[L] Clogging in Granular Flor through a Bottleneck

César Mejía [and Marnick Huisman]
(Dated: November 24, 2025)

This project investigates clogging phenomena in granular flows through a bottleneck. We aim to quantify how the probability of clogging and the statistics of particle discharge depend on the orifice diameter, grain size distribution, and particle-wall friction. We will explore a combination of molecular dynamics simulations and cellular automata models to capture both realistic contact interactions and rapid parameter sweeps. The study will provide insights into the mechanisms behind the formation of archs and flow interruptions in granular materials.

Project Topic: Granular Matter

Teaching Assistant: Agnese Callegari

I. INTRODUCTION

Granular flows through constrictions occur in many industrial and natural processes, such as hopper discharges, pedestrian evacuations, granular silo flows or even sand clocks. A key feature of these systems is the formation of arches that block flow, known as clogging. Understanding the statistical properties of clogging, including how it depends on particle and system parameters, is important for optimizing material handling and predicting jamming events. Previous work has shown that orifice size, particle size distribution, and frictional properties significantly affect clogging probability. In this project, we will try to model these effects using computational methods and look at the results to see what patterns appear. Some simpler models might not capture all the details, but they can still give a useful idea of how clogging behaves in different situations. The goal is to get a better sense of which parameters are most relevant for clogging and how they interact.

II. OVERVIEW

To study clogging, several computational methods are available. **Table I** summarizes three relevant approaches, detailing their use case, key features, and suitability for the project.

The chosen and combined application of these methods will allow the study of the clogging problem, ranging from detailed simulation of individual particles to the efficient exploration of the parameter space.

Method 1: Molecular Dynamics (Particle Simulation)

The Molecular Dynamics (MD) method, or specifically the Discrete Element Method (DEM) in the granular context, is the primary approach for reproducing realistic clogging dynamics in hopper or bottleneck flows. Its main use case is simulating the motion and interaction of individual grains in these systems. This method resolves direct particle contacts, which is crucial for capturing the formation of stable arches that lead to clogging. While it is computationally intensive, which can limit system size or duration, it is the most suitable method for obtaining high-fidelity results comparable to real experiments on the mechanics of clogging, such as those discussed in literature [**?**]. This makes it the main tool for the project.

Method 2: Cellular Automata (Rule-based)

The Cellular Automata (CA) approach, particularly rule-based variants, provides a computationally inexpensive alternative to detailed particle simulations. Its use case involves the rapid exploration of the parameter space using simplified lattice flow models. It is a grid-based model where cell states update based on local rules, allowing for very fast simulation and clear visual outputs of flow and clogging patterns. Its main drawback is the lack of mechanical detail, as it does not resolve real contact forces. However, it is an excellent complementary method for performing broad parameter sweeps to quickly identify regions of interest before resorting to more costly MD simulations.

Method 3: Brownian Dynamics / Stochastic Integration

Brownian Dynamics (BD), or the inclusion of Stochastic Integration in the equations of motion, is used to incorporate the effects of randomness and fluctuations. Its use case is the optional addition of stochastic noise to particle motion, modeling scenarios where small external vibrations or inherent randomness might affect the stability of a clogging arch. This feature allows it to model fluctuations and potentially smooth highly irregular flow behavior. The method is considered optional because, while it captures noise effects, the stochastic force must be carefully calibrated to avoid inaccurate representation of the granular contact mechanics. It may be used if the project requires the study of how kinetic or external noise influences clogging frequency and time.

TABLE I. **Overview of Simulation Methods/Models for Granular Flow Clogging.**

Method / Model	Use Case Scenario	Key Features (Summary)	Suitable for the Project?
Molecular Dynamics / Particle Simulations	Simulating individual grains in hopper or bottleneck flows	Resolves particle contacts, friction and normal forces, realistic arch formation; computationally intensive for large systems	**Yes** — main method to reproduce realistic clogging dynamics.
Cellular Automata / Rule-based CA	Rapid exploration of parameter space using simplified grid-based dynamics	Computationally cheap, easy to visualize clog/no-clog behavior; lacks force realism and detailed contact modelling	**Yes** — complementary method for wide parameter sweeps.
Brownian Dynamics / Stochastic Integration	Addition of stochastic driving or thermal-like perturbations	Captures fluctuations, simple to implement; does not model contact mechanics accurately	**Optional** — only if exploring noise-induced effects.

III. METHOD

In this project, we will use a combination of computational approaches to study clogging in granular flows. The main method will be Molecular Dynamics (MD), which allows us to simulate individual grains and their interactions. This will let us observe how arches form at the bottleneck and how flow is interrupted, providing realistic information on particle contacts and forces. To complement MD, we will implement a rule-based Cellular Automata (CA) model. The CA approach is simpler and computationally cheaper, allowing us to quickly explore a wide range of parameters, such as different orifice sizes, particle size distributions, and friction values. Using CA, we can identify general trends and regions of interest before running more time-consuming MD simulations. Optionally, we might include stochastic effects using Brownian Dynamics (BD) if we decide to investigate how random perturbations, like small vibrations or fluctuations, influence clogging probability. This will help us understand whether noise plays a significant role in flow interruptions.

Overall, our approach will start with CA simulations to map the parameter space efficiently and highlight interesting scenarios. Then, we will focus on selected cases using MD to obtain detailed results on arch formation and flow dynamics. By combining both methods, we aim to balance computational efficiency and physical realism, providing a comprehensive analysis of clogging phenomena in granular flows.