Complexity DTC Miniproject

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Image Analysis and Numerical Analysis

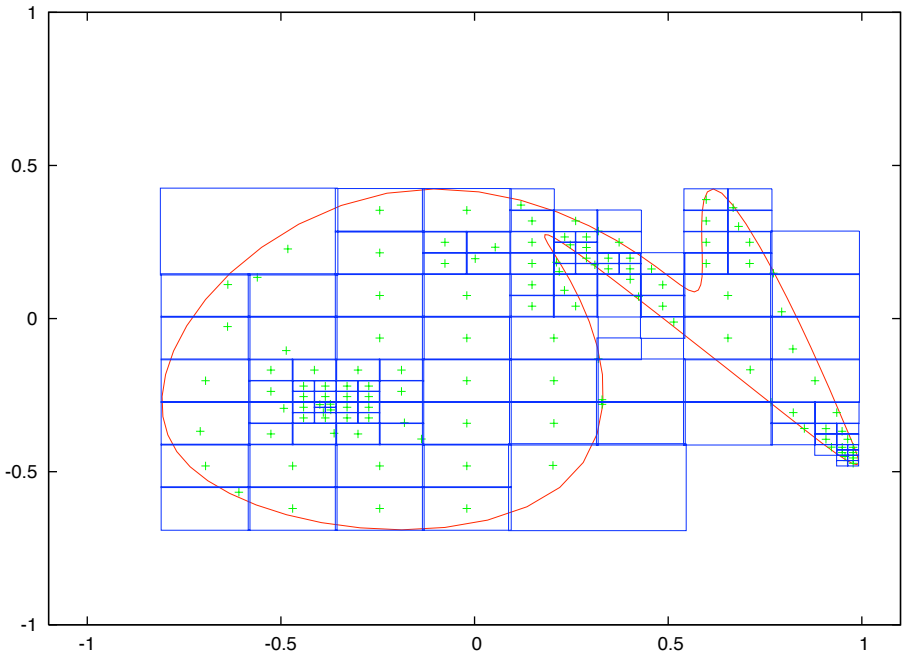
Research objectives

The main overall objective of this research is to find (a) mathematical models describing dynamical processes in images, possibly an approximation (in case some parts of a model are not formulated as discrete objects or events) which can be implemented and simulated on a digital computer. We will in particular try to achieve the following goals:

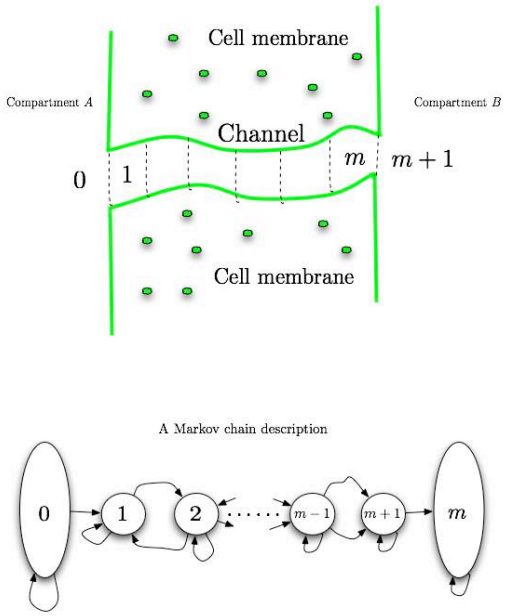
- Develop a computational theory that allows us to consider various combinations of multi-level complex systems applied to biological transport phenomena, partly formulated as discrete and continuum objects, and either formulated in discrete or continuum time (in case a dynamic process is considered).
- Formulate numerical discretisations and algorithms adapted to describe a large class of complex systems in the context of aggregation, as biological processes are usually too cumbersome to study in every molecular detail. Test the computational theory by way of real-world case studies inside the complex systems DTC.

We need efficient simulations of multi-scale systems in many scientific applications, but focus here on biological transport:

- What fine-level structures or temporal processes of a simulation model can be aggregated during the modelling process without changing the solution too much, or inside a well-defined error bounds? The solution will be defined on a relatively coarser scale of observation.
- How does the aggregation method change the simulation model when another scale of observational resolution is chosen?
- Once the computational model is implemented it will typically incorporate a mix of discrete objects (such as lower-dimensional manifolds defining the boundaries of computational sub-domains, i.e. biological membranes) and temporal processes (such as transport processes) defined on these structures, such as the cytoskelleton. In order to gain more accuracy of the solution, refinements of the computational grid at all these defining structures have to be made. Can aggregation methods help to determine when grid refinements (including those in time) lead to a change of the computational model defined on relative micro-structures?



A cover of a complex domain. It could possibly have several holes.



A biological example of a discrete dynamic object triggering dynamical changes in live imaging: a n ion channel.

• In case the computational domain is very heterogeneous (such as in porous media), the multi-scale character of the computational domain should be exploited in order to find an iteratively convergent and stable solution algorithm. One successful class of algorithms are the Algebraic Multi-Grids (AMG) [1], [2] which in a broad sense rely on stochastic sampling and aggregation on different scales of the problem. Can we define similar methods efficiently on computational domains with a mix of random and non-random structures, such as multi-scale transport networks?

- An overall question is whether complex multi-scale systems can be simulated in a stable way, using the latest advances in software methodology? There are many issues involved, such as the interplay of domains and surfaces in such problems,

interaction with discrete objects such as obstacles in different dimensions etc. Any such multi-scale structure imposes severe difficulties on the discretisation part of an algorithm, i.e. the construction of the computational grid at different scales.

- In complex systems theory, but also in economics and finance, so-called **agent-based models** [5] are frequently used. They can be implemented on digital computers directly, because (a) they are based on discrete objects (the agents), and (b) their updates in state (such as their 'opinion' or 'strategy') are following a discrete event statistics. It is clear that combinations of PDE (Partial Differential Equations) based models with agent-based models make perfect sense. Just think for example of agents that are acting in some kind of field (of 'information', or of a 'force') influencing their state, and that this field is having different effects than interaction with other agents. Such models will allow to model more advanced social systems, and are also occurring in reaction systems where some of the molecules are large enough in order to be described as discrete objects. We will aim at finding a basis for a computational theory combining numerical analysis with agent-based modelling.
- Often aggregation of a mathematical model induced by time-scaling can change the computational 'type' of the model. A good example is agents or molecules modelled by discrete states with the help of Markov Chains. In case the agents' switching behaviour between discrete states is on a faster scale than their interaction with their continuum environment one can collapse the discrete state dynamics to the invariant measure of the Markov Chain, i.e. their states' equilibrium distribution. Under this assumption one can reduce a reaction system (also if modelled in space) to a pure 'weighted' continuum model. [6]
- A computational theory of hierarchical modelling and aggregation must account for compatibility between aggregation methods and respective data structures. The aggregation method is essentially a compression of algorithmic speed or increase of efficiency. This triggers usually at the same time a data compression where the data structure itself becomes of structured type.

Why is it interesting?

The research leads towards the latest developments in biological and medical research, which is more and more often image-based.

Techniques required.

- Mathematical Modelling
- Numerical Analysis
- Computing and Programming

Prospective deliverables.

- A simulation based on the DUNE software (contact proposer).

Who should benefit from this research?

- Complex systems scientists
- Biologists and Medical Science

Outline of avenues for a follow-up PhD project.

The project has potential for several PhD so a thesis must focus on some aspect of this research. A very fruitful research direction is to implement a simple membrane-cytoskeleton-cytosol protein exchange model.

References:

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