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Brief communication

Filter width and uncertainty estimation in continuum modeling of particle phases

Julian A. Simeonov *, Samuel Bateman, Joseph Calantoni

Marine Geosciences Division, Naval Research Laboratory, Stennis Space Center, MS 39529, United States

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Continuum models for two-phase and granular flows have been derived from the microscopic equations of motion using either volume averaging (Anderson and Jackson, 1967; Drew, 1971; Whitaker, 1973; Elghobashi and Abou-Arab, 1983) or ensemble averaging (Batchelor, 1976; Reeks, 1992; Zhang and Prosperetti, 1994; Lun et al., 1984) to obtain the macroscopic fields. The general form of the multiphase momentum equations (Drew, 1971; Whitaker, 1973) contain stress terms that require detailed knowledge of the physics of the microscale interactions of the phases. For particle suspensions, progress is usually made by assuming linearized relationships between the hydrodynamic force and the local flow based on viscous (Anderson and Jackson, 1967; Batchelor, 1976; Reeks, 1992) or inviscid (Zhang and Prosperetti, 1994) theory. Alternatively, closures for the stress terms have been postulated using gradient transport relationships (e.g. Elghobashi and Abou-Arab, 1983). In granular flow, model closures have been obtained for rapid dilute granular flows (Lun et al., 1984) where the interactions are predominantly collisional and frictional effects or enduring contact is negligible. The theoretical studies have described the conditions under which the volume averaging procedure would produce smooth well-behaved continuum fields, but provide little detail beyond the general requirement that the averaging length scale, L, is much larger than the particle diameter, D (e.g. Whitaker, 1973; Jackson, 1997).

Discrete particle simulations where the microscale interactions are fully resolved provide an attractive tool for investigating the bulk rheological properties of particle-laden and granular flows as a function of the particle volumetric concentration, ϕ. Such fully resolved simulations are now possible as a result of recent advances in Cartesian grid moving boundary numerical methods that track the inter-phase Lagrangian boundaries and model the effect of the no-slip boundary condition by adding terms to the equations of motion. For example, in the immersed boundary method (Peskin, 2003), the solid boundary is replaced by a deformable boundary that exerts a frictional force on the surrounding fluid. In the distributed Lagrange multiplier method (Glowinski et al., 1999) and the Lagrangian tensorial penalty method (Vincent et al., 2014), a fictitious stress is added to maintain the fictitious fluid inside particles in solid body rotation. In the PHYSALIS method (e.g. Zhang and Prosperetti, 2005), the numerical solution in the vicinity of particles is corrected by an analytical solution of the Stokes equations. Finally, in the pressure boundary integral method (Simeonov and Calantoni, 2011), the pressure field of hydrodynamically interacting particles is computed from a discontinuous extension of the pressure Poisson equation inside particles that relates the pressure gradient jump condition (essentially a single layer potential) to the pressure Neumann boundary condition on the particle surface. The numerical advances have recently made possible fully resolved hydrodynamic simulations of various practical problems such as the interaction of particles with turbulence (Apte et al., 2009), sediment entrainment in turbulent channel flow (Ji et al., 2013), concentration waves in fluidized beds (Derksen and Sundaresan, 2007) and turbulent particle-laden flow in a vertical channel (Uhlmann, 2008).

Despite significant progress, fully resolved simulations of particle-laden flow remain computationally expensive and are still

* Corresponding author.
E-mail address: julian.simeonov@nrlssc.navy.mil (J.A. Simeonov).

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limited to relatively small domains and $O(1000)$ particles. The question then arises as to what is the minimum acceptable averaging length scale necessary to derive valid continuum model statistics from particle-laden flow simulations. In comparison, much larger systems with $O(100000)$ particles are now typical in DEM simulations of granular flow (Silbert et al., 2001; Jop et al., 2006). However, certain granular flows with convection patterns (e.g. Forterre and Pouliquen, 2001; Börzsönyi and Ecke, 2006) and particle-laden flow with large particles lack a well-defined separation between macroscopic flows and grain-size motions. Thus, a minimum averaging scale is essential to ensure that important macroscopic behavior of complex flows is not being filtered by the averaging process.

Here we will discuss practical considerations regarding the choice of a volume averaging scale and the relationship of this scale to the uncertainty of the filtered continuum fields. We limit our discussion to the microscopic binary volume fraction field,

$$\phi(\mathbf{r}) = \lim_{\delta V \to 0} \frac{\delta V_s(\mathbf{r})}{\delta V(\mathbf{r})}, \tag{1}$$

where δV_s is the volume of the solid phase in the elementary volume δV. The corresponding continuous macroscopic (volume averaged) volume fraction field is given by

$$\phi_L(\mathbf{r}) = \frac{1}{L^3}\int_{-L/2}^{L/2} \phi(\mathbf{r}')d^3r', \tag{2}$$

where L varies as the length of the side of cubes used for volume averaging to approximate the continuum field variable of the particle phase.

Deriving empirical continuum models from particle resolving simulations requires sufficiently smooth spatial variation of the volume averaged fields. Here, the spatial noisiness of the macroscopic volume fraction field, ϕ_L, will be quantified using its variance, σ_L^2, over a macroscopically homogeneous sample that consists of a collection of N averaging cubes centered at $\mathbf{r}_j$ $(j = 1, N)$,

$$\sigma_L^2 = \frac{1}{N}\sum_{j=1}^{N}\left(\phi_L(\mathbf{r}_j) - \overline{\phi}_L\right)^2, \tag{3}$$

where $\overline{\phi}_L$, the averaged macroscopic volume fraction over the entire sample, is given by

$$\overline{\phi}_L = \frac{1}{N}\sum_{j=1}^{N}\phi_L(\mathbf{r}_j). \tag{4}$$

By dividing the standard deviation by the mean we obtain a non-dimensional noise metric, $v = \sigma_L/\overline{\phi}_L$, which is essentially an inverse signal-to-noise ratio. We note that the noisiness of the volume averaged field is controlled by two factors, namely, the ratio of the averaging scale, L, to the particle diameter, D, and the mean volumetric concentration, $\overline{\phi}$. As the averaging scale becomes comparable to D, the integral in (2) will be less effective in smoothing the variation of the binary volume fraction field. Choosing an averaging scale larger than the particle size may still not be sufficient for smooth variability at low volume fractions when there are few particles inside the averaging volume. Thus, for a specified noise tolerance, v, the averaging scale will be expected to increase inversely with the concentration. In summary, the goal of this letter is to investigate the functional dependence of L on the specified noise tolerance, v, and the given sample volume fraction.

Using the Discrete Element Method (e.g. Cundall and Strack, 1979), we produced a macroscopically homogenous cubic sample with 1,844,818 identical spherical particles each having diameter, $D = 1$ mm and the density of quartz, 2.65 g/cm^3. The simulations were performed with LIGGGHTS (Kloss et al., 2012) using a Hertzian–Mindlin–Coulomb contact law with Young's modulus of 70 GPa, Poisson ratio of 0.08, coefficient of restitution of 0.2, and coefficient of friction of 0.5. LIGGGHTS is based on the molecular dynamics solver LAMMPS (http://lammps.sandia.gov, Plimpton, 1995) which includes granular packages that solve the linear and angular momentum equations for the motion of Lagrangian particles. Except for the coefficient of restitution, the above contact parameters correspond to the material properties of quartz. We used a reduced coefficient of restitution to speed up the kinetic energy dissipation and the packing of the particles. We show below that the coefficient of restitution does not have a significant effect on the noise statistics.

Initially non-overlapping particles with random coordinates were settled under gravity for a period of 0.5 s in a 350 D tall container with a 100 D square hard-bottom base using periodic boundary conditions in the horizontal. The hard bottom consisted of slightly overlapping fixed particles having a random vertical displacement with a maximum value of 0.5 D. The density of the initial random loose packing produced by the settling was increased by vibrating the hard-bottom base for 2 s with an amplitude of 0.1 mm at 100 Hz. Subsequently, the particles were allowed to resettle for another 0.5 s. During resettling, most of the energy dissipation (six orders of magnitude decrease) took place in the initial period of 0.2 s. The rough bottom boundary reduced undesirable effects such as local ordering of particle distributions near plane walls. Consequently, the procedure resulted in an approximately random close packing sample. Any local effects of the bottom wall on the mean concentration were mitigated further by choosing a cubic sub-sample of size $H = 96$ mm whose lower boundary started 20 D above the hard-bottom base. The mean volume fraction of the cubic sub-sample was $\overline{\phi}_L = 0.628$ and the mean coordination number (number of contacts per particle) was $Z = 4.44$.

To investigate the effect of the mean concentration on the volume averaging scale, we produced samples with lower concentration/larger size H (Table 1) by keeping the particle diameter D fixed while uniformly stretching all coordinates of the initial (96 mm)^3 sample. We constructed an approximation of the binary volume fraction field (1) by dividing each H sample into N_{vox}^3 cubic voxels of size $D/100$ and set $\phi(\mathbf{r}_i) = 1(0)$ if the voxel center, $\mathbf{r}_i$, is inside (outside) a particle. Given the large $O(10000^3)$ number of voxels, we used a "bucket" algorithm (adapted from Munjiza and Andrews, 1988) to perform efficient voxel-in-particle searches and efficient computation of the binary concentration and derived macroscopic concentration fields. The bucket algorithm subdivides the domain into cubes of size D called "buckets" and generates a list of particles whose center is contained in each bucket by integerizing the particle coordinates with respect to D. Thus, the voxels in a given bucket are only checked against the limited number of particles in the current bucket and its immediate neighbors. Once the binary concentration field is known, the macroscopic concentration fields are computed hierarchically by starting with the smallest boxes of size $L = D/10$. Since the box size, $D/10$, is an integer multiple of the voxel size, the box-integrated volume fraction, $\phi_L(\mathbf{r}_j)$, is simply the mean of $\phi(\mathbf{r}_i)$ for voxels contained in the j-th box. The hierarchical computation utilizes a larger box whose L is an integer multiple of the smaller box L. From the

Table 1
Cubical particle sample of size H of $D = 1$ mm particles.

Stretch factor	1	1.5	2.0	2.5	3.0	4.0
H/D	96	144	192	240	288	384
N_{vox}	9600	14,400	19,200	24,000	28,800	38,400
$\overline{\phi}_L$	0.6277	0.1860	0.0785	0.0402	0.0244	0.0098