

Institution: University of Dundee
Unit of Assessment: UoA 10 Mathematical Sciences
1. Unit context and structure, research and impact strategy

1.1 Unit structure and context

Research in the School of Science & Engineering (SSEN) is founded on four overarching *themes* that straddle UOAs10, 11 and 12: *Mathematical Sciences*, *Engineering and Physical Sciences*, *Computing Sciences* and *Science and Justice*. The *Mathematical Sciences* theme aligns with REF UOA10. Mathematical Sciences (the Unit) comprises 17 category A staff and is structured as three *clusters* (each with a lead, underlined):

- *Mathematical and Computational Biology* (MCB) (Davidson, Eftimie, Lin, Murray, Pisliakov, Sknepnek, Trucu, Zachariae) focuses on developing a wide range of mathematical, physical and computational tools and techniques that are applied to quantify and better understand complex biological problems.
- *Magnetohydrodynamics and Astrophysics* (MHDA) (Sicilia-Aguilar, Gregory, Hornig, Matsumura, Meyer, Russell) combines innovative computational and mathematical modelling with state-of-the-art observations to address problems from solar, stellar and exoplanetary physics that cannot be solved by any one of these approaches alone.
- *Numerical Analysis and Scientific Computing* (NASC) (Athanassoulis, Eftimie, Hall, Hornig, Kyza, Lin, Pisliakov, Russell, Sknepnek, Trucu, Zachariae) develop numerical methods and algorithms that are accurate, efficient and robust with respect to challenges that manifest in the simulation of complex phenomena arising in biological and physical applications.

Former staff (previously Category A eligible) who also contributed to the Unit over the reporting period are **Chaplain** (MCB until 2015), **Janvier** (MHDA until 2015), **Fletcher** (NASC until 2016), **Ptashnyk** (MCB until 2017) and **Pontin** (MHDA until 2019). Moreover, each cluster has affiliated postdoctoral and postgraduate researchers, and staff leading research-focussed teaching. Researchers can affiliate with multiple clusters to facilitate interdisciplinary working and build capacity. Clusters benefit from members of other Schools (e.g. MCB and NASC have members from Life Sciences).

Research within SSEN aligns with the core mission of the University to **Transform Lives Locally and Globally** through the societal and economic impact of its research. Fundamental to this mission is the concept of interdisciplinarity leading to impact across four key institutional themes of which Mathematical Sciences research is focused on two:

- Understanding and improving health and wellbeing (IT1)
- Innovating technological solutions to tomorrow's problems (IT2)

Mathematical and Computational Biology (MCB) [IT1, IT2] comprises mathematicians, physicists, and computational biologists who develop and implement a wide range of mathematical, physical and computational tools and techniques. Working closely with colleagues in the Schools of Dentistry, Medicine, Life Sciences and Social Sciences these tools are applied to quantify and better understand complex biological, medical, and ecological problems. The technical focus is on the development of tools used to study dynamics across temporal and spatial scales ranging from state-of-the-art molecular dynamics and agent-based systems, through multi-

scale models to continuum descriptions based on the functional analytic representation of ordinary and partial differential equations. Both deterministic and stochastic approaches are woven through the work of this cluster. Applications cover a diverse range of fundamentally important and topical issues including epidemiology, cancer, drug metabolism, the immune system, developmental biology including oral deformities, cell and tissue mechanics, cell physiology and microbiology. The MCB cluster is characterised by its pursuit of interdisciplinary impact through innovation. By working across discipline boundaries both locally and globally, the aim is to make significant progress on problems that are resistant to solution by experimental approaches alone.

Magnetohydrodynamics and Astrophysics (MHDA) [IT2] combines innovative computational and mathematical modelling with state-of-the-art observations to address problems that cannot be solved by any one of these approaches alone. By focussing on understanding fundamental processes, the results obtained have cross-disciplinary impact in areas such as laboratory plasmas, classical fluids, and superfluids. A key focus is plasma dynamics in the Sun's atmosphere, including the heating of the solar coronal plasma, acceleration of the solar wind, and processes important in solar flares such as magnetic reconnection. This work contributes to the international effort to develop reliable forecasting systems for "space-weather", essential for enabling space exploration and protecting services in our increasingly technological society. A second focus of the cluster is the formation, evolution, and dynamics of planetary systems, as well as star formation, accretion, magnetism and stellar activity in young stars. The approach to addressing the above problems combines numerical simulations (high performance computing) – such as N-body simulations, Computational Fluid Dynamics and Monte Carlo radiative transfer – with mathematical methods and observational studies. The mathematical methods range from dynamical systems theory and differential equations to braid theory, differential geometry, and statistical analysis. Observational methods combine multi-wavelength observations from ground- and space-based telescopes.

Numerical Analysis & Scientific Computing (NASC) [IT1, IT2] develops and analyses high-performance numerical methods designed to meet exacting demands regarding complexity, stability, convergence, error control and preservation of selected mathematical and physical laws. Moreover, this cluster applies numerical methods and develops computational tools and software for engineering, physical, biological and medical problems. The NASC algorithms have been applied to a wide range of problems such as caustics and dark matter streams, complex fluids, multiphase flows, magnetohydrodynamics, fluid-structure interaction, multiscale modelling of solid materials with defects, proton transfer process in cell physiology, biological and medical image processing, calibration with incomplete data of cancer invasion, chick embryo gastrulation, collective dynamics in ecology and cell biology, atomistic molecular dynamics simulation of proteins, and measuring clinical outcomes on digital dental models. Due to the interdisciplinary nature of the area, the NASC cluster has significant and productive intersections with the two other clusters within Mathematical Sciences and other clusters from UOA11 and 12 within SSSEN.

1.2 Implementation of plans from REF 2014 and future strategy

The plan for Mathematical Sciences at REF 2014 was to *build on excellence in areas of existing strength* and to *broaden the research portfolio from this strong base*. Going forward, the aim has been to build on the excellent results of REF 2014, increase the staff base in terms of FTE and research expertise, increase PhD student numbers, increase research income and improve impact, both academic and societal. The Unit has achieved these goals:

- Strategic investment has seen the Unit grow from 12.7 to 17 FTE staff since REF 2014. Three research clusters based on research strengths within the Unit at REF 2014 have been formed and all three clusters have been strengthened by this growth (details in Section 1.1).
- Broadening of research expertise to include the development and application of molecular dynamics (**Pisliakov, Zachariae** – MCB), soft matter physics (**Sknepnek** – MCB), stochastic processes (**Athanassoulis, Hall** – NACS) and astrophysics (**Matsumura, Sicilia-Aguilar, Gregory** – MHDA) (Section 2.1)
- Increased number of PhD students and research income per FTE (Section 2.3)
- Enhanced contribution to the academic community (Section 4.2)
- Sustained quantity, quality and breadth of public engagement activities (Section 4.3)

The strategy for Mathematical Sciences was refined at a mid-REF-term review, which highlighted that the Unit could benefit from further expansion. Two potential areas were identified as particularly promising, both in the way they would tie in with the existing research clusters and in their potential to open up new academic and industrial collaborations. The two areas identified were (i) *Stochastic Processes and Probability* and (ii) *Optimisation and Operational Research*. Both areas are a priority for UKRI, as subjects in their own right (EPSRC, Mathematical Sciences) and indirectly via major UKRI themes such as *Energy*, *Global Uncertainty* and *Health Care Technologies*.

Stochastic Processes and Probability (building from NASC, MCB)

Developing strength in this area builds on the existing expertise in stochastic PDEs (**Lin** and **Athanassoulis**) and carries significant potential for applications in technology and engineering such as image processing, signal processing, information theory, cryptography and telecommunications. Broadening this area also facilitates connections to existing research groups in the Schools of Business (e.g., Finance), Life Sciences and Medicine and thus opens further routes to collaboration with industry. In line with this strategy, research in this area has recently been strengthened by the appointment of **Hall** under the Institution's *Baxter Fellow* scheme instigated to attract Early Career Researchers of exceptional promise. **Hall's** work, centred around predictive data science, uncertainty quantification and stochastic numerics, includes applications to biology, engineering and finance. Future hires will further develop the Unit's interface with these areas.

Optimisation and Operational Research (building from NASC)

Reinvigorating this impactful research area (see **Fletcher** REF 2021 Impact Case Study) by building on growing strength and breadth in numerical analysis will further strengthen research links to the Schools of Business (Finance and Economics), Life Sciences and Medicine (drug discovery; parameter estimation in biochemical pathways), as well as within SSEN (e.g. medical image analysis in Biomedical Engineering and Computing).

1.3 Impact strategy

Core to the impact strategy of Mathematical Sciences is the commitment to interdisciplinarity to maximise the potential impact of concepts, ideas, and discoveries. The organisation of research in the Unit is deliberately designed around areas of application rather than the underlying mathematical concepts. This fosters the use and development of a range of mathematical tools to solve important problems in science and engineering. This approach has successfully delivered the submitted impact case studies (**Lin** and **Fletcher**, respectively). Examples of how this strategy is facilitating an effective pathway to future impact are as follows:

- **Eftimie's** work on epidemiological modelling has been recognised by the Ministry of Defence and confidential contract research was undertaken. She is also collaborating with colleagues in the School of Medicine and has already published work on the effect of bed placements in hospital wards on the spread of COVID-19 (Moreno-Martos *et al.*, *Math. Biosci. Eng.* 17, 2020).
- **Zachariae** is internationally renowned for the development of computational methods used to better understand the physiology of cell membranes and in particular their interaction with external active agents. He has experience of working with major pharmaceutical companies (e.g. BBSRC CASE award with Boehringer-Ingelheim completed in 2019). In 2019 he secured an MRC iCASE award with Helperby Therapeutics to develop novel antibiotic combination therapies. This reputation led to an invitation to apply to the UKRI-BBSRC COVID-19 Agile Response Call (31 March 2020). [Award subsequently made to **Zachariae** (PI) working with the Drug Discovery Unit, UoD: c. £330K].
- **Zachariae's** work with a colleague in Molecular Microbiology, UoD, and others (Brandani *et al.*, *Langmuir*, 31 2015; Bromley *et al.*, *PNAS* 112, 2015) contributed to the development of a patent for the biotechnological use of a bacterial protein, BslA, and its variants as surfactants to stabilise multiphase synthetic mixtures for use as pharmaceuticals, personal care or food products (Patent Publication Number EP3182836B8; Publication Date 25.02.2020).
- **Pisliakov's** work with colleagues in the Drug Discovery Unit, UoD (Baragana *et al.*, *PNAS* 116, 2019) contributed to ongoing developments of a potentially significant advance in the treatment of malaria (Lysyl-tRNA synthetase as a drug target in malaria and cryptosporidiosis - Patent Publication Number WO/2017/221002; Submitted 28.12.2017).

These and other outcomes give confidence that Mathematical Sciences' strategy of actively engaging in interdisciplinary research can deliver significant impact outside academia and is providing promising indicators for future development.

Connecting to Industry and Business

To enhance our impact and contribute to today's societal and economic challenges, the Unit aims to engage further in research and development of innovative technology in collaboration with industry and businesses. The appointment of a new Associate Dean for Industrial Engagement supports this aim and the many existing industry connections within SSEN e.g. Industrial Advisory Boards and the Graduate Apprentice Scheme form a strong basis for growth of this activity. This will enable us to take advantage of opportunities from the UK R&D Roadmap and Industrial Strategy, including training the next generation of researchers through PhD programmes in applied mathematics, (increasing the employability of MSc and PhD students) and securing future collaborative research grants. The research areas selected for targeted growth (Section 1.2) will facilitate these connections by providing high value tools and expertise.

1.4 Research culture

Connectedness - Mathematical Sciences is part of an international community and remains engaged with scientific and cultural developments by attending conferences, workshops, and seminars as well as inviting academics to Dundee for seminars, workshops, and research collaborations (further details in Section 4). During the reporting period a Mathematical Sciences seminar series has brought more than 160 UK and international researchers to Dundee. These regular meetings foster the exchange of knowledge and ideas (i) between the Unit and the international research community and (ii) within the Unit to trigger innovative ideas and new directions. This seminar series concentrates on the mathematical and computational foundations common across Mathematical Sciences. Individual clusters also run seminars and workshops,

often in conjunction with groups from other disciplines where the focus is on the relevant application.

The Mathematical Sciences Unit is represented in all relevant learned societies, professional bodies and organisations including the London Mathematical Society, the Edinburgh Mathematical Society, the European Mathematical Society, the Institute for Mathematics and its Applications, Heads of Department of Mathematical Sciences, the Isaac Newton Institute, the International Centre for Mathematical Sciences as well as more specialised organisations (further details under Section 4.2). Information from these organisations is shared by representatives with other members of the Unit and includes conference, workshop or seminar announcements, funding opportunities, policies, job adverts, relevant surveys or calls for proposals or actions. This stream of external information complements that provided by the School and University.

Inclusiveness – see EDI Section 2.4.

Openness - Mathematical Sciences has a long-established culture of sharing research and helping others within the research community and, in line with Institutional policy, is committed to fostering an open research environment through increased advocacy and support for all staff, including postgraduate researchers. Researchers routinely provide preprints of publications on preprint servers (e.g. arXiv.org, bioRxiv.org) as well as on the University's *Discovery* repository to ensure open access compliance (<https://discovery.dundee.ac.uk/>). Datasets generated are also deposited in appropriate international databases and/or distributed from local servers. All staff within the Unit are guided to publish in journals compliant with the Open Access policy set out by UKRI and to leverage expertise and advice from the University's Library and Learning Centre regarding data management planning and compliance with the Concordat for Open Research Data.

Integrity - Mathematical Sciences is an active participant in the School-wide Research Integrity structure through which a Research Integrity Lead provides (i) an independent point of contact for staff and research students outside their immediate research environment, (ii) impartial advice on responsible conduct of research and (iii) advice on making misconduct allegations. Research staff and students are provided with online video-based training in Responsible and Ethical Practice in Research and Publication, which is mandatory for research students. The Director of Postgraduate Research oversees rigorous procedures that ensure all postgraduate research students benefit from the appropriate research integrity training and all data created for PhD theses and publications are archived in an appropriate and accessible form.

2. People

2.1 Staffing strategy

Mathematical Sciences' staffing strategy is to recruit researchers with an outstanding research track record and the potential for achievement at the highest level. Emphasis is placed on recruiting staff who demonstrate excellence with impact and interdisciplinary collaborations or the potential to do so. Since REF 2014, the Unit has recruited staff from high profile international institutions (e.g. RIKEN Institute, Syracuse University, Universities of Maryland, Edinburgh and St Andrews) and in combination with strategic realignment following the creation of research clusters has grown from 12.7 to 17 Category A FTE. All Category A staff are on permanent contracts. The Unit has a comparatively young age profile with 41% in the age bracket 30-39 years, 41% in 40-49 years and 18% in 50-59 years. Succession planning in the medium term is therefore focussed on career progression for individual staff and building a strong future for the Unit rather than necessitated by imminent retiral. To grow capacity in existing areas, we will continue to invest in

recruitment of ECRs and support their development within the cluster, Unit, School and Institutional contexts. The development of new areas of research will require targeting the appointment of more senior staff.

In 2013, the University introduced the *Dundee Fellows Scheme* to bring the next generation of research-intensive ECRs to the institution. Targeted support for the Unit led to four appointments (from a total of 15 available posts) through this scheme: **Janvier** and **Matsumura** to the MHDA cluster; **Pisliakov** and **Sknepnek** to the MCB cluster. The School also took advantage of funding from the Scottish University's Physics Alliance (SUPA), to recruit in the same year **Zachariae**, to further strengthen and broaden the work now clustered under MCB. **Matsumura**, **Pisliakov**, **Sknepnek** and **Zachariae** remain in post as key contributors to Mathematical Sciences. Each has been promoted – **Matsumura**, **Pisliakov**, **Sknepnek** to Senior Lecturer and **Zachariae** to Chair.

Additional appointments have been made at Lecturer level to further strengthen Mathematical Sciences: **Sicilia-Aguilar** (2017, now Reader), **Russell** (2016), **Gregory** (2019) and **Meyer** (2020) to MHDA as well as **Athanassoulis** (2017) to NASC.

Building on the success of the *Dundee Fellows* and SUPA schemes, Mathematical Sciences has benefited from the University's investment in the *Baxter Fellowships Programme* (2019). Four out of 18 Fellowships in the institution were secured by the School with **Hall** (RWTH Aachen, 2020) appointed to further strengthen and broaden expertise in NASC.

2.2 Career development

The University is committed to the Concordat to Support the Career Development of Researchers. As such, the Unit provides a supportive environment that is aligned with the University's strategic aims to enable staff to flourish and promote a high-performance community. All staff including Postdoctoral Researchers benefit from annual, individual reviews of their research progress by their line manager as part of the Objective-Setting & Review (OSaR) process that delivers the University's strategic aim of embedding and supporting a culture of performance management and improvement. OSaR takes a holistic view of research, teaching and administrative duties, and is a data-driven process informed by:

- (i) **Workload Allocation Model** (WAM), to ensure that research, development and impact-generation activities can be accounted for in assigning teaching and administrative duties, and in developing future staffing strategy. The cluster lead role is recognised in the WAM, as is the supervision of postgraduate research students, time on external research projects and impact generating activities such as consultancy, which support the generation of new avenues of research and strong contribution to the wider academic community.
- (ii) **Annual Research Review** (ARR). This was introduced in 2016 with the principal aim of providing peer feed-forward to research-active staff to maximise the impact and visibility of their research, to provide guidance in developing plans for securing resources and to support career development (via feed-in to OSaR). The ARR, which in SSEN is conducted across all four themes as a single exercise, maximises the identification of interdisciplinary opportunities.

New lecturers are supported by line managers, the Associate Dean for Research and senior colleagues through the University's three-year probation period, which on successful completion results in confirmation in post and the award of a Postgraduate Certificate in Academic Practice in Higher Education. All newly appointed staff are assigned a mentor - a senior colleague typically within the Unit - to help formulate and achieve personal performance goals and deliver the

School's objectives. They also enjoy a reduced teaching load to provide additional time to establish sustainable research activities at the University. Newly appointed staff have access to start-up funding from the School Research Committee to support network establishment, dissemination activities and integration of their research activities within the cluster. In addition, they are guided through their probationary period by cluster leads and established research staff, who provide peer review of research proposals and e.g. convene mock interview panels for Fellowship applications. Postdoctoral Researchers are similarly supported in progressing their career and are mentored to apply for fellowships and/or ECR positions. Furthermore, ECRs are preferentially allocated PhD studentships (both at School and Institutional level) to aid the rapid establishment of their research profile.

All staff are encouraged to make use of TRAM (**T**eaching, **R**esearch and **A**cademic **M**entoring scheme), set up jointly with five other HEIs, to ensure that researchers (including postdoctoral researchers) are supported in developing their careers. Staff are encouraged to plan for promotion and are supported through the process by line managers and senior colleagues. Measures of research performance are captured through the ARR and OSaR processes and include quality of publications and research funding, PhD supervision, contributions to the wider academic community, indicators of esteem and activities leading to impact.

2.3 Research students

During the REF assessment, 25 PhD students completed under the supervision of staff within the Unit with a further 22 students studying in Mathematical Sciences (at 31st July 2020). Students have been financially supported by UKRI (c. £0.5M mainly EPSRC and STFC DTP), the Chinese Scholarship Council, the Northern Research Partnership (SFC Pooling Initiative), the Leverhulme Trust and Government Scholarships (the last totalling over £1M).

The School's Director of Postgraduate Research coordinates the recruitment, support and development activities for PhD students across all research themes along with quality assurance and mentoring of research staff in supervision (particularly for early career staff). Research student recruitment and supervision is framed by the University's commitment to the *QAA Code of Practice for Research Degree Programmes* and governed by the *University Code of Practice for Supervised Postgraduate Research*, supplemented by the School's own *Postgraduate Research Guide*. For each student, a Thesis Monitoring Committee (TMC) meets twice per year. These individual TMC meetings are held with two non-supervisory research staff to whom both student and supervisor provide information on progress and can identify, in a confidential manner, any issues that arise. A feed-forward mechanism operates with the TMC providing suggestions and guidance to the supervisory team. The composition of the TMCs remains set throughout the student's study period to ensure continuity of oversight and guidance.

At an institutional level, the Doctoral Academy provides generic support and research development training for students, bespoke training for supervisors (particularly those at ECR level) and has embedded an interdisciplinary research ethos. Students can also access the full academic and transferrable skills training programme offered by Organisational and Professional Development at the Institutional level.

Training specific to Mathematical Sciences students is provided mainly by the Scottish Mathematical Training Centre (SMSTC) and for some aspects also by SUPA. Specific postgraduate courses are offered by members of the Unit. New PhD students within the Unit are encouraged and supported to attend the Scotland-wide introductory SMSTC meetings organised by **Trucu** and **Eftimie**. An annual postgraduate research symposium within the School provides

opportunities to all students for dissemination of results across the research themes. In addition, the Mathematical Sciences seminar programme also enables discussions of research projects and the identification of cross-cluster research opportunities. Funding is available to all research students to facilitate participation in national and international conferences. For computational projects research students are provided with full access to School computing facilities and core-funded technical support.

2.4 Equality, diversity and inclusion (EDI)

The University is a member of the Race Equality Charter and both the University and the School hold an Athena SWAN Bronze Award (most recent renewals 2017 and 2018, respectively). Mathematical Sciences rigorously adheres to the principles of these Charters and is committed to the advancement of equality, diversity and inclusion. The School's Athena SWAN application received significant input from members of the Unit. The first application in 2015 was led by **Hornig**, together with **Matsumura** and **Russell** who were part of the application team. The School is currently working towards a Silver Award application for 2022 and **Kyza** represents Mathematical Sciences on the School-wide working group. The School's Athena SWAN self-assessment committee focuses on actions that maintain and further enhance an inclusive culture and collegiate working practices. School and University level EDI and Athena SWAN action plans guide ongoing improvements in support of all staff and students; these are informed by the University's biennial staff survey.

Mathematical Sciences fully engages with the range of University level work-life balance policies, including coverage for those with changed circumstances. These include compassionate leave, parental leave, adoption/fostering and carer's leave. A nursery is available on campus for children of staff and students. Line managers maintain regular contact with the member of staff during their leave. Discussions related to return to work are held prior to return, in line with the University's Flexible Working Policy. Voluntary declaration of any mitigating circumstances is part of the standard academic promotions process. A full-time counsellor for mental-health issues has recently been appointed by the University. Harassment Advisers have been appointed to support staff and students and among these is a member of Mathematical Sciences (**Eftimie**). Working with the School and University the Unit are supportive of the many staff with young families (currently seven members) by offering flexible working and distributed workloads.

The School appoints staff on merit alone and is committed to equality, diversity and inclusion. Appointing and shortlisting panels are always mixed gender; all panellists must have undertaken unconscious bias training. Online training in equality and diversity is mandatory for all staff and includes modules on *Diversity in the Workplace*, *Disability*, *Stress in the Workplace*, *Diversity in Learning & Teaching* and *A Manager's Guide to Stress*. Additionally, a module on *Recruitment and Selection* is taken by staff involved in those activities. Completion is monitored centrally as part of ensuring EDI is embedded in the institutional culture. Unconscious bias training sessions are delivered regularly and available to all in the School.

Twelve different nationalities are represented within the 17 Category A staff in Mathematical Sciences and the gender balance is currently five females to twelve males. This ratio is higher than the national average of academics in mathematics, but continued efforts are made to combat the "leaky pipeline", that is the decreasing proportion of women progressing to higher academic positions. For example, we encourage applications from women (and other under-represented groups) for academic positions highlighting flexible working, we promote the use of networking opportunities such as the Aurora Leadership programme (recent participant **Eftimie**) and special funding schemes such as the Emmy Noether Fellowships (**Kyza**) and provide support and

guidance to facilitate successful promotion applications. Over the REF assessment period four of the five Category A female staff have received promotion, including to Reader (**Sicilia-Aguilar**) and to Chair (**Eftimie**). Two of the 17 Category A staff identify as BAME and one of them (**Matsumura**) was promoted during the assessment period.

It is part of the University strategy to minimise the number of fixed-term contracts and the Unit is exemplary in that it has no academic staff on fixed-term contracts; all contracts are open-ended. Efforts are made to provide PDRAs, who are on fixed-term contracts, with the required skills and opportunities to apply for academic positions or personal fellowships and the Unit was successful in this in the past (see Section 3.1).

Construction of REF submission

All UOA10 Planning Group members completed institution level unconscious bias training in addition to equality, diversity and inclusion, and information security awareness training prior to contributing to output selection and Planning Group discussions. Outputs have been selected through a rigorous process of internal and external review and attributed to individual staff by the UOA10 Planning Group following the University's REF 2021 Code of Practice. All staff were invited to submit impact case studies and those selected reflect the strongest impacts arising over the REF period. Of the 43 outputs submitted 26% are attributed to female and 74% to male staff. This is in line with the gender balance of 30% female to 70% male staff who contributed to the submission. Two submitting staff identify as BAME (10%). The number of selected outputs attributed to BAME staff is seven (16%).

3. Income, infrastructure and facilities

3.1 Research funding

The Mathematical Sciences Unit was successful in attracting over £2.4M research grant income over the REF period, principally from UKRI (EPSRC, BBSRC and STFC) but also including support from the Leverhulme Trust, EU, the Ministry of Defence and the Northern Research Partnership (Scottish Funding Council Pooling). Highlights include:

- **MHDA cluster:** three separate awards from STFC to **Hornig & Pontin** (ST/K000993/1, ST/N000714/1, ST/S000267/1) totalling over £1.3M, together with an STFC award for **Sicilia-Aguilar & Matsumura**, (ST/S000399/1, £130K) and two Leverhulme awards (**Pontin**, RPG-2015-075, PLP-2011-074 totalling £100K), led to over 30 publications, six of which are part of the Unit's REF 2021 submission. Of the six Postdoctoral Researchers funded by these grants, three now have academic positions - UoD (**Russell**), Glasgow (S. Candelaresi) and Durham (P. Wyper) - one took up a prestigious fellowship position at the US Naval Research Laboratory (R.B. Scott) and one is employed in industry (J. Thurgood, NCTech Imaging). A further five PhD positions can be linked to these awards.
- **MCB cluster:** BBSRC awards to **Davidson** (Co-I on £2.6M sLoLa grant BB/P001335), **Sknepnek** (Co-I on £427K award BB/N009789), three EPSRC first grants (**Eftimie**, **Ptashnyk**, **Sknepnek**: EP/K033689/1, EP/K036521/1, EP/M009599/1, £90K each), EPSRC award to **Davidson** (Co-I, £501K, EP/P00301X), as well as a contribution from ERC Advanced Grant PE1, ERC-2008-AdG (**Chaplain**), collectively led to five Postdoctoral Researchers directly linked to the Unit (three of which have moved onto substantive academic posts: D. Matoz-Fernandez, Northwestern University; M. Pineda, UCL and B. Seguin, Loyola University) and five publications that form part of the Unit's submission.

3.2 Infrastructure and facilities

Support structure

Mathematical Sciences is supported in research both administratively and in terms of impact generation at an institutional level by the University Research Office, which operates under the strategic leadership of the Vice-Principal for Research, Knowledge Exchange and Wider Impact (VPR). Working as part of the Research Office, Research Finance Services provide pre- and post-award management of non-commercial grant applications and awards, and Research and Innovation Services support research strategy, consortia building, industrial engagement and issues pertaining to intellectual property, licensing, contracts and knowledge exchange.

Research strategy in SSEN, is led by the Associate Dean for Research (ADR), who chairs the School Research Committee comprising all cluster leads and the Director of Postgraduate Research. The ADR holds a budget that is used to support staff development and networking as well as other research-related expenses approved by the Research Committee (such as pump-priming activities), with priority given to supporting ECRs. The ADR is a member of the University's Research and Knowledge Exchange Committee and other groups convened by the VPR formed to contribute to the development and monitoring of the implementation of University-wide strategic objectives. The ADR works closely with the Associate Dean for Industrial Engagement, whose role is to provide additional leadership in relation to the School's engagement with industrial partners and organisations, contributing to the economic and social progress of the city, the region and beyond. This includes creating and nurturing partnerships with local enterprises, developing opportunities for industry-led innovative research and encouraging pathways for impact and commercialisation of research. The Research Administrative Lead coordinates a team that supports the ADR in sustaining a research-driven culture within the School.

Leadership provided by the AD Research and AD Industrial Engagement and support at institutional level has minimised the impact of the COVID-19 pandemic on Mathematical Sciences research. During lockdown, academic and research staff were supported to work effectively from home and computational resources were fully accessible to support remote working on research. Collaborations and supervision were optimised via the use of complementary online platforms.

Computing infrastructure

A substantial part of the research in Mathematical Sciences is based on numerical simulations of physical or biological systems, either to gain a better understanding of these systems or, in case of the Numerical Analysis and Scientific Computing cluster, to test and demonstrate the efficiency and accuracy of new numerical algorithms. High Performance Computing (HPC) requirements across all clusters are supported via scalable infrastructure. In 2014 SSEN established a local cluster, which now has 768 cores (640GB RAM) and is principally used by researchers in UOA10 and 12 for day-to-day research computing needs. A larger, institutional cluster is based in the School of Life Sciences and is a high-end facility that currently includes over 4PB of data storage with associated offsite backup systems, and over 3,000 CPU cores and 61 NVIDIA TESLA K80/GTX1080 GPGPU cards. The GPGPU cards are used by members of the MCB cluster for molecular dynamics simulations and simulation of biophysics at the cell-scale.

The Unit also has access to a smaller machine with high performance graphics cards that provides a test bed for GPU computing. As one example of the impact of these facilities, this infrastructure allowed for the development of a GPU-based Lagrangian magnetic relaxation solver using mimetic operators leading to the publication by Candelaresi *et al.*, (SIAM J. Sci. Comp., 36, 2014) submitted as part of the Unit's outputs. The software package (Glemur) has been released to the

public under the open-source GPL 2.0 licence on GitHub. The Glemur package not only runs significantly faster due to its use of GPUs but is also more accurate than its competitors due to the implementation of mimetic operators.

These facilities provide support for the genesis, development and up-scaling of large numerical simulations, prior to accessing national supercomputing resources such as the DiRAC HPC clusters in Cambridge and Durham and ARCHER in Edinburgh. Access to these national HPC facilities is supported by STFC funding for the UKMHD consortium (Royal Astronomical Society Group Achievement Award (G) for the quality of its work in 2013) of which the MHDA cluster is a member. The Unit benefits from support from a team of 18 HPC specialists within University of Dundee IT Services. Moreover, the School has a dedicated Computing Officer who maintains the facilities and provides hard and software support for staff and students in Mathematical Sciences.

The Unit's computing infrastructure proved to be a decisive lever in obtaining more than £1.5M of research funding from STFC and the Leverhulme Trust.

Physical infrastructure for staff and students

PhD students share a dedicated open plan space at the heart of the Mathematical Sciences footprint within one of the main School buildings. This colocation alongside Unit staff (who benefit from individual offices) helps to create a sense of communality and supports interaction as well as joint learning. This PhD space houses a dedicated reference library and an individual desk and personal computer is provided for each student. The SMSTC and SUPA courses for the students are delivered in two dedicated video conferencing suites with state-of-the-art large interactive flat panel displays.

4. Collaboration and contribution to the research base, economy and society

4.1 Research collaborations and networks

The work carried out by Mathematical Sciences is highly collaborative and interdisciplinary, both in its structure (see Section 1.1) and strategy (see Sections 1.4, 1.5). All members of the Unit are involved in collaborations and networks on either national or international levels. Such collaborations are supported by our research structure (see Sections 1.1, 1.5); pump-prime funds are provided by the School and special arrangements can be made regarding teaching schedules to enable visits during term time. The research cluster structure as well as the mentoring scheme are designed to help ECRs build their own successful collaborations and networks (see also Section 2.2). The success of this environment is evidenced in a high number of collaborations and networks; exemplars are:

- **Athanassoulis** is part of the *Scottish Numerical Methods Network* (Dundee with Strathclyde, Heriot-Watt and Edinburgh Universities). Support for the network has been awarded by LMS, EMS, IMA, RAS and others totalling c. £12K. (2017 - onwards) to organise a series of workshops, which led to a number of high-profile international speakers coming to the participating universities.
- **Hornig, Pontin & Russell** are part of an ongoing collaboration with Durham University (since 2013) on the dynamics of complex plasma, supported by STFC Consortium grants with over £1.3M (see Section 3.1 for details and impact).
- **Kyza** collaborated with cosmologists at Wolfgang Pauli Institute, Vienna on efficient numerical algorithms to describe the formation of galaxies, which led to a Carnegie Research Incentive Grant (2018).

- **Sicilia-Aguilar** is part of international, community-driven, public data projects to which Dundee is contributing via the development and application of the STAR-MELT code for emission line extraction and analysis in high-resolution, time-resolved spectra (funded by STFC grant ST/S000399/S).
- **Lin** is part of a collaboration with colleagues in China (USTB, Shanghai JTU) and Germany (U Magdeburg) on “Simulation and analysis of temporal multiscale problems” which obtained €360K funding from a collaborative NSFC-DFG fund.
- **Lin** collaborated with E Celiker (Cyprus) who worked as a PDRA in Dundee for one year funded by an EU Scholarship Programme, resulting in two publications.
- **Lin** collaborated with colleagues at USTB (China) resulting in funding from NSFC and CSC for four visits of researchers and PhD students.
- **Sicilia-Aguilar** is part of international project "Outflows and Disks around Young Stars: Synergies for the Exploration of ULLYSES Spectra (ODYSSEUS)", which is part of the Hubble Space Telescope "Ultraviolet Legacy Library of Young Stars as Essential Standards (ULLYSES)" project.
- **Matsumura** is collaborating with colleagues at the Earth-Life Science Institute (ELSI), Tokyo Institute of Technology in Japan, as an expert on numerical simulations of formation and dynamical evolution of planetary systems, leading to 12 joint publications so far including two papers attributed to the author in the Unit Output pool.
- **Meyer** collaborated with the Solar & Stellar X-Ray Group at the Harvard-Smithsonian Centre for Astrophysics, with research visits in 2015, 2017 and 2018 funded through NASA-ROSES grant “Studies of Reconnection in Coronal Jets Observed with IRIS”.
- **Meyer** collaborated with colleagues at the Royal Observatory of Belgium through three research visits in 2018-19 funded through the PROBA-2 Guest Investigator Program. This resulted in a publication and is the basis of a new grant application to STFC.
- **Hall** collaborated with colleagues at RWTH Aachen University and WIAS Berlin leading to a project concerning numerical methods for non-Markovian dynamics with applications in finance, which is currently funded by the Alexander von Humboldt Foundation (June 2020).
- **Hall** is participating in an ongoing collaboration concerning stochastic and predictive modelling with applications to nano-porous metamaterials with colleagues from University of Massachusetts Amherst and Stanford University leading to recent grant support from the AFOSR under grant FA-9550-18-1-0214 (June 2020) and six publications so far.
- **Russell** led a team at the International Space Science Institute on “Magnetic Waves in Solar Flares” leading to three publications and code development of HYDRAT and RADYN, used by the community.
- **Russell** is a collaborator on the project “IRIS Fe XXI line profiles as diagnostics for flare heating models” supported by NASA ROSES-2019 Heliophysics Guest Investigator grant.
- **Pontin** collaborated with colleagues at Northumbria University on the project “*Revealing the fundamental nature of time-dependent, wave generating reconnection*” leading to a successful Leverhulme grant with funding for a PDRA (2015-18).
- **Murray** visited a world leading developmental biologist/dermatologist in the US supported by funding from the Northern Research Partnership, which led to two papers in *Cell* that received international publicity (e.g., Science Daily, BBC, Guardian, LA Times, Daily Mail).

The Unit is also part of the Scottish Mathematical Sciences Training Centre and the Scottish Universities Physics Alliance, both are networks that contribute to the training of our PhD students (see Sections 2.3, 3.2 for further details).

4.2 Contributions to and recognition by the research base

Relative to its size, the Unit has a significant presence in the national and international research community. More than 250 invited talks/seminars were delivered by staff in Mathematical Sciences over the reporting period. Major awards and their impact are included under Section 3.1. Other indicators listed below, including editorial roles, conference organisation and membership of grant committees, provide further evidence of the active input to, and recognition by, the international research community.

Membership of societies, workgroups, and committees

- American Geophysical Union (**Russell**)
- Edinburgh Mathematical Society (**Athanassoulis, Trucu, Davidson, Pontin, Kyza, Hornig, Eftimie, Lin**) in various roles including Representative, Treasurer and Member of the General Committee
- Society for Mathematical Biology (**Eftimie, Trucu, Murray**)
- British Society for Immunology (**Eftimie**)
- London Mathematical Society (**Athanassoulis, Eftimie, Trucu, Kyza**)
- Institute of Mathematics and its Applications (**Athanassoulis, Davidson**)
- Society for Industrial and Applied Mathematics (**Eftimie**)
- EPSRC Early Career Forum Member (**Kyza**, 2014 – 2016)
- Royal Astronomical Society (**Sicilia-Aguilar, Russell**)
- International Astronomical Union (**Sicilia-Aguilar, Russell**)
- European Astrobiology Institute Project Team on Protoplanetary disks (**Sicilia-Aguilar**, since 2020)
- UK Solar Physics Council member (**Pontin** 2016 – 2019, **Russell** 2012-16, **Hornig** 2011-15)
- International Space Science Institute, team “New Diagnostics of Particle Acceleration in Solar Coronal Nanoflares from Chromospheric Observations and Modelling” (**Russell** invited member 2015-18)
- International Space Science Institute, team “Magnetosphere and Ionosphere as a Coupled System: Theory and Observations” (**Russell** invited member 2013-14)
- NASA Chandra satellite proposal peer review member (**Gregory**, Deputy Chair, 2015)
- Mills Observatory Advisory Committee (**Sicilia-Aguilar**, 2018-present)
- Marie Skłodowska- Curie fellowships, European Commission (**Zachariae** member of the evaluating panel)
- Young Stars Working Group for the Arago Space Mission proposed to the European Space Agency (**Sicilia-Aguilar**, 2015-2016)

Editorial roles

- Frontiers in Applied Mathematics and Statistics, Editorial Board (**Eftimie**)
- Frontiers in Medical Technology, Editorial Board (**Pisliakov** since 2019)
- Fungal Ecology, Editorial Board (**Davidson** since 2010)
- International Journal of Computer Mathematics, Editorial Board (**Lin** since 2018)
- Journal of Mathematical Biology, Editorial Board (**Eftimie**)
- Journal of Applied Mathematics, IMA Editorial Board (**Davidson** since 2007)
- Journal of Structural Biology, Editorial Board (**Zachariae**)
- Journal of Theoretical Biology, Associate Editor (**Eftimie**)
- Mathematical Biosciences and Engineering, Advisory Editor (**Eftimie**)
- Mathematics in Applied Science and Engineering, Associate Editor (**Eftimie**)
- Numerical Mathematics: Theory, Methods and Applications, Editorial Board (**Lin** since 2007)

Unit-level environment template (REF5b)

- PLOS Computational Biology, Guest Editor (**Zachariae**)
- Proceedings of the Royal Society of Edinburgh Series A, Editorial Board (**Davidson** since 2013)
- PLOS ONE, Editorial Board (**Eftimie, Trucu**)
- Scientific Reports - Nature, Editorial Board (**Zachariae, Matsumura**, since August 2016)

Conference organisation

Mathematical Sciences at Dundee actively promoted the exchange of scientific knowledge and ideas by organising 29 conferences, workshops or mini-symposia over the reporting period. Among those were mini-symposia at the International Congress on Industrial and Applied Mathematics (2019, **Trucu**), the British Applied Mathematics Colloquia (2018, **Athanassoulis, Pontin, Russell, Trucu, Kyza, Ptashnyk**), Annual Society for Mathematical Biology Meeting (2017, **Eftimie, Trucu**), European Conference on Mathematical and Theoretical Biology (2014, 2016, **Ptashnyk**), AIMS Conference on Dynamical Systems, Differential Equations and Applications (2014, **Ptashnyk**) and the Royal Astronomical Society National Astronomy Meeting (2014, **Gregory**). A prominent example for workshops organised for the regional community is a series of workshops under the title “Scottish Numerical Methods Network” (2017, 2018, **Athannassoulis**), which brought a range of international experts to the region and was supported by grants from the LMS, EMS, IMA and RAS.

Grant committees/ funding bodies

- EPSRC Peer Review College Member (**Davidson, Eftimie, Lin**)
- EPSRC Mathematics Prioritisation Panel Meeting (**Kyza**, 2015, 2018, **Murray**, 2019)
- STFC Peer Review Member (**Hornig, Pontin, Sicilia-Aguilar, Russell**)
- DiRAC Panel on Astronomy and Cosmology for the evaluation of computational programmes in UK universities (**Matsumura**, 2015-2017, **Sicilia-Aguilar**, 2018-2020).
- STFC, Ernest Rutherford Fellowships panel member, (**Hornig** 2016, **Pontin** 2018)
- INSERM (Paris, France) for the call “Interdisciplinary approaches in oncogenic processes and therapeutic perspectives: contributions of mathematics and informatics to oncology” (**Eftimie**)
- Volkswagen Stiftung (largest German private foundation), grant panel member (**Hornig**, since 2018)
- NASA “Living with a Star” grant panel member (**Pontin**, 2018)
- NASA Research Opportunities in Space and Earth Sciences programme, Grant panel member (**Russell**, 2016)
- NASA Solar System Workings, grants panellist (**Matsumura**, 2014)
- NASA Heliophysics Supporting Research panel member (**Meyer**, 2018)
- NASA grants panels, external examiner (**Matsumura**, 2014, 2015, 2016)
- MINECO Research Grants (main Spanish public funding body) External Referee (**Sicilia-Aguilar**, since 2017)
- Lise Meitner Position and the Erwin Schrödinger Fellowship, Austria (**Sicilia-Aguilar**, 2015-16).
- Research Grant Council of Hong Kong External Referee (**Lin**, since 2012)
- UKRI Future Leaders Fellowships, external examiner (**Sicilia-Aguilar**)

Keynote/plenary/public talks at conferences (selection only)

- Keynote Speaker **Davidson**, MiCom14 4th International Conference on Microbiology for Young Scientists, Jena, Germany, April 2014.
- Mentor and Plenary Speaker **Lin**, British Council Researcher Link Workshop on Soft Matter, Daejeon South Korea, March 2014.

Unit-level environment template (REF5b)

- Plenary Speaker **Trucu**, International Conference on Mathematics for the Natural and Life Sciences, University of Tlemcen, Algeria, November 2014.
- Keynote Speaker **Lin**, 9th International Conference on Computational Physics, National University of Singapore, January 2015.
- Plenary Speaker **Trucu**, International Conference on Perspectives in Environmental and System Biology, Universite Joseph Fourier, Grenoble, April 2015.
- Keynote Public Lecture **Davidson**, British Association of Science Lecture Series, Dundee, January 2016.
- Plenary Speaker, **Zachariae**, Annual Meeting, Biophysical Society, Los Angeles, February 2016.
- Keynote Speaker **Lin**, Bi-annual Conference of the East Asia Section of SIAM, University of Macau, June 2016.
- Public Talk **Sicilia-Aguilar**, Jöst Bürgi International Symposium, Lichtenstein, April 2018.
- Keynote Speaker **Eftimie**, BIOMATH 2018: International Conference on Mathematical Methods and Models in Bioscience, Sofia, Bulgaria, June 2018.
- Keynote Speaker **Eftimie**, Workshop PDE Models for Cancer Invasion, Belfast, Northern Ireland, December 2019.
- Plenary Speaker **Trucu**, International conference “Intensive Research Programme: Recent Progress in Mathematical Biology”, Centre de Recerca Matematica Barcelona, Spain, June 2018.
- Plenary speaker **Lin**, Annual Conference of the Computational Mathematics Association of Beijing and surrounding provinces, Henshui, China, August 2018.
- Plenary Speaker **Lin**, 16th International Conference for Mesoscopic Methods in Engineering & Science, Heriot-Watt University, July 2019.

4.3 Contributions to the wider community

The Unit actively responded to calls to address local and global challenges. For example, **Lin's** collaboration with colleagues in India led to pump-prime funding from the Global Challenges Research Fund in 2017. **Eftimie's** collaborations with colleagues across the University resulted in two projects awarded to Dundee (c. £500K) from the Chief Scientist Office (Scotland) as part of the Rapid Research in Covid-19 Programme. **Zachariae** was selected to apply to the UKRI-BBSRC COVID-19 Agile Response Call (award made – see Section 1.3).

Public Engagement activities directly related to Mathematical Sciences are co-ordinated by **Russell** and **Sicilia-Aguilar**, who work closely with other outreach leads across the School. School-wide coordination and support is provided by the School's Director of Public Outreach and Engagement. Activities benefit from close links with key stakeholders locally and nationally and strong links exist with local high schools, the Dundee Science Centre, the V&A Museum Dundee, and the Mills Observatory, all of which provide accessible, well-known and well-connected platforms for events.

Throughout the recording period, Unit staff contributed to 22 separate outreach events. These included regular workshops at local high schools as contributions to national initiatives like *Maths Week Scotland*. Other activities initiated by the Unit were designed to enthuse and engage young adults in mathematics and its applications through the research it conducts. A particular aim of the Unit's public engagement activities was to encourage more females to engage with mathematics. The Unit contributed to the Women in Science Festivals e.g. *Meet the Expert* (2015) and *Family Fun with Women in STEM* (2020) as well as *Girls in Physics* events hosted by the Institute of Physics (several events in Tayside and Fife in 2019, 2020). Staff contributed focussed activities as

part of event series e.g. the *Saturday Science and Wednesday Wonders* series at the local Mills Observatory (MHDA) as well as organising special events such as *Life and Light* (2014) (MHDA and MCB) and *Nature's Equations – D'Arcy Thompson and the Beauty of Mathematics* (2015) (MCB) both at the Dundee Science Centre.

The Unit has also designed and run two major public engagement activities during the reporting period:

Travel Through a Solar Storm: an immersive virtual reality experience (2016 onwards) This STFC funded outreach project (**Janvier**) provided a virtual reality (VR) experience through which participants could witness the birth of a solar storm, its journey across space and its impact with Earth (<http://www.solarstormvr.com/>). The project was first presented at SMASHfestUK in February 2016 and since then at the Edinburgh International Science Festival, the Cheltenham Science Festival, and the Dundee Science Centre.

Dundee Science Festival 2014. Mathematics was awarded the main auditorium at the Dundee Science Centre and in total 16 staff manned 10 separate display stations with 681 guests passing through the centre. Each hands-on exhibit presented an interesting phenomenon related to our research, including examples for chaos, biofilms, fungal growth, magnetic fields, and the dynamics of interfaces of rising bubbles. Feedback highlighted the popularity and effectiveness of our approach of using hands-on exhibits to introduce mathematical concepts in an interactive way and provide a starting point to explore and discuss mathematical ideas and how these impact our daily lives.