



# Uncertainty Quantification and Computational Imaging workshop

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International Centre for Mathematical Sciences, Edinburgh

## Abstracts

**Atlmann, Yoann**

*Bayesian cluster analysis for Atom Probe Tomography*

In this talk, we will discuss a novel Bayesian approach to modelling and extracting information for atom probe tomography (ATP) data. ATP is a microscopy technique that provides positions and chemical properties of atoms in 3D volumes and that can be used for material characterisation at an atomic scale. However, high point cloud density, complex cluster structures and high level of observation noise makes the analysis of such data particularly challenging. By adopting a flexible Bayesian model coupled with advanced Markov chain Monte Carlo simulation methods for high-dimensional problems, we illustrate how such methods can be used to enhance ATP data analysis, e.g., by providing more robust and complete cluster characterisation, which can in turn be used for a better sample and probe characterisation.

**Durmus, Alain**

*The Langevin MCMC: theory and methods*

In machine learning and computational imaging literature, a large number of problems amount to simulate a density which is log-concave (at least in the tails) and perhaps non smooth. Most of the research efforts so far has been devoted to the Maximum A posteriori problem, which amounts to solve a high-dimensional convex (perhaps non smooth) program. However, in order to perform more complex analyses, for example uncertainty quantification or model selection, it is necessary to be able to simulate the density of interest and therefore computationally intensive techniques such as Markov chain Monte Carlo methods have to be used. The purpose of this talk is to understand how we can use ideas which have proven very useful in signal processing community to solve large scale (non-smooth) optimization problems to design efficient sampling algorithms, with convergence guarantees (and possibly « usable » convergence bounds »). In high dimension, only first order method (exploiting exclusively gradient information) is a must. Most of the efficient algorithms known so far may be seen as variants of the gradient descent algorithms. This of course suggests to study methods derived from Euler discretization of the Langevin diffusion, which may be seen as a noisy version of the gradient descent. This algorithm may be generalized in the non-smooth case by « regularizing » the objective function. The Moreau-Yosida inf-convolution algorithm is an appropriate candidate in such case, because it does not modify the minimum value of the criterion while transforming a non-smooth optimization problem in a smooth one. We will prove convergence results for these algorithms with explicit convergence bounds both in Wasserstein distance and in total variation.

## **Kennedy, Anthony**

### *HMC on symmetric spaces*

It is often desirable to sample from a distribution over a symmetric or homogeneous space, such as a sphere or the space of symmetric positive matrices. I shall explain how Hamiltonian Monte Carlo may be used to do so efficiently by constructing symplectic integrators that satisfy these geometric constraints automatically and exactly.

## **McEwan, Jason**

### *Uncertainty quantification for radio interferometric Imaging*

In many fields high-dimensional Inverse Imaging problems are encountered. For example, imaging the raw data acquired by radio interferometric telescopes involves solving an ill-posed inverse problem to recover an image of the sky from noisy and incomplete Fourier measurements. Future telescopes, such as the Square Kilometre Array (SKA), will usher in a new big-data era for radio interferometry, with data rates comparable to world-wide internet traffic today. Sparse regularisation techniques are a powerful approach for solving these problems, typically yielding excellent reconstruction fidelity (e.g. Pratley et al. 2016). However, such approaches typically recover point estimators only and uncertainty information is not quantified. Standard Markov Chain Monte Carlo (MCMC) techniques that scale to high-dimensional settings cannot support the sparsity-promoting (non-differentiable) priors that have been shown to be highly effective in practice. We present work adapting proximal MCMC algorithms developed recently by Pereyra (2016a), for radio interferometric imaging with sparse priors (Cal, Pereyra & McEwen 2017a). While such an approach provides critical uncertainty information, scaling to extremely large data-sets, such as those anticipated from the SKA, remains challenging. To address this issue we develop a technique to compute approximate local Bayesian credible intervals by post-processing the point (maximum a-posteriori) estimator recovered by solving the associated sparse regularisation problem (Cal, Pereyra & McEwen 2017b), leveraging recent results by Pereyra (2016b). This approach inherits the computational scalability of sparse regularisation techniques, while also providing critical uncertainty information. We demonstrate these techniques on simulated observations made by radio interferometric telescopes.

## **Papaspilipoulos, Omiros**

### *Gradient-based samplers*

I will provide an overview of state of the art MCMC sampling using gradient information and introduce a new approach that empirically beats the state of the art often by an order of magnitude while it is entirely automatic.

## **Pereyra, Marcelo**

### *Bayesian statistical inference in computational imaging*

This mini-course will give an introduction to high-dimensional Bayesian analysis and computation methods to solve computational imaging inverse problems, with a focus on uncertainty quantification analyses and on problems involving unknown model parameters.

**Teckentrup, Aretha**

*Sampling methods for uncertainty quantification*

This mini-course will give an Introduction to sampling methods for uncertainty quantification, where the probability distributions of interest are typically high-dimensional. We will discuss methods based on Monte Carlo and Markov chain Monte Carlo, as well as the use of these methods on a typical inverse problem in uncertainty quantification.