

## EDWARD R. SMITH MEng PhD DIC afHEA

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### ACADEMIC HISTORY

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

### EMPLOYMENT HISTORY

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- Present* **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* **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 (*G*) AND AWARDS (*A*)

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- G* → 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) currently under review with very positive reviews (6 6 5).
- A* → **Dame Julia Higgins** Engineering Postdoc Collaborative Research Fund 2018 award providing £2,213, **a competition at Imperial for best grant writing.**
- A* → Software Sustainability Institute 2017 **Fellowship** providing £3,000.
- A* → Associate **Fellowship** of the Higher Education Academy.
- G* → Named researcher on proposal for collaboration with Australian collaborators "TWINNING: Confined Liquids and Smart Surfaces (P73161)".
- G* → Academic PI on **Innovate UK grant** with eDrive providing £46,778 for six months postdoctoral time to develop motor optimisation software (TSB Ref. 132767).
- G* → Co-PI for successful **eCSE** application providing £91,630 for a year of postdoctoral time for research software engineering (eCSE08-3).

- $\mathcal{G}$  → Contributed to successful **EPSRC** proposal *Particle-Scale Investigation Of Seepage Induced Geotechnical Instability* for £387,936 (EP/P010393/1).
- $\mathcal{G}$  → Helped write the multi-scale theory section of an **EPSRC** establish career fellowship grant covering £1,205,330 for tribological modelling (EP/N025954/1) .
- $\mathcal{A}$  → Margaret Fishenden Centenary Memorial **Prize for best PhD thesis over the last five years** in the Department of Mechanical Engineering, Imperial College, 2016.
- $\mathcal{G}$  → EPSRC Doctoral Prize Fellowship, Imperial College, 2014 providing £43,720 funding.
- $\mathcal{G}$  → 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).
- $\mathcal{A}$  → **Silver prize** in the UK wide prestigious Osborne Reynolds Student Award for work on *Reynolds' Transport Theorem Applied to a Discrete System*.
- $\mathcal{G}$  → Wrote first draft of re-application to **EPSRC** for a further six months of **dcSE** funding.
- $\mathcal{G}$  → Co-authored application to **EPSRC** for **dcSE** support providing six months funding.
- $\mathcal{A}$  → Sir Bruce White **Best Project Prize** in Mechanical Engineering, Imperial College for Master's dissertation on *Thermal Modelling using the Lattice Boltzmann Method*.

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#### **TEACHING – Created 2 new courses, 35+ hours lecturing and 80+ hours tutoring experience**

- Nov 2018 Teaching 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 solving differential equations (1 hour) and Mathematics (3 hours) 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-based solutions in Mechanical Engineering (20 hrs).

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#### **SUPERVISION – Supervised 1 postdoc, 2 PhD, 2 masters and 2 undergrad projects**

- 2015-present Second supervisor of 1 PhD student sponsored by BP, including quarterly meetings, reporting, academic and personal supervision.
  - Apr 2018 Master's projects on granular packing, obtaining first class marks.
  - Sep 2017 Academic supervisor of a postdoctoral researcher for 6 months, including management of finance, quarterly reporting, meetings with companies and academic overview.
  - Nov 2015 Two undergraduate projects obtaining first class marks.
- 2012-2015 One previous PhD student finishing with minor corrections.
  - 2012 One previous Master's student finishing in 2012.

## PUBLICATIONS – 13 Publications first/second author (significant contributions). 1 single author

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- 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 Article, 10.1021/acs.langmuir.8b00466 (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](http://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](http://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).

## CONFERENCES – Organised 1 conference, chaired 1 session, 8 invited and 11 conference talks

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- Organised, promoted and chaired a workshop at Imperial for twenty people on Continuous Integration in High Performance Computing.
- Invited to chair the general turbulence session at the 2016 APS Division of Fluid Dynamics, the biggest conference in the field of fluid dynamics.
- Invited talks: 1) *ESI/CECAM Workshop on Physics at Fluid/Fluid Interfaces* Vienna, Austria (2017). 2) *Coupling molecular to continuum for fluid mechanics* Aston Uni., UK (2017). 3) Invited keynote speaker, multi-scale modelling special interest group, 2017. Edinburgh Uni. 4) *Towards an exact coupling of Continuum Fluid Dynamics and Molecular Dynamics* Edinburgh Uni., (2016). 5) *Molecular Simulation of Turbulent Couette Flow* Swinburne Uni., Australia (2014). 6) *The Control Volume for Molecular Dynamics* RMIT Uni., Australia (2014). 7) *Linking the Continuous and the Discrete* Cavendish Laboratory, Cambridge UK (2013). 8) *Continuum to Molecular Coupling for Fluid Mechanics* ZCAM workshop, Spain (2011).