Multi-scale simulations with complex automata: in-stent restenosis and suspension flow

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Chapter 1

Introduction

How does Nature process information? Can we detect and describe the computational structure in natural processes and can we provide a quantitative characterization of essential aspects of this structure?

(Prof. Peter M.A. Sloot defining his research motivation and that of the whole Computational Science research group.)

These are the essential questions behind this thesis. They are the driving force behind Computational Science which does not only assist the solution of mathematical descriptions of natural systems by numerical methods. In fact, the aim of Computational Science is to develop means which can lead to a better study and understanding of natural systems by modeling the various interactions between individual components which give rise to endless signatures of order, disorder, self-organization and self-annihilation. The challenge in this field is that processes studied by natural scientists involve systems that are each described best in a different modeling language from continuous mathematical models to fully discretized cellular automata. Besides the challenges in modeling every single of such systems, the study of information processing between such systems in complex dynamical multi-scale problems is still in the early stages.

1.1 Distinct Entities

Our way to look at natural systems is based on entities appearing on distinct scales: to describe a part of nature we assume the entities of a particular subsystem not to change their properties nor the rules in which they interact with the other entities in such an extent that the concept of "object" is not applicable anymore. One might argue that this concept is merely a very successful workaround developed by the impressive, but still very limited, cognitive capacity of humans in processing the input from the outer world by means of very compressed representations. However, assuming the most objective view of science, we cannot neglect that nature tends to do the same, or, at least, that we can successfully apply the same approach by mathematical means or that of other modeling languages. The matter of our universe organizes in structures we characterize as cosmic objects, also life on earth expresses itself in relatively independent creatures whose internal dynamics can be neglected when we want to study their social behavior. When we focus on only one of such entities we find that it is made of other entities. Atomistic theories have been revised a few times in the history of science and the current candidate of an a-tom, the ultimate particle on the ultimately lowest scale, the quark, might be found to consist of smaller structures in the future. All those things are found to behave as entities (in a strange way, though) and from Quantum Field Theory we learn that also fields can be best described by a finite number of dynamical degrees and that these can only assume discrete states (so that even interaction between particles is mediated by particles - photons, vector bosons, gluons, gravitons (postulated but not found yet)). The discretization of space, time and state space has been successfully translated into a theory of Cellular Automata (CA) which successfully applies to most diverse systems (see for example [1] and the very recent [2]). Although it gives rise to a number of inconsistencies, particularly with the debatable probability interpretation of quantum mechanics, the theory of CA has been extended to extreme variants like the ideas of the Calculating Space (Zuse [3]) and Digital Philosophy (Fredkin [4], Wolfram [5]). Particularly Stephen Wolfram promotes the idea that below the Planck scale, thus "below" quantum mechanics, there exists an informational substrate that allows the build-up of time, space, and energy. Such ideas can even be traced back to Einstein [6] who stated: "One can give good reasons why reality cannot at all be represented by a continuous field. From the quantum phenomena it appears to follow with certainty that a finite system of finite energy can be completely described by a finite set of numbers (quantum numbers). This does not seem to be in accordance with a continuum theory, and must lead to attempts to find a purely algebraic theory for the description of reality."

1.2 Distinct Scales

Typically, there is no continuous crossover between the definitions of an object on one scale and another on another scale being composed from the former. When we go up or down the scales we find different structures for which other descriptions of the system are more applicable. A drastic case is that of going from a microscopical quantum mechanical description of a physical system to a description according to classical mechanics. The dynamics of quantum mechanical entities cannot always be described as deterministic, a system containing a large number of such entities like a macroscopical particle however shows classical time-reversible dynamics thus actually contradicting the former observation. Another example is that of the Ising model where the interaction of a large number of entities of binary state gives rise to rather complex order-disorder phenomena on the material scale that is easier described by continuous variables but its macroscopical state might as well be binary again (magnetization at $T = 0$) comparable to the phenomenon of a diverging correlation length in a Bose-Einstein condensate. The phenomenon of condensation as an example of order-disorder transitions can be found throughout all sciences and represents only one of the various phenomenons that are displayed by complex systems. Another, but much more accessible example is that of an ant-colony where, aside from the possible differentiation of workers, soldiers and a egg-laying mother of all, despite the absence of a global control entity the limited responses on external stimuli and local pair-communication give rise to impressive collective behavior that makes it valid to describe the whole colony as one entity when it comes to building home structures, growing food, hunting behavior, migration, defense, and the interaction with other ant colonies. There are endless other examples of complex systems showing a tremendous ability of the small-scale entities to form structures on the larger-scale by purely local interaction and a limited set of states they can assume. The so-called *emergence* describes exactly this phenomena: the occurrence of a new quality operating at a higher level than at which the system units are operating. Besides the mentioned examples of quantum mechanical entities that form as a classical particle and the ant-colony relation, numerous other examples for this can be found: flying birds group into V-shaped formations optimizing their aerodynamic conditions, the global economy may display a long-lasting crisis as response to short-term actions on sub-markets, in a Belousov-Zhabotinsky reaction (and other excitable media) locally interacting entities with a resting-time dynamics give rise to waves and spirals of activation on the macro-scale, and the human body representing a whole cascade of such emergent scales from amino acids, DNA, cells, tissues, organs, the whole body, and beyond that societies, ecosystems, etc.

1.3 Interaction between Scales

If physics, biology, sociology, and other sciences too, are so successful in applying the concept of distinguishable structures on different scales to describe the system under study, can we bring the introductory questions to a more specific level and ask: How do those structures on different scales interact?

In some of these examples mentioned so far we find counteracting tendencies with different correlation/interaction range between the small scale entities themselves leading to some form of pattern formation on the larger scale as a consequence of collective behavior. This emergent behavior and other forms of self-organization can also be a response to external stimuli. The range of interactions between different structures on different scales is wide as structures can also be induced by external influences as boundary conditions, for example waves on the ocean that appear on different spatial scales, all of them induced by streams of air that not necessarily shows structures on the same spatio-temporal scale. Another example, where also a feedback can be detected are periodic flow structures in cardiovascular subsystems induced by the cardiac cycle setting the pressure boundaries which than, in turn, act back to the heart which, as a regulatory system, adjusts the pressure to the flow resistance to maintain constant blood flux through the body. When Darwin published his theory of the evolution of the species on earth, for the first time a reasonable approach to understand the interrelation between biological creatures on the time scale of a life span and the dynamics of a whole species on a large time scale has been offered taking spatial boundaries into account. When Hodgkin and Huxley drafted their model of ion channels in neuronal dendrites, fast local processes on the molecular level could be related to the formation and dynamics of action potentials traveling on a much larger spatio-temporal scale. In turn, action potentials, in an abstract form, are the basic entities of information which can be related to a global computational capacity by artificial neuronal network models. For the example of a QM description for the structures on the micro-scale and the classical object on the macro-scale given earlier, laws of classical mechanics can be derived from the laws of quantum mechanics at the limit of large systems or large quantum numbers (correspondence principle). We thus can apply a mathematical (statistical) model to couple these two structures in an analytical way. Considering the simple example of ideal gas particles, statistical physics gives us means to extract the properties of a macroscopic system of such particles. Another rare example for an analytical solution is the thermodynamics of the Ising model solved by Onsager. In most cases numerical methods have to be used, e.g. Molecular Dynamics (MD) to connect the particle level with the phenomena on the macroscopic level where the system can be described with the help of quantities that do not take individual particles into account. Information about individual particles is transformed into information on structures at an other scale. And, structures on the macro-scale act back on individual particles, e.g. in the form of external fields etc. If they are able to consider as many entities and as large time spans to reveal the emergent spatio-temporal structures, mathematically formulated theories and any other type of models like a CA help us in understanding the correlation between two scales: the entity scale and the scale of the emergent structures. Of course, solutions should be available in a reasonable computation time to allow models to make sense as a tool to study a phenomenon.

1.4 Multiple Scales

The multi-scale aspect of nature is a recognized fact reflected by the numerous publications under this topic in the last two decades. Especially in the field of physiology which covers a vast amount of scales from DNA to health the need for a better understanding of multi-scale interaction between multi-science subsystems has been recognized. However, seldom systems consisting of more than two processes have been considered so far. Some phenomena, and in principle all of them if we want to study them on a higher level of realism, are the consequence of a number of processes that act on very different spatio-temporal scales and interact not only via a single micro-macro type of coupling in the same domain like a MD process giving local quantities on the Navier-Stokes level describing the same gas or fluid.

For example, to implement and test the theory of Darwin in a model that is able to compute the outcome of the evolution of the full range of species on earth to understand the fauna and flora as we know it now starting from an initial condition set billions of years ago, it would be necessary to incorporate not only the behavioral dynamics of individuals and the macroscopic behavior of a species. Also geological processes, the whole weather system from the evaporation of water from the surface of certain types of leaves to the global temperature changes, the change of the intensity of solar radiation, the dynamics of extraterrestrial bodies, the mutation process in relation to the presence of chemicals or radiation - the whole range of physics, chemistry and biology - would have to be taken into account. It is clear that we won't be able to do that in the foreseeable future.

It is not only the computational power that would limit such huge kind of projects. The computational complexity of models could always be reduced by orders of magnitude by some smarter more advanced algorithm. It is therefore useful to investigate how processes on different scales interact to be able to reduce the information processed between the scales to a minimum that still carries all relevant aspects of the interaction. In the way scientists have studied the interaction of entities on one scale so far and elaborated useful classifications of all possible interactions where much insight in universality of could be gained, the study of interactions between processes on different scales and a systematic classifications of them is promising in gaining insight in the multi-scale aspect of nature. Similarly to how we study the interaction of particles by their position x_i at a certain time t_i to model the interaction of a large number of them in a macroscopic system we can also identify whole processes occupying a distinct volume in this spatio-temporal space. Doing so, either an overlap (sharing the same domain), shared boundary (spatial interface, temporal successiveness) or separation of the two processes in either or both space and time can be found. Although this sounds trivial we can also apply this concept of classification in a space spanned by the spatial scales ξ_i and temporal scales τ_i where the processes occupy a certain volume defined by the spatio-temporal scales of its entities and that of the emergent structures. The identification of overlap, shared boundary, or full separation can be repeated in such a space. Many types of single scale systems have been studied so far and the study of the coupling between two scales has begun (most of which are of the typical micro-macro coupling). However no systematic classification of coupling types has been done yet considering all possible relative positions in such a space with the aim to recognize similarities/universalities or fundamental differences in multi-scale multi-science interactions.

We are only at the beginning of understanding of how information is processed over the scales. We cannot yet treat information in the strict sense of the word as defined in information theory. We first need a common concept when it comes to multi-scale modeling. And we need many examples of implementations of multi-scale systems that are studied in the view of this concept. This thesis is meant to be a contribution to satisfy this need. Within the COAST project we had the chance to closely collaborate with bio-medical scientists to work on modeling of in-stent restenosis (ISR), a serious cardiovascular disease involving processes on multiple scales and that poses a great challenge to understand. Originating from initial plans to resolve the blood flow in an ISR model on the cellular level, we worked on modeling suspensions with the Lattice-Boltzmann method. However, to understand the multi-scale nature of blood rheology itself we realized that it was necessary to study the simplest suspension system, monodisperse suspensions of hard spheres in two dimensions, in more detail first. It turned out that suspension rheology and its dependence on the involved scales is very complex in itself requiring knowledge on the very details of the involved interactions. Additionally, it takes substantial work to develop numerical methods that allow such a study. Weinan E phrased it this way [7]:

> We should emphasize that HMM[1] is not a specific method, it is a framework for designing methods. For any particular problem, there is usually a considerable amount of work, such as designing the constrained microscopic solvers, that is necessary in order to turn HMM into a specific numerical method.

Consequently, the work described in this thesis involves a large part on the method-

[1]Heterogeneous Multi-scale Method, the multi-scale approach used to model the suspension flow in this work.

ological level, particularly in improving Lattice-Boltzmann method for suspension flow.

1.5 Outline of this Thesis

Addressing the need of a classification of multi-scale systems and their internal coupling, in chapter 2 we motivate and propose an appropriate methodology to classify multi-scale problems based on the concept of CA's. In this theory of Complex Automata (CxA) we further elaborate the idea of a scale separation map sketched in the last paragraph and identify possible relative positions of two processes on it and discuss the consequences for their coupling. We also classify multi-scale coupling in regard to the relative position of two processes in space which leads to a full classification of multi-scale problems that can be reduced to two single-scale processes. Based on this full classification we discuss possible modeling strategies resulting from it. However, we do not leave it at describing the consequences of the classification in a general language. We also describe how this can be implemented in a simulation framework that allows researchers to couple single-scale models in a generic way by so-called smart conduits that are the software realizations of the coupling templates elaborated in this chapter. We also discuss the reduction of computational effort in applying the concept of a CxA that makes it very attractive to be applied to complex systems which could not be studied so far due to their computational complexity. Besides that, an estimation of the error that might be introduced by splitting a multi-scale system into sub-systems and replacing their coupling by one of the coupling templates is provided.

In chapter 3, as a first example of a multi-scale multi-science system, a model for the biomedical problem of in-stent restenosis (ISR) is described. Making use of the MUSCLE library the model was developed to study the influence of blood flow properties on the process. The involved subprocesses are identified on the scale map together with the type of their coupling. The implemented submodels will be described in detail, particularly that for the formation of thrombus in the early stages of ISR. Existing approaches to thrombus modeling will be discussed and a new simplified thrombus model will be proposed. At the end of this chapter results from runs of the 2D and 3D ISR CxA's are discussed.

Chapter 4 describes a second multi-scale system: the macroscopic flow of non-Brownian hard-sphere suspensions. The macroscopically emergent rheology is dictated by details of fluid-particle, and particle-particle interactions. In systems where the typical spatial scale on the particle level is much smaller than that of macroscopic properties the scales can be split using a hierarchical multi-scale method (HMM) approach. In that, on the macro-scale the suspension is treated as a non-Newtonian fluid whereas local properties of macroscopic fields are input to a fully resolved suspension simulation. Down- and upward mapping of viscosity and diffusivity related quantities will be discussed. The coupling of the sub-models has not been implemented by means of MUSCLE. However, the coupling is discussed in the light of the CxA theory.

Developing concepts and models on a rather high level is one thing, realizing a model down to the very detail of the methods another. Consequently the research presented in this thesis addresses the improvement of existing methods as well as the development of new ones necessary to realize the intended models.

In the HMM model of suspension flow the lattice-Boltzmann method (LBM) is applied to model the fluid phase on both levels. In this thesis two major improvements in simulating fully resolved suspensions with the help of LBM are proposed. First, Lees-Edwards boundary conditions (LEbc) are developed to remove the side-effects that walls have in a Couette type of shear flow on the microstructure. It can be shown that using LEbc's the shear-thickening behavior of hard-sphere suspensions is prolonged in comparison to Couette-flow results. Second, a correction to the momentum exchange algorithm (MEA) used in commonly applied LBM suspension methods is proposed that restores Galileian invariance of the particle dynamics. Furthermore, a database has been developed including inter- and extrapolation functionalities that effectively reduces the redundancy in executing the micro-model the way initially described in the HMM model. The reduction of the suspension's local properties to a mean solid-fluid volume fraction, and a scalar shear rate under exploitation of rotational and Galileian invariance maps many different local states of the macroscopical suspension to one realization of boundary conditions on the micro-scale.

In chapter 5 the improved LBM methods are then used to investigate the behavior of the spatial scale in hard-sphere suspensions under increasing shear for different solid-fluid volume ratios. Typically at higher shear rates hydrodynamically interacting particles form clusters which give rise to shear-thickening. Cluster size distributions are measured and compared with experimental findings and theoretical models. A scaling of the apparent viscosity with the typical cluster size can be found supporting the assumption that clustering is the prominent process leading to shear-thickening. A statistical model for the development of cluster size distributions in dependence on $\dot{\gamma}$, ϕ, and solid-fluid mass density ratio is proposed. Based on the findings from a two-particle collision model the formation and breaking of particle clusters are modeled and relax to cluster size distributions that are in very good agreement with measurements in fully resolved LBM suspensions. Although this study has not been carried out in relation to the concepts of CxA's, it returns to the motivation presented in the introduction chapter by presenting a study of a system in which new scales and objects on it emerge from the interaction of objects on a smaller scale. This study offered insight into the rheology of sheared suspensions absolutely necessary to realize the HMM suspension model in the previous chapter.