Institution: Edinburgh Research Partnership in Engineering (ERPE: Edinburgh and Heriot-Watt Universities joint submission)		
Unit of Assessment: UoA12 Engineering		
Title of case study: dsmcFoam+ Software: Advancing global microchip manufacturing and aerospace sectors		
Period when the underpinning research was undertaken: October 2013 – April 2018		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Matthew Borg	Reader	18/08/2015 – present
Jason Reese	Professor, Regius Chair of Engineering, RAE Chair in Emerging Technologies	01/10/2013 – 08/03/2019 (deceased)
Period when the claimed impact occurred: 2014 - 2020		
Is this case study continued from a case study submitted in 2014? No		

1. Summary of the impact

EPSRC funded research supported ERPE researchers Borg and Reese to develop new complex fluid dynamic engineering solvers and deliver extensive impact, as follows:

(A) The solvers have been incorporated into dsmcFoam+ open-source software, enabling accurate simulation of the physical behaviour of rarefied gases, which is essential for companies to design-engineer products and systems that operate in low-pressure, micro/nano scale or hypersonic environments. dsmcFoam+ was further incorporated within OpenFOAM software by OpenCFD Ltd in 2018, now with an international user-base and 200,000 annual downloads;

(B) In 2018 the full software was described as 'ground breaking' by multi-national company ASML in their adoption to design, model and manufacture Extreme Ultra Violet (EUV) photolithography machines of huge complexity (unit cost up to USD200M) used by the world's largest manufacturers of advanced integrated circuits, including Samsung and Intel;

(C) The software was utilised by aerospace engineering consultancy FGE to model jet propulsion designs in planetary atmospheres for European Space Agency missions since 2014;

(D) It was also used in the design of the CERN Beam Gas Curtain to model the continuous and molecular flows in the electron beam gun nozzle.

2. Underpinning research

Direct Simulation Monte Carlo (DSMC) modelling is a methodology for predicting the behaviour of gases in many different types of environments. The late Professor JM Reese was a pre-eminent developer of DSMC and joined the University of Edinburgh in 2013. From 2013-2019 he carried out EPSRC-funded research [P1] and collaborated in multi-institutional national and international partnerships, with groups including Strathclyde, Warwick, Glasgow, Michigan, US Air Force Office of Scientific Research and Brazilian aerospace research institutes, that made use of the EPSRC-funded ARCHIE WeST High-Performance Computer.

Key research drivers were defined by the silicon fabrication industries who required gas simulation capability in the design and development of their multi-million dollar facilities. Examples included being able to model the behaviour of rarefied gases to prevent deformation of silicon wafers or to prevent re-entry of gases into the process machines and avoid contamination of the expensive optical systems and masks. Other drivers included being able to model the gas plumes from satellite rocket motors, or to measure aerodynamic lift on a 'drag body in motion' in rarefied gas conditions, such as the Martian atmosphere.

In 2014, Reese and Borg proposed a new hybrid method to simulate heat transfer in dilute gas flows that coupled a continuum-fluid description to the DSMC solver [3.1]. It provided a local correction to a continuum sub-region, enabling the correct flow physics to be maintained over the entire continuum domain. Key advantages over existing techniques included its suitability for assessing complex flow problems at a fraction of the computational cost.

In 2014-15, a new coupling approach [3.2] for the time-advancement of multi-physics models of multi-scale systems was reported. A number of applications were tested, including a comparison with experiments of thermally-driven rarefied gas flow in a micro capillary. This new approach unlocked a key advance in the ability to model and produce analysis results almost 50,000 times faster than a conventionally-coupled solver, while achieving very similar results,.

Reese led the design and development and several applications of open-source software, specifically dsmcFoam code, where he and colleagues improved its code using their research findings and outputs. They tested the application of new developments of their work in the dsmcFoam software platform. Using DSMC procedures, based on microscopic gas information, they applied the quantum-kinetic (Q-K) model and demonstrated its validity when compared with analytical solutions for both inert and reacting conditions [3.3]. Early version test cases were also applied (2014-15) to design and model hypersonic flow benchmarks that would be of significant value to the aerospace sector.

Reese and team investigated the direct simulation of dsmcFoam and its ability to solve low and high speed non-reacting gas flows in simple and complex geometries. The test cases included the Mars Pathfinder probe, a micro-channel with heated internal steps and a simple micro-channel. The findings published in 2015 [3.4] showed that, for every case investigated, adopting this new approach within the dsmcFoam methodology resulted in significantly improved performance compared with experimental and numerical data available in the literature.

Borg joined the University of Edinburgh in 2015 and, funded by EPSRC, worked with Reese to research the validation of the transport of mass, momentum and heat in hybrid DSMC methods. Their work achieved a considerable speed-up for the 2D problem of gas flowing through a microscale crack. Their hybrid method accurately predicted the velocity and temperature variation over the cross-section as well as mass flow rates. They worked closely on the development of the dsmcFoam upgrades (dsmcFoam+) to ensure that the mathematical findings of their research could be embedded in an open software platform and made available to the user community through future upgrades. dsmcFoam+ is now able to rapidly analyse and successfully model 3D examples using OpenFOAM's functionality. A powerful tracking algorithm ensures that the modelled gas behaves in a physically realistic manner. The software is designed to handle new efficient multiscale parallel simulation and its novelty and originality is its ability to simulate a wide range of physics required by companies developing products in low pressure, micro/nano scale or hypersonic and aerospace engineering environments.

In 2018, the new full version software dsmcFoam+ was launched via OpenFOAM and in parallel, Reese and Borg published an appraisal of the latest contents, methodologies and research applications of *dsmcFoam+* [3.6]. This work proved to be key for the future gas modelling within Extreme Ultra Violet (EUV) photolithography machines. [3.6] was the 5th most downloaded paper from *Computer Physics Communications* in April 2018 and by February 2019 had become the 2nd most downloaded paper within the previous 90 days.

The very high potential for Reese's ongoing research to deliver further economic, scientific and social benefit to the UK and internationally was recognised in 2018 with the award of a prestigious GBP1.3M Royal Academy of Engineering Chair in Emerging Technologies.

3. References to the research

[3.1] **Journal**. Docherty, S., Borg, M., Lockerby, D. and Reese, J. (2014) Multiscale simulation of heat transfer in a rarefied gas. International Journal of Heat and Fluid Flow, Vol. 50, pp114-125. https://doi.org/10.1016/j.ijheatfluidflow.2014.06.003

[3.2] **Journal**. Lockerby, D., Patronis, A., Borg, M. and Reese, J. (2015) Asynchronous coupling of hybrid models for efficient simulation of multiscale systems. Journal of Computational Physics, 284, pp261–272 https://doi.org/10.1016/j.jcp.2014.12.035

[3.3] **Journal**. Scanlon, T., White, C., Borg, M., Palharini, R., Farbar, E., Boyd, I., Reese, J. and Brown, R. (2015) Open-source direct simulation Monte Carlo chemistry modelling for hypersonic flows. AIAA Journal, Vol. 53, (Issue 6), pp1670-1680. https://doi.org/10.2514/1.J053370

[3.4] **Journal**. Palharini, R., White, C., Scanlon, T., Brown, R., Borg, M. and Reese, J. (2015) Benchmark numerical simulations of rarefied non-reacting gas flows using an open-source DSMC code. Computers and Fluids. Vol. 120, pp140-157. https://doi.org/10.1016/j.compfluid.2015.07.021

[3.5] **Journal**. Docherty, S., Borg, M., Lockerby D. and Reese, J. (2016) Coupling heterogeneous continuum-particle fields to simulate non-isothermal microscale gas flows. International Journal of Heat and Mass Transfer, 98, pp712-727 https://doi.org/10.1016/j.ijheatmasstransfer.2016.03.040

[3.6] **Journal**. White, C., Borg, M., Scanlon, T., Longshaw, S., Emerson, D. and Reese, J. (2018). dsmcFoam+: An OpenFOAM based direct simulation Monte Carlo solver. Computer Physics Communications, 224, pp22-43 URL: https://doi.org/10.1016/j.cpc.2017.09.030

P1 - EPSRC funded project. EP/K038621/1. The First Open-Source Software for Non-Continuum Flows in Engineering. (PI) Reece, J., GBP344,848 (1/10/13 - 31/03/18).

4. Details of the impact

The multiple impacts arising from Reese and Borg's research include:

(A) Open-source software which incorporates dsmcFoam+ code

Reese and Borg's collaboration with ESI's OpenCFD Ltd led to the incorporation of their engineering design calculations into the development of the unique dsmcFoam+ code to create a state-of-the-art simulation tool that is now embedded within the internationally used software package OpenFOAM [5.1]. The dsmcFoam+ code includes the research findings from [3.6] and uses complex engineering fluid dynamic simulation solvers designed by Reese [3.3], and Reese and Borg [3.4, 3.5], including unsteady, rarefied, reacting flows in complex-3D geometries within the OpenFOAM framework.

The Managing Director of OpenCFD Ltd, owners of ESI-OpenFOAM, stated "*There is a big need for rarefied gas dynamics modelling in the community*" [5.1]. The Managing Director of ESI-OpenCFD also acknowledged the impact from Reese and Borg's work as "*This DSMC software that you and Jason develop is used by some of our big clients in the silicon-wafer industry (e.g. Samsung and ASML), other consultancy businesses in the aerospace industry (e.g. Fluid Gravity Engineering Ltd) and many other academics around the world*." [5.1]

(B) Enabling the mass manufacture of the world's most advanced microchips - ASML

ASML is a key user of the dsmcFoam+ design modelling software. A multinational company, based in 60 cities in 16 countries worldwide [5.2] and employing over 24,000 staff, it is a global innovation leader in technology for the microchip industry. It provides all of the major integrated circuit (IC) micro-fabricators with the hardware, software and services to use photolithography to mass-produce patterns on silicon [5.2]. The dsmcFoam+ code is essential for the optimal design of ASML's Extreme Ultra Violet (EUV) photolithography machines that are at the heart of the world's most advanced IC manufacturing systems. The EUV photolithography machines comprise 100,000 parts [5.2] and cost up to USD200,000,000 each, with the company selling 10

EUVs in the third quarter of 2020 [5.3]. ASML affirmed that the EUVs "*play a vital role in the manufacture of computer chips, mapping out their circuitry*" [5.2]. After winning the coveted SEMI Americas award (July, 2020) for their EUV machine, which is designed using the dsmcFoam+ software, their Chief Technology Officer stated "*moving to the extreme ultraviolet (EUV) wavelength of 13.5 nm represented a true paradigm shift, extending to all aspects of light generation, reflective optics, vacuum environment management, wafer stage alignment and a host of other fields*" [5.4].

ASML acknowledged Borg's impact on the development of dsmcFoam+ software and how this had benefitted ASML and their EUV machines, stating "*What we do increases the value and lowers the cost of a chip, which advances us all towards a smarter, more connected world*" [5.2]. To enable the fabrication of ever-smaller features in ICs (below the 2nm logic node), lithography machines utilise the shorter EUV light source. Careful control and mixing of gas-flows is critical, however, to avoid temperature variations, wafer deformation and fracture. ASML confirmed "*The use of the software has enabled improved design thinking, related to rarefied gas flows, in sensitive regions of the EUV machine … The ground-breaking research software developed at UoE by Prof Jason Reese and yourself has allowed us to meet some of these scientific challenges in ASML, specifically of modelling non-conventional rarefied gas dynamic physics in complex 3D geometries"* [5.2].

ASML supplies [5.5] to the world's top three IC fabricators including Samsung, Intel and Taiwan Semiconductor Manufacturing Company (TSMC) and their chips are used in Samsung S10 and iPhone X models (which had combined sales of over 50,000,000 in launch years). In the article '*EUV lithography: the brave new nanochip era'* [5.5], the advancements in the EUV machines, which were enabled by the new software, were described as "*Think of the old technology as a large paint brush, and a EUV light source as a fountain pen*" and how these also supported Moore's Law [5.5]. Moore's Law states that as the continual reduction in the size of transistors doubles, about every two years, the number of transistors that can be made (per unit area) on a microchip doubles, while at the same time halving the cost of computing power. The ever-increasing component density makes extreme demands on wafer fabrication technology. ASML stated "*Providing highest-resolution lithography in high-volume manufacturing, ASML's EUV machines are pushing Moore's Law forward*" [5.6]. This has impacted widely on society by enabling the rise of ever more affordable consumer, industry and business electronics including ubiquitous mobile communications, systems on chips, satellite navigation and medical electronics.

(C) Utilisation by Aerospace Industry and CERN

UK companies such as Fluid Gravity Engineering Ltd (FGE), who undertake space research modelling and aerospace consultancy for the European Space Agency have used dsmcFoam+. They described its use as having a "*substantial impact"* on the company [5.7] via consultancy projects they delivered which "*enabled FGE to establish a capability in computing rarefied flows relating to high speed aerodynamics and aerothermodynamics as well as spacecraft propulsion*". FGE utilised since 2014 the early versions of the Borg and Reece dsmcFoam software in projects to model interactions with rarefied gases in the following European Space Agency projects [5.7]:

- plume impingement studies for Mars Phobos and Lunar regolith, supporting both engineering aspects of descent module soft landing and scientific analysis of regolith samples,
- plume expansion calculations for in-space satellite propulsion, assisting to define the contamination environment, forces and moments from the spacecraft's control thruster,
- ENVISION Aerobraking scenarios: aerodynamic and aerothermodynamic calculations for a prospective Venus orbiter.

In October 2018 the Beam Gas Curtain project at CERN acknowledged the use of dsmcFoam+ to model continuous and molecular flows in an electron beam gun nozzle [5.8].

(D) Supporting Knowledge Networks and Advancing Reach

OpenFOAM is owned and operated by UK company ESI-OpenCFD Ltd [5.1] and has over 200,000 downloads per year with an approximate user-base of 25,000 advanced modellers [5.1]. Incorporating the dsmcFoam+ code into OpenFOAM made it accessible to tens of thousands of people around the world who download and use this software package. The dsmcFoam+, accessible downloads, has been promoted by the multi-institution online network for '*Micro and Nano Flows in Engineering*' funded by EPSRC [5.9]. This helped it to reach multi-institution researchers and international industry R&D staff working in this field to improve research capacity and engineering practice. UK and international universities and research institutes that utilise the dsmcFoam+ software to support fundamental and applied research projects include Warwick, Glasgow, Strathclyde, STFC Daresbury Lab, Xi'an Jiaotong and Beihang Universities in China [5.1, 5.9].

5. Sources to corroborate the impact

[5.1] Letter of impact from Managing Director of OpenCFD Ltd (Sept, 2020)

- about incorporation of dsmcFoam+ within OpenFOAM owned by ESI-OpenCFD Ltd
- stating number of annual downloads and users of OpenFOAM (which includes the dsmcFoam+ version)
- diversity of users of dsmcFoam and industry 'big need' for this modelling tool for gas flows.

[5.2] Letter from ASML multinational company on significance (ground breaking) of Borg/Reese dsmcFoam software used in the design of high value EUV machines. (Sept, 2020)

[5.3] CGTN News article, Comparative sales by ASML 2020 versus 2019 and sales of EUV 2020 showing 24% increase and value of EUV machines up to USD200,000,000 per unit. (Oct, 2020)

https://news.cgtn.com/news/2020-10-14/ASML-Q3-profit-beats-expects-China-s-annual-sales-to-exceed-1b-euros-UAcrbKHmjC/index.html

[5.4] Statement by ASML Chief Technology Officer, SEMI Americas Award and role of EUV machines enabling a paradigm shift, (used dsmcFoam+ in their design) (July, 2020) https://www.asml.com/en/news/stories/2020/asml-wins-semi-americas-award-for-euv

[5.5] Article by European patent law firm - describing the impact of EUV lithography, key global market users, advancing Moore's Law and technology advancements. (10th June, 2019) https://www.newelectronics.co.uk/electronics-technology/euv-lithography-the-brave-new-nanochip-era/216160/

[5.6] ASML website stating how the EUV machines are pushing Moore's Law forward https://www.asml.com/en/products/euv-lithography-systems (ASML website, 2020)

[5.7] Letter from Fluid Gravity Engineering Ltd, aerospace consultancy company on the impact of early versions of the dsmcFoam+ in ESA projects since 2014. (7th January, 2021)

[5.8] Application of the dsmcFoam+ for the CERN Beam Gas Curtain electron beam nozzle design. See Slide 9 (Oct, 2018) https://indico.cern.ch/event/763536/contributions/3183622/attachments/1737571/2810881/Gas_expansion_into_low_pressure_volume_-_intermediate_1.pdf

[5.9] Online Network for Micro and Nano Flows in Engineering supported by EPSRC – promoting access to open-source dsmcFoam+ to researchers and industry R&D working in this field. (Website - Dec, 2020) https://www.micronanoflows.ac.uk/links-and-downloads/