CURRICULUM VITAE

Name Prof. Dr. Matej Praprotnik

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Education

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

Professional Experience

2017-present	Acting Head of Department, Department of Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia
2016-present	Senior Research Adviser, Department of Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia
2013-present	Associate Professor of Physics, Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia
2011-2016	Senior Research Associate, Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia
2008-2013	Assistant Professor of Physics, Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia
2006-2011	Research Associate, Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia
2004-2008	Postdoctoral Researcher, Theory Group, Max Planck Institute for Polymer Research, Mainz, Germany
2003-2006	Postdoctoral Associate, Laboratory for Molecular Modelling and NMR Spectroscopy, 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

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

Teaching Experience

Supervision	4 Ph.D. and 2 undergraduate students

Fellowships and Grants

2017-present	Program Leader, 5-year Basic Research Program P1-0002: "Mathematical and Simulation Methods in Studies of Molecular Structure and Dynamics and Non-Equilibrium Statistical Mechanics" funded by Slovenian Research Agency (ARRS)
2011-2015	Project Leader, 3-year Basic Research Project J1-4134: "Computer Simulations of Fluid Flow - Matter Interactions at Multiple Length Scales" funded by Slovenian Research Agency (ARRS)
2011-2012	Principal Investigator, 2-year Bilateral Project BI-DK/11-12-002: "Multiscale Simulations of Fluid Flows" between Slovenia and Denmark funded by Slovenian Research Agency (ARRS)
2009-2012	Project Leader, 3-year Basic Research Project J1-2281: "Development and Application of Multiscale Modeling Approaches for Simulation of Soft Matter" funded by Slovenian Research Agency (ARRS)

Honors and Awards

2004	The National Institute of Chemistry Award for Exceptional Doctoral Work

Professional Activities

2016-present	Member, PRACE Scientific Steering Committee (SSC)
2015-present	President of the Slovenian Biophysical Society
2011-2015	Member, Executive Board of the Slovenian Biophysical Society

Membership in Professional 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)

Refereeing

- *Journals*: Phys. Rev. Lett, Phys. Rev. E, EPL, EPJP, EPJST, J. Chem. Phys., J. Comput. Phys., JACS, J. Chem. Theory Comput., PCCP, J. Comput. Chem., Soft Matter, Mol. Sim., J. Chem. Inf. Model, Microfluid Nanofluid., ChemPhysChem, RSC Advances, Mathematics, Sci. Rep., Phil. Trans. R. Soc. A, Chem. Sci.
- *Funding Agencies*: German Academic Exchange Service (DAAD), Swiss National Science Foundation (SNSF), ETH Zurich Research Commission.
- *Promotions*: University of Ljubljana (Slovenia), National Institute of Chemistry (Slovenia), University of Grenoble (France).

Research Interest

At present, my research is focused on computer simulation of soft and biological matter. The focus is both on developing new simulation techniques and their application to complex molecular systems.

Invited Talks and Lectures

1. *Adaptive resolution simulations coupling atomistic models to MARTINI.* Multiscale Simulation Methods in Soft Matter Systems II, Darmstadt, Germany, October 4-6, 2016.

2. *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.

3. *Adaptive resolution simulation of polarizable supramolecular water models.* 13th US National Congress on Computational Mechanics, San Diego, CA, USA, July 26-30, 2015.

4. *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.

5. *Napredne metode simulacij molekulske dinamike - vecskalne 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.

6. *Simulacije z uporabo metode AdResS: sklopitev atomisticne in grobozrnate resolucije.* 2. mednarodna spomladanska šola fizike - delavnice iz biofizike, Maribor, Slovenia, May 5-12, 2015.

7. *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.

8. *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.

9. *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.

10. *Open molecular dynamics simulation of star polymers*, ASPM 2013 Austrian-Slovenian Polymer Meeting, Bled, Slovenia, April 3-5, 2013.

11. *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.

12. *Multiscale simulation of liquids*. 12th International Conference Computational and Mathematical Methods in Science and Engineering (CMMSE), La Manga - Murcia, Spain, July 2-5, 2012.

13. *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.

14. *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.

15. *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.

17. *Hybrid methods for multiscale simulation of liquids*. ETHZ - CECAM - ESF Workshop in Multiscale Modeling and Simulation, Kartause Ittingen, Switzerland, October 19-22, 2010.

18. *Linking atomistic and continuum hydrodynamics*. Novel Simulation Approaches to Soft Matter Systems Workshop, Dresden, Germany, September 20-24, 2010.

19. *Hybrid methods for multiscale flow simulations*. Regional Biophysics Conference 2010, Primošten, Croatia, September 15-18, 2010.

20. *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.

21. *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.

22. *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.

23. *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.

24. *Adaptive resolution simulation.* The 3rd Adriatic Meeting On Computational Solutions in the Life Sciences, Primošten, Croatia, September 1-5, 2009.

25. *Adaptive resolution molecular dynamics simulation.* EPSRC Symposium Workshop on Molecular Dynamics, Mathematics Research Centre, University of Warwick, Coventry, UK, June 1-5, 2009.

26. *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.

27. *Adaptive resolution simulation of molecular liquids*. Sonderforschungsbereich (SFB) 716: Summer School "Hybridsimulationen" und Statusseminar, Universität Stuttgart, Pforzheim-Hohenwart, Germany, September 8-10, 2008.

28. *Concurrent triple-scale simulation of molecular liquids*. Computational Science & Engineering Laboratory, ETH Zürich, Zürich, Switzerland, May 14, 2008.

29. *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.

30. *Adaptive resolution molecular dynamics simulations*. Departamento de Fisica Teoretica de la Materia Condensada, Universidad Autonoma de Madrid, Madrid, Spain, May 26, 2007.

31. *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

1. 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.

2. 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.

3. J. Sablic, **M. Praprotnik**, R. Delgado-Buscalioni. Open boundary molecular dynamics of sheared star-polymer melts. *Soft Matter* **12**, 2416-2439, 2016.

4. J. Zavadlav, R. Podgornik, **M. Praprotnik**. Adaptive resolution simulation of a DNA molecule in salt solution. *J. Chem. Theory Comput.* **11**, 5035-5044, 2015.

5. R. Delgado-Buscalioni, J. Sablic, **M. Praprotnik**. Open boundary molecular dynamics. *Eur. Phys. J. Special Topics* **224**, 2331-2349, 2015.

6. R. Delgado-Buscalioni, J. Sablic, **M. Praprotnik**. Reply to comments by R. Klein on "Open boundary molecular dynamics". *Eur. Phys. J. Special Topics* **224**, 2511-2513, 2015.

7. A. Popadic, **M. Praprotnik**, P. Koumoutsakos, J. H. Walther. Continuum simulations of water flow past fullerene molecules. *Eur. Phys. J. Special Topics* **224**, 2321-2330, 2015.

8. 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.

9. S. Bevc, C. Junghans, **M. Praprotnik**. STOCK: Structure mapper and online coarse-graining kit for molecular simulations. *J. Comput. Chem.* **36**, 467-477, 2015.

10. A. Popadic, J. H. Walther, P. Koumoutsakos, **M. Praprotnik**. Continuum simulations of water flow in carbon nanotube membranes. *New J. Phys.* **16**, 082001, 2014.

11. 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.

12. 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.

13. S. Bevc, C. Junghans, K. Kremer, **M. Praprotnik**. Adaptive resolution simulation of salt solutions. *New J. Phys.* **15**, 105007, 2013.

14. 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.

15. **M. Praprotnik**, S. Poblete, K. Kremer. Statistical physics problems in adaptive resolution computer simulations of complex fluids. *J. Stat. Phys.* **145**, 946-966, 2011.

16. **M. Praprotnik**, S. Poblete, L. Delle Site, K. Kremer. Comment on "Adaptive multiscale molecular dynamics of macromolecular fluids". *Phys. Rev. Lett.* **107**, 099801, 2011.

17. 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.

18. S. Poblete, **M. Praprotnik**, K. Kremer, L. Delle Site. Coupling different levels of resolution in molecular simulations. *J. Chem. Phys.* **132**, 114101, 2010.

19. 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.

20. **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.

21. R. Delgado-Buscalioni, K. Kremer, **M. Praprotnik**. Concurrent triple-scale simulation of molecular liquids. *J. Chem. Phys.* **128**, 114110, 2008.

22. **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.

23. **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.

24. 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.

25. C. Junghans, **M. Praprotnik**, K. Kremer. Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. *Soft Matter* **4**, 156-161, 2008.

26. **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.

27. **M. Praprotnik**, S. Matysiak, L. Delle Site, K. Kremer, C. Clementi. Adaptive resolution simulation of liquid water. *J. Phys.: Condens. Matter* **19**, 292201, 2007.

28. **M. Praprotnik**, L. Delle Site, K. Kremer. A macromolecule in a solvent: Adaptive resolution molecular dynamics simulation. *J. Chem. Phys.* **126**, 134902, 2007.

29. **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.

30. **M. Praprotnik**, K. Kremer, L. Delle Site. Adaptive molecular resolution via a continous change of phase space dimensionality. *Phys. Rev. E* **75**, 017701, 2007.

31. **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.

32. **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.

33. **M. Praprotnik**, D. Janežič. Molecular dynamics integration meets standard theory of molecular vibrations. *J. Chem. Inf. Model* **45**, 1571-1579, 2005.

34. D. Janežič, **M. Praprotnik**, F. Merzel. Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. *J. Chem. Phys.* **122**, 174101, 2005.

35. **M. Praprotnik**, D. Janežič. Molecular dynamics integration and molecular vibrational theory. II. Simulation of non-linear molecules. *J. Chem. Phys.* **122**, 174102, 2005.

36. **M. Praprotnik**, D. Janežič. Molecular dynamics integration and molecular vibrational theory. III. The IR spectrum of water. *J. Chem. Phys.* **122**, 174103, 2005.

37. **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.

38. R. Trobec, M. Šterk, **M. Praprotnik**, D. Janežič. Parallel programming library for molecular dynamics simulations. *Int. J. Quant. Chem.* **96**, 530-536, 2004.

39. **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.

40. 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.

41. 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.

42. **M. Praprotnik**, D. Janežič. The Split Integration Symplectic Method. *Cell. Mol. Biol. Lett.* **7**, 147-148, 2002.

43. 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.

44. D. Janežič, **M. Praprotnik**. Symplectic molecular dynamics integration using normal mode analysis. *Int. J. Quant. Chem.* **84**, 2-12, 2001.

Book Chapters

1. **M. Praprotnik**, L. Delle Site. Multiscale molecular modeling. *Biomolecular simulations: methods and protocols*, L. Monticelli, E. Salonen (Eds.), **924**, pp. 567-583, Springer, New York, 2013.

2. D. Janežič, U. Borštnik, **M. Praprotnik**. Parallel approaches in molecular dynamics simulations. *Parallel computing : numerics, applications, and trends*, R. Trobec, M. Vajteršič, P. Zinterhof (Eds.), pp. 281-305, Springer, Dordrecht, 2009.

3. C. Junghans, **M. Praprotnik**, L. Delle Site. Adaptive resolution schemes. *Multi-scale simulation methods in molecular sciences*, J. Grotendorst, N. Attig, S. Blügel, D. Marx (Eds.), NIC series, Vol. **42**, pp. 359-379, Institute for Advanced Simulation, Forschungszentrum Jülich, 2009.

4. M. Šterk, R. Trobec, **M. Praprotnik**. Comparison of incompressible fluid flow simulation methods. *Parallel numerics '02 : theory and applications.*, R. Trobec, P. Zinterhof, M. Vajteršic, A. Uhl (Eds.), pp. 149-162, Institut Jožef Stefan; University of Salzburg, Ljubljana, 2002.

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

Ljubljana, January 19, 2017