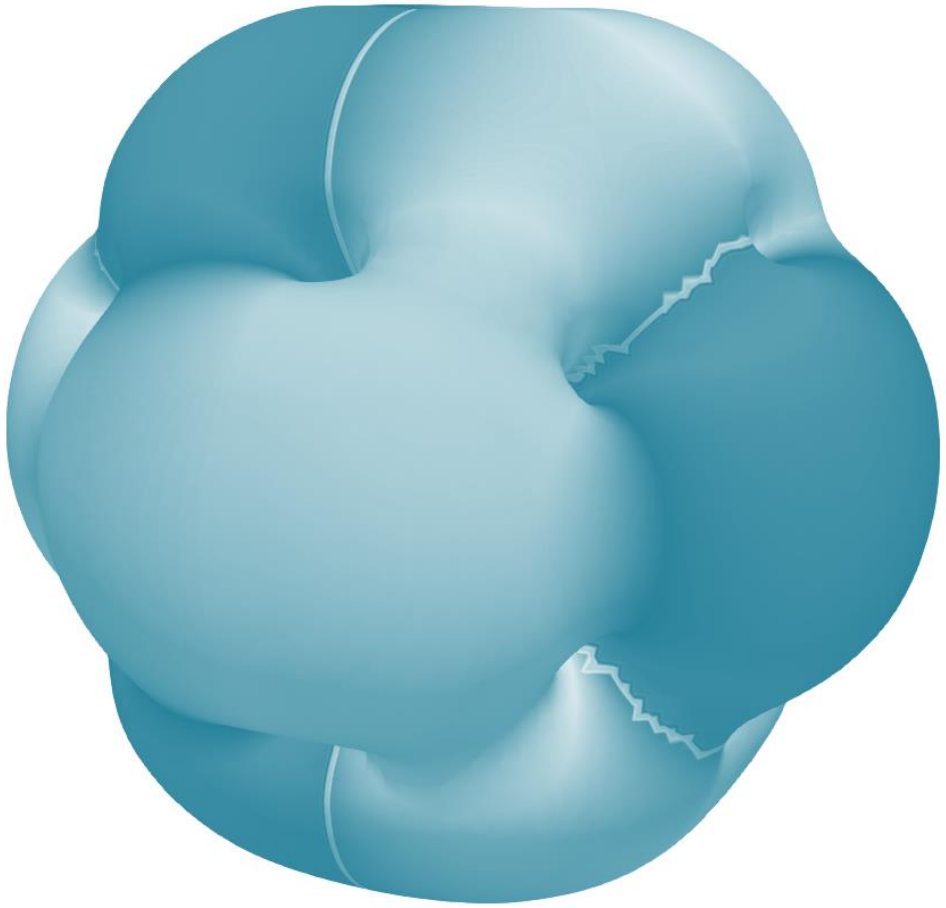
Prism

Platform for Research in Simulation Methods



The PRISM team are leading experts in developing advanced numerical methods for industrial, environmental and biomedical applications.

Report
May 2020 - December 2021

Imperial College London

UNIVERSITY OF OXFORD

UKRI Engineering and Physical Sciences Research Council

KING'S College LONDON

ABOUT US

ABOUT US

Highlights

Communication

86
Published journal articles

36
Website updates

3
Impact and case studies

Collaboration

The **UK Met Office** uses **Firedrake** as the principal dynamics prototyping platform for its next generation weather and climate simulation system.

McLaren Formula 1 Racing and **Rolls Royce** use **Nektar++** to guide their race car and engine design, respectively.

DUG Technologies Ltd uses **Devito** in production. DUG provides seismic imaging services to the oil and gas industry.

Zenotech has added a flux reconstruction solver based on **PyFr** to its proprietary zCFD codebase, complementing the existing finite volume solver.

Networking

£30.5M
Leveraged funding

8
Events and activities organised by the PRISM community.

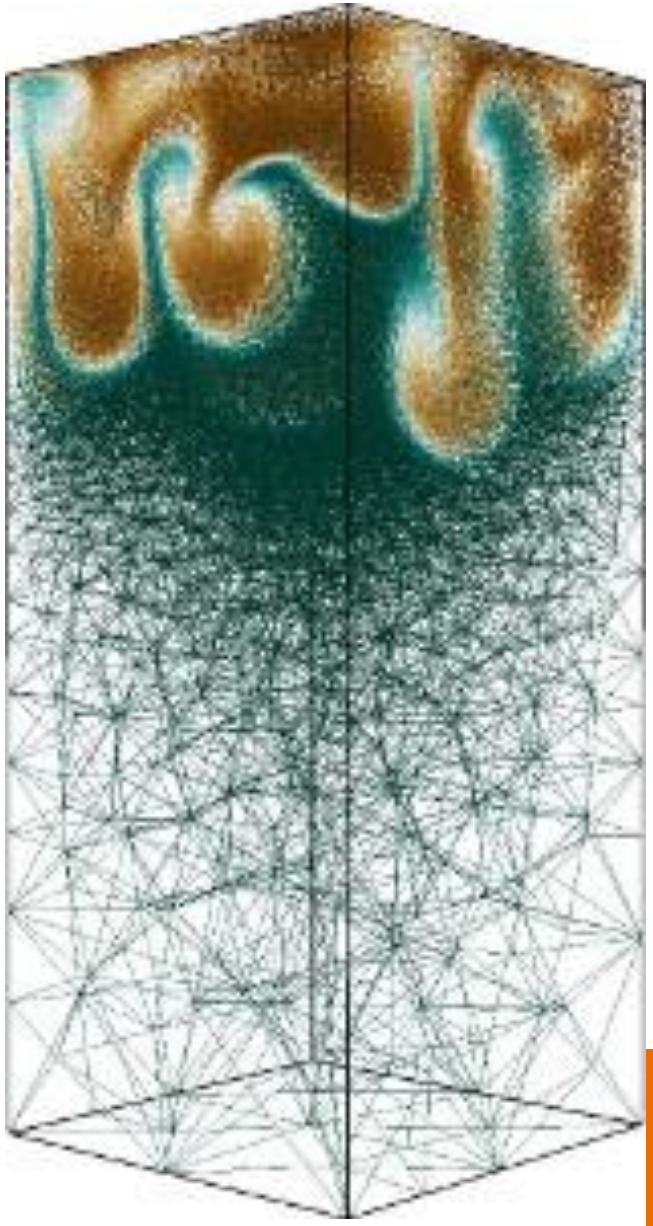
~150 Groups in 23 countries using our software with notable activity in UK, China and US.

5
Software updates

3
New funded PRISM projects

ABOUT US

PRISM Mission



The aim of the renewed platform is to build on the success of our first Platform Grant, to extend our impact further, and to extend the impact beyond simulation by delivering software tools that answer the science and engineering questions that underpin what users and applications collaborators really need.

Impact through people: The nature of a Platform Grant is that we focus on people, and on the support mechanisms that can be provided to enable them to succeed in pursuing not only the research plans we have now, but also the opportunities that emerge as the work of the group progresses. Scientific computing has been recognised by EPSRC as a “critical and valuable resource” via the Research Software Engineer program. We continue to furnish highly trained researchers in this field. In addition to the researchers directly supported by the grant, we are also able to influence the wider community of PhD and MSc students at Imperial, Oxford and King's College London who benefit from the sustained critical mass of expertise that this funding enables and the open-source codes we distribute.

As a result, a large body of individuals is being deployed to industry and academia with a deep appreciation of the possibilities of computational modelling and the expertise to exploit them. Finally, we have previously mentioned Prof. Sherwin’s role as Director of Research Computing Service at Imperial College which spans all faculties and departments. This complementary activity continue to grow and has recently appointed Dr Jeremy Cohen, a central member of our team, to the leadership team as the Director of Research Software Engineering Strategy.

Impact through open software: We strive to develop robust software that enables us to achieve academically excellent advances as well as publish these advances so that they can influence and be adopted by others, working on different codes. We empower new applications based on automated simulation capability, incorporating new methods and new technologies, embodied in open-source software.

Impact through widening engagement: We will continue to engage with users of our tools, and to develop applications projects and collaborations that realise the benefits of the technology we develop.

Multiphase flow

ABOUT US

PRISM at a Glance

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COLLABORATIVE SITES

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PRINCIPAL INVESTIGATORS

8
SOFTWARE PROJECTS DEVELOPED

Our Locations

UNIVERSITY OF OXFORD
MATHEMATICAL INSTITUTE

Imperial College London

IMPERIAL COLLEGE LONDON:

- DEPARTMENT OF AERONAUTICS
- DEPARTMENT OF MATHEMATICS
- DEPARTMENT OF COMPUTING
- DEPARTMENT OF EARTH SCIENCE AND ENGINEERING

KING'S College LONDON
DEPARTMENT OF ENGINEERING

ABOUT US

Platform for Research in Simulation Methods

Our Available Software

DEVITO	FIREDRAKE	FLUIDITY	NEKTAR++
A Domain-specific Language (DSL) and code generation framework for the design of highly optimised finite difference kernels for use in inversion methods.	A compiler for a domain-specific language for the finite element methods, that uses runtime code generation (via PyOP2) to deliver performance portability across CPUs and GPUs.	An open source, general purpose, multi-phase computational fluid dynamics code capable of numerically solving the Navier-Stokes equation and accompanying field equations on arbitrary unstructured finite element meshes in one, two and three dimensions.	A tensor product based finite element package designed to allow one to construct efficient classical low polynomial order h-type solvers (where h is the size of the finite element) as well as higher p-order piecewise polynomial order solvers.
https://www.devitoproject.org/	https://www.firedrakeproject.org/	http://fluidityproject.github.io/	https://www.nektar.info/
OPENTIDALFARM	**PYFR**	**PYOP2**	**THETIS**
OpenTidalFarm is an open source tidal modelling framework which utilises a range of array, turbine and wake parameterisations with advanced optimisation algorithms in order to design large tidal turbine arrays that maximise power or profit, and/or minimise environmental impacts.	An open-source framework for solving advection-diffusion type problems on streaming architectures using the flux reconstruction approach.	A framework for performance-portable parallel computations on unstructured meshes.	Unstructured mesh coastal ocean model in 2D and 3D, built using Firdrake and including adaptive mesh and adjoint capabilities.
https://opentidalfarm.readthedocs.io/en/latest/	http://www.pyfr.org/	https://github.com/OP2/PyOP2	https://thetisproject.org/

ABOUT US

Executive Summary

THE PRISM PURPOSE

In 2020, COVID-19 created disruption and uncertainty, but it also made it abundantly clear that everything in the world is truly interconnected and more than ever research needs to be adaptable, relevant, and resilient to thrive. For a scientific project to be successful in the long-term, its purpose needs to go beyond short-term stakeholder profit.

EXECUTING OUR MISSION

The period since our last report has clearly been dominated by the emergence of COVID-19 and the associated disruption at so many levels. The flexibility of the PRISM funding has been extremely useful in underpinning our combined research efforts providing essential bridging and underpinning funds whilst travel and visits have obviously been highly restricted.

Nevertheless, there have also been unexpected benefits most notably in virtual communication allowing opportunities for rapid and flexible workshops that you will see we have utilised. We are however very pleased to have just hosted in January an in-person PRISM workshop to allow researchers from all institution to interact and collaborate.

We have also continued to push forward delivering world class research software and engaging with industry through our multi-institute platform as is highlighted in the following report.

GROWING OUR DIVERSE TEAM

Finally, we continue to embrace the growth of our interdisciplinary team. Following the promotion of Prof Cotter and Peiro in 2019 we were pleased to celebrate the promotion to Reader of David Moxey and David Ham as well as the appointment of one of our supported research Jemma Shipton as a lecturer at Exeter.

THE PRISM' GOAL:

DELIVERING SOFTWARE TOOLS THAT ANSWER THE SCIENCE AND ENGINEERING

PROF SPENCER SHERWIN
PRISM's Principal Investigator

ACTIVITIES

THE PRISM ACTIVITIES

The following pages of the report include detailed information on PRISM activities in the period between May 2020 - December 2021

The PRISM team are leading experts in developing advanced numerical methods for industrial (multiphase flows and nuclear engineering, train aerodynamics, flow control, road and racing car aerodynamics, marine renewables), environmental (ocean modelling, numerical weather prediction, coastal engineering) and biomedical (cardiovascular flows, electrophysiology modelling in the heart, image registration) applications.

Our team draws together expertise in designing, analysing and implementing sophisticated finite element methods, deploying these methods in a broad range of industrial, biomedical and environmental applications, and developing software tools that deliver portable parallel performance. They form the UK's largest group of experts in developing finite element methods and software, with international reputations in high-order methods, adaptivity, mesh generation. Combining these aspects allows simulations of highly complex multiscale problems that are otherwise inaccessible on available computational resources, leading to new capabilities across a broad range of engineering applications.

The work of the PRISM team is focused on agile synthesis of modelling techniques: flexibly selecting a combination of discretization method, polynomial order, mesh, equation assembly algorithm, linear/nonlinear equation solver etc. to meet application-driven problem requirements and to match available hardware.

PRISM run regular training events and user and research workshops.

Technology made it possible for PRISM to rapidly transfer to teleworking for their staff. Standalone video conferencing programs like Zoom, virtual productivity suites like Microsoft Teams allowed PRISM team to efficiently work from home while collaborating with others.

Exclusively organised by entire PRISM team

3rd PRISM Workshop on Application of Time-Stepping Techniques
Date: 26th February 2021
In this workshop we shared experiences on application of time-stepping techniques, for example parallel time integration, encapsulation of time integration and implicit time integration.
The event's programme included:
3.00pm-3.15pm Scott MacLachlan (Memorial University of Newfoundland) on Parallel time integration
3.20pm-3.35pm Rob Kirby (Baylor University) on Encapsulation of time integration Encapsulation of time integration
3.40pm-3.55pm Zhenguo Yan (Imperial College London) on Implicit time integration Implicit time integration
4.00pm-4.30pm Group discussions
4.30pm-4.45pm Summary

2nd PRISM workshop on applications: Beyond CFD
Date: 30 September 2020
In this workshop we wish to share experiences on application of PDE solvers which go beyond CFD tools, for example composable solvers, stability analysis, inverse problems, data assimilation and uncertainty quantification.
The event's programme included:
2.00pm-2.15pm Matt Knepley (University at Buffalo) on "Building Complex Solvers in PETSc"
2.15pm-2.30pm Patrick Farrell (University of Oxford) on "Computing multiple solutions of PDEs"
2.30pm-2.45pm Koki Sagiyama (Imperial College London) on "Firedrake: Solving equations on subspaces "
2.45pm-3.30pm Small group discussions/Panel meeting
3.30pm-3.45pm Summary session

THE PRISM ACTIVITIES
LIST OF EVENTS *CONTINUES*

1st PRISM workshop on best practices for software training and workshops: Exploring online teaching in a post-pandemic era!
Date: 21st May 2020
Location: on-line
Summary: In this workshop we wish to share experiences and best practices on the use of workshops and tutorials for the PRISM related software. In light of the currently changes due to the Covid-19 pandemic it is also interesting to ask how our training experiences are likely to change at a broader level including all forms of remote teaching. The format of the on-line workshop will involve a series of 3 or 4 short 10-minutes talks followed by small group discussions and a summary session.
The programme includes presentations by:
2.00pm-2.15pm David Ham on Firedrake
2.15pm-2.30pm Spencer Sherwin / David Moxey on Nektar ++
2.30pm-2.45pm Matt Piggott / Gerard Gorman on Jupiter notebook
2.45pm-3pm Katerina Michalickova on Software Carpentry
3pm-4pm Brainstorming session on establishing best practices.

PRISM led events received excellent feedback from the audience. An example is provided below:

"Thanks for inviting me to the PRISM workshop, I found it very interesting, the topics and discussion was quite informative and interesting to me. It would be great if I can attend similar events in future, particularly those related to Nektar++."

Workshops organised by individual development teams

5th Nektar++ Workshop
13-15 Date: December 2021
The 5th annual Nektar++ Workshop brough together developers and users of all experiences to hear about new and future developments in Nektar++ and the exciting science and engineering being undertaken with the code. As part of this year's workshop PRISM also offered some introductory training on spectral/hp element methods and high order meshing as part of the ITN on Stability and Sensitivity Methds for Flow Control and Industrial Design (SSeCoID). The workshop was organised remotely. The main talks were run in the afternoons (GMT) to allow as many remote attendees to join as possible across different time zones. The three day event included a comprehensive programme of talks and training sessions.
The main workshop was followed by parallel informal group sessions allowing developers and users to discuss and work on specific aspects of the code and influence the future direction of Nektar++. Further information on the event is provided here.

PyFR Seminar Series
The series comprises invited talks on a range of topics related to the theory of high-order Flux Reconstruction schemes, their implementation in the PyFR (www.pyfr.org) flow solver, and their application to industrially relevant flow problems. The overarching objective of the series is to help bridge the gap between academic research activities and real-world industrial requirements. Further information on this Seminar Series is available here.

The PyFR Symposium 2020
The PyFR Symposium 2020 comprised talks from industry and the PyFR team on a range of topics related to the theory of high-order Flux Reconstruction schemes, their implementation in PyFR, and their application to industrially relevant flow problems. The overarching objective of the symposium was to help bridge the gap between industrial requirements and academic research activities.

5th Firedrake Workshop 2021
Date: 15-17 September 2021
The fifth Firedrake user and developer workshop was held online.The workshop was an opportunity for Firedrake users and developers to engage with each other to communicate the ways that Firedrake can be used in simulation science, the latest developments in the project, and the future developments anticipated. The event provided Firedrake users with the opportunity to interact directly with developers and other users.
Programme:
The full programme is available here: on EasyChair.
The recorded talks are available on Vimeo.

THE PRISM ACTIVITIES
LIST OF EVENTS *CONTINUES*

An active participation at the events organised by another organization

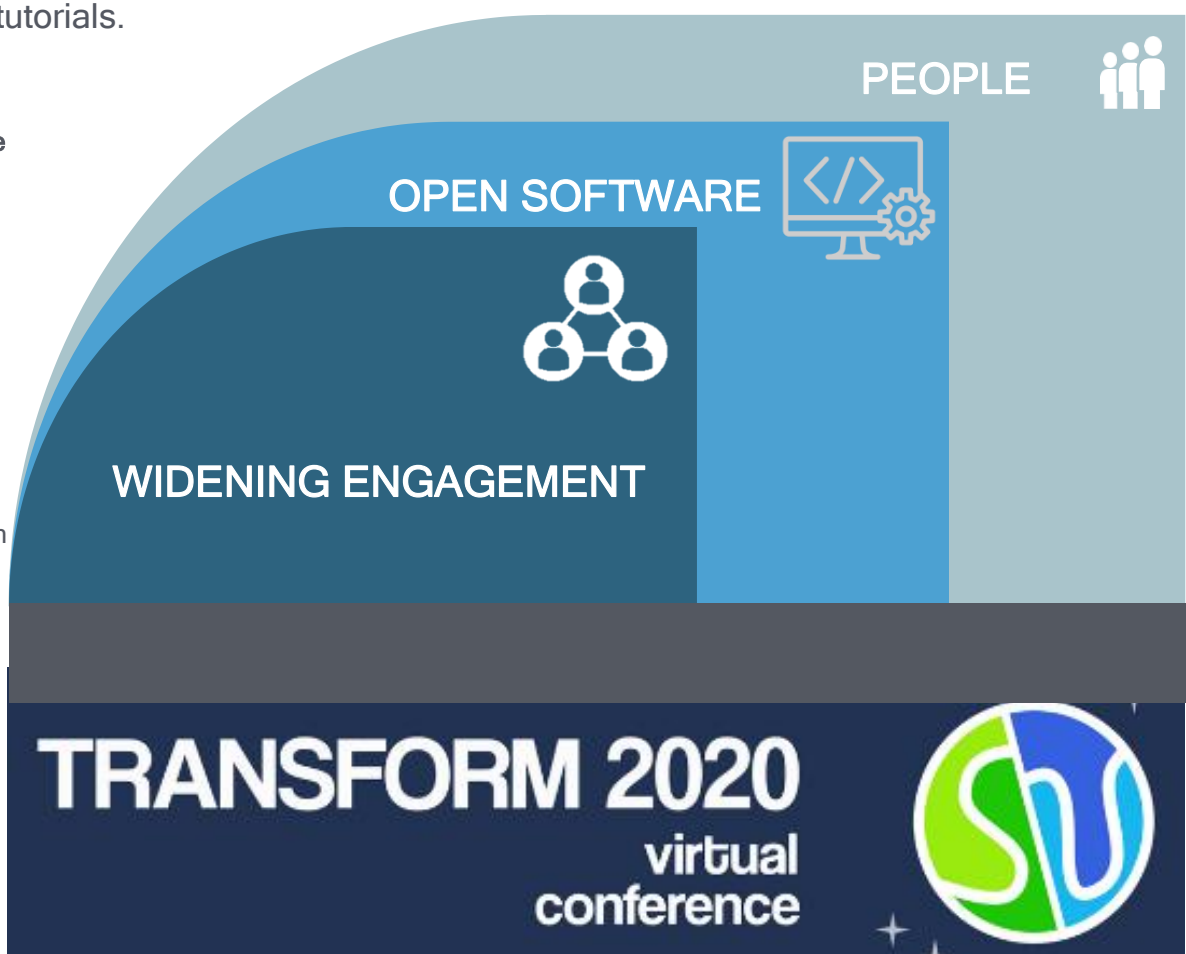
This prepares staff members to adopt their software naturally to the needs of different communities.

The below summarizes an active participation of PRISM team members at community level, through organization of mini-symposium and tutorials.

Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-16)
Date: 6 - 10 September 2021
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-16) took place in Germany. This conference was devoted to all numerical aspects of time-dependent differential equations and differential-algebraic equations. PRISM's team member, **Colin Cotter**, organised mini-symposum during this event which was dedicated to "Fluid dynamics: innovative discretisations and algorithms". Further information is available here.

Participation in the the Software Underground's annual virtual conference TRANSFORM!
The first global, virtual TRANSFORM took place in September 2020 (TRANSFORM 2020: Schedule). The Software Underground brought lots of interesting and useful sessions on the digital subsurface. This event was a bit different from most conferences: the sessions were fully participatory and interactive.
Rhodri Nelson from Imperial College London gave a tutorial on "Geophysical Modeling with Devito" which can be seen in full here: Tutorial: Geophysical Modeling with Devito – YouTube
In the following year, in April 2021 another Transform 2021 event took place. A week-long celebration of open subsurface code and data included a hackathon, 21 tutorials, 20 lightning talks, and an annual general meeting. The heart of the conference week itself was the 21 amazing tutorials including the one from Devito team: Tutorial: Synthetic seismic models with GemPy, Devito, and Pyvista.

PRISM impact through



THE PRISM ACTIVITIES
LIST OF EVENTS *CONTINUES*

Nuclear Institute Evening talk: Can Nuclear Modelling Techniques Help National Efforts to Combat COVID-19?
Date: 28 September 2021
Presenters: **Christopher Pain, Paul Smith**
Further details are available here

Chongqing University
Date: 2 June 2021,
Christopher Pain and Fangxin Fang presented an invited talk entitled "CFD, reduced-order models and neural networks for Urban and Indoor flows: Results from INHALE, MAGIC, PREMIERE consortia"

Fluids & AI modelling methods and applications, Computational Fluid Dynamic and Artificial Intelligence Workshop 2021,
Shanghai University,
Date: 30 August 2021
Presenters: **Christopher Pain**

The ANSWERS Seminar
Date: 9-11 November 2021
The ANSWERS Seminar is the annual get-together of ANSWERS customers and staff associated with the development and use of ANSWERS software products.
The three-day event covered radiation shielding, reactor physics and nuclear criticality topics including presentations on recent software developments and applications of ANSWERS software to practical problems.
Christopher Pain was an invited speaker and introduced to the audience the following topic: "Trends in nuclear modelling: fluids, solids, coupling and AI"
https://www.answerssoftwareservice.com/seminar.html

The 9th edition of the International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2021)
Date: 14 - 16 June 2021
Spencer Sherwin gave a plenary lecture on "The thick strip method for slender body fluid structure interaction"
The objectives of COUPLED PROBLEMS 2021 were to present and discuss state of the art, mathematical models, numerical methods and computational techniques for solving coupling problems of multidisciplinary character in science and engineering. The conference goal was to make step forward in the formulation and solution of real life problems with a multidisciplinary vision, accounting for all the complex couplings involved in the physical description of the problem.
The conference was one of the Thematic Conferences of the European Community on Computational Methods in Applied Sciences (ECCOMAS) and a Special Interest Conference of the International Association for Computational Mechanics (IACM). It is also supported by other scientific organizations in Europe and worldwide.

10th International Conference on Sustainable Development in the Building and Environment (SuDBE2021)
Date: 4-7 November 2021.
The aim of this event is to encourage academics, designers and engineers, policy-makers to share the most up-to-date research outcomes and practical experience in green buildings and low-carbon eco-cities.
Christopher Pain was talking about "Multi-physics and multi-scale adaptive mesh AI-modelling for the urban environment"
http://www.sudbeconference.com/

SIAM Conference on Mathematical & Computational Issues in the Geosciences
Date: 21-24 June
https://www.siam.org/conferences/cm/conference/gs21
This is the meeting of the SIAM Activity Group on Geosciences.
Christopher Pain presenting at conference aimed to stimulate the exchange of ideas among geoscientific modelers, applied mathematicians, statisticians, and other scientists, fostering new research in the mathematical foundations with an impact on geoscience applications.

THE PRISM ACTIVITIES

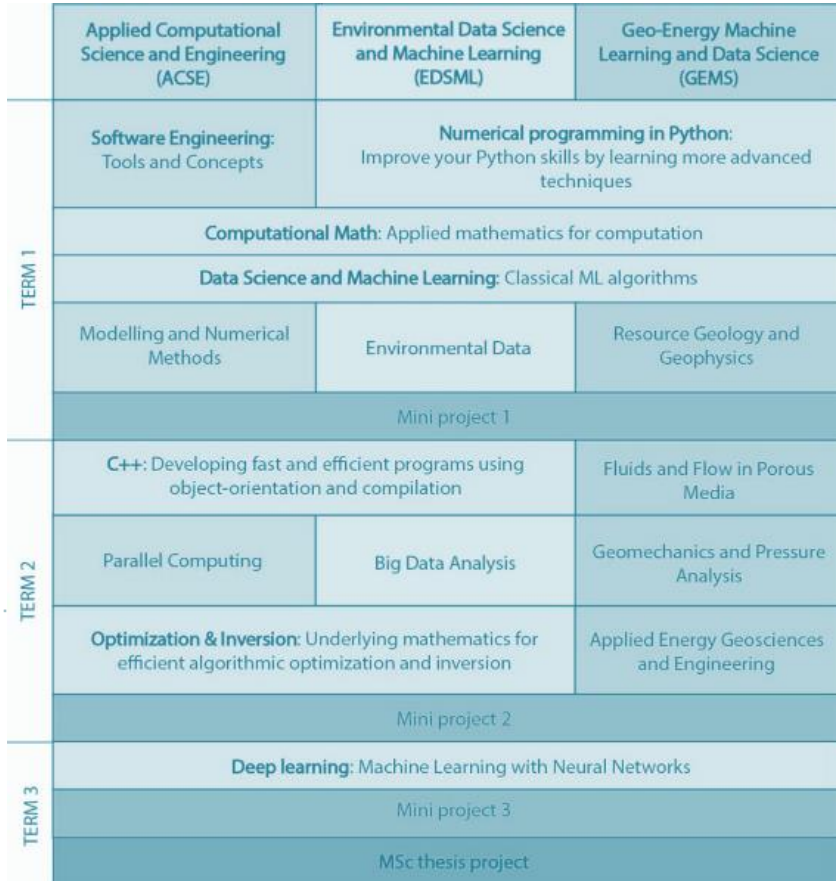
This project has resulted in the development of new training opportunities and materials to rain students in fundamental computational and data science skills.

Development of new training opportunities and resources

New MSc Programme started in October 2021: This programme focuses on Environmental Data Science and Machine Learning MSc. PRISM's PI **Matt Piggott** is a Director of this programme. The MSc Environmental Data Science and Machine Learning at Imperial College London will train students in fundamental computational and data science skills for application across the environmental sciences.

The course is led by expert computational scientists in the Department of Earth Science and Engineering. The programme offers a focus on environmental big data in addition to established modules in machine learning, computational science and modern programming skills that run in the Applied Computational Science and Engineering MSc. Graduates of this course will be well placed to fill the significant market demand for those with applied, hands-on computational and data science experience.

Many of the skills you learn are applicable broadly across all of science and engineering and so potential career paths are hugely diverse. The additional knowledge of environmental science and associated engineering solutions you will be exposed to in this course will make you particularly attractive to anything from relatively small environmental and engineering consultancies to large multi-national organisations including those in the energy and big tech sectors.

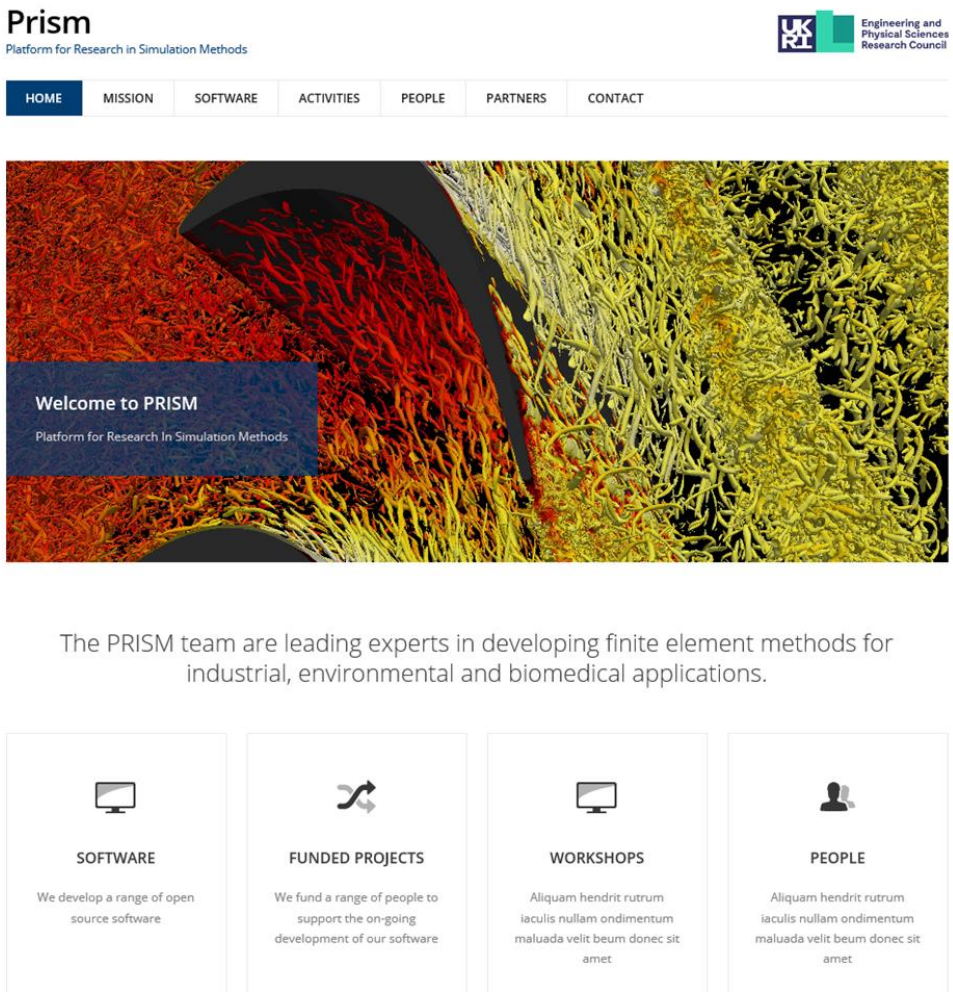


Devito Book Summer Project with Imperial College London: Great work by Rini Banerjee, a student of Joint Mathematics and Computer Science at Imperial College London who spent summer 2020 doing a remote research internship on the Devito Project, under the supervision of **Paul Kelly** and **Gerard Gorman**. Rini has been working on the Devito Book: a set of Jupyter Notebook tutorials that teach the finite difference method for solving partial differential equations using Devito, based on the textbook "Finite Difference Computing with PDEs – A Modern Software Approach" by H. P. Langtangen and S. Linge. More information can be found here: Devito Book Summer Project with Imperial College London – Microsoft Tech Community.

THE PRISM ACTIVITIES

Wider dissemination

The project website represents a reference point for partners, stakeholders and public audience who want to get informed on project activities and results. The PRISM website is hosted on the following URL: https://prism.ac.uk/.



REGULAR WEBSITE UPDATES

1	Blog items
1.1	The wake passing effect in LPTs with Nektar++
1.2	Research Software Engineering
1.3	Impactful PRISM research
2	Awards and promotions
2.1	ECCOMAS Prandtl Medal
2.2	Whitehead Prize
3	Events
3.1	5th Nektar++ Workshop 2021
3.2	5th Firedrake Workshop 2021
3.3	PyFR Symposium 2020
3.4	PRISM workshop on best practices for software training and workshops

The website has become an important tool for the project's interaction with the public and so a determined effort is made to present information in a manner that can be understood by members of the public. The portal also publicise opportunities for public and stakeholder participation in the project's events and activities as well as related events, calls, conferences and activities.

The PRISM team is committed to making its website accessible in accordance with the Public Sector Bodies (Websites and Mobile Applications) (No. 2) Accessibility Regulations 2018 and is partially compliant with the Web Content Accessibility Guidelines version 2.1 AA standards.

THE PRISM ACTIVITIES

Publications

Each project partner ensures that results are published in peer reviewed scientific publications. List of PRISM publications is presented below:

1. Gianmarco Mengaldo, David Moxey , Michael Turner, Rodrigo Costa Moura, Ayad Jassim, Mark Taylor, Joaquim Peiró , and Spencer Sherwin (2021). Relevant Implicit Large-Eddy Simulation of a High-Performance Road Car via Spectral/hp Element Methods. SIAM Review, Volume 63, Issue 4.
DOI
2. Cooke E, Mughal S, Sherwin S, Ashworth R, Rolston S. (2022). Destabilisation of Stationary and Travelling Crossflow Disturbances Due to Forward and Backward Facing Steps over a Swept Wing. IUTAM Laminar-Turbulent Transition - 9th IUTAM Symposium, London, UK, September 2-6, 2019. (pp. 713-723).
DOI
3. Pan W, Kramer S, Piggott M. (2021). A σ -coordinate non-hydrostatic discontinuous finite element coastal ocean model. Ocean Modelling,
DOI
4. Clare M, Percival J, Angeloudis A, Cotter C, Piggott M. (2021). Hydro-morphodynamics 2D modelling using a discontinuous Galerkin discretisation. Computers & Geosciences,
DOI
5. Arshad M, Rowland EM, Riemer K, Sherwin SJ, Weinberg PD. (2021). Improvement and validation of a computational model of flow in the swirling well cell culture model.. Biotechnology and bioengineering,
PubMed DOI
6. Basso R, Hwang Y, Assi G, Sherwin S. (2021). Instabilities and sensitivities in a flow over a rotationally flexible cylinder with a rigid splitter plate. Journal of Fluid Mechanics,
DOI

Recently, PRISM's team article published and featured on cover of SIAM Review.

THE PRISM ACTIVITIES

LIST OF PUBLICATIONS *CONTINUES*

7. Hossain M, Cantwell C, Sherwin S. (2021). A spectral/ hp element method for thermal convection. International Journal for Numerical Methods in Fluids, DOI
8. Pan Y, Yan Z, Peiró J, Sherwin S. (2021). Development of a Balanced Adaptive Time-Stepping Strategy Based on an Implicit JFNK-DG Compressible Flow Solver. Communications on Applied Mathematics and Computation, DOI
9. Wang R, Wu F, Xu H, Sherwin S. (2021). Implicit large-eddy simulations of turbulent flow in a channel via spectral/ hp element methods. Physics of Fluids, DOI
10. Farrell P, Gatica L, Lamichhane B, Oyarzúa R, Ruiz-Baier R. (2021). Mixed Kirchhoff stress-displacement-pressure formulations for incompressible hyperelasticity. Computer Methods in Applied Mechanics and Engineering, DOI
11. Clare M, Piggott M, Cotter C. (2021). WITHDRAWN: Assessing erosion and flood risk in the coastal zone through the application of multilevel Monte Carlo methods. Coastal Engineering, DOI
12. Yan Z, Pan Y, Castiglioni G, Hillewaert K, Peiró J, Moxey D, Sherwin S. (2021). Nektar++: Design and implementation of an implicit, spectral/ h p element, compressible flow solver using a Jacobian-free Newton Krylov approach. Computers & Mathematics with Applications, DOI
13. Buscariolo F, Assi G, Sherwin S. (2021). Computational study on an Ahmed Body equipped with simplified underbody diffuser. Journal of Wind Engineering and Industrial Aerodynamics, DOI
14. Lahooti M, Palacios R, Sherwin S. (2021). Thick Strip Method for Efficient Large-Eddy Simulations of Flexible Wings in Stall. DOI
15. Arshad M, Ghim M, Mohamied Y, Sherwin SJ, Weinberg PD. (2021). Endothelial cells do not align with the mean wall shear stress vector.. Journal of the Royal Society, Interface, 18 (174), pp. 20200772 PubMed DOI
16. Mariscal-Harana J, Charlton PH, Vennin S, Aramburu J, Florkow MC, van Engelen A, Schneider T. Alastruey J. (2021). Estimating central blood pressure from aortic flow: development and assessment of algorithms. American journal of physiology. Heart and circulatory physiology, 320 (2), pp. H494-H510 PubMed DOI
17. Tůma K, Rezaee-Hajidehi M, Hron J, Farrell P, Stupkiewicz S. (2021). Phase-field modeling of multivariant martensitic transformation at finite-strain: Computational aspects and large-scale finite-element simulations. Computer Methods in Applied Mechanics and Engineering, DOI
18. Adler J, Benson T, Cyr E, Farrell P, MacLachlan S, Tuminaro R. (2021). Monolithic Multigrid Methods for Magnetohydrodynamics. SIAM Journal on Scientific Computing, DOI
19. Boullé N, Charalampidis E, Farrell P, Kevrekidis P. (2020). Deflation-based identification of nonlinear excitations of the three-dimensional Gross-Pitaevskii equation. Physical Review A, DOI
20. Baker A, Craighead R, Jarvis E, Stenton H, Angeloudis A, Mackie L..... Hill J, (2020). Modelling the impact of tidal range energy on species communities. Ocean & Coastal Management, DOI
21. Spencer J. Sherwin, (2020). Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2018. External Link
22. Reavette RM, Sherwin SJ, Tang M, Weinberg PD. (2020). Comparison of arterial wave intensity analysis by pressure-velocity and diameter-velocity methods in a virtual population of adult subjects.. Proceedings of the Institution of Mechanical Engineers. Part H, Journal of engineering in medicine, 234 (11), pp. 1260-1276 PubMed DOI
23. Buscariolo F, Sherwin S, Assi G, Meneghini J. (2020). Spectral/hp Methodology Study for iLES-SVV on an Ahmed Body. Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2018 - Selected Papers from the ICOSAHOM Conference, London, UK, July 9-13, 2018. (pp. 297-311). DOI

THE PRISM ACTIVITIES

LIST OF PUBLICATIONS *CONTINUES*

24. Charalampidis E, Boullé N, Farrell P, Kevrekidis P, (2020). Bifurcation analysis of stationary solutions of two-dimensional coupled Gross-Pitaevskii equations using deflated continuation. Communications in Nonlinear Science and Numerical Simulation,
DOI
25. Moura R, Aman M, Peiró J, Sherwin S. (2020). Spatial eigenanalysis of spectral/hp continuous Galerkin schemes and their stabilisation via DG-mimicking spectral vanishing viscosity for high Reynolds number flows. Journal of Computational Physics,
DOI
26. Kukreja N, Hückelheim J, Louboutin M, Washbourne J, Kelly P, Gorman G. (2020). Lossy Checkpoint Compression in Full Waveform Inversion.
DOI
27. Farrell P, He Y, MacLachlan S. (2020). A local Fourier analysis of additive Vanka relaxation for the Stokes equations. Numerical Linear Algebra with Applications,
DOI
28. Marcon J, Castiglioni G, Moxey D, Sherwin S, Peiró J. (2020). rp -adaptation for compressible flows. International Journal for Numerical Methods in Engineering,
DOI
29. Alawiye H, Farrell P, Goriely A. (2020). Revisiting the wrinkling of elastic bilayers II: Post-bifurcation analysis. Journal of the Mechanics and Physics of Solids,
DOI
30. Mackie L, Coles D, Piggott M, Angeloudis A. (2020). The Potential for Tidal Range Energy Systems to Provide Continuous Power: A UK Case Study. Journal of Marine Science and Engineering,
DOI
31. Dargaville S, Smedley-Stevenson R, Smith P, Pain C. (2020). Goal-based angular adaptivity for Boltzmann transport in the presence of ray-effects. Journal of Computational Physics,
DOI
32. Xia J, Farrell P, Castro S. (2020). Nonlinear bifurcation analysis of stiffener profiles via deflation techniques. Thin-Walled Structures,
DOI
33. Goss ZL, Coles DS, Piggott MD. (2020). Identifying economically viable tidal sites within the Alderney Race through optimization of levelized cost of energy.. Philosophical transactions. Series A, Mathematical, physical, and engineering sciences, 378 (2178), pp. 20190500
DOI
34. Moxey D, Amici R, Kirby M. (2020). Efficient Matrix-Free High-Order Finite Element Evaluation for Simplicial Elements. SIAM Journal on Scientific Computing,
DOI
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THE PRISM ACTIVITIES

Collaborations

PRISM is involved with regional, national and international collaborations. Academic and industrial users of computational fluid dynamics software benefit from this research since the outputs of the platform give them access to robust performance-portable implementations of advanced methods.

10th year anniversary of the GungHo project

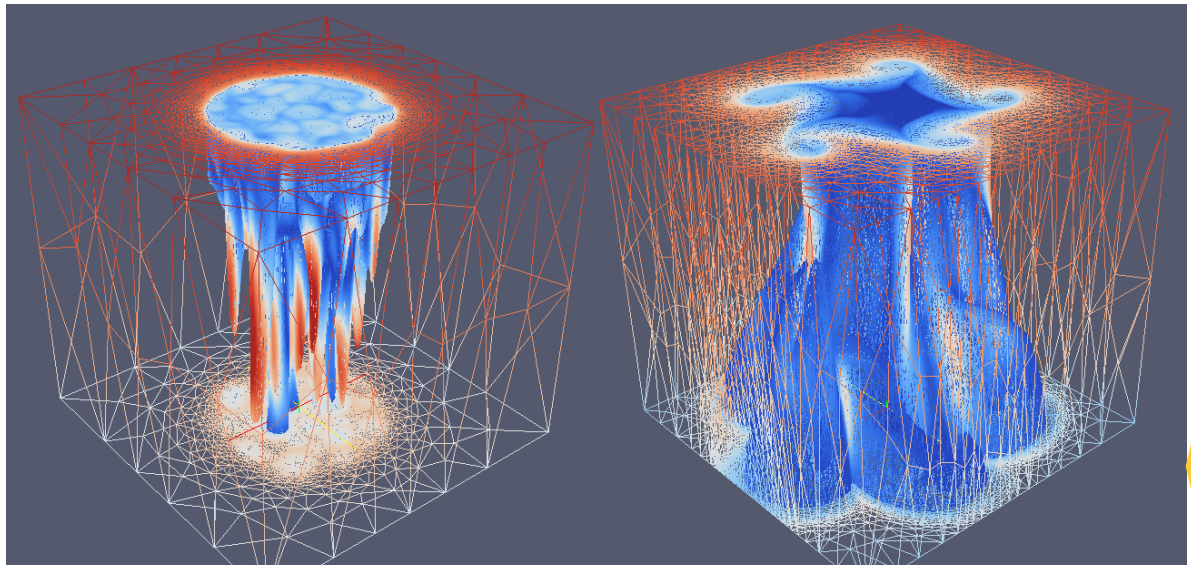
This year is the 10th year anniversary of the GungHo project, a NERC/STFC/Met Office funded project to develop the next generation dynamical core (the resolved fluid dynamics component) for their climate/weather modelling system, which incorporates research by Colin Cotter and David Ham. GungHo has recently started to run its first global weather and climate simulations, as described in the linked article:
https://www.metoffice.gov.uk/research/news/2021/gungho-and-lfric-10th-anniversary

Nektar++ on ARCHER2

The ARCHER2 national supercomputer is a world class advanced computing resource and is the successor to ARCHER. This guide is intended to provide basic instructions for compiling the Nektar++ stable release or master branch on the ARCHER2 system. Compilation instructions are available here: Nektar++ on ARCHER2 - Nektar++

Texas A&M University

New collaboration with Prof Kumbakonam Rajagopal (Texas A&M University). Prof Patrick Farrell started working with Prof Kumbakonam Rajagopal from Texas A&M University on implicitly constituted models in elast



Deep Ocean Convection Fluidity

THE PRISM ACTIVITIES

Funded projects

The PRISM platform provides PDRA funding to support a range of activities within the remit of the grant. This includes: 1-year fellowship; short projects; retention funding. Short projects are intended to provide short-term funding to test and try out ideas in preparation for writing full fellowship or grant applications. PDRAs are invited to apply for funding, in particular to buy out 3-6 months of their time to work on their own projects or to undertake secondments in international labs and industrial companies. An important aspect of this secondment activity is the translation of software so that it can be used robustly and reliably in industry.
A list of projects already funded under PRISM can be found below.

PDRA	Duration	Title	Objective
Mohsen Lahooti	7 months	Implementation of Fluid-Structure Interaction Solver in Nektar++	The end goal of this project of extend the Nektar++/SHARPy FSI solver which is currently under development by the same researcher for VIV of slender structure, to include the more general case of FSI of multi-body and incorporate the effect of rotating frame of reference with applications in simulation of turbomachinery and wind turbines.
Simon Warder	6 months	Multi-scale adjoint tidal and storm surge modelling with Thetis	This project performed further work, testing the applicability of calibrated parameter sets for a broader set of modelling case studies and numerical models. This aspect of the proposed work aimed to increase the impact of Thetis in the wider coastal ocean modelling community.
Christian Jane	3 months	Software Engineer	This short-term project had the objective of strengthening the maintenance/robustness aspects of the computational fluid dynamics software Nektar++, focusing on addressing some of the outstanding software-related issues present in the current version of the code. During this time, Christian has been integrated into the Nektar++ community and has been exposed to the complete continuous integration process.

THE PRISM ACTIVITIES

Software updates

PRISM continued to release software updates to our community in the same manner as we would prior to lockdown.

2021 Software Releases

Nektar++ v5.0.2

Version of Nektar++, v5.0.1, was released on the 21st January 2021.

The latest version of Nektar++, v5.0.2, was released on the 22nd of April 2021. It can be downloaded from the downloads page. This release included a range of bug fixes to the 5.0.1 release. A full list of the changes is available in the CHANGELOG.md file distributed with the source code.

Devito v4.6

Devito v4.2 supports multi-node-multi-GPU domain-decomposition parallelization and became a NumFOCUS affiliated project: https://github.com/devitocodes/devito/releases/tag/v4.2

The latest version of Devito is now at v4.6 https://github.com/devitocodes/devito/releases/tag/v4.6

PyFR 1.12.2

https://github.com/PyFR/PyFR/archive/v1.12.2.zip
Fixed issue with ac-euler solver.
Fixed issue with anti-aliasing and OpenMP backend.
Performance improvements for HIP backend.

Towards Green Aviation with Python at Petascale - Simulations with PyFR on Piz Daint and Titan shortlisted for 2016 Gordon Bell Prize
PyFR

SUSTAINABILITY

SUSTAINABILITY

New and on-going funding opportunities

It is crucial that PRISM uses an understanding of the evolving UK and international sustainability landscape to shape its strategy and manage its impacts accordingly.

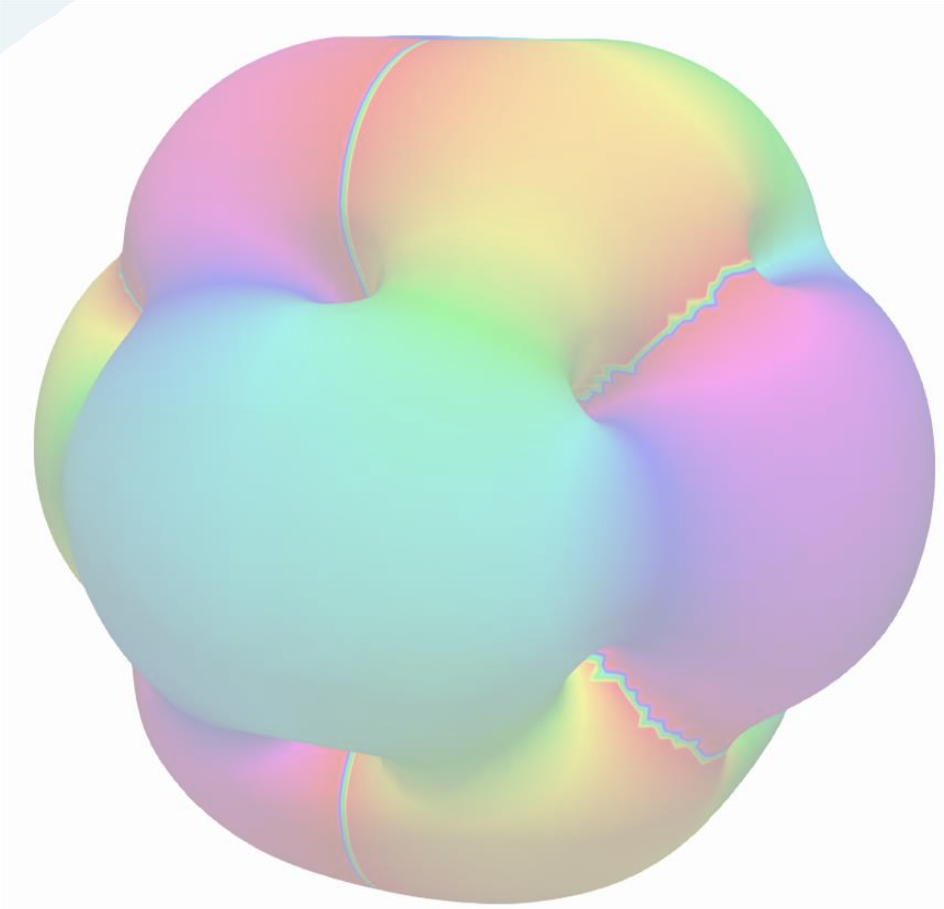
Funding opportunities have been identified and attracted through a number of diverse streams e.g., EPSRC, ERC and ARCHER2 eCSE Programm.

Exploring additional funding opportunities

The PRISM team is seeking additional funding opportunities through **European Research Council** sources. PRISM was pleased to announce an ERC grant award on Stability and Sensitivity Methods for Flow Control and Industrial Design (SSeCoID).SSECOID is Innovative Training Network (ITN) funded by the EU under program the European Union's Horizon 2020 research and innovation programme. SSECOID consists of 11 host institutions (employing Early-Stage Researchers) and 4 partner organizations (offering secondments and training) from seven different countries (Spain, UK, France, Belgium, Germany, Sweden, United States), and from both sectors: academic and industrial. Early Stage Researchers (ESR) employed within the project will undertake individual research projects leading to PhD degree at one of the host institutions. In addition, all the Early-Stage Researchers will benefit from network's training programme. **Prof Spencer Sherwin and Prof Joaquim Peiro** are the Imperial Investigators who are supervising two of the ESRs based at Imperial College London. In addition to that, they are also co-supervising two ERSs that are at **McLaren** (EU contribution for ICL: **~£500K**).

Further ERC grants on-going funding opportunities have been identified:

- EU grant HPCWE (**Prof Sherwin**) ~£300K
- EU grant DJINN (**Prof Sherwin**) ~£300K



Isosurfaces of solutions of the three dimensional nonlinear Schrödinger equation, solved using Firedrake

SUSTAINABILITY
NEW AND ON-GOING FUNDING OPPORTUNITIES *CONTINUES*

EPSRC funding

Principal Investigator	Grant Title	Total Value (£)
Dr Gorman / Prof Pain	• "Managing Air for Green Inner Cities"	4,173,134
Prof Kelly	• "EPSRC Centre for Doctoral Training in High Performance Embedded and Distributed Systems" • "Application Customisation: Enhancing Design Quality and Developer Productivity"	4,081,693 1,263,356
Prof Cotter	• "Parallel-in-time Computation for Sedimentary Landscapes", as part of the Mathematics Small Grant Scheme. • EPSRC Impact Acceleration award • "On the way to the asymptotic limit: mathematics of slow-fast coupling in PDEs" • "ESPRC Centre for Doctoral Training in the Mathematics of Planet Earth"	99,965 25,349 849,609 5,500,000
Prof Piggott	• EPSRC Impact Acceleration award "Multi-scale adjoint-enabled modelling to improve operational storm surge forecasting at the Flood Forecasting Centre (FFC) and support the wider modelling community" • EPSRC iCASE PhD project with **Shell** "Computational / data science techniques to improve and integrate weather forecasting in business decision-making"	66,000 100,000
Prof Farrell	• PhD studentship from the EPSRC Centre for Doctoral Training in Partial Differential Equations	58,000
Prof Pain	• "PREdictive Modelling with QuantIfication of UncERtainty for MultiphasE Systems (PREMIERE)" • "Health assessment across biological length scales for personal pollution exposure and its mitigation (INHALE)" • "JUNO: A Network for Japan - UK Nuclear Opportunities "	6,560,538 2,793,915 488,145
Prof Sherwin	• UK Turbulence Consortium	693,229
Prof Sherwin/ Dr Cantwell	• "Three dimensionality and Instabilities of Leading-Edge Vortices"	450,000
	Total EPSRC contribution	£27M

SUSTAINABILITY
NEW AND ON-GOING FUNDING OPPORTUNITIES *CONTINUES*

ExCALIBUR is a programme within the UK Research and Innovation (UKRI) Strategic Priorities Fund (SPF)

ExCALIBUR is delivering research and innovative algorithmic development to redesign the UK's high priority simulation codes to fully harness the power of future supercomputers across scientific and engineering applications. It is committed to bringing together an unprecedented range of UK domain/subject-matter experts, mathematicians and computational scientists who will identify common issues and opportunities and focus their combined scientific expertise and resources to accelerate toward interdisciplinary solutions.

Prof Cotter is taking part in a successful grant led by **Dr Jemma Shipton (University of Exeter)** The grant has been awarded to study Advanced Parallel in Time Algorithms for Partial Differential Equations, funded by UKRI in a directed call managed by the **Met Office**. The total grant value is £1.15M FEC with £375K FEC allocated to Mathematics at Imperial.
Other recipients of this funding include:

- **Dr Moxey/ Prof Sherwin/Prof Peiro:** ELEMENT - Exascale Mesh Network (Total Value (£): 245K)
- **Dr Moxey/Dr Cantwell/Prof Sherwin**: on "Examining the performance of Nektar++ for fusion applications." (Total Value (£): £252k)
- **Dr Cantwell/Dr Moxey/Prof Sherwin**: on "Solving high-dimensional plasma kinetics using Nektar++" (Total Value (£): £156K)
- **Dr Gorman / Prof Kelly**: Efficient Cross-Domain DSL Development for Exascale (Total Value (£): 430K)
- **Dr Ham/Prof Farrell/Prof Kelly**: ExCALIBUR phase 1b SysGenX: Composable software generation for system-level simulation at exascale (The Imperial/Oxford part grant value ~£1M)
- **Dr Ham/ Dr Vincent/ Prof Kelly / Prof Farrell/ Dr Gorman**: ExCALIBUR working group on Exascale continuum mechanics through code generation. (Total Value (£): 159K)

Total ExCALIBUR contribution for PRISM Principal Investigators

~£2.6M

ARCHER2 eCSE Programme

ECSE PROGRAMME OVERVIEW
Through a series of regular calls, Embedded CSE (eCSE) support provides funding to the ARCHER2 user community to develop software in a sustainable manner to improve research on the ARCHER2 service. The funding allows the employment of a Research Software Engineer (RSE) to carry out software development of ARCHER2 software. This development work may include the implementation of algorithmic improvements, improvements to scalability, portability, sustainability or maintainability, or may include the addition of new functionality to a code which in turn will allow new science to be carried out.

Prof Piggott has been awarded an ARCHER2 eCSE grant to fund a Research Associate (Joe Wallwork) for one year from 1st August 2021 to 31st July 2022. The project is entitled "Goal-Oriented Mesh Adaptation for Firedrake" and will make this advanced discretisation approach available to the Firedrake user community. Goal-oriented mesh adaptation seeks discretisations of the spatial and temporal domain which minimise the error accrued in evaluating a user-provided output diagnostic (such as the power output of a tidal turbine farm or the drag on an aeroplane wing), whilst maintaining low computational resource requirements.
Other beneficiaries of this financing were:

- **Dr Ham** for ARCHER2 eCSE Scalable I/O and checkpointing for Firedrake (Total Value (£): £96,390).
- **Dr Ham/Prof Farrell** for ARCHER2 eCSE Scalable and robust Firedrake deployment on ARCHER2 and beyond (Total Value (£): £54,876)

OTHER FUNDING

- **Air Force Office of Scientific Research** "Conference and Workshop Support" (**Prof Sherwin**) USD 7,5K
- **NSFPLR-NERC**: "Melting at Thwaites grounding zone and its control on sea level" (**Prof Piggott**) ~£200K
- **Research England GCRF** internal funding "Developing Ocean Modelling Capability in the Maldives: Ocean Economics and Sea Level Rise Related Hazards" (Prof Piggott)

STAFF DEVELOPMENT

STAFF DEVELOPMENT

Staff development opportunities

Career Management

Staff development is a key contributor to the success of individuals and, ultimately, to the success of PRISM as a whole initiative.

Promotions

Dr David Moxey was promoted to Reader in Engineering at King's College London.

Dr David Ham was promoted to Reader in Computational Mathematics at Imperial College London.

Former PRISM PDRA **Dr Jemma Shipton** has been promoted to a lecturer position at University of Exeter. This is a fantastic achievement warmly welcomed by the PRISM team.

Dr Jeremy Cohen has recently taken on the part-time role of "Director of Research Software Engineering (RSE) Strategy" at Imperial, which he will undertake alongside his EPSRC RSE Fellowship. The role will help to support the research software engineering activities being undertaken within the research community at the College and look to develop a wider strategy for RSE and stronger links with the College's Research Computing Service and central IT groups."

Awards/Prizes

PRISM's Principal Investigator **Prof Spencer Sherwin** was awarded a 2020 **ECCOMAS Prandtl medal**.
The Prandtl Medal is awarded for outstanding and sustained contributions to the area of computational fluid dynamics. ECCOMAS, the European Community on Computational Methods in Applied Sciences, is a scientific organization grouping together European associations with interests in the development and applications of computational methods in science and technology. Nominations for **the ECCOMAS awards** were submitted by members of the ECCOMAS community. The final selection was carried out by an independent awards committee assembled specifically for this purpose, comprising the previous awardees of the ECCOMAS medals, the previous recipients of the young investigator awards, and representatives of the ECCOMAS technical committees. More information on this year's awardees can be found here.

Prof Patrick Farrell was awarded a **Whitehead Prize** in recognition of his broad, creative and impactful work as a computational mathematical scientist. Farrell's contributions to the general area of the numerical solution of partial differential equations span algorithm development, rigorous analysis, high performance software implementation, and applications in scientific computation. See the full citation here.
The Whitehead Prize is awarded yearly by the London Mathematical Society to multiple mathematicians working in the United Kingdom who are at an early stage of their career.

Departing staff destinations

Ioannis Papadopoulos (supervised by Prof Farrell) has finished his PhD and started a postdoc at Imperial (with Sheehan Olver).
Jingmin Xia (supervised by Prof Farrell) has finished her PhD and won a permanent lectureship at the National University of Defense Technology, Changsha, China

IMPACT AND CASE STUDIES

IMPACT AND CASE STUDIES
IMPACTFUL PRISM RESEARCH

CASE STUDY

Impactful PRISM research

The Platform for Research in Simulation Methods (PRISM, https://prism.ac.uk) is a major research programme based at Imperial encompassing activity in computational science. The main outputs of PRISM are frameworks for encoding composable mathematical abstractions as software, making advances in numerical mathematics practically applicable to a wide range of high-performance real-world applications across industry and in government. PRISM software is used to benchmark modelling technology in industrial fluid mechanics at **McLaren Formula 1 and Rolls Royce**, is in operational use by **DUG Technologies** to provide seismic imaging services to many oil and gas majors, is the prototyping platform for the advanced numerics in the **Met Office's** next generation climate and weather model, and forms the core of the Finnish Meteorological Institute's development of a new operational capability for sea level forecasting.

ROLLS ROYCE

Met Office

IMPACT AND CASE STUDIES

IMPACTFUL PRISM RESEARCH *CONTINUES*

CASE STUDY

PRISM software

Computer software of fluids and solids underpin much of modern engineering, as well as forming the basis of the weather and climate forecasts that inform daily life and national policy. Advances in the numerical mathematics underpinning these simulations can enable higher fidelity simulations at larger scale. However advanced techniques are also harder to implement, with the result that sophisticated mathematics is often only applied to toy problems while real applications are limited to simpler but less capable techniques. The contribution of PRISM is to create software abstractions for the fundamental mathematics describing advanced numerical algorithms which can be composed together by scientists and engineers to create bespoke simulation capabilities. With PRISM-created software, the sophistication of the numerical discretisations and solvers available to scientists and engineers is no longer limited to the (typically simple) set that they can implement themselves. This mathematical composability of operators lets users easily make substantial changes to the algorithm, to discover the best approach for their current science challenge and available hardware. PRISM researchers take this automation and composability approach much further than other systems, so that many advanced approaches which are often regarded as too difficult in practice become straightforward.

Two EPSRC Platform Grants with classifications in the mathematical topics of Continuum Mechanics and Fluid Mechanics, have supported PRISM in the development of a suite of computational modelling software, which has been widely applied in industry and public sector science and engineering.

We now describe the software encapsulated by PRISM.

Firedrake [1] and Devito [2] replace the hand-derivation of the computation by computer algebra compiler processes which automatically apply the required series of symbolic transformations. This results in the automatic generation of the program which conducts the calculations. The scientist or engineer writes equations, and the computation occurs automatically, in parallel, achieving much higher computational performance than typical hand coding. Firedrake provides this capability for a vast range of finite element methods, while Devito provides high order finite difference capabilities for the wave equations critical to the oil and gas industries. The ability to effectively exploit complex finite element discretisations has underpinned numerics research led by Cotter [3] into compatible finite element methods which effectively capture the dynamics of atmospheric circulation. This work has provided an accurate numerical scheme for weather and climate prediction which avoids the catastrophic resolution singularities at the Earth's poles which plague the previous methods.

PyFR [4] is a compressible flow simulation framework using high order flux reconstruction techniques to exploit modern massively parallel hardware such as GPUs. PyFR's domain specific language separates the specification of the flux reconstruction algorithm from its implementation, which is generated by a specialised compiler. This enables the code to exploit the different brands and generations of GPUs available on different supercomputers without rewriting the core software.

Nektar++ [5] employs inheritance and template metaprogramming to enable the application of finite element techniques which combine spatial and polynomial refinement. This delivers unmatched levels of accuracy at the cost of complexity which would be infeasible to deliver in a more conventional software framework.

IMPACT AND CASE STUDIES

IMPACTFUL PRISM RESEARCH *CONTINUES*

PRISM software and the underpinning innovative numerical methods have been widely adopted by industrial and public sector users. The impacts are as diverse as the beneficiaries: whole new weather and climate simulation capabilities, commercial advantages in the seismic Impact imaging sector, and competitive edge in Formula 1 racing to name but a few. In the following, we detail examples impacts of each PRISM component.

Firedrake and UK Met Office

The **UK Met Office** uses Firedrake as the principal dynamics prototyping platform for its next generation weather and climate simulation system. The Firedrake high productivity development environment has enabled Cotter's advanced compatible finite element discretisations (and related solvers) to be demonstrated at scale as a solution to the Met Office's current parallel performance limitations. The Met Office decision to go ahead with the new model development, and to base it on these numerics, rests on Firedrake and the research it underpinned. "The capability of compatible FEM in the GungHo dynamical core is a key element of our strategy in developing a model that will be fit for the mid-life upgrade of our new supercomputer. This is currently expected to be in 2025 and up to £1.2 billion investment has been approved for this new machine."

The Met Office has now committed to a 180 FTE years project to turn these decisions into an improved forecasting system for the UK.

Firedrake and EDF

Firedrake plays a similar role for **EDF's** simulations in support of their geological storage of nuclear waste. The ability to rapidly combine sophisticated linear solvers and preconditioners has enabled them to overcome the scaling limitations of their current approaches, and they have committed resources to implement the improvements in their production code.

Firedrake and Finnish Meteorological Institute

The **Finnish Meteorological Institute** have built a coastal ocean modelling system, Thetis, directly using Firedrake. They use the 3D version of this model to develop their understanding of the complex internal processes that characterise the coastal ocean. The 2D version of the model enables sea level simulation over a wide area and has been chosen as the basis for their next generation operational forecasting capability.

"We would not be developing simulation capabilities at this level without Firedrake."

Devito and DUG Technologies Ltd

DUG Technologies Ltd (a public company with market capitalisation A$112.40M as 27 Jan 2021) uses Devito in production. DUG provides seismic imaging services to the oil and gas industry. Seismic imaging is a computational process which creates images of subsurface structures from acoustic survey data. Accurate seismic imaging enables fewer survey wells to be drilled, reducing the financial and environmental cost of this activity. Seismic imaging is a petascale problem in which the ability to rapidly translate numerical advances into operational use is key to the competitiveness of this technology. The agility that the code generation approach provides is the reason DUG adopted Devito. DUG have rebuilt the core computational engine for their DUG Wave waveform inversion software around Devito, achieving a factor of 10 improvement in performance scalability. Over the past year, DUG Wave has been running continuously using Devito on computing resources equivalent to the 100-200 range of the world's Top500 supercomputer 2020 list. The code now scales to tens of petaflops, translating to a cost reduction of millions of dollars for their customers.

CASE STUDY

"Without Devito, the same amount of processing with previous technology would have exceeded our total compute capacity."

IMPACT AND CASE STUDIES
IMPACTFUL PRISM RESEARCH *CONTINUES*

Nektar++ and McLaren Formula 1 Racing

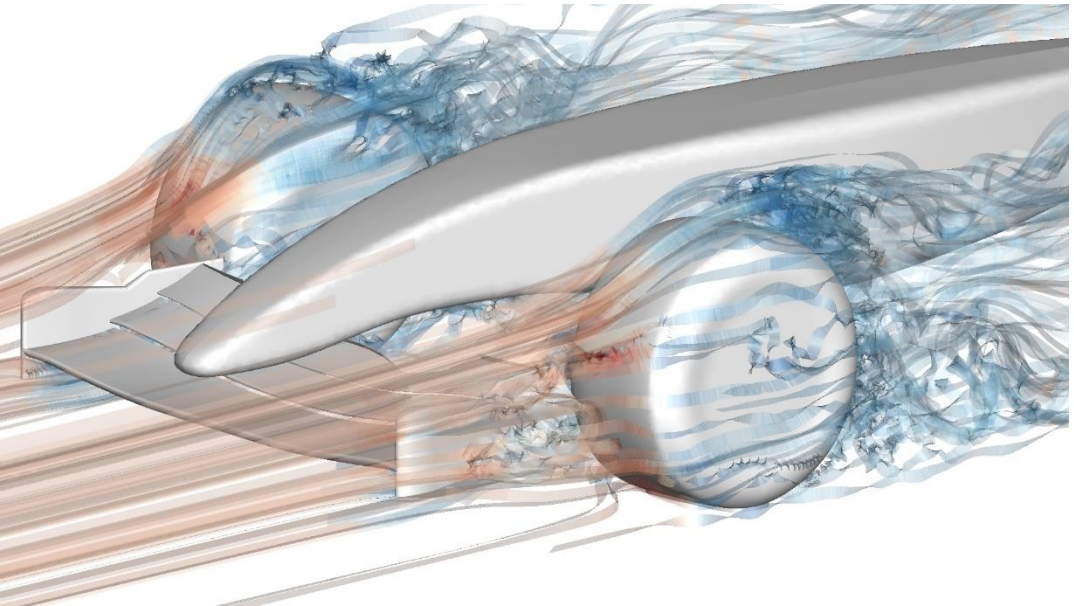
McLaren Formula 1 Racing uses Nektar++ to guide their race car design. Their standard tool is a Reynolds Averaged Navier Stokes (RANS) solver code which is fast but has limited applicability in terms of flow conditions (particularly during breakdown of vortical flows which are a key component of maintaining aerodynamics performance of racing cars). Nektar++ is a high-fidelity tool that has much broader applicability. Competition regulations prevent the direct application of high-fidelity tools during the race car season, so it is critical to understand the conditions where RANS loses reliability. McLaren use Nektar++ to develop protocols to decide whether given RANS simulations are reliable or not, and therefore whether the results suggest useful improvements to make to the car's aerodynamic shape.

Nektar++ and Rolls Royce

Rolls Royce uses Nektar++ for similar purposes in their next-generation turbomachinery design. Their RANS code is used as a crucial part of their design cycle, and they compare RANS predictions with those made by Nektar++ in order to guide their design process.

PyFr and Zenotech

Zenotech, based in Bristol, delivers market-leading high-performance computing tool and consultancy services for businesses in the aerospace, automotive, civil and renewable energy sectors. Zenotech has added a flux reconstruction solver based on PyFr to its proprietary zCFD codebase, complementing the existing finite volume solver. The resulting high order solver is being used by Zenotech to simulate aircraft parts and in acoustic problems for the rail sector.



Formula 1 Aerodynamics Nektar++

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IMPACT AND CASE STUDIES
RSE

Research Software Engineering and PRISM

The PRISM platform is characterised by its group of advanced scientific research software and the teams that build and maintain this software. Software engineering expertise is therefore a significant part of PRISM. The term Research Software Engineering or RSE is becoming increasingly common within the research community. Indeed, the acronym "RSE" may be something that you are already familiar with or have encountered as it becomes more widely used.

The RSE movement, which has developed over recent years, goes beyond purely considering expertise in building research software to include aspects such as best practices, careers, training, policy development and various other areas. Why is this so important? How does it relate to PRISM? And how are the PRISM team working with, contributing to and learning from the research software community? In this section we provide some background on what Research Software Engineering (RSE) is, why it's important not just to PRISM but to research more generally, and some of the resources that exist and may be of interest to you if you build, use or are interested in research software. Whether or not you're part of one of the PRISM groups, we hope this section of the website will provide useful information and links to some helpful resources.

Research Software Engineering: An Introduction

Software has been part of research for a long time, especially in the types of scientific domains represented by the PRISM platform. The unique mix of specialist research domain knowledge, and the ability to write code in often relatively low-level programming languages such as FORTRAN or C/C++, that is often found in these areas has become an increasingly valuable skill set as computational science has become an ever-more vital part of modern scientific research. As data volumes and the complexity of simulations increase, so the complexity of the software that is needed to support the science increases.

Photo by Glenn Carstens-Peters on Unsplash

IMPACT AND CASE STUDIES
RSE *CONTINUES*

Over the years a group of researchers started to emerge who were spending a significant amount of their time writing software, to the exclusion of other tasks such as writing papers or proposals or undertaking teaching duties.

Where these individuals were looking to go on to an academic career, this put them at a major disadvantage in terms of gaining the necessary experience and CV to support this. Where they enjoyed the focus on software development, their role was generally not recognised within the wider structure of university roles and they would often have limited job security, being supported through fixed-term funding, or no career advancement opportunities.

At the Software Sustainability Institute's Collaborations Workshop 2012, a group of individuals sat down to discuss this challenge and this led to the concept of the "Research Software Engineer" and ultimately the large (and still rapidly growing) RSE movement that we have today. You can read the full story in Simon Hettrick's **"A not-so-brief history of Research Software Engineers".**

RSEs in PRISM

Within the teams that are part of PRISM, there are many researchers and academics who spend much of their time writing code. In some cases, these individuals may identify themselves as Research Software Engineers while in other cases they may simply consider themselves as researchers who spend a lot of their time coding. Either way, there is lots that an active research software community can offer these people, from events at which to present their work and network with others developing software in different research fields through to offering training and offering opportunities to get involved with providing training to others.

Imperial College London has a Research Software Community in which there are members of PRISM who are active participants. This includes helping to run the community as part of its organisational committee and attending events and activities provided by the community. PRISM also has links with the wider London and South East of England regional research software community RSLondon.

One of UK Engineering and Physical Sciences Research Council (EPSRC)'s 11 Research Software Engineering Fellows is directly linked with PRISM through a work programme that includes continuation of a previous collaboration with the Nektar++ team. This work is developing tools and services to support bridging the gap between the code and growing user communities. These user communities include individuals who have limited technical computing knowledge but advanced scientific and mathematical knowledge to support their use of the code and its outputs.

Photo by Markus Spiske on Unsplash (modified)

IMPACT AND CASE STUDIES
RSE *CONTINUES*

Policy, Careers and Advocacy

One of the major opportunities for a community in the research software space is to bring together individuals who are often the only person (or one of a very small team) within a given research group focusing on developing software. These individuals could probably not, on their own, demonstrate the need to enhance support for RSEs or bring together a sufficiently large group to help with this. Whereas a larger community crossing many disciplines has more scope to demonstrate the wide-ranging need for change. The relatively large number of individuals within PRISM who work with and build research software ensure that PRISM is well-placed to help advance local research software capabilities in collaboration with existing research software communities.

Particular areas where RSE can make a difference include:

Policy	Careers	Advocacy
Helping to design, develop and implement new approaches to supporting research software. Working with a range of stakeholders either within a single organisation/institution or across multiple institutions to enhance the availability and awareness of research software services and/or support.	As highlighted above, individuals focusing on building research software often have limited job security or career advancement opportunities. This is beginning to change and developments such as the setting up of research software teams at academic organisations and institutions are helping to provide options for career progression. Groups of researchers and academics who understand research software are well-placed to make a case for the need for such groups.	Advocacy is, to some extent, encompassed within the previous two elements but it has significant importance in its own right. Research software that is developed according to best practices and that is sustainable, maintainable, robust and performant is a key element in ensuring high-quality outputs from computational research. This is highlighted by the Software Sustainability Institute's motto: "Better Software, Better Research". Getting this message out to people who have the capability to make a change to the way that RSEs are seen in the research community and ensuring that they have the necessary opportunities to realise the huge potential benefits their skills can offer is vital.

RSE Community

IMPACT AND CASE STUDIES
RSE *CONTINUES*

Links and Resources

General RSE links – groups (PRISM-related), organisations, blog posts, articles, etc.:

- Imperial's RSE Team
- Oxford Research Software Engineering
- Society of Research Software Engineering: A professional society for RSEs
- Software Sustainability Institute
- A not-so-brief history of Research Software Engineers
- The Four Pillars of Research Software Engineering

Training

- The Carpentries: Providing a wide range of training courses for researchers covering software development and data science among other areas.
- Imperial's Research Computing and Data Science Skills courses

Communities

- Imperial College Research Software Community
- Research Software London – A regional research software community for RSEs, researchers, systems professionals and anyone interested in research software within the London and South East of England region

Photo by Clark Tibbs on Unsplash (modified)

IMPACT AND CASE STUDIES
DEVITO CODES 4U

Devito Codes Ltd is the commercial arm of the open-source platform Devito. Devito makes it easy for scientists and engineers to write blazingly-fast performance-portable finite-difference software for CPUs and GPUs.

A brief history of Devito

Devito arose from an Imperial College London Intel Parallel Computer Centre started in 2014 by **Dr Gerard Gorman**. The goal was to develop open-source high-performance software for seismic imaging; taking as inspiration other code generation projects such as FEniCS and Firedrake. From the beginning, this initiative benefited from the industry guidance of Hamish McIntire and Charles Jones at BG Group and close academic collaboration with the SLIM group led by Prof Felix Herrmann.

The first incarnation of Devito used Python and symbolic computation at the primary programming interface for end-users. However, the underlying code generation technology was essentially a source-to-source translater which limited the range of optimizations that could be applied to the generated code. This changed in 2016 when Dr Fabio Luporini joined the project and rewrote the Devito backend as a true optimizing compiler.

In late 2017 Devito entered into a new phase of its evolution. We began working closely with DUG to mature Devito for commercial use as part of DUG Wave software infrastructure.

As of 2020, Devito has users from over 100 different organizations and companies. In January of this year, we established the first Devito open-source consortium with industrial partners BP, DUG, Microsoft and Shell. Microsoft sponsored an additional project to accelerate the development of GPU support in Devito, as well as performance and scalability on Microsoft Azure.

Devito Codes Ltd

In February 2020 **Dr Gerard Gorman** and Dr Fabio Luporini founded Devito Codes Ltd to secure the long-term future of Devito. Key to our strategy is drawing clear lines between the *open-source Devito* project and *DevitoPro*.

All general-purpose symbolic and compiler software technology will continue to be developed and maintained as open-source and patent-free. The basic research underpinning Devito will continue to be published in the open literature.

Devito Codes Ltd focuses on providing professional services including technical support, training, bespoke software development services and bespoke optimization for clients hardware. We are also developing a new software product called DevitoPro, which consists of proprietary extension packs such as a toolkit for integration with legacy codes.

Finally, we are also proud to announce that we have signed a partnership agreement with DUG to provide HPC software development services on DUG-McCloud. Over the last few years, we have significantly benefited from working with closely with our friends at DUG. We look forward to continuing this relationship into the future. In particular, to explore how the knowhow and disruptive software technologies developed within Devito can be reapplied to other compute-intense big-data problems.

We gratefully acknowledge the support received to develop Devito from industry and research council funding.

Open source Devito consortium runs from Jan 2020-Dec 2022.
Consortium members are:
BP,
Petrobras,
Shell
Other industry sponsors
AMD
DUG
Intel
Microsoft
NVidia
Fujitsu
Research Council grants
EP/W007789/1
EP/V001493/1
EP/R029423/1