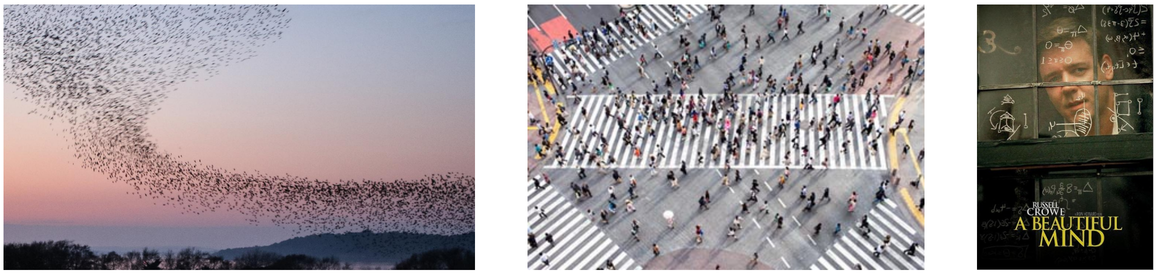
Master thesis proposal

Numerical approximation of cross-diffusion models for studying interacting species



(a) (b) (c)

(a) Formation of migrating birds; (b) A crowd formation during rush hour; (c) Russell Crowe potraying John Nash in the movie A Beautiful Mind, talks about governing dynamics.

Introduction. The study of pattern formation as a result of interaction between physical objects have long been an active area of theoretical research in the physical and mathematical sciences. It has been observed that when two physical objects (which we henceforth call *species*) interact, intricate patterns arise as a result of their mutual avoidance or attraction. Some examples of pattern formation in the physical world could be the development of an ecosystem for biological beings, which is formed when a variety of species arrange themselves spatially through postive interactions or through avoidance(5), or it could be the formation of thermodynamically stable physical structures such as snowflakes (3), membranes and micelles (1) or even the formation of galaxies (4).

In the context of mathematical modelling of such physical phenomena through partial differential equations, we rely on cross-diffusion models which are formulated as

$$\partial_t \rho_i = \nabla \cdot \left(\underbrace{\kappa_i \nabla \rho_i}_{Diffusion} + \sum_j \underbrace{\rho_i \nabla W * \rho_j}_{Interaction} \right), \qquad i = 1, \cdots, N,$$

for N interacting species. In the above model, the diffusion term plays a role of self-assembly and self-organisation, while the convolution term, to its right, is responsible for the interaction with other involved species. Typically, cross-diffusion systems are endowed with an dissipative energy functional which is minimized as the system reaches more stable energy states and the emergent patterns, mentioned previously, form as a result of local minimum energy states.

The project. In this master thesis, the primary focus will be to design numerical schemes that approximates complex interacting multispecies models and allow them to be understood through numerical simulation. Towards this goal, we aim to formulate a finite volume (FV) approximation for several cross-diffusion multispecies system found in the literature and study its properties against the theoretical analysis. An essential feature of the numerical schemes will be the use of the Scharfetter-Gummel (SG) flux (2) which will be used to design the FV scheme.

The candidate will be required to read through the literature and collect a set of simplified models that can be used as test cases. Furthermore, the candidate is expected to implement the multispecies numerical species using the SG flux and conduct analysis to arrive at a *structure-preserving* numerical scheme for the study of interacting species.

Skills to learn.

- A mathematical insight into the working of (interacting) dynamical systems.
- Numerical analysis using Finite Volume methods.
- Improved coding in Python and presentation skills.

Requirements.

- Strong knowledge in analysis and PDEs. Student must be familiar with courses 2MMA10 and 2MMA20.
- Good coding skills in Python. Course requirement 2MMN10 and 2MMS20.

Duration of the project. 4 to 6 months. Starting date end of 2023 or early 2024.

Master thesis supervisors. Interested candidates are encouraged to contact the supervisors at the below email addresses.

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References

[1] I.R. Epstein, J.A. Pojman and Q. Tran-Cong-Miyata. (2004). Nonlinear dynamics and polymeric systems: An overview.

[2] A. Schlichting and C. Seis. The Scharfetter–Gummel scheme for aggregation–diffusion equations. J. Numer. Anal. 42.3 (2022): 2361-2402.

[3] K. Libbrecht. (2003). The snowflake.

[4] J. Binney and S. Tremaine. Vol. 20 (2011). Galactic dynamics.

[5] V. Giunta, T. Hillen, M. Lewis and J.R. Potts. Local and global existence for nonlocal multispecies advection-diffusion models. SIAM J. Appl. Dyn. Sys. 21 (2022), pp.1686-1708.