Institution: University of Lincoln

Unit of Assessment: 9 Physics

1. Unit context and structure, research and impact strategy

Context

During the census period the University of Lincoln (UOL) has expanded dramatically in STEM areas, investing in the creation of several new Schools including Chemistry, Mathematics and Physics, Geography, and (most recently) Medicine. The new School of Mathematics and Physics (SOMP) is housed alongside Engineering and Computer Science in the purpose-built £28M Isaac Newton building (2017). The SOMP's founding in 2014 created the first totally new Physics department in the UK since the 1960s.

Before these new schools were opened, Physics research at UOL consisted solely of medical physics imaging (Medical Instrumentation Centre) and was submitted in REF 2014 under UOA 11. The SOMP was opened to extend and centralise research themes in physics. The initial strategy focused on computational materials research, with a distinct expertise portfolio in computational soft matter physics, soft/solid interfaces and chemical physics. Additional research themes were initiated as the school grew. The Physics return now consists of 15.2 FTE organised into the following research foci:

- *Healthcare* - Medical Instrumentation Centre (MIC)**,** Centre for Computational Physics (CCP***)***, Nanotechnology Team (NT***)***;
- *Green and sustainable materials* - CCP**,** NT;
- *Software Development for Materials Design* - CCP**,** High-Performance computing for Science, Technology and Environmental Research group, (HiPSTER);
- *Modelling of Interacting Systems* – CCP.

The UOL's research strategy emphasises complementary interdisciplinary units and these research themes have strong links with units in Engineering, Chemistry and Computer Science. Submitting staff are researchers drawn from across the UOL's Schools of Computer Science, Chemistry and Mathematics and Physics with global links (see Section 4).

Structure

These research groupings drive the research areas listed above:

‡: Centre for Computational Physics (CCP)

The nucleus of the CCP relocated to Lincoln in 2014 from another UK University to establish the SOMP. The CCP leads UOL research in computational and theoretical physics in the areas of soft-matter, soft/solid interfaces and chemical physics and their application in *Healthcare* and *Green and sustainable materials*. The ultimate goal of the CCP is computer-aided design of new materials. In June 2018, the CCP was formally inaugurated by Prof Daan Frenkel ForMemRS. Expertise includes modelling of planetary rings and exo-moon systems; nonlinear dynamical systems, perturbation theory and integrable systems; foundations of statistical mechanics such as efficient sampling, ergodicity probing and their applications in economics and materials, such as granular matter; and theoretical biophysics and colloidal science, including systems out of equilibrium such as active matter. The CCP develops and optimises High Performance Computing (HPC) software and numerical methods from continuum models to electronic structure methods. A recent highlight from 2019: An Institute of Physics (IOP) meeting on Machine Learning led to collaborations that proposed a reliable AI-based testing method which can outperform current RT-PCR testing methods for COVID-19.

†: Medical Instrumentation Centre (MIC)

The MIC is a hub for the development of new medical imaging instrumentation and part of its research is the application of medical physics. MIC's imaging work also includes extensive computations, complementing the UOA's high performance computing (HPC) based physics research. MIC's Monte Carlo simulator is the most advanced simulation platform for Proton Imaging.

The MIC is administered as part of the School of Computer Science, which connects to other areas of medical imaging research (e.g. algorithms, as a part of the Computer Science REF

submission). During the census period, MIC's work has focussed on the provision of proton CT for the enhancement of cancer treatment using Proton Beam Therapy (PBT). Many MIC members and associated members are based in other organisations – universities, hospitals, research institutes and industry. They work with medical and particle physicists, clinicians and electronic, device and computer engineers from leading research groups and companies across Europe and wider. Five NHS Trusts and Foundation Trusts and four UK universities are members of the Centre together with iThemba LABS, South Africa; Paul Scherrer Institute, Switzerland; and the Karolinska University Hospital, Sweden.
§: High Performance computing for Science Technology and Environmental Research (HiPSTER)
HiPSTER is an offshoot of the CCP to link expertise in HPC and simulations techniques across the UOL. Simulation software development expertise is found across the UOL, including engineers, geographers, pharmacists, robotics, agriTech and computer scientists. HiPSTER provides a mechanism for UOL's strengths in other areas to be fed back into UOA physics research, for instance, in machine learning (mLearn group in Computer Science and Power and Energy Group in Engineering) and fluid dynamics (e.g. the Physical Ecology Lab in the School of Lifesciences, and Intelligent Systems Research Group in the School of Engineering). Members contribute to the development of leading materials simulations codes,e.g. Quantum Espresso.
*****: Nanotechnology Team
The NT focuses on experimental research in nanophysics (e.g. quantum dots) and its application in nanotechnology (especially nanomedicine) contributing to the theme of Green and Sustainable Materials and with overlapping research interests to the CCP. A large part of the Nanotechnology Team's research involved national and international collaborations with pharmacy research (returned in the Allied Health UOA).

Achievement of Research Strategy
This is the first UOA Physics submission for UOL. The UOL STEM investment strategy was to build a strong, concentrated physics unit. Notable features of this new unit are: 1) four academics (Zvelindovsky, Vorselaars, Greenall, Pinna) are developing self-consistent field theory and phase field methods for polymer systems, especially block copolymers, which is the largest group of academics in this subfield in a single UK-based institution. 2) significant expertise in the development of massively parallel simulations (Watkins, Chulkov and Floris) contributing 4.5 person-years of software development in the atomistic simulation package CP2K, and to the development of (and to highly cited papers on) the Quantum Espresso (QE) software.
The research strategy of this UOA was two-fold: 1) continue the development of the existing MIC and 2) establish new research directions based on the core expertise in computational materials modelling. Here we detail our achievements.
Development of charged-particle imaging for Proton Beam Therapy
The main research activity during the current REF period was the development of charged-particle imaging for the optimisation of PBT in cancer treatment (Allinson[†], Esposito[†]). With Wellcome Trust funding, we led an international team to produce the first fully solid-state proton CT instrument, PRaVDA. PRaVDA has been called "the most complex medical imaging system ever conceived". Further work is supported by an EPSRC Healthcare Technologies award, developing a second-generation CT system for installation at the NHS Christie PBT Centre, Manchester. This will be the first time that a proton CT system will be set up in an operational clinic.
The standing of our proton imaging research is demonstrated by a number of awards; the Institute of Engineering and Technology (IET) Innovation Prize for Model-based Engineering (2014), runner-up in the British Engineering Excellence Awards for Design Team of the Year (2017) and being selected for the year-long IET exhibition of '100 Objects that Changed the World.' MIC Director, Professor Nigel Allinson was awarded the 2018 IET J. J. Thomson Medal for Electronics for his contributions to imaging technology.
Establishing new Physics research
The opening of the SOMP (Prof. Zvelindovsky[‡§], Founding Head of SOMP, Pinna[‡§], Mura[‡] and a PhD student, 2014) determined a new strategic focus for physics: computational and theoretical

physics of soft matter. In particular, polymeric materials including nanostructured soft matter (block copolymers), as well as colloids, bio-macromolecules and soft/solid nanomaterials. This led to further appointments in soft matter physics: Paillusson‡ (colloids, DNA, microemulsions, granular matter), Vorselaars‡§ (nucleation theory, polymers), Roccatano‡ (molecular dynamics, proteins) and Greenall‡ (polymers, vesicles). Thus, a critical mass was built, and two key themes have emerged, namely *Modelling Interacting Systems* and *Green and Sustainable materials*, in addition to the existing *Healthcare* research.
In the next expansion stage, appointments were made in the field of electronic structure of materials with Watkins‡§ and Floris§. As well as facilitating intra- and inter- school collaborations, these appointments increased our *Green and Sustainable materials* capacity and naturally the theme of *Software Development for Materials Design* emerged based on their software development work. A dedicated Research Software Engineer (RSE), Chulkov, was appointed to support the growing areas of computational physics research.
A senior appointment (Prof. Ahmed*) was made to lead a Nanotechnology Team, along with an early career researcher (Booth*) and a UOL funded researcher (Nourafkan). The team was to promote interdisciplinary research in experimentally and industrially-driven areas with applications in energy generation and storage, and healthcare (Ahmed's outputs are returned in the Allied Health UOA), in order to grow the Healthcare and Green and Sustainable Materials themes. Further expansion in computational astrophysics of planetary systems (Sutton‡) was chosen to strengthen the Modelling of Interacting Systems theme and bring links to external facilities and data sources - from the recent Cassini mission to Saturn, for instance. A recent paper by Sutton hit the top 5% of all research outputs as scored by Altmetric (with impact index of 175).

In 2019, McIlroy‡ and Christodoulidi‡ were appointed as lecturers. McIllroy was a holder of a 'Royal Commission for the Exhibition of 1851' Research Fellowship, who works in the field of polymer fluid dynamics tackling problems in additive manufacturing including development of leading models of 3D printing, and Christodoulidi‡ works on complex system dynamics. Further details of the staffing strategy are given in section 2.

Post-graduate student recruitment
Two PhD students have graduated in the census period. Dessi performed interdisciplinary work in applied mathematics with the PhD position funded by UOL as a pump-prime initiative (returned in UOA 10). Our first PhD completion in polymer physics, Diaz, received two national awards: the IOP Alexei Likhtman runner-up prize at 29th Biennial IOP Meeting "Physical Aspects of Polymer Science 2019" and the IOP Annual PhD Thesis Prize in Computational Physics. In order to attract excellent international candidates, we offer collaborative projects with top research universities. For instance, current PhD students have undertaken six-month placements at Cambridge Graphene Centre and the Stephenson Institute for Renewable Energy (Liverpool). The first experimental PhD (Amli, Nanotechnology Team) was funded by the Palestine Solidarity Initiative and UOL and is near completion. The PGR cohort is growing - 13 PGR enrolled at the submission date. Mechanisms to expand our PGR recruitment are outlined later in this section.

Creating a positive research environment
We have looked to build a lively research atmosphere and to make Lincoln recognisable on the international computational soft-matter and chemical physics research map. We hosted national and international conferences and workshops as detailed in section 4, found placements for our PGR students with extended visits to other institutions and joined networks (e.g., MMM Hub, see sections 2 and 4) that engage our students, post-doctoral researchers and staff with wider scientific communities. Joint PhD studentships with the School of Computer Science, "Collective behaviour of autonomous organisms: from bio-particles to robotics" and "Artificial intelligence for energy management optimisation in smart grid" are currently offered via a University DTP.
The UOL's Lincoln Institute of Advanced Studies (LIAS, see institutional statement) offered fellowships to build international collaboration. One the first two International LIAS Fellows was Professor Dick Bedeaux (NTU Norway, 2018), who delivered a set of research seminars and provided expert international mentorship during a one month stay. We also have visiting

appointments from small tech start-ups and local institutions, notably a Visiting Professor position for Martin Crawley, Head of Radiotherapy Physics at Lincolnshire NHS Trust.

Achievement of impact strategy

The impact strategy was: 1) build on the success of the PBT group as detailed in the accompanying impact case studies and 2) lay the groundwork for the future in the new research directions.

To commercialise Proton Beam Therapy

Following the success of the PRaVDA project (Allinson, Esposito, Watlham[†]), we are leading a £3.2m EPSRC Healthcare Technologies project to provide the next generation system for installation in the Research Room of the new NHS PBT Centre at The Christie, Manchester – the first time that a proton CT will be installed in an operational clinic. With existing commercial collaboration (Cosylab, the world's leading provider of control systems for cancer therapy systems), this work will be progressed through clinical trials and regulatory processes to market. The underlying philosophy is to develop technologies and methodologies from basic research, through prototyping and experimentation through to potential transfer to the commercial sphere. This is evidenced by our growing patent portfolio to protect essential IP, and by our associated ICS on the development of wafer-scale CMOS imagers for healthcare through the spin-out company ISDI Ltd, which has grown to become the third largest supplier of such devices and supporting systems worldwide.

To develop a basis for impact in new physics areas

Connections to local technological innovation companies were established using mechanisms including consultancy (Sutton with Pretorian Technologies Ltd.) and EU-funded Lincolnshire Innovation Programmes (Watkins with Foresight Data Systems) to build relations with local specialist companies based around our research specialisms: ranging from the smallest start-ups to large multinationals, e.g., Teledyne e2v. The school is engaging with companies involved in the Greater Lincolnshire Manufacturing Network (LEP) led by UOL to inform future applied physics research and seek ways to boost the sector including collaborative links through the Lincoln Institute of Agri-Tech (LIAT) and National Centre for Food Manufacturing (NCFM) where UOA soft-matter expertise can be strongly relevant.

Research and Impact Strategy for the next five years

Physics will continue to further the University of Lincoln's research strategy of prioritising research that is of relevance to our locality, has global significance, drives economic development and enhances social and cultural life both within and beyond our immediate community, feeding into the University's research themes of Health and Well-Being, Sustainability and Digitalisation (as set out in the Institutional environment statement). Lincoln physics development will build a powerful computational physics research centre able to design soft, bio-inspired and interface materials whilst developing a corresponding experimental capability.

Our priority research directions (PRD) are:

PRD1. Physics for healthcare

We will build capacity in medical care and advanced drug-delivery including,

- *Medical imaging* (Allinson, Esposito, Waltham): In parallel with providing the operational proton CT system for The Christie NHS Foundation Trust, MIC will continue to develop a pixelated proton probe, which is intended to provide direct measurement of proton stopping powers at the point of treatment and so enabling fully adaptive and personalised treatment regimes and an improvement of outcomes for tens of thousands of patients. In the longer term, the field of charged particle imaging will be developed into a new medical imaging modality. In parallel with producing new science, the commercialisation of our technologies will be pursued with our commercial partners. MIC development will be done in a synergetic way with the development of various image processing directions in the School of Computer Science (e.g. computer tomography), where MIC is an integral part;

- *Drug-delivery systems* (Vorselaars, McIlroy, Ahmed): We will build on our under-pinning research on the theory of nucleation and polymer dissolution for the development of novel drug-delivery systems using additive manufacturing techniques to provide a new approach to personalised healthcare. Collaborative research on nanomaterials for drug delivery for cancer and asthma will be developed further to build on research submitted in UOA 6; work will mature on modelling of block copolymer drug delivery systems, such as nanocontainers (Pinna, Zvelindovsky, Vorselaars) as well DNA complexes (Paillusson);
- *Machine Learning for diagnosis* (Vorselaars): build on developed AI-based testing methods. Potential uses, improvements and applications of this new method will be sought to help respond to new episodes of the Covid-19 epidemic. This direction will stimulate further work on machine learning applications, bridging powerful soft-matter computational techniques to healthcare applications;
- *Interfaces and coatings* (Mura, Roccatano, Ahmed): We use our computational methods and develop interdisciplinary links to investigate antimicrobial coatings and bio-interface designs for health-care applications. Our experimental research in coatings for surgical tools and instruments will be further enhanced by molecular modelling developments.

PRD2. Green and sustainable materials
We will build on modelling approaches developed over the current census period to aid the design of efficient and sustainable materials.
Fluid dynamics for industry: We will apply non-Newtonian fluid mechanics together with molecularly-aware modelling beyond continuum models to develop more easily-recycled plastic products using additive manufacturing technology (McIlroy, Vorselaars).

- *Energy:* Modelling to understand responsive polymer capsules for smart energy applications (Greenall), block copolymer nanoscaffolds for energy materials (Pinna, Zvelindovsky, Vorselaars), and the development of experimental methods to understand quantum dot nanoparticle structures for energy harvesting (Booth). Further theoretical approaches will be pursued to understand thermofluids for energy storage (Floris). These developments will be in close collaboration with the University's new Bridge Lab initiative, which involves Chemistry, Engineering and Computer Science and will seek to develop closer links between university research in battery technologies and energy from waste systems with industrial companies (Ahmed).

PRD3. Model and Software development for material design
We develop multiscale physics software to enable collaborative research in materials modelling, applied to areas including additive manufacturing and full anti-microbial protein simulation. The extensive knowledge of soft-matter modelling techniques present in CCP provides a rare opportunity to develop these models successfully.
Examples of development areas include molecular force fields refining (Roccatano), self-consistent field theory and field-theoretic codes for soft matter (Vorselaars, Zvelindovsky). Our emphasis will be on software solutions with a world-wide user base, and to include open access, for materials design which comprises development of more efficient computational methods but also seeks more accurate and transferable models (force field, DFT, polymer SCFT, etc.) and coupling between them.
We will contribute to the development of world leading materials simulation software: *CP2K* software suite (Watkins, particularly optical properties of materials and coupling to macroscopic environments); *Quantum Espresso* software (Floris, spectroscopic methods); and *SUSHI/OCTA* (Zvelindovsky, Pinna, block copolymer/nano-particle composites) in collaboration with leading groups from Japanese industry and academia.

PRD4. Modelling of Interacting Systems
Our speciality is theoretical and mathematical physics research in soft matter, biophysics, foundations in statistical physics and dynamic systems, as well as planetary astrophysics. Research in these areas will be supported and strengthened including:

- modelling of planetary rings and exo-moon systems (Sutton);
- nonlinear dynamical systems, perturbation theory and integrable systems (Christodoulidi);

- foundations of statistical mechanics such as efficient sampling, ergodicity probing and their applications in economics and materials, such as granular matter, (Paillusson);
- theoretical biophysics (DNA) and colloidal science (Paillusson);
- systems out of equilibrium such as active matter (Zvelindovsky, Paillusson).

Strategic Actions

To achieve an impactful and sustainable research environment within the UOA we will take the series of actions outlined below to mature and advance the technological readiness level of core research carried out in the current period.

A1. Diversify income generation

We will build a strong and sustainable research effort by accessing a diverse range of funding streams to support our priority research areas bringing our funding up to around £2.5m in the next REF period. The main driver to accomplish this will be the increase in research bidding activity following the successful establishment of the SOMP's internal infrastructure. The PRD directions are those where the UOA has an existing presence and can successfully compete for external income.

A2. Mature the technological level of research lines

McIlroy is working with Natureworks through the AM-Bench initiative to develop biodegradable polymers for 3D printing applications; McIlroy, Vorselaars and Ahmed will seek industrial connections in the pharmaceutical industry through the School of Pharmacy and external academic collaborators (King's College, London) to build on published proof of concept work and models. Software development knowledge in HPC can be channelled via project partners in the Excalibur network and contribute to RSE development policy.

A3. Connect to the UOL led £6.5m Bridge commercial analytical suite

The Bridge Initiative provides a commercial route to access our academic expertise in materials research. The Physics involvement in the Bridge Initiative also seeks to build on the Greater Lincolnshire (LEP) Manufacturing Network by focussing on industrially relevant research.

A4. Expand PGR recruitment

PGR recruitment will be expanded through targeted recruitment from international channels and matched funding to support large fellowship applications up to around two PhD or researchers per FTE. The CCP is working towards teaming with other universities for joint submission of an EPSRC doctoral training centre in materials modelling, including biomaterials for medical applications.

A5. Broaden research outreach

We will popularise our public lecture series; increase our public communication, aiming to reach at least 10,000 attendees in the next REF cycle; massively expand our online delivery to widen the reach and accessibility following recent experience such as the recent "International Nanotechnology Workshop" (Ahmed, McIlroy, Mura); expand our student placements, support and host Newton Academy events to increase uptake of STEM to female students and work with the IOP to deliver more physics outreach activities.

Approach to Interdisciplinary Research

Most of our research is inherently interdisciplinary or is strengthened by collaborations outside the UOA. Examples include; charged particle imaging (Allinson) where our consortia include Co-Is from leading particle physics groups, directors of national PBT facilities, bodies of international standing such as the Karolinska Institute, and NHS clinicians and medical physicists; 3D-printed drug-delivery systems (McIlroy, Vorselaars) bring together non-Newtonian fluid mechanics, polymer physics, engineering technology, pharmaceutical science and computational modelling. We will also seek expertise from Lincoln's National Centre for Food Manufacturing to utilise soft-matter domain knowledge usefully.

We benefit from close links with research in the Schools of Chemistry, Computer Science, Engineering, Pharmacy and Life Sciences and share analytical facilities housed in the purpose-built Joseph Banks Laboratory and The Bridge Lab (see Section 3). New facilities in the Bridge Lab will also promote interdisciplinary soft-matter and other materials projects, especially with

business. Conference organization is key to our approach to interdisciplinary research, see section 4 for further details of conference organisation.

Research Integrity and Open Research Environment

We follow the University's Code of Practice for Research, as well as the University's Ethics Policy, as the main instruments for the creation of a comprehensive framework for good research conduct.

The HiPSTER group is committed to work on international open-source and open-development codes, for instance long-term contributions to CP2K and Quantum Espresso. These initiatives are augmented by providing support to the user and developer communities via dedicated forums, regular tutorial workshops, and user/developer meetings aiming to up-skill users and widen participation in scientific open-source development. The principle audience is PGR and post-docs UK and internationally but includes SMEs and other industry.

MIC provides an on-line proton imaging database that allows the worldwide research community to research new proton CT reconstruction methods. The CCP (Pinna and Zvelindovsky) have for many years contributed to the development of the Japanese open-source software SUSHI/OCTA for soft-matter systems.

We financially support open-access publication schemes wherever possible via green/gold open access pathways or engaging with innovative publication models such as full open-access/open-review journals. For example, Roccatano is an Associate Editor for the open-access journal PLOS ONE and Paillusson is on the Board of Reviewers for the open-access mathematical physics journal Entropy.

2. People

Staffing strategy

Since 2014, the School of Mathematics and Physics has invested in developing strength in computational and theoretical physics. The aim was to build a powerful computational physics team supported by a growing experimental and analytical capacity as evidenced by the £640,179 staff investment from the UOL in this UOA. UOA 9 also includes returns from the established MIC based in the School of Computer Science and a chemical physicist based in the School of Chemistry.

The strategy was implemented by the appointment of seven academics (Prof., three Senior Lecturers and three Lecturers) in soft matter theory/modelling, reinforced with the appointment of experts (two SL) in chemical physics materials modelling and, more recently, in astrophysics, computational fluid dynamics and complex dynamical systems (three Lecturers). These appointments have created a distinctive materials-modelling portfolio comprised of a wide range of knowledge and technical skills, from its fundamentals to its more applied components. Further appointments in the SOMP and inclusion of the Medical Instrumentation Centre (Prof., SL, design engineer), bring the total to 15.2 academics in the UOA.

The appointment strategy targeted the employment of early career researchers (Paillusson, Vorselaars, Floris and Greenall in 2015, Booth in 2016, Sutton in 2017, McIlroy and Christodoulidi in 2019) supported by senior lecturer appointments (Pinna and Mura in 2014, Watkins and Roccatano in 2015). More details of the research drivers for the appointments were given in Section 1. Beyond 2021, we aim to strengthen the smaller research branches that have begun in the present period by:

- Appointments in astrophysics, e.g. plasmaspheres around celestial objects, to complement the existing modelling expertise of the CCP and promote cross-fertilisation between research areas;
- Appointments in materials development to increase opportunities for partnership with industry and the possibilities offered by the new Bridge Lab facility. The over-arching aim is to achieve full materials design "in house": from model to experimental validation and commercialisation.

Staff Development
Physics research is supported by the University of Lincoln's comprehensive range of policies concerning employment, equal opportunities, research management and ethics, each with an element designed to support research activity. The staffing strategy is strongly linked to the unit's research strategy through increasing research capability (see above) and providing continuous professional development and mentoring support. All academics participate in the annual appraisal scheme and can apply for a promotion annually. In the REF period two academics were promoted to Associate Professor (Watkins, Pinna, both promoted 2018). Leadership training is also offered to staff via appropriate ILM management courses.
The SOMP runs an annual travel grants scheme for all academics to visit / host collaborators to foster national and international collaborations. We organize regular Research Away Days for developing joint research projects. All early-career researchers have a mentor as well as their line manager and we have used initiatives like the LIAS International Fellow scheme to bring in mentors of international stature.
College away days are organised to enable early-career, mid-career and senior staff from different schools to get to know each other and develop plans to work together. The College runs an annual Research Showcase event at which researchers from all Schools within the College can see their colleagues' research and develop knowledge of what research expertise is available for interdisciplinary projects.

Support for PGR Students
The Lincoln physics community is committed to developing the next generation of researchers through its PGR students. All PhD students have at least two active supervisors providing a broad view to develop the students. Following UoL's Institutional Environment Statement PGR students participate in weekly meetings and presentations at Group / Laboratory level, seminars and open days across UOA 9, and talks by academics in events organised by LIAS. International students have access to peer support in events hosted via the International Postgraduate Society.

To expand their experience, we have connected our PGR students to external institutions and infrastructure through the following initiatives:

- Engagement with the MMM-hub (EPSRC) is encouraged and we promote their journal clubs, conferences, and lecture series aimed at PGR and early career researchers to our students;
- PGR students with an experimental focus are given opportunities to collaborate with external organisations, e.g, Stephenson Institute for Renewable Energy at Liverpool and Cambridge Graphene Institute via three-month student placements (Amli). Several PhD students benefited from the placements in industry (Boukari at Inciner8 Ltd for his PhD studies on Incineration Systems for Energy from Waste, and Walwyn at MSS Products for Advanced Energy Systems);
- Computational physics PhD student Díaz benefited from three extended research visits to the University of Barcelona (2016, 2017 and 2018), supported by two Santander travel awards and a BritishSpanish Society award;
- Engagement with the School's RSE allows students to develop advanced computational methods in the context of their projects;
- Students also benefit from access to and training on the use of local cluster computing facilities and the tier-2 MMM-hub Young supercomputer (we also contribute to the training).

Experimental physics research students also have access to the pool of centrally managed laboratory equipment and training, as detailed in section 3.

Equality, Diversity and Inclusion
The school supports the university's position on equality, diversity and inclusion, see the institutional statement. SOMP operates an EDI Committee chaired by the Equalities Officer to develop strategy, oversee effective implementation and monitor equalities policies in all functions of the School. The EDI Committee leads the work on applying for a Juno Award, an IOP initiative designed to develop an equitable working culture in which all students and staff

can achieve their full potential. Of the UOA's 15.2 members, 25% identify as female, 0% are BAME and 0% disabled. Currently, senior research academic staff are few, with all Professors (2) and Associate Professors (2) identifying as male.
Key objectives in the School's EDI action plan are to support staff promotion and encourage the presentation of female role models in research - ECR staff are encouraged to participate in the Aurora AdvanceHE leadership development scheme for female academics. Mura sits on the committee for the Eleanor Glanville Centre (EGC), which is a central hub for the University's equality and diversity policy research. Through the EGC, one of the School's academics and one MRes student secured 'Back to Science' research support (£15k) as part of the University's support for academics returning from maternity leave. Additionally, the School provides flexible working arrangements for academics actively supporting parenting and caring responsibilities and the working space is fully accessible.
As well as involvement in the University wide EGC, Pipeline mentoring scheme, and other institutional policies, the School of Mathematics and Physics is an IOP Juno supporter. The School is working with the IOP towards obtaining Juno practitioner status and will be submitting its application this year and building on this to move towards the school's aspiration to acquire Athena Swan awards.

3. Income, infrastructure and facilities

Research Income
The School of Mathematics and Physics was founded in 2014 and MIC's interdisciplinary work was returned in the Computer Science UOA in REF2014. Hence, there was no research income reported pre-2014.
During the census period, major grant awards have come from:

- the Wellcome Trust and EPSRC for the development of charged-particle imaging for the optimisation of PBT in cancer treatment. With £1.8m Wellcome Trust funding to produce the first fully solid-state proton CT instrument in the world, PRaVDA. Following the success of this project, MIC are leading a £3.2m EPSRC Healthcare Technologies project to provide the next generation system;
- Another prestigious grant was to McIlroy of a Royal Commission for the Exhibition of 1851 independent research fellowship to investigate semi-crystalline polymer materials in additive manufacturing;
- Specialised computational software development grants have come from three person years of software development ARCHER, an EPSRC and NERC funding stream for software development for the National Supercomputer (*Watkins £212,000*) and one and a half person years of software development from EPSRC High End Computing flagship and Excalibur exascale computing initiative (*Watkins £123,000)*.

We have secured numerous smaller grants and awards not reported in the HESA figures including a Royal Society International Exchange Scheme with the University of Genoa (*McIlroy)*, HPC computer time, travel grants (Santander, British-Spanish Society) and small equipment grants (RSC). Total research income for this UOA is £2.1m.

Infrastructure and Facilities
Computational physics research is enabled by an excellent computing infrastructure developed over the census period. We have a growing local CPU/GPU cluster (currently ~600 cores) with expert support from an RSE (Chulkov). We are one of three new partners (along with Reading and Brunel) joining a refresh of the Tier 2 EPSRC HPC resource the MMM-Hub (Young supercomputer ~30,000 cores of which ~1000 cores are dedicated to UOL), which is led from UCL. This facility provides a springboard to national tier-1 resources, national collaborations and to international initiatives. Additionally, we have access to national tier-1 (Archer and Archer-2) and other tier-2 resources (Thomas, Jade) via membership of Materials Chemistry Consortium (Watkins, Floris) and Biomolecular Simulation Consortium (Roccatano).
The MIC works with long-standing OEM companies (ISDI Ltd, a CMOS design house that spun-out of Professor Allinson's research on large-area CMOS imagers), and aSpect Design Systems

(Dresden), a specialised scientific data acquisition company. Such arrangements allow us to design and fabricate custom CMOS circuits and imagers, as well as start-of-the-art electronics built to an industrial standard.
Modern purpose designed wet-lab space is available within the Joseph Banks Laboratory (JBL, which also houses the School of Chemistry). In the JBL we also have access to analysis tools, including research grade NMR (500MHz including broad band solution and solid state probes), X-Ray Diffraction (dual-source SCD, multi-stage PXRD), Mass Spectrometry-Chromatography (GC- triple quadrupole, LC-Orbitrap, LC-triple quadrupole), Elemental Analysis (XRF, ICP-OES), Thermal Analysis (STA-MS, STA-IR, Thermomicroscopy, ITC) and Nanoscience (DLS, Zeta-potential, Nano-sight). These facilities were combined with existing resources including PVD apparatus, machining and SEM. Dedicated instrument scientist support is available for characterisation work. Further instrumentation will be become available as part of the £6.5m Bridge Lab project that will provide opportunities for collaboration with industry and facilitate an expansion of staff expertise into experimental areas.

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

Research collaborations, networks and partnerships

Research Consortia and Networks

The MIC is leading two major research consortia funded by the Wellcome Trust (£1.8m) and the EPSRC Investigator-led Healthcare Technologies (£3.2m) project, OPTIma. Both consortia have partnerships with up to five UK and two overseas universities, five NHS Trusts and Foundation Trusts and PBT centres worldwide (e.g., Switzerland and South Africa). Due to their complexity, these consortia are managed by an experienced project manager.
Watkins is on the steering committee of the Materials Chemistry Consortium, one of the largest EPSRC-supported High End Computing consortia which allocates a significant amount of time (~15% in 2019) on the national supercomputer. The CCP led UOL in joining the Materials and Molecular Modelling (MMM) Hub (EPSRC), along with ten other UK institutions, gaining access to significant computing resources.
McIlroy is on the polymers scientific committee for AM-Bench, a joint academic and industrial initiative led by the US NIST, which guides best practice in developing additive manufacturing methods.

HiPSTER and CCP participate in the national networking programme Excalibur (Met Office/ EPSRC) combining the effort of over 100 research groups UK-wide in order to roadmap the development of UK exascale computing using materials simulation codes.

Research Collaborations

We have grown strong networks of research collaborations with other UK universities, as evidenced by our publications record. These include:
Universities of Nottingham and Leeds, see submitted papers from McIlroy;
Universities of Warwick and Aston, collaboration on an MCSA individual fellowship and publications, Greenall;
University of York, papers (McKenna, Physics) and joint supervision of student (Avestro, chemistry); UCL long standing collaborations with Woodley and Shluger (Watkins);
UCL, KCL (Ahmed, Floris, Watkins, Mura)
University of Liverpool and Anglia Ruskin University (Ahmed);
University of East Anglia, (Roccatano).
We also have extensive ongoing international collaborations with researchers at institutions including:

- Tohoku University, Japan (SUSHI/OCTA soft matter code co-development, Zvelindovsky, Pinna; MD modelling, Roccatano);
- Norwegian University of Science and Technology (Dick Bedeaux, Visiting LIAS International Fellow);
- Kanazawa University, Japan (Atomic Force Microscopy in liquid, Watkins, Nanoscale 2016);
- Aix-Marseille Université, (collaboration on synthesis of molecularly fused nano-meshes for light harvesting, Watkins, Nature Chemistry 2018);

- Sorbonne Universités, UPMC Univ Paris 06 (Paillusson, Journal of Chemical Physics 2019);
- University of Zurich and ETH Zurich, ongoing CP2K development, Watkins, editor's highlight in Journal of Chemical Physics;
- University of Waterloo, Canada, publications, extended visits, Vorselaars;
- Centro Brasileiro de Pesquisas Físicas, Brazil, a paper in this REF submission - Christodoulidi;
- University of Padua, Italy, Christodoulidi's collaborators;
- Universitat de Barcelona, several papers in this REF submission (Pinna, Zvelindovsky);
- CECAM, Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lausanne, several papers in this REF submission (Pinna, Zvelindovsky);
- Universitat Rovira i Virgili, Tarragona, Spain (a paper in this REF submission – Pinna, Zvelindovsky);
- University of Genoa, Italy (via Royal Society International Exchange Scheme, McIlroy);
- Purdue University and Kansas State University, USA, BZ Multan University, Pakistan, Qatar University and Dhofar University, Oman) (Ahmed's collaborators);
- RWTH Aachen University, DECHEMA Research Institute, Germany (a paper in this REF submission – Roccatano);
- University of the Basque Country UPV/EHU, Spain (a paper in this REF submission – Roccatano);
- Johannes Gutenberg University Mainz, Germany (Floris' collaboration).

Industrial Partnerships
MIC has two long-term industrial partners, aSpect Systems GmbH and ISDI Ltd – the latter is a spin-off CMOS design and supply company that provides large-scale CMOS imagers chiefly to the healthcare industry. Both companies market products based on research undertaken by MIC.

Relationships with users, beneficiaries and society
Users of Medical Imaging*:*
Research conducted by MIC directly benefits UK healthcare in relation to cancer treatment using proton beams. Through our research consortia and relationships with NHS trusts, our research outputs are directly beneficial to patients. Through our industrial partnerships (aSpect Systems GmbH, ISDI Ltd), we continue to inform development of imaging technology for the healthcare industry. The OPTIma instrument at The Christie Foundation Trust will form part of the UK national research facility to enable access to other UK and overseas groups.
Users of Computational Physics Software
Watkins and Floris contribute to the development of CP2K and Quantum Espresso (QE), respectively. They are two of the most widely used materials simulation codes internationally and UOL has contributed around five person years of software development as well as user support and training as part of the larger international effort. CP2K was used for £1.7m and QE £470k of calculations on the national supercomputer between November 2014 and October 2019 by EPSRC and NERC users - typically occupying ~10% of the machine combined. 100s of groups are using these codes internationally with >20,000 papers citing the core development papers over the census period. We have co-organised annual CP2K summer-workshops and user-group meetings since 2014 - co-organisers have included EPCC, KCL, Imperial, STFC Daresbury, University of Zurich - as part of a five-year EPSRC network grant (CP2K-UK). We are actively developing online resources to supplement workshop delivery.
Public Engagement and Outreach
Our public lecture series, established in 2014, has hosted leading international speakers to deliver compelling research at a non-specialist level to audiences including academics, schoolteachers and children, leaders and technical experts from industry and NHS. A 500+ person lecture theatre in the Isaac Newton Building allows the hosting of large conferences and talks, greatly enhancing our research outreach. Since its inception this series has been attended by over 3,000 people from around the UK.
Staff actively disseminate their research to the public, examples include:

- Paillusson's research on entropy was presented in two public IOP talks in Lincoln and during a tour of four other UK cities;
- SOMP launched its own series of Christmas Lectures, two of which were about research on physics of the dynamics of self-propelling particles (Zvelindovsky), protein dynamics (Roccatano) and physics of DNA (Paillusson);
- Roccatano, Zvelindovsky, Paillusson and Sutton presented their research results at the highly popular Grantham Gravity Fields Festivals in 2016 and 2018;
- McIlroy and Christodoulidi presented their research to MPs at STEM for Britain 2018 and 2020;

In March 2021 the members of the unit will deliver eight research outreach talks online as a part of British Science Week 2021;

The MIC team are very active in public engagement because cancer treatment is a topic of great interest to the public. An interactive display on PRaVDA was exhibited at The Royal Society Summer Exhibition (2014), GravityFields Festival (2014) and Spark Engineering Festival (2015) as well as in the Wellcome Trust HQ. The display has been visited by an estimated 25,000 people;

- The Annual Edmund Weaver Lectures in Astronomy, focussing on Sutton's research on Saturn Cassini mission data and exoplanets, were attended by over 600 people. He also presented his research to a wider community on 12 talks in various Astronomical Societies, and popular science clubs like Cafe Scientifique and Pint of Science;

Sutton's paper on exoplanet J1407b, in Monthly Notices of the Royal Astronomical Society, was featured in 18 news outlets, such as Forbes, Fox News and MSN, as well as Russian news outlets and BBC Radio 5.

Wider Contributions to the research base

Contribution to Learned Societies

We are actively involved with physics learned societies:

- Vorselaars (Treasurer) and Pinna (Chair) of the IOP Computational Physics Group;
- Greenall (term finished in 2019) and Zvelindovsky (current) ordinary committee members of the IOP Polymer Physics Group;
- McIlroy is the Secretary of the British Society of Rheology, and a member of the Institute of Non-Newtonian Fluid Mechanics.

Contribution to Research Quality

All researchers within the UOA are involved in peer-reviewing for internationally-recognised journals, and many review grant applications for major award bodies both in the UK and internationally. We also contribute to journal editorship:

- Zvelindovsky is on the International Advisory Board of *Macromolecular Theory and Simulations* (Wiley) and the Editorial Advisory Board of *Advanced Theory and Simulations* (Wiley);
- Roccatano is an Associate Editor of *PLOS ONE*;
- Sutton is on the Editorial Board of *Journal of International Astrophysics;*
- McIlroy is an Associate Editor for the journal of *Additive Manufacturing* (Elsevier).

Contribution to Conferences and Workshops

Conference organisation is our main driver for instigating international collaborations, which have contributed to many of our best publications. International meetings we have organised include:

- International symposium and workshop 'Computational condensed matter: advances and challenges' (CompMat2014), (2014, Zvelindovsky, Pinna, Mura);
- Annual Meeting of the Crystallize COST Action CM1402 group, involving scientists from 27 different countries (2017, Vorselaars);
- International CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop: 'Nano-structured soft matter: a synergy of approaches to amphiphilic and block copolymer systems', (2018, Zvelindovsky, Vorselaars, Paillusson, Greenall);
- International CECAM workshop: 'Emerging behaviour in active matter: computational challenges', (2019, Paillusson, Zvelindovsky, Pinna);

- The 29th biennial meeting “Physical Aspects of Polymer Science”, IOP, (2019, Greenall);
- The Biannual Materials Chemistry Consortium Conference (2018, Watkins);
- Non-Newtonian Club meeting on “Rheology for Processing” (2019, McIlroy);
- Machine Learning in Physics meeting by the IOP CPG, (2019, Vorselaars).