Institution: Sheffield Hallam University

Unit of Assessment: 13 Electrical and Electronic Engineering, Metallurgy and Materials

Title of case study: Fluid Modelling - Expertise and Software

1. Summary of the impact

Fluid modelling approaches devised by the Materials and Engineering Research Institute's (MERI's) materials and fluid flow modelling group have impacted on **industrial partners**, **research professionals** and **outreach recipients**. This case study focuses on **economic impacts arising from improved understanding** which this modelling work has given of commercial products and processes. These include: metal particulate decontamination methods developed by the UK small company *Fluid Maintenance Solutions*; liquid crystal devices (LCDs) manufactured by the UK SME *ZBD Displays*; and an ink-droplet dispenser module originally invented at the multinational *Kodak*. Additionally, the modelling group's computer simulation algorithms have been **adopted by industrial research professionals** and made available via *STFC Daresbury*'s internationally distributed software package DL_MESO. Finally, the group has developed, presented and disseminated simulation-based materials and visualisations at major **public understanding of science** (PUS) events.

2. Underpinning research

Materials modelling has been a continuous element in MERI's research activity through the work of Care (1988-2012), Halliday (1985-present) and Cleaver (1994-present). Particular areas of specialisation have been: coarse-grained molecular simulation of ordered fluids; Lattice Boltzmann (LB) simulation of multi-component fluids; and mesoscopic modelling of liquid crystals (LCs). As set out below, much of this work has been undertaken in collaboration with industrial partners.

The simulation methodologies developed by the MERI modelling group over the last ~20 years represent an unrivalled suite of modelling tools for LCD design and optimisation: no other group in the world can offer molecular, coarse-grained, LB and mesh-free modelling of LCs. The group's standing in this field originates from the period 1994-2002 when, in collaboration with the then Displays and Devices group at *DERA*/*QinetiQ* in Malvern, Care and Cleaver led a series of research projects relating to molecular and mesoscopic computer simulation of LC behaviour. This comprised four PhD projects partially supported by *DERA*/*QinetiQ* [i] and one by EPSRC [ii], and included innovations on the modelling of, for instance, LC mixtures [1] and tilted smectic phases. Within this collaboration, Cleaver and Care, working with senior scientists from *DERA*/*QinetiQ*, identified an industrial need for a methodology capable of modelling the switching behaviour of LCDs. This triggered two projects (1998-2002) with *DERA*/*QinetiQ* within which a generalised LB simulation approach for LCs was developed [2]. This also built on Halliday's previous expertise on LB modelling of isotropic fluids (see below). The first of these projects [iii] concentrated on a director-based LB model. The second [iv], which focused on a prototype display device then being developed by *QinetiQ*, prompted the development of algorithms for a more comprehensive Qian-Shen Q-matrix description of LB nemato-dynamics [2]. This was particularly progressive since it aligned the simulations with the continuum descriptions employed by *QinetiQ*'s LCD designers. Equipped with this designer-oriented technology, the MERI modelling group secured EPSRC support [v] and a significant research contract with *SEIKO-Epson* (2001-3) to develop, evaluate and document a mesoscopic LCD simulator [vi]. However, *SEIKO-Epson* would not disclose its motivations or intended usage of this simulator, so any impact arising from [vi] remains uncaptured.

As documented in **section 4**, Care went on to lead a DTI-supported [vii] project (2005-08) with *ZBD Displays*, an SME which had been spun out from *QinetiQ*. This required the modelling group's LB nemato-dynamics methods to be extended to incorporate realistic representations of electromagnetism, dielectric inhomogeneity and complex boundaries. The result was the first full device solver capable of modelling the switching behaviour of a LCD [3]. Further innovations led by Cleaver (2004-09) included simulations of LC anchoring at patterned substrates [viii], which led to a joint publication with *Sharp Labs Europe*, and the development of a fundamentally different "mesh-free" approach for LCD modelling based on inherently multi-scale Modified Smooth Particle Hydrodynamics methods. This approach was rolled out and tested in an industrial context in 2009 through a collaboration with *Hewlett-Packard Labs*, Bristol [4,ix].

In parallel with their developments on LC modelling, from 1997 the MERI modelling group also established an expertise in LB simulation of isotropic fluids, particularly immiscible multiphaseflows. Here, using support from both industry [x-xii] and research councils [v,xiii] Care and Halliday focussed on the development of mathematical descriptions and simulation algorithms for fluid-fluid interfaces [5]. Achieving more singular and isotropic representations of these interfaces enabled descriptions of model systems whereby deformable particles suspended in an ambient fluid were represented as multiple immiscible droplets. The resultant algorithms subsequently found application in simulation of a range of complex flows involving high-volume-fraction suspensions [6]. In the context of engineering flows, this led to collaborative projects with: *BNFL* on radioactive sludges; *Rolls Royce Associates* on thermal fluids [x]; Fluent on algorithm refinement [xi]; *Cadbury* on food systems; and *Kodak* on ink droplet formation [xii]. The developments made with Fluent went on to form the basis of a collaboration on haemodynamics with Harvard Medical School and another on biofluid flows with UK experimental groups [xiii]. The modelling group's LB expertise was also used in Knowledge Transfer interventions with *Fluid Maintenance Solutions* and *Nestlé*.

3. References to the research

[1] D.J. Cleaver, C.M. Care, M.P. Allen and M.P. Neal "Extension and generalization of the Gay-Berne potential "*Phys. Rev. E* **54,** 559 (1996)
DOI: 10.1103/PhysRevE.54.559 118 citations (WoS Sept 2013)

[2] C.M Care, I. Halliday, K. Good and S.V. Lishchuck, "Generalized lattice Boltzmann algorithm for the flow of a nematic liquid crystal with variable order parameter" *Phys. Rev. E* **67**, 061703 (2003) DOI: 10.1103/PhysRevE.67.061703 17 citations (WoS Sept 2013)
KEY REFERENCE

[3] T.J. Spencer, C.M. Care, R.M. Amos and J.C. Jones**, "**Zenithal bistable device: comparison of modelling and experiment" *Phys. Rev. E* **82**, 021702 (2010)
DOI: 10.1103/PhysRevE.82.021702 5 citations (WoS Sept 2013)

[4] M.M. Yakutovich, C.J.P. Newton, C.M. Care and D.J. Cleaver, "Mesh-free modelling of liquid crystals using modified smoothed particle hydrodynamics" *Phys. Rev. E* **82**, 041703 (2010)
DOI: 10.1103/PhysRevE.82.041703 1 citation (WoS Sept 2013)

[5] S.V. Lishchuk, C.M. Care and I. Halliday, "Lattice Boltzmann algorithm for surface tension with greatly reduced microcurrents" *Phys. Rev. E* **67**, 036701 (2003)
DOI: 10.1103/PhysRevE.67.036701 53 citations (WoS Sept 2013)
KEY REFERENCE

[6] T.J. Spencer, I. Halliday and C.M. Care, "Lattice Boltzmann method for multiple immiscible continuum fluids" *Phys. Rev. E* **82**, 066701 (2010)
DOI: 10.1103/PhysRevE.82.066701 3 citations (WoS Sept 2013)
KEY REFERENCE

[i] DERA, Malvern, PI Cleaver "Molecular simulations of liquid crystals" £31,000 (1995-'99)

[ii] EPSRC GR/L86135, PI Care "JREI funding for computer equipment" £33,838 (1998-'01); EPSRC GR/M16023, PI Cleaver "Molecular modelling of liquid crystalline materials" £39,000 Plus £63,288 national facility time (1998-'01)

[iii] DERA, Malvern, PI Care "Mesoscopic simulations of liquid crystals" £15,000 (1998-'01)

[iv] Qinetiq, Malvern, PI Care "Lattice Boltzmann modelling of a display device" £62,000 (2001-'02)

[v] EPSRC GR/R41170/01, PI Care "Modelling phase separation and flow in mixtures of nematic and isotropic fluids" £57,300 (2001-'03)

[vi] Seiko-EPSON (Japan), PI Cleaver "Mesoscopic simulator for liquid crystal devices" £191,000 (2001-'03)

[vii] DTI TP/2/ED/6/1/10260 with ZBD Displays Ltd, PI Care "ZBD Simulations" £146,625 (£128,662 from DTI, remainder from ZBD Displays) (2005-'07)

[viii] EPSRC GR/S59833/01, PI Cleaver "Anchoring of liquid crystals on self-assembled monolayers" £85,355 (2004-'07)

[ix] Hewlett Packard, PI Cleaver "Mesoscopic Liquid Crystal simulation" £2,000 (2008)

[x] Rolls Royce Associates, PI Halliday "LB simulation of thermofluids" £10,000 (1997-2000);

[xi] Fluent, PI Care "LB algorithms for immiscible fluids" £23,000 (2000-'02);

[xii] Kodak, PI Care "LB simulations of a flow-focussing device" £13,927 (2007-'08)

[xiii] BBSRC BB/F013744/1, PI Care "Optimisation of perfusion bioreactor for bone tissue growth" £298,755 (2008-'11)

REF2014 Research Excellence Framework

4. Details of the impact

In the REF impact period, the MERI modelling group's simulation expertise has achieved **economic impact** through **improved product and process understanding**. This range of outward-facing activities undertaken by the group is illustrated here in the contexts of a small company (*Fluid Maintenance Solutions*), an SME (*ZBD Displays*) and a multinational (*Kodak*).

Fluid Maintenance Solutions (*FMS*) [A] is a South-Yorkshire-Based small company specialising in the recovery of high value metals contained within sump sludges. *FMS*'s core activity is a recycling process in which thin contaminant films of hydrocarbon are removed from poly-disperse metallic particulates. *FMS* first engaged with the MERI modelling group in 2008 via the coordinated Knowledge Transfer activity Nanofactory (**REF3a(b)**). This enabled a sustained intervention in which Halliday determined the key decontamination mechanism in *FMS*'s recycling process and developed a LB-based model, based on reference [5], with which to simulate it. *FMS* had no in-house expertise capable of undertaking such work. In 2010, Halliday delivered a final report setting out simulations performed to investigate the viscous shear stress effects underpinning the decontamination stage of *FMS*'s re-cycling process. The insight this gave *FMS* into the capabilities of its industrial methodology then aided in the development of its future business. Specifically, the credibility provided by Halliday's report enabled the company to substantiate its claims to customers. *FMS* went on to make two successful TSB funding applications and in 2012 it was shortlisted for an Advanced Manufacturing Award [A]. Beneficiaries from this impact are ***FMS* and its customers**.

ZBD Displays is a Malvern-based technology company which was spun out from *QinetiQ* in 2000 [B]. Its core business is based on a specialist LCD technology – a very-low-energy display requiring no battery power to retain its image – which it has successfully directed towards the niche market of shelf-edge labelling for retail. As a small company with limited funds or staff time for R&D, *ZBD Displays* nevertheless engaged the MERI modelling group on a 24 month (2005-7) DTI-funded project [vii] to develop a detailed LB nemato-dynamics simulation scheme and use it to investigate operational details of the *ZBD* device. Subsequently, the company fully funded a further 6 months of research and invested staff time to maintain the collaboration up to publication of a joint paper in 2010 [3]. Given the company's size and the capabilities of its staff-base, it would have been impossible for it to undertake such work other than through partnership with the MERI group. The work programme for this collaboration was designed to explore potential future device improvements and, so, enable *ZBD Displays* to make informed future strategic decisions. The simulations did, indeed, determine and quantify potential improvements as well as providing insights into certain failure mechanisms. However, the enhancements identified were ultimately judged insufficient to warrant disruption of a working production process. The key impact of MERI's interaction with *ZBD Displays* was, therefore, that it provided the company with unambiguous "capability limits" for its device hardware. This contributed to a fundamental shift in the company's focus from its hardware origins to systems processes and software [C]. *ZBD Displays* has thrived since its 2006-10 collaboration with MERI - in 2012 it achieved sales of £12m, was ranked 5th in the Sunday Times League Table of the UK's fastest growing technology firms, and named top of the Deloitte Fast 50 technology firms following 5-year growth of 17910% [B]. Beneficiaries from this impact are ***ZBD Displays*, their share-holders and customers**.

In 2007-08, the MERI modelling group worked with *Kodak*'s then European Research Lab in Cambridge to study an ink-droplet dispenser module developed to enhance the capabilities of high-speed digital printers [xii]. *Kodak* had a pre-existing patent on this module [D], but had identified a requirement for specialist simulation work to determine key operational processes and design parameters. Experimentally, the geometry of this module had been shown to achieve consistent droplet size uniformity, but ambiguities persisted regarding the underlying physics. Therefore, in a study led by Care, LB simulations of multiple droplet flow were performed using MERI's immiscible fluid algorithms [6] in *Kodak*'s module geometry. This succeeded in identifying the key droplet pinch mechanism [E] and, thus, the module's main design parameters. In particular it confirmed that there was a sound basis for the observed droplet uniformity. Whilst *Kodak* underwent global restructuring subsequent to this intervention, the relevant patent remained active because (i) as part of *Kodak*'s core printing portfolio it was retained during chapter 11 proceedings and (ii) the module's inventors (the *Kodak* employees who had worked with Care) negotiated rights to exploit the device outside of printing through a new spin-out *Imbrys*. Additionally, subsequent work on the module, involving the same inventors, elicited a new patent filing on a different feature of the droplet module [E]. Beneficiaries from the improved device understanding achieved here are, then, ***Kodak*** and ***Imbrys***, through their ongoing patent interests in [D].

As well as working with a range of industrial groups, the MERI modelling group also has a track record of achieving uptake of its simulation algorithms by **other modelling professionals**. Direct uptake includes that by modellers at *Kodak* (USA) and *Petrobras* (Brazil) who have utilised the MERI group's LB algorithms to simulate industrially-relevant systems. The former, which started through a direct email query, has developed into an extended interaction [F]. More systematically, the group has also contributed actively to the development DL_MESO a commercially-available simulation package developed and disseminated by the Computational Science Group at the *STFC Daresbury* laboratory [G]. Specifically, Care and Halliday have been advisory panel members for DL_MESO and the LB routines which comprise the bulk of DL_MESO, including the multi-component schemes for both "dipahsic" and many mutually immiscible fluids are, essentially, those developed in references [5,6]. Downloads of the DL_MESO software in the REF impact window total 637, of which 574 were from outside the UK [H]. Beneficiaries from this work include relevant sections of ***STFC Daresbury*** and **their sponsors**, due to the associated enhancements to their product, as well as **materials simulation professionals** gaining access to MERI-devised algorithms (either directly or through DL_MESO) and applying them in a non-academic context.

The final impact achieved by the MERI modelling group relates to **PUS** activities undertaken by Cleaver. In collaboration with partners from the Universities of Manchester, Southampton and York and *Sharp Labs Europe*, under the auspices of the British Liquid Crystal Society, Cleaver developed and presented LC simulation material for the PUS stand "Liquid Crystals: Living Cells and Flat Screen TVs" at the Royal Society tri-centennial Summer Science Exhibition (July 2010) [J]. As well as simulation-based display items and information sheets for teachers, Cleaver developed a live interactive computer simulation application for the event. The PUS stand was presented to Her Majesty the Queen, David Willets MP, and many other dignitaries and Fellows of the Royal Society at the Exhibition's opening event [J]. Over the following three weeks, the event, which occupied the ground floor exhibition space of London's Festival Hall, was attended by thousands of members of the public and school groups, with over 2000 specifically visiting the LC stand. The Royal Society gave a positive evaluation to Cleaver's stand and subsequently nominated it for inclusion in the 30,000 footfall Big Bang event (March 2011, Excel Arena, London). In this shorter, but larger, event, a slightly revised version of the original stand was presented and included in a Royal-Society-coordinated Family Tour called "Specially Selected". Big Bang evaluated the LC stand as "Excellent" [K]. Follow through on the events delivered in 2010 and '11 included write-ups in 'Liquid Crystals Today' and conference presentations. These were picked up in the 'Routes to Impact' sections of several RCUK applications and explicitly led to, for example, development of a PUS stand at Big Bang Scotland 2013 from Strathclyde University. Additionally, resources developed were shared with other PUS providers globally. For example, Cleaver's live interactive computer simulation application was posted on the high profile NSF-funded Soft Matter World website [L] where it has achieved downloads from 5 continents of ~80 per month. Beneficiaries of this impact were the **Royal Society** and **Big Bang 2011**; **school groups** who visited the stand (as independently evaluated by the Royal Society and Big Bang); and **family groups** who engaged in, for example, the "Specially Selected" Royal Society Family Tour.

5. Sources to corroborate the impact

[A] http://www.fluidmaintenancesolutions.com/
[B] http://www.zbdsolutions.com/
[C] Co-Founder and Chief Scientific Officer of *ZBD Displays Ltd*, corroborating source 1
[D] US patent US20100188466 A1 http://www.google.co.uk/patents/US20100188466
[E] Former lead researcher at *Kodak European Research* and co-owner of *Imbrys*, corroborating source 2
[F] Email trail from researcher at *Kodak USA*, corroborating source 3
[G] http://www.stfc.ac.uk/CSE/os/25522.aspx.
[H] Lead developer of DL_MESO, *STFC Daresbury*, corroborating source 4
[J] http://seefurtherfestival.org/exhibition/view/liquid-crystals-living-cells-and-flat-screen-tvs
[K] Email from Big Bang coordination team, corroborating source 5
[L] http://www.softmatterworld.org/education/index.html