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rete particles to continuum fields: Coarse-Graining
An accurate micro-macro mapping technique

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ABSTRACT Micro-macro transition methods can be used to, both, calibrate and validate continuum models from discrete data obtained via experiments or simulations. These methods generate continuum fields such as density, momentum, stress, etc., from discrete data, i.e. positions, velocity, orientations and forces of individual elements. Here, we present a brief overview of an existing micro-macro mapping technique called coarse-graining, which we have been developing since the past 7 years.

By construction, coarse-graining gives us macroscopic fields that are consistent with the continuum equations of mass, momentum, and energy balance. Additionally, boundary interaction forces are taken into account in a self-consistent way and thus allowing for the construction of continuous stress fields even within one element radius of the boundaries. Similarly, stress and drag forces can also be determined for individual constituents of a multi-component mixture, which is critical for several continuum applications, e.g. mixture theory based segregation models. Moreover, the method does not require ensemble-averaging and thus can be efficiently exploited to investigate static, steady, and time-dependent systems.

1. Introduction

Particulate media or granular materials are omnipresent, both, in nature and industry, where common examples range from planetary motion, landslides and avalanches to steel manufacturing and food processing. Due to a variety of factors such as varying size, shape, density, inelasticity and more, granular mixtures exhibit highly complex phenomena.

To understand these behaviours, besides experiments, discrete particle simulations have proved to be a very powerful computational tool that allow for the simulation of individual particles with complex interactions, arbitrary shapes, in arbitrary geometries, by solving Newton's laws of motion for each particle; however, it is computationally very expensive. Although, recent computational advances can easily simulate a few million particles; it is still a challenging task to simulate real-life scenarios found in nature and industry.

Continuum methods, on the other hand, are able to simulate the volume of real environmental and industrial flows, but need simplifying assumptions that often require effective macroscopic material parameters, closure relations or constitutive laws, etc. In order to correctly apply these continuum models, both the continuum assumptions must be validated and the effective material parameters must be determined for a given application; e.g., the Savage-Hutter model [1] for granular geophysical mass flows requires the effective basal friction for closure [2]. Therefore, in order to formulate accurate continuum models, one needs to accurately construct the macroscopic (averaged) fields from the available microscopic particle dynamics, e.g. particle position, velocity, stresses and more.

2. Micro-Macro mapping via coarse-graining

Mapping of particle data, i.e. microscopic scale dynamics, onto a macroscopic continuum scale has
been under focus since the classical studies by Irving and Kirkwood [3] and others [4,5]. Based on a variety of theoretical postulates, various methods for local averaging have been formulated to extract these macroscopic quantities efficiently, e.g., binning of the microscopic fields into small volumes [6] and method of planes [7]. However, most of them are restricted in terms of their application due to limitations, see [6] and the reference therein. One of the challenges or requirements for multi-scale methods is to efficiently map the microscopic particle dynamics onto a macroscopic field which in turn satisfy the classical equations of continuum mechanics i.e. the fundamental balance law of mass and momentum

\[ \frac{D (\rho)}{D t} + \rho \nabla \cdot \mathbf{u} = 0, \]
\[ \frac{D (\rho \mathbf{u})}{D t} + \rho \mathbf{u} \nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g}. \]

The \( D (\cdot) \) in the above equations denotes the material derivative and are stated in terms of the macroscopic quantities: mass density \( \rho(x, t) \), bulk velocity \( \mathbf{u}(x, t) \) and stress tensor \( \mathbf{\sigma}(x, t) \), where \( x \) and \( t \) denotes the spatial and temporal coordinate, respectively.

Coarse-graining (CG) approaches to granular materials first appeared in the work of Weber [8] and since then has been extended by several other studies listed in [9,10]. However, an exact and general coarse-graining formulation was first presented by Goldhirsch [10]. When compared with other simpler methods of performing the micro-macro transitions, the coarse-graining method has the following advantages: (i) the resulting macroscopic fields exactly satisfy the equations of continuum mechanics, (ii) the elements are neither assumed to be spherical or rigid, (iii) the resulting fields are even valid for a single element and a single time step, hence no ensemble-averaging is required, i.e. no averaging over several time steps or stamps. However, the coarse-graining method does assume that (i) each pair of elements has a single contact; i.e. elements are assumed to be convex in shape; (ii) the contact area can be replaced by a single contact point, implying that the overlaps are not too large; (iii) the collisions are enduring (i.e. not instantaneous). Often, micro-macro methods employ ensemble- or bulk-averaging to obtain accurate results; therefore, the methods are only valid for homogeneous, steady situations. The coarse-graining method overcomes these challenges by applying a local smoothing kernel, coarse-graining function, with a well-defined smoothing length, i.e. coarse-graining scale, that automatically generates fields satisfying the continuum equations. As an example, one could consider a Gaussian distribution function as a coarse-graining function with its standard deviation as a coarse-graining scale.

The coarse-graining formulation of Goldhirsch [10] was further extended to account for external boundaries, see Weinhart et al. [11]. This extension is vital as other mapping techniques lack consistency and are highly inefficient near the boundaries. Given this, the technique is further extended to account for polydisperse mixtures [15,16], where one can easily construct partial macroscopic quantities such as partial density, velocity, stresses corresponding to different species types. Moreover, through this extension, one can now efficiently compute the inter-particle drag forces, which are very important in understanding various granular phenomena. For more details, see Tunuguntla et al [15].

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1 Polydisperse mixture implies a granular mixture comprising different types of constituents. For example, a bidisperse mixture varying in size means a mixture comprising two types of constituents varying in size alone.
Fig. 1: A snapshot of a bidisperse mixture flowing in a periodic box inclined at 26 degrees to the horizontal (discrete particle simulation). Colours/shades indicate the base/boundary (yellowish green, \( P^b \)), species type-1 and type-2 (blue, \( P^1 \) and red, \( P^2 \)). We define the bulk as \( F^1 \cup F^2 \). Figure adapted from Tunuguntla et al. [15].

a) Idea behind coarse-graining

To illustrate the idea, let us consider a bidisperse mixture flowing over a rough inclined channel as shown in Fig. 1. From statistical mechanics, the partial microscopic (point) mass density for a system at the point \( x \) and time \( t \), is given as

\[
\rho^{\text{mic},v}(x, t) = \sum_{i \in F^v} m_i \delta(x - x_i(t)) \quad \text{with } v = 1, 2,
\]

where \( i \) denotes the particle index in a set of type-1 or type-2 constituent, \( x_i \) denote the particles’ centre of mass and \( \delta(x) \) is the Dirac delta function in \( \mathbb{R}^3 \). This definition complies with the basic requirement that the integral of the mass density over a volume in space equals the mass of all the particles in this volume. To extract the partial macroscopic mass density field, \( \rho^v(x, t) \), the partial microscopic mass density \( \rho^{\text{mic},v}(x, t) \) is convoluted with a spatial coarse-graining function \( \psi(x) \), e.g. uniform distributions, Gaussian distributions or a family of Lucy polynomials [28]. Thus, leading to

\[
\rho^v(x, t) := \int_{\mathbb{R}^3} \rho^{\text{mic},v}(x, t) \psi(x - x') dx',
\]

\[
:= \sum_{i \in F^v} m_i \psi(x - x_i(t)) = \sum_{i \in F^v} m_i \psi_i.
\]

The result is equivalent to replacing the delta-function with a spatial coarse-graining function (that is positive semi-definite, integrable, and has finite support), \( \psi(x) \). For simplicity, seen later, we define \( \psi_i \) as \( \psi_i = \psi(x - x_i(t)) \). For more details regarding the types of coarse-graining function and the choice of spatial and temporal coarse-graining scale please see Tunuguntla et al. [15].

b) Coarse-graining expressions

Using the same idea as explained above, expressions for the partial macroscopic quantities such as density, momentum, velocity and stresses are stated below

| Density          | \( \rho^v(x, t) := \sum_{i \in F^v} m_i \psi_i \) | Total Stress                        | \( \sigma^v(x, t) = \sigma^{\text{kin},v}(x, t) + \sigma^{\text{con},v}(x, t) \) |
where in the kinetic stress expression, \( \mathbf{u}'_i \) is the fluctuation velocity of particle \( i \), defined as \( \mathbf{u}'_i(x_t, t) = \mathbf{u}(x, t) - \mathbf{u}(t) \). Furthermore, in the partial contact stress expression, \( \mathbf{b}_{ij} \) is the branch vector\(^2\). \( \psi_{ij} \) denotes a line integral along the branch vector \( \mathbf{b}_{ij} \), \( \psi_{ij} = \int \psi(x - x_i + s \mathbf{b}_{ij}) ds \), which ensures the distribution of the force, \( f_{ij} \), between two constituents \( i \) and \( j \) to the partial stresses. The partial stresses are proportional to the length of the branch vectors. In other words, the stresses are distributed proportionally, based on the fraction of the branch vectors contained within each constituent. Thus, for contacts between a small and a large constituent, the larger-sized constituent receives a larger share of the stress. Moreover, the first term in the contact stress expression corresponds to the stresses originating due to contact between the same constituent type (e.g. small-small) whereas the second term corresponds to the stresses originating due to contact between two different constituent types (e.g. small-large). More importantly, all the above partial quantities are derived such that both the partial mass and momentum balance laws are exactly satisfied. For more details, see [15,16]. From the above expressions for the partial macroscopic quantities, the bulk macroscopic quantities are constructed as below,

\[
\begin{align*}
\rho(x, t) &:= \sum_{\nu} \rho^\nu(x, t), \\
P(x, t) &:= \sum_{\nu} P^\nu(x, t), \\
\mathbf{u}(x, t) &= \frac{P(x, t)}{\rho(x, t)}, \\
\sigma(x, t) &= \sum_{\nu} \sigma^{\mathrm{Kin,} \nu}(x, t) + \sigma^{\mathrm{Con,} \nu}(x, t).
\end{align*}
\]

Note again, the bulk macroscopic quantities also fundamentally satisfy the bulk mass and momentum balance laws, which is an invaluable asset of this technique.

### 3. Analysis or post-processing with coarse-graining

Given the above expressions, the coarse-graining approach has been utilised to analyse several simulations or experiments, e.g. 2D granular systems [18-21] and flows in hopper geometry [22,23], where the results have been characterised in terms of density, velocity, stress, strain, couple-stress and other fields. Given the numerous advantages of CG, the above CG expressions have been implemented in our in-house statistical toolbox called \textit{MercuryCG}. This tool is part of our robust software package called \textit{MercuryDPM}, which is also our in-house open-source discrete particle solver. \textit{MercuryCG} can be run either as a post-processing step, or live during the simulation. Where

\(^2\) Branch vector is defined as a vector pointing from the particle centre to contact point, see Fig. 2 in Tunuguntla et al. [15].
traditional techniques cannot accurately produce continuum fields near the edges of a system, *MercuryCG* uses advanced mathematics to allow continuum information to be extracted from microscopic data even within one particle diameter of a boundary [11,24]. Moreover, the CG technique is applicable valid for both static and dynamics situations, see Tunuguntla et al. [15] for intricate details regarding coarse-graining of unsteady granular systems.

Several studies have utilised *MercuryCG* to investigate granular systems, where applications include analysis of flows through silos [27] and mixture flows over inclined channels, with special focus on shallow flows [2,13] and segregation phenomenon in bidisperse granular mixtures [12,15,16,26]. As an example, an exemplary output of our statistics package is shown for a jet of particles impacting a rough inclined plane in Fig. 2. In order to obtain the height of the flow we assume that the density of the flow is constant over height, and that the flow is steady and uniform enough to have a lithostatic stress profile. Thus, the height can be defined using the depth-averaged stress and density, as plotted in Fig. 3. Once the height is known, a depth-averaged velocity and the Froude number can be defined. A Froude number larger than unity denotes supercritical flow; otherwise the flow is subcritical. This allows us to determine the location of the shock (black line in right panel of Fig. 3).

![Fig. 2](image1.png)  
**Fig. 2:** Top left shows the flow in the hopper, bottom left the impact region, middle schematic of the original experiment, right the top view of the full particle simulation (~500k particles). Black particles indicate fixed particles; all other colours indicate speed, with blue low and red high speed.

![Fig. 3](image2.png)  
**Fig. 3:** Coarse grained macroscopic fields created using *MercuryDPM*’s our own statistics toolbox, *MercuryCG*. Left shows the height of the flow in millimetres and right the local Froude number of the flow. The white lines indicate velocity streamlines; the black line indicates the location of a hydraulic jump/shock

4. Interested in *MercuryCG* or *MercuryDPM*?
Hopefully, by now you are interested in trying out MercuryCG for yourself. If you would like more information about the MercuryCG and its parent code MercuryDPM, it can be found at MercuryDPM.org. Alternatively, you can also subscribe to our mailing list. To do so, simply send an email to listserv@lists.utwente.nl with subject: subscribe and body: MERCURYDPM-USER <your full name>. This is a low volume mailing list and typically you will receive no more than one e-mail a month. The code itself is available through a public svn repository and details of how to obtain and install it can be found on the website, MercuryDPM.org. Once downloaded and installed, instructions to use MercuryCG are presented in Tunuguntla et al. [15].

Open-Source: MercuryDPM was originally started as a research code at the University of Twente, to meet a local need for a tool that was not available in any existing simulation codes. Since then it has grown and gained many external users in academia, research and industry. Therefore, we decided to make it freely available to both industry and academia via an open-source release (using the BSD license).

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5. References