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# Dynamical and structural self-organization : a study of friction, liquid-crystal nucleus growth, and supramolecular polymers through simple models

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# 1 General introduction

Processes in which the organization of a system with many, often very similar, elements increases in complexity or regularity without any external guidance are called self-organizing. In other words, the self-organization of the constituent elements is only driven by the interactions between the elements. These elements usually explore many configurations before reaching the one that is most stable.

Self-organizing systems are the subject of many fields of science. The structure of almost all materials is achieved by self-organization, patterns found in dynamical systems with many coupled elements often arise through it, and even quite complex biological structures emerge from this process. The reasons behind why the individual elements behave the way they do may be very different, and may constitute a field of science all of its own. However, the art of studying self-organization is to model these elements and their interactions in the simplest way possible, while still retaining the complexity of the structures and patterns they form.

In this thesis I study and use three simple models that describe a self-organizing system, or that exhibit self-organization. I study (i) a simple block and spring model representing multicontact friction, (ii) a set of partial differential equations describing the dynamics of the change of order in the isotropic-to-nematic transition of liquid crystals, and (iii) I use a patchy particle model to model linear supramolecular self-organization. Because each of the three subjects is introduced in a separate chapter, I will only give a short outline of my thesis in this general introduction.

In chapter 2 I will introduce the Burridge Knopoff (BK) model of multicontact friction. This is a model for two slowly moving, macroscopic objects that are pressed together by an external force. Although these objects are in relative motion, the surface separating the objects consists of many small contacts that move only occasionally and remain motionless the rest of the time. The BK model describes these rather complex sliding systems as a collection of blocks connected to neighboring

blocks and to one of the objects by springs, and to the other object by a simple velocity dependent friction law. Depending on the stiffness of the springs, and on the type of friction law that is used, this model can be applied to sliding systems of hugely different length scales. On the high end of the scale it has been used to describe the motion of the interface between two tectonic plates in an earthquake fault, whereas on the other end of the scale it has been proposed to describe the interface between two atomically flat sliding surfaces, lubricated by a locally solidifying liquid of only a few molecular layers thick. In Chapter 3 I study the BK model describing the latter situation, where a mode of motion arises in which every block only moves when its direct neighbors do not. I study the properties and stability of this special mode of motion, both computationally and analytically. In Chapter 4 I then use the properties of this solitary state of motion to better describe the relaxation of the average stress on the contacts at finite temperature, after the sliding objects suddenly stop moving.

In chapter 5 I introduce the concept of a first order phase transition by means of nucleus growth, applied to the growth of orientational order in a liquid crystal. In this phase transition an undercooled isotropic liquid, consisting of anisotropic liquid crystal molecules, suddenly aligns locally into an orientationally ordered, nematic, domain. If this nucleated domain is large enough it grows, so that eventually all the molecules are aligned. Latent heat caused by the change of order leads to a small temperature change at the growing domain interface. In chapter 6 I study the effect of this temperature change on the growth dynamics of a spherical domain. For the time and length scales I am interested in, I cannot keep track of the organization of the individual elements in this transition. Instead, I study the evolution of an order parameter that describes the *amount* of ordering at each position during the transition. For this order parameter I solve a partial differential equation in time and space, called the time dependent Landau-Ginzburg equation, that models the evolution of the order parameter as a function of temperature. By coupling this equation to a diffusive heat equation I can compute the effect of latent heat on domain growth dynamics. Because the time and length scales involved in orientational ordering and in thermal diffusion are so different in liquid crystals, I devised a semi-analytical approach to integrate the coupled equations efficiently.

In the last part of this thesis I address supramolecular self-assembly, a type of self-organization found in nature to result in highly complex biological structures such as virus capsids, membranes and fibers. Studying this type of self-assembly may not only lead to a better understanding of how these structures are formed, but may also lead to the design of new materials. In Chapter 7 I introduce the patchy particle, a promising approach to model the subunits that self-assemble into these supramolecular structures. Dealing with each individual atom in each individual molecule, and calculating all the interactions between all the atoms, quickly becomes too costly for the large assemblies that are formed. Therefore the patchy particle model separates the shape of a molecule from the interactions between the molecules. The shape of the molecule is modeled by one, or only a few simple impenetrable

beads, and the interactions between the molecules are modeled by only a few patches of interaction at the surface of these beads. In Chapter 8 I describe a discotic molecule by a single bead and two directionally dependent patches, and I study the linear self-assembly of these patchy particles numerically. I show that a small sideways interaction between the beads in different polymers causes these polymers to undergo a transition to a solid bundle, which may be a first step to understanding why many naturally forming polymers self-assemble further into bundles.

Each of these three subjects requires a different numerical approach. I integrate large systems of ordinary differential equations in Chapter 3, and solve a simplified version of these equations by means of a probabilistic automaton in Chapter 4. In Chapter 6 I integrate two coupled partial differential equations, and in Chapter 8 I perform Monte Carlo simulations of systems of many patchy particles. For each of the subjects I have combined my numerical simulations with theoretical studies, not only to explain my findings, but also to increase the efficiency of my simulations.