EDWARD R. SMITH MENG PHD DIC

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ACADEMIC HISTORY

PhD
2009 - 2013 Awarded: **01/01/14**
Date of viva: **13/11/13**

On The Coupling Of Molecular Dynamics To Continuum Computational Fluid Dynamics
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

- Civil Engineering eCSE funded Software Engineer, **2017-2018**
- Chemical Engineering Research Associate, **2014-2017**
- Mechanical Engineering EPSRC Doctoral Prize Fellow, **2013-2014**
- Mechanical Engineering PhD student, EPSRC Doctoral Training Award, **2009-2013**
- Arup building services mechanical engineer, **2004-2005** with three summer placements in Arup research and development, fire and communications, **2006-2008**

GRANTS

- Authored academic portion of **innovate UK** grant with my colleague from company eDrive giving six months postdoctoral time to develop motor optimisation software.
- Co-PI for successful **eCSE** application providing £100,000 for a year of postdoctoral time for research software engineering.
- PI for successful **EPSRC fellowship** application providing £49,000 funding.
- Co-PI of a successful application to BP to secure £210,000 funding for a fellow researcher and PhD student funded through the centre for doctoral training (CDT).
- Co-authored a successful application to **EPSRC** for distributed computational science and engineering (**dCSE**) support providing six months of direct employment costs and a contribution towards the indirect costs of a Nag computer scientist.
- Co-authored a successful re-application to **EPSRC** for a further six months of **dCSE** funding.

SOFTWARE

- CPL library – A software library to couple any two codes – massively parallel with a minimal unit-tested interface made freely available under the GNU GPL v3 open source licence (`http://www.cpl-library.org`).
- PyDataView – python based graphical user interface (gui) framework for rapid visualisation of scientific data (GNU GPL v3 licence `https://github.com/edwardsmith999/pyDataView`).
- *FlowMol* – a massively parallel molecular dynamics code, designed for non-equilibrium molecular dynamics and coupled simulation.

TEACHING

- Created and delivered a three-part Python course; hands-on sessions and lectures.
- Preparing to give again as a two-day segment of Imperial's HPC Summer School and invited teaching at Roll Royce Nuclear.

HONOURS AND AWARDS

- Software Sustainability Institute Fellowship, 2017.
- Margaret Fishenden Centenary Memorial Prize for best PhD thesis over the last five years in the Department of Mechanical Engineering, Imperial College, 2016.
- EPSRC Doctoral Prize Fellowship, Imperial College, 2014.
- Silver prize in the UK wide prestigious Osborne Reynolds Student Award for work on *Reynolds' Transport Theorem Applied to a Discrete System*.
- Sir Bruce White Best Project Prize in Mechanical Engineering, Imperial College for Master's dissertation on *Thermal Modelling using the Lattice Boltzmann Method*.

INVITED TALKS

1. *Direct Coupling of Computational Fluid Dynamics and Molecular Dynamics: Conservation, Computation and Timesteps* First meeting of Multiscale and molecular flows special interest group, (2017).
2. *Towards an exact coupling of Continuum Fluid Dynamics and Molecular Dynamics* Edinburgh University, (2016).
3. *Molecular Simulation of Turbulent Couette Flow* Swinburne University, Australia (2014).
4. *The Control Volume for Molecular Dynamics* RMIT University, Australia (2014).
5. *Linking the Continuous and the Discrete* Cavendish Laboratory, Cambridge UK (2013).
6. *Continuum to Molecular Coupling for Fluid Mechanics* ZCAM workshop, Spain (2011).

PUBLICATIONS

1. **E. R. Smith**, D. M. Heyes and D. Dini, Probability Distribution Functions of Pressure from Molecular Dynamics Simulation of a Lennard-Jones Fluid Under review in Physical Review E, EV11365 (2016)
2. **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 SM-ART-08-2016-001980 (2016)
3. D. M. Heyes, **E. R. Smith**, D. Dini, Equilibrium fluctuations of liquid state static properties in a subvolume by molecular dynamics. J. Chem. Phys. A16.05.0118R-A (2016)
4. **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) [**hdl.handle.net/10044/1/21849**].
6. 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).

7. **E. R. Smith**, D. Trevelyan and T. Zaki Scalable coupling of Molecular Dynamics (MD) and Direct Numerical Simulation (DNS) of Multi-scale Flows Part 2 Distributed CSE technical report (2013)
8. **E. R. Smith**, *On The Coupling Of Molecular Dynamics To Continuum Computational Fluid Dynamics* Thesis, Imperial College London, (2014).
9. L. Anton and **E. R. Smith**, Scalable coupling of Molecular Dynamics (MD) and Direct Numerical Simulation (DNS) of Multi-scale Flows Part 1 Distributed CSE technical report (2012)
10. **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**].
11. D. M. Heyes, **E. R. Smith**, D. Dini, H. A. Spikes, and T. A. Zaki, J. *Pressure dependence of confined liquid behaviour subjected to boundary driven shear* J. Chem. Phys. 136, 134705 (2012).
12. 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).

PRESENTATION AT CONFERENCES/WORKSHOPS

1. Software Sustainability Collaborations Workshop (2017) Leeds, UK.
2. APS Division of Fluid Dynamics (2016) Oregon, USA.
3. APS Division of Fluid Dynamics (2015) Boston, USA.
4. International Congress on Industrial and Applied Mathematics (2015) Beijing, China.
5. Computer Simulation of Confined Fluids (2014) the Shard London, UK.
6. APS Division of Fluid Dynamics (2014) San Francisco, USA.
7. CCP5-RSC Non-Equilibrium Molecular Dynamics workshop (2013) Imperial, UK.
8. HYBRID 2013 workshop (2013) Jülich supercomputing centre, Germany.
9. 21st International Discrete Simulation of Fluid Dynamics (2012) Bangalore, India.
10. GMSI nano-scale summer camp in Seoul (2011), South Korea.