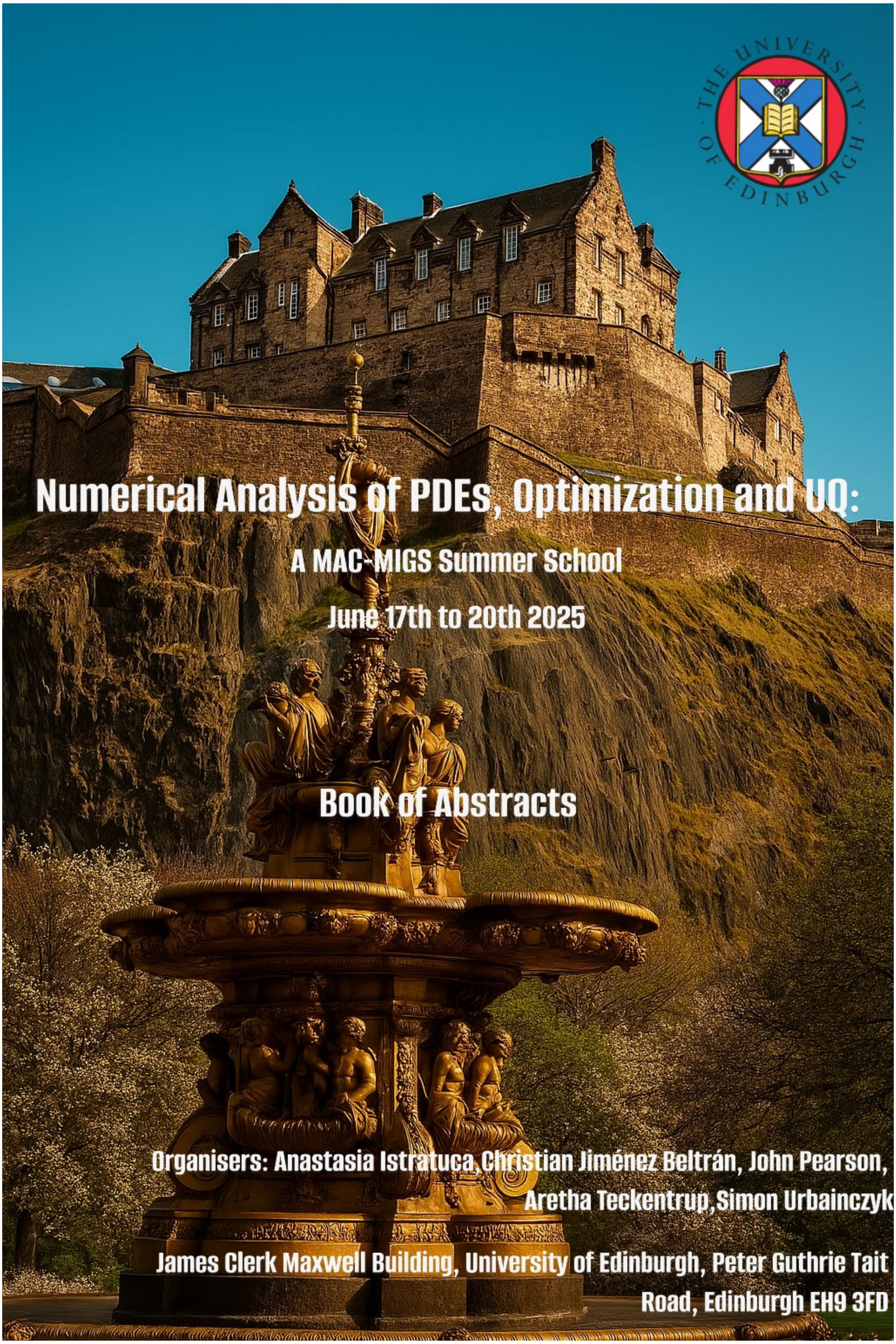


Numerical Analysis of PDEs, Optimization and UQ:

A MAC-MIGS Summer School

June 17th to 20th 2025

Book of Abstracts

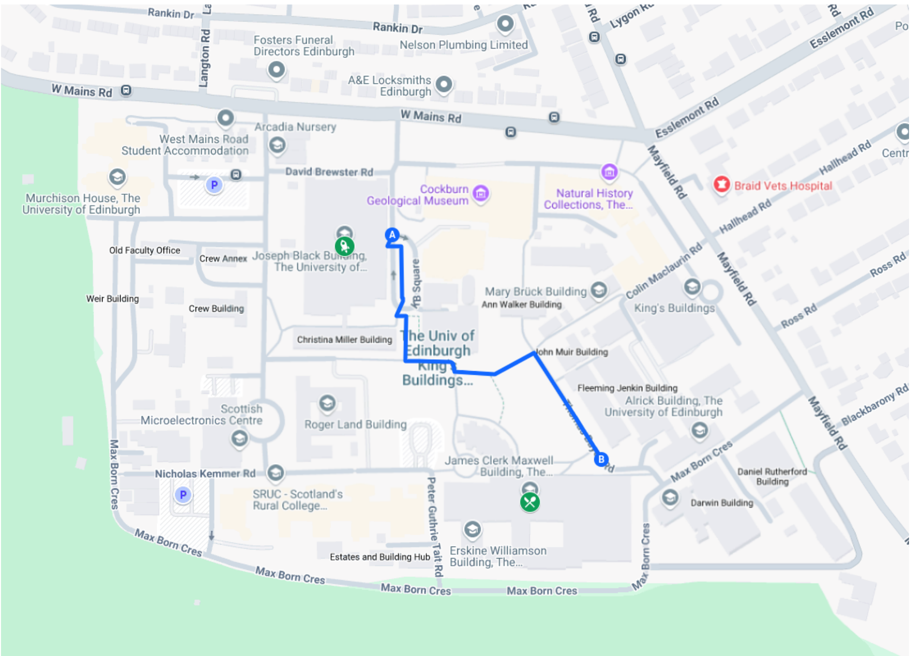
Organisers: Anastasia Istratuca, Christian Jiménez Beltrán, John Pearson, Aretha Teckentrup, Simon Urbainczyk

James Clerk Maxwell Building, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD

Schedule

	Tuesday (High-Dimensional PDEs)	Wednesday (Scientific ML)	Thursday (PDE-Constr. Optimization)	Friday (Data Assimilation)
09:00 - 10:15	–	Andrew Stuart	Roland Herzog	Jana de Wiljes
10:15 - 10:30	Registration	*Coffee Break*		
10:30 - 10:45			*Coffee Break*	*Coffee Break*
10:45 - 11:00	Welcome remarks	Andrew Stuart		
11:00 - 12:00	Catherine Powell		Roland Herzog	Jana de Wiljes
12:00 - 13:30	*Lunch*	Picture, *Lunch* & Poster Session	*Lunch*	Closing Remarks & *Lunch*
13:30 - 15:00	Catherine Powell	Konstantinos Zygalakis	Estefania Loayza R.	–
15:00 - 15:30	*Coffee Break*	–	*Coffee Break*	
15:30 - 17:00	Alison Ramage		ECR talks	
19:00 -	–	Conference dinner	–	

Time	ECR Talks Thursday
15:30 - 15:45	Panagiotis Paraschis
15:45 - 16:00	Jack Buckingham
16:00 - 16:15	Rowan Turner
16:15 - 16:30	Andrei Cataron
16:30 - 16:45	Heidi Wolles Ljósheim
16:45 - 17:00	Giacomo Borghi



King's Buildings Map

Contents

Lectures

High-dimensional PDEs (17/06/2025)

Parametric PDEs: An Introduction to Numerical Methods for Forward UQ and Surrogate Modelling

Speaker: Catherine Powell

Time: 11:00 – 12:00 and 13:30 – 15:00

Abstract: In applied mathematics we frequently encounter physics-based models consisting of partial differential equations (PDEs) with inputs such as material coefficients, boundary conditions and/or source terms that are uncertain in real-world settings. For example, in modelling the deformation of an elastic material, we might be uncertain about Young's modulus. In groundwater flow modelling, we might not have complete knowledge of the permeability of the rocks through which the water is flowing.

In uncertainty quantification (UQ), we represent uncertain model inputs as (functions of) random variables. The resulting PDEs may then be reformulated as parametric ones on a possibly high- (or even infinite-) dimensional parameter domain. In forward UQ, one aims to understand how uncertainty in model inputs affects uncertainty in model solutions. Naive sampling methods require the repeated numerical solution of the original PDE for different samples of the random inputs. When the cost of solving the problem for just one sample is already expensive (e.g. using a high-fidelity finite element method), obtaining accurate uncertainty assessments is infeasible.

Over the last three decades, many numerical schemes have been developed to tackle both forward and inverse problems involving PDEs with uncertain inputs. Some of these are known as surrogate modelling techniques because they produce approximations in a functional form that can be cheaply evaluated for new choices of input parameters of interest (without additional PDE solves). In this two-part session, we will first discuss appropriate ways to model spatially-varying uncertain PDE inputs, introduce the concept of parametric PDEs and review the basic Monte Carlo method. We will then give an overview of some of the most popular surrogate modelling methods for facilitating forward UQ in parametric PDEs, including stochastic collocation, reduced basis methods, and the so-called stochastic Galerkin method. We will focus on basic versions but if time permits, will also briefly mention more advanced adaptive and multi-level variants which are key to beating the curse of dimensionality, and the focus on ongoing research.

An Introduction to Iterative Solvers and Preconditioning

Speaker: Alison Ramage

Time: 15:30 – 17:00

Abstract: The efficient solution of large systems of linear equations arising from PDE models is of great practical importance in many areas of scientific computing and, as a result, impacts strongly on a wide range of disciplines in academia and technology-based industries. As the range and size of models has rapidly increased in the era of data science and high-performance computing, developing fast solvers for these new (and typically very challenging) problems continues to be extremely important.
This introductory lecture will give an overview of some popular iterative methods for solving the linear systems arising from numerical models of PDEs. The main ideas involved in choosing a suitable method and, where appropriate, an associated preconditioning technique, will be discussed and illustrated with some examples.

Scientific Machine Learning (18/06/2025)

Contrastive Learning and the Attention Mechanism

Speaker: Andrew Stuart

Time: 9:00 – 10:15

Abstract: A fundamental problem in artificial intelligence is the question of how to simultaneously deploy data from different sources such as audio, image, text and video; such data is known as multimodal. In this talk I will focus on the canonical problem of aligning image and text data, and describe some of the mathematical ideas underlying the challenge of allowing them to communicate. I will describe the encoding of text and image in Euclidean spaces and describe contrastive learning methods to identify and learn embeddings which align these two modalities; I will also describe the attention mechanism, a form of nonlinear correlation in vector-valued sequences. Attention turns out to be useful beyond this specific context, and I will show how it may be used to design and learn maps between Banach spaces or between spaces of probability measures.

Memorization in Diffusion-Based Generative Modeling

Speaker: Andrew Stuart

Time: 10:45 – 12:00

Abstract: Diffusion models have emerged as a powerful framework for generative modeling. At the heart of the methodology is score matching: learning gradients of families of log-densities for noisy versions of the data distribution at different scales. When the loss function adopted in score matching is evaluated using empirical data, rather than the population loss, the minimizer corresponds to the score of a time-dependent Gaussian mixture. However, use of this analytically tractable minimizer leads to data memorization: in both unconditioned and conditioned settings, the generative model returns the training samples. This talk overviews an analysis of the dynamical mechanism underlying memorization. The analysis highlights the need for regularization to avoid reproducing the analytically tractable minimizer; and, in so doing, lays the foundations for a principled understanding of how to regularize. Numerical experiments investigate the properties of: (i) Tikhonov regularization; (ii) regularization designed to promote asymptotic consistency; and (iii) regularizations induced by under-parameterization of a neural network or by early stopping when training a neural network. These experiments are evaluated in the context of memorization, and directions for future development of regularization are highlighted.

(Stochastic) Differential Equations, discrete approximations, and connections to optimization and sampling algorithms

Speaker: Konstantinos Zygalakis

Time: 13:30 – 15:00

Abstract: In this talk I will review some recent development that allow to analyse optimization and sampling algorithms through the lens of numerical analysis. In particular, many popular optimization and sampling algorithms can be cast in terms of numerical discretizing appropriate (stochastic) differential equations. Combining this view point together with appropriate ideas from control theory allows to analyse existing algorithms as well as understanding the structural conditions needed such that constructing algorithms with desired behaviour.

PDE-Constrained Optimization
(19/06/2025)

Introduction to PDE-Constrained Optimization

Speaker: Roland Herzog

Time: 9:00 – 10:30

Abstract: Optimization subject to PDE constraints comes in a variety of flavors, including optimal control, inverse problems, as well as shape and topology optimization. We give a brief overview over these problem types and then focus on optimal control problems for further discussion of the existence of solutions as well as optimality conditions. Concrete examples will be used to illustrate these concepts throughout the presentation.

Discretization in PDE-Constrained Optimization

Speaker: Roland Herzog

Time: 11:00 – 12:00

Abstract: While PDE-constrained optimization problems and algorithms for their solution can be discussed on the infinite-dimensional level, discretization must occur at some point in the solution procedure. A proper choice of this discretization is required in order for the discretized problems to inherit their properties from the infinite-dimensional counterpart. We will discuss some guidelines and caveats when carrying out these discretizations, with an emphasis on finite element approaches.

Computational Methods for PDE-Constrained Optimization Problems

Speaker: Estefania Loayza R.

Time: 13:30 – 15:00

Abstract: This lecture explores numerical methods for solving finite-dimensional unconstrained nonlinear optimization problems. We begin with a comprehensive examination of descent methods, which iteratively generate direction and step size information to decrease the objective function value using first and second-order derivatives.

The effectiveness of descent methods depends on two key factors: the choice of direction and the step size determination. We will analyze both elements, establishing properties that guarantee convergence. Four specific algorithms will be introduced, each characterized by a different choice of direction.

We will then apply these techniques to PDE-constrained optimization problems by utilizing the reduced functional approach, demonstrating how our algorithms can be adapted to handle discretized PDE-constrained problems effectively.

Finally, recognizing that many practical applications involve additional constraints on the control variables, we will develop the theoretical framework for box-constrained optimization problems. This section will feature two powerful solution techniques: the projected gradient method and semi-smooth Newton method.

Data Assimilation
(20/06/2025)

Modern Approaches in High-Dimensional Nonlinear Filtering

Speaker:	Jana de Wiljes
Time:	9:00 – 10:30 and 11:00 – 12:00

Abstract:

High-dimensional nonlinear filtering plays a crucial role in a wide range of applications, including atmospheric and oceanic data assimilation, robotics and autonomous systems, neuroscience, and personalized medicine. This lecture introduces modern strategies to overcome the challenges posed by high-dimensionality, highlighting methods such as ensemble-based techniques, particle filters, variational inference, and machine learning-inspired algorithms. We will discuss both theoretical underpinnings and practical implementations, illustrating key ideas through real-world examples. Participants will gain insight into current research trends and emerging directions in this rapidly evolving area.

Contributed Talks (19/06/2025)

hp-Version discontinuous Galerkin methods for the p-Laplacian

Speaker: Panagiotis Paraschis

Time: 15:30-15:45

Abstract: We consider the full discretization of the elliptic and parabolic p-Laplacian with discontinuous Galerkin methods. We analyze an hp-version interior penalty discontinuous Galerkin method for the elliptic p-Laplacian and a space-time discontinuous Galerkin method for the corresponding parabolic problem. With the help of new optimal hp-version quasi-norm trace-type inverse estimates, we derive stability and quasi-norm error bounds of optimal order with respect to the mesh-size and slightly suboptimal order with respect to the local polynomial degrees. The analysis of the interior penalty discontinuous Galerkin method for the elliptic p-Laplacian in meshes with curved polygonal/polyhedral elements with arbitrarily large numbers of faces, will also be discussed.
This is joint work with Konstantinos Chrysafinos and Emmanuil H. Georgoulis.

Bayesian Optimisation for Two-Stage Stochastic Problems

Speaker: Jack Buckingham

Time: 15:45-16:00

Abstract: Many real-world engineering problems involve designing the best 'something', and evaluating each possible design often requires slow and complex simulations. In this talk, I will introduce Bayesian optimisation, a method for efficiently solving such problems by using a probabilistic model – typically a Gaussian process – to predict the outcomes of unevaluated designs and guide the search. I will also show how this approach can be extended to solve two-stage stochastic optimisation problems. These are optimisations under uncertainty, where some design parameters must be chosen before the uncertainty is resolved while others can be chosen after. The result is a sample-efficient algorithm which can search simultaneously for the optimal design and the optimal control policy to accompany it.

A tailored, matrix free interior point method for fast optimization on gas networks

Speaker: Rowan Turner

Time: 16:00-16:15

Abstract:

We consider a PDE-constrained optimization problem arising from the prospective use of hydrogen as an energy carrier to support fully renewable electric grids. One important question is whether existing natural gas infrastructure can be reused for hydrogen to this end, and the challenges this brings for the control of these networks. We expect that a hydrogen network which uses gas generated from excess renewable electricity would be more difficult to control as the patterns of injection and withdrawal would be much less regular than today. Additional challenges arise from new operating parameters required for hydrogen – such as controlling for pressure fluctuations to prevent pipe-ageing. Motivated by a need for instationary optimization methods on networks at scale, we present a specialized, matrix free interior point method for gas problems. Our test problem is a line-pack optimization problem using a discretization of the 1d isothermal Euler equations, as a step towards understanding the important questions above. By incorporating a bespoke preconditioned iterative solver to tackle the linearized systems at each iteration of the interior point method, which form the key computational bottleneck in such a method, we utilize the highly structured nature of the problem to gain efficiency. The expectation is that the method will scale well with both network size and time windows, and be generalizable to broader PDE-constrained network optimization problems.

A regularising iterative algorithm for the Cauchy problem in elasticity

Speaker: Andrei Cataron

Time: 16:15-16:30

Abstract:

The numerical reconstruction of the solution to the system of linear (an)isotropic elasticity in a doubly-connected three-dimensional domain from overdetermined data, also referred to as Cauchy data, available on a part of the boundary is investigated. A regularising iterative method is employed to generate a stable numerical approximation to this severely ill-posed inverse problem. The method proposed herein is an extension of the Landweber iteration for an operator equation equivalent to the Cauchy problem. Numerical examples are presented in order to confirm the accuracy, convergence, stability and robustness of the algorithm.

Thinking in parallel: Preconditioning time-dependent mean field games

Speaker: Heidi Wolles Ljósheim

Time: 16:30-16:45

Abstract: Mean field games provide a powerful framework for modeling the collective behavior of large populations of interacting agents. In this talk, we present a class of time-dependent, variational mean field games formulated as PDE-constrained convex optimization problems. Using finite difference discretization in time, we solve the resulting finite-dimensional problem with a primal–dual algorithm.

A major computational challenge arises from repeatedly solving large, ill-conditioned linear systems at each iteration. We introduce a novel class of parallel-in-time preconditioners based on diagonalization via discrete Fourier transforms, enabling efficient and scalable solvers robust across a wide range of parameters. Numerical experiments demonstrate the improved performance and parallel scalability of the approach, highlighting its potential in large-scale PDE-constrained optimization.

Multi-agent optimization in the space of Gaussian measures

Speaker: Giacomo Borghi

Time: 16:45-17:00

Abstract: Multi-agent systems are commonly employed in finite-dimensional optimization to identify global minima of potentially non-differentiable objective functions. In this talk, we extend this paradigm to address optimization problems in the space of Gaussian probability measures by introducing Gaussian-valued agents. These agents evolve according to stochastic consensus dynamics based on the Bures-Wasserstein geometry of the space. Numerical experiments on a Gaussian Variational Inference problem demonstrate the effectiveness of the approach and provide comparisons with gradient-based methods.

Poster Presentations (18/06/2025)

Least-squares p and hp-Spectral Element Methods for Two-dimensional Elliptic Boundary Layer Problems

Speaker: Sonia

Time: 12:00-13:30

Abstract:

Boundary layers are rapidly varying solution components that arise in singularly perturbed boundary value problems. These layers typically arise in narrow regions near the domain boundary and appear across a wide range of applications. Standard numerical methods fail to resolve these layers and specially designed numerical methods are required to resolve these layers accurately and efficiently with approximations in suitable sobolev spaces which accounts for the boundary layer parameter.

We propose non-conforming least-squares p and hp spectral element methods for two-dimensional elliptic boundary layer problems on rectangular domains. We derive stability estimates and numerical schemes based on minimizing a least-squares functional and prove parameter robust error estimates. The method is able to approximate boundary layers at a robust rate $O\left(\frac{\sqrt{\log W}}{W}\right)$ for the $p-$version and at the rate $O(\sqrt{\epsilon}\alpha^W)$ for the $hp-$version, where $0 < \epsilon \leq 1$ is the boundary layer parameter, $\alpha < 1$ is a constant and W denotes the degree of the approximating polynomial. Numerical results demonstrate that the proposed method captures boundary layers with high accuracy, confirming its effectiveness and stability, in the presence of sharp solution gradients.

Building a numerical solver for Dirac Solitons

Speaker: Felipe Arevalo Escobar

Time: 12:00-13:30

Abstract:

Dirac solitons (or Dirac Stars) describe the structures that form from the coupling of the Dirac equation to a set of classical gravitational field equations, like Einstein's general relativity or conformal gravity. We have worked towards building a numerical solver capable of obtaining solutions for a variety of such structures using techniques inspired by attempts at relaxation methods, transposed to standard function minimization methods. Aiming to encapsulate solutions across varying symmetries and theories of gravitation.

Online learning of stochastic closures of quasi-geostrophic turbulence

Speaker: Martin Brolly

Time: 12:00-13:30

Abstract:

Stochastic parameterisations are essential for representing the uncertainty introduced when numerical models neglect certain scales or components of the Earth system. Moreover, the specific structure of stochastic parameterisations is critical to representing this uncertainty accurately. A ubiquitous (though generally invalid) assumption is that of Markovianity. Computational constraints mean that Markovian parameterisations are much preferred in practice, but identifying optimal Markovian approximations is far from trivial. We propose an "online" data-driven approach to learning Markovian parameterisations, wherein the dynamics of the parameterised model feature explicitly in the loss function, which is based on a proper scoring rule. We apply the method to the problem of subgrid closure in an idealised model of geophysical turbulence. We find significant improvement over offline approaches in both the "weather" and "climate" paradigms.

Integrating Multimodal Cell Imaging with Mathematical and AI Models

Speaker: Kirsty Cowie

Time: 12:00-13:30

Abstract:

Integrating different imaging modalities provides a more comprehensive understanding of tissue at the cellular level, which is essential for understanding disease and advancing drug development. Hematoxylin and Eosin staining (H&E) is widely used in clinical practice and provides detailed tissue morphology. Mass Spectrometry Imaging (MSI) reveals the spatial distribution of metabolites and proteins while Spatial Transcriptomics (ST) maps gene expression patterns. MSI and ST are modalities which offer key molecular information however they are more expensive and less readily available than H&E. This project aims to develop mathematical and AI models to link these modalities, using H&E as a bridge to then predict MSI and ST data. A key part of this process is image registration, where the goal is to align a moving image (here MSI or ST) to a fixed image (H&E) by finding a transformation, denoted ϕ. Although many affine and non-rigid registration techniques exist, using a mixture of more classical mathematical models to more modern deep learning approaches, they often struggle with aligning multi-modal data due the differences in appearance and content. Current progress and future plans of integrating these modalities will be outlined with the aim of sparking discussions which could help shape the future directions of the work.

Adaptive sparse grid surrogate modeling for uncertainty quantification in large-scale vibroacoustic systems

Speaker: Robin Eßling

Time: 12:00-13:30

Abstract: This work presents an adaptive sparse grid surrogate modeling strategy for uncertainty quantification in large-scale vibroacoustic systems. In the frequency domain, the underlying linear systems depend on a large number of uncertain inputs, e.g. material parameters, in addition to frequency. As a result, computing statistical moments of the output quantities requires solving the underlying system so frequently, that it becomes practically infeasible – especially over a large frequency range. To overcome these challenges, we construct an accurate multi-moment matching reduced order model, based on a global projection matrix. While this approach can yield accurate surrogates for a small number of inputs, it becomes computationally expensive again in highdimensional settings due to the large number of resulting multi-moments. We therefore embed the construction of the global projection matrix within an adaptive sparse grid framework in order to refine only the expansion points corresponding to the sensitive input parameters.This enables the construction of a global sparse projection basis of moderate dimension with acceptable approximation errors. The method will be illustrated by numerical results for platecavity coupled models.

Development of Mathematical Models Based Deep Learning Algorithms for Selective Image Segmentation

Speaker: Jacqueline Fergusson

Time: 12:00-13:30

Abstract:

Image segmentation is the process of dividing an image up into separate meaningful regions with the goal of automatically identifying shapes or features. This is done by grouping together pixels that have similar characteristics such as intensity or texture. There are two main types of segmentation: global and selective. Global segmentation segments all objects within an image whereas selective segmentation segments a specific region of interest (ROI). Selective segmentation requires some user input and is an important task in medical imaging. Current variational methods struggle to segment noisy or cluttered images with histology images being amongst the most challenging. However, recent advancements in both deep learning methods and digital pathology provide potential opportunities for improvements.

This work will consider a new variational model for performing selective image segmentation which is based on the Roberts-Chen model (Journal of Math. Imaging & Vision, 61 (2019), pp. 482-503). The Roberts-Chen model uses a constrained convex variational approach which combines the edge-based approach of geodesic-active contours (International Journal of Computer Vision, 22 (1997), pp. 61-79) with the region-based approach of Chan-Vese (IEEE Transactions on Image Processing, 10 (2001), pp. 266-277). In addition, it also includes an edge-weighted geodesic distance penalty term which measures distance from the user input data.

We propose an alternative form of geodesic distance term based on the formula for arc length. A more insightful distance term means the extraction of more information from the user input data and thus a more accurate segmentation result. We will therefore present results from our preliminary experiments showing the advantages of this new method.

In future work, we plan to investigate how our model translates to the segmentation of 3D images, particularly for the analysis of MRI scans. Also, we will apply our model to the segmentation of histology images with the aim of producing labelled segmentation data which may be used to perform supervised learning with a deep learning model. Currently, acquiring labelled data for histology images is incredibly time and labour intensive so the automation of this process would be favourable.

Optimisation algorithms and surrogate models for drainage systems

Speaker: Emilie Herpain

Time: 12:00-13:30

Abstract: Due to climate change, extreme weather events are getting increasingly more frequent. Run-off phenomena and flooding pose a serious risk, especially in urban areas. Relying solely on resistance-based strategies does not suffice. Rather, a more holistic approach to flooding should be undertaken, encompassing prevention, protection, mitigation, preparation and recovery. Sustainable drainage systems (SuDS) and nature-based solutions can help in these respects and their benefits could outweigh traditional drainage features, such as cost, longevity and impact. This project aims to build a framework which optimises urban features such as drainage systems by looking at objectives such as cost, impact, longevity and bio-diversity. In doing this, we build a surrogate model which is computationally more efficient than traditional numerical methods in order to estimate the impact of the optimised drainage feature on the rest of the network. The computational efficiency aspect is crucial for drainage engineers who look at drainage networks of considerable size. This project is only in its very beginnings and draws on new research from sustainable drainage systems to nature-based solutions and ML techniques such as artificial neural networks.

Deep Operator Networks for data assimilation problems in PDEs

Speaker: Trung Hieu Hoang

Time: 12:00-13:30

Abstract: We study the solution of unique continuation problems using Deep Operator Networks. Given measurements of fluid flow in part of the domain, can we reconstruct the flow everywhere? We consider noisy, irregular or sparse measurements, generated from synthetic simulations using high-fidelity numerical solutions. Beyond the Stokes problem for fluid flows, we consider wider classes of elliptic and parabolic partial differential equations, with partially given data for the solution.

Improving Markov Chain Monte Carlo Estimates using a Reweighting Algorithm

Speaker: Joel Jones

Time: 12:00-13:30

Abstract:

Markov Chain Monte Carlo (MCMC) has been the golden standard in Bayesian inverse problems for sampling from a posterior distribution and thereby producing Monte Carlo (MC) estimates for key quantities of scientific interest and associated uncertainties. However, as is well-known, issues with slow convergence rate and poor mixing, particularly in the context of high per-sample cost, can lead to poor MC estimates. This is especially true in cases with a multimodal posterior.

While the distribution of posterior samples is often used in diagnosis and improvement of MCMC performance, the values of the target function (usually up to proportionality) evaluated at these samples is less commonly exploited. Here, we introduce an algorithm that uses such target function values to calculate a weight for each sample in order to produce more accurate MC estimates without requiring further sampling. The aim is to produce a continuous estimate for the posterior probability density and use it to reweight the discrete histogram estimate from the accepted MCMC samples.

Using Gaussian Process (GP) regression on the proposed samples and their densities from the MCMC algorithm - which are usually discarded - we can produce this estimate for the posterior probability density function that covers a larger part of the state space than the accepted samples. Then the weights can be found either by calculating the ratio between each bin height and the GP mean estimate or by an optimisation scheme to minimise some distance measure between the histogram and GP mean. Two main examples are shown, firstly in the case with a limited number of samples and secondly a bimodal distribution. In both cases the reduction in relative error for MC estimates is shown.

Steering Probability Distributions via PDE-Constrained Optimisation

Speaker: Lucas Machado Moschen

Time: 12:00-13:30

Abstract:

Fokker–Planck equations often arise as macroscopic descriptions of interacting particle systems in the mean-field limit. These models capture important collective phenomena, and due to non-convex confining potentials or small spectral gaps, their convergence to equilibrium can be slow. We investigate PDE-constrained optimisation strategies aimed at improving convergence rates in this setting. The first approach focuses on the linear Fokker–Planck equation, reformulated through a ground state transformation into a Schrödinger-type operator. We compute open-loop controls using a gradient-based method, aiming to attenuate slow-decaying modes. The second one targets the nonlinear and nonlocal Fokker–Planck equation, known as the McKean–Vlasov equation. By linearising the dynamics around a steady state, we derive a linear-quadratic optimal control problem whose solution provides a feedback law via an operator Riccati equation. This feedback has the goal of accelerating convergence or stabilising otherwise unstable equilibria. Preliminary numerical results based on spectral methods suggest that both strategies can enhance relaxation in models with challenging energy landscapes.

Deep Learning-Enhanced Algorithms for Efficient X-ray Ptychographic Reconstruction

Speaker: Alan Muriithi

Time: 12:00-13:30

Abstract:

X-ray ptychography is a scientific imaging technique which enables high resolution imaging of small-scale objects at the expense of solving an inverse problem to form an image. Recent growth in dataset size, dimensionality, and data throughput present significant computational challenges for traditional iterative reconstruction algorithms, which will exacerbate the delays already faced during inference. Additionally, existing reconstruction algorithms for ptychography often require experiment-specific hyperparameter tuning for meaningful convergence, creating bottlenecks in the research pipeline. This work introduces a novel framework that integrates deep learning techniques— including importance sampling, momentum-based optimization, and variance reduction methods—for ptychographic image reconstruction. My approach significantly reduces computational complexity while maintaining reconstruction quality, resulting in a robust algorithm with demonstrably compute requirements.

Computation of stabilization parameters using machine learning

Speaker: Manoj Prakash

Time: 12:00-13:30

Abstract: In convection-dominated regimes, traditional stabilization methods often encounter significant drawbacks: they are either computationally expensive or induce numerical oscillations. In this work, we propose a novel approach that integrates a machine learning model to predict a better stabilization parameter than the standard one used in SUPG. Our methodology employs a neural network that extracts important local features of the problem from a coupled SUPG-Tabata frame- work, predicting a more appropriate stabilization parameter for the SUPG method. This approach not only aims to reduce computational cost but also mitigates oscillatory inaccuracies, ultimately enhancing the reliability of numerical simulations in convection-dominated environments.

Neural Network Methods for Power Series Problems of Perron-Frobenius Operators

Speaker: Tanakorn Udomworarat

Time: 12:00-13:30

Abstract: Perron-Frobenius operators play an important role in capturing behaviors of dynamical systems. One particularly interesting problem involves finding the power series of these operators applied to a given initial density, which has direct applications in determining equilibrium energy distributions. In this work, we propose neural network methods for approximating the power series of Perron-Frobenius operators that are non-expansive under a given L^p-norm with a constant damping parameter in $(0, 1)$. We use Physics-Informed Neural Networks (PINNs) and Robust Variational PINNs (RVPINNs) to approximate solutions in their strong and variational forms, respectively. Additionally, we provide a priori error estimates for quasi-minimizers of the associated loss functions. Finally, we present some numerical results for 1D and 2D examples to support our theoretical results.

Bayesian Optimisation Techniques for PDE-Constrained Optimisation Under Uncertainty

Speaker: Eliott Van Dieren

Time: 12:00-13:30

Abstract: PDE-constrained optimisation under uncertainty arises in robust design applications, such as aeronautics, shape optimisation, and manufacturing. However, these problems often lead to non-convex cost functions, which challenge gradient-based optimisation algorithms due to local minima. Furthermore, the PDE-constrained setting implies a high computational cost, since a random PDE must be solved at each evaluation of the cost function. To address these issues, we explore Bayesian optimisation methods to identify optimal parameters that minimise the cost function. The adjoint state method provides computationally efficient gradient information, which can enhance Bayesian optimisation via gradient-enhanced Gaussian processes. We present numerical results using both standard and gradient-enhanced Bayesian optimisation for PDE-constrained problems.

Exponential Ergodicity of Path-Dependent McKean-Vlasov SDEs under Non-Uniform Dissipation

Speaker: Haitao Wang

Time: 12:00-13:30

Abstract: In this poster, we mainly explore the following stochastic differential equation (SDE):

$$dX(t) = \big(b_1(X(t), \mathcal{L}_{X(t)}) + b_2(X_t, \mathcal{L}_{X(t)})\big)\, dt + \alpha\, dB_1(t) + \sigma(X(t))\, dB_2(t),$$

where $(X_t)_{t\geq 0}$ is the segment process, and $\mathcal{L}_{X(t)}$ denotes the distribution of $X(t)$ for $t \geq 0$. Due to the non-Markovian property, traditional analytical methods face significant challenges.

We assess exponential contraction of the solution's distribution in the W_p distance under non-global dissipative conditions—positive within a certain radius from the origin, negative outside this localized region—for the drift coefficient b_1. Unlike the globally dissipative case, we construct a weighted Wasserstein distance equivalent to the traditional Wasserstein distance by designing a suitable weighting function, thereby overcoming the challenge posed by insufficient dissipativity in certain regions. Consequently, we establish the existence of a unique invariant probability measure, demonstrating exponential convergence property.

Semi-Supervised Medical Image Segmentation with ADMM-Based Energy Regularization

Speaker: Qian Wang

Time: 12:00-13:30

Abstract: This paper addresses the problem of data scarcity by choosing a suitable energy functional as a loss function in a semi-supervised framework. Inspired by the variational model proposed by Wei et al. (2017), in which the Potts Energy functional is minimized using a region force derived from the negative log-likelihood of the Bernoulli distribution, instead of assuming fore and background intensities are respectively constants, this study investigates which form of the loss function works well with a U-Net based deep learning. In contrast to the classical Chan–Vese model, which is susceptible to local minima due to its non-convex formulation, a convex relaxed Potts energy model enables global optimization. However, the energy function is still too nonlinear as a loss function and hence leads to poor results. An ADMM-based optimization strategy, as done in the work of Wei et al., is able to enhance convergence, stability, and computational efficiency. We found that when incorporated as a loss term into a deep neural network, the energy term serves as a regularization prior that mitigates the limitations of neural networks in enforcing spatial coherence and boundary consistency, particularly in the presence of irregular or noisy lesion boundaries. Furthermore, this integration alleviates the reliance on large-scale labeled data, thereby enhancing the applicability of deep learning models to semisupervised segmentation scenarios. Numerical experiments will be shown to demonstrate the advantages of the proposed semi-supervised algorithm for effective segmentation.

A Posteriori Error Control & Adaptivity for Vector-Valued Schrödinger Equations with Conical Crossings.

Speaker: Yilin Wang

Time: 12:00-13:30

Abstract: In this work, we aim to develop a posteriori error control and adaptive strategies for time-dependent two-level Schrödinger systems with conical crossings. As a foundational step, we begin by constructing a posteriori error estimators for the fully discrete scheme of the one-dimensional linear semiclassical Schrödinger equation using time-splitting spectral methods, specifically the Lie and Strang schemes. These methods are widely used for their efficiency and effectiveness in capturing the oscillatory behaviour of the semiclassical regime. By reconstructing a time-continuous approximation from the discrete time-splitting spectral solutions, we derive computable residual terms that quantify the deviation from the exact solution. These residuals are then used to obtain rigorous a posteriori error bounds, which provide guaranteed accuracy estimates without requiring knowledge of the exact solution. We further prove that the estimators decrease at the same rate as the true error, ensuring reliability and efficiency. This work lays the groundwork for future extensions to adaptive time-stepping strategies and more complex systems, such as the two-level Schrödinger equation with conical crossings.