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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 **Ph.D. Student**, *Laboratory for Molecular Modelling and NMR Spectroscopy*, National Institute of Chemistry, Ljubljana, Slovenia.

Visiting Positions

2025– **Member**, Universitat de Barcelona Institute of Complex Systems, University of Barcelona, Spain.

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

2022 **Zois Recognition for Important Achievements in Multiscale Modeling and Simulation of Soft and Biological Matter**.
Republic of Slovenia

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

2023– **Project Coordinator**, *Centre of Excellence in Exascale-Oriented Application Co-Design and Delivery for Multiscale Simulations*, 101093169 — MultiXscale — HORIZON-EUROHPC-JU-2021-COE-01, funding: EuroHPC JU.
6.0M EUR

2021– **Principal Investigator**, *Multiscale Modeling and Simulation Approaches for Biomedical Ultrasonic Applications*, ERC-2019-ADG MULTraSonicA, funding: European Research Council.
2.5M EUR

2021–2024 **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

2019–2022 **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

2018–2022 **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).

2018–2022 **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

2024– **Matevž Jug**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.

2024– **Dr. Petra Papež**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.

2023– **Dr. Brieuc Benvegnen**, *Postdoctoral Fellow*, Universitat de Barcelona Institute of Complex Systems, Barcelona.

2023–2025 **Dr. Nerea Alcazar Cano**, *Postdoctoral Fellow*, Universitat de Barcelona Institute of Complex Systems, Barcelona.

2023– **Urban Čoko**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.

2022– **Maša Lah**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.

2020–2024 **Dr. Jaka Sočan**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.

2020– **Nikolaos Ntarakas**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.

2020–2024 **Dr. Amaury Coste**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.
Currently: Postdoctoral Fellow, LEPMI laboratory, Grenoble, France

2020–2023 **Dr. Tilen Potisk**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.

2019– **Ema Slejko**, *Ph.D. Student*, Faculty of Mathematics and Physics, University of Ljubljana.

2018–2024 **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 Sablić**, *Postdoctoral Fellow*, National Institute of Chemistry, Ljubljana.
Currently: Postdoctoral Fellow, CECAM, EPFL, Lausanne, Switzerland

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 Sablić**, *Ph.D. Physics*, Faculty of Mathematics and Physics, University of Ljubljana.

2012 **Jurij Sablić**, *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^{nd} *Cycle Master Study Program in Physics*, Faculty of Mathematics and Physics, University of Ljubljana.

Organization of Scientific Meetings

2025 **Symposium Chair**, *EBSA2025 Symposium – Machine Learning and Agent-Based Models*, Rome, Italy.

2025 **Minisymposia & Posters Program Committee Member**, *PASC25*, Zurich, Switzerland.

2025 **Organizing Committee Member**, *CECAM Workshop – Modeling & Simulation of Fluid-Structure Interactions across Scales*, Ljubljana, Slovenia.

2024 **Organizing Committee Member**, *MMM11 Minisymposium – Multiscale Simulations of Polymers and Polymer Composites*, Prague, Czech Republic.

2024 **Program Committee Chair**, *Austrian-Slovenian HPC Meeting 2024 (ASHPC24)*, Grundlsee, Austria.

2024 **Minisymposia & Posters Program Committee Member**, *PASC24*, Zurich, Switzerland.

2023 **Organizing Committee Member**, *Symposium – Coarse-graining the Finer Structure of Macromolecular Interactions*, Ljubljana, Slovenia.

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 Commitee Member**, *Biophysical Days 2017*, Rogla, Slovenia.

2017 **Local Organizing Commitee Member**, *Liquids 2017 – 10th Liquid Matter Conference*, Ljubljana, Slovenia.

Institutional Responsibilities

2018– **Scientific Council Member**, *National Institute of Chemistry*.

2013–2021 **Pregl Award for Outstanding Doctoral Work Committee Member**, *National Institute of Chemistry*.

Commissions of Trust

2025– **Management Council Member**, *International Research Centre on Artificial Intelligence under the auspices of UNESCO (IRCAI)*, Jožef Stefan Institute.

2024– **Scientific Expert Panel Member**, *Computation-based Science and Technology Research Center (CaSToRC)*, Cyprus Institute.

2023– **Project Coordinator**, *MultiXscale — EuroHPC JU Center of Excellence*.

2022–2023 **Member**, *PRACE HPC Excellence Award Committee*.

2021–2022 **Member**, *CECAM Director Search Committee*.

2021– **Scientific Research Council Member**, *Natural and Mathematical Sciences*, Slovenian Research Agency.

2020–2021 **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*.

2019–2023 **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.

2016–2022 **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., Small, Nat. Commun.
- **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

68. *Sub-THz acoustic excitation of protein motion.* ESPResSo Summer School, CECAM-DE-SMSM, University of Stuttgart, Germany, October 7-11, 2024.
67. *Sub-THz acoustic excitation of protein motion.* Multiscale Materials Modeling (MMM11) Conference, Prague Congress Center, Prague, Czech Republic, September 22-27, 2024.
66. *MultiXscale, EuroHPC JU Centre of Excellence.* OpenModel Exploitation Workshop, Hamburg, Germany, September 17-18, 2024.
65. *Sub-THz acoustic excitation of protein motion.* Computational Modelling of Molecular Systems: from Atoms to the In-silico Design of Materials, SimEA workshop, The Cyprus Institute, Nicosia, Cyprus, May 20, 2024.
64. *Developing an implicit solvation machine learning model for molecular simulations of ionic media.* Machine Learning Modalities for Materials Science (ML4MS), Jožef Stefan Institute, Ljubljana, Slovenia, May 17, 2024.
63. *Sub-THz acoustic excitation of protein motion.* Colloquium CRC 1114, FU Berlin, Berlin, Germany, February 15, 2024.
62. **Keynote lecture**: *DPD simulation of ultrasound propagation through liquid water.* Slovenian Chemical Society Annual Meeting 2023, Portorož, Slovenia, September 13, 2023.
61. *DPD simulation of ultrasound propagation through liquid water.* 10th International Congress on Industrial

and Applied Mathematics (ICIAM 2023), Tokyo, Japan, August 24, 2023.

60. *Dissipative Particle Dynamics simulation of ultrasound propagation through liquid water.* CaSToRC - HPC National Competence Centre - EuroCC and SimEA Online Seminar Series, CaSToRC, The Cyprus Institute, Nicosia, Cyprus, November 8, 2022.
59. *Dissipative Particle Dynamics simulation of ultrasound propagation through liquid water.* Widely Applied Mathematics Seminar, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Boston, USA, October 13, 2022.
58. **Plenary lecture**: *Multiscale simulations of biomolecular systems.* Regional Biophysics Conference 2022, Pécs, Hungary, August 23, 2022.
57. *Multiscale modeling in soft and biological matter.* Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence, NOMAD-E-CAM Workshop and Hands-on Tutorial, IRIS Adlershof, Berlin, Germany, July 26, 2022.
56. *Multiscale simulations of open molecular systems.* Complex Fluids and Soft Matter (CFSM) Seminar Series, May 18, 2022.
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 Fisica 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

74. Rommie E. Amaro et al. The need to implement FAIR principles in biomolecular simulations. *Nature Methods* **22**, 641-645, 2025.
73. M. Lah, N. Ntarakas, T. Potisk, P. Papež, **M. Praprotnik**. Open-boundary molecular dynamics of ultrasound using supramolecular water models. *J. Chem. Phys.* **162**, 024103, 2025.
72. M. Jug, D. Svenšek, T. Potisk, **M. Praprotnik**. Learning macroscopic equations of motion from dissipative particle dynamics simulations of fluids. *Comput. Methods Appl. Engrg.* **432**, 117379, 2024.
71. D. Svenšek, J. Sočan, **M. Praprotnik**. Density–nematic coupling in isotropic solution of DNA: Multiscale model. *Macromol. Rapid Commun.* **45**, 2400382, 2024.
70. A. Coste, E. Slejko, J. Zavadlav, **M. Praprotnik**. Developing an implicit solvation machine learning model for molecular simulations of ionic media. *J. Chem. Theory Comput.* **20**, 411-420, 2024.
69. P. Papež, F. Merzel, **M. Praprotnik**. Sub-THz acoustic excitation of protein motion. *J. Chem. Phys.* **159**, 135101, 2023.
68. P. Papež, F. Merzel, **M. Praprotnik**. Rotational dynamics of a protein under shear flow studied by the Eckart frame formalism. *J. Phys. Chem. B* **127**, 7231-7243, 2023.
67. T. Potisk, J. Sablić, D. Svenšek, E. Sanz-de Diego, F. J. Teran, **M. Praprotnik**. Analyte-driven clustering of

bio-conjugated magnetic nanoparticles. *Adv. Theory Simul.* **6**, 2200796, 2023.
66. A. Draškovič-Bračun, T. Potisk, **M. Praprotnik**, D. Svenšek. Suspension of discrete microscopic oscillators as a model of an ultrasonic metafluid. *Phys. Rev. B* **105**, 224317, 2022.
65. P. Papež, **M. Praprotnik**. Dissipative Particle Dynamics simulation of ultrasound propagation through liquid water. *J. Chem. Theory Comput.* **18**, 1227-1240, 2022.
64. P. R. Vlachas, J. Zavadlav, **M. Praprotnik**, P. Koumoutsakos. Accelerated simulations of molecular systems through Learning of Effective Dynamics. *J. Chem. Theory Comput.* **18**, 538-549, 2022.
63. E. Papadopoulou, J. Zavadlav, R. Podgornik, **M. Praprotnik**, P. Koumoutsakos. Tuning the dielectric response of water in nanoconfinement through surface wettability. *ACS Nano* **15**, 20311-20318, 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. Kranzlmueller, 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.
38. A. Popadić, **M. Praprotnik**, P. Koumoutsakos, J. H. Walther. Continuum simulations of water flow past fullerene molecules. *Eur. Phys. J. Special Topics* **224**, 2321-2330, 2015.
37. J. Zavadlav, M. N. Melo, S. J. Marrink, **M. Praprotnik**. Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. *J. Chem. Phys.* **142**, 244118, 2015.
36. S. Bevc, C. Junghans, **M. Praprotnik**. STOCK: Structure mapper and online coarse-graining kit for molecular simulations. *J. Comput. Chem.* **36**, 467-477, 2015.
35. A. Popadić, J. H. Walther, P. Koumoutsakos, **M. Praprotnik**. Continuum simulations of water flow in carbon nanotube membranes. *New J. Phys.* **16**, 082001, 2014.
34. J. Zavadlav, M. N. Melo, A. V. Cunha, A. H. de Vries, S. J. Marrink, **M. Praprotnik**. Adaptive resolution simulation of MARTINI solvents. *J. Chem. Theory Comput.* **10**, 2591-2598, 2014.
33. J. Zavadlav, M. N. Melo, S. J. Marrink, **M. Praprotnik**. Adaptive resolution simulation of an atomistic protein in MARTINI water. *J. Chem. Phys.* **140**, 054114, 2014.
32. S. Bevc, C. Junghans, K. Kremer, **M. Praprotnik**. Adaptive resolution simulation of salt solutions. *New J. Phys.* **15**, 105007, 2013.
31. J. H. Walther, **M. Praprotnik**, E. M. Kotsalis, P. Koumoutsakos. Multiscale simulation of water flow past a C540 fullerene. *J. Comput. Phys.* **231**, 2677-2681, 2012.
30. **M. Praprotnik**, S. Poblete, K. Kremer. Statistical physics problems in adaptive resolution computer simulations of complex fluids. *J. Stat. Phys.* **145**, 946-966, 2011.
29. **M. Praprotnik**, S. Poblete, L. Delle Site, K. Kremer. Comment on "Adaptive multiscale molecular dynamics of macromolecular fluids". *Phys. Rev. Lett.* **107**, 099801, 2011.
28. S. Bevc, J. Konc, J. Stojan, M. Hodošček, M. Penca, **M. Praprotnik**, D. Janežič. ENZO: A web tool for derivation and evaluation of kinetic models of enzyme catalyzed reactions. *PLoS ONE* **6**, e22265, 2011.
27. S. Poblete, **M. Praprotnik**, K. Kremer, L. Delle Site. Coupling different levels of resolution in molecular simulations. *J. Chem. Phys.* **132**, 114101, 2010.
26. R. Delgado-Buscalioni, K. Kremer, **M. Praprotnik**. Coupling atomistic and continuum hydrodynamics through a mesoscopic model: Application to liquid water. *J. Chem. Phys.* **131**, 244107, 2009.
25. **M. Praprotnik**, S. Matysiak, L. Delle Site, K. Kremer, C. Clementi. Corrigendum: Adaptive resolution simulation of liquid water. *J. Phys.: Condens. Matter* **21**, 499801, 2009.
24. R. Delgado-Buscalioni, K. Kremer, **M. Praprotnik**. Concurrent triple-scale simulation of molecular liquids. *J. Chem. Phys.* **128**, 114110, 2008.
23. **M. Praprotnik**, L. Delle Site, K. Kremer. Multiscale simulation of soft matter: From scale bridging to adaptive resolution. *Annu. Rev. Phys. Chem.* **59**, 545-571, 2008.
22. **M. Praprotnik**, C. Junghans, L. Delle Site, K. Kremer. Simulation approaches to soft matter: Generic statistical properties vs. chemical details. *Comput. Phys. Commun.* **179**, 51-60, 2008.
21. S. Matysiak, C. Clementi, **M. Praprotnik**, K. Kremer, L. Delle Site. Modeling diffusive dynamics in adaptive resolution simulation of liquid water. *J. Chem. Phys.* **128**, 024503, 2008.
20. C. Junghans, **M. Praprotnik**, K. Kremer. Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. *Soft Matter* **4**, 156-161, 2008.
19. **M. Praprotnik**, S. Hočevar, M. Hodošček, M. Penca, D. Janežič. New all-atom force field for molecular dynamics simulation of an $AlPO_4$-34 molecular sieve. *J. Comput. Chem.* **29**, 122-129, 2008.
18. **M. Praprotnik**, S. Matysiak, L. Delle Site, K. Kremer, C. Clementi. Adaptive resolution simulation of liquid water. *J. Phys.: Condens. Matter* **19**, 292201, 2007.
17. **M. Praprotnik**, L. Delle Site, K. Kremer. A macromolecule in a solvent: Adaptive resolution molecular dynamics simulation. *J. Chem. Phys.* **126**, 134902, 2007.
16. **M. Praprotnik**, K. Kremer, L. Delle Site. Fractional dimensions of phase space variables: A tool for varying the degrees of freedom of a system in a multiscale treatment. *J. Phys. A: Math. Theor.* **40**, F281-F288, 2007.

15. **M. Praprotnik**, K. Kremer, L. Delle Site. Adaptive molecular resolution via a continous change of phase space dimensionality. *Phys. Rev. E* **75**, 017701, 2007.
14. **M. Praprotnik**, L. Delle Site, K. Kremer. Adaptive resolution scheme (AdResS) for efficient hybrid atomistic/mesoscale molecular dynamics simulations of dense liquids. *Phys. Rev. E* **73**, 066701, 2006.
13. **M. Praprotnik**, L. Delle Site, K. Kremer. Adaptive resolution molecular-dynamics simulation: Changing the degrees of freedom onthe fly. *J. Chem. Phys.* **123**, 224106, 2005.
12. **M. Praprotnik**, D. Janežič. Molecular dynamics integration meets standard theory of molecular vibrations. *J. Chem. Inf. Model* **45**, 1571-1579, 2005.
11. D. Janežič, **M. Praprotnik**, F. Merzel. Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. *J. Chem. Phys.* **122**, 174101, 2005.
10. **M. Praprotnik**, D. Janežič. Molecular dynamics integration and molecular vibrational theory. II. Simulation of non-linear molecules. *J. Chem. Phys.* **122**, 174102, 2005.
9. **M. Praprotnik**, D. Janežič. Molecular dynamics integration and molecular vibrational theory. III. The IR spectrum of water. *J. Chem. Phys.* **122**, 174103, 2005.
8. **M. Praprotnik**, D. Janežič, J. Mavri. Temperature dependence of water vibrational spectrum: A molecular dynamics simulation study. *J. Phys. Chem. A* **108**, 11056-11062, 2004.
7. R. Trobec, M. Šterk, **M. Praprotnik**, D. Janežič. Parallel programming library for molecular dynamics simulations. *Int. J. Quant. Chem.* **96**, 530-536, 2004.
6. **M. Praprotnik**, M. Šterk, R. Trobec. Inhomogeneous heat-conduction problems solved by a new explicit finite difference scheme. *International Journal of Pure and Applied Mathematics* **13**, 275-291, 2004.
5. D. Janežič, **M. Praprotnik**. Molecular dynamics integration time step dependence of the Split integration symplectic method on system density. *J. Chem. Inf. Comput. Sci.* **43**, 1922-1927, 2003.
4. M. Šterk, R. Trobec, **M. Praprotnik**. Numerical schemes for fluid flow and heat transfer in medical simulations. *Parallel and distributed computing practices* **5**, 321-329, 2002.
3. **M. Praprotnik**, D. Janežič. The Split Integration Symplectic Method. *Cell. Mol. Biol. Lett.* **7**, 147-148, 2002.
2. R. Trobec, M. Šterk, **M. Praprotnik**, D. Janežič. Implementation and evaluation of MPI-based parallel MD program. *Int. J. Quant. Chem.* **84**, 23-31, 2001.
1. D. Janežič, **M. Praprotnik**. Symplectic molecular dynamics integration using normal mode analysis. *Int. J. Quant. Chem.* **84**, 2-12, 2001.

Books and Book Chapters

8. **M. Praprotnik**, R. Cortes-Huerto, R. Potestio, L. Delle Site. Adaptive Resolution Molecular Dynamics Technique. In: W. Andreoni, S. Yip (Eds.) *Handbook of materials modeling. Volume 1 Methods: Theory and modeling*, pp. 1443-1457, Springer, Cham, 2020.
7. X. Bian, **M. Praprotnik**. Domain Decomposition Methods for Multiscale Modeling. In: W. Andreoni, S. Yip (Eds.) *Handbook of materials modeling. Volume 2 Applications: Current and emerging materials*, pp. 2551-2571, Springer, Cham, 2020.
6. Members of the PRACE SSC. Erik Lindhal (Editor-in-chief) *The scientific case for computing in Europe 2018-2026*, Insight Publishers, Bristol, 2018.
5. **M. Praprotnik**, L. Delle Site. Multiscale molecular modeling. In: L. Monticelli, E. Salonen (Eds.) *Biomolecular simulations. Methods in molecular biology (Methods and protocols)*, vol. **924**, pp. 567-583, Humana Press, Totowa, NJ, 2013.
4. D. Janežič, U. Borštnik, **M. Praprotnik**. Parallel approaches in molecular dynamics simulations. In: R. Trobec, M. Vajteršic, P. Zinterhof (Eds.) *Parallel computing: Numerics, applications, and trends*, pp. 281-305, Springer, London, 2009.
3. C. Junghans, **M. Praprotnik**, L. Delle Site. Adaptive resolution schemes. In: J. Grotendorst, N. Attig, S. Blügel, D. Marx (Eds.) *Multiscale simulation methods in molecular sciences*, NIC series, vol. **42**, pp. 359-379, Institute for Advanced Simulation, Forschungszentrum Jülich, 2009.
2. M. Šterk, R. Trobec, **M. Praprotnik**. Comparison of incompressible fluid flow simulation methods. In: R. Trobec, P. Zinterhof, M. Vajteršic, A. Uhl (Eds.) *Parallel numerics '02: Theory and applications*, pp. 149-162,

Institut Jožef Stefan; University of Salzburg, Ljubljana, 2002.

1. **M. Praprotnik**, M. Šterk, R. Trobec. A new explicit numerical scheme for nonlinear diffusion problems. In: R. Trobec, P. Zinterhof, M. Vajteršic, A. Uhl (Eds.) *Parallel numerics '02: Theory and applications*, pp. 163-176, Institut Jožef Stefan; University of Salzburg, Ljubljana, 2002.