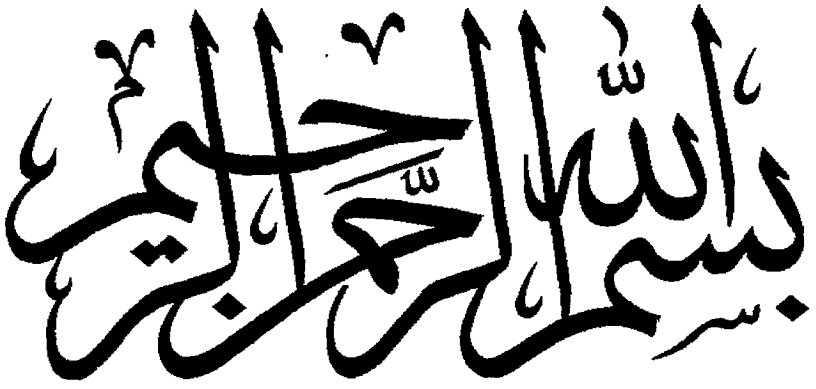

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Study of sediment transport in the saltation regime

Ph. D. Thesis

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To my parents and my husband

Table of Contents

Abstract

Sediment transport by laminar and turbulent flow are phenomena involved in the natural environment and industrial processes. We present a study of sediment transport in the creep and saltation regimes by laminar and turbulent flows. In our model the particles are supposed as hard disks in a two-dimensional domain with periodic boundary conditions in the horizontal direction. The motion of particles is calculated by the event driven molecular dynamics method. The flow of the fluid over the bed of particles is modeled by imposing a velocity dependent drag force on each particle that depends on the height above the bed. The fluid flows over the bed, so the particles can be entrained by the fluid and move under the influence of the drag force and gravity. We consider two velocity profiles for the fluid, parabolic and logarithmic. The first one models laminar flow and the second corresponds to turbulent flow. For each case we investigate the behavior of the saturated flux. For the logarithmic profile we compare our results to previous studies on turbulent flows. We find that for the logarithmic profile, the saturated flux shows a quadratic increase with the strength of the flow, and for parabolic profile, a cubic increase. We also find that for the parabolic profile, near the threshold velocity, saturated flux increases quadratically with the shear velocity. The velocity probability distribution functions of grains are used to interpret the results. The transverse velocity probability distribution function shows the same behavior for both the logarithmic and parabolic profiles.

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Chapter 1

Introduction

1.1 Granular matter

Granular matter is composed of many macroscopic grains. Examples of granular matter are all around us, sugar and salt in the kitchen or gravel in the garden. The size of the grains ranges from hundred microns to a few meters in diameter. So it is not surprising that various fields of research study granular matter; biologists, engineers, geologists, material scientists, and physicists. However, since the theoretical description of granular matter still contains many unsolved problems, this topic has also attracted many mathematicians and computer scientists [1, 2].

Many industries, such as the pharmaceutical industry depend on the processing of powders; the construction of highways depends on the manipulation of large amounts of gravel and sand, large amounts of grains from flour to coal are transported, processed, and then stored. In all these processes the study of the flow properties as well as the static properties of granular matter becomes necessary.

Granular materials are different from other materials, as they show very different behaviors under different circumstances. Sometimes they behave like a liquid: it flows through pipes, flows inside an hourglass, etc. In other situations it behaves more like a solid, for example a heap of sand. Also there are intermediate stages: If

we stand on the beach, we will sink through the sand as in a viscous liquid, but only for a few centimeters. Then the motion stops, almost independently of our weight. In some cases granular material can switch from a solid to fluid behavior, as we see in avalanches. Sometimes granular material resembles a gas (granular gas), but its energy is dissipated, as the collisions between the grains are inelastic. Therefore, the gas has a transition to fluid or solid state. In the absence of gravity, granular material can maintain its gaseous state for a long time, for example in the rings which encircle the planets.

Historically, Leonardo da Vinci (1452-1519) was first to devise a simple experiment demonstrating the laws of dry friction. It was not until the end of the eighteenth century, that Charles de Coulomb (1736-1806) wrote a definitive paper, which was based on a number of experimental observations on the equilibrium of earthen embankments, the stability of stone structures, and other edifices. Michael Faraday (1791-1867) was another scientist who had a strong interest in how vibrations induce the formation of sand piles. This phenomenon remained a mystery until recently. Osborn Reynolds (1842-1912) made observations on the puzzling effect of dilatancy. He introduced the concept of dilatancy, an effect one encounters while walking on a wet beach. When we exert a pressure on wet sand, a dry halo appears around our foot. Naively one would expect that the pressure of the foot would produce a hole in the sand which would then fill with water, but the opposite occurs. The physical reason for this effect is that the grains were so densely packed before pressure. The pressure causes the particle to move with respect to each other, separating them. Between 1940 and 1970 Ralph A. Bagnold made many important observations and wrote a book on desert sands [3]. Since that time, the number of scientific publications in the field has greatly increased.

Moving sand dunes are an example of granular flow, a poorly understanood

branch of physics. Imagine a little grain of sand in a moving sand dune. Each grain differs from all the other grains and each one is touching many others around it. As a grain moves, it is changing the position of the grains it touches. Its movement is determined by how all the surfaces respond to each other as they move. To write an equation which takes all the factors of sand's movement into account is difficult. Below we are going to review some studies about various kinds of sand movement.

1.2 Investigations into the sediment transport

Wind erosion is a serious environmental problem in arid and semi arid regions in the world. It occurs when a soil surface is unprotected by vegetation cover and is so dry that wind is able to pick up sand from the surface that usually contains some organic nutrients. The transport of soil by the wind causes structural and compositional changes of the soil. For instance, it reduces soil productivity and lead to land degradation, dust suspension reduces visibility, etc. so the control of wind erosion is important. These show the importances of the investigation about sediment transport. In the past decades research about the process of sand transport in desert has intensified to prevent desert sand from spreading and to protect soil from wind erosion. Such studies help to predict the shape of sand dunes [4, 5] and the evolution of a free sand surface.

Suspension, saltation and surface creep are the three distinct modes which occur during wind erosion [3]. In saltation individual grains ejected from the surface follow distinct trajectories under the influence of fluid flow and gravity. When the strength of the fluid is small the particles can move while still in continual contact with each other, and yet it could happen that every now and then, due to collisions, some particles jump by a distance of order of their diameter. This regime is called surface creep or reptation. Sediment transport as bed load usually moves in saltation or

reptation. In suspension the particles move in the fluid for long period of time, hardly colliding with the bed or each other. The bulk of total transport, roughly 50 to 80 percent, is by saltation.

In general, there are three ways in which particles can start their motion in a fluid: aerodynamics entrainment, rebound, and ejection. Aerodynamic entrainment is the process where particles initially lying on the ground, are picked by the fluid. Rebounding particles are the particles that already are in saltation, hit the surface and bounce of again, thus starting a new trajectory in saltation. The third possibility, ejection, takes place when a particle that is in saltation impacts onto the surface and ejects other particles from surface. This process sometime is called splash which comprises the complicated interaction between bed and impacting grain and is currently the subject of theoretical and experimental investigations [6, 7]. Study of the relative importance of the way a particle enters the fluid can be useful for the formulation of the saltation. The attention that several researchers have given to this problem, has not yet resolved the discussions about this topic [8, 9].

In order to understand the problem of sediment transport, studies have been done for a long time, ranging from the motion of a single grain [10] to the flux of sand as a continuum quantity [11]. One of the most important issues has been the relation between the shear velocity (u_*) of the fluid and the saturated sand flux ($q(u_*)$), or bed-load transport rate. An application of sand flux relation is in geomorphology where it becomes necessary to calculate the erosion rate in order to predict the evolution of a free sand surface or a dune. There has been a great effort to obtain experimentally [3, 12, 13], and theoretically [3, 14, 15, 11, 16] the relationship between the saturated granular flux over a bed and the shear velocity. Bagnold [3] was first to introduce a simple flux law, a cubic relation, expressing the dependence of sand flux on the shear velocity. Apart from the work by Ungar and

Haff, all the above theoretical studies give similar results: the saturated flux q scales at large shear velocity like the Bagnold description and vanishes below a threshold value. The model given by Ungar and Haff predicts that the flux increases at a rate that is slower than u_*^3. The velocity profile of the wind within the layer of grain has also been the object of investigation [12], but it is experimentally much more difficult to access than the flux. Numerical methods will be useful for this quantity [17]. Almeida *et al.* [17] also obtained numerically a quadratic relation near the threshold shear velocity. They simulated the saltation inside a two-dimensional channel with a mobile top wall. Jiang and Haff [18] made some simplifications and presented a model in which the fluid is a moving layer or slab which exerts a velocity dependent drag force on the embedded grains. However, the slab model does not consider the details of the vertical velocity structure and it is just the upper particles that experience the effect of the slab. Most of these studies analyze only the longitudinal, down-stream component of particle displacement, and neglect any lateral movement. Lateral motion of grains will be important in studying the grain trajectory in the intermediate range and in studying the diffusion of saltating particles [19].

Although there are many studies on the problem of the sediment transport, each model works under the conditions that the authors have imposed. If we can fully describe the sediment transport mechanism, we will then be able to apply it to any problem of sediment transport, for examples about dunes on Mars.

1.3 Methodology

This thesis constitutes a numerical effort to study the sediment transport in saltation and creep. In our model, a bed of particles is simulated with the conventional event-driven molecular dynamics method. We suppose that the particles are hard disks

in a two-dimensional domain with periodic boundary conditions in the horizontal direction. The flow of the fluid over this bed of particles is modeled by imposing a force on each particle, that depends on the velocity profile of the fluid, $u_f(y) = u_* f(y)$. Here f is a function of height, y. We investigate the sediment transport for two fluid profiles, parabolic and logarithmic. The first one models laminar flow and the second corresponds to turbulent flow.

The fluid with a certain strength flows over a bed at rest. The motion of the particles is caused by aerodynamic entrainment or collisions with other particles. We follow the trajectory of the particles with time, and study the flux, and the velocity probability distribution function (PDF) of the grains in the system.

1.4 Outline

In chapter 2 we study some conventional numerical methods for handling the granular material problems. In particular we explain the event-driven molecular dynamics method in detail because we use this method in chapter 4 to study the sediment transport in our model system.

Chapter 3 reviews the basic hydrodynamics that we need in studying the sediment transport. We are not going to review the literature on the hydrodynamics for sediment transport because this is a very wide topic. We pick up the information that we need to know in sediment transport, at the onset.

Due to the lack of understanding of the details of the physical processes involved, an analytical description of the sediment transport is often inaccurate. The majority of the works on this topic were derived from field or wind tunnel experiments, or numerical simulations. Also some analytical models have been proposed. Chapter 4, reviews the previous works relevant to this study.

In Chapter 5 we explain our model in detail and compare our results with those

of the previous works.

Finally, we summarize and discuss our results in chapter 6.

Chapter 2

Simulation methods for granular matter

2.1 Introduction

As granular media are composed of many grains, keeping the discrete nature of the medium and at the same time handling the related problems with theoretical methods is impossible. One way to study this media is numerical simulations, that can model various aspects of physics of granular materials. The numerical simulations are used to solve a number of practical problems in industry such as segregation and blockage of flows by arch effect. Also numerical simulations are of considerable interest from a more fundamental point of view: They offer the possibility to explore the effect of the many parameters which are not simply accessible to experiment.

There are some numerical methods for modeling the granular medium Each simulation method has its advantages and draw-back. Here we review the Molecular Dynamics method for both soft and hard spheres, via time-driven and event driven approaches, that are best suited for modeling granular systems. Special attention will be given to the event-driven method because we use it for our simulations of sediment transport.

2.2 Molecular dynamics simulation (time driven)

Molecular dynamics simulation (MD) is one of the well-developed techniques which is based on constant time stepping procedure [20, 21]. The principle of MD method is to solve in regular incremental step the equations governing the changes in linear and angular momentum of particles. It is widely used for granular media. In this method the duration of particle collisions is not zero.

The governing equation of motion of the particle is Newton's second law:

$$\mathbf{F}_i = m_i \mathbf{a}_i = m_i \frac{d\mathbf{x}_i^2}{dt^2}, \tag{2.2.1}$$

where $\mathbf{F}_i$ denotes the force acting on particle i, and $\mathbf{x}_i$ and $\mathbf{a}_i$ are its position and acceleration vector respectively. The time is discredited in steps of δt. The Taylor expansion for the particle position is:

$$\begin{aligned} \mathbf{x}_i(t+\delta t) &= \mathbf{x}_i(t) + \delta t \mathbf{v}_i(t) + \frac{1}{2}\delta t^2 \mathbf{a}_i(t) + ... \\ \mathbf{x}_i(t-\delta t) &= \mathbf{x}_i(t) - \delta t \mathbf{v}_i(t) + \frac{1}{2}\delta t^2 \mathbf{a}_i(t) + ... \end{aligned} \tag{2.2.2}$$

then the equation for advancing the positions is:

$$\mathbf{x}_i(t+\delta t) = 2\mathbf{x}_i(t) - \mathbf{x}_i(t-\delta t) + \delta t^2 \mathbf{a}_i(t). \tag{2.2.3}$$

The velocities are not needed except for calculating the kinetic energy. Velocities are obtained from the equation below,

$$\mathbf{v}_i(t) = \frac{\mathbf{x}_i(t+\delta t) - \mathbf{x}_i(t-\delta t)}{2\delta t}. \tag{2.2.4}$$

So, by knowing the positions of all particles for two times, we can derive the future behavior of system under the influence of the forces F_i acting on each particle.

One can use higher orders in the Taylor expansion for more accuracy, but it would require larger memory. Solving the above equations requires a knowledge of

the forces, and how they vary in time and also the duration of contact time. It is important to model as exactly as possible the forces of elastic restitution and friction during collision between particles. Here are the different types of behavior we might encounter in modeling the contact forces. Consider a system that is contained of N spherical particles with diameter d_i for particle i. The particles will contact when $d_i + d_j < 2r_{ij}$, where r_{ij} is the distance between the centers of two particles i and j. Neglecting the angular momentum, the forces are:

— A force of elastic restitution that is related to the elastic energy stored during the penetration of the two particles. This force is given by

$$f_{el}^{(i)} = -k[\frac{1}{2}(d_i + d_j) - r_{ij}]n_{ij}, \tag{2.2.5}$$

where n_{ij} is the unit vector along the line connecting the centers of the particles i and j. This is simply a linear expression like the Hookes's law for a spring with stiffness k. The general form of the elastic force is nonlinear as Hertz's penetration model or de Gennes model for inhomogeneous spheres. The general nonlinear expression is

$$f_{el}^{(i)} = -k[\frac{1}{2}(d_i + d_j) - r_{ij}]^{\nu}n_{ij}, \tag{2.2.6}$$

where $\nu = \frac{3}{2}$ in the Hertz model, and $\nu = \frac{1}{2}$ in the de Gennes models.

— A friction force that plays a dissipative role. It has two components; normal and tangential. The normal component is

$$f_n^{(i)} = -2D_n m_{ij}(v_{ij} \cdot n_{ij})n_{ij}, \tag{2.2.7}$$

where m_{ij} is the reduced mass of particles i and j, v_{ij} is the difference between their velocities, and D_n is a dissipative coefficient along the direction of n_{ij}. The general nonlinear form of the above equation can be written as:

$$f_n^{(i)} = -2D_n m_{ij}(v_{ij} \cdot n_{ij})[\frac{1}{2}(d_i + d_j) - r_{ij}]^{\gamma}n_{ij}, \tag{2.2.8}$$

that is valid when $\frac{1}{2}(d_i + d_j) > r_{ij}$.

The simple linear spring-dashpot model (with $\nu = 1$ *and* $\gamma = 0$) can be solved analytically and leads to a contact duration $t_c = \frac{\pi}{\omega}$ and a restitution coefficient $r = exp(\frac{D_n}{2m_{12}})t_c$, with $\omega = \sqrt{\omega_0^2 - D_n^2}$, $\omega_0^2 = \frac{k}{m_{12}}$ [22].

The tangential component of the friction force is

$$f_t^{(i)} = -2D_t m_{ij}(v_{ij} \cdot t_{ij})t_{ij}, \tag{2.2.9}$$

where t_{ij} is a vector tangential to the contact, normal to n_{ij}, and D_t is the dissipation coefficient in tangential direction. The present model applies to a dynamic analysis of granular pile. For many application (arching, heap formation) it is important to include real Coulomb's static friction [23]. Main source of static friction in real systems is the geometrical roughness of the surfaces.

2.3 Molecular dynamics for hard spheres (event driven method)

In the event driven (ED) method, the continuous time dynamic system can be approximated by a system whose components evolve independently all the time except for discrete asynchronous instances of pairwise interaction. This method already has been used for simulating the collisions of billiard balls [24]. This method is able to reconstruct the history of each component.

In this method, the particles move independently until a collision occurs. Using the velocities just before contact we can compute the particle velocities after the contact.

Suppose that $t_0 \leq t_1 \leq t_2 \leq ...$, where t_0 is the initialization time and t_{i+1} is the nearest next collision time seen at time t_i. In the first version of this method,

the state of all N particles were updated at each t_i. As in this method after each collision all of the particles are examined and updated, the same collision is repeatedly predicted an order of N times until it occurs. Also in a typical time duration most of the particles may not participate in a collision; nonetheless in the simulation they are examined. This makes the simulation inefficient for large N. The model proposed by Lubachevsky [24] is more efficient. This model updates only those particles which were involved in the previous collision. For this purpose it is enough to save the old state and new state of particles. The old state of particle i has to be saved in memory, in order to calculate the time of the next collision of particle i with any other particles. With this method, examining and updating the state of a ball is postponed until its collision.

In ED method it is not necessary to maintain the snapshot of the states of all simulated particles at a time t and change the state of them at time $t+\delta t$, as used in time-driven simulation. Only at $time = 0$ the state of the particles are known and if particle A has a collision with particle B at $time = t$, only the states of particles A and B are changed at t, and the states of other particles don't need to be known at t, also won't be examined by the algorithm.

Before explaining the details of the ED method, we derive the general form of the velocity of the two spheres after a collision, because in the ED method the evolution of the system is governed by collisions between particles. The following description of the collisions is based on the work by Foerster *et al.* [25].

2.3.1 Collision between two grains

For given velocities before contact, we need three coefficients to calculate the velocities after the collision. The first coefficient is the normal restitution coefficient, r, which defines the incomplete restitution of the normal component of the relative