High Performance Numerical Modelling: a Key Driver of Successful Space Missions (Helio)

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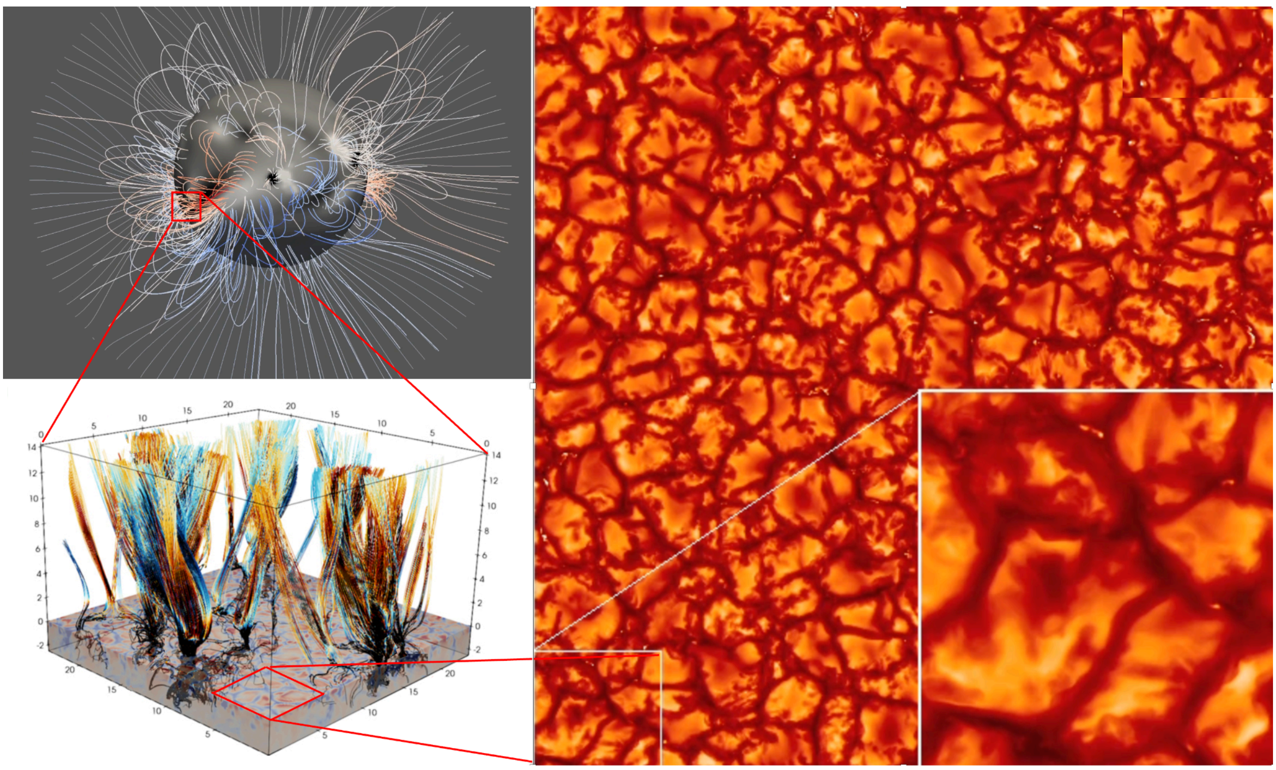

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Scientific motivation and objectives

The UK Heliophysics community has a long history of world-leading numerical modelling, both in terms of model/code development and in applying them to address the mysteries of our enigmatic Sun. With recent and likely future advances in Exascale High-Performance Computing (HPC) and Artificial Intelligence (AI), there are many potential avenues to push our capabilities further. As we look forward over the next 10 years, a coordinated strategy that embeds this expertise throughout the UKSA mission-funding process will ensure the greatest possible scientific return from mission data. Furthermore, advances in modelling capabilities contribute to the development of predictive tools and mission planning strategies that enhance the UK's position in international collaborations such as ESA's & NASA's heliophysics programmes.

The role of numerical modelling is fundamental to driving scientific advances in solar and space science, including in the key topics of the field: how the Sun's magnetic field cyclically regenerates in the solar interior; how this magnetic field rises to the surface and energises the solar atmosphere; what drives the dynamics and heating of the solar atmosphere; how solar activity influences the heliosphere; and how the heliosphere interacts with and drives changes in planetary magnetospheres. These have been recognised by the community as important areas of focus, as presented in the 2022 *Roadmap for Solar System Research* [1], particularly within "Theme 1: Solar Variability and its Impact on Us" and "Theme 3: Space Plasma Processes".

Recent advances and High-priority Science Questions

Solar Interior: The UK is at the forefront of modelling the solar interior, with internationally recognised expertise in solar dynamo theory, tachocline dynamics and the interaction of turbulent solar convection with rotation and stratification. These processes underpin our understanding of the long-term evolution of solar activity on decadal to millennial timescales, important not just for space weather prediction, but also because it increases our knowledge of the physics of stellar interiors. Recent successes include elucidation of the fundamental mechanisms by which large-scale magnetic fields can be generated in a turbulent rotating system [2], and how magnetically-driven instabilities in the solar tachocline [3] and in the Near Surface Shear Layer [4] can potentially contribute to the large-scale solar dynamo process. State-of-the-art theoretical and numerical models have provided key insights into the convective conundrum, demonstrating how refined treatments of convective turbulence and rotation can help reduce long-standing discrepancies between models and observations[5,6]. However, significant challenges remain. The scale gap between the global magnetic field and the turbulent processes that drive its evolution is beyond the scope of current HPC, making innovative new numerical approaches necessary [7].

The Dynamic Solar Atmosphere: The solar atmosphere still holds many mysteries, including identifying the dominant mechanisms that heat the chromosphere, corona and drive the solar wind [e.g. 8,9], determining how energy and momentum are transferred from the photosphere into higher layers[10]; clarifying how energy is dissipated through turbulence, magnetic reconnection [11] & magnetohydrodynamic (MHD) waves[12]; and understanding the non-local thermodynamic equilibrium (non-LTE), partially ionised chromosphere[13,14]. The origin and evolution of fine-scale magnetic structures, e.g. spicules, flux tubes, and current sheets, remain insufficiently understood. Similarly, additional research is needed to quantify how variations from solar parameters shape the physical processes and emission characteristics of stellar atmospheres.

Progress requires integrating next-generation observations with advanced numerical modelling. High-resolution spectropolarimetry, multi-wavelength imaging from ground-based and spaceborne facilities, and coordinated measurements from missions like Solar Orbiter, Polarimeter to Unify the Corona and Heliosphere (PUNCH), MUlti-slit Solar Explorer (MUSE) and SOLAR-C EUVST [15] will provide the required diagnostics. However, the mapping of thermodynamic parameters to the emission from each layer is non-trivial, and, in the cases of the strongest spectral lines, a non-local function of the plasma state over a wide region. Therefore, radiative MHD simulations and data-assimilative models will be essential to connect observations to plasma processes.

STFC has recently made a significant 5-year investment in the UK capabilities in modelling the solar atmosphere through the Large Award to develop the Solar Atmospheric Modelling Suite (SAMS). This fully modular, open source code will allow users to perform the complex radiative MHD modelling required to match directly with observations. Over the next decade, with SAMS, we will be in a position to routinely synthesise realistic solar atmospheric models and to start to realistically treat the radiative terms in 3D simulations of the solar atmosphere.

Magnetic Modelling of the Solar Atmosphere: Many chromospheric and coronal phenomena depend on the gradual build-up and storage of magnetic energy and helicity over periods too long to model fully with detailed multi-physics simulations (for example, those possible to perform using SAMS). Since energy and helicity are (highly) conserved quantities, they can be estimated using simpler approaches. UK researchers have played a strong international role in developing codes and promoting this “time-dependent” data-driven approach, using combined magneto-frictional and MHD techniques to demonstrate new emergent behaviour, including the hemispheric pattern of filaments [16], enhancement of the Sun’s open flux [17], self-consistent formation and eruption of flux ropes [18], and helicity condensation [19]. Recent work has focused on developing data-driven models to the point of making predictions: Is a particular active region likely to produce eruptions? Where is the magnetic field at a spacecraft connected back to the Sun? These questions depend fundamentally on how the coronal magnetic field is energised over time periods of days to months.

These time-evolving models are complemented by numerically modelled magnetic field extrapolations [e.g. 20,21,22], as these allow a more focused view on individual active regions. These models extrapolate from the observed photospheric magnetic field to calculate the coronal magnetic field and thus to provide estimates of the magnetic energy and helicity in active regions. Since direct measurements of the chromospheric and coronal magnetic fields are extremely limited, extrapolations from photospheric magnetograms provide the best available three-dimensional view of how magnetic energy is stored and where it is likely to be released. These models help identify stressed or twisted magnetic structures that are prone to instability, enabling forecasters to assess the likelihood, timing, and potential severity of eruptions. Research under the SAMNet programme has shown an up to 8-hour lead time in the prediction of eruptions using extrapolations [23], with these developments being important for space weather prediction.

Solar wind/space weather: Plasma and energetic particles released at the Sun play a fundamental role in determining the conditions in space. The solar wind couples the Sun with planetary magnetospheres. Transient solar events, including solar flares[24,25] and Coronal Mass Ejections (CMEs)[9], cause disturbances in near-Earth space that are a key component of Space Weather. With society’s increased reliance on satellites and ground-based infrastructure susceptible to space weather, scientific understanding of the interaction with the Earth’s magnetosphere and atmosphere, and the development of forecasting capabilities, are key priorities [26,27,28].

The UK has a long history in modelling the solar wind and space weather, with these efforts having application to the forecasting of space weather at the UK Met Office. This includes modelling Solar Energetic Particles (SEPs) [9,29], which are a key component of space weather due to the radiation risk to satellites and humans in space. As yet, we still do not know how SEPs are accelerated and propagate through the interplanetary magnetic field to reach Earth. Predicting the likelihood of an SEP radiation event occurring at Earth following a solar eruption is challenging and we do not know how the Earth’s magnetosphere shields us from these events.

The Earth’s magnetosphere represents a key structure that facilitates the transfer of energy into near-Earth space, in the form of energetic particles that form the hazardous radiation belts, and atmospheric heating visualised through aurorae and felt through increased satellite drag and satellite collisions [30,31]. Key unsolved questions include: what are the dominant modes of energy transfer through the dayside magnetopause? What defines the substorm cycle? How much energy is transported from the magnetosphere into the upper atmosphere?

Particle energization and energy transfer throughout the heliosphere involve fundamental plasma processes: shock waves, waves and turbulence, and magnetic reconnection [e.g. 32,33]. These are inherently multi-scale, with understanding the smaller-scale physics important for predicting global scales. For example, particle injection into diffusive shock acceleration ultimately depends on the shock kinetic-scale physics. Modelling plays an important role in bridging the scale gap.

Solving the key science questions of these research areas will go hand-in-hand with the modelling developments. The first breakthrough on the horizon is the arrival of exascale HPC facilities. However, effectively utilising these will require effective algorithms for both CPU and GPU facilities that bring performance portability across architectures to maximise the use of the resources.

Objective 1 - Through the development of the required skill base, develop high-performance algorithms that fully utilise the upcoming and future HPC facilities.

Even if we achieve this, some problems naturally involve so much computational power that they are even beyond the scale of exascale HPC. To supplement algorithm development, the use of machine learning to parameterise key physics like radiative transfer or turbulence at the grid scale will be necessary through the use of Physics-Informed Neural Networks (PINN) and techniques like running machine learning during calculations to drive speed-up.

Objective 2 - Develop the skills base to effectively utilise machine learning as a tool for effective and accurate modelling.

Machine learning sits as one aspect of model development [34], but it cannot flourish as a tool on its own. Broader investment is required in both the development of models and in nurturing the wide range of skills and expertise required to effectively develop and implement models.

Objective 3 - Investment in building and retaining the skill base of both researchers and research software engineers to develop the next numerical models for solar and space science.

Furthermore, numerical modelling is also a crucial tool for the development of future ground-based facilities (e.g., the UK-led SAMNet) and satellite missions. It allows us to assess whether planned observations and measurements can truly support understanding of the complex physical processes that govern the Sun and its interactions with the wider heliosphere and planets. This capability has been effectively utilised in recent & proposed NASA and ESA missions. The NASA Interface Region Imaging Spectrograph (IRIS) mission pioneered this approach for developing solar missions. With numerical models of the solar chromosphere and corona, we used to plan the required capabilities of the instruments and integrated all the way through the processes leading to numerical data cubes being released to the community to aid interpretation of the observations. This approach has continued with MUSE [35]. In the UK, the modelling community has had a significant involvement in supporting and justifying the design for the ESA Vigil mission.

Objective 4 - Develop modelling capabilities to support planning and enable maximal exploitation of future space missions.

Despite its significance, numerical modelling often remains an under-resourced component of the research pipeline, facing challenges related to computational infrastructure, software sustainability, and long-term career development for researchers. Addressing these gaps through targeted policy support and coordinated investment would strengthen the UK's capacity to lead in solar and space science, maximise the scientific impact of current and future missions, and reinforce the integration between data, theory, and simulation.

Strategic Context

Looking ahead, the improvement of numerical modelling with advances in exascale HPC and artificial intelligence will open new frontiers for exploration and application. These emerging capabilities align directly with UKRI's Digital Research Infrastructure and AI for Science initiatives, providing opportunities for shared investment and innovation across disciplines and driving forward developments that support the industrial strategy in these areas. This will connect with the training of PhD students and RIAs with these skills, creating a base of highly skilled, highly trained experts able to move between academic research and industry.

A significant focus of the heliophysics modelling community is enhancing our understanding of the physical processes underpinning space weather, from their origin in eruptions at the Sun to their effects at Earth. Significant involvement of academic researchers is aimed at producing better space weather forecasting tools, in cooperation with stakeholders such as the UK Met Office. Therefore, there is a clear societal benefit in funding research and research to operations (R2O) efforts in solar and heliospheric areas. Modelling plays a key role in space weather research, as a tool for linking together multi-point and multi-instrument observations and as part of forecasting.

By embedding numerical modelling within this broader technological and policy framework, STFC and UKSA can ensure that UK researchers are not only able to interpret existing data but can also design, predict, and optimise the missions and instruments of the 2030s and beyond. Ultimately, a forward-looking policy approach that embeds modelling at the core of solar and space science will secure the UK's long-term leadership in discovery and innovation. It will also ensure that the UK's contribution to international missions—scientific, operational, and strategic—continues to be defined not only by participation but by leadership in the theory and simulation that drive research.

Proposed Approach

Numerical modelling to underpin fundamental research

Modelling magnetic field evolution and dynamics of the solar interior, atmosphere and heliosphere requires capturing physical processes across a vast range of spatial and temporal scales. Over the next decade, major scientific progress will depend on the development of efficient algorithms that enable the accurate solution of equations on exascale machines in both global and local geometries. The development and refinement of such methods (such as spectral methods for modelling the solar interior or radiance cascades to model the radiative transfer of the solar atmosphere) tailored for modern CPU and GPU architectures will be essential going forward.

Even with the most efficient algorithms, the range of scales that must be solved for will simply be beyond computing facilities going forward. A key future research priority is therefore the development of models that couple these methods to subgrid scale models that accurately represent the unresolved scales. There are a number of elegant and promising approaches to developing these models, including: the use of Machine Learning, in which transport coefficients are learned from high-resolution local computations to improve global models; the development of methods that solve for the statistics of the unresolved scales (termed Direct Statistical Simulation), offering a fundamentally different route to capturing multiscale behaviour; the development of numerical techniques for the solution of a reduced set of equations that retain essential nonlinear interactions while enabling simulations on a vast range of scales.

For data-driven simulations, ongoing efforts are required to improve both the physics and parameter fitting on both active region and global scales. Major stakeholders include the Met Office Space Weather Operations Centre (MOSWOC), improving forecasts of both eruptions [36] and the background solar wind [37] and their interaction [38]. There is a role for the development of new simulation codes (global models) and use of machine learning for optimisation.

Modelling the solar atmosphere requires the coupling of the dynamics to atomic physics and to the radiative field of the solar atmosphere. Modelling this is the main goal of the SAMS project. SAMS will be developed with a modular structure allowing users to include all atmospheric layers or a subset of layers, e.g. the chromosphere and corona, running time-dependent non-LTE radiative transfer MHD simulations as either complex 3D models or faster 1D models with a clear pipeline from input, through simulation to observable. The code will be made available to the community as Open Source with detailed physics-based documentation to promote ease of use. Building a user base for this code that not only can perform cutting-edge science but also drive forward the development is an important goal over the next decade.

Support for numerical modelling through future missions

Modelling and observational data go hand-in-hand, as even the best theories need to be tied to observational data. To provide important constraints to models of the solar atmosphere, and to support their scientific development. A key aspect of this is high-resolution, high-time-cadence observations along with spectra that cover different layers of the solar atmosphere. With Solar Orbiter and the planned launch of MUSE, some of this requirement is met. But as new missions are developed, for example SOLAR-C EUVST [15], SPARK [39] or OSIRIS [40], it is key that they are pushing the boundaries in terms of the spatial and temporal resolution to open a new window into the physics of the solar atmosphere. Complementary to this are measurements of the chromospheric and coronal magnetic field which provide a key input and constraint on models [41].

The main limitation at the present time for models of the global magnetic field is input data, especially magnetograms. Recent and ongoing work is looking at how forecasts are affected by methods of driving the simulations [42] and with increased longitudinal range of magnetograms [43], e.g. simulations have been used to support/justify the ESA Vigil mission. A major advantage of the time-dependent approach is that it can be used with purely line-of-sight magnetograms rather than requiring more expensive and uncertain vector magnetograms. But it is essential to maintain access to synoptic programmes.

A priority is continued access to regular magnetogram coverage. Given the reliance on NASA's Solar Dynamics Observatory (SDO) for daily space-based magnetograms, support of upcoming missions with magnetographs is essential both for maintaining existing simulation support and for the development of improved capability. These missions also provide important observations for helioseismic inversions, which place important constraints on modelling the solar interior. Missions that continue the work of SDO are of high priority to the modelling community [44].

Numerical modelling to support future and upcoming missions

Radiative transfer postprocessing of modern advanced solar simulations during the mission design phase enables both careful selection and refinement of targets for maximal scientific return. For example, for SOLAR-C EUVST [15] forward modelling for the short-wavelength camera (λ = 17–21.2 nm, developed in the UK, funded by ESA) has been used iteratively to demonstrate likely performance and feed back into instrument design to improve performance. The forward modelling development will also enable the provision of software tools for users to optimise their observations, increasing science return (resources permitting). But it is not just remote sensing where modelling work is critical for shaping missions and their instrumentation. For the development of the Smile mission and in the proposal for Plasma Observatory to ESA, both focussed on the magnetosphere, modelling underpinned the development of the mission design to make sure the mission could most effectively answer the science questions.

Modelling is also crucial for fully interpreting observations of missions in flight. As an example, STFC provided funding for a PDRA and several workshops to support UK contributions to the Solar Orbiter modelling working group pre-launch. The tools developed by that group are routinely used and have increased science return.

The non-local nature of radiative transfer in many strong spectral lines (for example, the optically thick Mg II resonance lines observed by IRIS) has required significant investigation to determine the importance of competing terms affecting their formation in realistic solar conditions. These spectra contain a wealth of information, but it cannot be simply decoded. The development of specialised forward models, which, due to computational complexity, capture the necessary physics in the formation of a particular spectral region as efficiently as possible, can only be developed through a robust suite of end-to-end atmospheric modelling tools. These are a key component of inversion tools which infer potential thermodynamic (and magnetic, in the case of polarised observations) parameters from observations using iterative fitting techniques. In the Extreme Ultraviolet, the majority of spectral lines are optically thin, however they require careful atomic physics calculations to correctly determine their ion balance. Whilst a less computationally complex undertaking, there remains significant theoretical work to correctly model these lines to correctly interpret observations [e.g. 45]. A wide range of wavelength coverage throughout the ultraviolet and visible is needed to support different observatories simultaneously to provide a more comprehensive view of the plasma state.

Proposed Technical Solution and Required Development

To sustain the UK's leadership position, investment is required across computing and data storage infrastructure, skill development, and fundamental research efforts.

Historically, the UK has had an advantage in computational science. However, there are no British facilities in the top 10 supercomputers internationally, and only nine in the top 500. Continued investment in high-performance computing infrastructure in GPU and CPU architectures is essential to enable the multiscale simulations required for future breakthroughs. This investment should include a joined-up approach between UKSA and STFC so that development of exascale HPC systems supports the compute requirements that fall under both STFC and UKSA remits.

Equally important is investment in people. There is a clear need for dedicated training programmes in high-performance computing (on both GPU and CPU architectures) and machine learning techniques will ensure that early-career researchers develop the expertise needed to fully exploit emerging computational approaches. Strengthening the national cohort of Research Software Engineers is another key priority, providing the specialist expertise needed to optimise codes for new architectures, maintain software, and support scalable, long-term modelling efforts. Funding for early career researchers is required so that we can develop and retain the skill base we require.

Significant funding for fundamental theory, numerical methods, and code development is also crucial to maximise progress in this area. This funding should also include important support for the long-term development and maintenance of codes as well as data storage and accessibility.

Support to allow modelling to be effectively integrated into mission planning and development, both so that modelling can support instrument development and that the modelling tools are ready to aid interpretation at first light of an instrument. Numerical modelling creates a huge volume of data, but there needs to be investment in the storage and accessibility of this data to maximise the return from the investment made both into model development and the missions that connect with the modelling. This modelling work cannot be performed without high-quality atomic data, which must be calculated through, e.g. R-matrix calculations or measured as laboratory spectra. The SAMS project will perform some theoretical calculations, but laboratory data underpins our interpretation of radiation from a vast number of astrophysical sources, and cannot be ignored.

UK leadership and capability

The UK is world-leading in the theory and numerical modelling of magnetic field generation and interior dynamics in the Sun. This strength is underpinned by a network of internationally recognised research groups, including those at Durham, Edinburgh, Exeter, Glasgow, Leeds, Sheffield and Newcastle. These groups are not only advancing fundamental theory but are also at the forefront of developing and applying cutting-edge computational methods, including spectral approaches and contributions to major open-source codes such as Dedalus.

The UK has a long-established history of expertise in the numerical modelling of the Sun's atmosphere and has led development in a number of internationally-renowned codes (e.g. LareXd [46], GLoVaG [47,48], SAC [49], PIP [50,51]). The UK's commitment to such projects was recently re-emphasised by the funding of the SAMS; an ambitious project across four UK universities to develop an open-source next-generation code for modelling the Sun's atmosphere. This project will leverage the UK's numerical and technical expertise to implement state-of-the-art modelling techniques. This investment will push the UK to the forefront of solar atmospheric modelling with cutting-edge capabilities in simulating radiative transfer and non-equilibrium ionisation. The SAMS project is inherently community-driven and will reflect the evolving priorities of UK solar physicists.

The UK's position in radiative transfer modelling is advancing rapidly thanks to projects such as SAMS, which are connecting development in radiative transfer modelling with modelling of dynamics. This builds on expertise in developing an accessible and open-source framework for traditional radiative transfer techniques [52], along with recent pioneering efforts in GPU-accelerated non-LTE radiative transfer [53,54] building on cross-disciplinary knowledge exchange with the field of computer graphics. This development is complemented by the UK's world-leading status in the calculation and provision of atomic data for astrophysics, an area that, together with atomic modelling and laboratory astrophysics, is now continued at Cambridge by Del Zanna. This effort underpins some of the SAMS developments and several space missions (at their proposal or analysis stage).

The UK has established excellence in numerical modelling of the interactions of the solar wind with the Earth, through projects such as the NERC RadSat highlight topic, and the £20M SWIMMR programme. The group at the University of Lancashire has developed new approaches to SEP modelling [29] and these have been incorporated into Space Weather forecasting tools, including real-time SEP forecast tools and in-progress ground-level enhancement (GLE) forecast capability [55,56]. The UK has long-standing expertise at multiple institutions in kinetic plasma simulations used to study shock waves (HYPSI code [32,57]) and turbulence (CAMELIA code [33]). These simulations have provided strong support for the mission proposal of Plasma Observatory in the current ESA M7 call, highlighting their timeliness and leadership in the field.

Alongside the great numerical expertise present in the UK, there is a growing connection with international heliospheric missions. The UK has long-standing capability in solar/heliophysics instrumentation and observation, as is exemplified by the Mullard Space Science Laboratory at UCL, RAL Space and recent leading involvement in ESA missions. These partnerships facilitate the integration of modelling with real data, enabling validation, synthetic observables, and mission support. The convergence of observational, computational, and instrumental expertise means the UK can be a hub for model-to-observation validation for the global community.

Partnership Opportunities

There is a long-established partnership with the UK Met Office in space weather research. This gives scope to develop partnerships with space weather forecasting teams throughout the world. There is also the potential developing industrial partnerships, for example with EDF, in this space.

Space missions are typically multinational, multi-agency developments. Through the ESA subscription, the UK plays a central role in current ESA led missions, e.g. Solar Orbiter, but has involvement in other agency missions, either through ESA Missions of Opportunity, or bilateral agreements. Future opportunities for the UK modelling community to support UK hardware roles in missions in development or being proposed, include SOLAR-C (ESA, MoO, JAXA/NASA) [15], SPARK (ESA) [39], MESOM (UK, Australia, NASA) [58]; and ground-based facilities (SAMNet, EST) or industry (magneto-optical filters).

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