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# Matej Praprotnik

*Professor of Physics*

## Education

- 2003 **Ph.D. Physics**, *University of Ljubljana*.
- 1998 **B.S. Physics**, *University of Ljubljana*.

## Current Position(s)

- 2018– **Professor of Physics**, *Department of Physics*, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia.
- 2018– **Head of Laboratory**, *Laboratory for Molecular Modeling, Theory Department*, National Institute of Chemistry, Ljubljana, Slovenia.
- 2017– **Research Professor**, *Laboratory for Molecular Modeling*, National Institute of Chemistry, Ljubljana, Slovenia.

## Previous Positions

- 2019–2020 **Head of Department (Rotational)**, *Theory Department*, National Institute of Chemistry, Ljubljana, Slovenia.
- 2017–2018 **Acting Head of Department**, *Department of Molecular Modeling*, National Institute of Chemistry, Ljubljana, Slovenia.
- 2013–2018 **Associate Professor of Physics**, *Department of Physics*, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia.
- 2008–2013 **Assistant Professor of Physics**, *Department of Physics*, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia.
- 2004–2008 **Postdoctoral Researcher**, *Theory Group*, Max Planck Institute for Polymer Research, Mainz, Germany.
- 2003–2017 **(Senior, Postdoctoral) Research Associate**, *Laboratory for Molecular Modeling*, National Institute of Chemistry, Ljubljana, Slovenia.
- 2002–2005 **Teaching Assistant**, *Department of Physics*, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia.
- 1998–2003 **Young Researcher**, *Laboratory for Molecular Modelling and NMR Spectroscopy*, National Institute of Chemistry, Ljubljana, Slovenia.

## Visiting Positions

- 2017–2018 **Academic Guest**, *Computational Science & Engineering Laboratory*, ETH Zurich, Switzerland. (6 months)

- 2013 **Visiting Scientist**, *Kavli Institute for Theoretical Physics China*, Chinese Academy of Sciences, Beijing, China.  
(1 month)
- 2012 **Member**, *The Kavli Institute for Theoretical Physics*, University of California, Santa Barbara, USA.  
(2 months)
- 2009–2010 **Academic Guest**, *Computational Science & Engineering Laboratory*, ETH Zurich, Switzerland.  
(6 months)
- 2008 **General Member**, *Institute for Mathematics and its Applications*, University of Minnesota, Minneapolis, USA.  
(1 month)

## Honors and Awards

- 2020 **ERC Advanced Grant 2019**.  
European Research Council
- 2019 **Pregl Award for Exceptional Achievements in the Field of Chemistry and Related Disciplines**.  
National Institute of Chemistry
- 2004 **National Institute of Chemistry Award for Outstanding Doctoral Work**.  
National Institute of Chemistry

## Grants and Fellowships

- 2021– **Principal Investigator**, *Multiscale Modeling and Simulation Approaches for Biomedical Ultrasonic Applications*, ERC-2019-ADG MULTraSonicA, funding: European Research Council.  
2.5M EUR
- 2021– **Principal Investigator**, *Multiscale Simulations of Fluid Flows in Nanomaterials*, Basic Research Project J1-3027, funding: Slovenian Research Agency (ARRS).  
1.10 FTE/year
- 2020– **Program Leader**, *Multiscale Modeling and Simulation of Soft and Biological Matter in and out of Equilibrium*, Basic Research Program P1-0002, funding: Slovenian Research Agency (ARRS).  
3.68 FTE/year
- 2019– **Work-Package Leader**, *Advanced Magnetic Nanoparticles for Detection and Quantification of Biomarkers in Biological Fluids*, M-ERA.NET Consortium BIOMAG, funding: Ministry of Education, Science and Sport (MIZŠ), Slovenia.  
1.00 FTE/year
- 2018– **Principal Investigator**, *Supramolecular Self-Assembly in Open Molecular Systems*, Bilateral Project BI-US/18-20-043 between Slovenia and USA, funding: Slovenian Research Agency (ARRS).
- 2018– **Principal Investigator**, *Self-Assembly and Nonequilibrium Response in Polymer-Nanoparticle Mixtures*, Bilateral Project Bi-CN/18-20-014 between Slovenia and China, funding: Slovenian Research Agency (ARRS).
- 2017 **Visiting Researcher**, *Multiscale Modeling for Solvents*, Fellowship to visit ERC Grantee, funding: Slovenian Research Agency (ARRS).
- 2017–2019 **Program Leader**, *Mathematical and Simulation Methods in Studies of Molecular Structure and Dynamics and Non-Equilibrium Statistical Mechanics*, Basic Research Program P1-0002, funding: Slovenian Research Agency (ARRS).  
3.68 FTE/year

- 2011–2014 **Principal Investigator**, *Computer Simulations of Fluid Flow - Matter Interactions at Multiple Length Scales*, Basic Research Project J1-4134, funding: Slovenian Research Agency (ARRS).  
1.48 FTE/year
- 2011–2012 **Principal Investigator**, *Multiscale Simulations of Fluid Flows*, Bilateral Project BI-DK/11-12-002 between Slovenia and Denmark, funding: Slovenian Research Agency (ARRS).
- 2009–2012 **Principal Investigator**, *Development and Application of Multiscale Modeling Approaches for Simulation of Soft Matter*, Basic Research Project J1-2281, funding: Slovenian Research Agency (ARRS).  
0.81 FTE/year

## Supervision of Graduate Students and Postdoctoral Fellows

- 2020– **Dr. Jaka Sočan**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.
- 2020– **Nikolaos Ntarakas**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2020– **Dr. Amaury Coste**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.
- 2020– **Dr. Tilen Potisk**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.
- 2019– **Ema Slejko**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2018– **Petra Papež**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2018–2019 **Dr. Aleksandar Popadić**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.  
Currently: Software Developer, *freiheit.com technologies gmbh*, Hamburg, Germany
- 2017–2020 **Dr. Jurij Sablič**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.  
Currently: Postdoctoral Fellow, Department of Fundamental Physics, University of Barcelona, Spain
- 2016–2018 **Matija Kuclar**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.  
Currently: Research Assistant, Faculty of Medicine, University of Ljubljana, Slovenia
- 2015–2016 **Dr. Julija Zavadlav**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.  
Currently: Assistant Professor, Department of Mechanical Engineering, Technical University of Munich, Germany
- 2013–2018 **Aleksandar Popadić**, *Ph.D. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2013–2016 **Dr. Staš Bevc**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.  
Currently: Director of Gocan d.o.o., Parecag, Slovenia
- 2013 **Aleksandar Popadić**, *B.S. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2012–2017 **Jurij Sablič**, *Ph.D. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2012 **Jurij Sablič**, *B.S. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2011–2015 **Julija Zavadlav**, *Ph.D. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.
- 2009–2013 **Staš Bevc**, *Ph.D. Computer Science*, Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska.

## Teaching Activities

- 2013– **Lecturer – Molecular Biophysics**, *2<sup>nd</sup> Cycle Master Study Program in Physics*, Faculty of Mathematics and Physics, University of Ljubljana.

## Organization of Scientific Meetings

- 2022 **Minisymposia & Posters Program Committee Member**, *PASC22*, Basel, Switzerland.
- 2021 **Organisation & Programme Committee Member**, *EuroHPC Summit Week 2021*, Porto, Portugal.
- 2019 **Organizer**, *Get-to-know meeting CECAM: SISSA/Ljubljana*, Postojna, Slovenia.
- 2019 **Organizing Committee Member**, *CECAM & IUPAP Workshop – High Density DNA Arrays: Models, Theories and Multiscale Simulations*, Ljubljana, Slovenia.

- 2019 **Organisation & Programme Committee Member**, *EuroHPC Summit Week 2019*, Poznań, Poland.
- 2018 **Programme Committee Member**, *PRACE Autumn School 2018 – HPC for Engineering and Chemistry*, Ljubljana, Slovenia.
- 2018 **International Scientific Committee Member**, *32nd Conference of the European Colloid and Interface Society (ECIS)*, Ljubljana, Slovenia.
- 2018 **Organisation & Programme Committee Member**, *European HPC Summit Week 2018*, Ljubljana, Slovenia.
- 2018 **Scientific Committee Member**, *Regional Biophysical Conference (RBC 2018)*, Zreče, Slovenia.
- 2017 **Organizing Committee Member**, *Biophysical Days 2017*, Rogla, Slovenia.
- 2017 **Local Organizing Committee Member**, *Liquids 2017 – 10th Liquid Matter Conference*, Ljubljana, Slovenia.

### Institutional Responsibilities

- 2018– **Scientific Council Member**, *National Institute of Chemistry*.
- 2013–2017 **Pregl Award for Outstanding Doctoral Work Committee Member**, *National Institute of Chemistry*.

### Commissions of Trust

- 2021– **Member**, *Scientific Research Council*, Natural and Mathematical Sciences, Slovenian Research Agency.
- 2020– **Leadership Committee Member**, *International COVID-19 HPC Knowledge Exchange*, XSEDE-PRACE Webinar Series.
- 2020–2021 **Selection Committee Member**, *PRACE COVID-19 Fast Track Call for Proposals*.
- 2020–2021 **Member**, *PRACE Board of Directors*.
- 2020–2021 **Chair**, *PRACE Scientific Steering Committee*.
- 2019–2020 **Vice-Chair**, *PRACE Scientific Steering Committee*.
- 2019– **Supervisory Board Member**, *Slovenian Biophysical Society*.
- 2019– **Management Committee Member**, *COST Action CA18127: International Nucleome Consortium*.
- 2017– **Council Member**, *CECAM (Centre Européen de Calcul Atomique et Moléculaire)*.
- 2017–2019 **Review Panel Member**, *International Peer Review Panel in Mechanics, Materials and Mechatronics*, Independent Research Fund Denmark | Technology and Production Sciences.
- 2016– **Scientific Steering Committee Member**, *PRACE (Partnership for Advanced Computing in Europe)*.
- 2015–2019 **President**, *Slovenian Biophysical Society*.
- 2011–2019 **Executive Board Member**, *Slovenian Biophysical Society*.

### Editorial Boards

- 2019– **Editorial Board Member**, *Polymers*, MDPI.
- 2018– **Editorial Board Member**, *Scientific Reports*, Nature Research.

### Alternative Civilian Service

- 2001–2002 **Researcher**, *Department of Digital Communication and Computer Networks*, Jožef Stefan Institute, Ljubljana, Slovenia.  
7 months

## Reviewing Activities

- **Journals:** Phys. Rev. Lett., Phys. Rev. E, EPL, EPJP, EPJST, J. Chem. Phys., J. Comput. Phys., Comput. Phys. Commun., PNAS, JACS, J. Chem. Theory Comput., ACS Omega, PCCP, J. Comput. Chem., Chem. Phys. Lett., Soft Matter, Soft Materials, Mol. Sim., J. Chem. Inf. Model, Microfluid Nanofluid., ChemPhysChem, RSC Advances, Mathematics, Sci. Rep., Phil. Trans. R. Soc. A, Chem. Sci., CICP, Computation, Polymers, Symmetry, J. Mol. Liq., Comput. Mater. Sci., J. Biomol. Struct. Dyn.
- **Funding Agencies:** European Research Council (ERC), Swiss National Science Foundation (SNSF), ETH Zurich Research Commission, German Research Foundation (DFG), German Academic Exchange Service (DAAD), Croatian Science Foundation (HRZZ), Independent Research Fund Denmark (IRFD), National Science Centre (NCN) Poland, KU Leuven.
- **Ph.D. Examinations and other Promotions:** University of Ljubljana (Slovenia), National Institute of Chemistry (Slovenia), Jožef Stefan Institute (Slovenia), University of Grenoble (France), KU Leuven (Belgium), Queen Mary University of London (UK), University of Piemonte Orientale (Italy).
- **Research Group Evaluation:** Institute of Physics, Chinese Academy of Sciences (China).

## Memberships of Scientific Societies

- Slovenian Biophysical Society
- Society of Mathematicians, Physicists and Astronomers of Slovenia (DMFA)
- Slovenian Chemical Society
- German Physical Society (DPG)
- American Physical Society (APS)
- Society for Industrial and Applied Mathematics (SIAM)
- Biophysical Society

## Research Interests

At present, my research is focused on *computer simulation of soft & biological matter*. The focus is on developing and applying innovative *computational* and *theoretical* methods augmented by *machine learning* techniques to study complex molecular systems. My main research interests, which are at the interface of *computational (bio)physics*, *chemistry*, and *applied mathematics*, include: **multiscale modeling & simulation**, **open boundary molecular simulations**, and **nanofluidics**.

## Invited Talks and Lectures

55. *Multiscale simulations of open molecular systems*. JSI Colloquia, Jožef Stefan Institute, Slovenia, November 24, 2021.
54. *Use of urgent supercomputing in tackling the pandemic*. From Open Data to Innovation: 2nd NI4OS-Europe Dissemination Event in Slovenia collocated with the Network of Knowledge 2021 Conference, Slovenia, November 24, 2021.
53. *Multiscale simulations of open molecular systems*. CRC 1114, Scaling Cascades in Complex Systems, FU Berlin, Germany, March 3, 2021.
52. *Open Boundary Molecular Dynamics of DNA*. 9th Minisymposium of the SFB TRR 102, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany, February 5, 2021.
51. *Open Boundary Molecular Dynamics of DNA*. Theoretical and Computational Biophysics Group, Beckman Institute for Advanced Science & Technology, University of Illinois at Urbana-Champaign, USA, February 3, 2020.
50. **Plenary lecture:** *Scientific case for computing in Europe 2018-2026*. The 15th International Symposium on Operations Research in Slovenia - SOR'19, Bled, Slovenia, September 25-27, 2019.
49. *Mixed resolution schemes*. CECAM/IRTG school: Bio/Soft Matter Simulations across Multiple Scales, Crowne

- Plaza Hotel, Heidelberg, Germany, September 18-20, 2019.
48. *Rotation of star polymers under shear flow: Application of the Eckart frame to soft matter*. Public Seminar, Max Planck Institute for Polymer Research, Mainz, Germany, July 23, 2019.
  47. *Multi-resolution techniques*. Summer School in Multi-Scale Modelling, Lorentz Center, Leiden, the Netherlands, June 17-21, 2019.
  46. *Open Boundary Molecular Dynamics of biomolecular systems*. Out of Equilibrium Soft Matter Systems - From Driven to Active Systems, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, Beijing, China, May 19-24, 2019.
  45. *Open Boundary Molecular Dynamics of DNA*. Institute of Physics, Chinese Academy of Sciences, Beijing, China, January 23, 2019.
  44. *Concurrent coupling of MD and DPD*. Coupling and Linking Simulations - EMMC Expert Meeting and Roadmap, CECAM-HQ-EPFL, Lausanne, Switzerland, November 8-9, 2018.
  43. *Open Boundary Molecular Dynamics of a DNA molecule in a hybrid explicit/implicit salt solution*. Advances in Computational Statistical Physics, CIRM, Marseille, France, September 17-21, 2018.
  42. *Open Boundary Molecular Dynamics of DNA*. CECAM Workshop: Computational Biophysics on your Desktop: Is that Possible?, University of Trento, Trento, Italy, September 3-6, 2018.
  41. *Multiscale simulations of biomolecular systems*. CANES (Cross-Disciplinary Approaches to Non-Equilibrium Systems) Seminar Series, King's College London, London, UK, May 23, 2018.
  40. *Adaptive resolution simulations coupling atomistic water to dissipative particle dynamics*. "Multiscale and Non-Continuum Flows", Special Interest Group, Queen Mary University of London, London, UK, April 18, 2018.
  39. *Adaptive resolution simulations coupling atomistic to supramolecular water models*. PASC17 MS "Particle-based Methods for Simulations in Life Sciences, Fluids and Materials", Lugano, Switzerland, June 26-28, 2017.
  38. *Multiscale simulations of DNA*. Bioorigami - Designed Bionanostructures from Nucleic Acids to Proteins and beyond, National Institute of Chemistry, Ljubljana, Slovenia, June 21-23, 2017.
  37. *Open Boundary Molecular Dynamics Simulation*. Seminar SBP, SISSA, Trieste, Italy, June 8, 2017.
  36. *Adaptive resolution simulations of supramolecular water*. E-CAM Workshop: State of the Art in Mesoscale and Multiscale Modeling, CECAM-IRL, Dublin, Ireland, May 29-June 1, 2017.
  35. *Adaptive resolution simulations of DNA*. Multiscale Modeling and Experimental Approaches to Genome Organization, Ecole de Physique, Les Houches, France, April 2-7, 2017.
  34. *Adaptive resolution simulations of supramolecular water models*. First Workshop on Hybrid Methods in Molecular Simulation, University of Cagliari, Cagliari, Italy, April 3-4, 2017.
  33. *Open Boundary Molecular Dynamics*. Scaling Cascades in Complex Systems, FU Berlin, Berlin, Germany, March 27-29, 2017.
  32. *Concurrent coupling of atomistic and supramolecular water models*. COST Action MP1305 Flowing Matter WG2+WG3 Meeting, Erlangen, Germany, February 28-March 3, 2017.
  31. *Adaptive resolution simulations coupling atomistic models to MARTINI*. Multiscale Simulation Methods in Soft Matter Systems II, Darmstadt, Germany, October 4-6, 2016.
  30. *Open boundary molecular dynamics of sheared star-polymer melt*. 12th World Congress on Computational Mechanics (WCCM XII) in 6th Asia-Pacific Congress on Computational Mechanics (APCOM VI), Seoul, Korea, July 24-29, 2016.
  29. *Adaptive resolution simulation of polarizable supramolecular water models*. 13th US National Congress on Computational Mechanics, San Diego, CA, USA, July 26-30, 2015.
  28. *Adaptive resolution simulations of supramolecular coarse-grained water models*. ZCAM Workshop: Molecular Hydrodynamics Meets Fluctuating Hydrodynamics, Residencia La Cristalera, Miraflores de la Sierra, Madrid, Spain, May 10-14, 2015.
  27. *Napredne metode simulacij molekulske dinamike - večskalne simulacije z uporabo polja sil MARTINI, odprte simulacije molekulske dinamike in hibridne metode za simulacijo nanofluidike*. 2. mednarodna spomladanska šola fizike - delavnice iz biofizike, Maribor, Slovenia, May 5-12, 2015.
  26. *Simulacije z uporabo metode AdResS: sklopitev atomistične in grobozrnate resolucije*. 2. mednarodna spomladanska šola fizike - delavnice iz biofizike, Maribor, Slovenia, May 5-12, 2015.
  25. *Multiscale simulations of water flow past/through nanoscale objects*. CECAM Workshop: Scale-Bridging

- Techniques in Molecular Simulation: A Critical Appraisal, Zuse-Institut Berlin (ZIB), Berlin, Germany, August 25-27, 2014.
24. *Adaptive resolution simulation of atomistic protein in multiscale water*. 11th World Congress on Computational Mechanics (WCCM XI) and 5th European Conference on Computational Mechanics (ECCM V) and 6th European Conference on Computational Fluid Dynamics (ECFD VI), Barcelona, Spain, July 20-25, 2014.
  23. *Open molecular dynamics simulation of star polymers*. III International Conference on Particle-Based Methods. Fundamentals and Applications (Particles 2013), Stuttgart, Germany, September 18-20, 2013.
  22. *Open molecular dynamics simulation of star polymers*. ASPM 2013 Austrian-Slovenian Polymer Meeting, Bled, Slovenia, April 3-5, 2013.
  21. *Adaptive resolution simulations coupled to continuum*. IUTAM Symposium on Particle Methods in Fluid Mechanics, Technical University of Denmark, Kgs. Lyngby, Denmark, October 15-17, 2012.
  20. *Multiscale simulation of liquids*. 12th International Conference Computational and Mathematical Methods in Science and Engineering (CMMSE), La Manga - Murcia, Spain, July 2-5, 2012.
  19. *Coupling atomistic and continuum hydrodynamics*. Modeling Soft Matter: Linking Multiple Length and Time Scales, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA, June 4-8, 2012.
  18. *Concurrent multiscale simulation of molecular liquids*. CECAM Workshop: Multiscale Modeling of Simple and Complex Liquid Flow Using Particle-Continuum Hybrids, ZCAM, Zaragoza, Spain, October 5-7, 2011.
  17. *Multiscale simulation methods for liquids*. Cambridge-Edinburgh Meeting, Department of Chemistry, University of Cambridge, Cambridge, UK, April 26-27, 2011.
  16. *Multiscale simulations of fluids*. INRIA, Grenoble, France, April 20, 2011.
  15. *Hybrid methods for multiscale simulation of liquids*. ETHZ - CECAM - ESF Workshop in Multiscale Modeling and Simulation, Kartause Ittingen, Switzerland, October 19-22, 2010.
  14. *Linking atomistic and continuum hydrodynamics*. Novel Simulation Approaches to Soft Matter Systems Workshop, Dresden, Germany, September 20-24, 2010.
  13. *Hybrid methods for multiscale flow simulations*. Regional Biophysics Conference 2010, Primošten, Croatia, September 15-18, 2010.
  12. *AdResS: Concurrent coupling of different levels of resolution in molecular simulations*. 2010 Workshop on Multiscale Molecular Modelling: Molecular Dynamics, Computational Statistical Mechanics, and Simulation Algorithms, University of Edinburgh, Edinburgh, UK, June 30 - July 3, 2010.
  11. *Linking length scales in molecular simulations*. ACAM Workshop: Dynamic Coarse-Graining: Towards Quantitative Mesoscale Modeling of Complex Fluids, ACAM, Dublin, Ireland, May 19-21, 2010.
  10. *Hybrid atomistic-continuum methods for dense liquids*. Molecular Simulations at Different Scales - Future and Perspectives on Modeling Interfaces, International Autumn School, Technische Universität Darmstadt, Darmstadt, Germany, September 24-25, 2009.
  9. *Coupling MD with continuum through a mesoscopic model*. Molecular Simulations at Different Scales - Future and Perspectives on Modeling Interfaces, International Autumn School, Technische Universität Darmstadt, Darmstadt, Germany, September 24-25, 2009.
  8. *Adaptive resolution simulation*. The 3rd Adriatic Meeting On Computational Solutions in the Life Sciences, Primošten, Croatia, September 1-5, 2009.
  7. *Adaptive resolution molecular dynamics simulation*. EPSRC Symposium Workshop on Molecular Dynamics, Mathematics Research Centre, University of Warwick, Coventry, UK, June 1-5, 2009.
  6. *Coupling atomistic and continuum hydrodynamics through a mesoscopic model*. IWoM3 2009 - International Workshop on Multiscale Materials Modeling, Harnack House, Berlin, Germany, March 10-13, 2009.
  5. *Adaptive resolution simulation of molecular liquids*. Sonderforschungsbereich (SFB) 716: Summer School "Hybridsimulationen" und Statusseminar, Universität Stuttgart, Pforzheim-Hohenwart, Germany, September 8-10, 2008.
  4. *Concurrent triple-scale simulation of molecular liquids*. Computational Science & Engineering Laboratory, ETH Zürich, Zürich, Switzerland, May 14, 2008.
  3. *Adaptive resolution simulation of liquid water*. New Developments in Computational Physics: CompPhys07 - 8th International NTZ Workshop, Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany, November 29 - December 1, 2007.
  2. *Adaptive resolution molecular dynamics simulations*. Departamento de Física Teoretica de la Materia Condensada, Universidad Autonoma de Madrid, Madrid, Spain, May 26, 2007.

1. *Fast vibrational modes in molecular simulation studies*. Through Science to Stability: 1st South Eastern European Workshop on Practical Approaches to Computational Biology, Opatija, Croatia, September 1-4, 2005.

## Publications

### Articles in Refereed Scientific Journals

63. E. Papadopoulou, J. Zavadlav, R. Podgornik, **M. Praprotnik**, P. Koumoutsakos. Tuning the dielectric response of water in nanoconfinement through surface wettability. *ACS Nano*, 2021.
62. N. Lopez, L. Del Debbio, M. Baaden, **M. Praprotnik**, L. Grigori, C. Simoes, S. Bogaerts, F. Berberich, T. Lippert, J. Ignatius, P. Lavocat, Oriol Pineda, M. G. Giuffreda, S. Girona, D. Kranzmueller, M. M. Resch, G. Scipion, T. Schulthess. Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic. *Proc. Natl. Acad. Sci. USA* **118**, e2024891118, 2021.
61. R. Cortes-Huerto, **M. Praprotnik**, K. Kremer, L. Delle Site. From adaptive resolution to molecular dynamics of open systems. *Eur. Phys. J.* **94**, 189, 2021.
60. S. Thaler, **M. Praprotnik**, J. Zavadlav. Back-mapping augmented adaptive resolution simulation. *J. Chem. Phys.* **153**, 164118, 2020.
59. L. Delle Site, **M. Praprotnik**, J. B. Bell, R. Klein. Particle–continuum coupling and its scaling regimes: Theory and applications. *Adv. Theory Simul.* **3**, 1900232, 2020.
58. A. Popadić, D. Svenšek, R. Podgornik, **M. Praprotnik**. Density–nematic coupling in isotropic linear polymers: Acoustic and osmotic birefringence. *Adv. Theory Simul.* **2**, 1900019, 2019.
57. J. Zavadlav, S. J. Marrink, **M. Praprotnik**. SWINGER: A clustering algorithm for concurrent coupling of atomistic and supramolecular liquids. *Interface Focus* **9**, 20180075, 2019.
56. A. Popadić, D. Svenšek, R. Podgornik, K. Ch. Daoulas, **M. Praprotnik**. Splay-density coupling in semiflexible main-chain nematic polymers with hairpins. *Soft Matter* **14**, 5898-5905, 2018.
55. C. Krekeler, A. Agarwal, C. Junghans, **M. Praprotnik**, L. Delle Site. Adaptive resolution molecular dynamics technique: Down to the essential. *J. Chem. Phys.* **149**, 024104, 2018.
54. J. Zavadlav, J. Sablić, R. Podgornik, **M. Praprotnik**. Open-Boundary Molecular Dynamics of a DNA molecule in a hybrid explicit/implicit salt solution. *Biophys. J.* **114**, 2352-2362, 2018.
53. J. Zavadlav, S. J. Marrink, **M. Praprotnik**. Multiscale simulation of protein hydration using the SWINGER dynamical clustering algorithm. *J. Chem. Theory Comput.* **14**, 1754-1761, 2018.
52. R. Podgornik, J. Zavadlav, **M. Praprotnik**. Molecular dynamics simulation of high density DNA arrays. *Computation* **6**, 3, 2018.
51. E. R. Cruz-Chu, E. Papadopoulou, J. H. Walther, A. Popadić, G. Li, **M. Praprotnik**, P. Koumoutsakos. On phonons and water flow enhancement in carbon nanotubes. *Nat. Nanotechnol.* **12**, 1106-1108, 2017.
50. J. Zavadlav, **M. Praprotnik**. Adaptive resolution simulations coupling atomistic water to dissipative particle dynamics. *J. Chem. Phys.* **147**, 114110, 2017.
49. J. Sablić, R. Delgado-Buscalioni, **M. Praprotnik**. Application of the Eckart frame to soft matter: Rotation of star polymers under shear flow. *Soft Matter* **13**, 6988-7000, 2017.
48. J. Zavadlav, S. Bevc, **M. Praprotnik**. Adaptive resolution simulations of biomolecular systems. *Eur. Biophys. J.* **46**, 821-835, 2017.
47. J. Zavadlav, R. Podgornik, **M. Praprotnik**. Order and interactions in DNA arrays: Multiscale molecular dynamics simulation. *Sci. Rep.* **7**, 4775, 2017.
46. L. Delle Site, **M. Praprotnik**. Molecular systems with open boundaries: Theory and simulation. *Phys. Rep.* **693**, 1-56, 2017.
45. J. Sablić, **M. Praprotnik**, R. Delgado-Buscalioni. Deciphering the dynamics of star molecules in shear flow. *Soft Matter* **13**, 4971-4987, 2017.
44. J. Zavadlav, S. J. Marrink, **M. Praprotnik**. Adaptive resolution simulation of supramolecular water: The concurrent making, breaking, and remaking of water bundles. *J. Chem. Theory Comput.* **12**, 4138-4145, 2016.
43. J. Zavadlav, R. Podgornik, M. N. Melo, S. J. Marrink, **M. Praprotnik**. Adaptive resolution simulation of an



- atomistic DNA molecule in MARTINI salt solution. *Eur. Phys. J. Special Topics* **225**, 1595-1607, 2016.
42. J. Sablić, **M. Praprotnik**, R. Delgado-Buscalioni. Open boundary molecular dynamics of sheared star-polymer melts. *Soft Matter* **12**, 2416-2439, 2016.
  41. J. Zavadlav, R. Podgornik, **M. Praprotnik**. Adaptive resolution simulation of a DNA molecule in salt solution. *J. Chem. Theory Comput.* **11**, 5035-5044, 2015.
  40. R. Delgado-Buscalioni, J. Sablić, **M. Praprotnik**. Open boundary molecular dynamics. *Eur. Phys. J. Special Topics* **224**, 2331-2349, 2015.
  39. R. Delgado-Buscalioni, J. Sablić, **M. Praprotnik**. Reply to comments by R. Klein on "Open boundary molecular dynamics". *Eur. Phys. J. Special Topics* **224**, 2511-2513, 2015.
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