Antonia S J S Mey

email antonia.mey@gmail.com
github https://github.com/ppxasjsm
twitter @ppxasjsm
post David Brewster Road
Joseph Black Building
University of Edinburgh
EH9 3FJ

EDUCATION

July 2013 — University of Nottingham, Nottingham, UK
PhD in Physics (Thesis: *Trajectory ensemble methods for understanding complex stochastic systems, Supervisor: Prof. Juan P. Garrahan*)

July 2007 — Keele University, Keele, UK
Bachelor of Science in Physics with Chemistry 1st Class Honours
(Dissertation: Bose-Einstein Condensates)

PROFESSIONAL EXPERIENCE

Since April 2015 — University of Edinburgh, School of Chemistry
Postdoctoral Research Associate with Dr. Julien Michel
April 2019 - August 2019 Acting Group Leader during parental leave cover for Dr. Julien Michel
Research:
- Machine learning augmented identification of collective motions in complex biological time-series data
- Lead Scientist of the CCPBioSim Software Flagship project BioSimSpace; a software effort to produce a more interoperable software framework for biomolecular and quantum mechanical simulations, e.g. to predict free energies of binding of drug-like molecules.
- Clustering methods in time-series data
- Development and validation of new data analysis tools for alchemical free energy workflows through community challenges such as the blinded D3R grand challenges, allowing for rigorous statistical analysis of state-of-the-art computational techniques.

Jan 2013 - March 2015 — School of Mathematics, Freie Universität Berlin
Research Scientist, Computational Molecular Biology Group, Prof. Frank Noé
Research:
- Development of statistical estimator (xTRAM) which allows estimation of stationary and kinetic properties from enhanced sampling simulations using bayesian inference.
- Application of Markov State Models to investigate molecular forcefield dependence of kinetic properties in peptides and larger protein systems.

PUBLICATIONS

Google scholar: goo.gl/PaKuF3
h-index: 11
* equal contribution

Preprints

1. Geometric constraints in protein folding, N. Molkenthin, S. Mühle, **A.S.J.S. Mey**, M. Timme, arXiv (under review) **DOI**

2. Atomic Level Characterisation of Millisecond Time Scale Protein Motions through a Combined Molecular Simulations and NMR Approach, J. Juárez-Jiménez, A. Gupta, G. Karunanithy, **A.S.J.S. Mey**, et al. (under review) **DOI**

3. Modern Mathematics Communication — An Asian Focus, A.D. Matt, **A.S.J.S. Mey**, B. Violet, *Asia Pacific Mathematics Newsletter (accepted)*

Peer Reviewed

4. Allosteric effects in a catalytically impaired variant of the enzyme Cyclophilin A may be explained by changes in nano-microsecond time scale motions, P. Wapeesittipan, **A.S.J.S. Mey**, M. Walkinshaw, J. Michel, *Comms. Chem*. **2**, 41 (2019) **DOI**

5. Effect of automation on the accuracy of alchemical free energy calculation protocols over a set of ACK1 inhibitors, J.M. Granadino-Roldan*, **A.S.J.S. Mey*,** J.J. Perez, S. Bosisio, J. Rubio-Martinez, J. Michel, PloS One **14**, e0213217 (2019) **DOI**

6. Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations, **A.S.J.S. Mey**, J. Juárez-Jiménez, J. Michel, *J. Comput. Aided. Mol. Des.* **32**, 199 (2018) **DOI**

7. Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge, S. Bosisio, **A.S.J.S. Mey**, J. Michel, *J. Comput. Aided. Mol. Des.* **31**, 61 (2017) **DOI**

8. Analytical methods for structural ensembles and dynamics of intrinsically disordered proteins, M. Schor, **A.S.J.S. Mey**, C.E. MacPhee, *Biophys. Rev.* **8,** 429 (2016) **DOI**

9. Blinded predictions of distribution coefficients in the SAMPL5 challenge, S. Bosisio, **A.S.J.S. Mey**, J. Michel, *J. Comput. Aided. Mol. Des.* **30,** 1101 (2016) **DOI**

10. Blinded predictions of binding modes and energies of HSP90-α ligands for the 2015 D3R Grand Challenge, **A.S.J.S. Mey***, J. Juárez-Jiménez*, A. Hennessy, J. Michel, *Bioorg. Med. Chem.* **24,** 4890 (2016) **DOI**

11. Elucidation of Non-Additive Effects in Protein-Ligand Binding Energies: Thrombin as a Case Study, G. Calabrò, C.J. Woods, F. Powlesland, **A.S.J.S Mey**, A.J. Mulholland, J. Michel, *J. Phys. Chem. B* **120,** 5340 (2016) **DOI**

12. Shedding light on the dock-lock mechanism in amyloid fibril growth using Markov State Models, M. Schor, **A.S.J.S. Mey**, F. Noé, C.E. MacPhee, *J. Phys. Chem. Lett.* **6**, 1076 (2015) **DOI**

13. Dynamic Properties of Forcefields, F. Vitalini*, **A.S.J.S. Mey***, F. Noé and B.G. Keller, *J. Chem. Phys.* **142**, 084101 (2015) **DOI**

14. IMAGINARY – Mathematics Communication for the 21st Century, G.-M. Greuel, A.D. Matt, **A.S.J.S. Mey**, *Newsletter of the European Mathematical Society* **92**, 3 (2014) [http://www.ems-ph.org/journals/newsletter/pdf/2014-06-92.pdf] [invited contribution]

15. Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states, H. Wu, **A.S.J.S. Mey**, E. Rosta, F. Noé, *J. Chem. Phys.* **141,** 214106 (2014) **DOI**

16. xTRAM: Estimating equilibrium expectations from time-correlated simulation data at multiple thermodynamic states, **A.S.J.S. Mey**, H. Wu, and F. Noé, *Phys. Rev. X* **4,** 041018 (2014) **DOI**

17. Rare-event trajectory ensemble analysis reveals metastable dynamical phases in lattice proteins, **A.S.J.S. Mey**, P.L. Geissler and J.P. Garrahan, *Phys. Rev. E* **89**, 032109 (2014) **DOI**

18. Variational approach to molecular kinetics, F. Nüske, B.G. Keller, G. Pérez-Hernández, **A.S.J.S. Mey**, F. Noé, *J. Chem. Theory Comput.* **10**, 1739 (2014) **DOI**

19. EMMA - A software package for Markov model building and analysis, M. Senne, B. Trendelkamp-Schroer, **A.S.J.S. Mey**, C. Schütte, F. Noé, *J. Chem. Theory Comput.* **8**, 2223 (2012) **DOI**

20. Thermodynamics of trajectories of the one-dimensional Ising model, E.S. Loscar, **A.S.J.S. Mey**, J.P. Garrahan, *J. Stat. Mech.* **2011,** P12011 (2011) **DOI**

TEACHING EXPERIENCE AND TRAINING

2019: Enrolled on EdTA scheme to become an associate fellow of the AdvanceHE (AFHEA)
2019: Two 1-Day workshops at the CCP BioBioSim Training Week
Course content design on alchemical molecular simulations, using BioSimSpace and course instructor for Markov State modelling using pyemma here
2018: SUPA Computational Chemistry course, University of Edinburgh
Molecular Dynamics lecture for the SUPA computational chemistry course
2018: 1-Day workshop at the CCP BioBioSim Training Week
Course content design on alchemical molecular simulations, as well as course instructor, using a cloud based teaching infrastructure with material available here
2015 — 2017: Chemistry 1A and 1B co-tutor, University of Edinburgh
Running tutorials covering mainly introductory university level physical and quantum chemistry concepts

2014 — 2017: PyEMMA workshop lecturer, Freie Universität Berlin and King's College London
Lecturer and tutor for 1-day courses on Markov State Modelling using PyEMMA software
2014: MSc course organiser, Freie Universität Berlin
Co-organiser for "Computational Molecular Physics and Methods of molecular simulations" MSc module for students across chemistry, physics and mathematics
2014: Higher Education pedagogics training week
One week training workshop on higher education pedagogics at the Freie Universität Berlin — attendee
2010 — 2011: Private tutor
Private tuition for A-Level and AS-Level mathematics and physics
2008 — 2011: Tutor for problem classes University of Nottingham
Running problems classes on quantum mechanics, solid state physics, and mathematics for physicists

Supervision of master and bachelor students at the University of Edinburgh:
2018/19: *Calum Smart* (School of Chemistry) Comparative study of different docking tools, such as Flare and VINA and their performance on BACE-1 as part fo D3R Grand Challenge 4
2016/17: *Jason Klebes* (School of Physics) Investigating dynamics in small intrinsically disordered peptides using enhanced sampling methods and TRAM.
2016/17: *Clara Kelly* (School of Chemistry) Charging corrections in alchemical free energy protocols as part of the D3R Grand Challenge 2.
2015/16: *David Tiemessen* (School of Physics) Looking at coarse grained modelling of BSLA - a protein playing vital parts in Bacterial raincoats.
2015/16: *Alexis Hennessy* (School of Chemistry) Docking calculations and simple MD simulations of ligand molecules biding to HSP90 as part of the D3R Grand Challenge 2015.

AWARDS, GRANTS, SCHOLARSHIPS & INDUSTRY COLLABORATIONS

2018: Co-Investigator on: EPSRC Flagship Software - BioSimSpace: A shared space for the community development of biomolecular simulation workflows Grant: EP/P022138/1 (UK)
2018: Scientific Support for KTP project in partnership with Cresset to incorporate free energy methods into Cresset software Flare (UK)
2017: Institute for Academic Development New Network Award: Edinburgh MD Simulation day (UK)
2016: Computing time worth $10000 on Amazon Web services (AWS) (UK)
2016: Poster prize at the 1st UK Research Software Engineering conference (UK)
2014: 1st prize in the 'Fast-forward Science' short film competition (https://youtu.be/cyKb-P3mwDk) joint with G. Jouvet, Glacial mysteries (Germany)
2014: Computing time at the HLRN worth 3 million CPU hours (Germany)
2013: 3rd prize in a competition of the "Math of Planet Earth 2013" initiative (http://imaginary.org/film/the-future-of-glaciers) (France)
2009: BESTS Travelling Scholarship to fund a 2-month research visit to UC Berkeley (USA)
2007-2012: Doctoral scholarship from the University of Nottingham (UK)
2007: DESY Summer student programme (Germany)
2006: Nuffield Undergraduate Research Bursary (UK)

ORGANISED CONFERENCES, COMMITTEES & MEMBERSHIPS

since 2019: Member of the Inequality and Diversity Committee, Chemistry University of Edinburgh
2018: Organiser of the 3rd EaStChem early careers researcher conference (ECECR2018), University of Edinburgh, Edinburgh
2018: Organiser of '2018 Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design', at Silicon Therapeutics and Novartis, Boston
2017: Organiser of 'Edinburgh MD Simulation Day', a college of Science wide simulation day to encourage cross-departmental collaborations at the University of Edinburgh, Edinburgh
since 2017: Member of the Institute of Physics
2016: Organiser of joint Physical Chemistry meeting between University of Edinburgh and Heriot-Watt University, Edinburgh
2016: Organiser of IMAGINARY conference 2016, bringing mathematics outreach enthusiasts together, Berlin
2016/2017: Member of the American Chemical Society
2015-2018: Organiser of the Physical Chemistry Section Committee at the University of Edinburgh, organising seminars and social events for PhD students and postdocs, Edinburgh
2014: Organiser of 3 day IMAGINARY workshop at AIMS Institute South Africa, Cape Town
2010: Organiser of a 1-day CUDA training workshop University of Nottingham, Nottingham
2009-2011: Founder and Organiser of a "Scientific Computing Seminar" for PhD students across various departments at the University of Nottingham, Nottingham
2009-2011: Postgraduate committee member at the University of Nottingham, Nottingham

Member of the American Chemical Society (ACS) and **Institute of Physics** (IOP)

INVITED TALKS & CONFERENCES (SELECTED)

1. **Invited talk**, *Alchemical Free Energy Workshop,* Göttingen (May 2019),
2. **Invited talk,** Mathematics Seminar, Nottingham Trent University, Nottingham (February 2019)
3. Conference Talk, *Europython*, Edinburgh (July — 2018)
4. **Invited talk**, *Cresset User Meeting,* Cambridge (June — 2018)

5. **Invited talk**, *Kinetics and Markov State Models in Drug Design,* Boston (May — 2018)
6. **Invited talk**, *CECAM Multi-scale modelling meeting*, Université Paris-Est, Paris (May—2017)
7. **Invited talk**, Institute for Condensed Matter and Complex Systems, University of Edinburgh, Edinburgh (January — 2017)
8. **Invited talk**, *IOP Workshop: Self-Assembly, Recognition, and Application,* University of Edinburgh, Edinburgh (December — 2016)
9. **Invited lecturer** at *CCPBiosim Molecular Kinetics workshop,* King's College London, London (September — 2016)
10. **Invited talk**, *Kinetics and Markov State Models in Drug Design,* Boston (May — 2016)
11. Seminar talk, A. Mulholland group, University of Bristol, Bristol (April — 2016)
12. Conference talk, *ACS Annual Meeting*, San Diego (March — 2016)
13. **Invited talk**, *D3R Workshop*, UCSD, San Diego (March — 2016)
14. **Invited lecturer**, *CECAM Macromolecular Simulation Software Workshop,* Jülich (October — 2015)
15. Conference talk, *ScotChem*, Strathclyde University, Glasgow (June — 2015)
16. **Invited talk,** *the Non-linear Science Colloquium,* Münster (November —2014)
17. Seminar talk, Schrödinger, New York (September — 2014)
18. Seminar talk, MSKCC, John Chodera Lab, New York (September — 2014)
19. Conference talk, *Exploring energy landscapes Conference*, Durham (August — 2014)
20. Seminar talk, University of Edinburgh, (August — 2014)
21. **Invited talk**, *Roland Netz Group,* Freie Universität Berlin, Berlin (July — 2014)
22. Conference Talk, *Open Statistical Physics,* The Open University, Milton Keynes (March — 2013)
23. Conference Talk, *CCP BioSim Annual Meeting*, Nottingham (March — 2013)
24. Conference Talk, *Computer Simulations and Theory of Macromolecules*, Hünfeld (April — 2012)
25. Seminar talk, *Center for Soft Matter Research,* New York University, NY (September — 2011)
26. Conference Talk, *Open Statistical Physics,* Open University, Milton Keynes (March — 2011)
27. *MDnet conference*, University of Bath, Bath (November — 2010) (attended)
28. Autumn School, *Core Algorithms for High Performance Scientific Computing,* University of Warwick, Warwick (October — 2009) (attended)
29. 3-day meeting: *Aspects of Complexity,* University of Manchester, Manchester (July — 2009)

RESEARCH VISITS

August 2014 University of Edinburgh, Dr Marieke Schor
Collaboration on investigating the dock-lock mechanism for fibril formation
April 2011— February 2012 Freie Universität Berlin, Dr Frank Noé
Collaborative visit that initiated the development of Multi-ensemble transition based free energy estimators.
July — August 2010 UC Berkeley, Dr John D. Chodera
Collaborative visit to explore entropy in trajectory ensembles.
April 2010 Université Paris VII, Prof Frédéric van Wijland
Educational visit to gain insight into the mathematical background of trajectory ensemble methods.
October — December 2009 UC Berkeley, Prof Geissler
Collaborative visit, funded by the BESTS traveling scholarship to collaborate on understanding complex dynamical phases in lattice protein models.

PUBLIC ENGAGEMENT & OUTREACH

since 2019 STEM Ambassador with various 1-day activities, e.g. Edinburgh Science Festival
since 2014: Project manager for IMAGINARY gGmbH (www.imaginary.org)

IMAGINARY is a non-profit outreach organisation popularising modern mathematics, through exhibitions, workshops, and online-material

Selected List of outreach activities conducted as part of IMAGINARY:

2019 Contributor to Lala Lab and exhibition on maths and music and Artificial Intelligence

since 2015: IMAGINARY coordinator for Snapshots of modern mathematics, short articles on current mathematical research made available to a general audience (https://imaginary.org/snapshots)

since 2015: Technical Museum Berlin Germany, Exhibit: Future of Glaciers on display, Berlin

2017: 2-week IMAGINARY exhibition as part of the ENESCU music festival responsible for setup and training of local staff, Bucharest

2017: UNESCO funded teacher training workshop in Liberia, introducing 'Mathematics in a Suitcase' (designed and taught 2-day workshop), Monrovia

2016: 2-day IMAGINARY conference, bringing together mathematics outreach practitioners around the world, organiser and workshop leader, Berlin

2015 and 2016: Glasgow Science festival: pop-up stand with IMAGINARY exhibitions, Glasgow

2015: 3 month IMAGINARY exhibition at the Weizmann Institute, project coordinator, set-up, testing, and local staff training, Rehovot

2015: MATRIX conference, conference for community of mathematics museums, Dresden

2014/2015: Long Night of Sciences Berlin: 'Math of Planet Earth' exhibition, Berlin

2014: 3-day IMAGINARY workshop at AIMS Institute South Africa, coordinator for workshop content, exhibition setup, and local staff training, Cape Town

2014: Tanzania Pi day — 1-day pop-up workshop to celebrate 10th anniversary of pi day in Tanzania, Dar es Salaam

Funding:

2017: UNESCO funding for 2-day teacher training workshop (€7000)

2016: Co-author for VW foundation funding for IMAGINARY conference 2016 (€50 000)

2015: Co-author for Leibniz association funding for the founding of IMAGINARY as a non-profit organisation (€200 000)

2015: Co-author for Funding from Ministry of Science and Education, Germany for exhibition in Israel (€50 000)

PEER REVIEW

European Physics Letters, Journal of Chemical Theory and Computation, PloS One Computational Biology, Journal of Chemical Physics, Journal of Computer Aided Molecular Design, Journal of the American Chemical Society