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Bridging percolation and particle dynamics models of the granular rigidity transition

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HIGHLIGHTS

- Sheared Granular Lattice Gas (SGLG) model, an adapted lattice gas model.
- Includes an explicit description of force chains and granular shear.
- Recovers experimental measurements such as dilation and velocity profiles.
- Captures similar dependence of coordination number on density as in MD simulations.
- Transition of percolation network strength shown to have a 1st order transition.

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ABSTRACT

Percolation models are routinely used to study the rigidity transition. However, they cannot capture dynamics occurring in granular media. Molecular Dynamics can be used to model the rigidity transition, yet, they cannot represent realistic hard granular materials due to computational constraints. Contact Dynamics can be used instead; but only by assuming perfectly rigid particles where dissipation occurs by friction alone and deformation is excluded. We present an alternative dynamic approach to studying the solid–fluid granular rigidity transition for rigid particles, which is computationally faster than contact dynamics, and does not exclude particle deformation. Here we present an adaption of the Granular Medium Lattice Gas model of Károlyi and Kertész (1998) called the Sheared Granular Lattice Gas (SGLG) model which incorporates, for the first time in a lattice gas model, a description of force chains and granular shear. Significantly, we demonstrate that the SGLG model recovers typical experimental measurements such as dilation effects adjacent to the shearing boundary, the functional dependence of the velocity with depth near the transition, and qualitatively, granular anisotropy. The SGLG model also reproduces key results from simulations. Firstly, it exhibits similar functional dependence of particle coordination number on density as observed in Molecular Dynamics simulations. Secondly, the SGLG allows the transition of the percolation network strength to be calculated. It is found to be a first order transition and functionally equivalent to that observed for central force rigidity percolation. However, the exponents characterising the transition differ.

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1. Introduction

Granular materials, such as powders and aggregates, can change from a solid to a fluid granular state by simply pouring, vibrating, or by applying external shear. In a solid state a granular medium carries a load through a heterogeneous network of contact forces known as force chains [1–4], while in a fluid state particle motion is determined by collision dynamics. The solid–fluid jamming or rigidity transition that arises by applying external shear has been the subject of considerable recent study [5–11].

Molecular Dynamics (MD) can be used to study granular shear [11–13] but the efficiency of any MD code is determined by the efficiency of the computation of the inter-particle forces. While such computation may be optimised with Verlet lists or bounding box search algorithms [14] MD algorithms are not appropriate for the simulation of realistic hard grains where Young's modulus is of the order 10^9 Pa. This is due to the small integration time steps necessary to accurately resolve particle interactions. Contact dynamics [15–17] is a more efficient method of modelling the granular dynamics of rigid particles, but particles are assumed to be perfectly rigid, collisions are perfectly elastic, and dissipation occurs solely by friction. The model is therefore a limiting case, and excludes particle deformation, which has been shown to be integral to the response of granular media to external loading [2,11,18].

The granular phase transition is known to exhibit power laws in shear modulus, and the transition is thought to be critical [7,9,11]. The force chain network, is also a complex connectivity or topographical response to external loading [1–4]. On this basis it is reasonable to use a percolation based model [19] at the solid–fluid transition. While models have been used to explore rigidity [20–22] they are used in an instantaneous sense and the dynamic nature of a continually sheared granular medium and associated correlations in time are not accounted for. Lattice Gas (LG) models [23,24] have been extended to granular dynamics due to their computational efficiency. The Granular Medium Lattice Gas (GMLG) model of Károlyi and Kertész [25–27] incorporates inelastic particle collisions, dilatancy, gravity and friction and has been applied to simulate granular piles [25], hopper flow subject to gravity [27] and segregation effects [28]. In this paper, we present the Sheared Granular Lattice Gas (SGLG) model. The SGLG model is an application of the GMLG model to a sheared granular configuration that has been adapted to include force chain identification and dynamics. The main distinctions between the SGLG model and the GMLG model are that gravity is removed, a shear plane is included and rearrangements due to external shear (both adjacent to the shear plane and throughout the granular medium) are modelled. The dynamic rule set governing particle collisions has been expanded to include a greater number of possible particle outcome configurations, and average dissipative collisions have been added that allow the granular bed to dissipate artificial residual motion. Importantly, the SGLG model incorporates for the first time in an LG model of a granular packing, force chains identified by percolation methods and their response to external shear. The SGLG model is nevertheless a simplistic phenomenological description of particle interactions in a sheared granular bed that considers only a distilled set of particle interactions probabilistically. It lacks the physical details of molecular dynamics and contact dynamics, yet as will be seen it is still capable of capturing qualitative and quantitative aspects of the sheared granular medium. The lack of details also leads to improved computational speed.

The subsequent sections of the paper are structured as follows. In Section 2 we provide a brief overview of the SGLG model. In Section 3 we describe the details of the mechanisms for particle dynamics and the method for identifying the force chain network and the subsequent response of the network to shear. In Section 4 we present and compare results from the SGLG model with physical experiments. We find good agreement with a number of experimental observations such as dilation effects, the functional dependence of the velocity with depth near the jamming transition and qualitatively the contact network anisotropy. We also show the model exhibits similar functional dependence of coordination number on density observed in MD simulations, and observe a first order transition of percolation strength but with different exponents to those seen in central force rigidity percolation. Finally, in Section 5 we present our conclusions.

2. Sheared Granular Lattice Gas (SGLG) model

2.1. Physical motivation

The SGLG is a model that simulates a two dimensional granular medium subject to constant shear in a Couette style geometry [2]. In this geometry 2-D discs rotate between an inner and outer boundary colliding with each other and the boundaries. Heterogeneous networks of force emerge through the contacts between particles that form continuous links to the boundaries. To simulate the dynamics, particle–boundary and particle–particle collisions must be described. The collisions are governed by material properties which are captured by an energy coefficient of restitution, and in the case of the boundaries the collisions are directional. We also distinguish inter-particle collisions in terms of collisions with particles that bear and do not bear boundary force as the former can collectively dissipate momentum and energy to the boundaries, while the latter can be treated as isolated collisions. To distinguish these collisions the force bearing particles need to be identified. Simply identifying connected particles along paths that lead to both boundaries is insufficient as not all such particles are force bearing. Particles that form dangling end connections to a force chain are not load bearing, and forces around closed loops necessarily sum to zero. In sheared granular experiments force chains also constantly rearrange under the external shear, as particles react and shift position. The SGLG must also therefore capture the deformation of force chains as a result of shearing.

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