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Simulations of driven overdamped frictionless hard spheres

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ABSTRACT

We introduce an event-driven simulation scheme for overdamped dynamics of frictionless hard spheres subjected to external forces, neglecting hydrodynamic interactions. Our event-driven approach is based on an exact equation of motion which relates the driving force to the resulting velocities through the geometric information characterizing the underlying network of contacts between the hard spheres. Our method allows for a robust extraction of the instantaneous coordination of the particles as well as contact force statistics and dynamics, under any chosen driving force, in addition to shear flow and compression. It can also be used for generating high-precision jammed packings under shear, compression, or both. We present a number of additional applications of our method.

1. Introduction

Systems of frictionless hard spheres serve as prototypical models in statistical physics, displaying a variety of emergent complex phenomena [1–6]. Owing their popularity to their inherent simplicity, systems of frictionless hard spheres are used to model gases [7], supercooled liquids [6], dense suspensions [8–11] and granular media [4,12]. The simplicity of hard-sphere systems stems from the absence of energy scales in the hard-sphere interactions. It is this simplicity which makes these systems a preferred choice of model for the investigation of complex phenomena in particulate systems.

Perhaps the most extensively studied model of hard spheres is the fully inertial fluid, in which collisions between particles are entirely elastic. In these systems, collisions are instantaneous, i.e., colliding particles spend no time at all in contact, but instead conservation of energy and momentum determines the post-collision velocities as a function of the pre-collision velocities. Event-driven simulations of these systems are carried out by predicting the next collision time from the instantaneous velocities and positions of the particles [13]. Then, the system is evolved forward in time directly to the next collision.

Here we shall rather focus on non-Brownian hard particles immersed in a viscous fluid, in the overdamped limit where inertia is negligible. We shall assume further that hydrodynamic interactions are negligible. This assumption has been made in the context of flow near jamming [5,8–11], where it appears to capture at least qualitatively the critical behavior in the dense limit [11]. Within the framework of these assumptions, *contacts* are formed between the particles upon collisions, as they are pushed towards each other. These contacts persist for finite intervals of time, during which repulsive forces are exerted between the particles in contact.

Our simulational approach is based on the exactly derivable equations of motion of overdamped dynamics in the hard-sphere limit, neglecting hydrodynamic interactions. These equations are used to build an event-driven simulation. The equations of motion are entirely based on geometric information, which allows us to calculate the contact forces between the constituent hard particles, and hence their distribution and evolution [14]. The main idea is to evolve the system according to the equations of motion, while carefully handling the formation of new contacts and the opening of existing contacts between particles. Our method shares some similarities with the method of contact dynamics [15] used in dry granular materials, in which contact forces and velocities are resolved iteratively under a set of complementarity relations.

The simulational scheme presented below has merits and disadvantages with respect to existing methods. In terms of bare complexity, the method we present is far inferior to conventional molecular dynamics methods, in which the running time typically scales linearly with the number of particles, given that interactions are sufficiently short ranged. The running time of the scheme presented here scales at least quadratically with the number of particles. This is a consequence of the event-driven nature of the scheme, together with the effectively long-range interactions which can span the entire system at high packing fractions. However, when compared to existing methods in which hard-sphere dynamics is approached by reducing the loading rates in systems of soft-potential interactions [8–10], our method has the

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advantage of directly sampling the hard-sphere limit. Furthermore, our method requires essentially no adjustable parameters; particle trajectories are invariant when length and time are measured in the appropriate microscopic units.

The formalism presented here allows for useful extensions of the methods built in this work. For instance, it is straightforward to introduce hard boundaries (such as various container shapes, hoppers, or inclined planes), or constructing composite particles made of any number of beads, which can be floppy or constrained as rigid bodies. The method can also be used to generate jammed packings under various loading geometries, while maintaining complete control over the identity of particles in contact, in distinction from existing methods [16,17]. This control allows us to properly account for rattlers in jammed states, with no ambiguity whatsoever.

This paper is organized as follows. Section 2 derives the equations of motion for overdamped, frictionless hard spheres, either driven by external forces, or under imposed spatial deformations, neglecting hydrodynamic interactions. We also include an extension of our formalism for simple shear flow under fixed imposed pressure. Section 3 illustrates the concept of the instantaneous contact network, which is geometric information on which the equation of motion is based. Section 4 contains an elaborate description of our simulational scheme and ends with a prescription for generating jammed configurations under shear or compression. Section 5 describes applications of our simulation method and presents some results from our simulations, illustrating the utility of our event-driven approach. Section 6 presents concluding remarks.

2. Equations of motion for overdamped, frictionless, driven hard spheres

Consider a system of N frictionless hard spheres (referred to in the following as particles) in a volume Ω with periodic boundary conditions in d dimensions, such that there are no overlapping particles, and some of the particles are exactly in contact: the distance between their centers is equal to the sum of their radii. When the system is unjammed, the number of contacts N_c in the system remains smaller than the number of spatial degrees of freedom $Nd - d$. Note that we subtract d translations but not rotations due to the periodic boundary conditions. We denote the d-dimensional vector of the ith particle coordinates as $\vec{R}_i$, its time derivative as $\vec{V}_i$, and define the directional differences $\vec{R}_{ij} = \vec{R}_j - \vec{R}_i$, the pairwise distances $r_{ij} = \sqrt{\vec{R}_{ij}\cdot\vec{R}_{ij}}$, and the normalized directions $\vec{n}_{ij} = \vec{R}_{ij}/r_{ij}$. We will refer to the *contact network* as the set of all pairs of particles that are in contact at some instance in time, and the geometric information that accompanies the network, namely the directions $\vec{n}_{ij}$, and the pairwise distances r_{ij}.

We begin the derivation with accounting for the hard-sphere interactions; given some vector of particles' velocities $\vec{V}_k$, the rate of change induced on a pairwise distance r_{ij} is

$$\dot{r}_{ij} = \sum_k \frac{\partial r_{ij}}{\partial \vec{R}_k}\cdot\vec{V}_k = \sum_k (\delta_{jk} - \delta_{ik})\,\vec{n}_{ij}\cdot\vec{V}_k = (\vec{V}_j - \vec{V}_i)\cdot\vec{n}_{ij}. \tag{1}$$

The above relation consists of a linear transformation of vectors from *the space of the particles* (of dimension Nd) to vectors in *the space of contacts* (of dimension N_c). We define

$$\mathcal{S} \equiv \frac{\partial r_{ij}}{\partial \vec{R}_k}; \tag{2}$$

then Eq. (1) can be written in bra-ket notation as

$$|\dot{r}\rangle = \mathcal{S}|V\rangle. \tag{3}$$

Here and in the following we use bra-ket notations with upper-case letters to denote vectors from the space of the particles (e.g., $|V\rangle$ for particle velocities), and bra-ket notations with lower-case letters to denote vectors from the space of contacts (e.g., $|r\rangle$ for the vector of pairwise distances).

As the particles are completely rigid, they cannot penetrate each other. We thus impose a constraint on the particles' velocities: they must keep the distance between the pairs of particles that are in contact *unchanged*, if the contact force exerted between the pairs of particles is positive. We will see in Section 3 how a given set of contacts between the particles does not change except at discrete points in time. Except for at those discrete time points, the velocities must satisfy

$$|\dot{r}\rangle = \mathcal{S}|V\rangle = 0. \tag{4}$$

In the next two subsections we present the derivation of the equations of motion for the case of dynamics under external forces, and the case of spatial deformations of the system (e.g., compression or shear). Section 2.3 contains an extension of our formalism to systems of hard particles under simple shear, with fixed imposed pressure, as opposed to fixed volume.

2.1. Overdamped dynamics under external forces

In our framework, there are three forces acting upon each particle: a drag force $\vec{F}_k^{\text{drag}}$, the force exerted on a particle by its neighbors with which it is in contact $\vec{F}_k^{\text{cont}}$, and some external driving force $\vec{F}_k^{\text{ext}}$. Assuming that the dynamics is overdamped, and neglecting hydrodynamic interactions, the net force on each particle must always be zero:

$$\vec{F}_k^{\text{ext}} + \vec{F}_k^{\text{drag}} + \vec{F}_k^{\text{cont}} = 0. \tag{5}$$

We assume conventional Stokes drag forces acting upon particles, which are opposite in sign and proportional to their velocities:

$$\vec{F}_k^{\text{drag}} = -\xi_0^{-1}\vec{V}_k, \tag{6}$$

where ξ_0 has units of $\frac{\text{time}}{\text{mass}}$. ξ_0 may generally depend on the radius of the k'th particle; however, for the sake of brevity, we consider here mono-disperse spheres, as the extension to poly-disperse spheres is straightforward. Denoting the magnitude of the (purely repulsive) force exerted between the jth and kth particles as $f_{jk}(=f_{kj})$, the forces exerted on a particle by its neighbors with which it is in contact can be written as

$$\vec{F}_k^{\text{cont}} = \sum_{j \text{ in contact with } k} \vec{n}_{jk} f_{jk} = \sum_{\text{all pairs } i,j \text{ in contact}} (\delta_{jk} - \delta_{ik})\,\vec{n}_{ij} f_{ij} = \sum_{\text{all pairs } i,j \text{ in contact}} \frac{\partial r_{ij}}{\partial \vec{R}_k} f_{ij}. \tag{7}$$

The above equation, similarly to Eq. (1), also consists of a linear transformation, but this time from the space of contacts to the space of particles, with the *transpose* of the same linear operator $\mathcal{S}$ of Eq. (2); we thus write equation (7) as [12,18]

$$|F^{\text{cont}}\rangle = \mathcal{S}^T|f\rangle, \tag{8}$$

with $|f\rangle$ a vector of dimension N_c denoting the contact forces f_{ij}. Inserting Eqs. (6) and (7) in Eq. (5) and rearranging, we find

$$|V\rangle = \xi_0|F^{\text{ext}}\rangle + \xi_0\mathcal{S}^T|f\rangle. \tag{9}$$