1st CMM-Bath Workshop on Applied & Interdisciplinary Mathematics

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ABSTRACTS

Patricio Cumsille, UBB

"Parameter estimation and mathematical modeling for the quantitative description of drug resistance in gastrointestinal stromal tumor metastasis to the liver"

Abstract: In this work we develop mathematical modeling and devise a practical identifiability approach for gastrointestinal stromal tumor (GIST) metastasis to the liver, with the aim of quantitatively describing drug resistance. To this end, we have modeled metastatic growth and resistance to two standard treatments based on tyrosine kinase inhibitors (Imatinib and Sunitinib) that have been observed clinically in patients with GIST metastasis to the liver. The parameter identification problem is difficult to solve, since there are no general results on this issue for models based on ordinary differential equations (ODE) like the ones studied here. We propose a general modeling framework based on ODE for GIST metastatic growth and therapy resistance and analyzed five different model variants, using medical image observations (CT scans) from patients that exhibit drug resistance. The associated parameter estimation problem was solved using the Nelder-Mead simplex algorithm, by adding a regularization term to the objective function to address model instability, and assessing the agreement of either an absolute or proportional error in the objective function. We compared the goodness of fit to data for the proposed model variants, as well as evaluated both error forms in order to improve parameter estimation results. From the model variants analyzed, we identified the one that provides the best fit to all the available patient data sets, as well as the best assumption in computing the objective function (absolute or proportional error). This is the first work that reports mathematical models capable of capturing and quantitatively describing drug resistance based on clinical images in a patient-specific manner. Additional studies need to be conducted in order to elucidate the underlying mechanisms of resistance for developing mathematical models that may explain this phenomenon in a more accurate way.

Joaquín Fontbona, CMM/UChile

"Synchronization of stochastic mean field networks of Hodgkin–Huxley neurons with noisy channels"

Abstract: We are interested in a mathematical model of the collective behavior of a fully connected network of finitely many neurons, when their number and when time goes to infinity. We assume that every neuron follows a stochastic version of the Hodgkin–Huxley model, and that pairs of neurons interact through both electrical and chemical synapses, the global connectivity being of mean field type. When the leak conductance is strictly positive, we prove that if the initial voltages are uniformly bounded and the electrical interaction between neurons is strong enough, then, uniformly in the number of neurons, the whole system synchronizes exponentially fast as time goes to infinity, up to some error controlled by (and vanishing with) the channels noise level. Moreover, we prove that if the random initial condition is exchangeable, on every bounded time interval the propagation of chaos property for this system holds (regardless of the interaction intensities). Combining these results, we deduce that the nonlinear McKean–Vlasov equation describing the

evolution of an infinite network of such neurons concentrates, as time goes to infinity, around the dynamics of a single Hodgkin–Huxley neuron with chemical neurotransmitter channels. Our results are illustrated and complemented with numerical simulations. Joint work with Mireille Bossy (INRIA Sophia-Antipolis) and Héctor Olivero (U. of Valparaíso).

Silvia Gazzola, University of Bath
"Fast Iterative Regularization Methods"

Abstract: Inverse problems are ubiquitous in many areas of Science and Engineering and, once discretized, they lead to ill-conditioned linear systems, often of huge dimensions: regularization consists in replacing the original system by a nearby problem with better numerical properties, in order to find a meaningful approximation of its solution. After briefly addressing some classical regularization strategies (such as Tikhonov method) and surveying some standard iterative regularization methods (such as many Krylov methods), this talk will introduce the recent and promising class of the Krylov-Tikhonov iterative regularization methods. In particular, strategies for choosing the regularization parameter and the regularization matrix will be emphasized. Also, this talk will present a common framework that exploits a flexible version of well-known Krylov methods such as CGLS and GMRES to handle non-negativity constraints and regularization terms expressed with respect to the 1-norm, resulting in an efficient way to enforce sparse reconstructions of the solution. Numerical experiments and comparisons with other well-known methods for the computation of nonnegative and sparse solutions will be presented. These results have been obtained working jointly with James Nagy (Emory University), Yves Wiaux (Heriot-Watt University), Julianne Chung (Virginia Polytechnic Institute and State University), and Malena Sabate' Landman (University of Bath).

Sergio Gutiérrez, PUC
"Worst Case Optimal Design using Small Amplitude Homogenization"

Abstract: The Small Amplitude Homogenization idea is used to solve optimal design problems in the worst possible case when there is uncertainty in some of the information needed to formulate the state equation of the problem. To select the worst possible case, a first-order approximation of the objective function in terms of the quantity known with uncertainty is maximized over the set of admissible perturbations. Considering perturbations of the bounded norm, the worst possible case becomes explicit and the aforementioned first order approximation is minimized by a gradient method. Numerical examples for heat diffusion are shown, first when the internal heat source is known with uncertainty, and secondly, for solving an inverse problem.

Duván Henao, PUC
"Debonding of a gel from a rigid substrate"

Abstract: A variational model for the delamination of polymer gel thin films from rigid substrates is presented. A formal asymptotic analysis of a simplified 2D version of the underlying governing equations show that, as the film grows thinner, the absorption of the moisture of its surroundings tends to produce a homogeneous vertical stretch in the part of the film that remains bonded to the substrate and a state of free swelling in the debonded part. A transition layer, with a width comparable to the film thickness, is developed in order to connect the two swelling modes. This work is joint with Carme Calderer (U. Minnesota), Carlos Garavito (U. Minnesota), and Suping Lyu (Medtronic Inc.).

Daniel Hurtado, PUC

“Multiscale modeling of lung tissue biomechanics”

Abstract: The mechanical behavior of the lungs plays a key role in the process of respiration in mammals, as it continuously deforms to accommodate the air necessary for gas exchange in the respiratory system. Under certain chronic diseases, the mechanical properties of lung tissue can change dramatically, which results in a macroscopic change of lung elasticity that is strongly related to impaired lung function. More recently, highly prevalent chronic lung diseases such as pulmonary emphysema and lung fibrosis have been postulated to be the result of a biological response to unphysiological stress demands. Therefore, understanding the mechanics of lung tissue and relating its mechanical function to the underlying microstructure and microstructural properties are key to understand lung disease genesis and progression. In this work, we use non-linear asymptotic homogenization theory to develop a micromechanical model for the lung tissue. To this end, we consider a tetrakaidecahedral unit cell to represent the microstructure observed in alveolated tissue. Furthermore, we include the contribution of key structural biological elements in the definition of the constitutive relations that govern the micro-scale problem. We validate the proposed micromechanical model with experimental data obtained from uniaxial tension tests of lung tissue samples and discuss the relevance of the different parameters considered in our model on the macroscopic response, as well as their connection with certain chronic lung diseases.

Rodrigo Lecaros, UTFSM

“An inverse problem for Moore--Gibson--Thompson equation arising in high intensity ultrasound”

Abstract: It is well known that the use the classical Fourier's law to describe the heat flux leads to an infinite signal speed paradox. The use of other constitutive relations for the heat flux have been considered in the literature. One of these is the Maxwell--Cateneo law which, combined with fluid physics equations, leads to a third order (in time) partial differential equation, known as the Moore--Gibson--Thompson (MGT) equation:

$$\left\{\begin{array}{l} u_{ttt}+\alpha u_{tt}-c^2\Delta u-b\Delta u_t=f, \;\; \text{in } \Omega\times(0,T) \\ u=h, \;\; \text{on } \Gamma\times(0,T) \\ u(\cdot,0)=u_0, u_t(\cdot,0)=u_1, u_{tt}(\cdot,0)=u_2, \;\; \text{in } \Omega, \end{array}\right.$$

where Γ denotes the boundary of Ω, and $\alpha=\alpha(x)>0$ is a coefficient depending on a viscosity of the fluid, and the rest of the parameters are positive constants.

Rajesh Mahadevan, UdeC

“An optimization problem related to the nematic equilibrium of liquid crystals”

Abstract: In an ongoing work with A. Chorwadwala and A. Majumdar we consider the problem of determining the nematic equilibrium of a liquid crystal with a circular inclusion inside a circular domain. We present some results on the optimal configuration in the framework of the one-constant approximation of the Oseen-Frank model based on a sensitivity analysis of the shape functional.

References

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[2] A. H. Lewis, D. G. A. L. Aarts, P. D. Howell, and A. Majumdar, Nematic Equilibria on a Two-Dimensional Annulus, Studies In Appl. Math. **138** (2017), 438-466.
[3] A. Majumdar and A.H. Lewis, A Theoretician's Approach to Nematic Liquid Crystals and Their Applications, Variational Methods in Molecular Modeling, pp. 223-254, Springer, Singapore, 2017.

Apala Majumdar, Bath
"Pattern Formation in Confined Nematic Liquid Crystals"

Abstract: Nematic liquid crystals are classical examples of mesophases that have physical properties intermediate between those of conventional solids and liquids. Nematics are anisotropic liquids with long-range orientational order, with distinguished directions. Consequently, nematics have directional properties, making them suitable working materials for several opto-electronic devices and the multi-billion dollar display industry. In this colloquium, we discuss the hierarchy of continuum theories for nematics - the Oseen-Frank, the Ericksen and the Landau-de Gennes theories and illustrate their predictive powers by reviewing recent work on pattern formation in square wells filled with nematic liquid crystals, driven by geometrical, topological and energetic considerations. We discuss pattern formation in different asymptotic limits, with emphasis on multistability and the stabilizing/de-stabilizing effects of nematic defects and how this can lead to new optical and mechanical responses.

Paul Milewski, Bath
"The Complex Dynamics of Faraday Pilot Waves: A Hydrodynamic Quantum Analogue"

Abstract: Faraday pilot waves are a newly discovered hydrodynamic structure that consists a bouncing droplet which creates, and is propelled by, a Faraday wave. These pilot waves can behave in extremely complex ways exhibiting a classical form of wave-particle duality, and result in dynamics mimicking quantum mechanics, including multiple quantization, probabilistic particle distributions reminiscent of QM, single slit diffraction and tunneling. I will show some of this fascinating behaviour and will develop a surface wave-droplet fluid model that captures many of the features observed, and focus on rationalizing the emergence of the statistics of complex states.

Jaime Ortega, CMM/UChile
TBA

Axel Osses, CMM/UChile
"A mathematical direct & inverse model for light-sheet microscopy"

Abstract: We consider a mathematical model for light sheet microscopy based on the propagation of the laser as a Fermi pencil beam into the object. We also model the camera reception from the excited fluorescent material using the transport of photons. We prove the uniqueness of the recovery for the three-dimensional distribution of the fluorescent material using some non-standard backward uniqueness for the heat equation. We show some numerical examples of algebraic reconstruction using the proposed model.

Iván Rapaport, CMM/UChile
"The Congested Clique Model"

Abstract: The congested clique model is a message-passing model of distributed computation where the underlying communication network is the complete graph of n nodes. We consider the situation where the joint input to the nodes is an n-node labeled graph G. The reconstruction problem is defined as follows: if the input graph G doesn't belong to a particular graph class, then every node must reject; otherwise, every node must "reconstruct G" (i.e., must end up knowing all the edges of G). In this talk we are going to discuss some relations between particular graph classes and the corresponding complexity measures of the distributed algorithms for solving the reconstruction problem (these complexity measures are in fact time and bandwidth).

Johannes Zimmer, University of Bath
"From fluctuations in particle systems to their scaling limits and applications"

Abstract: We study particle systems and analyze their fluctuations. A motivation for this study work of Onsager, where he describes macroscopic systems by linear relations between forces and fluxes in this system. This Onsager structure is closely related to the modern mathematical theory of gradient flows. We consider dynamical fluctuations in systems described by Markov chains, and discuss a canonical structure that provides a unifying description of Markov chains, Onsager theory, and so-called macroscopic fluctuation theory. As Onsager theory, the theory involves a relation between probability currents (fluxes) and their conjugate forces. However, we will explain that on the level of Markov chains, the relation is non-linear. The tool will be dynamical large deviations, and the formulation is applicable to irreversible Markov chains. We discuss the resulting variational structure, which leads to generalized gradient flows. It is shown that various physically natural splittings can be introduced, which can help to derive applications such as an understanding of acceleration of convergence to equilibrium and dissipation bounds. We will sketch relations between the underlying variational structure on the particle level and its continuum counterpart, which describes the gradient flow of the macroscopic density associated with the particle system. This is joint work with Marcus Kaiser (Bath) and Rob Jack (Cambridge).