I use probability theory, dynamical systems, and differential geometry to investigate questions in mathematical physics. The broad objective is the development of simple and explicit models for stochastic behavior in certain mechanical systems; we seek a theory of probabilistic mechanics to compliment the success of statistical mechanics.

There has been much recent interest in non-equilibrium, steady-states [11] and stochastic thermodynamics [13]. We aim to provide a class of models that, while easy to understand and simulate, display interesting stochastic behavior.

Here, I will illustrate this broad research program using the specific example of the heat engine constructed in [3]. Though heat engines have long been central objects of study in thermodynamics, this one is built in a novel way. Its "parts" are randomized versions of simple billiard dynamical systems (*billiard Markov models* for short). One advantage of this novel approach is that billiard Markov models are easy to simulate and study; for example, figure 4 shows the efficiency of this heat engine, computed from simulation.

Though I will focus here on one specific, *simulation* based result, some of the rigorous *analytical* results arising from billiard Markov models and their connection to multiple areas of mathematics are demonstrated in [4, 6, 9].

We start with some background on billiard Markov models in section 1. In section 2, we introduce the notion of temperature for billiard Markov models established in [5]. In section 3, we will allow heat to flow and harness it to build the aforementioned heat engine. Finally, I will discuss some future research directions in section 4.

## 1 Background

The study of collisions certainly dates to the beginning of human-kind. The modern mathematical version of this ancient science is called billiard dynamics; it has enjoyed a period of great activity and success extending back to the middle of the last century; see [1, 10, 14] for example. More recently, [6, 8, 9] investigate randomized versions of billiard dynamical systems. These random billiards produce classes of Markov chains; thus we often call these billiard Markov models. Billiard Markov models have proven quite useful because they tend to have some properties that reflect the deterministic structure of dynamics and some properties that reflect the randomness inherent in the study of any real physical system.

For example, imagine a sample of gas particles enclosed by a tank. Many of the thermodynamically interesting quantities, like pressure, arise from the constant collisions between the gas particles and the interior wall of the tank. So, it is natural to investigate the characteristics of the particle-wall collisions. For example, the Danish physicist Martin Knudsen experimentally measured the distribution of post-collision gas particle trajectories [12]. Knudsen's Law says that this distribution depends on the cosine of the angle made with the wall's normal vector at the point of collision.

An early success for billiard Markov models came in [7], where it was shown that Knudsen's Law (an empirical observation) arises naturally within this theoretical framework. In this model, a geometric structure is imposed on the interior surface of the wall as in figure 1. Specifically, the model asserts that the wall is lined with tiny, identical chambers. One segment of each chamber is open to the interior of the tank. When a gas particle collides with the wall, it enters one of these chambers at a *random* point on the open segment. The random entry point is key; it reflects the idea that the chambers are much smaller than measurement error. Since we can't resolve position of the gas particle on the scale of the chamber, we simply treat it as random. After crossing the open segment at a random point, the particle performs *deterministic* billiard motion inside the chamber until it returns to, and passes through, the open segment. (Poincaré recurrence guarantees return to the open segment almost surely.)

The post-collision trajectory is completely determined by the chamber geometry (which we treat as fixed), the pre-collision trajectory, and the point of entry. By choosing the point of entry randomly (according to a known distribution), we obtain a Markov chain on the space of particle trajectories. It is a discrete time Markov chain with continuous state space. Importantly, the stationary state of this Markov chain gives Knudsen's Law.

The appearance of this noted experimental result within the theory of billiard Markov models motivated substantial further investigation, see [6, 8, 9].

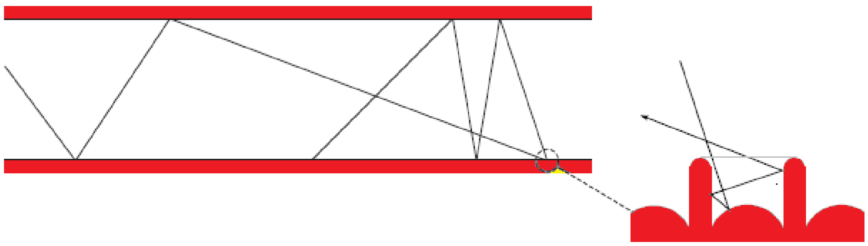

Figure 1: A gas particle confined to a tank. Macroscopically, the interior walls appear smooth, but the particle tends to rebound in surprising ways. By zooming in to the microscopic level, we see a geometric structure that causes this scattering behavior.

## 2 Temperature

In joint work with Renato Feres [5], we add a notion of temperature to this billiard Markov model. The gas particles in the above model move at constant speed. Recalling that the Kinetic Theory of Gasses relates temperature and average particle speed, a fast particle moving in a cold tank should slow down.

To the previous model, we add additional particles that are "bound" inside the chambers. We also allow "molecular" structure for the gas; see figure 2. Now, when a "free" gas particle collides with the wall of the tank, it enters (at a random point) a chamber containing one or more bound particles. The initial states of these bound particle are also chosen randomly. The system then evolves *deterministically*, with the possibility of elastic collisions between the free particle and the bound particles. These particle-particle collisions permit transfer of energy between the gas and the walls of the tank.

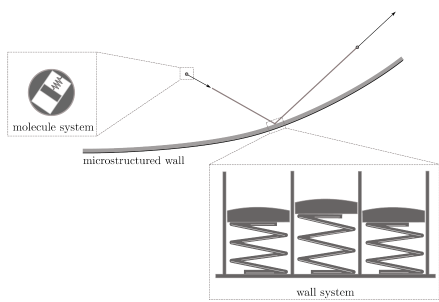


Figure 2: The microstructure now features bound particles. The particle-particle collisions allow transfer of energy between gas and tank.

It is natural to choose the initial velocity of the bound particles according to the normal distribution with mean 0 and a variance $\sigma^2$ that reflects the intended temperature of the tank. Under this (and other natural assumptions), we show that the stationary distribution of the resulting Markov chain

1. Gives Knudsen Law for angle of the outgoing gas particle.
2. Gives (a scaled) Maxwell-Boltzmann distribution for the speed of the outgoing particle. This is another fact which was well-known experimentally and arises naturally within our billiard Markov model.
3. The "temperature" of the gas particles given by this Maxwell-Boltzmann equals the "temperature" of the tank given by $\sigma^2$. Hence our billiard Markov model seeks thermal equilibrium. This is yet another empirically familiar phenomenon that is demonstrated by the model.

## 3 Heat Engines

With a notion of temperature established for our billiard Markov models, Tim Chumley, Renato Feres, and I show in [3] that these models can generate heat flow. Hence, we can build simple machines from billiard-like parts.

For example, consider the minimal heat engine in figure 3. It consists of two closely spaced parallel circular rails. Let us first consider just the top rail. It passes through a wall with temperature $T_1$ on one side and $T_2$ on the other. An obstacle is attached to the top rail at a certain point. As the rail rotates, the obstacle collides with the wall. These collisions are modeled using the billiard Markov models discussed above with the corresponding temperature.

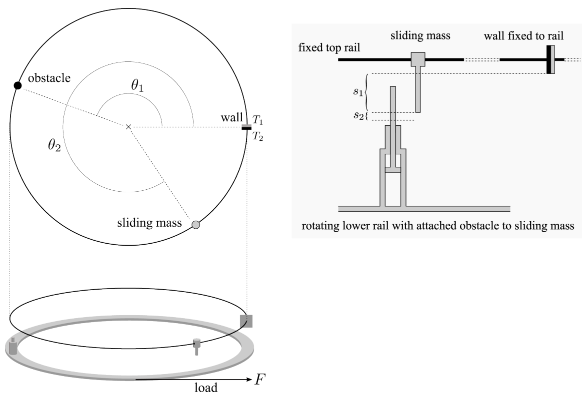


Figure 3: Our minimal billiard Markov heat engine. Top left shows the view from above. Top right shows the view from the side with the moving piston on the bottom rail and the fixed obstacle on the top rail.

The first noteworthy result from Matlab simulations of this system is that heat flows from the hot side of the wall to the cold side at the rate expected from classical thermodynamics. We saw a consistent linear dependence between the mean energy transfer per collision and the temperature differential across the wall.

Now, attach a piston to the bottom rail. This piston moves vertically within a fixed cylinder. As the two rails rotate and bring the piston and obstacle together, they will interfere if the piston is up, but slide past each other if the piston is down. There is no wall blocking the rotation of the bottom rail.

From simulation, we see that, if the temperature differential across the wall is small, the motion of the bottom rail is essentially Brownian with no drift. By contrast, a large temperature differential causes the bottom rail to rotate preferentially toward the cold wall. By adjusting the temperature differential, we adjust the strength of the drift, moving from a strongly stochastic motion to a rotation at nearly constant speed.

Finally, we attach a constant load to the bottom rail so that its rotation can be harnessed to do work. Through simulation, we investigate the affect of various parameters (like temperature differential) on the efficiency of this heat engine. As you can see in figure 4, while our first billiard Markov machine does work, there is a much room to improve its efficiency.

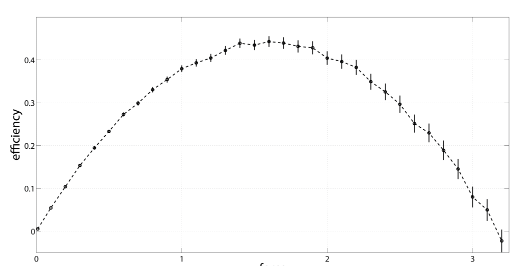


Figure 4: Efficiency our heat engine versus the opposing force (for a specific choice of model parameters)

# 4 Conclusion

Though I focused this discussion narrowly on the goal of presenting the heat engine of figure 3, the theory of billiard Markov models is both quite deep and flexible. It pulls from many mathematical disciplines (dynamical systems, probability theory, differential geometry) and addresses topics from physics and chemistry. The interdiscplinary nature of this research appeals strongly to my broad background in the sciences. As an undergraduate, I earned a major in chemistry and a major in physics before working as an aerospace engineer. In graduate school, I first explored combinatorics before I moved to billiard Markov models. I feel that this breadth is one of my strengths as a scholar and teacher; I love researching in an area that uses this breadth.

Chumley, Feres, and I have a substantial list of planned research directions, including building better and more interesting machines, establishing rates of convergence for these Markov chains, and systematically exploring some "concentration of measure" properties that have we sporadically observed during these studies.

Our current paper [2] is currently being edited and will be submitted shortly. It explores diffusion behavior of "Brownian" particles with temperature gradient using a billiard Markov models. In June 2015, we will participate in the *Stochastic methods for non-equilibrium dynamical systems workshop* at AIM (American Institute of Mathematics) in Palo Alto, CA `aimath.org/workshops/upcoming/noneqdynsys/`. We have also submitted a proposal for a SQuaRE workshop at AIM during the immediately following week. This will provide six of us a chance for focused research work on stochastic thermodynamics and random billiards `aimath.org/programs/squares/`.

I plan to involve a diversity of students in my research. Most of these research directions will combine computer simulation and theory from several of the disciplines mentioned above. So, I believe that I can find projects that appeal to students of diverse appetites and sophistication.

As I said in the cover letter, I want to do research with students because I matured through research. From three REU's and my years in graduate school, I learned that the path to success involves a few good ideas and a lot of hard work, confusion, frustration, and tenacity. Learning these lessons early as an undergraduate helped me succeed as a graduate student and early career mathematician; I'd like to share them with my students.

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