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EDUCATION

July 2013

University of Nottingham, Nottingham, UK
PhD in Physics (Thesis: *Trajectory ensemble methods for understanding complex stochastic systems, Supervisor: Professor 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

April 2015 — Present

School of Chemistry, University of Edinburgh
Postdoctoral Research Associate with Dr. Julien Michel

Research:
Development of alchemical free energy workflow methods to allow for a more reliable prediction of binding free energies as well as solvation free energies of small molecules. This involves the direct implementation of new algorithms and software packages to validate new protocols using community challenges such as D3R grand challenge 2, a blind challenge to asses state of the art computational methods to predict free energies of binding between proteins and small molecules.
Involvement in various projects in the group, such as using Markov state models in Cyclophilins to uncover druggable hidden protein conformations joint with Dr Juárez-Jiménez.

Supervision of master students:

- *Jason Klebes* (Physics) Investigating dynamics in small intrinsically disordered peptides using enhanced sampling methods and TRAM.
- *Clara Kelly* (Chemistry) Looking at the robustness of current free energy protocols in conjunction with D3R Grand Challenge 2.
- David Tiemessen (Physics) Looking at coarse grained modelling of BSLA - a protein playing vital parts in Bacterial raincoats.
- Alexis Hennessy (Chemistry) Docking calculations and simple MD simulations of ligand molecules biding to HSP90 as part of the D3R Grand Challenge 2015.

April 2012 — March 2015

Institute for Mathematics and Computer Science, Freie Universität Berlin
Research Scientist, Computational Molecular Biology Group, Prof. Frank Noé

Research:
Development of multi ensemble free energy estimator xTRAM.

Application of Markov state models to better understand the underlying dynamics of small peptide systems, such as elucidating the dock-lock mechanism for amyloid fibre formation as well as understanding forcefield dependence on small peptides stationary and dynamical properties.

PUBLICATIONS

Google scholar: goo.gl/PaKuF3
h-index: 8
* equal contribution

In preparation or Preprints

1. Combining enhanced sampling simulations and Markov state modelling to characterise the dynamics of the intrinsically disordered Aβ 1-42 peptide, **A.S.J.S. Mey**, J. Michel, C.E. MacPhee, M. Schor, *in preparation*

2. Markov State Models (and NMR) reveal hidden conformations of Cyclophiling A in the μs to ms timescale, J. Juárez-Jiménez, A. Gupta, H. Ioannidis, **A.S.J.S. Mey**, J. Michel *in preparation*

3. Changes in fast active site dynamics are sufficient to explain allosteric effects in the Cyclophillin A S99T mutant, Pattama Wapeesittipan, **A.S.J.S. Mey**, J. Michel *in preparation*

4. An open licensed Math-Art Showcase for non-formal education, B. Violet, **A.S.J.S. Mey,** A.D. Matt, J. Math. Arts, (2017), *submitted*

5. 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, *bioRxiv,* 150474 (2017) **DOI**

Peer Reviewed

6. 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**

7. 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**

8. 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**

9. 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**

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

11. 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**

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

13. 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**

14. 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**

15. 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**

16. 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**

17. 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**

18. 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**

INVITED TALKS & CONFERENCES

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

TEACHING EXPERIENCE

2015 — present

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

Summer semester 2014

MSc course organiser, Freie Universität Berlin
Joint course organiser for "Computational Molecular Physics and Methods of molecular simulations" MSc course for Chemistry, Physics and Mathematics covering topics of various simulation methods, running tutorials and 20% of the lectures.

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.

AWARDS, GRANTS & SCHOLARSHIPS

- **Computing time worth $10000** on Amazon Webservices (AWS) for prototyping using alchemical free energy calculations and cloud computing (UK — 2016)
- **Poster prize** at the 1st UK Research Software Engineering conference (UK — 2016)
- **1st prize** in the 'fast-forward science' competition (https://youtu.be/cyKb-P3mwDk) with a film by G. Jouvet, Glacial mysteries (Germany — 2014)
- **Computing time** at the HLRN worth 3 million CPU hours (Germany — 2014)
- **3rd prize** in a competition of the "Math of Planet Earth 2013" initiative (http://imaginary.org/film/the-future-of-glaciers) (France — 2013)
- **BESTS Travelling Scholarship** to finance 2 month research visit at UC Berkeley (USA — autumn 2009)
- **Doctoral scholarship** from the University of Nottingham (UK)
- **DESY Summer student** programme (Hamburg, Germany — summer 2007)
- **Nuffield Undergraduate Research Bursary** (Keele, UK — summer 2006)

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.

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

OTHER ACTIVITIES

Committees and Conferences:

- **Organiser of '2018 Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design'**, Boston at Silicon Therapeutics and Novartis (May 2018)
- **Organiser of 'Edinburgh MD Simulation Day'**, a college of Science wide simulation day to encourage cross-departmental collaborations at the University of Edinburgh (May 2017)
- **Organiser of joint Physical Chemistry meeting** between University of Edinburgh and Heriot-Watt University (December 2016)
- **President of the Physical Chemistry Section Committee** at the University of Edinburgh, organising seminars and social events for the Physical Chemistry Section. (2015 throughout)
- Organiser of a **1-day CUDA training workshop** University of Nottingham (2010)
- Founder and Organiser of a **"Scientific Computing Seminar"** for PhD students across various departments at the University of Nottingham (2009-2011)
- **Postgraduate committee member** at the University of Nottingham (2009-2011)

Outreach:

February 2014 — throughout

Project coordinator for IMAGINARY (www.imaginary.org)

IMAGINARY started as the outreach project of the Mathematische Forschungsinstitut Oberwolfach and has now developed into a non-profit company to promote mathematics outreach around the world.

My main roles involved coordinating various larger and smaller projects, amongst smaller projects were: Long Night of Sciences (Berlin —2014/2015), Glasgow Science festival (Glasgow — 2014/2015), IMAGINARY conference 2016 a conference aimed at mathematics communicators.

Larger Projects:

- UNESCO Funded **teacher training workshop** in Liberia
- Project coordinator for an **IMAGINARY exhibition** at the Weizmann Institute (Israel — Summer 2015)
- Organiser of 3 day **IMAGINARY workshop at AIMS Institute South Africa** (South Africa — November 2014)
- *Editorial: IMAGINARY – Mathematics Communication for the 21st Century,* G.-M. Greuel, A.D. Matt, A.S.J.S. Mey, EMS Newsletter [http://www.ems-ph.org/journals/newsletter/pdf/2014-06-92.pdf] (June 2014)
- **Co-author of various larger successfully funded proposals**:
  €50 000 from the VW foundation for IMAGINARY 2016 conference organisation
  €200 000 from the Leibniz foundation for the funding of the IMAGINARY non-profit company

Other:

- **Founding member of a postgraduate theatre group** at the University of Nottingham (2008-2010)

SKILLS

Computational:

- Good knowledge of various programming languages (Python, Java, C++)
- Contributor to various scientific software and maintainer of Sire (C++, Python) — https://github.com/michellab/Sire
- Experienced user of HPC facilities using CPU's and GPU's and cloud computing.
- Experience in administrating small Computing clusters (~ 10-32 nodes and a mix of GPU and CPU nodes using Slurm) (Rocks/Ubuntu).
- Experience with MD packages such as Gromacs and OpenMM.

Languages:

German (mother tongue), *English* (fluent), *French* (intermediate), *Hebrew* (intermediate), *Spanish* (basic)