INI Programme on Uncertainty Quantification (UNQ)

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Organisers: Catherine Powell (University of Manchester), Max Gunzburger (Florida State University), Peter Challenor (University of Exeter), Henry Wynn (London School of Economics).

Scientific Committee: Dave Woods (University of Southampton), Wolfgang Dahmen (University of South Carolina), Andrew Stuart (Caltech), Serge Guillas (University College London).

Rothschild Distinguished Visiting Fellow: Andrew Stuart (Caltech).

Simons Fellows: Claudia Schilling (Universität Mannheim), Masoumeh Dashti (University of Sussex), Catherine Powell (University of Manchester), Ron De Vore (Texas A&M University), Max Gunzburger (Florida State University), Peter Challenor (University of Exeter), Serge Guillas (University College London), Henry Wynn (London School of Economics), Lindsay Lee (University of Leeds).

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1. Background

In areas as diverse as climate, manufacturing, energy, life sciences, finance, geosciences and medicine, mathematical models and their discretizations into computer models (numerical algorithms) are routinely used to make forecasts, inform decisions and formulate policies. Naturally one asks: how accurate are the predictions made using such models? This crucial question lies at the heart of uncertainty quantification (UQ).

Today, UQ is a broad phrase used by scientists to describe methodologies for taking account of uncertainties when mathematical and computer models are used to describe real-world phenomena. When we use models to simulate real-world processes (e.g., the weather, the temperature in a jet engine), the quantities we compute have uncertainty in them due to (i) model error/discrepancy; (ii) uncertainty in inputs/parameters for the model(s); (iii) errors associated with the use of numerical algorithms (computer models) and (iv) measurement errors. UQ is vital for model-based science and associated decision making. Ignoring uncertainty can lead to overly confident (and potentially incorrect) decisions due to the underestimation of risk. At the same time, being too cautious when faced with uncertainty can also lead to bad decisions.

Modern society is challenging UQ science with the scale and complexity of the models required to solve real-world problems, and the rapidly growing amount of data available to help develop and validate models. Today, UQ involves far more than implementing Monte Carlo methods to propagate uncertainty from model inputs to computer model outputs. It includes the study of uncertainty in the form of models themselves; the careful design of physical experiments to collect informative data; developing numerical approximation schemes that result in cheap yet accurate computer models; model calibration and other inverse problems; the study of model bias and discrepancy as well as analysis of approximation errors. Thus, UQ is a highly interdisciplinary field which combines aspects of applied mathematics, numerical analysis, computational science, probability, statistics and applications.

Having a six-month research programme on UQ in the UK was long past due. There has been an explosion of UQ research activity over the last decade with new UQ-themed journals, research groups and conferences appearing all the time. There have been several international initiatives to try and build connections across the mathematical and statistical sciences on the topic of UQ, but few specifically in the UK. The biennial SIAM (Society for Industrial and Applied Mathematics) conference on UQ, which is held in cooperation with the ASA (American Statistical Association) and GAMM (Gesellschaft for Angewandte Mathematik und Mechanik) UQ Activity Group is now a large international event, attracting over a thousand participants. The jointly run SIAM/ASA journal on UQ is also well established, publishing papers across a range of mathematical disciplines. Large UQ research programmes have been held outside the UK at institutes such as SAMSI (The Statistical and Applied Mathematical Sciences Institute). Despite these efforts, it is widely acknowledged that significant barriers remain to establishing meaningful collaborations at the interface of applied mathematicians and statistics. This can be attributed in part to educational infrastructures (it is still the case that teaching and research is split up into applied mathematics, pure mathematics, and probability & statistics in many UK universities) but also due to fundamental differences in approaches to modelling and in the different criteria adopted by different groups of scientists to measure success/accuracy of results. It is not simply the case, as is often perceived, that different groups use different methods to perform the same UQ task. The culture and mindsets as well as the goals of researchers in each discipline are different.

The language of probability is used by most mathematicians and statisticians to express beliefs about uncertain quantities. This is a common point of understanding. However, there are fundamental differences between disciplines. For example, numerical error associated with 'simulators', unlike model error, often has an identifiable source and can in theory be controlled. Traditional numerical analysis approaches seek deterministic statements about errors in computer model outputs. Knowledge of the underlying continuous model and the adopted numerical scheme is heavily exploited to determine bounds for and computable estimates for the error. In contrast, statistical approaches often do not exploit such knowledge and simply treat numerical errors, together with other uncertainties, in a Bayesian fashion. However, because of this, statistical approaches can often be used in a more black-box way and may be more readily applicable to complex models, where traditional numerical analysis is less well developed or not available at all.

Thus, the primary objective of the research programme was: *to bring **applied mathematicians and statisticians together** to formulate a common foundation for UQ and to establish long-lasting interactions that will lead to advances in UQ theory and methodologies for complex systems.* A secondary objective was *to establish interdisciplinary UQ collaborations **within the UK**.*

2. Programme Outline

There were around 100 programme participants (PPs), with visits lasting between two weeks and six months. To prevent PPs retreating into their disciplinary silos, it was important to organise the programme around broad scientific themes of common interest. Thus, the core themes were: **Surrogate Modelling; Multilevel & Multifidelity Methods, Dimension Reduction Methods** and **Inverse UQ.** Workshops associated with these themes were held in January, February, March and April. There is clearly some overlap between these themes. For instance, surrogate modelling and dimension reduction techniques are required to help ameliorate the extreme computational burden of solving inverse problems involving complex forward models. The reason for delaying a workshop on inverse problems until April was so that progress made on topics addressed in earlier workshops could be directly fed into that workshop and its follow-on activities.

2.1 Programme Activities. Outside of workshop weeks, group activities such as seminars and focussed discussion/reading groups took place. Informal discussions also took place over coffee on most days which were both technical and philosophical in nature. At the start of each week, a group meeting was held over morning coffee. Informal discussions were held with new PPs to establish common research interests. This helped the organisers to plan appropriate activities and connect people working on similar issues. New PPs were also encouraged to give seminars.

Seminars. Seminars were held two or three times a week, depending on the number of PPs in residence. Many PPs reported that they found giving a seminar to be extremely beneficial (and exhausting!). Indeed, many seminars lasted for two hours or more, with the record being three and a half hours. Since the audience was far more diverse scientifically than would usually be the case when delivering a standard University seminar or conference talk, most seminars stimulated a lot of questions and scientific debate. Many speakers also found that giving a seminar led to further one-on-one conversations with other participants which have since proved fruitful in terms of developing ideas for new grants and joint publications.

Discussion Groups. At the start of the programme, following Workshop 1, participants organised themselves into working groups to discuss research directions of common interest. The themes that were identified (after a vote) as being of most interest to both the applied mathematicians and statisticians present were as follows.

- **Design:** including experimental design and possible connections to appropriate choices of training sets in the development of reduced basis methods for PDEs with uncertain/ parameter-dependent inputs, as well as space filling designs vs sparse grids and their appropriateness for different UQ tasks.

- **Multilevel & Multifidelity methods:** including connections between multilevel and multifidelity Monte Carlo methods and multilevel Gaussian process emulation and different strategies for variance reduction and controlling bias.

- **Surrogate Modelling:** including connections between stochastic collocation, stochastic Galerkin (or polynomial chaos) methods, and Gaussian process emulation, as well as the connections between Gaussian process emulation, radial basis function approximation and reproducing kernel Hilbert spaces, as well as reconciling deterministic and probabilistic statements about accuracy of surrogate models.

Attempts were made by the organisers and long-stay PPs to keep these discussion groups going throughout the programme. Other popular discussion sessions included: Foundations of UQ; Probabilistic Numerics and UQ education (especially new UQ MSc courses).

2.2 Workshops & Events. The programme included four week-long workshops (W1-W4) and two Open for Business Days. All events were held at the INI.

Workshops. These were well attended and were by far the busiest weeks of the programme. Each workshop attracted a new set of PPs who stayed on and then took part in other programme activities. In each workshop, half of the speakers were drawn from the statistics community and half from the applied mathematics/numerical analysis community. There were also poster sessions to provide PhD students and early career researchers with an opportunity to present their work. These were well attended and reported to be highly enjoyable. Each workshop organising committee was allocated £5K to support PhD students.

- *W1: Key UQ Methodologies and Motivating Applications (8th-12th January 2018).* Organisers: Dave Woods, Rob Scheichl, Ralph Smith, Richard Wilkinson, Henry Wynn.

  Since UQ scientists from the applied mathematics and statistics communities often approach modelling problems in very different ways, and consequently favour different methods and metrics for assessing uncertainty, it was important to start the programme with a workshop that had a significant educational component. There were tutorial talks on key mathematical and statistical UQ methodologies, such as: Gaussian process emulation, stochastic collocation and stochastic Galerkin approximation, multilevel Monte Carlo methods, design of experiments, the Bayesian approach to inverse problems etc. In addition, there were a few talks focused on applications (in areas such as climate, geosciences, energy and demography) to highlight current UQ challenges in those areas and open research questions.

- *W2: Surrogate Models for UQ in Complex Systems (5th-9th February 2018).* Organisers: Fabio Nobile, Serge Guillas, Linsday Lee, Clayton Webster, Max Gunzburger.

Simulating complex systems (eg through the numerical solution of continuous models consisting of coupled systems of differential equations) at a level of fidelity that predicts the solution to a high level of accurately, is infeasible except in idealized situations. To reduce the enormous computational effort required to perform UQ studies for complex systems (which might require, say, a million calls to a forward solver), surrogate models are commonly employed to quickly and efficiently predict the input-output map. Constructing provably accurate surrogates and computing their predictions along with the uncertainties they introduce can be hugely challenging. This workshop explored a variety of approaches that have been developed to address such challenges, including Gaussian processes, sparse interpolation, Galerkin approximation, discrete least squares approximation, compressed sensing, dimension reduction, multi-fidelity techniques and Bayesian inference.

- *W3: Reduced Dimensions and Cost for UQ in Complex Systems* (5th-9th March 2018). Organisers: Gianluigi Rozza, Elisabeth Ullmann, Alex Diaz, Jim Gattiker, Peter Challenor.

  Simple UQ tasks such as the estimation of statistical properties of system outputs often require multiple calls to a deterministic solver. A single solver call can already be very expensive for complex mathematical models. Advanced UQ tasks such as sensitivity and reliability analysis, parameter identification, or optimal control and design often involve several layers of increasing complexity where each layer requires the performance of a specific UQ task. This workshop was devoted to efficient numerical and statistical methods for reducing the overall cost of solving the discrete problems that arise in UQ studies, focusing on methodologies that reduce the dimension of the problems to be solved. Talks were organised around topics such as: multifidelity methods; reduced basis methods; dimension reduction strategies; low rank and tensor methods; challenges in Gaussian process emulation, and active subspaces.

- *W4: UQ for Inverse Problems in Complex Systems (9th--13th April 2018)*. Organisers: Don Estep, Claudia Schillings, Derek Bingham, Danny Williamson, Catherine Powell.

  In many real-world situations, quantities that can be measured experimentally are related through mathematical models to quantities of interest that are not directly observable. The formulation and solution of inverse problems is a fundamental task in UQ, since uncertainty and stochastic error affects both the observable quantities and the (computer) models used. The challenge and computational expense of solving inverse problems becomes very severe when the systems involved are complex, e.g. those incorporating multiple physical processes or scales. This workshop explored the following themes: (1) formulation, solution, and use of inverse problems for large complex systems; (2) Bayesian model calibration; (3) efficiency and accuracy in computational methods for inverse problems; and (4) experimental design.

Open for Business Days. These one-day workshops were organised by the Turing Gateway for Mathematics, with audience members drawn from the public and private sectors as well as from government and academia. One event was held at the start of the programme and one towards the end to disseminate findings and give an overview of the programme.

- *Taming Uncertainty in Mathematical Models Used in the Private & Public Sectors (1st Feb 2018).* At this event, two of the programme organisers (Challenor, Powell) gave overview talks on the different approaches to UQ and the different perspectives in the statistics and applied mathematics communities. Speakers from the engineering, aerospace, finance and insurance sectors also gave talks about the UQ challenges faced in their respective fields.

- *UQ for Complex Systems: Development in Theory and Methodologies (15th June 2018).* At this event Gunzburger, Wilkinson, Teckentrup and Woods (all PPs) delivered talks on Surrogate Modelling, Multilevel & Multi-fidelity Methods, Inverse Problems and Design, drawing attention to state of the art mathematical and statistical methods, scientific issues that had been discussed by PPs during the programme, and future research directions.

Rothschild Lecture. The Rothschild Lecture was delivered by Professor Andrew Stuart on *"The Legacy of Rudolph Kalman"* on 5th April 2018. In this talk, Professor Stuart gave an overview of Kalman's pioneering work in blending data and mathematical models.

Other Events. Two other events that took place at the INI involved PPs from the UQ programme.

- *LMS Women in Mathematics Days 2018 (30th April-1st May).* This two-day event was well attended by PPs. Powell, Schillings, Dashti (all Simons Fellows) were invited to be speakers and gave UQ-themed talks. Marianne Freiberger subsequently wrote two articles for plus magazine (www.plus.maths.org) about UQ, using these talks as inspiration.

- *M2D 2nd Annual Conference on Decision Making Under Uncertainty*. The Models to Decisions (M2D) network (http://www.models2decisions.org), led by Challenor and Powell, is one of two RCUK-funded networks on decision making under uncertainty. Since UQ plays an essential role in decision making in situations where the decisions are informed by outputs obtained from models, it was natural to hold the conference at the INI and involve PPs from the UQ programme. Their input was invaluable in drafting a research agenda on UQ (see below).

3. Scientific Outcomes & Future Directions

It was certainly challenging to bring the two communities together, and discussions were sometimes slow and frustrating. Indeed, one PP stated that *"[The] program was slightly too focussed on [the] issue of bringing together statisticians and applied mathematicians. Would rather have focussed on people from both communities who are versed in one another's work ….",* while another one stated that *"[…] there is much work required to cross the divide as the starting points for defining the problems and the criteria for success are so very different."*

Despite this, most PPs stated that they gained valuable insight into how researchers in other fields approach UQ problems. The programme has certainly helped to connect researchers who generally would not meet or interact at conferences or other events. PPs have reported that the programme has led them to have a better understanding and a greater respect for other PPs' disciplines. Some sample quotes from PPs supporting these claims are as follows:

"As a statistician, I gained some helpful insights into how numerical analysts tackled problems of similar form to those I am involved with";

"I had a number of interesting 1-1 discussions where I learned about alternative viewpoints of reduced-order modelling in a UQ context";

"I had a good number of discussions with statisticians about connections between sparse grids approximation and experimental design";

"I talked with several other participants [...], in particular with researchers from the statistics community. I have understood some of their thinking and identified where my own research could possibly help solve problems arising in model-based statistics";

"The programme enabled me to have my first serious conversations with Applied Mathematicians. I learnt lots about the problems they address, and the methods they develop and apply. It has led directly to a new grant proposal between Statisticians, Applied Mathematicians and Engineers"

More than half of those PPs who filled in the questionnaire stated that their participation had had a significant effect in opening up new research directions, with the remainder agreeing that this was at least partially true.

Discussions were held with PPs in May/June to summarise ideas for **future directions**. These ideas were used to form a **draft research agenda** which was further refined at the M2D Network's Annual Conference through roundtable discussion sessions. The research agenda will be presented to RCUK/UKRI (by Challenor and Powell) at the end of 2018, to help establish the need for future funding calls relating to Decision Making Under Uncertainty. Work on this is ongoing. However, PPs identified the following questions as being particularly important for future research.

- *How can we develop a rigorous mathematical framework for treating model error?* No model is a perfect description of reality. The discrepancy between a model and the real-world process it represents is vitally important but often neglected. Indeed, if it was known in what way a model was deficient, steps could be taken to improve it. Instead, such discrepancies are often identified from data, which is linked to the inverse problem of parameter estimation. When the model cannot be solved exactly, and computer models are required, the total discrepancy involves numerical error. Currently, it is not clear how to systematically exploit knowledge about this. More interactions between numerical analysts and statisticians could help here.

- *How can we reconcile probabilistic statements about uncertainty with deterministic bounds for numerical error?* Can we meaningfully combine them? Different mathematical communities approach the quantification of numerical error in different ways. Numerical analysis exploits the structure of models and their numerical implementations to produce deterministic bounds for, and computable estimates of such errors. Statistical approaches more commonly treat models as black-boxes and model the input-output map using stochastic processes. What are the limitations of both approaches, and when is one approach more appropriate than another?

- *How can we design surrogate models that (i) have guaranteed error control, (ii) satisfy important physical constraints?* The construction of surrogates (also known as emulators or meta-models) is a key step in the solution of UQ problems involving computationally expensive (high-fidelity) computer models. A surrogate model is a cheaper computer model that can be run more quickly than the high-fidelity one, usually resulting in loss of accuracy. While many approaches to building surrogates exist, it is often difficult to make statements about the errors between the high-fidelity model output and the surrogate model output, and about the impact of these errors on quantities of interest that are computed using surrogate models. When the computer model simulates a physical process, important features (e.g., conservation of mass, positivity, monotonicity) are often not satisfied by solutions of surrogate models. Moreover, it is often not clear how to incorporate available data, into the construction of surrogate models.

- *How can we quantify and manage uncertainty well when we have chains/ensembles of models?* Modern decision-making rarely relies on the results from a single model. Multiple models may be chained, with outputs (and uncertainties) from earlier models defining the (uncertain) inputs into later models. Multiple models may also operate in parallel, all feeding into a decision-making process or providing alternative (perhaps competing) descriptions of the same process. Even when there is a single preferred computer model, recent advances in numerical analysis (e.g. multilevel, multi-fidelity and multi-index methods) have shown that, for some simple classes of models, substantial computational savings can be achieved by combining hierarchies of different models in the right way.

With the rapidly growing expansion of Data Science, Machine Learning and AI, another crucially important question is: *How can we better fuse data, models and algorithms in UQ studies, and provide rigorous underpinning mathematics?* Finally, while it is acknowledged that UQ is well established in applications like engineering, there is a clear need for new UQ research in biology, healthcare and finance.

4. Online & Multimedia Resources.

The following educational resources were generated from the activities of the UQ programme.

- **Workshops talks.** Most workshop talks (those where presenters gave permission) were streamed live. Slides and videos of such presentations continue to made available through the following web links and will provide a valuable resource for early career researchers.

  Workshop 1: https://www.newton.ac.uk/event/unqw01/timetable
  Workshop 2: https://www.newton.ac.uk/event/unqw02/timetable
  Workshop 3: https://www.newton.ac.uk/event/unqw03/timetable
  Workshop 4: https://www.newton.ac.uk/event/unqw04/timetable

- **Seminars.** As mentioned above, seminars were typically informal in nature and included in promptu and often lengthy discussions amongst participants. To enable full and frank discussions with audience members, many seminar talks were not recorded. Videos of those that were recorded are available at the following link, which also lists workshop talks in chronological order.

  https://www.newton.ac.uk/event/unq/seminars

- **Discussion Groups**. Github pages relating to some of the discussion groups were set up. These include suggested reading lists and links to other potentially useful online resources.

  Design: https://github.com/statsdavew/UQdesign
  Multilevel & Multi-fidelity: https://github.com/rich-d-wilkinson/Multilevel
  Surrogate Modelling: https://github.com/ceapowell/Surrogate-Modelling
  UQ Education: https://github.com/ceapowell/UQ_Education

  The organisers would like to thank Dave Woods and Richard Wilkinson in particular for their help in setting up these pages.

5. Publications

Almost all participants reported that they worked on some form of publication during their stay in Cambridge, and/or developed new ideas for work that could form the basis for future publications. A list of preprints associated with completed work is available at the following link.

https://www.newton.ac.uk/event/unq/preprints

These works cover topics such as:

- **Stochastic Galerkin approximation:**
  - Efficient linear algebra for computing stochastic Galerkin approximations to linear elasticity problems with uncertain Young's modulus.
  - Computable a posteriori error estimates for stochastic Galerkin approximations to solutions of elliptic PDEs with uncertain coefficients, leading to multilevel and goal-oriented adaptive numerical algorithms that deliver surrogates with controlled errors.

- **Gaussian Random Fields/Processes:**
  - Reduced basis models for the fast numerical simulation of Gaussian random fields.
  - Kernels for Gaussian process metamodels with categorical inputs.

- **Emulation of Computer Models:**
  - Calibration-optimal bases for expensive computer models with high-dimensional spatial outputs.

New items will be added as time progresses and works currently in progress are completed.