MSc. Projects 2009

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Numerical methods and solvers for PDEs with random data

In traditional mathematical modelling of physical processes all the input parameters in the PDEs to be solved are assumed to be known *exactly*. That is, we assume full knowledge of the geometry of the domain, the boundary terms, the source functions, the PDE coefficients etc. Once the problem has been explicitly defined, we then put all our computational effort into finding a solution, if it exists, to high accuracy.

In realistic modelling situations, we never have access to all this information. For example, we can write down a system of PDEs that describes the flow of groundwater in porous rocks but we will never have a complete deterministic description of the porosity properties of the rocks at every point in space. We could choose many different realisations of sets of porosity coefficients (four possibilities are given below, taken from a particular statistical distribution) and solve the governing PDEs to find the flow field corresponding to each one.

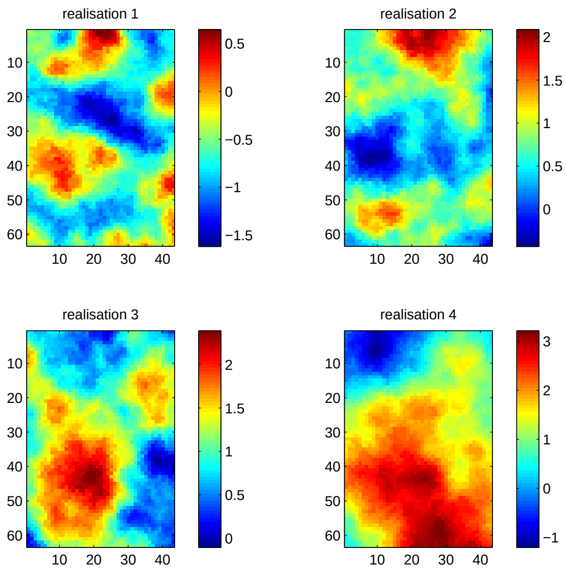

Figure 1: Four simulations of porosity values of rocks in a rectangular domain with Bessel covariance function. Red zones have high permeability and blue zones have low permeability.

Since there are uncertainties in our input data, we are in fact faced with solving stochastic PDEs and we have to ask probabilistic questions such as 'What is the expected solution?' rather than what is *the* solution. 'Can we compute probabilities of unfavourable events?' An important application is modelling the storage of nuclear waste in underground repositories. In the event that radioactive particles escape and enter groundwater, we need mathematical models that allow us to make reliable predictions about contamination scenarios. The porosity values of the rocks in the repository will never be known at more than a few scattered locations and so we must treat them as a random quantity and seek probabilistic solutions to the flow equations.

The traditional way of dealing with this type of uncertainty in input parameters is to use Monte Carlo methods, in which large numbers of realisations of the random inputs are first generated and then the solutions to the corresponding deterministic PDEs are post-processed to approximate their statistics. The expected flow, for a simple model groundwater flow problem, computed by averaging solutions to the flow equations obtained with 1,000 different sets of porosity coefficients is shown in Figure 3. Although the Monte Carlo method is simple, and very widely used, it is notoriously slow to convergence. Realistic flow problems require many hundreds of thousands of simulations to be performed before we get sensible approximations to the statistics of the solution. This requires significant computational resources.

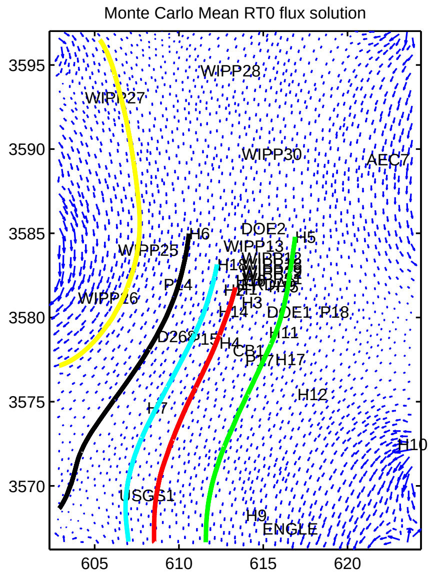

Figure 2: Expectation of the flow field, for a model problem, averaged over 1000 Monte Carlo simulations

Recently, more elegant mathematical techniques have been proposed to solve PDEs with random inputs including so-called stochastic Galerkin methods, stochastic collocation methods, stochastic reduced basis methods, the non-intrusive polynomial chaos method etc. Starting from the assumption that the unknown inputs can be approximated by a finite set of random parameters, the key idea behind these methods is that the spatial components and the random components of the unknown quantities in our PDEs are discretised separately. In physical space, we can use traditional **finite element methods** (which you learn about on the MSc program). Additionally, we then need to introduce the concept of a probability space and investigate how to discretise it.

Two projects are offered on this topic in 2009. Students can choose to work on one of the following types of numerical discretisation schemes:

1. **stochastic reduced basis methods** (SRBMs) (see or [4] and [5] for an introduction)

   or

2. the **non-intrusive polynomial chaos method** (NIPC) (see [2] or [3] for an introduction)

Potential model problems to be solved include:

a) groundwater flow problems with uncertain porosity coefficients

b) convection-diffusion problems with uncertain boundary conditions eg the double-glazing problem with stochastic heating condition on one wall

Initially, students will examine the relevant literature on the existence of solutions to PDEs with stochastic coefficients, and on the chosen family of discretisation schemes. The student(s) will write MATLAB codes to implement the chosen numerical methods for model problems, investigate efficient linear algebra techniques for solving the resulting linear systems, and compare the results with the traditional Monte Carlo approach based on solving many deterministic problems.

Pre-requisites

To carry out a project in this area, students will need to have completed courses in functional analysis, finite elements and numerical linear algebra (and have a liking for those subjects), and have experience of coding in MATLAB. A knowledge of basic probability theory is desirable but not essential. The following references give an idea about the type and range of mathematics that will be involved.

References

[1] M.K. Deb, I.M. Babuška and J.T. Oden, Solution of stochastic partial differential equations using Galerkin finite element techniques, *Comput. Methods Appl. Mech. Engrg.,* 90, 48(2001), pp.6359–6372.

[2] B.J. Debusschere, H.N. Najm, P.P. Pebay, O.M Knio, R.G. Ghanem and O. Le Maitre, Numerical Challenges in the use of Polynomial Chaos Representations for Stochastic Processes, *SIAM J. Sci. Comp.,* 26, 2(2005), pp.698–719.

[3] O.P. Le Maitre, M. T. Reagan, H.N. Najm, R.G. Ghanem and O. M. Knio, A stochastic projection method for fluid flow II: random process, *J. Comp. Physics,* 181 (2002), pp.9–44.

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[5] P. S. Mohan, P.B. Nair and A.J. Keane, Multi-element stochastic reduced basis methods, *Comput. Methods Appl. Mech. Engrg.,* 197 (2008), pp. 1495–1506.