

# **PRISM REPORT**

PRISM- Platform for Research in Simulation

**Prepared for** 

**PRISM Advisory Board** 

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Engineering and Physical Sciences Research Council

# 1. EXECUTIVE SUMMARY

In this report we outline our activities during the first eighteen months into our renewed EPSRC platform grant which continues to build on the success of our previous award. Whilst our focus firmly remains on making impact through promoting and training people to develop and apply state of the art, open source, simulation tools; we are also exploring how to have impact beyond our traditional industrial interactions and to see how our tools can be used beyond traditional "computational fluid dynamics". We have currently funded four researchers on short term placements and are establishing workshops focused on how best to train young researchers/students to utilise our software thereby also encouraging a wider impact in academia and industry. We continue to release our software, publish in internationally leading journals and seek new funding opportunities. Since the start of the grant we have secured £7M in related funding as well as engaging with UK related research activities such as the recent EPSRC/MET Office/AEAUK call ExCALIBUR (Exascale Computing Algorithms and Infrastructures Benefiting UK Research).

PROF SPENCER SHERWIN, Principal Investigator

# 2. NEW 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 Exeter who benefit from the sustained critical mass of expertise that this funding enables and the open source codes we distribute.

# Ø

As a result, a large body of individuals will be deployed to industry and academia with a deep appreciation of the possibilities of computational modelling and the expertise to exploit them.

Finally, Imperial has recently established a central research computing service and appointed Prof. Sherwin as the director. This activity spans all faculties and departments at Imperial and provides an excellent opportunity for us to engage with the Research Software Engineering community at Imperial and around the UK.

#### WHAT WE ARE

**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.

#### WHAT WE DO

The quality of our software engineering processes is: crucial to our success:

- We continue to use the most effective available disciplines and tools for developing high quality computational science software on which others can build with confidence.
- We continue to advocate good practice by using revision control, continuous integration and testing, systematic code review, regular releases, and coordinated sprints to achieve major milestones and refactoring projects.



**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.

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#### TRAINING EVENTS

We regularly run regular training events and user and research workshops, building on the success of our Nektar++, Fluidity and Firedrake user events inviting international experts as appropriate.

#### PUBLICATIONS

In addition to academic publications, we continue to focus on publishing and expanding training materials, including targeted tutorials for particular applications domains, such as geophysical fluid dynamics, tidal energy, surgery planning, motor racing, and seismic inversion.

#### SOFTWARE DEVELOPMENT

- We maintain online software development community-building tools through Github, Bitbucket and Slack as well as mailing lists, and use them to provide a rapid and supported "on ramp" for users and collaborators.
- We develop the creation of packaged application tools targeting domains, building on our experience with Thetis (<u>thetisproject.org</u>) Gusto (<u>firedrakeproject.org/gusto</u>) and using Python.

#### ENGAGEMENT

- We work with our Advisory Board to deliver the new application areas and to add to the group as application opportunities emerge.
- We continue to engage with policy makers as we have under our roles in the EPSRC e-Infrastructure Strategic Advisory Committee, the EPSRC High Performance Computing Science Advisory Board and the Blackett Government office review on modelling.
- We engaged with the Great Exhibition Road Festival, which in 2019, attracted more than 60,000 visitors with workshops, tours, talks and, performances to give the public an insight into the research that goes at Imperial College London and in the UK.
- We strengthen and deepen continuing engagement with our current collaborators, including McLaren Racing, Airbus, Rolls Royce, BG/Shell, BAE Systems, Nvidia, Intel, AMEC Foster Wheeler, BP, the Met Office, Tidal Lagoon Power, Atlantis Resources, and The Weir Group ITI Global.

# 3. ACTIVITIES AND OUTCOMES

*This section of the report presents PRISM progress and performance towards delivering the strategic outcomes and priorities between July 2018 – April 2020.* 



# WORKSHOPS

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*Firedrake* is an automated system for the solution of partial differential equations using the finite element method (FEM).

https://www.firedrakeproject.org/

Firedrake run regular training events and user and research workshops such as:



#### 2<sup>ND</sup> FIREDRAKE WORKSHOP 2018

7<sup>th</sup> -8<sup>th</sup> June 2018, ICL The second workshop provided the 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.



FIREDRAKE TUTORIAL – UK

11<sup>th</sup> January 2019, ICL The Firedrake team once again offered a half day Firedrake tutorial aimed at new Firedrake users. The tutorial was an introduction to solving PDEs using the finite element method with Firedrake. The lecture was pitched at new MRes and PhD students just starting to use or develop Firedrake.



#### FIREDRAKE TUTORIAL - USA

1st March 2019, USA The Firedrake team presented a live cloud tutorial at the SIAM Conference on Computational Science and Engineering in Spokane Washington.



#### FIREDRAKE TUTORIAL -GERMANY

18<sup>th</sup> June 2019, Germany There was a hands-on Firedrake tutorial at the Aachen Institute for Advanced Study in Computational Engineering Science (AICES).



#### **3<sup>RD</sup> FIREDRAKE WORKSHOP 2019**

26<sup>th</sup>-27<sup>th</sup> September 2019, Durham The workshop began with a half day Firedrake tutorial for interested new users. See the programme for detailed timings: <u>https://firedrakeproject.org/firedra ke\_19.html</u>.



#### 4<sup>TH</sup> FIREDRAKE WORKSHOP 2020

10<sup>th</sup>-11<sup>th</sup> February 2020, USA This was a first workshop in North America at the University of Washington.



**PyFR** is an open-source Python based framework for solving advectiondiffusion type problems on streaming architectures using the Flux Reconstruction approach of Huynh. The framework is designed to solve a range of governing systems on mixed unstructured grids containing various element types. It is also designed to target a range of hardware platforms via use of an in-built domain specific language derived from the Mako templating engine.

www.pyfr.org

# Y Devito

**Devito** is a Domain-specific Language (DSL) and code generation framework for the design of highly optimised finite difference kernels for use in inversion methods.

#### RSE HACK EVENT WITH MICROSOFT AND THE ALAN TURING INSTITUTE

January 2020, London This event focused on the theory and practise of automated testing and verification of research software and is critical reproducible research.

#### 2020 RICE OIL & GAS HPC CONFERENCE, Workshop: From Zero-to-Devito

4<sup>th</sup> March 2020, USA

The Devito workshop participants learnt how to implement finite difference and inverse solvers using Devito.

https://www.devitoproject.org/



**Thetis** is an unstructured grid coastal ocean model built using the Firedrake finite element framework. Currently Thetis consists of 2D depth averaged and full 3D baroclinic models.

TRAINING:

July 2019, Maldives National University 4-day workshop

November 2019, Korean Institute of Ocean Science and Technology 5-day finite element training

https://thetisproject.org/













**Fluidity** is an open source, general purpose, multiphase 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.

These are some of the projects that the computational platform has helped to develop.

MAGIC and INHALE consortia looking at pollution within urban environments and the KAUST sustainability centre which also develops similar modelling. Our work will address within MAGIC, KAUST and INHALE projects: (i) effective ventilation of urban environment at inside building, street and city scales; (ii) thermal and wet environmental conditions; (iii) impact of architectural design; (iv) integrated vehicle traffic, cyclist and pedestrian pathways; (v) incorporation of local power and thermal energy plants (such as Combined Heat and Power plant, CHP); (vi) emergency response following a release of toxic material (e.g. fire or terrorist attack); (vii) transport and removal of pollutants (i.e. through rainfall and other depletion processes); (viii) tree, greening and water system placement; (ix) transfer of critical information (via clear visual interfaces) on pollution levels, winds and temperatures to city planners, administrators, emergency services and the general public; and viiii) impact of pollutants on health. This is a complex modelling problem that can only be satisfactorily treated through an innovative and fully integrated model framework.

**Fluidity**, a finite element -based flow simulator incorporating an anisotropic mesh adaptivity capability as well as the Large Eddy Simulation (LES) methodology (Aristodemou et al. 2009).

#### **Boltzmann Transport and Lattice Boltzmann methods**

As part of the Lattice Boltzmann (LB) work on PREMIER, we will be working to bring a suite of cutting-edge numerical tools developed for other Boltzmann applications into the field. These include adaptivity in the complete phase space and large-scale parallelism in order to tackle a range of problems in LB. These problems include resolving flow in boundary layers next to walls, using unstructured grids and enabling stable simulations with multi-scale discretisations. An initial prototype o this technology has been developed based on previous work with Prof. Spencer Sherwin. This prototype is built on top of established code at Imperial used in other Boltzmann applications (like radiation transport and spectral wave modelling) and supported by Fluidity. In PREMIER development on this prototype will continue, with the goal of providing new tools for large-scale fluid simulations with far greater flexibility and accuracy than is currently available. In an effort to further integrate different Boltzmann communities, we also ran a one-day workshop in early December at Imperial College (Boltzmann Transport and Applications Meeting 2019), attending by over 30 different academics and industrial partners. As part of **PREMIER** we are hoping to run this workshop again in 2020 and engage with the wider group of Lattice-Boltzmann and CFD communities in the UK.





**Nektar++** is a tensor product based finite element package designed to allow 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. <u>https://www.nektar.info/</u> Nektar++ run the following events:



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#### **NEKTAR++WORKSHOP**

#### 10<sup>th</sup> - 12<sup>th</sup> June 2019, Exeter

The 4th annual Nektar++ Workshop brought 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. The first two days included a comprehensive programme of talks, which were followed by a number of parallel informal group sessions allowing developers and users to discuss and work on specific aspects of the code.

HIFICOMA 2019: WORKSHOP ON SPECTRAL/HP ELEMENT METHOD USING NEKTAR++

#### 14<sup>th</sup> - 16<sup>th</sup> December 2019, China

We are delighted to report that the following members of the PRISM team: Chris Cantwell, Dave Moxey, Joaquim Peiro, Spencer Sherwin were invited to organise workshop on Spectral/hp element method using Nektar++ during the symposium International Symposium on High-Fidelity Computational Methods & Applications 2019, HiFiCoMa 2019, which was held in Shanghai. The objective of this symposium was to bring together experts in computational science and experts in engineering application to exchange new ideas and discuss development perspectives of high-fidelity methods. It also offered a platform to show the exciting scientific and engineering study undertaken in this area. The symposium ended with a Nektar++ workshop to provide a more opportunity to understand how to apply high order spectral/hp element software. More information on the event is available here: <a href="https://www.ishfcma.org/">https://www.ishfcma.org/</a>

# CONFERENCES

We have also organised two large international conferences. The details are provided below:

INTERNATIONAL CONFERENCE ON SPECTRAL AND HIGH ORDER METHODS (ICOSAHOM) 2018

**Date:** 9<sup>th</sup>-13<sup>th</sup> July 2018 **Location:** Imperial College London, UK **Scientific scope:** The purpose of this conference series was to bring together researchers and practitioners with an interest in the theoretical, computational and applied aspects of high-order and spectral methods for the solution of differential equations





**Subjects included, but were not limited to:** spectral methods, high-order finite difference methods, p and hp finite element methods, discontinuous Galerkin methods, ENO/WENO methods, high order methods for integral equations, wavelet-based methods, stochastic methods, efficient solvers and preconditioners for high order methods, efficient time-stepping methods, parallel and computational aspects, flux reconstruction.

#### **Outcomes:**

- The Christine Bernardi Award was given for her outstanding contributions in the area of "high-order approximations for the solution of PDE's". The 2018 Christine Bernardi Award was presented with a €1,000 cash prize during the celebration of the 50th anniversary of the Laboratoire Jacques Louis Lions where she was working. The Laureate was invited to give a talk at this occasion. The award was presented to honor Christine Bernardi, CNRS senior researcher at Laboratoire Jacques-Louis Lions at Sorbonne University (formerly known as Université Pierre et Marie Curie) in numerical analysis, who prematurely passed away on March 10, 2018. She was a leading figure in the domain of finite element and spectral methods and had contributions both in delicate a priori and posteriori estimates and in new numerical approaches in fluid flows and electromagnetism.
- The live streams of all the conference plenary talks can be found on the plenary speakers' page. <u>http://icosahom2018.org/programme/plenaryspeakers/</u>
- WINASc reception for female participants: there was a special drinks reception for women participants on Tuesday evening, 18:30-19:45, at 170 Queens Gate in the Drawing Room. This reception was hosted by Fengyan Li, Jennifer Ryan, and Beth Wingate, in conjunction with WINASc (Women in Numerical Analysis and Scientific Computing) and was made possible through the ICOSAHOM organization and their sponsors (EPSRC, Rolls-Royce, PRISM, AFOSR, and Imperial College London).



THE IUTAM SYMPOSIUM ON LAMINAR-TURBULENT TRANSITION 2019

Date: 2<sup>nd</sup>-6<sup>th</sup> September 2019

**Location:** Imperial College London, UK **Scientific scope:** The objectives of the symposium was to present and discuss novel developments in fundamental and applied aspects of stability and laminar-turbulent transition in complex flows, at all speed regimes, and to provide a forum for the free exchange of ideas for their implementation in an industrial setting.

**The scientific programme covered a range of fundamental topic areas, including:** Global analysis of instabilities and receptivities for complex configurations; Nonlinear dynamical-systems approaches to minimal seeds and transition to turbulence; Influence of multi-physics phenomena on transition: reactive flows, non-Newtonian material behaviour, interfacial flows, flows with interacting structures; Novel experimental measurement and evaluation techniques for transition in complex flows; Roughness-induced transition; transition from steps, gaps, junctions and other geometric imperfections; Transition in hypersonic flows; prediction of thermal loads; Active and passive control of flows undergoing transition; transition delay; Transition mechanisms in natural and controlled environments; receptivity techniques and studies; Late stages of transition and the breakdown to fully developed turbulence; Transient growth problems and bypass mechanisms and their role in the transition process.

#### **Outcomes:**

- We received very positive feedback from attendees on the well organised and attended meeting.
- Symposium was well attended by early-career academics, post-graduate students, industry representatives, senior members of the community and invited guests.
- 175 registered delegates of which 40% are PhDs
- Evening reception (Monday, 2nd September) and conference dinner (on the 5th September) provided networking opportunities for attendees to discuss future collaborations.



# NEW WEBSITE

<image>



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



PROJECTNAME

Web design project

CLIENT prism.ac.uk

**DELIVERY** Jakub Mysona from 56 Degrees

#### OVERVIEW

The official PRISM website has been completely redesigned. The new website features a clean design, improved functionality and enhanced content. It aims to provide clear, up-to-date information on all PRISM activities.

#### PROJECT STAGES

STAGE 1. PLANNING AND DESIGN

Completed

STAGE 2. BUILD AND HANDOVER FOR TESTING WITH KEY AUDIENCES

Completed

## SOFTWARE UPDATE

The following software updates have been delivered:



#### 01 || DEVITO V4.0

Devito v4.0 has been released in December 2019. More information can be found here:

https://github.com/devitocodes/devi to/releases/tag/v4.0



#### 03 || NEKTAR++V5.0.0



The latest version of Nektar++, v5.0.0, was released on the 9th December 2019. It can be downloaded from the <u>downloads</u> <u>page</u>.This release includes a wide range of new library features as well as many other improvements and bug fixes. Many of the solvers and utilities have also received major improvements.

#### 02 || PYFR 1.9.0

Latest release of PyFR 1.9.0 includes:

- Improved strong scaling.
- Added support for Gmsh v4.1.
- Fixed performance issue with OpenCL backend.

http://pyfr.org/download.php



#### 04 || THETIS



A new (coastal) ocean model, in 2D and 3D, using finite element methods, and implemented via the Firedrake framework. Includes an adjoint capability for sensitivity analyses and optimisation. Also includes a preliminary mesh adaptivity capability. https://thetisproject.org/

#### KEY PROJECT STATISTICS AND FACTS

Summary of the outputs and outcomes that demonstrate project's impact:

~80 GROUPS IN 23 COUNTRIES USING OUR SOFTWARE WITH NOTABLE ACTIVITY IN THE UK, USA AND CHINA







PUBLICATIONS

# PRISM FUNDED PROJECTS

#### OVERVIEW

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:



**JULIAN MARCON,** Research Postgraduate, Department of Aeronautics (ICL)

**GIACOMO CASTIGLIONI,** Research Associate, Department of Aeronautics (ICL)

**YAN ZHANG,** Research Associate, Department of Aeronautics (ICL)

**CHRIS CAVE AGLAND,** Senior Research Software Engineer, ITC (ICL)

JAN EICHSTADT, Research Postgraduate, Department of Aeronautics (ICL)



Automating forward and adjoint coupling in finite element geoscience simulations

NekMesh: towards industrial high-order mesh generation

Implementation of high-performance SIMD kernels in Nektar++

DG methods for the Galerkin-Boltzmann equations in Nektar++

Continuous Integration/Research Software Engineer (RSE)

Implementation of high-performance GPU kernels inNektar++



# PUBLICATIONS

- Xia J, Farrell PE, Castro SGP. (2020). Nonlinear bifurcation analysis of stiffener profiles via deflation techniques. Thin Walled Structures. https://www.sciencedirect.com/science/article/pii/S0263823119316404
  - Medina E, Farrell P, Bertoldi K, Rycroft C. (2020). Navigating the landscape of nonlinear mechanical metamaterials for advanced programmability. Physical Review B.

https://doi.org/10.1103/PhysRevB.101.064101

 Farrell PE, Gazca-Orozco PA, Suli E. (2020). Numerical analysis of unsteady implicitly constituted incompressible fluids: three-field formulation.
SIAM Journal on Numerical Analysis.

https://www.researchgate.net/publication/332564404\_Numerical\_Analysis\_of\_Unsteady\_Implicitly\_Constituted \_Incompressible\_Fluids\_Three-Field\_Formulation

- Charalampidisa E, Boulléb N, Farrell P, Kevrekidis P. (2020). Pitaevskii equations using deflated continuation. Communications in Nonlinear Science and Numerical Simulation
- https://doi.org/10.1016/j.cnsns.2020.105255

• Croci M, Farrell P. (2020). Complexity bounds on supermesh construction for quasi-uniform meshes. https://arxiv.org/abs/1911.11589

- Clare M, Percival J, Angeloudis A, Cotter C, & Piggott M. (2020). Hydro-morphodynamics 2D modelling using a discontinuous Galerkin discretisation. EarthArXiv
- https://doi.org/10.31223/osf.io/tpqvy
  - Wallwork J, Barral N, Kramer S., Ham D, & Piggott M. (2019). Goal-Oriented Error Estimation and Mesh Adaptation for Shallow Water Modelling. EarthArXiv

https://doi.org/10.31223/osf.io/cs4we

- Farrell P, Croci M, Surowiec T. (2019). Deflation for semismooth equations. Optimization Methods and Software.
- https://doi.org/10.1080/10556788.2019.1613655
  - Moxey, D., Sastry, S.P. & Kirby, R.M. (2019). Interpolation Error Bounds for Curvilinear Finite Elements and Their Implications on Adaptive Mesh Refinement. Journal of Scientific Computing.
- https://doi.org/10.1007/s10915-018-0795-6
  - Luporini F, Lange M, Jacobs C, Gorman G, Ramanujam J, Kelly P. (2019). Automated Tiling of Unstructured Mesh Computations with Application to Seismological Modeling. ACM Transactions on Mathematical Software

http://dx.doi.org/10.1145/3302256

• Louboutin M, Lange M, Luporini F, Kukreja N, Witte P, Herrmann F, Velesko P, Gorman G. (2019). Devito (v3.1.0): an embedded domain-specific language for finite differences and geophysical exploration. Geoscientific Model Development

http://dx.doi.org/10.5194/gmd-12-1165-2019

- Witte P, Louboutin M, Kukreja N, Luporini F, Lange M, Gorman G, Herrmann F. (2019). A large-scale framework for symbolic implementations of seismic inversion algorithms in Julia. GEOPHYSICS <a href="http://dx.doi.org/10.1190/geo2018-0174.1">http://dx.doi.org/10.1190/geo2018-0174.1</a>
  - Paganini A, Sturm K. (2018). Weakly-normal basis vector fields in RKHS with an application to shape Newton methods. SIAM Journal on Numerical Analysis, 57 (1), pp. 1-26

https://doi.org/10.1137/17M1131623

• Harcourt F, Angeloudis A, Piggott M. (2019). Utilising the flexible generation potential of tidal range power plants to optimise economic value. Applied Energy,

http://dx.doi.org/10.1016/j.apenergy.2018.12.091

• Pan W, Kramer S, Piggott M. (2019). Multi-layer non-hydrostatic free surface modelling using the discontinuous Galerkin method. Ocean Modelling

http://dx.doi.org/10.1016/j.ocemod.2019.01.003

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#### **SPRINGER BRIEFS**

- The ICOSAHOM proceedings were published by Springer as a special volume of the book series Lecture Notes in Computational Science and Engineering.
- The IUTAM Transition 2019 peer-reviewed conference proceedings will be published also by Springer.



Melvin T, Benacchio T, Shipway B, Wood N, Thuburn J, Cotter C. (2019). A mixed finite-element, finite-volume, semi-implicit discretization for atmospheric dynamics: Cartesian geometry. Quarterly Journal of the Royal Meteorological Society

#### https://doi.org/10.1002/qj.3501

Luporini F; Lange M; Louboutin M; Kukreja N; Hückelheim J; Yount Ch; Witte P; Kelly P; Gorman G.; Herrmann F. (2019) Architecture and performance of Devito, a system for automated stencilcomputation. ACM Transactions on Mathematical Software

#### http://arxiv.org/abs/1807.03032v2

Kukreja N; Hückelheim J; Louboutin M; Hovland P; Gorman G. (2019). Combining Checkpointing and Data Compression to Accelerate Adjoint-Based Optimization Problems. Euro-Par 2019: Parallel Processing

#### 10.1007/978-3-030-29400-7 7

- Yakhot A; Feldman Y; Moxey D; Sherwin S; Karniadakis G. (2019). Near-Wall Turbulence in a Localized Puffin a Pipe. Springer Proceedings in Physics. 10.1007/978-3-030-22196-6\_3
- - Wallwork J, Barral N, Ham D, Piggott M. (2019). Anisotropic Goal-Oriented Mesh Adaptation in Firedrake International Meshing Roundtable
- https://imr.sandia.gov/\_assets/documents/2019\_IMR\_Papers/2.3-Wallwork.pdf
  - Moura R; Aman M; Peiró J; Sherwin, Spencer (2019). Spatial eigenanalysis of spectral/hp continuous Galerkin schemes and their stabilisation via DGmimicking spectral vanishing viscosity: Application to high Reynolds number flows. Journal of Computational Physics
- 10.1016/j.jcp.2019.109112
- Vouriot CVM, Angeloudis A, Kramer SC, Piggott MD. (2018). Fate of largescale vortices in idealized tidal lagoons. Environmental Fluid Mechanics https://link.springer.com/article/10.1007/s10652-018-9626-4
  - Paganini A, Wechsung F, Farrell P. (2018). Higher-Order Moving Mesh Methods for PDE-Constrained Shape Optimization. SIAM Journal on Scientific Computing
- http://dx.doi.org/10.1137/17M1133956
  - Melvin T, Benacchio T, Thuburn J, Cotter C. (2018). Choice of function spaces for thermodynamic variables in mixed finite-element methods MELVIN et al. Quarterly Journal of the Royal Meteorological Society
- http://dx.doi.org/10.1002/qj.3268
  - Kyrke-Smith T, Gudmundsson G, Farrell P. (2018). Relevance of Detail in Basal Topography for Basal Slipperiness Inversions: A Case Study on Pine Island Glacier, Antarctica. Frontiers in Earth Science

#### http://dx.doi.org/10.3389/feart.2018.00033

Shipton J, Gibson T, Cotter C. (2018). Higher-order compatible finite element schemes for the nonlinear rotating shallow water equations on the sphere. Journal of Computational Physics

#### http://dx.doi.org/10.1016/j.jcp.2018.08.027

Croci M, Giles M, Rognes M, Farrell P. (2018). Efficient White Noise Sampling and Coupling for Multilevel Monte Carlo with Nonnested Meshes. SIAM/ASA Journal on Uncertainty Quantification

#### http://dx.doi.org/10.1137/18M1175239

Koch MK, Kelly PHJ, Vincent PE (2019). Towards In-Situ Vortex Identification for Peta-Scale CFD Using Contour Trees. (2018) 2018 IEEE 8th Symposium on Large Data Analysis and Visualization (LDAV)

10.1109/LDAV.2018.8739233

## OTHER ACTIVITIES

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Several other activities took place in addition to those described earlier.

NEW COLLABORATIONS

- Rolls Royce we have been exploring the application of the Nektar++ software to turbo-machinery problem. Access to data and expert knowledge of the field as well as exposure to other researcher supported by Rolls Royce.
- McLaren Racing we have transferred fundamental ideas behind vortex stability and identification to their design practice. More recently we are been applying computational modelling tools developed in an academic setting to example flow problems of direct interest to McLaren.
- Centre Beijing Aeronautical Science & Technology Research Institute (BASTRI) of Commercial Aircraft Corporation of China (COMAC). The key objective of Imperial College London - Beijing Aeronautical Science & Technology Research Institute (BASTRI) of Commercial Aircraft Corporation of China (COMAC) collaboration is innovative wing design for commercial manned aircraft. Supported jointly by the Department of Aeronautics and Department of Mechanical Engineering, the Centre's focus is on manufacturing, performance and application of lightweight materials, including composites. The aim will be to underpin COMAC, and other aircraft manufacturers, with more effective solutions for wing design for commercial manned aircraft.
- University of São Paulo: Researchers at the university of São Paulo are using Firedrake for a variety of challenges related to seismic inversion. Dr Ham visited in November 2019 and gave a Firedrake tutorial.
- Met Office: Scientists in the dynamics research group at the Met Office are using Firedrake to develop new numerics and solvers for weather and climate simulation.
- University of Durham (Lawrence Mitchell Assistant Professor in the Department of Computer Science).
- Naval Postgraduate School (Thomas Gibson NRC fellow)

#### VISITORS

02

- November 5th-7<sup>th</sup>, 2018: Prof Koen Hillewaert (Cenaero)
- October 3<sup>rd</sup>, 2019: Prof Kenneth Morgan (Chairman of the PRISM Advisory Board, Swansea University)
- Prof Jan Pech (Multiple trips in 2019)
- Prof Kak-Choon (Malaysia University (1 year))
- Prof Mike Kirby (Multiple visits)
- January 23<sup>rd</sup>-24<sup>th</sup>, 2020: Prof Ram Ramanujam (Louisiana State University) <u>https://www.ece.lsu.edu/jxr/index.html</u>
- December 2019: Sebastian Mitusch and Dr Simon Funke (Simula Research Laboratory)

#### APPOINTMENT OF A NEW ADVISORY BOARD

- Prof Mike Kirby (School of Computing and Scientific Computing and Imaging Institute, University of Utah), prof Robert Kirby (Baylor University), prof Kenneth Morgan (Chairman, Swansea University), Mark Taylor (Deputy Director Energy Innovation at BEIS), Dr Julien Hoessler (McLaren).
- Identifying a broader group of experts that would serve as Advisory Board members has been discussed. Possible non-academic included: McLaren representative, ITI representative, Rolls-Royce representative.

04

05

03

#### **GUSTO: THE FIREDRAKE DYNAMICAL CORE TOOLKIT**

 Gusto is a dynamical core library using compatible finite element methods developed in the Gung Ho project, and built using the Firedrake finite element code generation library. Gusto is a core Firedrake application package. <u>https://firedrakeproject.org/gusto/</u>

#### OUTREACH

#### Great Exhibition Festival 2019

The Great Exhibition Road Festival is a free three-day celebration of curiosity, discovery and exploration in South Kensington. Over the summer, Imperial partnerec with 20 neighbours across Exhibition Road and South Kensington, including some of the world's most iconic museums, to create a unique new festival. Over 60,000 people attended the first ever Great Exhibition Road Festival at the end of June to enjoy a mixture of art and science, culture and local history, technology and curiosity.

#### Aerodynamics Showcase Event 2020

In a strategic move to embolden our aerodynamics research, the Department of Aeronautics announced the Aerodynamics Research Showcase event in 2020. Over the last few years, Imperial College's Department of Aeronautics has made significant investments in facilities for computational and experimental research, enabling us to focus our expertise on key research goals and to develop novel technology platforms. We will be displaying the range of our research, facilities and expertise to industrial and sponsor organisations. At our showcase, you'll have the chance to meet our Academics and to see first-hand how our research extends across several engineering sectors using the full range of expertise in computational and experimental methods.



# 4. ON-GOING FUNDING

The following on-going funding opportunities have been identified:



#### 01. EPSRC

- Three dimensionality and Instabilities of Leading-Edge Vortices (Sherwin/Cantwell) ~£450K
- ExCALIBUR High Priority Use Cases: Phase 1 (Ham/Farrell/Kelly) ~£200K
- ExCALIBUR High Priority Use Cases: Phase 1 (Sherwin/Peiro) ~£230K
- On the way to the asymptotic limit: mathematics of slow-fast coupling in PDEs (Cotter) ~£850K
- ESPRC Centre for Doctoral Training in the Mathematics of Planet Earth (Cotter) ~£550M

#### 02. EU

- EU grant HPCWE (Sherwin) ~£300K
- EU grant DINN (Sherwin) ~£300K
- Innovative Training Networks (Peiro/Sherwin) \*

#### 03. INDUSTRY

- COMAC Centre Beijing Aeronautical Science& Technology Research Institute (BASTRI) of Commercial Aircraft Corporation of China (Sherwin) ~£3M
- ATI/Rolls-Royce (Sherwin) ~1M

#### 04. OTHER

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

PLEASE NOTE: \* indicates pending grant application

# 5. STAFF DEVELOPMENT

The following colleagues were recently promoted to new roles:





#### PRISM has provided a stimulating academic environment and financial support to explore innovative research ideas in high-order mesh generation and adaptation. The work carried out in this project has been instrumental in releasing the open-source mesh generation code Nekmesh, in generating the ideas for a bid to support the adoption of emerging frameworks and, more importantly, in increasing my research output and raising my research profile.

JOAQUIM PEIRO

Professor of Engineering Computation

Professor of Computational Mathematics



**COLIN COTTER** 

# 66

PRISM allowed us to retain our PDRA Dr Jemma Shipton, developing our time-parallel algorithm capability to a level where we were successful in securing one NERC and one EPSRC grant. The publications Jemma developed led to her being appointed as a lecturer at the University of Exeter.





PRISM underpinned my position as a senior post-doctoral researcher for three years, enabling me to strengthen my publication record, bid for further research funding and ultimately secure a Senior Lectureship position at Imperial College London.

#### CHRIS CANTWELL

Senior Lecturer in Aeronautics



DAVID MOXEY

Senior Lecturer in Engineering



The support I received as a PDRA from PRISM allowed me to develop as an independent researcher, establish a track record of publications and ultimately secure a lectureship and promotion to senior lecturer at the University of Exeter.

## 6. DEPARTING STAFF DESTINATION

The following data on staff destination after leaving was recorded:

#### DR THOMAS GIBSON

01

03

NRC fellow at the Naval Postaraduate School

Currently his research interests lie where applied mathematics and computer science meets the physical sciences, namely the multidisciplinary field of computational science. He actively develops for the Firedrake Project: an open-source software package for automating the solution of PDEs using the finite element method.

#### DR SIMON FUNKE

Research Director for Scientific Computing Simula Research Laboratory

Researcher and programmer with 10 years' experience with Python, C/C++ and Ruby and Rails. Loves technological challenges and hackathons. Currently, leads a research team of 30+ people at Simula Research Laboratory.

#### -

05

#### DR JEMMA SHIPTON

Lecturer at the University of Exeter

Jemma Shipton was Prof Colin's Cotter PDRA from 2010 until August 2019.

#### 07

#### **DR JULIAN MARCON**

NPP Fellow at NASA Ames Research Center

His research focuses on high-order mesh generation and adaptation, within the team led by Scott Murman in the NASA Advanced Supercomputing division.

### 02

#### **DR LAWRENCE MITCHELL**

Assistant Professor at University of Durham

His research is in high performance computing and computational mathematics. Much of his recent focus has been in the development of compilers and software abstractions for the development of numerical models implemented using the finite element method. This research is concretely realised in the open source Firedrake project.



#### **DR MICHAEL LANGE** Scientist at ECMWF

He is currently working on utilising modern

software engineering techniques, such as automated code generation and symbolic computation, to enhance numerical weather prediction using novel and emerging HPC architectures. He has extensive experience in developing numerical software packages and domain-specific languages.

## 06

08

#### DR FLORIAN RATHGEBER

Site Reliability Engineer at Google

He was the lead developer of the open source projects PyOP2, a framework for performanceportable parallel computations on unstructured meshes, and Firedrake, an automated system for the portable solution of partial differential equations using the finite element method (FEM), built on top of PyOP2.

#### DR ALBERTO PAGANINI

Lecturer at the University of Leicester

Alberto is numerical analyst and study numerical methods for solar physics and PDE-constrained shape optimization. He is also interested in numerical software. His main project is the open source library <u>Fireshape</u>.

# 7. FORWARD-THINKING

We want to ensure our scientific software is taken up by the international community and used to benefit academia and industry, by building collaborative links through visits, placements and events. Software is best disseminated through hands-on activities: we will provide this access through regular workshops and by establishing on-line tutorial systems for our open-source software.



STAFF DEVELOPMENT

We will aim to influence and keep up with the latest innovations from hardware vendors. The type of multidisciplinary experience that we provide to researchers on this project will make them experts in both numerical modelling and the necessary computer science and software engineering foundations, ensuring they become very employable within both academia and industry.



EDUCATION

We will enable training in multiple disciplines to address this demand from both industry and academia. Organisation of 3 workshops has been proposed as the way forward to consolidate the available materials.

**Workshop 1** on Establishing best practices for MSc and PhD students training.

**Workshop 2** on flow stability. **Workshop 3** on optimisation, data simulation and uncertainty.



INDUSTRY ENAGEMENT

We will aim to translate advanced mathematical algorithms for the real-life problems beyond proof-ofconcept examples to real-world complex models used in science and industry. By doing this, we will expand our world-leading research into important new application areas, give our industrial collaborators a competitive edge, and contribute to the UK's national strategic needs. We will be holding regular events where we showcase our work and share ideas with industrial collaborators.