

EDWARD R. SMITH MEng PhD fHEA

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ACADEMIC HISTORY

PhD 2009 - 2013 Awarded: 01/01/14 Date of viva: 13/11/13	<i>On The Coupling Of Molecular Dynamics To Continuum Computational Fluid Dynamics</i> Mechanical Engineering, Imperial College London , UK
Masters in Engineering 2005 - 2009 Awarded: 01/10/09	Overall Grade: 1st Class Honours Mechanical Engineering, Imperial College London , UK

EMPLOYMENT HISTORY

- 2019-Present* **Lecturer, Brunel University London**
Multiscale fluid dynamics Lecturer in Aerospace and Mechanical Engineering.
- 2018-2019* **Mechanical Engineering Research Associate, Imperial**
Named researcher on fellowship to apply coupling to Tribological models.
- 2017-2018* **Civil Engineering Research Associate, Imperial,**
Developed my software, CPL library, for granular mechanics modelling of seepage instabilities, funded by eCSE grant I co-authored.
- 2014-2017* **Chemical Engineering Research Associate, Imperial,**
Applying coupled simulation techniques to model the impact of super-spreading surfactants on the moving contact line in droplets.
- 2014-2014* **Academic Visitor, Swinburne University, Melbourne, Australia,**
Visited Australia for two months to establish a new collaboration between Imperial and Swinburne university.
- 2013-2014* **Mechanical Engineering EPSRC Doctoral Prize Fellow, Imperial,**
Extended mathematical and computational framework for coupling and wrote single author paper on the first ever turbulent simulation using molecular dynamics.
- 2009-2013* **Mechanical Engineering PhD EPSRC Doctoral Training Award, Imperial,**
Centre of a collaboration between researchers in Tribology, fluid dynamics and molecular dynamics to establish a new multi-scale research area at Imperial, developing new molecular dynamics code and coupled to Computational Fluid Dynamics (CFD).

GRANTS AND AWARDS

- Grant* → Research Co-I on **EPSRC** application for a new supercomputer Young, a 12 university consortium Materials and Molecular Modelling Hub £4.5 million, (EP/T022213/1).
- Grant* → Funding for Special Interest Group (SIG) by the **UK Fluids Network (UKFN)** on Non-Equilibrium Molecular Dynamics (<https://fluids.ac.uk/sig/NonEqmMD>).
- Grant* → Research Co-I on an **EPSRC** Multiscale Surfaces Optimisation proposal worth £1.5 million, with £431k for Imperial, £561K for Brunel and £511k for Edinburgh (EP/S019545/1).
- Award* → **Dame Julia Higgins** Engineering Postdoc Collaborative Research Fund 2018 award providing £2,213, **a competition at Imperial for best grant writing.**
- Award* → Software Sustainability Institute 2017 **Fellowship** providing £3,000.
- Award* → Associate **Fellowship** of the Higher Education Academy.

- Grant* → Established contacts and named researcher on Royal Society International Exchange Grant IES/R3/170233 for £12k.
- Grant* → Academic PI on **Innovate UK grant** with eDrive providing £46,778 for six months postdoctoral time to develop motor optimisation software (TSB Ref. 132767).
- Grant* → Co-PI for successful **eCSE** application providing £91,630 for a year of postdoctoral time for research software engineering (eCSE08-3).
- Grant* → Contributed to successful **EPSRC** proposal *Particle-Scale Investigation Of Seepage Induced Geotechnical Instability* for £387,936 (EP/P010393/1).
- Grant* → Helped write the multi-scale theory section of an **EPSRC** establish career fellowship grant covering £1,205,330 for tribological modelling (EP/N025954/1) .
- Award* → Margaret Fishenden Centenary Memorial **Prize for best PhD thesis over the last five years** in the Department of Mechanical Engineering, Imperial College, 2016.
- Grant* → EPSRC Doctoral Prize Fellowship, Imperial College, 2014 providing £43,720 funding.
- Grant* → Assisted writing of a BP ICAM application to secure £210,000 funding for a postdoc and PhD student through the centre for doctoral training (CDT).
- Award* → **Silver prize** in the UK wide prestigious Osborne Reynolds Student Award for work on *Reynolds' Transport Theorem Applied to a Discrete System*.
- Grant* → Wrote first draft of re-application to **EPSRC** for a further six months of **dcSE** funding.
- Grant* → Co-authored application to **EPSRC** for **dcSE** support providing six months funding.
- Award* → Sir Bruce White **Best Project Prize** in Mechanical Engineering, Imperial College for Master's dissertation on *Thermal Modelling using the Lattice Boltzmann Method*.

TEACHING – Created 3 new courses, ~90 hours lecturing and ~160 hours tutoring experience

- Oct 2020 Taught the FEA Masters Course 12 hrs lectures and 12 hrs tutorials for ~50 students, again with excellent feedback
- Oct 2020 Module Leader developing 12 hrs of lectures and 12 hrs of tutorial content to modernise a second year course on Aerodynamics to include CFD (computational fluid dynamics) for 70 students. This included course organisation for remote delivery and critical alignment of questions for online group work tutorials, coursework and exams. Feedback was positive for the lectured content and delivery.
- Oct 2020 Developed and delivered 12 hrs of lectures in an entirely new second year programming course for ~200 students as part of mathematics and programming course. I ran 26 hrs of tutorials which included multiple breakout rooms for group work and a central seminar session where I solved problems interactively. This was supported by weekly automarked programming submissions using unit-testing concepts to continually engage students during COVID-19 pandemic lockdown, finishing with a software development exercise with report. Despite weekly deadlines, the course had very positive student feedback.
- Jan 2020 Ran 12 hrs team-based learning sessions and Labs for a first year dynamics course
- Oct 2019 Developed and taught the Finite Element Analysis (FEA) Masters Course at Brunel University where ~50 student are given 12 hrs lectures on fundamentals of FEA and write a code from scratch in 12 hrs of tutorials, testing and verifying their results. Course received excellent student feedback
- Nov 2018 Taught the CFD part of multi-scale modelling IMSE Masters program.
- Sep 2018 Delivered Python matplotlib course, 1 hr, ~40 students at HPC summer school.

- May 2018 Designed and lectured 4 hrs Git and best practice in software course to ~ 15 people.
- Nov 2017 Created a new for-credit computational fluid dynamics (CFD) course for the IMSE multi-scale Masters program with board derivations, hands-on sessions and lectures over 6 hrs including exam/course work development and marking.
- Oct 2017 Paid by Rolls-Royce to deliver two days of Python and software best practice teaching, with 12 hrs of material, to 40 professional engineers on site in Derby.
- Sep 2017 Developed a 2 day Python course, with 10 hrs lectures and hands-on, ~ 60 students.
- March 2017 Created and delivered a new 6 hrs Python course, for ~40 students, to address the shortage for Python teaching I observed at Imperial including surveying attendees to design lectures, creating exercises and recruiting tutors.
- 2011-2017 Extensive tutoring experience, including Mathematics (3 hours) and differential equations (1 hour) in Civil Engineering; MATLAB in both Chemical (36 hours) and Mechanical Engineering (16 hours); Polymer Simulation labs in Materials (6 hrs) and Fluid Mechanics board derivations in Mechanical Engineering (20 hrs).

SUPERVISION – Supervised 3 postdoc, 2 PhD, 7 masters and 14 undergrad projects

- 2020 Six third year projects, one group project and three Masters projects.
- 2020-present Numerical supervisor of a PhD student working on simulation of flow over an aerofoil.
- 2019-present Supervisor of a postdoctoral researcher on the EMBOSS project.
- 2018-present Supervisor of a postdoctoral researcher on the particle seepage project.
- 2019 Six third year projects and two masters project
- 2015-present Second supervisor of a PhD student sponsored by BP, including quarterly meetings, reporting, academic and personal supervision.
- Sep 2017 Academic supervisor of Innovate UK funder postdoctoral researcher for 6 months, including management of finance, quarterly reporting, meetings with companies and academic overview.
- 2012-2018 Two Master's student and two undergraduate projects at Imperial.

PUBLICATIONS – 21 Publications (14 significant contributions) including a single author

- 21 D. M. Heyes, D. Dini, and **E. R. Smith**, *Single trajectory transport coefficients [...] by molecular dynamics simulations*, J. Chem. Phys. 152(19):194504, (2020)
- 20 D. M. Heyes, D. Dini, and **E. R. Smith**, *Statistical analysis and molecular dynamics simulations of the thermal conductivity of Lennard-Jones solids including pressure and temperature dependencies*, Physica Status Solidi (b), 257(10):2000344, (2020)
- 19 **E. R. Smith** and C. Braga. *Hydrodynamics across a fluctuating interface*, J. Chem. Phys., 153(13):134705, (2020).
- 18 P. E. Theodorakis, **E. R. Smith**, R. V. Craster, E. A. Muller, O. K. Matar *Molecular dynamics simulation of the superspreading of surfactant-laden droplets. A review* Fluids 4 (4), 176 (2019)
- 17 P. E. Theodorakis, **E. R. Smith**, E. A. Muller *Spreading of aqueous droplets with common and superspreading surfactants. A molecular dynamics study*, Colloids and Surfaces A: Physicochemical and Engineering Aspects 581, 123810 (2019)
- 16 D. M. Heyes, D. Dini, and **E. R. Smith**, *Shear stress relaxation and diffusion in simple liquids by molecular dynamics simulations: Analytic expressions and paths to viscosity*, J. Chem. Phys. 150 (17), 174504 (2019)
- 15 **E. R. Smith**, E. Ramos-Fernandez, D. Trevelyan, C. O'Sullivan, D. M. Heyes and D. Dini, *CPL library - A computational framework for coupled molecular dynamics and computational fluid dynamics simulation* J. Comp. Phys. Comms. 250, 107068 , (2019)
- 14 **E. R. Smith**, P. Daivis, B. Todd *Measuring Heat Flux Beyond Fourier's law* Under review by J. Chem. Phys, 150, 064103 (2019)
- 13 C. Braga, **E. R. Smith**, A. Nold, D. N. Sibley, S. Kalliadasis *The pressure tensor across a liquid-vapour interface* J. Chem. Phys. 149, 044705 (2018)
- 12 D. M. Heyes, D. Dini, **E. R. Smith** *Incremental viscosity by non-equilibrium molecular dynamics and the Eyring model* Editors-pick J. Chem. Phys. 148, 194506 (2018)
- 11 **E. R. Smith**, P. E. Theodorakis, R. V. Craster, O. K. Matar *Moving contact lines: linking molecular dynamics and continuum-scale modelling* Langmuir Invited Feature and Journal Cover, 34, 12501 (2018).
- 10 D. M. Heyes, **E. R. Smith**, A. Branka and D. Dini, *Nanowire stretching by Non-equilibrium Molecular Dynamics*, Physica Status Solidi B, 160086 (2017)
- 9 **E. R. Smith**, D. M. Heyes and D. Dini, *Towards The Irving Kirkwood Limit Of The Mechanical Stress Tensor*, J. Chem. Phys. 146 , 224109 (2017)
- 8 **E. R. Smith**, E. A. Muller, R. V. Craster and O. K. Matar, *A Langevin Model for Fluctuating Contact Angle Behaviour Parametrised using Molecular Dynamics*, Front Cover Soft Matter 12(48):9604-9615 (2016)
- 7 D. M. Heyes, **E. R. Smith**, D. Dini, *Equilibrium fluctuations of liquid state static properties in a subvolume by molecular dynamics*. J. Chem. Phys. 145, 104504 (2016)
- 6 **E. R. Smith** *A Molecular Dynamics Simulation of the Turbulent Couette Minimal Flow Unit* Phys. Fluids 27, 115105 (2015) [www.arxiv.org/abs/1508.01163].
- 5 **E. R. Smith**, D. M. Heyes, D. Dini, and T. A. Zaki, J. *A localized momentum constraint for non-equilibrium molecular dynamics simulations* J.Chem.Phys. 142, 074110 (2015)

- 4 D. M. Heyes, **E. R. Smith**, D. Dini, and T. A. Zaki, J. *The method of planes pressure tensor for a spherical subvolume* J. Chem. Phys. 140, 054506 (2014).
- 3 **E. R. Smith**, D. M. Heyes, D. Dini, and T. A. Zaki, *Control Volume Representation of Molecular Dynamics* Phys. Rev. E, 85, 056705 (2012) [www.arxiv.org/pdf/1203.2453v2].
- 2 D. M. Heyes, **E. R. Smith**, D. Dini, H. A. Spikes, and T. A. Zaki, J. *Pressure dependence of confined liquid behaviour* J. Chem. Phys. 136, 134705 (2012).
- 1 D. M. Heyes, **E. R. Smith**, D. Dini, and T. A. Zaki, J. *The equivalence between volume averaging and method of planes definitions of the pressure tensor at a plane* J. Chem. Phys. 135, 024512 (2011).

SOFTWARE – Extensive software development with both open and close source projects

- CPL library – A software library to couple any two codes on high performance computing platforms (HPC) – massively parallel using MPI with a minimal interface and a full unit-testing and novel mocking framework, freely available under the GNU GPL v3 open source licence (<http://www.cpl-library.org>) with DOI: (10.5281/zenodo.56208).
- *FlowMol* – A massively parallel molecular dynamics code, designed for non-equilibrium molecular dynamics and coupled simulation. Written entirely from scratch, full details of validation and features on http://www.edwardsmith.co.uk/content/flowmol/MD_coding.html.
- PyDataView – Python based graphical user interface (GUI) framework for rapid visualisation of scientific data, open source under the GNU GPL v3 licence (<https://github.com/edwardsmith999/pyDataView>).
- SimWrapPy – A job running framework in Python for parallel and distributed parameter studies both locally and on HPC platforms, allowing runs of *FlowMol*, LAMMPS, OpenFOAM and Python scripts. Open source under the GNU GPL v3 licence (<https://github.com/edwardsmith999/SimWrapPy>).

CONFERENCES – Organised 2 conferences, 15 invited talks and 15 conference talks

- Secured funding, organised and ran the first special interest group meeting on non-equilibrium molecular dynamics at Brunel for thirty people.
- Organised, promoted and chaired a workshop at Imperial for twenty people on Continuous Integration in High Performance Computing.
- Invited talks: **1) Plenary Lecture**, Surface Wettability Effects on Phase Change Phenomena, Brighton, UK (2020) **2) Multiscale Fluid Dynamics with Molecules**, University of East Anglia (2020) **3) A Molecular Simulation of the Turbulent Minimal Channel Flow**, Southampton University (2019) **4) A Tutorial of Boiling Simulation using Coupled Simulation**, Royal Society-DFID Africa Capacity Building Initiative, Imperial College London (2019) **5) Coupling Molecular Dynamics to the Continuum for Fluid Dynamics Simulation**, Unimore, Modena (2019) (slides). **6) Heatflux Beyond Fourier's Law**, Swinburne University, (2019) (slides). **7) Molecular Fluid Dynamics**, University of Melbourne (2019) (slides). **8) ESI/CECAM Workshop on Physics at Fluid/Fluid Interfaces** Vienna, Austria (2017). **9) Coupling molecular to continuum for fluid mechanics** Aston Uni., UK (2017). **10)** Invited keynote speaker, multi-scale modelling special interest group, 2017. Edinburgh Uni. **11) Towards an exact coupling of Continuum Fluid Dynamics and Molecular Dynamics** Edinburgh Uni., (2016). **12)**

Molecular Simulation of Turbulent Couette Flow Swinburne Uni., Australia (2014). **13)**
The Control Volume for Molecular Dynamics RMIT Uni., Australia (2014). **14)** *Linking
the Continuous and the Discrete* Cavendish Laboratory, Cambridge UK (2013). **15)**
Continuum to Molecular Coupling Fluid Mechanics ZCAM workshop, Spain (2011).

REF 2021 Summaries for selected papers

Smith et al 2019 [15] This paper presents an overview of CPL library, software designed for coupling of computational fluid dynamics to molecular dynamics. The multiscale approach presented in this work was designed to directly benefit industry as part of a BP ICAM grant for £210k and two six month dCSE projects. The software has allowed a new collaboration with Civil Engineer including an eCSE grants which paid for my previous post doctoral position (eCSE08-3) as well as being a key component in the successful EPSRC grant (EPP0103931) for £388k. The users/collaborations base includes academics at Imperial, Japan, Glasgow and Melbourne.

Smith, Braga 2020 [19] In this work, we applied my control volume framework to a moving interface, providing a technique which allowed unrepresented insight into the nature of the fluid-liquid interface. The work resulted in me being an invited speaker at a Faraday format conference in Austria. The multiphase framework is the basis for an EPSRC grant (EP/S019545/1) between Imperial, Edinburgh and Brunel for £1.5 million, currently with very good reviews (6-6-5).

Smith et al 2016 [8] In this work, the moving contact line motion is simulated using molecular dynamics (MD) and the results parametrised using probability density functions used to design a Langevin model for coupling to a continuum solver. The reviews were favourable so the editor chose this article as the cover of *Soft Matter*. After seeing this work and meeting, Mirco Magnini came to Imperial to work and we wrote the Dame Julia Higgins engineering grant award together. The expertise demonstrated resulted in a paid BP challenge day on upstream oil recovery and an invitation to write a review article in *Langmuir*.

Smith et al 2015 [6] This single author paper presents the first ever simulation of turbulence using an all molecular dynamics (MD) simulation. Previously, such simulation scales were assumed to be impossible but it was achieved through a combination of careful parameter studies, heavily optimisation of my custom MD software for large scale computing and a year of running on a supercomputer. This work lead to me being asked to chair the general turbulence session at the 2017 APS Division of fluid dynamics conference, a number of invited talks and a meeting and email exchange with the father of MD, Prof. Berni Alder, who believes that this is the future of molecular simulation.

Smith et al 2015 [5] This paper builds on my mathematical framework, [Smith et al (2012)[3], with minimisation principles from classical physics to derive an exact method for coupling which generalises and unifies much of the existing literature. This work provides a complete underpinning framework for coupling and was a major factor in the award of the Margaret Fishenden prize for best thesis in the last 5 years. Based on this work, I was invited to Australia, establishing collaborations with Billy Todd and Peter Davis, obtaining a Royal Society Grant [IESR3170233] and publishing [14], as well as with Carlos Braga at Imperial publishing [13]. In addition, this fundamental contribution resulted in my invite to give the young researcher keynote at the first ever UK multiscale Special Interest Group.