Lorenzo Rovigatti

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Date of birth: December 17, 1985

Place of birth: Rome, Italy

Citizenship: Italian

My profile on scientific databases: Scopus, ResearcherlD, Google Scholar Number of published items: 56 refereed papers + 2 book chapters

H-index (Scopus, 09/09/2021): 24

Total citations (Scopus, 09/09/2021): 1582

Current address

Dipartimento di Fisica Sapienza Università di Roma P.le A. Moro 5, 00185 Roma, Italy

Education and Career

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C 0001	Associate Professor,	C - '	11
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Sep 2018 – Aug 2021 Rita Levi Montalcini fellow, tenure-track researcher (RTDB), Sapienza Università di Roma.

May 2017 – Aug 2018 Non-tenure researcher (RTDA), CNR-ISC, with Dr. E. Zaccarelli.

Apr 2016 – Apr 2017 **Marie Skłodowska-Curie Individual Fellow**, *University of Oxford*, with Prof. A. Louis.

Mar 2016 Post-doctoral fellow, University of Vienna, with Prof. C. Likos.

Mar 2014 - Feb 2016 Lise Meitner fellow, University of Vienna, with Prof. C. Likos.

Dec 2012 - Feb 2014 Post-doctoral fellow, Sapienza Università di Roma, with Prof. F. Sciortino.

Nov 2009 – Dic 2012 **Dottorato di Ricerca (Ph.D.) in Materials Science**, *Sapienza Università di Roma*, under the supervision of Prof. F. Sciortino.

Apr – May 2012 **HPC-Europa visitor**, *University of Edinburgh*, with Dr. P. J. Camp.

Jun 2011 Visiting scientist, University of Oxford, with Prof. J. P. K. Doye.

Oct 2007 – Oct 2009 Laurea Specialistica (Master Degree) in Physics, Sapienza Università di Roma, 110/110 cum laude.

Mar - May 2009 Visiting scientist, University of Montpellier 2, with Prof. W. Kob.

Oct 2004 – Oct 2007 Laurea Triennale (Bachelor Degree) in Physics, Sapienza Università di Roma, 110/110 cum laude.

Fellowships, Grants & Awards

- 2020 Italian Scientific Qualification (Abilitazione Scientifica Nazionale), as Full Professor in Theoretical Condensed Matter Physics.
- 2019 "Alfredo di Braccio" Prize, awarded by Accademia dei Lincei.
- 2018 Rita Levi Montalcini Fellowship, $(211,173.66 \in)$.
- 2017 Italian Scientific Qualification (Abilitazione Scientifica Nazionale), as Associate Professor in Theoretical Condensed Matter Physics.
- 2016 "Marie Skłodowska-Curie" Individual Fellowship, (183,454.80 €).

- 2016 "Young Investigator Training Program" Award, ECIS 2016.
- 2016 ESG-Nano-Prize 2016, Erwin Schrödinger Symposium.
- 2014 "Lise Meitner" Fellowship, (144,420.00 €).
- 2012 **HPC-Europa 2 Fellowship**.

Student Supervisions and Co-supervisions

- 2019 Marco Spinaci, Master candidate, Dipartimento di Fisica, Sapienza Università di Roma.
- 2017 **Mariarita Paciolla, Master candidate**, *Dipartimento di Fisica, Sapienza Università di Roma*, with Dr. E. Zaccarelli and Dr. N. Gnan.
- 2016 2018 **Ferdinando Randisi, Ph.D. student**, *Rudolph Peierls Centre for Theoretical Physics, Oxford University*, with Prof. A. Louis.
 - 2016 **Michele Fava, Summer intern**, Rudolph Peierls Centre for Theoretical Physics, Oxford University, with Prof. A. Louis.
 - 2015 **Maud Formanek, Master candidate**, *Faculty of Physics, University of Vienna*, with Prof. C. N. Likos.
 - 2014 **Manfredo di Porcia, Master candidate**, *Dipartimento di Fisica, Sapienza Università di Roma*, with Prof. F. Sciortino.
- 2012 2016 **Sofia Biagi, Ph.D. student**, *Dipartimento di Fisica, Sapienza Università di Roma*, with Prof. F. Sciortino.
 - 2012 **Simone Dussi, Master candidate**, *Dipartimento di Fisica, Sapienza Università di Roma*, with Prof. F. Sciortino.

Teaching activity

- 2018 today **Titolare del corso "Fisica 2" per Chimici Industriali (9 CFU)**, Sapienza Università di Roma.
- 2019 today **Co-docente del corso "Laboratorio di Calcolo" per Fisici (3 CFU)**, Sapienza Università di Roma.

Research interests

- Structure, dynamics and elastic properties of polymer-based materials.
- Hierarchical self-assembly in polymer- and DNA-based materials.
- Self-assembly in colloidal systems.
- Phase behaviour and dynamics of patchy particles and dipolar fluids.

Talks (invited talks are marked with a *)

*Designer protein assemblies with tunable phase diagrams in living cells, Workshop on Molecular Dynamics and its Applications to Biological Systems (invited talk), ICTP/Sissa - Italy (online webinar).

The effect of chain polydispersity and chain preparation state on the elasticity of disordered polymer networks, *Italian Soft Days*, Bari University - Italy (online webinar).

2019 *A perspective on oxDNA, OxDNA users and developers workshop (invited talk), Oxford - UK.

- *Elastic Properties and Effective Interactions of In Silico Realistic Polymer Networks, *Invited talk at University of Vienna*, Vienna Austria.
- *Elastic Properties and Effective Interactions of In Silico Realistic Polymer Networks, Invited talk at the Wageningen University & Research, Wageningen The Netherlands.
- Elastic Properties and Effective Interactions of In Silico Realistic Microgels, 2019 MRS Spring Meeting, Phoenix USA.
- 2018 Elastic properties and effective interactions of in silico realistic microgels, 9th International Conference on Multiscale Materials Modeling, Osaka Japan.
 - *The importance of softness and deformability, from DNA origami to microgels, Computational biophysics on your desktop: is that possible? (invited talk), Trento Italy.
 - Elastic properties and effective interactions of in silico realistic microgels, *Multiscale Materials Modeling*, Osaka Japan.
 - **Computer-generated realistic microgels**, *Soft Matter Forefronts*, Atlanta USA.
 - * *In silico* modelling of microgels, *Invited talk at the CMF*, San Sebastian Spain.
- 2017 **Computer-generated realistic microgels**, *EMLG/JMLG Meeting*, Vienna Austria.
 - *Beyond patchy colloids: patchy models at the atomic and molecular scale, "Self-assembly: theory and simulations" workshop at SISSA (invited talk), Trieste Italy.
 - *Hierarchical self-assembly of DNA nanostars: from theory to experiment, "Fluids and Materials seminars" at the Department of Applied Mathematics (invited talk), Bristol United Kingdom.
 - *Hierarchical self-assembly made easy: DNA nanostars as a new class of model systems for complex fluids, Soft Matter, Biomaterials and Interfaces seminar series (invited talk), Oxford United Kingdom.
 - *Hierarchical self-assembly made easy: DNA nanostars as a new class of model systems for complex fluids, *Invited talk at the MPIPKS*, Dresden Germany.
- 2016 **Bottom-Up Colloidal Crystal Assembly with a Twist**, *ECIS 2016*, Rome Italy.
 - **S**oft self-assembled nanoparticles with temperature-dependent properties, *Italian Soft Days*, Milan Italy.
- 2015 **Soft self-assembled nanoparticles with temperature-dependent properties**, *FisMat 2015*, Palermo Italy.
 - **Soft self-assembled nanoparticles with temperature-dependent properties**, *101*° *Congresso SIF*, Rome Italy.
 - *Tetravalent DNA Nanostars as Valence-limited Building Blocks, *Invited talk at the IIT*, Genova Italy.
- 2014 **Tetravalent DNA Constructs as Valence-limited Soft Building Blocks**, *Mini Workshop in Molecular and Statistical Biophysics at SISSA*, Trieste Italy.

*Dipolar hard spheres at low temperature and density: structure, thermodynamics and magnetic properties, *Invited talk*, Montpellier – France.

Gels of DNA nanostars never crystallise, Italian Soft Days, Rome - Italy.

Investigating the Phase Behaviour of Valence-limited DNA Constructs on GPUs, Perspective of GPU Computing in Physics and Astrophysics, Rome – Italy.

- *Closing the loop: a single-component system with two critical points, Central European Statistical Mechanics Mini-Meeting (invited talk), Budapest – Hungary.
- *Tetravalent DNA Constructs as Valence-limited, Patchy-like Building Blocks, DNA-based self-assembly: theory, simulations and experiments, CECAM workshop (invited talk), Vienna Austria.
 - **Branching in the low-temperature dipolar hard sphere fluid**, *International Soft Matter Conference*, Roma Italy.
- 2012 *A coarse-grained DNA model: sequence dependence and some applications, DNA in a material world (invited talk), Roma Italy.
- 2011 The phase diagram of dipolar hard spheres: a new look, SoftComp Annual Meeting, Heraklion Crete.

Papers

2021 **Gel Formation in Reversibly Cross-Linking Polymers**, by M. Formanek, <u>L. Rovigatti</u>, E. Zaccarelli, F. Sciortino and A. J. Moreno, Macromolecules, **54**, (2021) p. 6613.

OxDNA.org: A public webserver for coarse-grained simulations of DNA and RNA nanostructures, by E. Poppleton, R. Romero, A. Mallaya, <u>L. Rovigatti</u> and P. Šulc, Nucleic Acid Research, **49**, (2021) p. W491.

A Primer on the oxDNA Model of DNA: When to Use it, How to Simulate it and How to Interpret the Results, by A. Sengar, T. E. Ouldridge, O. Henrich, L. Rovigatti and P. Šulc, Frontiers in Molecular Biosciences, **8**, (2021) p. 693710.

Effect of Chain Polydispersity on the Elasticity of Disordered Polymer Networks, by V. Sorichetti, A. Ninarello, J. M. Ruiz-Franco, V. Hugovieux, W. Kob, E. Zaccarelli and L. Rovigatti, Macromolecules, **54**, (2021) p. 3769.

Effect of Internal Architecture on the Assembly of Soft Particles at Fluid Interfaces, by J. Vialetto, F. Camerin, F. Grillo, S. N. Ramakrishna, L. Rovigatti, E. Zaccarelli and L. Isa, ACS Nano, 15, (2021) p. 13105.

2020 Designer protein assemblies with tunable phase diagrams in living cells, by M. Heidenreich, J. Georgeson, E. Locatelli, L. Rovigatti, S. K. Nandi, A. Steinberg, Y. Nadav, E. Shimoni, S. A. Safran, J. P. K. Doye, E. D. Levy, Nature Chem. Biol., 16, (2020) p. 939.

Designer protein assemblies with tunable phase diagrams in living cells, by F. Camerin, N. Gnan, J. Ruiz-Franco, A. Ninarello, <u>L. Rovigatti</u>, E. Zaccarelli, Phys. Rev. X, **10**, (2020) p. 031012.

Shape control of soft patchy nanoparticles under confinement, by I. E. Ventura-Rosales, L. Rovigatti, E. Bianchi, C. N. Likos, E. Locatelli, Nanoscale, , (2020).

- Charge affinity and solvent effects in numerical simulations of ionic microgels, by G. Del Monte, F. Camerin, A. Ninarello, N. Gnan, <u>L. Rovigatti</u>, E. Zaccarelli, J. Phys.: Condens. Matter, , (2020).
- 2019 TacoxDNA: A user-friendly web server for simulations of complex DNA structures, from single strands to origami, by A. Suma, E., Poppleton, M., Matthies, P., Šulc, F., Romano, A. A. Louis, J. P. K. Doye, C., Micheletti, L. Rovigatti, Macromolecules, 52, (2019) p. 7584.

Modeling Microgels with a Controlled Structure across the Volume Phase Transition, by A. Ninarello, J. J. Crassous, D. Paloli, F. Camerin, N. Gnan, L. Rovigatti, P. Schurtenberger, N., Zaccarelli, Macromolecules, **52**, (2019) p. 7584.

Numerical insights on ionic microgels: structure and swelling behaviour, by G. Del Monte, A. Ninarello, F. Camerin, L. Rovigatti, N. Gnan, E. Zaccarelli, Soft Matter, **15**, (2019) p. 8113.

Connecting Elasticity and Effective Interactions of Neutral Microgels: The Validity of the Hertzian Model, by <u>L. Rovigatti</u>, N. Gnan, A. Ninarello, E. Zaccarelli, Macromolecules, **52**, (2019) p. 4895.

q-Independent Slow Dynamics in Atomic and Molecular Systems, by P. H. Handle, L. Rovigatti, F. Sciortino, Phys. Rev. Lett., **122**, (2019) p. 175501.

Microgels Adsorbed at Liquid–Liquid Interfaces: A Joint Numerical and Experimental Study, by F. Camerin, M. Á. Fernández-Rodríguez, L. Rovigatti, M.-N. Antonopoulou, N. Gnan, A. Ninarello, L. Isa, E. Zaccarelli, ACS Nano, 13 (2019) p. 4548.

Numerical modelling of non-ionic microgels: an overview, by <u>L. Rovigatti,</u> N. Gnan, L. Tavagnacco, J. A. Moreno, E. Zaccarelli, Soft Matter, **15**, (2019) p. 1108.

2018 A new look at effective interactions between microgel particles, by M. J. Bergman, N. Gnan, M. Obiols-Rabasa, J.-M. Meijer, L. Rovigatti, E. Zaccarelli, P. Schurtenberger, Nat. Commun., 9, (2018) p. 5039.

How to Simulate Patchy Particles, by <u>L. Rovigatti</u>, J. Russo and F. Romano, Eur. Phys. J. E, **41**, (2018) p. 59.

Modelling realistic microgels in an explicit solvent, by F. Camerin, N. Gnan, L. Rovigatti and E. Zaccarelli, Sci. Rep., 8, (2018) p. 14426.

Force-Induced Unravelling of DNA Origami, by M. C. Engel, D. M. Smith, M. A. Jobst, M. Sajfutdinow, T. Liedl, F. Romano, L. Rovigatti, A. A. Louis, J. P. K. Doye, ACS Nano, **12**, (2018) p. 6734.

On the effect of the thermostat in non-equilibrium molecular dynamics simulations, by J. Ruiz-Franco, <u>L. Rovigatti</u>, E. Zaccarelli, Eur. Phys. J. E, **41**, (2018) p. 80.

An Accurate Estimate of the Free Energy and Phase Diagram of All-DNA Bulk Fluids, by E. Locatelli and L. Rovigatti, Polymers, 10, (2018) p. 447.

Self-Dynamics and Collective Swap-Driven Dynamics in a Particle Model for Vitrimers, by <u>L. Rovigatti</u>, G. Nava, T. Bellini and F. Sciortino, Macromolecules, **51**, (2018) p. 1232.

Internal structure and swelling behaviour of in silico microgel particles, by <u>L. Rovigatti</u>, N. Gnan and E. Zaccarelli, J. Phys.: Condens. Matter, **30**, (2018) p. 044001.

2017 In Silico Synthesis of Microgel Particles, by N. Gnan, <u>L. Rovigatti</u>, M. Bergman and E. Zaccarelli, Macromolecules, **50**, (2017) p. 8777.

Free energy calculations for rings and chains formed by dipolar hard spheres, by M. Ronti, <u>L. Rovigatti</u>, J. M. Tavares, A. O. Ivanov, S. S. Kantorovich and F. Sciortino, Soft Matter, **13**, (2017) p. 7870.

Void-Based Assembly of Colloidal Crystals, by N. Mahynski, <u>L. Rovigatti</u>, C. N. Likos and A. Z. Panagiotopoulos, G.I.T. Laboratory Journal, **5-6**, (2017) p. 32.

Limiting the valence: advancements and new perspectives on patchy colloids, soft functionalized nanoparticles and biomolecules, by E. Bianchi, B. Capone, I. Coluzza, L. Rovigatti and P. D. J. van Oostrum, Phys. Chem. Chem. Phys., 19, (2017) p. 19847.

The role of directional interactions in the designability of generalized heteropolymers, by C. Cardelli, V. Bianco, <u>L. Rovigatti</u>, F. Nerattini, L. Tubiana, C. Dellago and I. Coluzza, Sci. Rep., **7**, (2017) p. 4986.

Hierarchical self-organization of soft patchy nanoparticles into morphologically diverse aggregates, by I. C. Gârlea, E. Bianchi, B. Capone, L. Rovigatti and C. N. Likos, Curr. Opin. Colloid Interface Sci., 30, (2017) p. 1.

Condensation and Demixing in Solutions of DNA Nanostars and Their Mixtures, by E. Locatelli, P. H. Handle, C. N. Likos, F. Sciortino and L. Rovigatti, ACS Nano, 11, (2017) p. 2094.

Re-entrant limits of stability of the liquid phase and the Speedy scenario in colloidal model systems, by <u>L. Rovigatti</u>, V. Bianco, J. M. Tavares and F. Sciortino, J. Chem. Phys., **146**, (2017) p. 041103.

Connectivity, Dynamics, and Structure in a Tetrahedral Network Liquid, by S. Roldán-Vargas, L. Rovigatti and F. Sciortino, Soft Matter, 13, (2017) p. 514.

2016 Small-angle neutron scattering and molecular dynamics structural study of gelling DNA nanostars, by J. Fernandez-Castanon, F. Bomboi, L. Rovigatti, M. Zanatta, A. Paciaroni, L. Comez, L. Porcar, C. J. Jafta, G. C. Fadda, T. Bellini and F. Sciortino, J. Chem. Phys., 145, (2016) p. 084910.

Bottom-Up Colloidal Crystal Assembly with a Twist, by N. Mahynski, L. Rovigatti, C. N. Likos and A. Z. Panagiotopoulos, ACS Nano, 10, (2016) p. 5459.

Surface wave excitations and backflow effect over dense polymer brushes, by S. Biagi, <u>L. Rovigatti</u>, F. Sciortino and C. Misbah, Scientific Reports, **6**, (2016) p. 22257.

Direct Simulation of the Self-Assembly of a Small DNA Origami, by B. E. K. Snodin, F. Romano, L. Rovigatti, T. E. Ouldridge, A. A. Louis and J. P. K. Doye, ACS Nano, 10, (2016) p. 1724.

Soft self-assembled nanoparticles with temperature-dependent properties, by L. Rovigatti, B. Capone and C. N. Likos, Nanoscale, **8**, (2016) p. 3288.

- 2015 How soft repulsion enhances the depletion mechanism, by <u>L. Rovigatti</u>, N. Gnan, A. Parola and E. Zaccarelli, Soft Matter, **11**, (2015) p. 692.
 - Temperature-induced structural transitions in self-assembling magnetic nanocolloids, by S. S. Kantorovich, A. O. Ivanov, <u>L. Rovigatti</u>, J. M. Tavares, F. Sciortino, Phys. Chem. Chem. Phys., **17**, (2015) p. 16601.
 - Low temperature structural transitions in dipolar hard spheres: The influence on magnetic properties, by S. S. Kantorovich, A. O. Ivanov, <u>L. Rovigatti</u>, J. M. Tavares, F. Sciortino, J. Magn. Magn. Mater., **383**, (2015) p. 272.
 - A comparison between parallelization approaches in molecular dynamics simulations on GPUs, by <u>L. Rovigatti</u>, P. Šulc, I. Z. Reguly and F. Romano, J. Comput. Chem., **36**, (2015) p. 1.
- 2014 **Gels of DNA Nanostars Never Crystallize**, by <u>L. Rovigatti</u>, F. Smallenburg, F. Romano and F. Sciortino, ACS Nano, **8**, (2014) p. 3567.
 - Accurate phase diagram of tetravalent DNA nanostars, by <u>L. Rovigatti</u>, F. Bomboi and F. Sciortino, J. Chem. Phys., **140**, (2014) p. 154903.
- 2013 Coarse-graining DNA for simulations of DNA nanotechnology, by J. P. K. Doye, T. E. Ouldridge, A. A. Louis, F. Romano, P. Šulc, C. Matek, B. E. K. Snodin, <u>L. Rovigatti</u>, J. S. Schreck, R. M. Harrison and W. P. J. Smith, Phys. Chem. Chem. Phys., 15, (2013), p. 20395.
 - Self-assembly in chains, rings and branches: a single component system with two critical points, by <u>L. Rovigatti</u>, J. M. Tavares and F. Sciortino, Phys. Rev. Lett., **111**, (2013) p. 168302.
 - Branching points in the low-temperature dipolar hard sphere fluid, by <u>L. Rovigatti</u>, S. Kantorovich, A. O. Ivanov, J. M. Tavares and F. Sciortino, J. Chem. Phys., **139**, (2013) p. 134901.
 - On the gas-liquid phase-separation and the self-assembly of charged soft dumbbells, by S. Dussi, <u>L. Rovigatti</u>, F. Sciortino, Mol. Phys., **111**, (2013) p. 3608.
 - Nonmonotonic Magnetic Susceptibility of Dipolar Hard-Spheres at Low Temperature and Density, by S. Kantorovich, A. O. Ivanov, <u>L. Rovigatti</u>, J. M. Tavares, F. Sciortino, Phys. Rev. Lett., **110**, (2013) p. 148306.
 - Computing the phase diagram of binary mixtures: A patchy particle case study, by <u>L. Rovigatti</u>, D. de las Heras, J. M. Tavares, M. M. Telo da Gama, F. Sciortino, J. Chem. Phys., **138** (16), (2013) p. 164904.
- 2012 Sequence-dependent thermodynamics of a coarse-grained DNA model, P. Šulc, F. Romano, T. E. Ouldridge, L. Rovigatti, A. A. Louis, and J. P. K. Doye, J. Chem. Phys., 137 (13), (2012) p. 135101.
 - Quantitative description of the self-assembly of patchy particles into chains and rings, by J. M. Tavares, <u>L. Rovigatti</u>, and F. Sciortino, J. Chem. Phys., **137** (4), (2012) p. 044901.
 - Self-assembly of short DNA duplexes: from a coarse-grained model to experiments through a theoretical link, by C. De Michele, <u>L. Rovigatti</u>, T. Bellini, and F. Sciortino, Soft Matter, **8**, (2012) pp. 8388–8398.

Structural properties of the dipolar hard-sphere fluid at low temperatures and densities, by <u>L. Rovigatti</u>, J. Russo, and F. Sciortino, Soft Matter, **8**, (2012) pp. 6310–6319.

No Evidence of Gas-Liquid Coexistence in Dipolar Hard Spheres, by L. Rovigatti, J. Russo, and F. Sciortino, Phys. Rev. Lett., 107, (2011) p. 237801.
Self and collective correlation functions in a gel of tetrahedral patchy particles, by L. Rovigatti and F. Sciortino, Mol. Phys., 109 (23-24), (2011) pp. 2889–2896.

The vibrational density of states of a disordered gel model, by <u>L. Rovigatti</u>, W. Kob, and F. Sciortino, J. Chem. Phys., **135** (10), (2011) p. 104502.

Book contributions

- 2017 A Nucleotide-Level Computational Approach to DNA-Based Materials, by F. Romano and L. Rovigatti, in Design of Self-Assembling Materials, edited by I. Coluzza, Cham (2017), ISBN: 978-3-319-71576-6.
- Accurate Coarse-Grained Potentials for Soft Matter Systems, by R. Blaak, B. Capone, C. N. Likos and L. Rovigatti, in Computational Trends in Solvation and Transport in Liquids, of the IAS Series 28, edited by G. Sutmann, J. Grotendorst, G. Gompper and D. Marx. Forschungszentrum, Juelich (2015), ISBN: 978-3-95806-030-2.

Organised events

- 2016 Local committee member and editor of the book of abstracts, *ECIS 2016*, Rome Italy.
- 2013 Local committee member and editor of the book of abstracts, *ISMC 2013*, Rome Italy.

Institutional Responsibilities

2017 – 2018 Member of the "ISC Committee for Research Project Management and Evaluation" (Commissione ISC per la Valutazione e la Gestione dei Progetti di Ricerca), Institute of Complex Systems (CNR-ISC).

Editorial activities

Guest editor of the special issue on "Advances in Computational Methods for Soft Matter Systems" for *The European Physical Journal E.*

Languages

Italian (native), English (proficient) and German (elementary)

Other activities

Reviewer for Nanoscale, Nature Communications, Physical Review Applied Letters, Physical Review B, Physical Review E, Physical Review Letters, Polymers, Soft Matter, The European Physical Journal E and The Journal of Chemical Physics.

Lead developer of oxDNA, an open-source simulation package for coarse-grained simulations of DNA and RNA, and of cogli2, a tool for the visualisation and rendering of configurations of coarse-grained systems.