M.Sc. in Mathematical Modelling and Scientific Computing Dissertation Projects

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Contents

1 Projects with the Industrial Sponsors of the M.Sc.

1.1 NAG — L1 Approximation Problems Using the NAG Library

Supervisor: Dr Andy Wathen (Numerical Analysis)
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For various reasons there is a growing interest in the approximation of data in the ℓ_1 norm rather than more common least squares (ℓ_2) approximation. One particular reason is the relatively recent observation that such approximations can be sparse in the sense that a best ℓ_1 approximation often has very many zeros in it: this is helpful in getting simpler or less expensive approximations.

The NAG software library has for several decades been one of the leading sources of mathematical solution techniques and has some existing capability for solving ℓ_1 approximation problems. This project would be to investigate the 'sparse' approximation properties of ℓ_1 approximation and to consider how the NAG library routines for related problems might be employed for solving these problems.

This project would involve some Approximation Theory, computational methods and hopefully some useful interaction with our highly knowledgable colleagues at NAG Ltd up the Banbury Road in North Oxford. (I have suggested this project and not them!)

1.2 NAG — Multi-Criteria Optimisation

Supervisor: Dr Raphael Hauser (Numerical Analysis)
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Background and Problem Statement: Numerical optimisation are mathematical problems of the form

$$\begin{aligned} &\min_x f(x) \\ &\text{s.t. } g(x) \le 0, \quad \text{(inequality constraints)}, \\ &\quad\;\; h(x) = 0, \quad \text{(equality constraints)}, \end{aligned}$$

that is, the minimisation or maximisation of an objective function in n variables over an implicitly defined set of feasible values for the decision variables. This is a well studied and rich class of problems for which powerful algorithmic approaches have been developed. In many practical applications, one would like to minimise or maximise several functions at once. For example, an investor might aim to maximise return and minimise risk, or an engineer might aim to minimise the cost and weight and maximise the strength of a material. Conceptually, such problems can be thought of as taking the form

$$\begin{aligned} &\min_x f_1(x), \ldots, f_k(x) \\ &\text{s.t. } g(x) \le 0, \quad \text{(inequality constraints)}, \\ &\quad\;\; h(x) = 0, \quad \text{(equality constraints)}, \end{aligned}$$

although this is not a mathematically coherent formulation, as optimising one criterion often renders other criteria suboptimal. In this situation one is interested in finding Pareto optimal solutions which are characterised by the property that none of the criteria can be further improved without worsening one of the other criteria. The industrial sponsor would a student to work out an survey of different approaches to solving multi-criteria optimisation problems and to compare the different approaches numerically.

Description of the Planned Approach and the Techniques Needed: Typical approaches to multi-criteria optimisation include the following:

1. Forming a merit function as a weighted sum of the different objectives.
2. Prioritise the relative importance of different objectives.
3. Formulating constraints that guarantee that some of the objectives satisfy a chosen "budget".

In a first phase we will focus on computing Pareto optimal solutions, which can be done by either approach 1 or 3 from the above list. In a second phase, different approaches to striking a compromise between the different criteria will be investigated on a number of numerical examples to be determined in collaboration with the industrial partner. In a third phase, we aim to produce a tool that allows users to explore the Pareto optimal surface. In principle, this surface can be computed by varying the parameters, but in practice this may be too time consuming and not required. Instead, we aim to provide an interactive tool that allows users to propose changes to the solution to which an improved Pareto optimal solution is then computed.

References

Starting points:

- Raphael Hauser's HT course "Continuous Optimisation".
- Literature on filter methods in continuous optimisation.

1.3 NAG — Knapsack Problems

Supervisor: Dr Raphael Hauser (Numerical Analysis)
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Background and Problem Statement: Knapsack problems are an important type of integer optimisation problem that deal with the problem of filling a back pack of volume b with n objects of volumes a_i $(i = 1, \dots, n)$ so that the total volume $\sum_{i=1}^{n} a_i$ surpasses b. One is therefore forced to prioritise and make a decision as to which objects to take along. Each object i is associated with a value or utility c_i, and the objective is to maximise the total value of the objects that end up being packed. Mathematically, the problem can be formulated as follows,

$$\max_x \sum_{i=1}^{n} c_i x_i$$
$$\text{s.t.} \sum_{i=1}^{n} a_i x_i \leq b$$
$$x_i \in \{0, 1\}, \quad \forall i.$$

Note that the x_i are simply flag variables that indicate whether or not we pack object i. In real applications, a truck or a container can replace the back pack, or the problem can be to cut a wide roll of paper or an expensive type of cable into smaller sections so as to minimise waste. Other applications occur in scheduling jobs on a machine to complete before a certain time. The industrial sponsor would like a student to identify a good general method for solving or approximately solving such problems and produce a prototype implementation.

Description of the Planned Approach and the Techniques Needed: Knapsack problems are a classical class of problems on which a wide literature has been published. Good heuristics are also known. The student will start with LP and integer-knapsack relaxation based branch-and-bound approaches for which they can use the supervisor's Part B lecture notes. They will then compare the performance of these implementations with off-the shelf software such as ipsolve and work out possible improvements and refinements. The third phase comprises a wider literature study on the subject, give an overview of the most widely used approaches, and investigation into how the approach described above could be further refined. Time permitting, the project may end with an outlook of how the algorithm might be extended to the related bin packing problem.

References

Starting points:

- Raphael Hauser's lecture notes on Integer Programming (Part B course available from the web site of the Mathematical Institute).
- Laurence Wolsey, "Integer Programming" (Wiley).

1.4 Thales Aerospace — Sparse Sampling and Gabor Atoms

Supervisor: Dr Andy Wathen (Numerical Analysis)
Industrial Collaborator: Dr Andy Stove
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In the past 5 years or so there has been much mathematical interest in the idea of Compressed Sensing. The idea is roughly as follows: all images (TV, photos, ...) are these days compressed before they are saved or transmitted. The savings in terms of the datasize can be considerable. But for many years the compression of an image was done after its capture as a dense 2 dimensional array of pixel values. The idea of Compressed Sensing is to be able to sample the image only sparsely in the first place, but so that it can be recovered essentially exactly from the data. That is, it is like the approach described above but without having to obtain the whole image before compressing it. Magically (or Mathematically) such 'compressed sampling' or 'compressed sensing' can be achieved almost certainly for most images of interest.

There are many possible applications of such a technology, particularly where there is limited time or possibility to capture an image, but significant processing 'back at base' is feasible — consider images taken by spacecraft for example.

Thales have an interest in considering the new mathematical techniques which allow such compressive sampling and their possible applicability for a number of sensing problems. In particular they have wondered if an old idea, the Gabor Atom (devised by the inventor of the hologram, Dennis Gabor) has some relevance.

The project would commence with the student learning about the technique or Compressed Sensing and the related questions of sparse representation. Consideration of whether Gabor Atoms or other structures (such as Wavelets) might allow for such sparse representation would follow.

1.5 Thales Underwater Systems — In-Plane Dynamic Response of a Thin Elastic Disc with Circular Holes

Supervisor: Dr David Allwright (OCIAM) Industrial Collaborator: Dr Robert Harter

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Thales Underwater Systems need to analyse the vibration properties of various underwater structures, which are generally built from flat and curved plates of various kinds, coupled together along the edges in various ways. In connection with this, Thales would like to have an efficient way to compute the in-plane harmonic point-forced vibration of a thin flat circular plate containing circular holes. The problem is to be addressed for small forcing and small displacements, so linear models can be used. An M.Sc. project last year considered the corresponding problem for the out-of-plane (bending) motion. It is expected that similar methods will be suitable for the in-plane problem. Forcing at a point on the edge of the disc or the edge of a hole is to be included.

Mathematical background: A general interest in vibration is useful. If you are not familiar with the mathematical theory of elasticity you will easily be able to pick up the material relevant to this project. You will need to do some Matlab programming.

1.6 Thales Aerospace — Information Theory and Radar Detection

Supervisor: Dr David Allwright (OCIAM) Industrial Collaborator: Dr Andy Stove

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How does Shannon's theory of information relate to the information content in a radar return? When a radar pulse is sent out, and the echo received, we aim to learn something about the object that caused the echo: e.g. its range, speed, size, structure etc. Shannon's theory says that the information rate in a signal should be $\log_2(1+\text{SNR})$ bits per second, where SNR is the signal-to-noise ratio. In the 1950s P.M. Woodward showed that at low SNR the information obtained is related to the radar range accuracy in an efficient way, but that at high SNR it is not. Relatively little work has been done since then. Can the power of a radar be reduced while still giving the required information? Can additional information be extracted from the return? Can the nature of the radar pulse be optimized for the information we wish to learn from the echo?

Mathematical background: A general background in either waves or information theory or both would be useful.

1.7 Thales Underwater Systems — Dimensionality Reduction and Covariance Matrix Estimation

Supervisor: Dr Raphael Hauser (Numerical Analysis)

Contact: hauser@maths.ox.ac.uk

Background and Problem Statement: This problem concerns the detection of an acoustic signal from noisy data measured by an array of microphones. The majority of the statistical array signal processing methods require the estimation of second order statistics

$$\hat{R} = \frac{1}{K}\sum_{k=1}^{K} x_k x_k^H, \quad x_k \in \mathbf{C}^{M\times 1},$$

and to solve linear systems of equations involving this matrix. Unfortunately, to get a good estimate $\hat{R}$, one would have to use data that range too far in the past to be of relevance to the signal one would like to detect. A very similar problem occurs in mathematical finance, where the data relevant to current market conditions is not sufficient to compute a good estimate of the covariance matrix of returns for large baskets of assets. By reducing the degrees of freedom one can get faster convergence and computationally simpler algorithms. Take adaptive algorithms (MVDR/Capon) as an example,

$$x_k = s_k a_\theta + n_k,$$

where x_k is measured, s_k is the source signal, a_θ is a phase vector associated with the direction of search for the signal source and n_k is a noise. The aim is now to design spatial filters to reject noise but to pass signals of interest. The performance criterion is the output Signal to Noise Ratio (SNR). Mathematically, this problem reduces to designing a complex $M \times N$ matrix D such that $N \ll M$ and

$$D^H x_k = s_k D^H a_\theta + D^H n_k$$

That is, given x_k, we want to find s_k and n_k, and we dont know the noise statistics. (We may assume that s_k is uncorrelated.) Another way to formulate the problem is as a covariance-fitting problem.

Description of the Planned Approach and the Techniques Needed: There is existing work on regular/uniform arrays of sensors that the project students would study in the first phase of the project. In a second phase, we would investigate more general formulation for non-uniform arrays, with the aim to achieve the following:

- protect signals;
- provide good performance in terms of output SNR;
- work in variable noise environments;
- work in the presence of nulled elements.

References

Starting points:

- Existing literature on Capon.

1.8 Radius Health — Imaging with X-Ray Emitter Arrays

Supervisors: Dr Raphael Hauser (Numerical Analysis) and Prof. Jon Chapman (OCIAM)
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Background and Problem Statement: Current X-ray machines in hospitals consist of heavy equipment that require small cranes as support structure. The vision of the industrial partner - an American-British startup company - is to reduce the cost and space requirements of such equipment drastically by replacing the traditional point source of X-rays by an array of small small X-ray emittors that could be hand held and fired from close proximity to the patient. They developed a prototype of such a device. While traditional point sources immediately yield an interpretable picture, the detected information obtained in the process of firing an array needs to be processed to yield easily interpretable information: In effect, the picture needs to be inferred from indirect observations. The project investigates certain aspects of this process.

Description of the Planned Approach and the Techniques Needed: The supervisors have developed a conceptual approach to solve this problem via compressed sensing. In the situation where groups of emittors are fired so that their emitted radiation does not overlap, an underdetermined system

$$
\begin{aligned}
Ax &= b + \varepsilon \\
x &\leq 0
\end{aligned}
$$

can be identified from the measurements taken by the device, and the relevant information for inferring the picture is contained from x, which should be chosen so that the set of its nonzero entries has minimum cardinality. This is an NP-hard problem, but it is known from the literature that the convex relaxation

$$
\begin{aligned}
&\min_x \|x\|_1 \\
&Ax = b + \varepsilon \\
&x \leq 0
\end{aligned}
$$

often solves the cardinality minimisation problem exactly. In the situation where cones of radiation emitted by several emittors overlap, the approach is to use a sequence of problems of the above form. The project student will study several design options that relate to the choice of matrix A in this approach and compare the results numerically:

- The spatial discretisation of the specimen that is to be X-rayed.
- The choice of groups of emittors to be fired together.
- The influence of parameter choice on the convergence of the algorithm in the case with overlap.

References

Starting points:

- Matousek's lecture notes on compressed sensing.

2 Numerical Analysis Projects

2.1 Iterative Numerical Linear Algebra

Supervisor: Dr Andy Wathen (Numerical Analysis)
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For linear systems of equations of very large dimension such as arise from finite difference and finite element approximation of PDE boundary value problems, it is often necessary to employ iterative solution methods to obtain numerical solutions in feasible computational time. There are a number of very good approaches, notably those of Krylov subspace type, but also many remaining difficult matrix problems.

This project will be to investigate the use of iterative methods with preconditioning for the solution of certain types of linear equations systems. Since this is one of my main areas of research, I am happy to choose a particular focus which appeals to any student who might be interested.

2.2 Numerical Methods in Fluid Mechanics

Supervisor: Dr Ian Sobey (Numerical Analysis)
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I am interested in most aspects of fluid mechanics and particularly applications in physiology and CFD and am happy to discuss possible projects in these areas. Some example fluid dynamic problems are:

1. Flow through a symmetric channel can become asymmetric (Coanda effect). Asymptotic expansions using boundary layer theory ("triple deck theory") have not predicted this effect, I have speculated on a possible way asymptotic boundary layer theory might be modified to predict this by numerically solving two unsteady boundary layer equations which interact non-linearly to give the Coanda bifurcation. The project would involve adapting my existing CFD codes or developing new ones to solve time evolving interactive boundary layer equations.

2. Each human adult has around 150ml of cerebrospinal fluid surrounding the brain and spinal chord. This fluid is continually produced and absorbed, the production rate is around 0.35ml/min and the main site of production is in the choroid plexus in the centre of the brain. In working on CSF movement over the last decade, I have not seen any quantitative model for CSF production. The general biochemical mechanism seems understood, see for example [1] for an illustration of one chemical pathway in CSF studies. This is a speculative project: survey the present state of knowledge of CSF production and the consider whether we can, I assume by a system of ordinary differential equations in time, develop a quantitative model for CSF production that might ultimately allow, for example, quantitative prediction of how different treatment strategies will affect CSF production.

Reference

[1] Smith, D.E. Johanson, C.E. & Keep, R.F. Peptide and peptide analog transport systems at the blood-CSF barrier, Advanced Drug Delivery Reviews 56(2004)pp1765-1791, doi:10.1016/j.addr.2004.07.008

2.3 Parallel Computing for ODEs/PDEs with Constraints

Supervisor: Dr Colin Macdonald (OCCAM)
Collaborators: Prof. Raymond Spiteri (Saskatchewan), Prof. Ping Lin (Dundee)
Contact: macdonald@maths.ox.ac.uk

This project proposes a parallel time-stepping routine for differential equation with constraints. The incompressible Navier–Stokes are an example of constrained PDEs where the divergence free condition (the constraint) is enforced by the pressure [3]. A multicore idea for ODEs and time-dependent PDEs was developed in [2] where parallelism was exploited to obtain higher-order accuracy. Here we propose to exploit parallelism to impose the constraint, in an iterative fashion where all iterations happen in parallel.

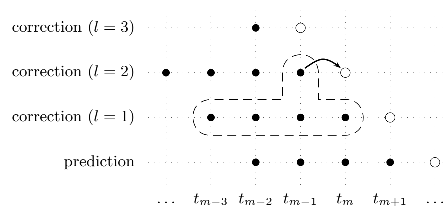

Figure 1: Each row of computations happens in parallel.

The project would begin with a brief review of differential-algebraic equations (DAEs) which are a framework for dealing with differential equations with constraints. The proposed numerical algorithm is the Sequential Regularization Method [1]. An implementation, in OpenMP, Python (using the `multiprocessing` module), or perhaps Matlab would be programmed. Applications would include multi-body systems (e.g., the pendulum and slider-crank mechanisms) and incompressible Navier–Stokes, and these would form the test cases.

The anticipated achievements include improving a DAE solver, a projection-free incompressible fluid solver and experience in multicore and parallel computing.

References

[1] U. Ascher and P. Lin. Sequential regularization methods for nonlinear higher-index DAEs. SIAM J. Sci. Comput., 18(1):160–181, 1997.

[2] A. Christlieb, C. B. Macdonald, and B. Ong. Parallel high-order integrators. SIAM J. Sci. Comput., 32(2):818–835, 2010.

[3] P. Lin. A sequential regularization method for time-dependent incompressible Navier–Stokes equations. SIAM J. Numer. Anal., 34(3):1051–1071, 1997.

[4] C. B. Macdonald and R. J. Spiteri. The predicted sequential regularization method for differen- tial-algebraic equations. In C. D'Attellis, V. Kluev, and N. Mastorakis,

editors, Mathematics and Simulation with Biological, Economic, and Musicoacoustical Applications, pages 107–112. WSES Press, 2001.

2.4 Multi-Structures and Computing in Mixed Dimensions

Supervisor: Dr Colin Macdonald (OCCAM)
Contact: macdonald@maths.ox.ac.uk

The Closest Point Method is a recently developed simple technique for computing the numerical solution of PDEs on general surfaces [2,4]. It is so general that it can compute on surfaces where I don't understand the results. For example, it can compute on problems with variable dimension just as easily as a simple sphere. In the figure, the pig and sphere are connected with a one dimensional filament and heat flow is solved over the composite domain. But what does such a calculation *mean*? What is the correct solution to such a problem?

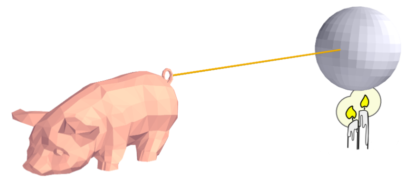

Figure 2: Heat equation in mixed dimensions.

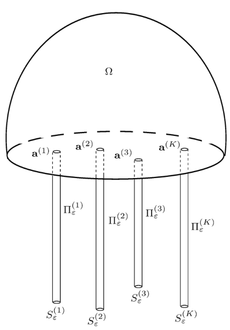

Figure 3: A multi-structure from [3].

A presentation by Prof. Vladimir Maz'ya (Liverpool) introduced me to *multi-structures* [1,3]. An example of a multi-structure problem would to be determine the eigenvalues of a bridge consisting of solid structures coupled to thin cables. The aim of this project is to learn about multi-structure problems and do some calculations (e.g, heat equation or Laplace–Beltrami eigenvalues) using the Closest Point Method. There are also asymptotic techniques that can be applied here, letting ϵ represent the "radius" of the one-dimensional parts (e.g., [3]).

A reasonable achievement would be showing that the Closest Point Method computes a solution which is consistent with an asymptotic analysis for some mixed-dimension multi-structures. Or maybe it is not consistent: that would be equally interesting!

References

[1] V. Kozlov, V. G. Maz'ya, and A. B. Movchan. Asymptotic analysis of fields in multi-structures. Oxford University Press, 1999.

[2] C. B. Macdonald and S. J. Ruuth. The implicit Closest Point Method for the numerical solution of partial differential equations on surfaces. SIAM J. Sci. Comput., 31(6):4330–4350, 2009.

[3] A. B. Movchan. Multi-structures: asymptotic analysis and singular perturbation problems. European Journal of Mechanics/A Solids, 25(4):677–694, 2006.

[4] S. J. Ruuth and B. Merriman. A simple embedding method for solving partial differential equations on surfaces. J. Comput. Phys., 227(3):1943–1961, 2008.

2.5 Chebfun Dissertation Topics

Supervisors: Prof. Nick Trefethen (Numerical Analysis) and Dr Nick Hale (OCCAM and Numerical Analysis)
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Chebfun is an algorithmic and software project based on the idea that Matlab's vectors and matrices are overloaded to functions and operators. It is very powerful, at least for computations in one space variable, and a lot of fun to use. Check it out at http://www.maths.ox.ac.uk/chebfun, especially the Guide and Examples.

For these last few years, a couple of M.Sc. dissertations have been related to Chebfun each year. There are many possibilities here and we can tailor the project to the student's interests and expertise. Here are three specific possibilities with the flavor of ODEs, approximation, and linear algebra:

(1) Solving ODEs on unbounded intervals. The technology here involves rational changes of variable to reduce the domain to a finite interval, where Chebyshev spectral methods are applied.

(2) The Remez algorithm for rational best approximation. Chebfun's existing REMEZ command is far from robust, but we have ideas about where the problem may lie.

(3) Computing Singular Value Decompositions of operators. Chebfun has some initial capabilities in this area but there are exciting additional possibilities.

The leaders of the Chebfun project at Oxford are Prof. Nick Trefethen and Dr Nick Hale, and they would be the likely supervisors of a project in this area. The Chebfun team consists of 8–10 people, and an M.Sc. student doing a project in this area would be welcome to participate in our weekly team meetings.

Any student wishing to do a project related to Chebfun is urged to take the Approximation course in Hilary Term. Other areas of interest include PDEs, complex analysis, quadrature,...

2.6 Adaptive Finite Element Methods for Convection Dominated Diffusion Problems

Supervisor: Dr Kathryn Gillow (Numerical Analysis)
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The standard finite element method applied to convection dominated diffusion problems is known to generate a numerical solution with non-physical oscillations unless a very small mesh size is used. One of the standard remedies is to use the streamline diffusion finite element method (SDFEM) in order to remove the oscillations. Suppose we then wish to compute a linear functional of the solution to this partial differential equation. It can be shown that the error in computing this solution depends on the solution to this PDE and also to its adjoint. Problems arise when the adjoint of the numerical scheme does not correspond to the adjoint of the original PDE. In this case convergence rates are not optimal and the SDFEM can be shown to suffer from this problem.

The aim of this project is to compare the use of SDFEM with other methods for convection diffusion problems (e.g. local projection stabilization, discontinuous finite element methods) to see which achieve optimal convergence rates and hence work better in adaptive algorithms. The project will include both theory and numerical experiments.

3 Biological and Medical Application Projects

3.1 Multiscale Reaction-Diffusion Simulations in Biology

Supervisors: Dr Radek Erban and Dr Mark Flegg (OCCAM)
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There are three common approaches to mathematically simulating chemical reactions in the presence of spatial heterogeneity (reaction-diffusion processes):

(i) macroscopic deterministic models which are writen as partial differential equations (PDEs) for concentrations;

(ii) mesoscopic stochastic simulation on a lattice in space (compartment-based models);

(iii) microscopic molecular-based stochastic algorithms which simulate trajectories of individual molecules.

Stochastic approaches (ii) and (iii) provide detail about the state of a chemical system that is not observable with a deterministic model (i). The fluctuation in these possible states become significant when the numbers of chemical molecules are small. Stochastic simulation is therefore common on small scales such as intracellular biological chemical systems [1].

Compartment-based models (ii) involve partitioning the spatial domain into small connected regions called compartments or computational cells [2]. Algorithms for mesh generation (developed for finite element computations) can be used for partitioning the spatial domain [2]. Diffusion is modelled as a jump process between the compartments. Chemical reactions are then considered in each compartment individually. This approach is fundamentally different from Brownian (off lattice) models (iii) which assign continuous spatial coordinates to each chemical molecule. Diffusion is modelled by displacing each molecule a random normally distributed distance. Implementation of boundary conditions and reactions for the methods (ii) and (iii) are also fundamentally different [3,4].

In this project, we will consider how modelling approaches (ii) and (iii) compare on a fundamental level. This is important for development of efficient multiscale algorithms for simulating reaction-diffusion processes. A method of coupling the two different regimes (ii) and (iii) spatially has recently been published in [5] where cubic structured mesh was considered for the compartment-based model. The student will study the generalization of the method [5] to hexagonal (honeycomb) meshes. Hexagonal meshes are not only of theoretical interest, but have been used in algorithms developed in the computational biology community [6]. This project will combine partial differential equations, asymptotic analysis, numerical methods and stochastic simulations.

References

[1] R. Erban, J. Chapman, P. Maini, Lecture Notes, available as http://arxiv.org/abs/0704.1908 [arxiv.org] (2007)

[2] S. Engblom, L. Ferm, A. Hellander and P. Lötstedt, SIAM Journal on Scientific Computing 31(3), pp. 1774-1797 (2009)

[3] R. Erban and J. Chapman, Physical Biology 4(1), pp. 16-28 (2007)

[4] R. Erban and J. Chapman, Physical Biology 6(4), 046001 (2009)

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[6] S. Arjunan, M. Tomita, Systems and Synthetic Biology 4(1), pp. 35-53 (2010)

3.2 Multiscale Modelling of Chemical Systems: Coupling Differential Equation Models with Stochastic Algorithms

Supervisors: Dr Radek Erban and Dr Simon Cotter (OCCAM)
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It is important in many chemical systems, where the copy numbers of the reactants are relatively small, to take into account the effect of intrinsic noise. We can model well mixed systems exactly, through the Gillespie [1] or Gibson-Bruck algorithms [2]. However, these algorithms simulate every single reaction in the system, and so for some systems their use become intractable.

When the copy numbers of a given species remain high enough, Gillespie trajectories can be approximated well by stochastic differential equations (SDEs) [3]. Species which are even more abundant can be well approximated by ordinary differential equations (ODEs). There are also other approximate stochastic methods which can be used to speed up the Gillespie algorithm in certain situations [4]. The aim of this project is to study multiscale methods where different approaches are used for different species, in an optimal way such that the error incurred is kept to a minimum, while the computational demands of the problem are greatly reduced [5].

We will consider test model systems for which we can alter the degree of multiscale separation, and the average abundance of each species. Comparison with standard algorithms [1,2] and analytic solutions will provide insight into the appropriateness of the chosen coupling of regimes. If time permits, we will also apply these approaches to the simulation of biological systems of interest, such as oscillations in circadian rhythms or cell cycles.

This project will combine numerical methods for differential equations with stochastic simulation algorithms.

References

[1] D. Gillespie, Journal of Physical Chemistry 81(25), pp. 2340-2361 (1977)

[2] M. Gibson and J. Bruck, Journal of Physical Chemistry A 104, pp. 1876-1889 (2000)

[3] S. Cotter, K. Zygalakis, I. Kevrekidis and R. Erban, Journal of Chemical Physics 135, 094102 (2011)

[4] D. Gillespie, Journal of Chemical Physics 115(4), pp. 1716-1733 (2001)

[5] Andreas Hellander, Per Ltstedt, Journal of Computational Physics 227(1), pp. 100-122 (2007)

3.3 Modelling Collagen Distribution in Gel Constructs for Tissue Engineering Applications

Supervisor: Dr Ian Griffiths (OCCAM) and Dr Rebecca Shipley (OCIAM)
Collaborator: Professor Robert Brown (UCL)
Contact: griffit4@maths.ox.ac.uk

Tissue engineering involves growing new tissues to replace those that have become defective due to ageing, trauma or disease. This is usually achieved by seeding a sample of cells on a scaffold, which provides a template for the tissue structure as it grows. The scaffold must be carefully designed to promote cell function and mimic the architecture, biomechanical and biochemical environment of in-vivo tissue. One scaffold design involves seeding cells in a gel containing native protein matrix such as collagen. Our collaborator Professor Robert Brown's laboratory at UCL has developed a plastic compression (PC) technique for the controlled fabrication of scaffolds by rapid removal of fluid from hyper-hydrated collagen gel constructs. Reconstituted collagen gels comprise a random mesh of collagen fibrils supporting a large amount of excess fluid (99%) which is expelled upon compression. This may be achieved by application of a mechanical load and/or capillary suction into porous layers, as illustrated in Figure 4. In this way, compressed collagen gels can be produced with a range of predictably controlled collagen and cell densities (typically 11% collagen), with functional mechanical properties (in terms of strength and compliance), and with no substantial reduction in cell viability. The goal is to achieve a spatially uniform distribution of collagen throughout the scaffold. However, the aforementioned process results in the undesirable accumulation of collagen in a thin layer at the fluid-leaving surface which subsequently alters the cell behaviour in these regions.

The aim of this project is to develop a mathematical model to quantify the connection between the load applied, the resulting flow, and the build-up of the high-density collagen layer at the fluid-leaving surface. The model will be used to predict optimal operating regimes for the set-up that promote a spatially uniform distribution of collagen within the gel. A key component of the project will involve the development of models for particle filtration and aggregation [2] under an imposed flow and will involve an array of modelling, asymptotics and numerical techniques.

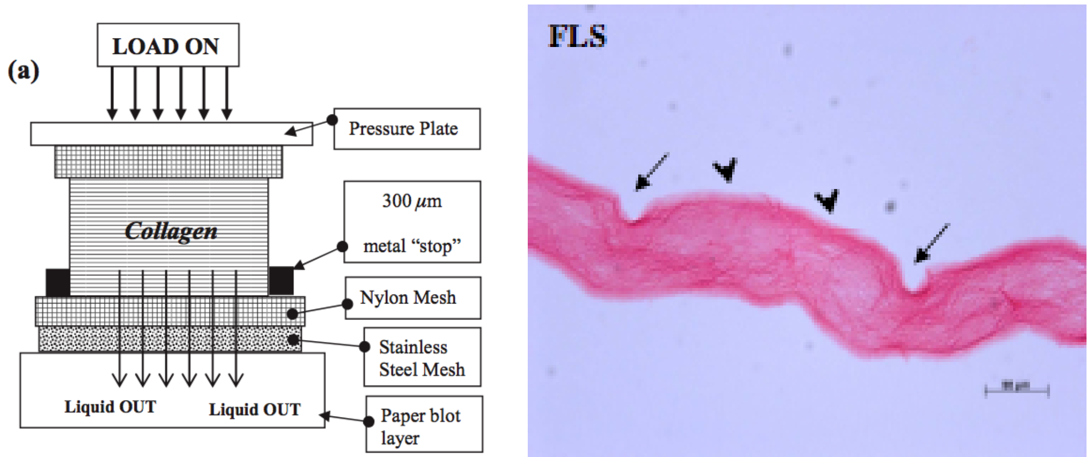

Figure 4: (a) The plastic compression of preformed collagen gels, including both loading (mass) and paper blotting. (b) A collagen-stained gel showing the higher concentration of collagen near the fluid-leaving surface.

A particularly exciting aspect of this project is the opportunity for the student to visit the Tissue Repair and Engineering Centre at UCL to gain first-hand experience of working in a laboratory, and use the modelling outcomes to inform the experimental programmes.

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3.4 Quantifying the Relationship Between Fluid Flow and Matrix Deposition in a Novel *In Vitro* Tissue Engineering Device

Supervisors: Dr Cameron Hall (OCCAM), Dr Peter Howell, Dr James Oliver, Dr Rebecca Shipley and Dr Sarah Waters (OCIAM), Dr Mark Thompson, Dr Russell Tucker (Department of Engineering Science)
Contact: waters@maths.ox.ac.uk

Project background: Mechanical forces play a fundamental role in regulating the activities of cells when building mechanically important tissues — this is exemplified by the fact that athletes build bone and muscle in training, while astronauts lose bone and muscle in microgravity. To harness this powerful helpful effect in engineering replacement tissues for the treatment of major disabling, painful diseases such as osteoarthritis, osteoporosis and tendinopathy, we need to develop a detailed and quantitative understanding of mechanotransduction, the method by which cells sense and respond to mechanical signals.

Cells in muscle, bone and tendon are sensitive to fluid shear stresses that arise due to interstitial flows. Indeed, these cells are equipped with specialised organelles that respond to fluid shear stress. In our experimental work, we are using a novel in vitro stimulation device to mimic the cell environment in vivo. In particular we are interesting in understanding how fluid flows influence the process by which cells put down protein matrix, and also how this process can be controlled *in vitro* when growing new tissues. Our device consists of a petri dish mounted on a platform that see-saws through an angle of around 7 degrees at a frequency of around 0.5 Hz (see Figure 5). The petri dish contains a monolayer of tenocytes (tendon cells), around 10 μm thick, seeded on the base; the cells are bathed in a thin layer of fluid (with density and viscosity similar to water) so that the imposed rocking motion forces waves in the fluid, which in turn impart periodic tangential and normal stresses on the cells.

Our experimental research to date shows that the applied shear stresses from the fluid flow result in upregulated levels of collagen and glycosaminoglycan secretion (these are important protein components of cellular matrix *in vivo*). Importantly, the device is cheap to run and can be used to map the parameter space (cyclic frequency, duration, viscosity etc.) affecting the secretion of these proteins. Preliminary computational fluid dynamics modelling, validated with particle image velocimetry, has also been exploited to establish a direct link between local shear stresses and local protein secretion.

However, in order to translate these basic science results into useful tissue engineering, we need to be able to predict the interaction between the build up of newly secreted matrix and the mechanotransduction capabilities of the cultured cells. This requires multi-scale modelling to connect behaviour at the level of a single cell and its mechanosensory apparatus (in particular, the cell cilia), to that at the level of the cell stimulation device.

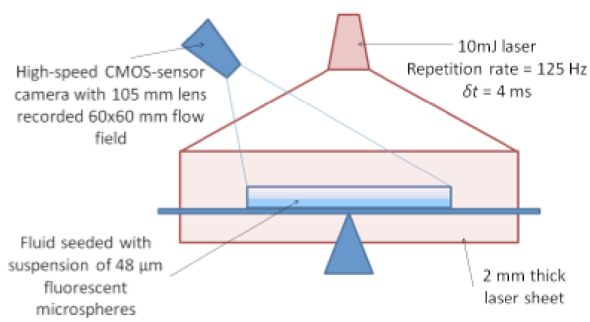

Figure 5: Sketch of the experimental set-up and its validation using laser illuminated particle image velocimetry.

Project aims: The aim of this project is to develop novel theoretical models that describe how the local fluid shear stress environment of the cells evolves as the cells produce extra-cellular matrix. These models will provide insights into the role of mechanotransduction in the developing tissue construct, and also enable the operation of our device to be adapted to promote functional tissue development (e.g. the models will enable the optimum frequency of oscillation to be determine). This research is timely, as on-going experiments at the Engineering Department can be used to validate the outputs of the theoretical models. Once validated, we will have a predictive and quantitative theoretical tool that can be used to inform experimental protocols and will stimulate new experiments.

In addition to the development of the theoretical models, the student will also have the opportunity to spend time in the experimental laboratories and, if willing, can also undertake some simple experimental work.

Project summary: Possible avenues of research are described below, although this is by no means exhaustive, and other research avenues can also be explored.

Preliminary dimensional analysis reveals that the fluid dynamics is well captured by the shallow water equations subject to a time-periodic horizontal forcing, and hence is parameterised purely by the amplitude and dimensionless frequency of the imposed oscillation. Numerical and, where possible, approximate analytical solution of these equations will reveal the regions of parameter space to be avoided experimentally to prevent sloshing instabilities, as well as enabling the stresses experienced by the tissue placed in the device to be quantified.

Once the fluid dynamics of the experimental device are determined (both theoretically and using computational fluid dynamics tools), we will develop models that couple the fluid dynamics to cell matrix secretion. Initially, we will focus at the level of a single cell, and investigate the role of the primary cilium in sensing the local shear stress field. We will then consider a macroscale model, in which the interaction between the local flow environment, mechanotransduction by the cells, and matrix deposition will be considered, with the aim of determining experimental protocols that will be favourable to the engineering of a viable tissue construct.

3.5 Discrete/Hybrid Modelling of Lymphangionesis

Supervisors: Dr Sarah Waters (OCIAM), Prof. Helen Byrne (OCCAM), and Dr Jonathan Whiteley (Computer Science)
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The lymphatic and vascular systems are coupled: fluid and nutrients are delivered by the vasculature while extracellular fluid flows from the capillaries into the lymphatic microvessels and is returned to the vascular system via the thoracic ducts. Failure of the lymphatic system can result in conditions such as lymphoedema.

Although both transport systems interact and are similar, comprising large networks of vessels with an endothelial lining, experimental and theoretical research has focused on the blood system. A variety of theoretical frameworks have been used to study aspects of angiogenesis and vasculogenesis (the de novo formation of new blood vessels) [Perfahl et al, 2011]. Modelling of the lymphatic system is less advanced. Roose & Fowler, (2008) considered the prepatterning of lymphatic vessel morphology within collagen gels, via the establishment of a fluid flow network (no cells present), while Friendman & Lolas (2004) considered a reaction-diffusion equation for lymphangiogenesis which neglects biomechanical stimuli.

Recently, Swartz and coworkers have developed novel assays for the detailed investigation of network formation from blood endothelial cells (BECs) and lymph endothelial cells (LECs). Ng, Helm & Swartz (2004) exposed ECs to interstitial flow in collagen gels, and found key differences between the two cell types in their cell-cell and cell-matrix interactions, and their responses to the local biophysical environment. Through combined experimental and theoretical work, Helm et al. (2005) and Fleury et al. (2006) showed that interstitial flow affects LEC and BEC organization in a fibrin matrix with matrix-bound vascular endothelial growth factor (VEGF). Helm, Zisch & Swartz (2006) found that extracellular matrix composition (fibrin versus collagen) differentially influences the organisation of the two endothelial cell types, with LECs showing the most extensive organisation in fibrin-only matrix and BECs preferring a collagen matrix. These differences are also observed in vivo and it is hypothesised that during dermal wound healing the tissue matrix remodels so that initially it is optimised for angiogenesis and at later stages for lymphangiogenesis.

In this project, we will use a discrete/hybrid modelling approach, similar to that developed in (Owen et al, 2009) and (Perfahl et al, 2011), to study lymphangiogenesis and the interplay between the lymph and vascular networks. In more detail, a discrete model that accounts for the evolving spatial structure of the vascular network will be coupled to reaction-diffusion equations describing the distribution of key growth factors. The models will be informed by the experimental results of Swartz and co-workers, and once formulated, will be validated against the experimental data. The aim is to generate a predictive tool that can be used to inform network formation from lymph endothelial cells in vivo (with applications to wound healing) and in vitro (with applications to tissue engineering for example).

3.6 The Electric-Fluidic Brain

Supervisor: Dr Nick Jones (Physics)
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There is an accepted view that information processing within the brain occurs as a result of electrical activity in our neurons. It is assumed that the blood vessels of the brain tissue have a passive role supplying oxygen. However, while electrical signals are slow to propagate from neuron to neuron, hydraulic effects can propagate through fluid filled vessels at the speed of sound in the fluid. A constriction of a blood vessel in one part of the brain can thus have nearly instantaneous effects elsewhere. There is now increasing evidence that neural activity can serve to control the width of blood vessels and that blood vessel width can affect neural activity. The student will investigate simple models of (fractal) networks of fluid filled vessels penetrating an excitable medium. We will investigate assorted mechanisms in which the neural activity controls the vessels and vice versa. We may investigate whether epilepsy can be reinterpreted as a vascular phenomenon in the context of fluctuations in blood pressure and fluctuations in smaller vessels.

This work will attempt to take existing models of the excitable brain http://www.scholarpedia.org/article/Models_of_epilepsy and establish treatments using excitable media and couple them to a treatment of the vasculature in terms of simple circuit theory.

Outcomes will include an alternative view of brain function and an alternative view of an excitable medium inter-penetrated by an incompressible medium (from which nutrients diffuse).

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4 Physical Application Projects

4.1 Violent Surface Motion: The Entry of a Free Falling Wedge

Supervisors: Dr Jim Oliver (OCIAM) and Dr Dominic Vella (OCCAM)
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Violent surface motion is an important evolving area of fluid dynamics and beyond its fundamental scientific interest it has applications in a number of diverse fields, including industrial coating, cleaning and combustion processes; soil erosion; aircraft icing; the locomotion of animals through or over water (e.g. swimmers and the Basilisk lizard); ship slamming; wave impact on offshore structures and land-slides. All of these impact scenarios require reliable predictions for the fluid flow and/or stress on the impactor.

Even in the simplest two-dimensional inviscid, incompressible water-entry problems (in which a solid body impacts on an initially stationary half-space of liquid, and the effects of gravity, surface tension and air cushioning are neglected), the nonlinearities involved lead to considerable analytical and numerical difficulties in obtaining useful predictions for the liquid flow.

Theoretical efforts have focused almost entirely on the simplifications afforded by the existence of disparate lengthscales, with the majority of work focusing on the "small deadrise angle" regime in which the normals to the impactor and liquid surface are nearly parallel near to the point of impact. This theory is based on the pioneering ideas of Wagner (1932) on the alighting of seaplanes, and has proved to be extremely useful because of its applicability during a small initial time interval to the impact of an arbitrary blunt body and its success in describing many salient features of the flow.

The aims of this project are to (i) develop and analyse a model for the two-dimensional normal symmetric impact of a free falling wedge on a half-space of ideal and incompressible liquid using the methodology described in [1]; (ii) compare the modelling predictions to the experimental data presented in [2] (see Figure 6) and elsewhere.

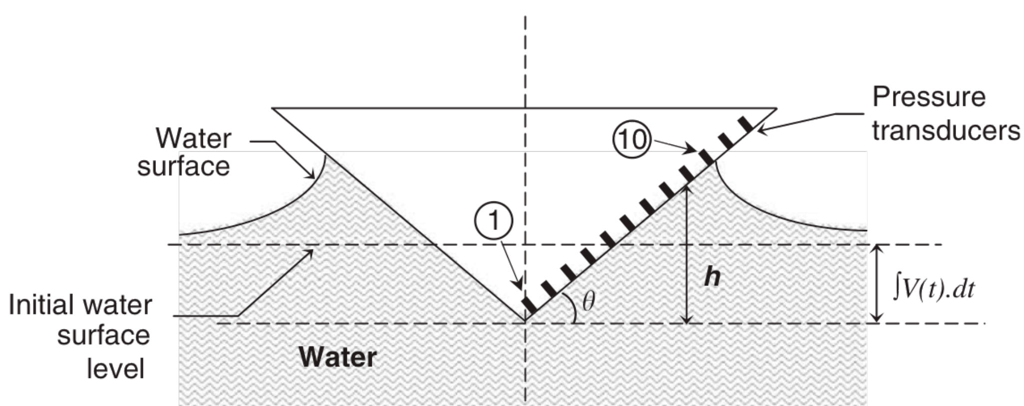

Figure 6: Schematic of experimental setup used in [2].

The project will identify the regimes in which Wagner's theory may be applied successfully to a free falling wedge, as well as those in which additional physical effects (e.g. air cushioning) must be taken into account.

Keywords: Water entry, matched asymptotic expansions, complex variable methods.

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4.2 Mathematics of Freezing Water

Supervisors: Dr Apala Majumdar, Dr Stephen Peppin (OCCAM) and Dr Dirk Aarts (Chemistry)
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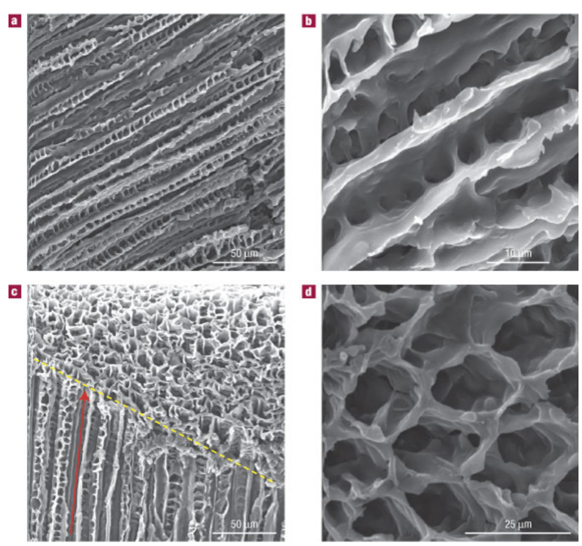
Ice growth in the presence of small particles (colloids) is an example of a nonequilibrium dissipative system with applications in geophysics (glaciers, permafrost), materials science (tissue scaffolds) and biological science (cryobiology). The particles affect the ice growth rate leading to instabilities and pattern formation. In this project we will study, using analytical and numerical methods, the morphological stability of an initially planar ice interface as it interacts with a colloidal suspension. Predicted instabilities will be compared with experiments undertaken at the Department of Chemistry. There is also opportunity to do some simple freezing experiments in the OCCAM Laboratory. This project is motivated by results reported in [1], [2], [3].



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4.3 Liquid Snowflakes

Supervisors: Stephen Peppin (OCCAM), Sam Howison (OCIAM), John Ockendon (OCIAM) and Rich Katz (Earth Sciences)
Presented by: Matt Hennessy (OCCAM)
Contact: peppin@maths.ox.ac.uk

Liquid snowflakes, also called Tyndall figures, are small volumes of water that resemble the classical shape of a snowflake that is composed of ice. They initially form as cylindrical discs of liquid in superheated crystals of ice. Several experimental studies have shown that liquid snowflakes acquire their shape through an instability that occurs in the circular interface. This project will involve mathematical investigation of the evolution of liquid snowflakes. In particular, linear stability analysis will be carried out in order to gain insight into the physical mechanisms that drive the instability of the circular interface. The nonlinear evolution of liquid snowflakes will be studied via direct numerical simulation. The results from the mathematical analysis will be compared with experimental results undertaken in the Earth Sciences and OCCAM Laboratories.

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4.4 On Strong Collision-Free Hydromagnetic Solitary Waves

Supervisor: Prof. John Allen (OCIAM)
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An early paper on large amplitude collision-free hydrodynamic waves was published in 1958 by Adlam and Allen [1]. The term “hydrodynamic” could be misleading because we are not dealing with a fluid model here, but a situation in which electrons and ions interact through macroscopic electric and magnetic fields. The authors obtained a solution for a solitary wave of large amplitude for wave velocities between the Alfvén speed and twice the Alfvén speed. Recent work by Nairn et al [5] has shown that the equations used could be reduced to a single non-linear equation, namely the Korteweg-de Vries equation. Their analysis, however, dealt with finite but limited wave amplitudes. The subject of this dissertation is to find the more general equation corresponding to the large amplitude solutions found in the original work.

A subsequent paper by Adlam and Allen dealt with the excitation of a train of such waves by the magnetic compression of a plasma containing a magnetic field [2]. The solitary wave referred to above predated the nomenclature "soliton", a term coined by Zabusky and Kruskal [3] who studied the collision of such waves. After colliding, the waves do not lose their identity, which led to the adoption of the term "soliton". A semi-popular paper on solitons is cited below [4].

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4.5 Modelling the Onset of Menisci

Supervisors: Dr Dominic Vella (OCCAM), Dr Jim Oliver (OCIAM) and Dr Jonathan Whiteley (Department of Computer Science)
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Whenever a solid object touches a liquid's surface a meniscus forms. The equilibrium shape of this meniscus has been understood for more than two hundred years — its shape is determined by a balance between surface tension and the hydrostatic pressure within the liquid. However, it is only more recently that experimentalists have started to address the question of *how fast* this meniscus develops; how quickly does an interface go from being flat to curved? A series of careful experiments have been reported by Clanet and Quéré [1] along with some simple scaling arguments to understand the growth of the meniscus height with time (see images in Figure 7). However, a more mathematical understanding of these scalings, starting from the Euler equations for fluid flow, remains elusive. Such an understanding would not only confirm the scaling results already obtained but also elucidate how the rate of meniscus growth is affected by, among other things, the wettability of the solid. The aim of this project is to develop such a mathematical model. A key outcome of the model would be a prediction of the rise height as a function of time around vertical cylinders of differing radii and wettability. Such a prediction should then be compared to the experimental results presented in [1].

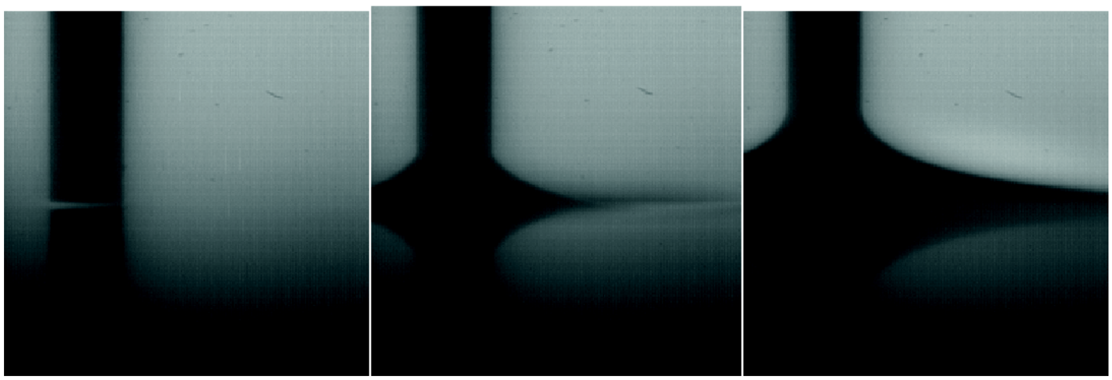

Figure 7: Rise of a meniscus of hexame around a cylinder of diameter 0.45mm.

The project will begin by applying the model of Keller and Miksis [2] which was developed for a related problem, to the case of a cylinder of infinite radius, i.e. a planar wall. This would involve the development of a numerical code using a finite element method (or similar technique) as well as the use of asymptotic methods (e.g. WKB) to understand the behaviour of the solutions. This model should then be modified to account for a finite cylinder radius to understand the role of the cylinder's curvature in determining the dynamics. Again a similar combination of numerical and asymptotic methods will be used in this model. Finally, experimental images similar to those in Figure 7 will be analysed to test the relationship between contact angle and speed of meniscus growth determined from the model.

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4.6 Cooperation versus Dominance Hierarchies in Animal Groups

Supervisors: Dr Mason Porter (OCIAM), Dr Cameron Hall (OCCAM) and Prof. Marian Dawkins (Zoology)
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Various models based on game theory have been used in attempts to describe social interactions among animals. For example, a series of iterated games between "hawks" (who always fight) and "doves" (who always reteat) leads to a an evolutionarily stable state (ESS) composed of a mixture of hawks and doves. A related but slightly more realistic idea is a series of games between "conditional hawks", who act like a hawk if the opponent is smaller but like a dove if the opponent is bigger, which results in an ESS composed entirely of conditional hawks.

To give another example, the iterated prisoner's dilemma has been used to explain why animals that regularly encounter each other might be expected to cooperate, while animals that rarely encounter each other might be expected to defect. However, this model is flawed: true cooperation is rare, even among animals who live together in groups, whereas dominance hierarchies (such as the pecking order in chickens) are much more common. A slightly more realistic variant, in which symmetries between individuals are built into the prisoner's dilemma game, could perhaps provide a sufficient base for a simplistic model of observed behaviors. Just as a conditional hawk does much better than either a hawk or a dove, one would expect a "conditional cooperator" to perform better than pure defectors or pure cooperators.

The aim of this project is to use ideas from game theory and dynamical systems to develop and investigate simple models that account for individual asymmetries and hence allow both dominance hierarchies and co-operation as possible outcomes. By introducing ideas like conditional cooperators, the student will investigate how much asymmetry is needed to make qualitative and quantitative differences in the relative frequencies of altruism versus dominance hierarchies. The student will also investigate the different observed behavior based on the ability of animals to detect and exploit such asymmetries.

4.7 Mathematical Modelling of Surface Tension-Driven Boats

Supervisors: Dr Ian Griffiths and Dr Dominic Vella (OCCAM)
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When a small amount of soap is added to the back of a "soap boat" the surface tension of the water is lowered, inducing Marangoni flows that propel the boat forward. This technique is also employed by some water-walking insects who release chemicals (surfactants) to propel themselves on the water surface [1]. Surface tension gradients can also be generated by temperature differences. This property has led to the recent suggestion that solar-powered boats or "solar ships" may be used to convert sunlight directly into mechanical work [2]. Since relatively few strategies exist that convert light directly to work there are clear implications of such a technology for energy production. (Usually, solar-powered devices rely on the conversion of light to electrical energy, which is then transferred into work.) This concept also provides a novel solution to the challenging problem of remotely controlling the motion of small objects on the surface of water.

Carbon nanotubes are the key component of a solar ship. These strongly radiation-absorbent tubes are attached to the back of the boat. As they absorb light they heat the surrounding water, thereby reducing the surface tension locally and inducing the boat motion. The aim of this project is to develop a mathematical model that describes the underlying mechanism in thermo-capillary and chemical-driven Marangoni flows. Models that incorporate fluid dynamics, surfactant chemistry, and heat and chemical transport will be developed. A combination of analytical, asymptotic and numerical methods will be employed to understand and quantify the behaviour of soap boats and solar ships. In particular, these techniques will allow us to develop an understanding of the balances that determine the speed of translation of the boat, as well as the way in which light causes the development of a temperature gradient.

This project will provide a mathematical theory that allows for the control and guidance of small objects in fluids. The influence of fluid surface tension on boat propulsion will be examined, and the effect of combining both surfactant and heat-absorbing material will be considered. The current solar-ship technology is size-independent and can be extended into both the microscopic and macroscopic regimes. However, the fluid mechanics is very different in these regimes. We will therefore also address the question of the optimal module size for effective energy production.

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4.8 Ordering in Anisotropic Systems

Supervisors: Dr Apala Majumdar, Dr Radek Erban and Dr Stephen Peppin (OCCAM)
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This project aims to build mathematical models for systems of vibrating anisotropic particles where symmetry breaking instabilities lead to pattern formation. A prototype example is a nematic liquid crystalline system with constituent rod-like molecules. This project will involve a combination of mathematical modelling, numerical methods and simple table-top experiments. The student will study systems of vibrating pins or ellipsoid-shaped particles and analyze phase transitions from disordered to ordered states as a function of the vibration frequency, amplitude, packing fraction and geometrical features. These transitions will be modelled via partial differential equations-based models and simulations based on discrete individual-based models simultaneously. The two approaches will be compared and the coefficients of the partial differential equations-based model will be computed from the discrete model simulations. The student will undertake all related experiments in the newly established OCCAM Applied Mathematics Laboratory. This project is motivated by the results reported in [1],[2], [3] and [4].

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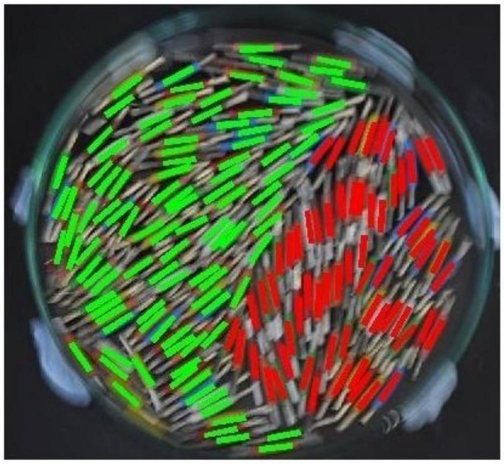

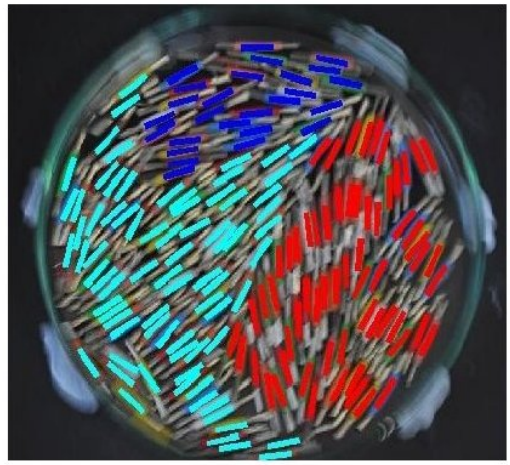

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4.9 Carbon and Climate

Supervisors: Dr Andrew Fowler (OCIAM) and Dr Ros Rickaby (Earth Sciences)
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Carbon is thought to be very important for the climate of the future, as well as the climate of the past. Carbon dioxide is produced volcanically (and recently, anthropogenically), and it controls temperature through its action as a greenhouse gas. It is removed from the atmosphere by weak acid rainfall and by dissolution in the ocean, where most of it resides. To understand the variation of carbon, we therefore need to describe the buffering system of carbon in te ocean, and this brings in additional considerations involving acidity, calcium, biomass and phosphorus. In addition, the climate since the Eocene requires a prescription for ice sheet growth.

The simplest such models are box models describing the evolution of these variables in compartments representing the ocean, atmosphere, etc., and comprise a sequence of ordinary differential equations. The formulation, anaysis and solution of these represent the starting point for the project, based on recent work of the supervisors, and there are a number of applications: ice ages, global warming, post-Eocene cooling. The main part of the project will lie in the extension of this box model to allow for either or both of transport in the vertical in the ocean, and poleward transport in the ocean and atmosphere. Other extensions are also possible, notably to account for the uptake of CO2 by biomass on land.

4.10 Liesegang Rings

Supervisors: Dr Andrew Fowler (OCIAM) and Dr Rich Katz (Earth Sciences)
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Liesegang rings form when a solution od silver nitrate is placed at the centre of a gel impregnated with potassium dichromate. The chemical species diffuse and react, forming a product which then precipitates. However, the precipitate is not continuous, but forms a series of rings (in a petri dish) or layers (in a test tube). A classical explanation for this behaviour lies in the necessity for supersaturation of the solution before precipitation can occur, and it is straightforward to write down simple mathematical models to describe this.

The aim of this project will be to understand and analyse the mechanism for the periodic precipitation bands, and to solve the consequent model numerically. The project will also involve experimental work, and the data will be compared with the anaytic results. Possible extensions of the mode structure lie in the formation of orbicular plagioclases, cloud layers and layered igneous intrusions, and some initisl investigation of some of these phenomena may also be possible.

4.11 Structure Stability Diagram for Nanoparticle Embedded in Amorphous Matrix

Supervisors: Prof. Alain Goriely and Dr Victor Burlakov (OCCAM)
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Nanoparticles of a material embedded in a matrix of another material form a composite nanomaterial useful for many applications ranging from quantum opto-electronics to automotive industry. An example of such nanocomposite is Si nanocrystals in SiO_2 matrix (PRB 83, 235303 (2011)). Both electro-optical and mechanical properties of this system significantly depend on the adhesive interactions between the constituent materials and their structural stability. Structure stability is especially important for embedded nanoparticles. There are experimental evidences that these nanoparticles may have amorphous or crystalline structure depending on their size and ambient temperature. The current project is aimed at the development of a generic theory of structural stability of nanoparticles in an amorphous matrix. Possible approach will be based on a phenomenological analysis of the phase stability taking into account both cohesive and interface energies and their temperature dependence. The latter will be estimated considering thermal expansion of the materials and associated stress distributions.

4.12 Ostwald Ripening in the System of Concentric Rings

Supervisors: Prof. Alain Goriely and Dr Victor Burlakov (OCCAM)
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Phase separation of polymer mixtures is a very common phenomenon during fabrication of photo-voltaic devices by spin coating (Eur. Phys. J. E 31, 369 (2010); E 33, 283 (2010)). The final structures are often represented by a set of concentric rings. Such systems have still very high interface energy, which can be reduced via coarsening (Ostwald ripening) phenomenon. The project is focused on developments of the phenomenological theory of Ostwald ripening for the geometry represented by a set of concentric rings. The problem could not be approached in a way similar to classical Lifshitz-Slyozov-Wagner theory of Ostwald ripening, as the mean field approximation cannot be used in such a system. The main question to be addressed is related to the time evolution of average ring radius.

5 Networks

5.1 Temporal Networks

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A network, usually modelled as a graph, consists of a set of entities and the connections between them. The study of networks has exploded during the past twenty years, and techniques from subjects such as statistical mechanics, graph theory, information theory, and computer science have played major roles in these investigations. Most of this work, however, has concentrated on static networks even though most networks in the real world depend on time. This is starting to change, as scientists attempt to generalize concepts applied to static networks for time-dependent situations. In particular, concepts like centrality, social balance, clustering, and community structure need to be pursued in time-dependent contexts. In this this project, the student will study "simple" dynamical systems on temporal networks in order to investigate the interplay between dynamics on networks and dynamics of networks. One possible type of problem to study are social or biological contagion models on temporal networks.

5.2 Network Modelling of Coronary Microcirculation

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The coronary microcirculation consists of vessels with dimensions less than about 200 mm and contains more than 95% of the total coronary vasculature segments. These vessels are responsible for the major resistance to vascular flow, as well as short-term regulation and long-term adaptations that ensure that the cardiac demands are satisfied at both local and global levels. However, despite years of research, a complete and concise description of the coronary microcirculation remains elusive: the vessel networks exhibit a heterogeneous and anisotropic 3D mesh-like organisation, with a vascular density that is some 5–10 times higher compared to other organs, which makes quantitative characterization of its structure technically challenging.

In this project, we will attempt to characterize this structure using ideas from networks. In one part of the project, the student will examine the structure of networks taken from experimental data. Simultaneously, the student will develop generative network models – e.g. in the form of random-graph ensembles – that produce similar values for network characteristics. Time-permitting, the student will also examine appropriate dynamics on these networks to determine what observable differences might result from using different network descriptions.