MSN 514 - Computational Methods for Material Science and Complex Systems

Homework 06

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I. INTRODUCTION

Friction is a common phenomenon in nature, from macroscopic to large scale mechanical contacts. However, understanding friction at the atomic scale is not always direct. One well-known model that explains many basic features of atomic-scale friction is the Prandtl-Tomlinson (PT) model . This model considers a small "tip" of mass m, which is pulled across a potential that represents the surface. The tip is attached to a spring of stiffness k, and the other end of the spring moves at a constant velocity v_0.

A. Original Form of the Prandtl-Tomlinson Equation

In Dr. Jahangirov's [1?] work, the PT model is introduced as follows:

$$m\frac{d^2x}{dt^2} = -\,m\,\gamma\,\frac{dx}{dt} \;+\; k\,(v_0\,t - x) \;-\; f\,\sin\!\Big(\frac{x}{a}\Big), \tag{1}$$

where the parameters in the equation are as follows: $x(t)$ represents the position of the tip, m is the tip mass, γ is the damping (friction) coefficient, k denotes the stiffness of the pulling spring, and v_0 is the pulling speed of the other end of the spring. Additionally, f is the amplitude of the sinusoidal potential, while a corresponds to the wavelength of the potential.

The term $-\,f\,\sin\big(\frac{x}{a}\big)$ comes from the derivative of a sinusoidal potential $V(x) = f\,a\,\big[1 - \cos(x/a)\big]$, which is a simple way to represent the tip-surface interaction.

B. Equation (4.2) in Dr. Jahangirov's Thesis and the Sign Mistake

In Dr. Jahangirov's PhD thesis, the dimensionless form of the PT model is given as Equation (4.2). However, in the original text, there is a small sign error in front of the $\sin(\tilde{x})$ term. Specifically, the thesis shows a "$+\sin(\tilde{x})$" on the right-hand side instead of a minus sign. Figure 1 illustrates the uncorrected version. The correct version should have a "$-$" sign before the sine term, in line with the force being $-\,\partial V/\partial x$.

The corrected dimensionless equation can be written as:

$$\frac{d^2\tilde{x}}{d\tilde{t}^2} = -\,\tilde{\gamma}\,\frac{d\tilde{x}}{d\tilde{t}} \;+\; \tilde{k}\,\big(\tilde{v}_0\,\tilde{t} - \tilde{x}\big) \;-\; \sin(\tilde{x}), \tag{2}$$

where hats denote dimensionless variables. This correction ensures that the tip feels a restoring force from the sinusoidal potential in the proper direction. Using the plus sign would change the force direction and lead to inconsistent friction loops.

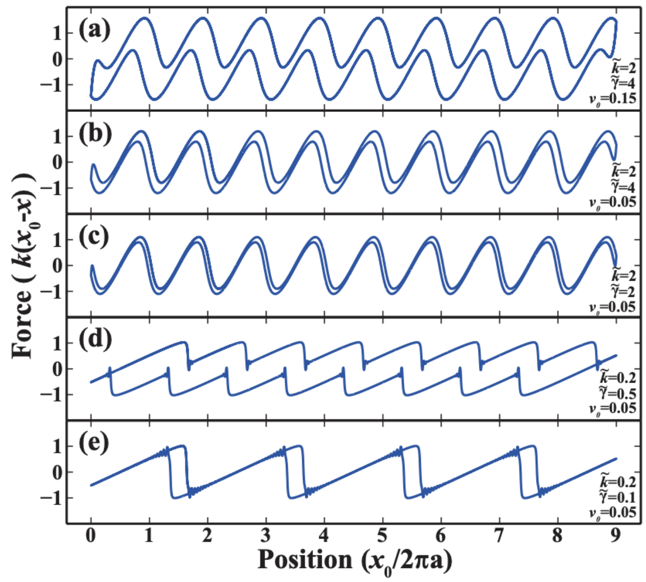

FIG. 1. Fig. 4.2 from Dr. Jahangirov's PhD thesis. Each panel has different γ, k, and v_0 for the corrected equation (4.2). We observe smooth loops (no big jumps) when $\tilde{k} > 1$ and sharp jumps when $\tilde{k} < 1$.

C. Langevin Extension: Force Effects

Real surfaces at finite temperature also cause random collisions on the tip. We can model this by adding a normally distributed random force that would mimic the effect of being connected to a thermal bath at a certain temperature to Eq. (2). This leads to a *Langevin* form:

$$m\frac{d^2x}{dt^2} = -\,m\,\gamma\,\frac{dx}{dt} \;+\; k\,(v_0\,t - x) \;-\; f\,\sin\!\left(\frac{x}{a}\right) \;+\; \eta(t), \tag{3}$$

where $\eta(t)$ is a normally distributed random force with zero mean. Its variance depends on temperature T, according to the fluctuation-dissipation theorem. Physically, this means the tip will experience small kicks from the environment, allowing it to jump over potential barriers more easily, especially if the temperature is high.

D. Scope of This Study

In this homework, we do two main things:

1. **Reproduce Figure 4.2 and Figure 4.3(a) from the thesis** using the *corrected* version of Eq. (2). These figures show friction loops (Fig. 4.2) and average friction force versus velocity (Fig. 4.3(a)).

2. **Study the effect of adding a thermal force** (Langevin dynamics) on the average friction. We see how temperature modifies the friction loops and velocity dependence.

Below, we present the details of our code and the numerical results. For reference, Figure 2 shows the original Figure 4.3(a) from the thesis. We will compare our results with that figure later.

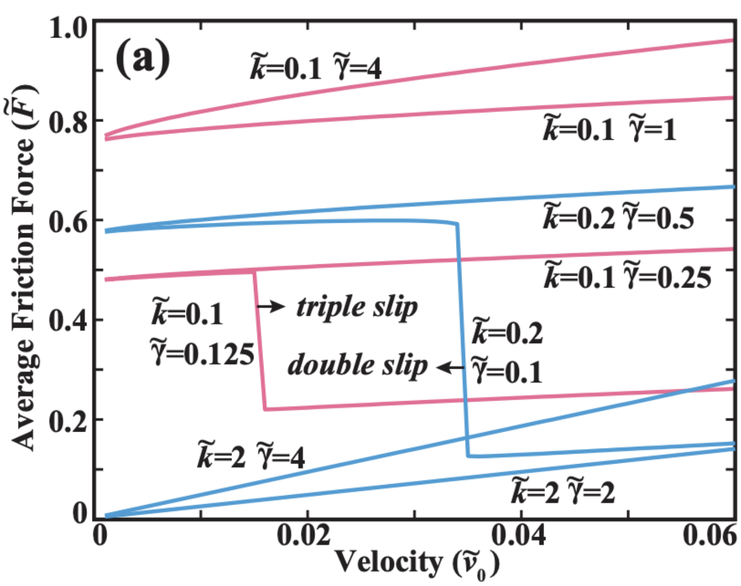

FIG. 2. Fig. 4.2(a) from the thesis. It shows the average friction force versus velocity for different values of $\tilde{k}$ and $\tilde{\gamma}$. We will reproduce a similar figure with the corrected sign in Eq. (2).

II. RESULTS

A. Numerical Method

We implemented a simple time-integration (finite difference) approach in Python. We split the simulation into small time steps Δt. At each step:

1. We calculate the total force on the tip:

$$F_{\text{tot}} = -\, m\,\gamma\,v \;+\; k\,(v_0\,t - x) \;-\; f\,\sin\!\left(\frac{x}{a}\right) \;+\; F_{\text{rand}},$$

   where F_{rand} is zero in the deterministic case and is a random Gaussian number in the Langevin case.

2. We update velocity: $v \leftarrow v + (F_{\text{tot}}/m)\,\Delta t$.

3. We update position: $x \leftarrow x + v\,\Delta t$.

When $F_{\text{rand}} \neq 0$, we use $\sigma = \sqrt{2\,m\,\gamma\,k_B T/\Delta t}$ for the standard deviation of the random force.

B. Reproducing Figure 4.2: Friction Loops

Figure 3 shows our reproduction of the friction loops (the force $F = k(x_0 - x)$ versus $x_0/(2\pi)$). We scan the pulling point x_0 forward and backward to form a loop. We match the same parameters as in the thesis: different γ, k, and v_0 values.

Observations:

- For large $\tilde{k}$ (i.e. stiff spring compared to the substrate potential), the motion is continuous and the loop is smoother.

- For small $\tilde{k}$, the tip gets pinned in the potential minima and then "slips" suddenly, creating a bigger hysteresis loop (larger energy loss).

- Lower damping (γ) can cause multiple slips per period (the tip overshoots and comes back).

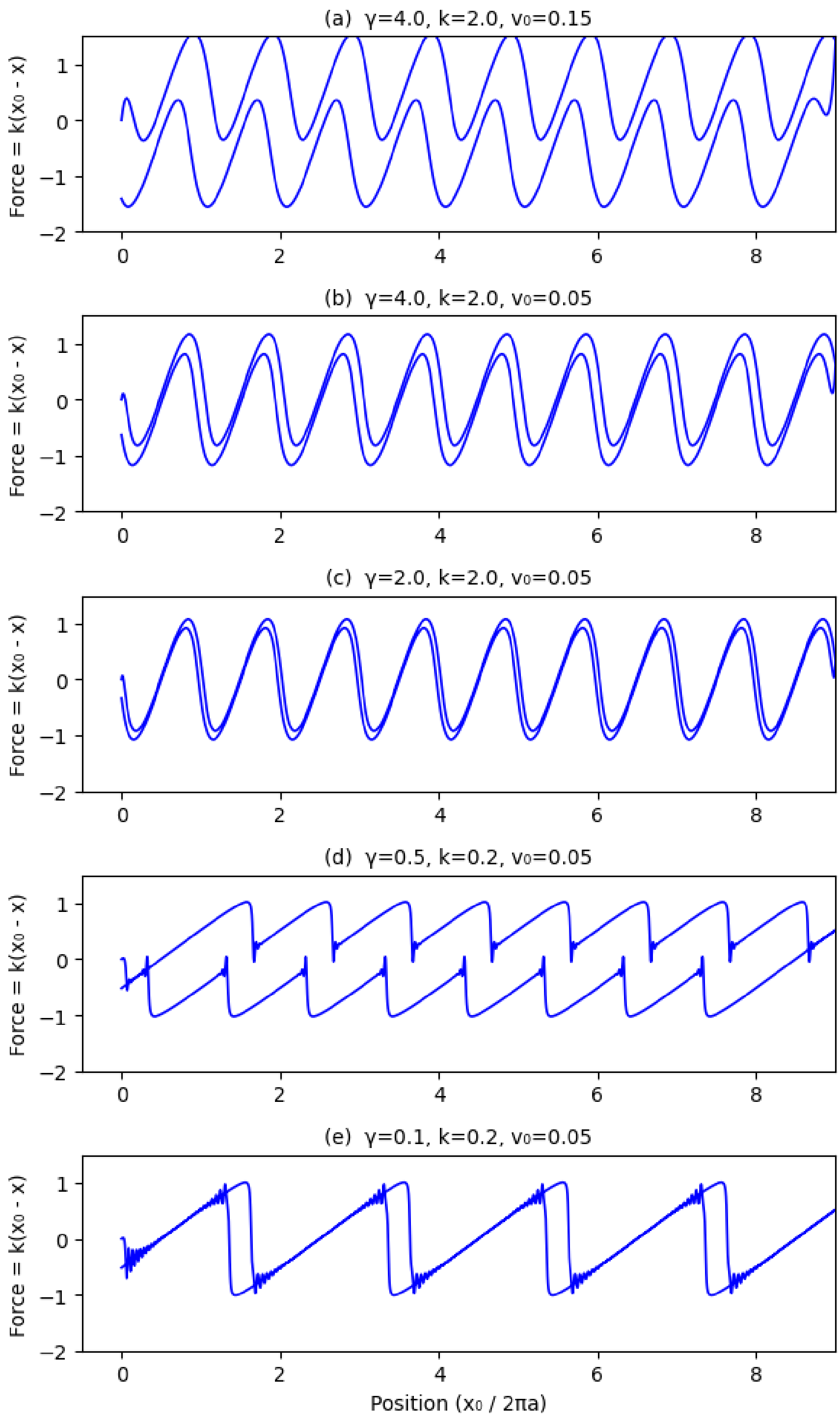

FIG. 3. Our reproduction of Figure 4.2. Each panel has different γ, k, and v_0. We see smooth loops (no big jumps) when $\tilde{k} > 1$ and stick-slip loops (sharp jumps) when $\tilde{k} < 1$. This matches the thesis results

C. Reproducing Figure 4.3(a): Average Friction vs. Velocity

We now fix the pulling velocity v_0 and let the system reach steady state. Then we measure the time-averaged friction force, $\overline{F} = \langle k(x_0 - x) \rangle$, for a range of velocities. Figure 4 compares to the original Figure 4.3(a) in the thesis.

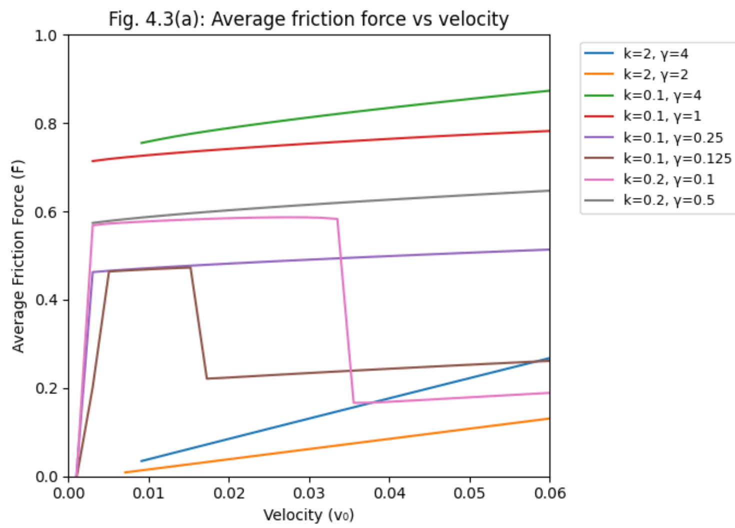

FIG. 4. Our version of Figure 4.3(a). The average friction force is plotted versus velocity. Different curves correspond to different (k, γ). Note that for $\tilde{k} < 1$, the friction does not go to zero at low velocity. For $\tilde{k} > 1$, the friction is roughly linear with v_0 and goes to zero as $v_0 \to 0$.

Key points:

- If $\tilde{k} > 1$, the system slides smoothly, so friction grows with velocity and approaches zero as $v_0 \to 0$.
- If $\tilde{k} < 1$, the system shows stick-slip. Even at very slow speeds, there is a finite friction due to the repeated "stick and slip" process.
- For certain γ values, one can see "double slip" or "triple slip" patterns that lower the average friction at intermediate velocities.

D. Force Effects with Langevin Dynamics

To investigate the role of force fluctuations, we add a random force term to the Prandtl-Tomlinson model and run simulations at different temperatures ($T = 0.0$, 0.01, 0.05, 0.1 in dimensionless units). The resulting average friction force $\overline{F}$ as a function of velocity v_0 is shown in Figure 5.

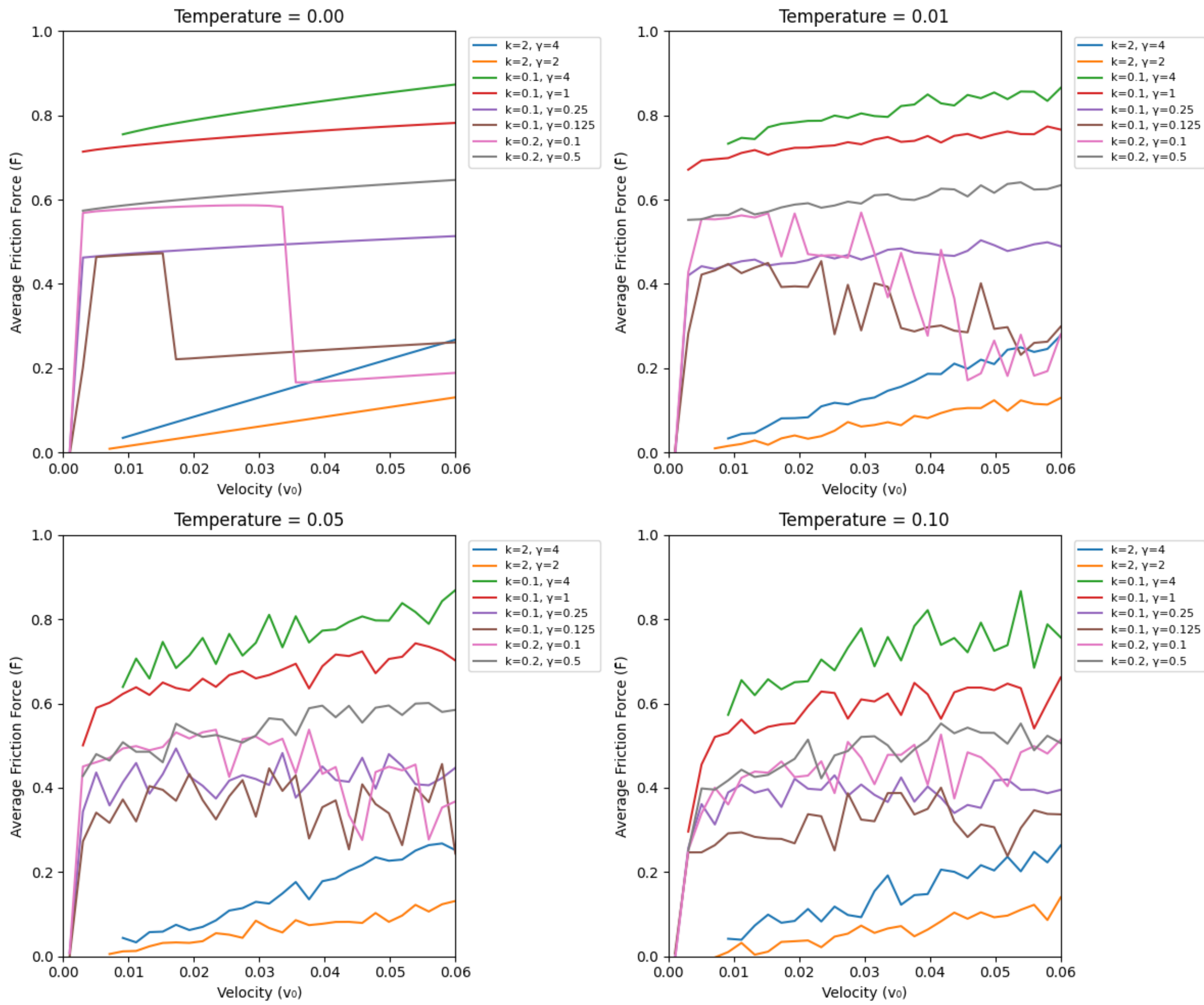

FIG. 5. Average friction force versus velocity at different temperatures. Unlike a simple smoothing effect, force introduces fluctuations that amplify deviations from the deterministic trend. While stick-slip motion is altered, thermal noise increases force variability, leading to irregular friction force behavior.

Effects of Thermal Noise:

- At $T = 0$, the system behaves deterministically, following the expected trends from the Prandtl-Tomlinson model. The curves match those obtained in the previous section without any random force.
- As T increases, thermal noise causes the tip to escape from potential wells earlier

than in the deterministic case. However, rather than simply reducing friction, this effect introduces **randomness** into the motion. As a result, the friction force does not decrease smoothly but fluctuates more due to increased probability of multiple slips.

- We observe that fluctuations **increase** with temperature. The presence of thermal kicks does not remove stick-slip motion but makes it more irregular. This behavior is especially prominent in the stick-slip regime ($\tilde{k} < 1$), where the force response becomes noisier.

- At higher temperatures, the friction force no longer follows a monotonic trend. Instead of a systematic reduction, we observe unpredictable force variations due to competing effects of thermal activation and barrier-induced resistance. The fundamental shape of the friction-velocity relationship remains, but the increased randomness causes deviations from the deterministic predictions.

III. CONCLUSION

In this homework, we analyzed the Prandtl-Tomlinson (PT) model for atomic-scale friction by reproducing key results from Dr. Jahangirov's PhD thesis and extending the model with Langevin dynamics to investigate the role of thermal fluctuations. Our work focused on two main objectives: (1) accurately reproducing Figures 4.2 and 4.3(a) while correcting a sign mistake in Equation (4.2), and (2) studying the effects of a thermal bath on friction loops and velocity dependence.

Key Findings:

1. Our numerical implementation successfully reproduced Figure 4.2, showing distinct regimes of **continuous sliding and stick-slip motion. When the dimensionless stiffness $\tilde{k}$ is greater than 1, the system moves smoothly, and the force loop is relatively small. When $\tilde{k} < 1$, the system enters a stick-slip regime, where the tip gets pinned in local potential wells and jumps abruptly, leading to a larger hysteresis loop and greater energy dissipation.

2. Our reproduction of Figure 4.3(a) confirmed the characteristic dependence of average friction force on velocity. When $\tilde{k} > 1$, the friction force grows approximately linearly

with velocity and approaches zero as $v_0 \to 0$. In contrast, when $\tilde{k} < 1$, the friction force saturates to a finite value at low velocities, reflecting persistent stick-slip dissipation.

3. Introducing Langevin forces revealed that thermal fluctuations introduce irregular variations in friction force rather than simply smoothing out the curves. At moderate temperatures, thermal kicks help the tip overcome potential barriers more frequently, slightly reducing friction in some velocity regimes. However, as temperature increases further, the friction force exhibits random deviations rather than following a clear trend. This suggests that at high temperatures, thermal effects disrupt the predictable stick-slip pattern rather than merely lowering friction.

These results contribute to a deeper understanding of how microscopic interactions shape macroscopic friction behavior, providing valuable insight for the design of nanoscale devices and materials with tailored frictional properties.

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[1] L. Prandtl, "Ein Gedankenmodell zur kinetischen Theorie der festen Körper," Z. Angew. Math. Mech. **8**, 85 (1928).

[2] J. Jahangirov, "PhD Thesis, FRICTIONAL AND VIBRATIONAL PROPERTIES OF NANOSTRUCTURES" University Repository (2012).