Reaction-diffusion equations
modelling, analysis and simulations

April 5, 2024 - Room 5.5, DM-UC

Abstracts

Title: Reaction-diffusion systems: the effects of cross-diffusion and domain growth

Speaker: Raquel Barreira[1,2]

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Abstract

Reaction-diffusion systems have been extensively studied as a class of the prominent models for investigating the pattern generation in various biological and chemical processes. Cross-diffusion refers to a special type of diffusion process in which one of the species influences the flux of the concentration gradient of others. Some applications of cross-diffusive systems include pattern formation and bacterial chemotaxis. Another application relevant to cross-diffusive systems is illustrated by the process of electrodeposition experimentally.

In this talk we will present an overview of the studies on the influence of cross-diffusion and domain growth in expanding the range of mechanisms that can give rise to spatial patterns away from the classical short-range activation, long-range inhibition paradigm of reaction-diffusion systems on static domains with no cross-diffusion.

References

[1] Yigit, G., Sarfaraz, W., Barreira, R., Madzvamuse, A. (2024). Unravelling the geometric influence on the spatiotemporal pattern formation of cross-diffusive reaction-diffusion system on annular regions (Manuscript in preparation)

[2] Yigit, G., Sarfaraz, W., Barreira, R., Remaki, L., Alhazmi, M., Madzvamuse, A. (2024). Understanding the dual effects of linear cross-diffusion and geometry on reaction-diffusion systems for pattern formation (submitted)

[3] Yigit, G., Sarfaraz, W., Barreira, R., Madzvamuse, A. (2024). A domain-dependent stability analysis of reaction–diffusion systems with linear cross-diffusion on circular domains. *Nonlinear Analysis: Real World Applications*, 77

[4] Madzvamuse A., Barreira R. (2018). Domain-growth-induced patterning for reaction-diffusion systems with linear cross-diffusion. *Discrete and Continuous Dynamical Systems –B*, 22

[5] Madzvamuse, A., Ndakwo, H.S., Barreira, R. (2016). Stability analysis of reaction-diffusion models on evolving domains: the effects of cross-diffusion. *Discrete and Continuous Dynamical Systems - A*, 36

[6] Madzvamuse A., Ndakwo, H.S. , Barreira, R. (2015). Cross-diffusion-driven instability for reaction-diffusion systems: Analysis and simulations.*J. Math. Biol.*, 70

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Title: On the design of discrete cross-diffusion filters

Speaker: Sílvia Barbeiro, CMUC, Department of Mathematics, University of Coimbra

Abstract:

Image restoration is one of the major concerns in image processing with many interesting applications. In the last decades there has been intensive research around the topic and hence new approaches are constantly emerging. Partial differential equation based models, namely of non-linear diffusion type, are well-known and widely used for image noise removal.
In this talk we will focus on nonlinear cross-diffusion systems for image filtering. Some attention will be given to the numerical discretization of the models. Then we will explore fully-discrete filters which reveal similar features as their continuous counterparts as scale-space invariances as well as the existence of Lyapunov functions. Finally, we will discuss a flexible learning framework in order to optimize the parameters of the model improving the quality of the denoising process.

Title: Deep Learning for parameter estimation in reaction-diffusion PDEs for battery modeling

Speaker: Maria Grazia Quarta [1,2]

(1) Università del Salento

(2) visiting PhD student at Instituto Politécnico de Setúbal

Abstract

One of the key development areas in battery research is finding ways to use metallic anodes, like Zn and Mg, but avoiding lithium, which is pyrophoric and sourced only in potentially critical geopolitical areas. Unfortunately, use of post-Li batteries is impaired by poorly understood shape changes, responsible for various failure modes.

Over the past decade, in the framework of the RD-PDEs, a powerful mathematical approach has been developed in [1], able to capture the essential features of unstable material growth in electrochemical systems in terms of Turing pattern formation. Recharge instability problems in batteries with metal anodes are a special case of this phenomenon. On the other hand, the difficulty of studying materials in real-life battery context leads to a methodological gap between theory and experiments. For this reason, parameter identification in the above PDE modelling is crucial for advancement in this direction.

In this research, based on [2], we propose to apply Deep-Learning as a new approach for parameter estimation, instead of the more traditional PDE constrained optimization, as for example in [3]. In the seminar we will discuss the Convolutional Neural Network devised for our goals, trained with the numerical solutions [4] of the morphochemical PDE model that is able to capture the essential features of unstable material growth in electrochemical systems.

We will show that the CNN carries out three tasks:

i. automatic partitioning of the parameter space associated to the PDE model, according to the types of patterns generated;

ii. classification of simulated and experimental patterns;

iii. identification of the model parameters for experimental electrode images.

References

[1] D. Lacitignola, B. Bozzini, I. Sgura, Spatio-temporal organization in a morphochemical electrodeposition model: Hopf and Turing instabilities and their interplay, EJAM, 2015.

[2] I. Sgura, L. Mainetti, F. Negro, M. G. Quarta, B. Bozzini, Deep-Learning based parameter identification enables rationalization of battery material evolution in complex electrochemical systems. J. of Computational Science (2023).

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[4] M.C. D'Autilia, I. Sgura, V. Simoncini, Matrix-oriented discretization methods for reaction–diffusion PDEs: Comparisons and applications, Computers and Mathematics with Applications (2020).

Title: A Crank-Nicolson approach for drug delivery from Maxwell-Wiechert viscoelastic devices

Speaker: Gonçalo Pena, CMUC, Department of Mathematics, University of Coimbra

Abstract: Polymeric drug delivery platforms offer promising capabilities for controlled drug release thanks to their ability to be custom-designed with specific properties. When a spherical polymeric platform containing a drug is placed in a solvent reservoir, a series of complex phenomena occur: solvent absorption, polymer swelling, drug dissolution and diffusion. As the fluid permeates the polymeric structure, the polymer chains start building up stress, leading to an anti-convective flux. To account for the polymer's relaxation and stress development, we incorporate a Maxwell-Wiechert model. This introduces a memory effect in the system where the flux depends not only on the current fluid concentration gradient but also on the history of this gradient through a time integral. This phenomenon is mathematically described by a system of integro-differential partial differential equations, as detailed in [1].

From a numerical standpoint, this integro-differential system presents interesting challenges. When developing numerical methods for these equations, due to the presence of the memory term in the form of an integral over time, the standard approach is to directly discretize the time integral with some quadrature formula. However, in general, this leads to a scheme that, in each timestep, requires the approximate solution at all previous timesteps.

In this talk, we propose a novel approach to overcome this drawback. We introduce a new differential equation that effectively replaces the memory term, avoiding the integral formulation. This enables the development of a new numerical scheme that does not require storing information from all previous timesteps, significantly improving computational efficiency. The proposed scheme utilizes the Crank-Nicolson approach for time integration and incorporates suitable nonuniform finite differences in space.

The main results of this talk focus on the scheme's stability and its second-order accuracy for non-smooth solutions.

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