

## **MIGSAA Industry Stream**

### **Fully funded 4-year projects.**

Students on this stream of MIGSAA are admitted to work on a pre-arranged project in collaboration with industry or a non-university body. The studentship is fully-funded for 4 years, sometimes by the external partner. Students follow the same programme of mathematical and generic skills training as the other MIGSAA students during their first and later years, and are based together with the rest of the MIGSAA cohort. Work on the project itself usually starts in the Spring of the first year at the same time as the projects for the other students. The main differences are that the main project topic and supervisory team are fixed from the start, and the project includes work with the external partners. This provides a very valuable experience for future careers.

Students can get further information about these projects by contacting the supervisors directly.

Applications should be made by the standard MIGSAA mechanism, but note on your application that you are interested in the Industry Stream and give the name of the project.

## **Projects for Entry in 2018**

### ***1. Energetic Materials and Blow-up***

**Supervisors:** Dr H Gimperlein <[H.Gimperlein@hw.ac.uk](mailto:H.Gimperlein@hw.ac.uk)> and  
Prof A A Lacey <[A.A.Lacey@hw.ac.uk](mailto:A.A.Lacey@hw.ac.uk)>, Heriot-Watt University  
**Company:** A UK defence company

Highly energetic materials can undergo dramatic temperature change, due to the interplay of exothermic chemical reactions with material deformations, when they are subjected to some external forcing. This can lead to a possible explosion.

To lower the risk of damaging accidental explosions during handling, coupled models for the mechanical motion and the chemical reactions need to be investigated, ideally both analytically and numerically. The equations governing the behaviour of the material itself, as found from experiments, must also be better understood. It is then especially important to study experiments, which can involve simple geometries, on such energetic materials mathematically, through modelling, analysis and numerical methods. Cases where temperature blows up will be of particular interest.

This project and funding is only available to UK-based applicants, which includes EU nationals who have been resident in the UK for the last 3 years or more.

## **2. Incorporating Deep Learning Approaches in High-Dimensional Bayesian Inference Methods. Application to Satellite Imaging.**

### **Supervisors:**

Dr Marcelo Peyera <M.peyera@hw.ac.uk> Heriot-Watt University, and

Dr Kostas Zygalakis <kzygalak@ed.ac.uk> University of Edinburgh

**External Agency:** CNES, the French space agency

Modern data science relies strongly on probability and statistics to solve challenging problems. In this context, statistical models are used to represent the raw data observation process and the prior knowledge available; and solutions are obtained by performing (often Bayesian) statistical inference analyses, computed by using sophisticated computational statistics techniques. Traditionally the prior knowledge is incorporated into the Bayesian model by a function with a specific functional form.

In this PhD project we will investigate new Bayesian methods that use Deep Learning approaches, particularly neural networks, to incorporate prior knowledge in the form of training examples or datasets. More precisely, our starting point will be the Langevin stochastic differential equation (SDE) which will be used as a computational engine in order to obtain Monte Carlo samples from the Bayesian posterior distribution [2]. However, instead of using the traditional approach of explicitly defining the functional form of the SDE, here the terms of the SDE related to the prior distribution will be represented implicitly by using neural networks. This is a paradigm shift to the conventional modelling approach that raises important mathematical questions of fundamental nature, such as well-posedness, stability and long term behaviour of the SDE, and of practical nature related to its numerical solution [1].

This project will be done in close collaboration with the French space agency (CNES), with the aim of applying the novel framework developed to mathematical imaging problems related to satellite imaging, using real satellite data provided by CNES. In addition, another collaborator in the project will be Prof. Jean-Yves Tournet from the University of Toulouse, who is a world-leading expert in Bayesian image processing and has worked extensively in satellite image analysis. It is expected that the PhD student will spend some portion of his time visiting CNES Toulouse and Prof. Tournet, working in a strongly interdisciplinary environment at the interface of statistics, probability, numerical analysis, optimisation, computer science, physics, and image processing engineering.

[1] A. Abdulle, G. Vilmart, and K.C. Zygalakis, High order numerical approximation of the invariant measure of ergodic SDEs. *SIAM J. Numer. Anal.*, 52(4):1600-1622, (2014).

[2] A. Durmus, E. Moulines, and M. Peyera, Efficient Bayesian computation by proximal Markov chain Monte Carlo: when Langevin meets Moreau. *SIAM J. Imaging Sci.*, 11(1): 473-506, (2018).

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### **3. A New Generation of Explicit, Numerical Algorithms for Stochastic Systems**

**Supervisor:** Dr Sotirios Sabanis <[S.Sabanis@ed.ac.uk](mailto:S.Sabanis@ed.ac.uk)> University of Edinburgh

**Company:** Aberdeen Standard Investments

The aim of the project is to develop and implement a new generation of explicit, numerical algorithms for stochastic systems (including those with non-linear coefficients) so as to tackle challenging data science problems in high-dimensional settings and, specifically: (i) within the framework of MCMC algorithms with emphasis on unadjusted Langevin algorithms; (ii) in stochastic gradient methods for a wide class of data, not necessarily Markovian, in the context of global optimization for non-convex functionals, and, (iii) with a particular focus in benchmark examples in Finance (such as portfolio optimization) in collaboration with the industrial partner Aberdeen Standard Investments.

In particular, with the recent breakthrough (Brosse et al, 2017) in unadjusted Langevin (MCMC) algorithms for sampling from high-dimensional distributions, a new avenue is open for developing new methodology, which can play an important role in Bayesian inference. The use of this new technique enables a much larger variety of target distributions, since we can now include terms (i.e. coefficients of stochastic systems) which are superlinear at infinity. The new version of the unadjusted Langevin algorithm also has the desirable feature to include a kind of “self-normalisation”, which makes the algorithm much more robust to the choice of the stepsize/gain/learning rate which is otherwise rather difficult to identify.

We aim to study these desired properties under different regimes and scenarios which will include for example discontinuities for the gradient term or partial information. Further, we aim to present concrete theoretical results in the aforementioned direction which will crucially help the implementation of such algorithms, e.g. optimal selection of stepsize/gains/learning rates. Moreover, the interplay between the newly developed theory and the framework of stochastic gradient Langevin dynamics will be examined under the influence of the newly developed techniques.

Particular attention will be given to the practical implementation of the new algorithms as they are naturally parallelizable and thus ideal to be used in a cloud computing environment. Further, suitable problems will be identified in economics/finance and machine learning with the help of the industrial partner (Aberdeen Standard Investments) so as to serve as benchmark examples for the quality of our findings.

[1] Brosse, N., Durmus, A., Moulines, E. and Sabanis, S.: “The Tamed Unadjusted Langevin Algorithm,” (2017) ArXiv:1710.05559 [stat.ME].

[2] Chau, H. N., Kumar, C., Rásonyi, M. and Sabanis, S.: “On fixed gain recursive estimators with discontinuity in the parameters,” (2016) ArXiv:1609.05166 [math.PR]

[3] Durmus, Alain; Moulines, Éric.: Nonasymptotic convergence analysis for the unadjusted Langevin algorithm. *Annals of Applied Probability* 27 (2017), no. 3, 1551--1587. doi:10.1214/16-AAP1238

[4] G. Fort, E. Moulines, A. Schreck, and M. Vihola, Convergence of Markovian stochastic approximation with discontinuous dynamics, *SIAM J. Control Optim.* 54 (2016), pp. 866–893

[5] Sabanis, S. : Euler approximations with varying coefficients: the case of superlinearly growing diffusion coefficients, *Annals of Applied Probability*, Vol. 26, No. 4 (2016), pp. 2083-2105

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#### **4. Smart Energy Storage and Uncertainty**

**Supervisor:** Dr Markus Schmuck, Heriot-Watt University  
**Company:** Denchi Power Ltd.

The increasing global awareness of the need to reduce CO<sub>2</sub> leads to a growing interest in renewable energy (renewables) and associated alternative transport and production technologies. Such developments require novel and efficient strategies to store, deliver, and price energy from sustainable sources such as solar and wind. The main challenges are uncertainties in demand and weather. Batteries are playing an increasingly important role in this context and hence are the main focus of this project. We will develop an optimal control framework for maximising the performance of application specific, battery banks based on the information about usage and uncertainties in demand and in the availability of renewable energy. This leads to a complex optimisation problem relying on entirely different systems operating on different and multiple scales. We will resolve these challenges by combining mathematical optimal control strategies with novel data-driven methods extending state of the art techniques such as time series and machine learning methods based on neural networks (deep learning).

The project is in association with Denchi Power Ltd. They are a leading producer of batteries operating in extreme conditions as well as a provider of large battery systems for grid, industry, residential, and marine usage. This project will also stimulate the interaction and collaboration with existing collaborators from Imperial College (Chem. Eng. & Maths), ETH Zurich (Materials Science), MIT Boston (Chem. Eng. & Maths), and University of Alberta (Department of Science) just to mention a few.

The project requires strong programming skills (C, C++, Python, or Java), preferably Python. Good mathematical knowledge in machine learning, statistical methods, and probability theory. Of advantage will also be experience in one or more of the following topics, i.e. numerical methods for PDEs, optimal control, time series, dynamical systems, and uncertainty quantification.

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## **5. Deep-Learning Reduced Order Models for Uncertainty Quantification of Subsurface Reservoirs**

**Supervisors:** A.H. Elsheikh and G. Lord, Heriot-Watt University

The aim of this project is to develop data-driven Reduced Order Models (ROM) as a replacement to physics-based subsurface flow models for statistical forecasting tasks. Data-driven ROMs will be built using Deep-learning (DL) techniques. The developed ROMs will be built (i.e. learned) using a set of full physics simulation runs representing the various sources of geological and model uncertainties. Further, the reduced order model will be iteratively enriched with more training samples (i.e. simulation runs) close to the target distribution mimicking importance sampling techniques (aka. active learning). The proposed framework will build on recent advances in deep learning for real-time fluid simulation and the recently introduced deep residual recurrent neural networks.

**Note:** This project is available to both national and international students. It also involves spending some time at the sponsor research offices in Houston, USA.

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## **6. Multiscale Diffusion Modelling for Swarm Robotics**

**Supervisor:** H. Gimperlein, Heriot-Watt University

Biological organisms have found efficient strategies to move and disperse in search of randomly located targets, like food. Swarm robotics aims at developing bio-inspired computational models usually combined with machine learning techniques to allow robots to autonomously explore areas for tasks like search-rescue missions, monitoring, surveillance, forest fire combat and agricultural applications, just to name a few. The use of robotic agents instead of human beings may add security, reliability and efficiency.

A main mathematical approach for understanding the biological organisms' movement or robots' movement relates it to diffusion problems. This project derives macroscopic diffusion equations for the dispersion of robot swarms and uses them to develop efficient search strategies. The strategies are evaluated in numerical simulations, with physical simulation tools as well as with real robots.

Diffusion equations are long-studied for biological or physical systems, such as the Keller-Segel model for cell movement in the presence of chemical cues. Robotic systems open up new possibilities of interaction, coordination and control. They lead to challenges in the mathematical analysis and the development of algorithms. In particular, the macroscopic description allows the efficient optimisation of movement rules and real-time learning and evaluation of strategies.

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