Role of solitons in sliding friction models

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Matricola n° 656298
A.A. 2006/2007

Codice PACS: 68.35.-p
Role of solitons in sliding friction models

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December 11, 2007

Abstract

We construct a computer code to solve the (Nosé Hoover) finite-temperature classical dynamics of a Lennard-Jones solid lubricant slab between two rigid solid substrates. The code is based on a standard periodically repeated supercell scheme, which imposes relative substrates/lubricant densities. We investigate the possible occurrence of Moiré patterns due to incommensurability, and for the dragging of such Moiré patterns producing a state of ”quantized” lubricant velocity. In the few numerical experiments we run due to limited time, we do not find such special states, but observe standard stick-slip friction.

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Bibliography
1 Introduction

Recent investigations of lubricated friction have discovered a special sliding state, where the lubricant velocity relative to the velocity of one the sliding remains constant (on average) as many physical parameters are changed. This "quantized" velocity state was interpreted \[1, 2, 3, 4, 5, 6, 7\] in terms of solitonic waves, the so called Kinks in the 1-dimensional model of that initial research, being dragged by the sliding "top" layer.

The purpose of the present thesis is to verify if some mechanism operates in the more realistic framework of a 3D Lennard-Jones lubricant. The incommensuracy of the solid lubricant layer with the underlying rigid substrate should provide a Moiré pattern of lattice deformations that should be easily dragged along by the sliding top layer.

2 The model

The model is composed by two sliding solid surfaces that we indicate with "top" and "bottom", between which a layer of lubricant atoms is placed. The two substrates are composed of periodic triangular lattices. This lattices may have different spacings and may be rotated around the vertical \(z\)-axis by different angles. The atoms of the lubricant interact with those of the top and bottom layers through action of the Lennard-Jones potentials. For the LJ interaction energy we use the expression:

\[
\Phi_{LJ}(r) = \epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - 2 \left( \frac{\sigma}{r} \right)^{6} \right]
\]

which has a dimer equilibrium distance at \(r = \sigma\). The Lennard-Jones potential has an infinite range, but after a certain distance it’s influence on the atoms is very weak. In order to reduce the number of interactions that must be calculated, we introduce a cutoff radius \(R_C\) and decide to ignore the effect of the LJ potential between atoms separated by more than \(R_C\). A truncation of the potential would create energy jumps when distance between particles crosses the cutoff value. In order to avoid energy discontinuity in \(R_C\) we shift the 2-body potential energy by the fixed quantity \(\Phi_{LJ}(R_C)\):

\[
\Phi(r) = \begin{cases} 
\Phi_{LJ}(r) - \Phi_{LJ}(R_C) & r < R_C \\
0 & r > R_C 
\end{cases}
\]
We set a cutoff radius $R_C = 2.5\sigma$, where $\Phi_{LJ}(R_C) \simeq -8.17510^{-3}\epsilon$.

The particles of the lubricant can move along the $x$, $y$ and $z$-axes, they interact with other lubricant particles and with top and bottom atoms. The force acting on the $j$-th lubricant particle is the following:

$$\vec{F}_j = -\sum_{i=1}^{N_t} \frac{\partial}{\partial \vec{r}_j} \Phi_{tp}(|\vec{r}_j - \vec{r}_{ti}|) - \sum_{i,j'=1,j'
eq j}^{N_t,N_p} \frac{\partial}{\partial \vec{r}_j} \Phi_{pp}(|\vec{r}_j - \vec{r}_{j'}|) - \sum_{i=1}^{N_t} \frac{\partial}{\partial \vec{r}_j} \Phi_{bp}(|\vec{r}_j - \vec{r}_{bi}|)$$

(3)

where $\vec{r}_j$ is the position of the lubricant $j$-th particle; $\vec{r}_{ti}$ and $\vec{r}_{bi}$ are the positions of the top and bottom atoms. $N_b$, $N_p$ and $N_t$ are the numbers of bottom, lubricant and top particles. $\Phi_{tp}$, $\Phi_{pp}$ and $\Phi_{bp}$ are the truncated 2-body potential energy for the interactions between top-lubricant, lubricant-lubricant and bottom-lubricant particles, respectively. There are all LJ potentials, characterized by different values of $\sigma$.

The three-dimensional components of the gradient of the central potential in Eq. (3) yield:

$$\frac{\partial}{\partial \vec{r}_j} \Phi(|\vec{r}_j - \vec{r}_{j'}|) = \frac{\vec{r}_j - \vec{r}_{j'}}{|\vec{r}_j - \vec{r}_{j'}|} \frac{\partial \Phi(r)}{\partial r}$$

(4)

By convention, we choose the frame of reference where the bottom layer is static. The top layer can move both horizontally and vertically under an external force $F_{ext}$ applied on each particle of the layer, the force due to the interaction with the lubricant particles, and the force caused by a spring with an elastic constant $K$ connected to a rigid stage moving at a constant velocity $v_{ext}$ in the $\hat{x}$ direction. Thus the dynamics of the top layer is described by the following equations:

$$N_t m \ddot{r}_{tx} = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial \Phi_{tp}}{\partial r_{ti'x}} (|\vec{r}_{ti'} - \vec{r}_j|) - K [r_{tx}(t) - r_{tx}(t_0) - v_{ext}(t - t_0)]$$

(5)

$$N_t m \ddot{v}_{tx}(t) = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial \Phi_{pt}}{\partial r_{ti'x}} (|\vec{r}_{ti'} - \vec{r}_j|)$$

(6)

$$N_t m \ddot{r}_{tz}(t) = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial \Phi_{pt}}{\partial r_{ti'z}} (|\vec{r}_{ti'} - \vec{r}_j|) - N_t F$$

(7)

$$\vec{r}_{ti} = \vec{r}_t + \vec{R}_{ti}$$

(8)
Physical quantity & Natural units \\ 
length & $a_p$ \\ 
mass & $m$ \\ 
energy & $\epsilon$ \\ 
force & $\epsilon a_p^{-1}$ \\ 
velocity $v$ & $\epsilon^{1/2}m^{-1/2}$ \\ 
time & $m^{1/2}\epsilon^{-1/2}a_p$ \\ 

Table 1: Natural units for several physical quantities in a system where length, mass and energy are measured in units of $a_0, m, \epsilon$, respectively.

where $\vec{R}_{ti}$ are fixed relative positions of the rigid top layer, which are defined below.

2.1 The Nosé-Hoover thermostat

To simulate at fixed temperature we use a Nosé-Hoover thermostat chain \[8\]. As shown in Ref. \[9\], the Nosé-Hoover chain method is described by the following equations of motion:

$$m r_{ji} = \vec{F}_{ji} - \xi_i m r_{ji},$$

(9)

$$\dot{\xi}_1 = \frac{1}{Q_1} \left( \sum_{j=1}^{N_p} |\vec{r}_j|^2 - gK_B T \right) - \xi_1 \xi_2,$$

(10)

$$\dot{\xi}_i = \frac{1}{Q_i} \left( Q_{i-1} \xi_{i-1}^2 - K_B T \right) - \xi_i \xi_{i+1}$$

(11)

$$\dot{\xi}_M = \frac{1}{Q_M} \left( Q_{M-1} \xi_{M-1}^2 - K_B T \right),$$

(12)

with $1 \leq j \leq N_p$ and $1 \leq i \leq M$, where $M$ is the number of the thermostats, that we take $M = 3$; we take $Q_i$, the effective ”mass” of each thermostat, and the coefficient $g = \frac{3}{2}N_p$ of the same order of $N_p$. $\xi_i$ is a set of auxiliary variables that keep the kinetic energy of the system close to its classical value $\frac{3}{2}N_p K_B T$. In our calculations, we take all $Q_i = 2N_p$ and $g = 3(N_p - 1)$. We measure the thermal energy scale $K_B T$ in units of the LJ energy $\epsilon$. 

7
3 Technical implementation

We integrate the equation of motion using a standard 4th order of Runge-Kutta method. We measure all quantities in a system of units where length is measured of the equilibrium separation $a_p$ of nearest neighbor lubricant atoms, mass is measured in units of the mass $m$ of all particles, and energy is measured in units of the LJ cell depth. This system of units is summarized in Table 1. We also set $\sigma_{pp} = a_p$, $\sigma_{tp} = a_t$, $\sigma_{tb} = a_b$.

3.1 The linked-cell method

The linked-cell method allows to reduce substantially the computing time required, by avoiding to compute the interaction between $N^2$ pairs of particles as required by Eq. 3, and considering for each particle $j$ only the finite number of other particles $j'$ separated by less than $R_C$. This method consists in dividing the initial cell into smaller cells with both sides slightly larger than the cutoff radius $R_C$. This is realized in practice by mapping the supercell into a unitary box centered in the origin. Given the flat geometry of the present problem, we only consider linked cells in 2D ($\hat{x}, \hat{y}$), not $\hat{z}$. The calculation of forces is performed by considering only atoms within each cell and neighboring cells. An atom of a particular cell interacts with all the atoms in the same cell, which are kept in a suitable "list" of the indexes of all the particles in the cell. An atom also interacts with the atoms of neighboring cells. In this case, to avoid double counting of these forces, we consider only 4 out the 8 neighboring cells.

To fix the small cell we first divide each side of the initial cell by $R_C$. Then we sort all particles in their appropriate cells. Two arrays are created during the sorting process. The 'head-of-chain' array (head) has one element per each cell. This element contains the identification number of one of the atoms sorted into that cell. This number is used to address the element of a linked-list array (list), which contains the number of the next atom in the index of the next atom in the cell, and so on. If we follow the trail of link-list references, we will eventually reach an element of the list which is zero. This indicates that there are no more atoms in that cell, and that it is time to move on to the head-of-chain atom in the next cell. The lists of atoms in each cell are updated at each step in the integration.
3.2 Periodic Boundary Conditions

The number of atoms $N_p$ of the simulated system is negligible compared to a realistic number of atoms at the surface of contact of a macroscopic piece of matter (easily of the order of $10^{11}$ in a mm$^2$): the finite size of the simulation produces unphysical boundary effects. To alleviate this problem we use periodic boundary conditions (PBC). We choose a cell, that we call supercell, that replicates infinitely, and we study only the dynamics of the particles contained in the supercell. Thus we assume that these particles really represent an infinite set of particles that occupy the same position in all other supercells of the model. All these ”image” particles move together and, in fact, only one copy of each of them is represented in the computer program, but each particle $j$ in the cell should be thought as interacting not only with other particles $j'$ in the cell, but also with their images in nearby cells. However, the size of the supercell is much larger than $R_M$ so that in practice this interactions vanish.

3.3 Matching Conditions

When three different layers of periodic triangular lattices are superimposed it is not unlikely that the combined system is periodic. To find the combinations of angles and lattice spacings for which we obtain a periodic situation we must impose as a condition that there are (infinite) points where we can find a particle of each of the three substrate. Let us call these particular points nodes. The positions of the particles of the three lattices, $\vec{R}_b$, $\vec{R}_p$, and $\vec{R}_t$ are described by the equations:

$$\vec{R}_b = n_{1b}a_b \left( \frac{\cos \theta_b}{\sin \theta_b} \right) + n_{2b}a_b \left( \frac{1}{2} \cos \theta_b - \frac{\sqrt{3}}{2} \sin \theta_b \right)$$  \hspace{1cm} (13)$$

$$\vec{R}_p = n_{1p}a_p \left( \frac{\cos \theta_p}{\sin \theta_p} \right) + n_{2p}a_p \left( \frac{1}{2} \cos \theta_p - \frac{\sqrt{3}}{2} \sin \theta_p \right)$$ \hspace{1cm} (14)$$

$$\vec{R}_t = n_{1t}a_t \left( \frac{\cos \theta_t}{\sin \theta_t} \right) + n_{2t}a_t \left( \frac{1}{2} \cos \theta_t - \frac{\sqrt{3}}{2} \sin \theta_t \right)$$ \hspace{1cm} (15)$$

where $\theta_p$ and $\theta_t$ are respectively the lubricant and top angles of rotation with respect to the bottom.
Thus we choose angles $\theta_b$, $\theta_p$ and $\theta_t$ and lattice spacings $a_p$, $a_b$ and $a_t$ that satisfy the following equation:

$$\vec{R}_b = \vec{R}_p = \vec{R}_t \quad (16)$$

for nonzero $n_{1b}$, $n_{2b}$, $n_{1p}$, $n_{2p}$, $n_{1t}$, and $n_{2t}$ to find a periodic system.

If the system is periodic we can select a supercell and apply the boundary conditions. As illustrated in Fig. 1 the nodes form a regular lattice that we can take as the periodicity of the 3-layer system. Thus if we choose a cell identified by four nodes we are sure that it replicates infinitely. The positions of the nodes are found for particular values of $n_{1b}$, $n_{2b}$, $n_{1p}$, $n_{2p}$, $n_{1t}$, and $n_{2t}$ that satisfy the equality (16).

The fixed top relative positions $\vec{R}_{ti} = \begin{pmatrix} R_t \\ r_{tz}(0) \end{pmatrix}$ are defined by selecting $N_t$ vectors out of those defined in Eq. (15) such that they all belong to the supercell. An analogous expression holds for $\vec{R}_{bi}$.

4 The dynamics of the model

We study three particular configurations of the model described in Sect. 2: Equal Spaced (ES), Less Dense Top (LDT), Incommensurate (IN). In the Equal Spaced system the Lubricant is rotated and all three substrates have the same lattice spacings. The Less Dense Top situation is the same of the Equal Space but the top has a double lattice spacings compared with those of lubricant and bottom. In the Incommensurate case the top and bottom are rotated by the same angle and the three layers have three different lattice spacings. The geometric parameters of the three configurations are listed in Tab. 2.

In both the Equal Spaced and the Less Dense Top configurations the lubricant has the same lattice spacing as the bottom and is free to rotate. The difference is that the LDT has doubled lattice spacing $a_t$. As a result the minimal supercell to hold the lattice is twice as large in the LDT than in the ES geometry, as shown in Figs. 1, 2. In the Incommensurate situation the lattice spacings of the three substrates are all different as illustrated in Fig. 3.
Figure 1: The top, bottom and lubricant layers in their initial perfect-lattice configuration. In this configuration the bottom and the top are perfectly overlapped as they have the same lattice spacing and are not rotated around the $z$-axis. The lubricant lattice is rotated by an angle of $27.8099^\circ$ with respect to the $x$-axis. For this particular angle the overlap of the three substrates originates a periodic figure where we select a cell that replicates infinitely as drawn. Observing the selected cell we can notice that a particle that exits from one side of the cell, reenters from the opposite side at the right position.
Figure 2: The top, bottom and lubricant layers, in their initial perfect-lattice configuration. The lubricant lattice is rotated by an angle of $27.8099^\circ$ with respect to the $x$-axis and has a lattice spacing $a_t = 2a_p = 2a_b$. 
Figure 3: The top, bottom and lubricant layer in the IN geometry. The top and bottom are rotated by an angle of $-19.1066^\circ$ with respect of the $x$-axis. The lattice spacing of the bottom is $1.32a_p$ and the one of the top is $1.76a_p$. 
Figure 4: Positions of the particles of the lubricant at $t = 0$ and at $t = 100$ in the Equal Spacing situation. The lattice spacings of the top, bottom and lubricant layer are the same. Initially the lubricant is rotated by $27.8099^\circ$ but as the simulation starts the atoms rearrange so that the lubricant effectively rotates rather quickly, so after a rather short time $t = 100$ in practice the lubricant rearrange at an angle of $0^\circ$ with respect of the $x$-axis. In this simulation we use $K = 10$ and $T = 0.01$ and $v_{ext} = 0.1$. 
Figure 5: Positions of the particles of the lubricant at three successive times when starting from the Less Dense Top situation. The lattice spacings of the bottom and lubricant layers are the same. Initially the lubricant is rotated by 27.8099° but as the simulation starts the atoms rearrange so that the lubricant rotates rather quickly, thus after a rather short time \( t = 500 \) in practice the lubricant forms a definitive lattice at an angle of 0° with respect of the \( x \)-axis. The configuration is irregular, but comparing the particles positions at successive times we observe that as the disorder decreases. In this simulation we use \( K = 10 \) and \( T = 0.01 \).
Figure 6: Position of the particles of the lubricant at $t = 0$ and at $t = 100$ in the Incommensurate situation. Initially the lubricant is not rotated and all its particles are well sorted in a lattice configuration. As the simulation starts its regularity is broken and at $t = 100$ seems to don’t have any particular configuration. In this simulation we use $K = 10$ and $T = 0.01$. 
### Table 2: The lattice parameters and supercell parameters in the three considered geometries: ES, LDT, IN.

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Equal Spaced</th>
<th>Less Dense Top</th>
<th>Incommensurate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_p$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$a_b$</td>
<td>1</td>
<td>1</td>
<td>$\sqrt{7}/3 = 1.32$</td>
</tr>
<tr>
<td>$a_t$</td>
<td>1</td>
<td>2</td>
<td>$\sqrt{28}/3 = 1.76$</td>
</tr>
<tr>
<td>$\theta_p$</td>
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<td>$\arctan[3\sqrt{3}/13]$</td>
<td>$0^\circ$</td>
</tr>
<tr>
<td></td>
<td>$= 27.8099^\circ$</td>
<td>$= 27.8099^\circ$</td>
<td></td>
</tr>
<tr>
<td>$\theta_b$</td>
<td>$0^\circ$</td>
<td>$0^\circ$</td>
<td>$\arctan[-\sqrt{3}/5]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$= -19.1066^\circ$</td>
</tr>
<tr>
<td>$\theta_t$</td>
<td>$0^\circ$</td>
<td>$0^\circ$</td>
<td>$\arctan[-\sqrt{3}/5]$</td>
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<td></td>
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<td>$= -19.1066^\circ$</td>
</tr>
<tr>
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</tr>
<tr>
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<td>112</td>
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</tr>
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<tr>
<td>$a_{2y}$</td>
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<td>15.588</td>
<td>3.464</td>
</tr>
</tbody>
</table>

Table 2: The lattice parameters and supercell parameters in the three considered geometries: ES, LDT, IN. Where $a_p$, $a_b$ and $a_t$ are the particles nearest-neighbor distances of respectively the lubricant, bottom, and top layer and $\theta_p$, $\theta_b$ and $\theta_t$ are the angles between the lattice and the $x$-axis of the lubricant, bottom, and top. $N_p$, $N_b$ and $N_t$ are the number of bottom, lubricant and top particles in the supercell and $(a_{1x}, a_{1y}), (a_{2x}, a_{2y})$ are the components of the two primitive vectors that define the supercell.

### 4.1 The time evolution: the stick-slip phenomenon

We integrate the equations of motion described in Sec. 2 and 3 starting from the initial states described above. We use a rather large value of $K = 10$ for the spring used for the dragging of the top layer. Different phenomena are observed in different simulations. Figure 4 shows that the rotated lubricant of the ES rotates rapidly to re-align to the top and bottom principal lattice directions. A similar behavior occurs in the LDT geometry, but as shown in Fig. 5, the configuration after $t = 500$ is not perfectly regular, where defects heal slowly as time goes by. In the IN geometry instead the regular arrangement is rapidly destroyed, and a disordered configuration is realized as shown in Fig. 6. Figures 4, 5, and
represents the time-evolved lubricant reported back inside the simulation cell, thus the drift motion does not show.

Stick-slip between top and bottom substrates is caused by an alternation of sticking to each other and sliding over each other. This phenomenon is due to the fact that traction at velocity $v_{ext}$ is applied through a spring. As shown in Fig. 7 and 8, the stick-slip phenomenon occurs in all three systems, but Fig. 8 shows that in the Equal Spaced configuration stick-slip involves also the lubricant layer. Figure 9 compares the pattern of the lubricant center of mass in the Equal Spaced situation and in the LDT configuration: observe that in the first case the lubricant center of mass also moves with a step-like pattern while in the second case the lubricant remains almost stationary, as expected by full pinning being established in the fully commensurate configuration. The patterns of the top center of mass are also different in these two situations: they are both step-like but in the first case the steps are wider. This result suggests that in the Equal Spaced system the lubricant tends to pin to both the top and the bottom substrate: as a consequence it moves with the top but is obstructed by the bottom and so the width of the steps is larger.

The stick-slip phenomenon is less evident in the IN situation. As Fig. 7 shows, the pattern of the top center of mass is more straight than the one of the Equal Spaced and Less Dense Top. In the Incommensurate case the lubricant cannot pin to the bottom or the top because the lattice spacings are different. As a result the lubricant moves irregularly and alleviates the stick-slip effect.

Figure 10 shows that the stick-slip effect becomes less evident as $v_{ext}$ increases. For the Incommensurate configuration, we also elaborate the ratio of the center-mass velocity of the lubricant in the $x$ and $y$ directions (Fig. 11), and find a very irregular time dependency. Moreover once we execute a time average we find a fairly constant pattern for the time-averaged $x$ component (Fig. 12). Given the disorder of the lubricant it is however unlikely that this regularity can be related to solitonic patterns being dragged by the top substrate.

5 Discussion and Conclusion

The present work deals mostly with coding a correct implementation of the periodic box and linked-cell method in a general geometry. The time devoted to simulations was too short to come to definite conclusions about a possible soli-
Figure 7: Top center of mass pattern in the configurations of Equal Spaced and Incommensurate. In the first case the stick-slip phenomenon is more evident than in the second. Both simulations are carried out at $v_{ext} = 0.1$, $T = 0$ and $K = 10$. 
Figure 8: The top center of mass pattern for the Equal Spaced and the Less Dense Top situations. In both cases the stick-slip effect is evident, but in the ES system the step width are larger. Both the simulation are carried out at $v_{ext} = 0.1, T = 0$ and $K = 10$. 

![Graph showing equal spaced and less dense top situations](image-url)
Figure 9: Time evolution of the lubricant center of mass in the case of Equal Spaced and Less Dense Top. The simulation are both carried out at $v_{ext} = 0.1$, $T = 0.01$, and $K = 10$. 
Figure 10: The pattern of the top center of mass for three different $v_{ext}$ for the Incommensurate model. As the external velocity increase the stick-slip effect decreases. These simulations are carried out at $T = 0.01$ and $K = 10$. 

\[ v_{ext} = 0.1 \quad v_{ext} = 0.2 \quad v_{ext} = 0.5 \]
Figure 11: The velocity ratio $v_{cm}/v_{ext}$ for the $x$ and $y$ components of the lubricant center of mass velocity. Despite the very wide fluctuations, on average the $x$-component of the center-of-mass velocity ratio is almost constant for the three different values of $v_{ext}$, see Fig. [12]. These simulations are carried out at $T = 0.01$ and $K = 10$, for the Incommensurate configuration.
Figure 12: The time-averaged velocity ratio $\langle v_{cm} \rangle / v_{ext}$ for the $x$ and $y$ components of the lubricant center-of-mass average velocity and for the top transverse velocity. These simulations are done at $T = 0.01$ and $K = 10$, for the Incommensurate configuration.
tonic quantized velocity regime for the lubricant. This analysis will be the object of further studies. In the few simulations we could carry out here, however, we demonstrated full pinning in the commensurate case, the instability of the rotated geometry when it involves only the lubricant, and characteristic stick-slip motion.
References


