Paul Smith

LINKEDIN p-j-smith **SCHOLAR** Paul Smith

Background

My research over the past few years has focused on the use of molecular dynamics (MD) simulations to help understand emergent biological phenomena. I have become increasingly interested in the use of statistical and machine learning methods — such as Hidden Markov Models (HMM), dimensionality reduction and unsupervised clustering — in the analysis of MD simulations.

Education

PhD Physics 10/2017 - Present
KING'S COLLEGE LONDON

I am using MD simulations to study the biophysics of lipid membranes and proteins. Projects include:

- using HMMs to study the effects of cholesterol oxidation on model lipid membranes
- using unsupervised ML to study cholesterol-sphingomyelin interactions in lipid bilayers
- studying the denaturation of apolipoproteins by graphene oxide

MSc Physics (Distinction) 10/2015 - 09/2017
KING'S COLLEGE LONDON

MSc Project: I used atomistic molecular dynamics simulations to study the interactions of hyaluronic acid with lipid membranes, which govern the lubricating properties of synovial fluid.

BEng Mechanical Engineering (2.1 Hons) 10/2009 - 07/2012
KING'S COLLEGE LONDON

BEng Project: I used coarse-grained molecular dynamics simulations to study the formation and structural characteristics of a chemically cross-linked hydrogel derived from fish collagen.

Experience

Teaching Assistant 10/2018 - Present
BIO- AND NANO-MATERIALS IN THE VIRTUAL LAB

This graduate course teaches students how to: implement simple, two-dimensional molecular dynamics and Monte Carlo simulations using Python; perform biomolecular simulations on high-performace computers; and analyse simulation trajectories using Python and and the scientific Python stack.

Research Intern 06/2019 - 09/2019
IBM RESEARCH UK

I worked on the development of a Python package for setting up, running and analysing high-throughput molecular dynamics simulations from a Jupyter Notebook environment. I subsequently used this package to study the conformational landscape of a series of cyclic peptides. I presented the findings to our industrial collaborators (a multinational pharmaceutical company), and a paper of the results is in press.

Warren L. DeLano Memorial PyMOL Open-Source Fellow 11/2018 - 11/2019
SCHRÖDINGER

As a co-fellow, I implemented various proof-of-concept functionalities in PyMOL, a molecular visualisation tool with a Python interface for the analysis of molecular dynamics simulations. Schrödinger have since incorporated some of these functionalities into their flagship software, Maestro.

Teaching Assisstant (King's College London) 10/2018 - 06/2019
MATHEMATICS AND COMPUTATION FOR PHYSICISTS

I introduced undergraduates to programming with Python, with a focus on using Python to numerically solve mathematical problems. I was also responsible for reviewing the students' code and marking their Jupyter Notebook reports.

Research Intern 2014
KING'S COLLEGE LONDON

I used atomistic molecular dynamics simulations to study the role of water-mediation in the formation of β-turns in polypeptides.

Publications

[10] "Unsupervised Learning Unravels the Structure of Four-Arm and Linear Block Copolymer Micelles", R. M. Ziolek, P. Smith, D. L. Pink, C. A. Dreiss, C. D. Lorenz (submitted).

[9] "Asymmetric phospholipids impart novel biophysical properties to lipid bilayers allowing environmental adaptation", P. Smith, D. M. Owen, C. D. Lorenz, M. Makarova (sumitted).

[8] "Membrane permeability in cyclic peptides is modulated by core conformations", F. Cipcigan, P. Smith, J. Crain, A. Hogner, L. De Maria, A. Llinas, E. Ratkova (2020) J. Chem. Inf. Model., In Press.

[7] "Accurate large scale modelling of Graphene Oxide: ion trapping and chaotropic potential at the interface", M. A. al-Badri, P. Smith, R. C. Sinclair, K. T. al-Jamal, C. D. Lorenz (2020) Carbon, In Press.

[6] "Supramolecular Architecture of a Multicomponent Biomimetic Lipid Barrier Formulation", D. Ahmadi, R. Ledder, N. Mahmoudi, P. Li, J. Tellam, D. Robinson, R. Heenan, P. Smith, C. D. Lorenz, D. Barlow, J. M. Lawrence (2020) J. Colloid Interface Sci., In Press.

[5] "Two Coexisting Membrane Structures are Defined by Lateral and Transbilayer Interactions Between Sphingomyelin and Cholesterol", P. Smith, P. J. Quinn, C. D. Lorenz (2020) Langmuir, 36, 33, 9786–9799.

[4] "Time-Resolved Fluorescence Anisotropy of a Molecular Rotor Resolves Microscopic Viscosity Parameters in Complex Environments", I. E. Steinmark, P-H. Chung, R. M. Ziolek, B. Cornell, P. Smith, J. A. Levitt, C. Tregidgo, C. Molteni, G. Yahioglu, C. D. Lorenz, K. Suhling (2020) Small, 1907139.

[3] "On the interaction of hyaluronic acid with synovial fluid lipid membranes", P. Smith, R. M. Ziolek, E. Gazzarrini, D. M. Owen and C. D. Lorenz (2019) Phys. Chem. Chem. Phys., 21, 9845-9857.

[2] "On the hydration structure of the pro-drug GPG-NH2 and its derivatives", P. Smith, N. Steinke, J. F. C. Turner, S. E. McLain & C. D. Lorenz (2018) Chem. Phys. Lett. 706, 228-236.

[1] "Hybrid gelation processes in enzymatically gelled gelatin: impact on nanostructure, macroscopic properties and cellular response", F. Bode, M. A. da Silva, P. Smith, C. D. Lorenz, S. McCullen, M. M. Stevens, & C. A. Dreiss (2013) Soft Matter, 9, 6986-6999.

Awards

[3] Mitacs Globalink Research Award (2020) - £15 k

[2] Warren L. DeLano Open-Source Fellowship (2018) - £6 k

[1] Best talk - CPP5 Summer School (2018)

Societies

[3] Member of the Institute of Physics

[2] Member of the British Biophysical Association

[1] Member of the Biophysical Society

Open-Source Projects

MDAnalysis (Contributor) 2018 - Present

github.com/mdanalysis/mdanalysis

- Developed a new module for finding hydrogen bonds in molecular dynamics simulations that is orders of magnitude faster, more modular, and with a simpler API than the previous implementation.
- Collaborated on the development of an analysis tool that calculates dynamical properties of water at interfaces from molecular dynamics trajectories.
- Used scientific Python libraries, including numpy, to achieve a speedup of two orders of magnitude compared to previous implementation.
- Became familiar with git, github, pull requests and unit testing using pytest.