Coarse-grained computations of demixing in dense gas-fluidized beds

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We use an “equation-free”, coarse-grained computational approach to accelerate molecular dynamics-based computations of demixing (segregation) of dissimilar particles subject to an upward gas flow (gas-fluidized beds). We explore the coarse-grained dynamics of these phenomena in gently fluidized beds of solid mixtures of different densities, typically a slow process for which reasonable continuum models are currently unavailable.

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Particulate flows, even for experimental systems of small size (∼10 cm), consist of a very large number of discrete dissipative particles. Molecular dynamics (MD) simulations often serve as a quantitative modeling tool for such flows; however, such simulations for realistically large temporal and/or spatial scale problems are challenging even with modern computers. Navier-Stokes-like, macroscopic continuum models have been developed by many authors based on the kinetic theory of granular materials (see Refs. [1, 2] and references therein); however, quantitative continuum models for realistic particles (accounting for frictional interactions, heterogeneity among particles, and/or other inter-particle forces, such as van der Waals forces) in many regimes of practical interest (e.g. dense and/or cohesive flows where enduring contacts between particles occur) are currently unavailable.

In this paper, we consider well-known phenomena for which the derivation of continuum models is still in flux; mixing and demixing (segregation) can occur when dissimilar particle mixtures of different sizes and/or densities are subject to a strong enough upward fluid flow [3]. A few different continuum models, more phenomenological or more rigorous, have been proposed [4, 5], which often reproduce the phenomena in a qualitatively correct manner; however, quantitative agreement is generally elusive [2]. Furthermore, kinetic theory-based continuum models for binary mixtures are much more complicated than those for uniform particles, and numerical simulation becomes more time-consuming (e.g. by an order of magnitude in Ref. [5]). Accelerating the computation using (quantitative) microscopic models would become more pronounced in such narrow beds. The equation of motion for each particle can be simplified to be [10]:

\[ m_p \frac{d \mathbf{v}_p}{dt} = m_p \mathbf{g} + \mathbf{F}_{\text{cont}} + \frac{V_p}{\phi} \beta(\phi) \times \left[ \mathbf{u}_s - \mathbf{v}_p \right] - \frac{1}{(1 - \phi)^2} (\mathbf{u}_s - \mathbf{U}_s) ] , \]

where \( m_p \) and \( \mathbf{v}_p \) are individual particle mass and velocity, respectively; \( \mathbf{g} \) is the gravitational acceleration; \( V_p \) is the volume of each particle; \( \phi \) is the locally-averaged solid phase volume fraction; \( \beta \) is the interphase momentum transfer coefficient [11, 12]; \( \mathbf{u}_s \) is the coarse-grained solid phase velocity; and \( \mathbf{U}_s \) is the superficial gas flow velocity, in the direction opposite to that of the gravity. In our study, the Reynolds number based on the particle size is generally very small (<\sim 0.1), and \( \beta \) is approximated to be

\[ \beta(\phi) = 18 \frac{\mu_g}{d_p} (1 - \phi)^{-2.65} , \]

where \( \mu_g \) is the gas phase viscosity. We nondimensionalize quantities by using \( \rho_s \), \( d_p \), \( \sqrt{d_p} \), and \( d_p/g \) as characteristic density, length, velocity, and time scales, where \( \rho_s \) is the solid phase mass density of the lighter particles. More details of the model can be found in Refs. [11, 12].

Direct simulations. Demixing is typically a slow process, whose occurrence and duration depend on the density difference and the gas flow rate. Direct simulation with a sufficiently large \( U_s \) (≡ \( |U_s| \)), starting from a homogeneously mixed, packed (static) state (Fig. [1], illustrates that particles of different densities gradually demix.

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spontaneously. When \( U_s \) is well above the minimum fluidization rate of both species (as in Fig. 1), the bed exhibits 1D traveling waves (TWs) \([13]\), and demixing occurs superposed on the persistent oscillatory motion driven by 1D-TWs. A typical computation of an entire demixing process in the above “tiny” system \((2 \times 10^7)\) integration steps of 12,500 particles shown in Fig. 1 takes nearly two days, or more than a week for smaller gas flow rates, on a single-processor PC with 1.7 GHz CPU. Obtaining an ensemble of long simulations for statistical averaging purposes can be extremely time-consuming.

Coarse-grained description and “observables”. In the literature, the degree of mixing/demixing is often characterized by various lumped indices (or “order parameters”) \([14, 15, 16]\) such as the so-called Lacey mixing index \([14]\) (e.g. see its use in Ref. \([8]\)). Here we seek coarse-grained variables (or “observables”) that could be used in continuum descriptions.

As in the two-fluid modeling approach \([1]\), it is natural to think of hydrodynamic variables as candidate coarse observables. From direct simulations, we observe that in the course of demixing in quasi-1D beds, the process strongly depends on the local density, which makes the 1D volume fraction profiles themselves sufficient coarse observables; when we suddenly randomize only the individual particle velocities (hence the granular temperature as well) and continue the simulation, the demixing progresses essentially undisturbed. We further recognize that cumulative particle distribution functions (CDFs, and more precisely, their inverses which are bounded by 0 and 1) are more convenient coarse observables: CDFs are smoother than volume fraction profiles, suffer from less noise, and facilitate the lifting (see below) procedure.

We consider both discretized inverse CDFs (ICDFs; Fig. 2) and their compact parametric representations (finite element or expansion coefficients in convenient polynomial sets; Fig. 3) as our actual coarse observables. For a narrow range of \( U_s \)’s slightly above the minimum fluidization rate, the time evolution of ICDFs does not exhibit any waviness (thin lines in Fig. 2 (a)), and demixing occurs very slowly (complete demixing is hardly achieved). In the presence of 1D-TWs \((U_s = 0.19)\), the bed hardly expands and no 1D-TWs form. Projective steps of \( \Delta t = 80 \) were taken through forward Euler, after direct integration for \( \delta t = 20 \) (the latter half of data were used to estimate the local slope). (b) In the presence of 1D-TWs \((U_s = 0.41)\); \( \delta t = 30 \), and \( \Delta t = 2T \), where \( T \) is the average period estimated during short bursts of direct integrations; the last two periods of the locally oscillating data were used to estimate the coarse slope.
ables, one can actually accelerate the overall computation. This simple idea underpins coarse projective integration \cite{17,18}.

In equation-free computations, traditional continuum numerical techniques are directly applied to the outcome of appropriately initialized short bursts of microscopic simulation, and the macroscopic equations are “integrated” or “solved” without ever being written down \cite{13,20,21}. The essential steps are: (i) Identify coarse observables (which are discretized ICDFs or their parameterization coefficients in our study). For convenience, we denote the microscopic description (here the individual particle positions) by $\mathbf{x}$, and the macroscopic description (here the ICDFs) by $X$. (ii) Choose an appropriate lifting operator $\mu_L$, which maps $X$ (ICDFs) to one (or more, for the purposes of variance reduction and ensemble-averaging,) consistent description(s) $\mathbf{x}$ (here, particle positions). Figuring out an efficient lifting operator is essential. (iii) Starting from lifted initial condition(s) $\mathbf{x}(t_0) = \mu_L(X(t_0))$, run the detailed simulator for some time horizon ($T_h > 0$) to obtain $\mathbf{x}(t_0 + T_h)$. (iv) Use an appropriate restriction operator $\mathcal{M}_R$ which maps the microscopic state(s) to the macroscopic description $X(t_0 + T_h) = \mathcal{M}_R(\mathbf{x}(t_0 + T_h))$, resulting in time series of the coarse observables (ICDFs), or a coarse time-stepper $\Phi_{T_h}$ for them: $X(t_0 + T_h) = \Phi_{T_h}(X(t_0))$. (v) Apply desired numerical techniques (forward Euler, in our study) to the coarsely observed results in step (iv), and repeat.

Lifting. Given an ICDF as the coarse observable, we need to construct particle configurations consistent with it. Arranging particles (i.e. sphere packing) in three-dimensional space with an arbitrarily prescribed ICDF (or local volume fraction, especially dense) profile is non-trivial and generally time-consuming \cite{22}, as excessive particle-particle overlap has to be avoided; it would be less difficult for dilute particulate flows. In our study, the total height of a bed remains virtually the same, even in the presence of 1D-TWs (see the second and later frames in Fig. 1). Therefore, we do not reassign particle locations from scratch in each lifting step. Instead, we utilize particle locations which are already obtained from an earlier step, and switch only particle indices (or “colors”, whether “red” or “yellow”) until the prescribed ICDF becomes satisfied. When a system of polydisperse particles is considered, this scheme should be modified; this would be a subject of future research.

Our lifting operator for single realization computations requires additional consideration when 1D-TWs are present: particle locations obtained from earlier simulation at the same “phase angle” during the wave propagation have to be used. In ensemble-averaged computations, the oscillatory motion becomes smoothed, requiring no special attention.

Coarse projective integration. We choose discretized ICDFs of the lighter particles as the coarse observables, and accelerate the demixing computation using coarse projective forward Euler scheme \cite{17,18}. For smaller $U$, where the bed hardly expands and ICDFs do not oscillate, the projection step size is determined by only the temporal smoothness (accuracy of the local linearization) of ICDF evolution. The demixing occurs very slowly in this case (Fig. 2 (a)), and these computations can achieve high computational speedup. Excessively large projection steps can cause inaccuracies, similar to large time steps in normal integration. In the presence of 1D-TWs, the projection step size is chosen to be an integral multiple of the local oscillation period (Fig. 2 (b)).

Projected integrator values (thick lines in Fig. 2) follow the trajectories of direct, full integrations (thin lines in Fig. 2) well, confirming that these coarse observables are good continuum variables. Ensemble-averaging of ICDFs over different realizations (of different phase angles during wave propagation) smoothens local oscillations arising from 1D-TWs. Projective integration of ensemble-averaged ICDFs, both in the presence and absence of 1D-TWs, can be applied in the same way.

A more compact description. The difference between the ICDF of particles located in the upper half of the bed (irrespective of their densities) and that of the lighter ones can serve as a useful coarse observable: ICDFs of the lighter particles are bounded by those of the (total) top half particles, and their difference is positive definite (Fig. 3). Furthermore, once nearly-full local demixing occurs, the ICDF difference there becomes virtually zero. The difference of the two ICDFs can be fit by the following simple functional form (dashed lines in Fig. 3):

$$y = \max[Ax + B + C \exp(Dx), 0],$$

where $A(t), B(t), C(t)$, and $D(t)$ are our new coarse observables, determined on the fly by functional fitting, and $x$ and $y$ represent the abscissa and the ordinate in Fig. 3 respectively. Other basis functions, such as high-order polynomials also can fit the functional form reasonably well, but they require many more terms and the time evo-
lution of their expansion coefficients is not generally slow. Lifting for these new coarse observables involves a minor intermediate step: mapping between these four variables and an ICDF discretization through the functional form in Eq. (3).

We use these four coarse observables to perform ensemble-averaged coarse projective integration over a number of realizations (Fig. 4). These observables vary slowly and smoothly in time (occasional oscillations disappear for larger ensembles); in a sense, this is a pseudospectral solution of the unknown governing equations for ICDF evolution.

Conclusions. We have used an “equation-free” coarse-grained approach to accelerate (by a factor of two to ten; the lifting step in our study involves minimal computational effort) computations of dense particulate flows and, in particular, of demixing occurring in gas-fluidized beds of dissimilar particles. This approach holds promise for the prediction of coarse-grained behavior at practically relevant spatial and temporal scales.

We deliberately considered a quasi-1D illustrative problem in our study, in order to demonstrate the viability of the approach. As a consequence of the problem considered in this study, the coarse observables were one-dimensional discretized ICDFs. For systems involving higher dimensional flows, candidates for coarse observables may include marginal and conditional ICDFs. More work for such systems has to be done to identify proper coarse observables and an efficient lifting operator, vital components of this approach. Ensemble averaging reduces fluctuations among the realizations, giving better quantitative representations; the computation of each realization readily parallels across computational nodes.

More sophisticated equation-free algorithms (e.g. coarse fixed point algorithms) can be used to find stable as well as unstable steady states; quantify their stability; and perform numerical bifurcation analysis. Exploiting such tools to investigate the coarse-grained dynamics of mixing and demixing (and other particulate flow problems) is the subject of current research.

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