Integral Representation for Continuous Matter Fields in Granular Dynamics

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Abstract We introduce a mathematical formalism towards the construction of a continuum-field theory for particulate fluids and solids. We briefly outline a research program aimed at unifying the fundamentals of the coarse-graining theory and the numerical method of Smoothed Particle Hydrodynamics (SPH). We show that the coarse-graining functions must satisfy well defined mathematical properties that comply with those of the SPH kernel integral representation of continuous fields. Given the appropriate dynamics for the macroscopic response, the present formalism is able to describe both the solid and fluid-like behaviour of granular materials.

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1 Introduction

Continuum mechanics in its simplest form has been the paragon of field theory to describe the response of solid bodies and fluids. The mathematical robustness of continuum theories rests on the field of partial differential equations (PDEs), which is one of the main and mature cores of mathematical physics. These mathematical models rationalize, explain, and predict very well the macroscopic behaviour of isotropic and homogeneous solid bodies. However, there is still no general continuum model for the description of discrete microscopic, mesoscopic, and nanoscale systems. For example, granular materials are composed of large collections of small grains and exhibit many interesting collective phenomena emerging from the many-body classical dynamics of their constituents (Jaeger et al. 1996). This kind of materials can exhibit solid-like as well as fluid-like behaviours. Nevertheless, a complete theoretical description of granular materials as well as particulate amorphous and heterogeneous solids is still missing (Jaeger et al. 1996; Kadanoff 1999; de Gennes 1999; Goldhirsch 2003). An analytical framework is required to bridge the gap between the experimental and theoretical studies in this area, and develop numerical algorithms for new and more efficient simulation techniques.

The study of continuum concepts and field values related to local (scale-dependent) space-time averages began in 1946 with the celebrated statistical mechanical theory of transport processes by Kirkwood (1946) and Irving and Kirkwood (1950). They assumed that any ensemble average of space-time averages could be equated with a space-time average of an ensemble average computed at given scales of length and time. This approach represents an alternative to the Gibbs measure (Murdoch and Bedeaux 1994; Babic 1997) (associated with the Boltzmann distribution and the notion of canonical ensemble in equilibrium statistical thermodynamics, connecting measurable macroscopic properties of materials to the properties of their constituent particles and the interactions between them).[1] Another interesting development was reported by Glasser and Goldhirsch (2001), who based on the ideas worked out in Kirkwood (1946); Irving and Kirkwood (1950) and Murdoch and Bedeaux (1994), constructed a field theory for granular fluids.

The purpose of this paper is to present a further step towards the construction of a macroscopic continuous-field mathematical description of granular materials that fulfils the condition of reproducing microscopic properties in a macroscopic representation of physical quantities. We address the problem of the estimation of coarse-graining functions and show that they must satisfy well-defined mathematical conditions for the requirement of compact support of the smoothing function.

[1] For granular systems this approach seems doomed from the outset: because energy is lost through internal friction, and gained by a non-thermal source such as tapping or shearing, the dynamical equations do not leave the canonical or any other known ensemble invariant.

2 Starting Definitions and Postulates of the Theory

2.1 Domains and Observables

Consider a physical system whose properties may vary in time and space. Denoting by $\mathbb{R}^3$ the three-dimensional coordinate space (and by $\mathbf{r}$ its elements), we shall then simply denote by $\mathbb{R}^4$ the four-dimensional space-time vector field whose elements $\mathbf{R}$ have three spatial coordinates and a time-coordinate t:

$$\mathbf{R} = (\mathbf{r}, t) \in \mathbb{R}^4. \tag{1}$$

This space is the stage on which our theory is developed, so herein we will refer to such a space as the *physical domain*:

Definition 1 *(**Physical domain**). The* physical domain Ω *of any problem is the set of all points in* $\mathbb{R}^4$.

In a discrete solid, for instance, the physical domain consists of all points occupied by the grains of the solid as well as the empty spaces (pores) inside the material.

Following Murdoch and Bedeaux (1994), we introduce the next definition:

Definition 2 *(**Material system**). A material system* $\mathscr{M} \subseteq \Omega$ *is an instant-by-instant identifiable set of fundamental discrete entities.*

In other words, a material system is a set of fundamental disjoint sets in space that belongs to the geometrical locus of the material to be described (atoms, ions, molecules, pores, etc). In our problem of granular materials, such discrete entities are modelled as interacting particles (grains), indexed by $\{i\}$. Since a granular material is a large system of grains with macroscopic sizes ($> 1\,\mu$m), we have for such materials that $\mathscr{M} \subset \Omega$. In the case of a continuous solid or fluid, there will be a unique identifiable discrete entity, for which we have $\mathscr{M} = \Omega$.

Definition 3 *(**Observable**). An observable is any real square-integrable function defined over the entire physical domain or a subset of it:*[2]

$$\begin{aligned} &f : \mathscr{D} \subseteq \Omega \to \mathbb{R}, \\ &f \in L^2[\mathscr{D}]. \end{aligned} \tag{2}$$

Definition 4 *(**Microscopic field**). Any function* ψ *is a microscopic field if it is an observable defined only in the material system, i. e.:*

[2] *Remark* 1 In general, an n-rank tensor function $G : \mathscr{D} \to \mathbb{R}^4 \otimes^{[n]} \mathbb{R}^4$ (where $\otimes^{[n]}$ denotes the n-rank tensor product) is not an observable. Nevertheless, each component of the tensor is an observable. Typical examples are the components of the stress tensor ($\sigma^{\alpha\beta}$, where Greek indices denote Cartesian coordinates), or the components of the velocity field (v^{α}).

$$\begin{array}{l} \psi : \mathscr{M} \to \mathbb{R}, \\ \psi \in L^2[\mathscr{M}]. \end{array} \quad (\mathscr{M} \subseteq \Omega) \tag{3}$$

Definition 5 ***(Macroscopic field)****. Any function $\tilde{\psi}$ is a macroscopic field if it is an observable defined over the entire physical domain, i. e.:*

$$\begin{array}{l} \tilde{\psi} : \Omega \to \mathbb{R}, \\ \psi \in L^2[\Omega]. \end{array} \tag{4}$$

We may characterize a granular material with the set of fundamental microscopic fields: $\{m_i\ ;\ \rho_i\ ;\ r_{\alpha_i}(t)\}$, which denote the mass, the density, and the α-component of the centre-of-mass position of the ith grain at time t, respectively. Obviously, in such a fundamental set, there are as many components of the centre-of-mass positions as spatial dimensions of the physical domain (which, for the sake of generality, we have taken as three-dimensional).

2.2 Principles

Consider the problem of building a *macroscopic field* $\tilde{\psi} : \Omega \to \mathbb{R}$ from a microscopic one $\psi(\mathbf{r}_i, t)$ (with $i = 1, 2, \ldots, N$; where N is the total number of grains). This has to be done in such a way that the microscopic information of the material is accurately represented in the macroscopic field. This problem can be formally stated as:

$$\mathscr{L}\tilde{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t), \tag{5}$$

where $\mathscr{L} : L^2[\Omega] \to L^2[\mathscr{M}]$ is some operator that when applied to a macroscopic field, returns the microscopic field. Thus, the sources of the macroscopic field $\tilde{\psi}(\mathbf{R})$ are the values of the microscopic field $\psi(\mathbf{R})$ evaluated in each grain.

Postulate 1 *(Linearity) The problem* (5) *satisfies the superposition principle.*

The above postulate allows us to write the output of Eq. (5) (the macroscopic field) as a linear functional of the input (the microscopic field), i. e.:

$$\tilde{\psi}(\mathbf{R}) = \int_{\mathscr{M}} \Phi(\mathbf{R}, \mathbf{R}')\psi(\mathbf{R}')d\mathbf{R}', \tag{6}$$

where Φ must belong to $L^2[\Omega]$.

Postulate 2 *(Space-time translation invariance) The problem* (5) *is space-time translation invariant.*

So, if the input (the microscopic field) is shifted along some displacement vector $\mathbf{D} = (\Delta\mathbf{r}, \Delta t)$ in $\mathscr{M}$, the output (macroscopic field) is also shifted in the same

manner: if $\tilde{\psi}(\mathbf{R})$ corresponds to $\psi(\mathbf{R})$, then $\tilde{\psi}(\mathbf{R}+\mathbf{D})$ corresponds to $\psi(\mathbf{R}+\mathbf{D})$. This can only be possible if the function Φ in Eq. (6) depends on the difference $\mathbf{R}-\mathbf{R}'$ of its arguments: $\Phi(\mathbf{R},\mathbf{R}') = \Phi(\mathbf{R}-\mathbf{R}')$. Then, Eq. (6) turns into the convolution product:

$$\tilde{\psi}(\mathbf{R}) = \int_{\mathscr{M}} \Phi(\mathbf{R}-\mathbf{R}')\psi(\mathbf{R}')d\mathbf{R}' = (\Phi \times \psi)_{(\mathbf{R})}. \tag{7}$$

Setting $\Phi(\mathbf{R}) = \Phi(\mathbf{r},t) \equiv \phi(\mathbf{r})F(t)$, where $F(t)$ and $\phi(\mathbf{r})$ are the temporal and spatial parts of Φ, respectively, Eq. (7) becomes:

$$\tilde{\psi}(\mathbf{r},t) = \int_{T} dt' F(t-t') \int_{\mathscr{M}_s} d\mathbf{r}'\phi(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}',t), \tag{8}$$

where $T \subset \Omega$ is the time subspace of $\mathscr{M}$ and $\mathscr{M}_s \subseteq \mathbb{R}^3$ is the spatial subspace of $\mathscr{M}$:

$$\begin{aligned} &\mathscr{M}_s = \{\mathbf{r} \in \mathbb{R}^3 : (\mathbf{r},t) \in \mathscr{M}\}, \\ &\qquad\qquad\qquad\qquad (\mathscr{M}_s \otimes T = \mathscr{M}) \\ &T = \{t \in \mathbb{R} : (\mathbf{r},t) \in \mathscr{M}\}. \end{aligned} \tag{9}$$

We see that the solution of problem (5) is given by Eq. (8), where $\phi : \mathscr{V} \to \mathbb{R}$ and $F : \mathscr{T} \to \mathbb{R}$ are the *spatial and temporal parts of the Green's function* Φ associated to the operator $\mathscr{L}$, respectively, with $\mathscr{V}$ and $\mathscr{T}$ being the spaces of all possible displacements in the Euclidean spaces $\mathbb{R}^3$ and $\mathbb{R}$, respectively. We see that ϕ has dimensions of the inverse of volume and F of the inverse of time. For a granular material, $\mathscr{M}_s$ is a disconnected subset of $\mathbb{R}^3$, and so the integral over $\mathscr{M}_s$ in Eq. (8) is, in fact, a discrete sum. Since the infinitesimal volume elements of size $d\mathbf{r}'$ in Eq. (8) lies in $\mathscr{M}_s$, such a sum must be taken over the small volumes ΔV_i of each disconnected set (i.e. over the volume of each particle). Setting $\Delta V_i = m_i/\rho_i$, Eq. (8) can be written as:

$$\tilde{\psi}(\mathbf{r},t) = \int_{T} dt' F(t-t') \sum_{i=1}^{N} \frac{m_i}{\rho_i}\psi(\mathbf{r}_i,t)\phi(\mathbf{r}-\mathbf{r}_i). \tag{10}$$

For static granular systems (granular packings in which the grains remain static but the fields could still vary in time), we have that $F(t-t') = \delta(t-t')$ and Eq. (10) becomes the weighted average sum:

$$\tilde{\psi}(\mathbf{r},t) = \sum_{i=1}^{N} \frac{m_i}{\rho_i}\psi(\mathbf{r}_i,t)\phi(\mathbf{r}-\mathbf{r}_i). \tag{11}$$

Postulates 1 and 2 has led us to a formulation via weighted-average sums of the same kind as those introduced heuristically by Irving and Kirkwood (1950); Murdoch

and Bedeaux (1994); Babic (1997) and Glasser and Goldhirsch (2001), referring to the Green's function Φ either as the *coarse-graining function*, the *probability density function*, or simply as the *weighting function*. The continuous representation of fields like the density, velocity, and stress tensor field components obtained using Eq. (11) are, indeed, identical to those obtained by Murdoch and Kowalski (1992); Babic (1997) and Glasser and Goldhirsch (2001). For instance, for the mass density we have from Eq. (10) that:

$$\tilde{\rho}(\mathbf{r}, t) = \int_T dt' F(t - t') \sum_{i=1}^{N} m_i \phi(\mathbf{r} - \mathbf{r}_i), \tag{12}$$

which is the well-known *coarse-grained mass density formula* (Babic 1997; Glasser and Goldhirsch 2001).

3 Properties of the Spatial Green's Function

The solution of problem (5) is then given by Eq. (8). The next step is to find the Green's function. Since we do not know in advance the exact form of the operator $\mathscr{L}$, we require an alternative method to the conventional one using delta-type sources for calculating the Green's function. This is exactly the same kind of mathematical problem that was solved by Lucy (1977) and Gingold and Monaghan (1977) when they developed the method of *Smoothed Particle Hydrodynamics* (SPH) for the discretization of PDEs. Here, we postulate that *one can use the method employed for constructing SPH smoothing functions to calculate the spatial Green's function*.

A kernel interpolant, as in Eq. (8), with $F(t - t') = \delta(t - t')$ is also used in SPH (called *smoothed* or *integral representation*) and the domain of the PDE is discretized using a particle generator, leading to a sum over particles of masses m_i and densities ρ_i identical to Eq. (11). This defines a Lagrangian mesh-free, semi-discrete version of the PDE (Monaghan 1992; Liu and Liu 2003, 2010; Li and Liu 2007). For the integral macroscopic representation $\tilde{\psi}$ in Eq. (8) to be consistent with the microscopic field ψ, the kernel ϕ must satisfy some well established mathematical conditions. In establishing such properties, one needs to consider some additional information about the macroscopic behaviour of the system (this is due to the lack of information about the exact form of the operator $\mathscr{L}$). For granular flows, we require the system to satisfy macroscopically the equations of granular hydrodynamics derived in Glasser and Goldhirsch (2001). Assuming that the macroscopic behaviour of the system is described by a second-order PDE (as is the case for granular hydrodynamics), Liu et al. (2003) demonstrated that the integral representation will have a consistency of order n if the kernel ϕ fulfils the following conditions:

$$\begin{cases} \phi(\mathbf{r}-\mathbf{r}')\big|_{\partial\mathbb{S}(\mathbf{r})} = 0, \\ \phi'(\mathbf{r}-\mathbf{r}')\big|_{\partial\mathbb{S}(\mathbf{r})} = 0, \\ M_i = \delta_{i0} \quad i = 0, 1, 2, \ldots, n\ , \end{cases} \tag{13}$$

where:

$$M_i \equiv \int_{\mathbb{S}(\mathbf{r})} \left(\mathbf{r}-\mathbf{r}'\right)^i \phi\left(\mathbf{r}-\mathbf{r}'\right) d\mathbf{r}', \tag{14}$$

is the ith momentum of the kernel, and $\mathbb{S}(\mathbf{r})$ is a *support domain of the point* $\mathbf{r}$, a subset of $\mathscr{M}_s$ outside of which the kernel's value is zero. The first and second of Eqs. (13) are referred to as the *compactness condition* for the kernel and its first derivative. Without such conditions, much more conditions would be needed over ϕ to guarantee consistency between the discrete and the continuous description, as was shown explicitly in Liu et al. (2003) and Liu and Liu (2006). The domain of the spatial Green's function is no longer the space of all possible displacements in Euclidean space (as was stated in Sect. 2.2), but rather the space of those displacements such that the argument of ϕ lies within the support domain $\mathbb{S}(\mathbf{r})$. When this support domain is spherically symmetric, its radius is called the *smoothing length* or *spatial resolution* in the SPH literature. We note that by considering this compactness property of the Green's function in the sum (11), only those particles that are within the support domain of the point $\mathbf{r}$ makes a contribution to the value of the macroscopic field. We also note that the kernel's momentum equation for $i = 0$ imposes a normalization condition over ϕ, while for $i = 1$ it establishes a parity condition. Note that all these properties were imposed heuristically over the spatial coarse-graining function by Glasser and Goldhirsch (2001), while here we have given a formal justification of them.

4 Conclusions

In this paper, we have given, by means of physical and mathematical arguments, a formal justification of the description of discrete complex systems using weighted average sums. This leads to a unification of the various formulations that have been separately treated so far, namely the *weighted average sums* introduced by Irving and Kirkwood (1950), the *coarse-graining* representation by Glasser and Goldhirsch (2001), and the *SPH integral representation* by Lucy (1977) and Gingold and Monaghan (1977). With this formulation we can guarantee that the macroscopic fields are consistent with the microscopic properties of the material, satisfying the equations of granular hydrodynamics in its macroscopic description up to a certain order n in its Taylor's series expansion around any point in the material system $\mathscr{M}$. The method developed by Liu et al. (2003) and Liu and Liu (2006) becomes one for the estimation of the spatial Green's function of the unknown operator $\mathscr{L}$. Using this method for the calculation of such kernels, we can assure that (8) interpolates the microscopic (discrete) field ψ. We propose that, given the appropriate macroscopic

dynamics, this representation can be used to successfully model both the liquid and the solid phase of a granular material. This is tightly connected to the fact that the SPH method is able to model the dynamics of fluids and elastic solids the same way (Gray et al. 2001).

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