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

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Friction

2.1 Introduction to sliding friction

Newton's first law states that objects do not change their velocity unless a force is acting on them. This law is not so intuitive as one might think, as in every day life it takes quite some effort to keep objects moving at the same, finite velocity. Newton's first law therefore also implies that in every day life there must be some invisible force that opposes the motion of objects. In the case of a falling leaf for instance, it is the drag, i.e. the force exerted by the gas or liquid surrounding the object, that is working against gravity to slow the leaf down. For a book sliding on a table it is the friction at the contact surface that slows the book down. In this and the next two chapters I will report our results for a microscopic model of boundary lubricated friction, a very specific type of sliding friction. In this chapter I will introduce this type of friction, and discuss the applicability to actual sliding systems.

Sliding friction is exerted at the contact interface between two objects, the place where the surfaces of the two objects touch each other. The objects always move in the direction parallel to this interface and it is convenient to consider one of the objects as a large stationary surface and the other one as the sliding object. The amount of friction force depends strongly on the force with which the sliding object is pressed onto the surface, i.e. the load in the direction perpendicular to the surface. In the case of a book on a table, this perpendicular force is caused by the gravitational pull on the book. Before an object starts sliding due to an externally applied force, this force must exceed a threshold value, called the static friction force F_s. Below this threshold the objects are literally glued together. The static friction force is what keeps us from sliding when we stand on a slightly inclined surface. Once the external force exceeds the threshold the object starts to move and the friction force decreases

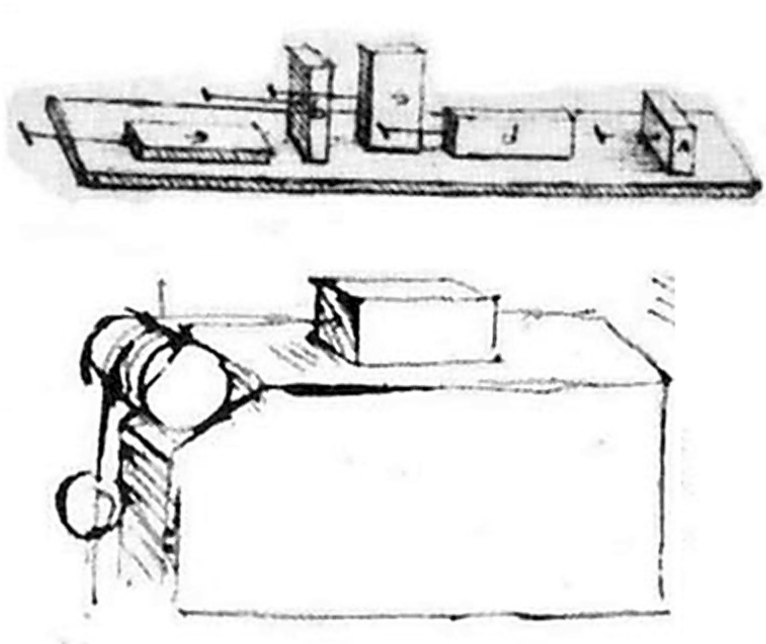

Figure 2.1: Sketches by Leonardo Da Vinci (Codex Atlanticus)[1], describing his studies on sliding friction. Top: Several ways of dragging the same block over a surface. Da Vinci observed that in all these situations the static friction force was the same, namely that the static friction force is independent of the contact area. Bottom: A way of exerting a constant force on a sliding block.

to what is called the dynamic (or kinetic) friction force F_d.

There are a few empirical relations, already observed by Da Vinci and collectively called the Amontons-Coulomb law, that describe sliding friction between macroscopic objects for not too extreme situations. Firstly, the static friction force is proportional to the force perpendicular to the surface. Secondly, the static friction force is higher than the dynamic friction force, and thirdly the dynamic friction force is largely independent of the sliding velocity. The last relation is often called dry friction, as opposed to viscous friction, where the dynamic friction force is proportional to velocity. When you consider the large differences between possible sliding systems, from rock-on-rock sliding in earthquake faults to the sliding of a book on a table, it is remarkable that these assumptions work reasonably well in all cases of dry friction. The mechanisms underlying the friction forces are very different for these sliding systems, and the study of the origins of friction defines the research field of tribology. Understanding what causes friction in a particular set-up might take you from studying the elasticity of the object on a scale of millimeters, to studying the electrons at the surface, on the scale of Ångstroms or less. This large difference in the time and length scales of the processes that result in the friction force is typical of the seemingly simple problems we have yet to solve in science today. There are two approaches to frictional problems today. One in which the surface atoms, and sometimes even electrons, of a very small

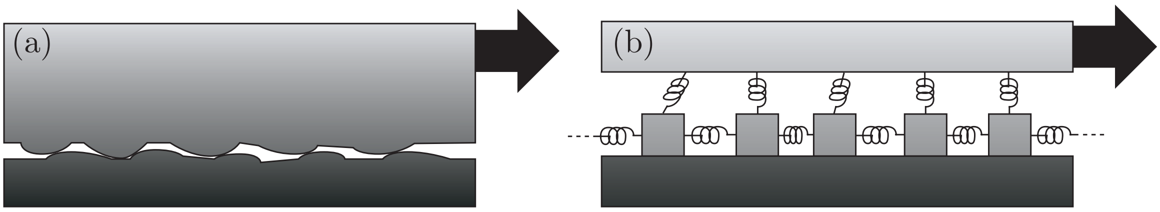

Figure 2.2: Sliding tectonic plates in an earthquake fault. (a) Two rough tectonic plates are locked at several positions. (b) The Burridge-Knopoff model representation of an earthquake fault.

patch of contact surface are modeled and simulated, and one in which one tries to capture the basic physics of the surface in a simple mechanical model. In the latter the smallest length scales are discarded, an approximation called *coarse graining*, where one replaces large collections of these surface atoms by simple mechanical objects such as blocks and springs. It is remarkable that the model I will introduce in the next section not only captures the basic physics of the motion of two tectonic plates in an earthquake fault, but can also be used to describe the motion of two flat surfaces lubricated by a very thin layer of liquid.

2.2 The Burridge-Knopoff model

In the fifties Bowden and Tabor[3] suggested that surface roughness was the key to explain friction. The real contact area, they proposed, was only a fraction of the apparent contact area, and was made up by the asperities (protrusions) of both surfaces. These asperities would interlock and hinder the sliding motion. Increasing the perpendicular force would cause more asperities to touch, and this gives rise to the load-dependent behavior described by the Amontons-Coulomb law. In 1967 R. Burridge and L. Knopoff argued that a simple block and spring model [2] could capture the physics of two slowly moving tectonic plates in an earthquake fault. Like Bowden and Tabor they suggested that the tectonic plates are in contact only at specific places. Although far from the interface the tectonic plates move slowly but steadily, most of the time at the interface the tectonic plates remain still. They suggested that these contacts build up stress until their static friction force is reached, after which they move. If neighboring contacts are also very close to the static friction threshold, the motion of one contact could set off an avalanche of moving contacts, resulting in an earthquake that can extend throughout the system.

In the Burridge-Knopoff (BK) model of Figure 2.2(b) the two tectonic plates are described as elastic materials that, at rest, are in contact at equidistant places. The contact points are modeled by blocks that connect to one of the plates by springs, modeling the transverse elasticity of the material, and to the other by static friction, modeling the lateral sliding friction of the contacts. The lateral elasticity is represented by springs between neighboring blocks. If the force on a block exceeds the

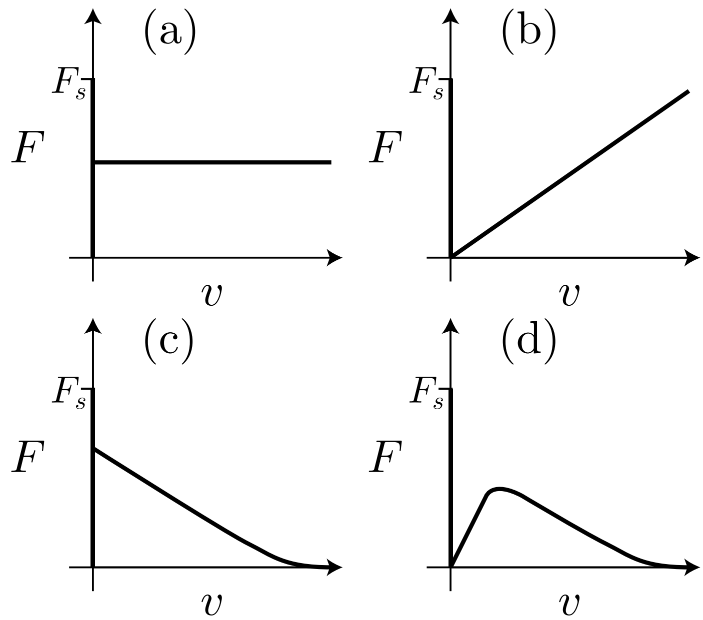

Figure 2.3: Friction force as a function of velocity. At rest the static friction force F_s applies. (a) Dry (Coulomb law) friction. (b) The viscous friction I have used to describe multicontact friction. (c) Velocity weakening friction (found in e.g. rock-on-rock sliding in earthquake faults) $F_i = F_0/(1 + \dot{q}_i)$. (d) A combination between velocity weakening and viscous friction.

static friction force a block is allowed to move according to newton's laws of motion, subject to the spring forces and to an empirical, velocity dependent dynamical friction force (Fig. 2.3). Once the force or velocity reaches some lower threshold a block is subjected to the static friction force again and the block stops. One such motion is called a slip event. To model rock-on-rock sliding, which is known to exhibit velocity weakening friction (Fig. 2.3(c)), the empirical, dynamic friction force is chosen to decrease with velocity. This suppresses small slip events and promotes larger and faster ones. Furthermore, the springs in the lateral direction are chosen to be at least a hundred times stronger than in the transverse direction. This increases the influence neighboring blocks have on one another and promotes the occurrence of avalanches, or earthquakes [4].

This model has been used in the last decade at a very different length scale to model the sliding friction between solids in the so called boundary lubrication regime[5]. In boundary lubrication two flat surfaces are separated by just a few layers of lubricant molecules. In the absence of sheer stress this layer solidifies, and the static friction force corresponds to the sheer stress needed to melt this layer. If the sliding velocity is small enough the liquid layer may solidify at some places, see Figure 2.4(a-b), locally gluing the two sliding objects together, much like the tectonic plates between avalanches. Locally then, the stress on such a solid island increases, until the island melts again and the elastic energy stored near this contact island dissipates. Bo

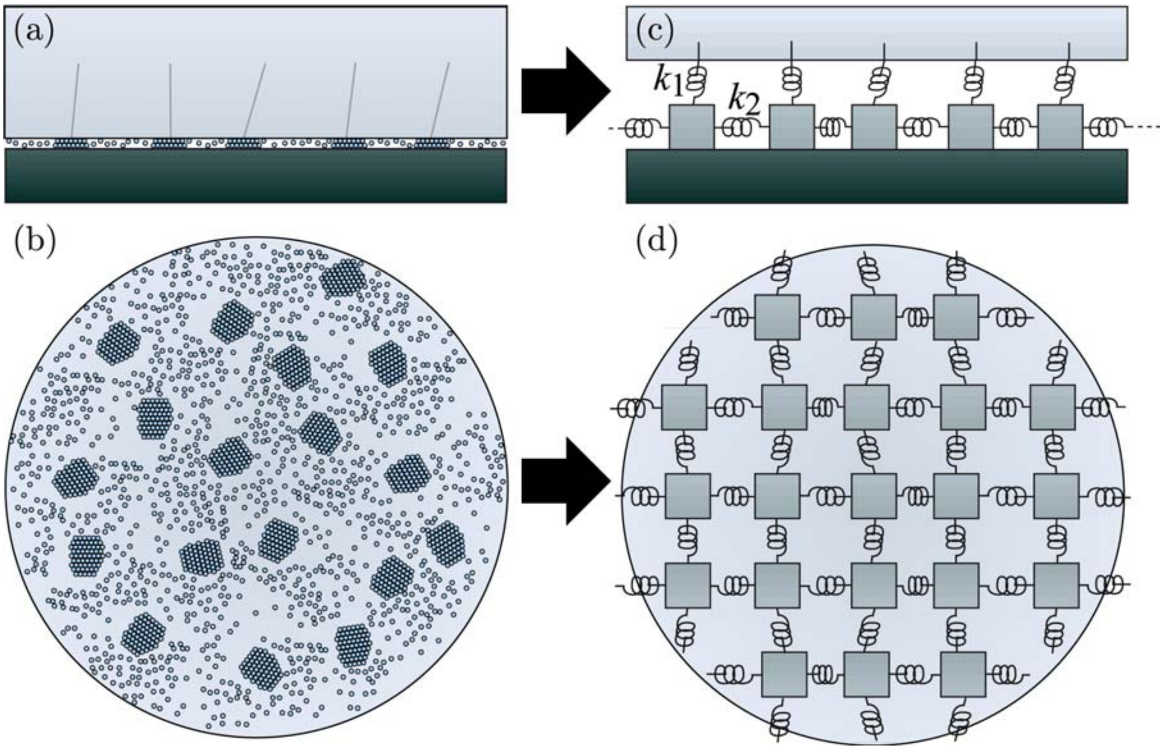

Figure 2.4: Lateral (a,c) and corresponding top view (b,d), of the Burridge-Knopoff model of multicontact friction. (a-b) Parts of the lubrication layer have frozen into solid islands. These islands locally glue the upper to the lower surface. (c-d) Burridge-Knopoff model representation of (a) and (b).

Persson pointed out that what causes friction in boundary lubricated surfaces is much like what causes earthquakes around tectonic plates. He suggested that the BK model, with some small alterations, would be equally good in describing boundary lubricated friction. Contrary to the earthquake models, he proposed a viscous friction force to slow down a slipping block, and chose the same strength for both the transverse and lateral springs. In this thesis I will call this version of the Burridge-Knopoff model the BK model of multicontact friction.

As Persson applies the BK model to describe the freezing and melting of a lubrication layer just a few molecules thick, temperature effects cannot be disregarded. Therefore Persson also added random thermal fluctuations to the BK model. The inclusion of temperature in the model allows blocks to slip by thermal excitation alone, in situations where, at zero temperature, they could not have slipped. Inclusion of temperature changes the properties of the BK model in many ways. First of all, as sliding of the upper surface at a lower velocity increases the time between slip-events of the blocks, the probability of a thermal excitation increases. This has the effect of decreasing the friction force for decreasing sliding velocities. A second effect of temperature is that when the top surface stops sliding, the stress on the blocks can relax due to thermal fluctuations alone. The thermal excitation probability is higher when the blocks are under a higher stress, and so the process of stress relaxation due to thermal excitations slows down in time. This ever slower relaxation of the system to a more energetically favorable state resembles the relaxation of glasses. In real sliding systems this stress relaxation of the surface layer is well known, and presents itself as the slow increase of the static friction with the time passed since the surfaces were in motion. The BK model shows the same behavior.

In Chapter 3 I show the results of the BK model of multicontact friction, where I drive the upper surface with a very low, constant velocity v_s. I identify a mode of microscopic motion specific of the BK model in the regime I considered (the unit ratio of the spring constants and the viscous friction of the blocks) that we have called *solitary motion*. In solitary motion a block always moves when its neighbors do not move. If all blocks are in solitary motion, the system is in the solitary state, and all observables will become periodic over time. I study the occurrence of the solitary state for different boundary conditions and show that it is stable for small thermal fluctuations.

In the Appendices of Chapter 3 I have added some supplementary material on the BK model of multicontact friction and the solitary state. In Appendix 3.A I describe how the problem of boundary lubrication can be translated to the Burridge-Knopoff model, and I determine the ratio of the lateral and transverse spring strengths and the viscous damping constant for this specific problem. Then, in Appendix 3.B, I describe in more detail how I integrate the equations of motion of the blocks. Appendix 3.C is dedicated to the solitary state. I first analytically calculate the motion of one block during a solitary slip event, and from these results determine the macroscopic friction force in the solitary state. For a large collection of blocks to be in the solitary state the blocks must be spatially organized in a very specific way. In the last part of Appendix 3.C I discuss how the forces acting on the individual blocks must be arranged for a system in the solitary state. The equations of motion show how to calculate the forces on the blocks from the block positions, but as I know the rules for the forces in the solitary state, not the positions, I invert the equations of motion in Appendix 3.D. This way one can generate a solitary state without performing a lengthy simulation. Finally, in Appendix 3.E, I give an outlook on the importance of the solitary state for fields outside of the friction community, most notably as a system that may exhibit directed percolation.

In chapter 4 I use the solitary state to revisit the problem of stress relaxation in the BK model of multicontact friction. The notion of the solitary state allows us to cast the problem into a simplified automaton model that perfectly reproduces the relaxation curve in exponentially less time than the full BK model. A further simplification then allows a refinement of the approximate analytical derivation of the stress relaxation, initially proposed by Persson. The analytical derivation and its results are exactly the same as proposed for the relaxation of a hierarchically constrained, glassy system and to my knowledge the BK model is the first model to exhibit exactly this type of glassy behavior without the proposed hierarchy[6].

2.3 References

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