** M. Giulini and R. Potestio, A deep learning approach to the structural analysis of proteins, Royal Society Interface Focus (2019)
42. **[ERC]** E. Riccardi, S. Pantano and R. Potestio, Envisioning data sharing for the biocomputing community, Royal Society Interface Focus (2019)

41. R. Erban, S. Harris and R. Potestio, Multi-resolution simulations of intracellular processes, Royal Society Interface Focus (2019) [Introduction to the Interface Focus theme issue Multi-resolution simulations of intracellular processes organised by Radek Erban, Sarah Harris and Raffaello Potestio]

40. **[ERC]** T. Tarenzi, V. Calandrini, R. Potestio, P. Carloni, Open-Boundary Molecular Mechanics/Coarse-Grained Framework for Simulations of Low-Resolution G-Protein-Coupled Receptor-Ligand Complexes, J. Chem. Theor. Comput. (2019)

39. **[ERC]** P. Diggins, C. Liu, M. Deserno, R. Potestio, Optimal coarse-grained site selection in elastic network models of biomolecules, J. Chem. Theor. Comput. (2019)

38. M. Heidari, K. Kremer, R. Cortes-Huerto, R. Potestio, Spatially Resolved Thermodynamic Integration: An Efficient Method To Compute Chemical Potentials of Dense Fluids, J. Chem. Theor. Comput. (2018)

37. **[OA]** M. Heidari, K. Kremer, R. Potestio, R. Cortes-Huerto, Fluctuations, finite size effects and the thermodynamic limit in computer simulations: Revisiting the spatial block analysis method, Entropy (2018)

36. **[OA]** M. Heidari, K. Kremer, R. Potestio, R. Cortes-Huerto, Finite-size integral equations in the theory of liquids and the thermodynamic limit in computer simulations, Mol. Phys. 1–10 (2018)

35. **[OA]** M. Heidari, R. Cortes-Huerto, K. Kremer, R. Potestio, Concurrent coupling of realistic and ideal models of liquids and solids in hamiltonian adaptive resolution simulations, Eur. Phys. J. E, 41 (2018)

34. K. Kreis, K. Kremer, R. Potestio, M. E. Tuckerman, From classical to quantum and back: Hamiltonian adaptive resolution path integral, ring polymer, and centroid molecular dynamics, J. Chem. Phys. 147, 244104 (2017)

33. H. Sharifi Dehsari, M. Heidari, A. Halda Ribeiro, W. Tremel , G. Jakob , D. Donadio, R. Potestio, K. Asadi, Combined Experimental and Theoretical Investigation of Heating Rate on Growth of Iron Oxide Nanoparticles, Chem. Mater. 29 (22) (2017)

32. **[OA]** T. Tarenzi, V. Calandrini, R. Potestio, A. Giorgetti, P. Carloni, Open Boundary Simulations of Proteins and Their Hydration Shells by Hamiltonian Adaptive Resolution Scheme, J. Chem. Theory Comput. 13 (11) (2017)

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. **[OA]** 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. **[OA]** 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]** M. Giulini, M. Rigoli, G. Matiotti, R. Menichetti, T. Tarenzi, R. Fiorentini and R. Potestio, From system modelling to system analysis: the impact of resolution level and resolution distribution in the computer-aided investigation of biomolecules, Front. Mol. Biosci. (2021)
- **[OA]** C. Perego and R. Potestio, Computational methods in the study of self-entangled proteins: a critical appraisal, Journal of Physics: Condensed Matter (2019)
- M. Praprotnik, R. Cortes-Huerto, R. Potestio, L. Delle Site, Adaptive Resolution Molecular Dynamics Technique, *Handbook of Materials Modeling: Methods: Theory and Modeling*, 1-15 (2018)
- **[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)

GRANTS AND AWARDS

May 2021	Partner of the project *CheEntropia!* funded by CARITRO - Cassa di Risparmio di Trento e Rovereto
October 2020	Co-PI of the project *AIACE - Artificial Intelligence Tracking Algorithms of Covid-19 Epidemics* funded by the University of Trento
June 2020	Project *HAMMOCK - Hybrid atomistic / coarse-grained molecular modelling with consistent kinetics* funded by the call FARE (Italian Ministry of University and Research)

August 2019	Partner of the EUREGIO Mobility Fund for the project *HPCDSI - High performance computing in computational data science* funded by the Euroregion Trentino - South Tyrol - Tyrol
July 2019	Partner of the project *SPGAS - Smart and Parallel Graph Analytics System* funded by the Free University of Bozen
January 2018	Recipient and PI of the ERC Starting Grant *VARIAMOLS - variable resolution algorithms for macromolecular simulations*
February 2016	Project contributor of a project proposal for HPC Access to the JURECA supercomputer at the Forschungszentrum Jülich
May 2014	Co-PI of a Project (B4) of the Collaborative Research Center / Transregio TRR 146 (4 years time window, 165,400 euro assigned to the B4 project)
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

Supervision of graduate students and postdocs

2013 - 2020	Supervision of 7 PhD students (4 graduated, 3 running), supervision of 5 Postdocs (3 running)

Reviewing and editorial Activity

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

June 2020	Review Editor on the Editorial Board of Polymer Chemistry (specialty section of Frontiers in Chemistry and Frontiers in Materials)

Workshop organisation

January 2020	Co-organiser of the winter school Physics of the Cell, University of Trento, Italy
September 2019	Scientific and high performance computing school 2019, University of Trento, Italy
November 2018	Scientific and high performance computing school 2018, University of Trento, Italy
September 2018	Royal Society Theo Murphy meeting Multi-resolution simulations of intracellular processes in Newport Pagnell, Buckinghamshire, United Kingdom
September 2018	CECAM workshop Computational biophysics on your desktop: is that possible? at the University of Trento, Italy
March 2017	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	MPIP Theory Group Retreat in Berlin
June 2015	6th Mainz Materials Simulation Days (MMSD) workshop, focussing on *Non-equilibrium Processes in Soft Matter*

TEACHING ACTIVITY

WS 2020-2021	Full master course on *Statistical Mechanics*, Physics dept., University of Trento (Italy)
SS 2020-2021	Full master course on *Multi-Scale Methods in Soft Matter Physics*, Physics dept., University of Trento (Italy)
Nov. 2020	4 lectures on *Applications of Statistical Mechanics to Biology* (PAF - Percorso di Approfondimento in Fisica), Physics dept., University of Trento (Italy)
WS 2020-2021	Full master course on *Statistical Mechanics*, Physics dept., University of Trento (Italy)
SS 2019-2020	Full master course on *Multi-Scale Methods in Soft Matter Physics*, Physics dept., University of Trento (Italy)
WS 2019-2020	Full master course on *Statistical Mechanics*, Physics dept., University of Trento (Italy)
SS 2018-2019	Full master course on *Multi-Scale Methods in Soft Matter Physics*, Physics dept., University of Trento (Italy)
Nov.-Dec. 2018	4 lectures on *Applications of Statistical Mechanics to Biology* (PAF - Percorso di Approfondimento in Fisica), Physics dept., University of Trento (Italy)
Jun. 2017	4 lectures on *Theoretical and Computational Methods in Soft Matter Physics*, Physics dept., University of Trento (Italy)
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

September 2021	*Communication pathways in an IgG4 antibody: a multiscale study*, invited online talk at the *ICTP-SISSA-CECAM Workshop on Molecular Dynamics and its Applications to Biological Systems*, Trieste (Italy)
September 2021	*Optimal reduced representations and multiple resolution models of biomolecules*, invited online talk at the *Mathematics of Life* conference, Hisarya (Bulgaria)
June 2020	*Exploring the crossroad between information theory, statistical mechanics, and biology* - invited online talk at the GSSI-Gran Sasso Science Institute - L'Aquila (Italy)

February 2020 *On the algorithmic identification of optimal coarse-grained representations of biomolecules* - invited talk at the *Biophysical Society Meeting* - San Diego, California (USA)

February 2020 *Simple, but not simpler - On representation, information, and molecular modelling* - invited talk at the University of California Davis, Chemistry Dept. (USAs)

February 2020 *Simple, but not simpler - In search of the optimal level of coarse-graining* - invited talk at the conference *Physics of biomolecules: structure, dynamics and function* - Bressanone (Italy)

December 2019 *Variable resolution models for multi-scale simulations of complex biomolecules* - invited talk at the conference *Photonic reservoir computing and information processing in complex networks* - Trento (Italy)

June 2019 *On the algorithmic identification of optimal coarse-grained representations of biomolecular structures* - invited talk at the *X Brazilian Meeting on Simulational Physics* - Ouro Preto (Brazil)

June 2019 *Searching the optimal folding routes of a complex lasso protein* - invited talk at the *Integrative Approaches to Protein Folding and Aggregation* workshop -Lisbon (Portugal)

December 2018 *Systematic and non-uniform coarse-graining of biopolymers* - invited talk at the Free University of Bozen, Faculty of Computer Science - Bozen (Italy)

September 2018 *Uniform vs. position-dependent coarse-graining: challenges and opportunities from variable resolution biomolecular modelling* - invited talk at the Royal Society meeting *Multi-resolution simulations of intracellular processes* - Newport Pagnell, Buckinghamshire (United Kingdom)

September 2018 *Fifty shades of coarse-grain - The hot topic of multiple resolution models* - invited talk at the CECAM workshop *New frontiers in particle-based multiscale and coarse-grained modeling*, MPIP Mainz (Germany)

June 2018 *Coarse-graining in soft matter - from practical tool to philosophical viewpoint* - invited talk at the *Physics and Chemistry of Biological Systems alumni workshop*, SISSA, Trieste (Italy)

March 2018 *Characterisation of the free energy landscape of self-entangled polymers* - invited talk at the University of Padua (Italy)

March 2018 *The devil is in the atomistic detail - Problems and solutions in computational soft matter*, invited talk at the University of Pavia (Italy)

February 2018 *Multi-scale approaches to the study of topological self-entanglement in biopolymers* - invited talk at the *IUPAC MODSIM workshop 2018*, Milan (Italy)

February 2018 *50 shades of coarse-grain - multiple resolution protein modeling* - invited talk at the *5th workshop Physics of biomolecules: structure, dynamics, and function*, Bressanone (Italy)

November 2017 *Looking at Nature with bifocal glasses - The problems of representation, mapping, and multiple resolution in computational soft and biological matter modeling* - invited talk at the University of Freiburg (Germany)

June 2017 *Adaptive resolution methods in soft matter simulations* - invited talk at the University of Trento (Italy)

April 2017 *Multi-resolution approaches for simulations of biomolecules: from simple liquids to proteins* - invited talk at the Bioexcel workshop *Hybrid methods in molecular simulation* in Cagliari (Italy)

February 2017 *Multi-resolution modelling for biomolecular simulations* - invited talk at the CECAM workshop *Challenges across Large-Scale Biomolecular and Polymer Simulations* at the University of Vienna (Austria)

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)