UNIVERSITY OF TWENTE.

From Discrete Particles to Continuum Fields in Mixtures

Thomas Weinhart,
Stefan Luding,
Anthony Thornton

Jan 23, 2014

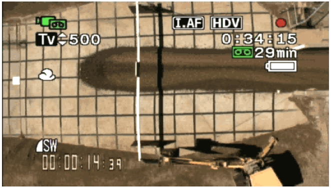
Size segregation in shallow granular flows

Size segregation
AR Thornton, PhD thesis

Size segregation in shallow granular flows

Size segregation

AR Thornton, PhD thesis



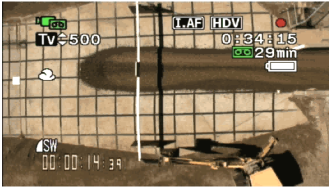
Elongated runoff

Johnson et al., J. Geophys. Res. (2012)

Size segregation in shallow granular flows

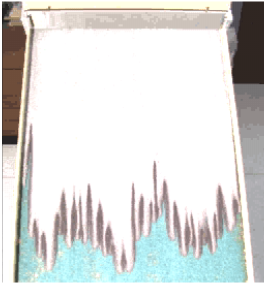
Size segregation

AR Thornton, PhD thesis



Elongated runoff

Johnson et al., J. Geophys. Res. (2012)



Fingering instabilities

Woodhouse et al., JFM (2012).

The Discrete Particle Method

- Particles have position $\mathbf{r}_i$, velocity $\mathbf{v}_i$, angular velocity $\boldsymbol{\omega}_i$, diameter d_i, mass m_i
- Governed by Newtonian mechanics:

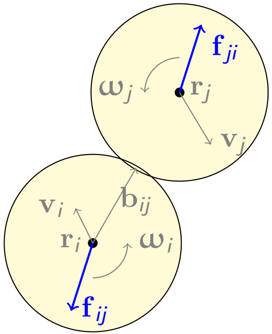
$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{f}_i,$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \mathbf{t}_i$$

- Contact forces and body forces:

$$\mathbf{f}_i = \sum_j \mathbf{f}_{ij} + m_i \mathbf{g}_i,$$

$$\mathbf{t}_i = \sum_j \mathbf{b}_{ij} \times \mathbf{f}_{ij}$$



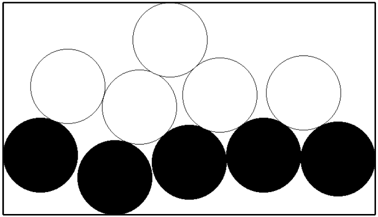
Coarse graining

Objective

Define continuous macroscopic fields such as mass density ρ, velocity $\mathbf{V}$, stress $\boldsymbol{\sigma}$, based on particle data $\{\mathbf{r}_i, \mathbf{v}_i, m_i, \mathbf{f}_i, \ldots\}_{i=1}^{N}$.

The fields should satisfy mass and momentum balance exactly.

Example: A static system of 5 fixed and 5 free particles.



Coarse graining: density ρ and mass balance

A) We define the macro-density using a coarse-graining function ϕ,

$$\rho(\mathbf{r}) = \sum_{i=1}^{n} m_i \phi(\mathbf{r} - \mathbf{r}_i).$$

Coarse graining: density ρ and mass balance

A) We define the macro-density using a coarse-graining function ϕ,

$$\rho(\mathbf{r}) = \sum_{i=1}^{n} m_i \phi(\mathbf{r} - \mathbf{r}_i).$$

B) We define the velocity s.t. mass balance,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

is satisfied:

$$\mathbf{v} = \frac{\mathbf{p}}{\rho}, \text{ where } \mathbf{p} = \sum_{i=1}^{n} m_i \mathbf{v}_i \phi(\mathbf{r} - \mathbf{r}_i).$$

Coarse graining: momentum balance

C) We define stress $\boldsymbol{\sigma}$ and boundary interaction force density $\mathbf{t}$ such that momentum balance,

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} + \mathbf{t},$$

is satisfied ($\mathbf{t}$ can be modelled as a boundary condition):

$$\boldsymbol{\sigma}^k = -\sum_{i=1}^{n} m_i \mathbf{v}_i' \mathbf{v}_i' \phi(\mathbf{r} - \mathbf{r}_i),$$

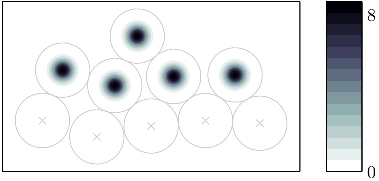
$$\boldsymbol{\sigma}^c = -\sum_{\text{contacts } \{i,j\}} \mathbf{f}_{ij} \mathbf{r}_{ij} \int_0^1 \phi(\mathbf{r} - (\mathbf{r}_i + s\mathbf{r}_{ij}))\, ds$$

$$- \sum_{\text{wall contacts } \{i,k\}} \mathbf{f}_{ik} \mathbf{b}_{ik} \int_0^1 \phi(\mathbf{r} - (\mathbf{r}_i + s\underset{\substack{\uparrow \\ \text{branch vector } b_{ik} = \mathbf{r}_i - \mathbf{c}_{ik}}}{\mathbf{b}_{ik}}))\, ds,$$

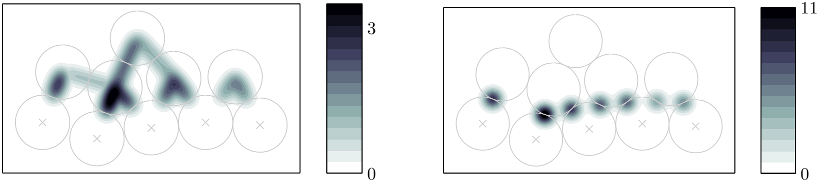
$$\mathbf{t} = -\sum_{\text{wall contacts } \{i,k\}} \mathbf{f}_{ik} \phi(\mathbf{r} - \mathbf{c}_{ik}),$$

Weinhart, Thornton, Luding, Bokhove, GranMat (2012) 14:289

A static system of 5 fixed and 5 free particles.



Density ρ *for Gaussian coarse-graining function of width* $w = d/8$.



Magnitude of stress $|\boldsymbol{\sigma}|_2$ *and boundary interaction force* $|\mathbf{t}|_2$.

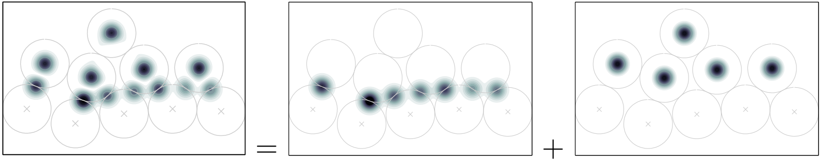
Satisfying mass and momentum balance

- Mass balance in a static system is trivial.

Satisfying mass and momentum balance

- Mass balance in a static system is trivial.
- Satisfying the momentum balance in a static system requires

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{t} + \rho \mathbf{g}.$$

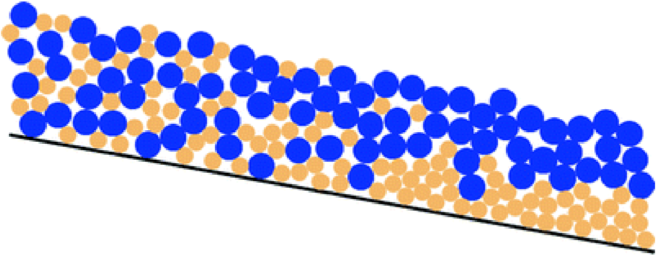


Magnitudes of stress divergence $|\nabla \cdot \boldsymbol{\sigma}|_2$ *(left), boundary interaction force density* $|\mathbf{t}|_2$ *(centre), and weight density* $|\rho \mathbf{g}|$ *(right).*

Important result

Mass/mom. bal. is satisfied locally for any coarse-graining function.

How do we define stress and interspecies drag in mixtures?



bidisperse mixture of small and large particles

from Marks, Einav, Rognon, Geomat. Proc., (2011)

Coarse graining in mixtures

For both species $\nu = s, l$, we define

- partial densities $\rho^\nu = \sum_{i\in\mathcal{F}^\nu} m_i \phi(\mathbf{r}-\mathbf{r}_i)$, so $\rho = \rho^l + \rho^s$.
- partial momenta $\rho^\nu \mathbf{v}^\nu = \sum_{i\in\mathcal{F}^\nu} m_i \mathbf{v}_i \phi(\mathbf{r}-\mathbf{r}_i)$, so $\rho\mathbf{v} = \rho^l\mathbf{v}^l + \rho^s\mathbf{v}^s$,

Coarse graining in mixtures

For both species $\nu = s, l$, we define

- partial densities $\rho^\nu = \sum_{i \in \mathcal{F}^\nu} m_i \phi(\mathbf{r} - \mathbf{r}_i)$, so $\rho = \rho^l + \rho^s$.
- partial momenta $\rho^\nu \mathbf{v}^\nu = \sum_{i \in \mathcal{F}^\nu} m_i \mathbf{v}_i \phi(\mathbf{r} - \mathbf{r}_i)$, so $\rho \mathbf{v} = \rho^l \mathbf{v}^l + \rho^s \mathbf{v}^s$,
- partial stresses $\boldsymbol{\sigma}^{c,\nu} = \sum_{i \in \mathcal{F}^\nu} \sum_{j \in \mathcal{F}} \mathbf{f}_{ij} \mathbf{b}_{ij} \int_0^1 \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{b}_{ij})\, ds$, so

  $\boldsymbol{\sigma} = \boldsymbol{\sigma}^l + \boldsymbol{\sigma}^s$,
- interspecies drag $\boldsymbol{\beta}^l = -\boldsymbol{\beta}^s = \sum_{i \in \mathcal{F}^l} \sum_{j \in \mathcal{F}^s} \mathbf{f}_{ij} \phi(\mathbf{r} - \mathbf{c}_{ij})$.

Coarse graining in mixtures

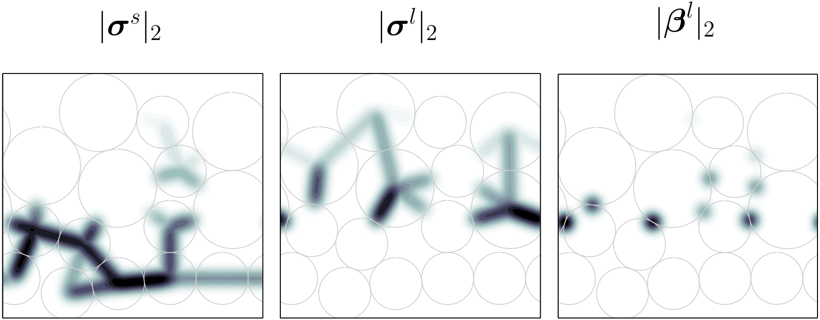
For both species $\nu = s, l$, we define

- partial densities $\rho^\nu = \sum_{i \in \mathcal{F}^\nu} m_i \phi(\mathbf{r} - \mathbf{r}_i)$, so $\rho = \rho^l + \rho^s$.
- partial momenta $\rho^\nu \mathbf{v}^\nu = \sum_{i \in \mathcal{F}^\nu} m_i \mathbf{v}_i \phi(\mathbf{r} - \mathbf{r}_i)$, so $\rho \mathbf{v} = \rho^l \mathbf{v}^l + \rho^s \mathbf{v}^s$,
- partial stresses $\boldsymbol{\sigma}^{c,\nu} = \sum_{i \in \mathcal{F}^\nu} \sum_{j \in \mathcal{F}} \mathbf{f}_{ij} \mathbf{b}_{ij} \int_0^1 \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{b}_{ij})\, ds$, so $\boldsymbol{\sigma} = \boldsymbol{\sigma}^l + \boldsymbol{\sigma}^s$,
- interspecies drag $\boldsymbol{\beta}^l = -\boldsymbol{\beta}^s = \sum_{i \in \mathcal{F}^l} \sum_{j \in \mathcal{F}^s} \mathbf{f}_{ij} \phi(\mathbf{r} - \mathbf{c}_{ij})$.

Then mass and momentum equations are satisfied:

$$
\begin{aligned}
&\frac{\partial \rho^\nu}{\partial t} + \nabla \cdot (\rho^\nu \mathbf{v}^\nu) = 0, \\
&\rho^\nu \frac{D\mathbf{v}^\nu}{Dt} = -\nabla \boldsymbol{\sigma}^\nu + \rho^\nu \mathbf{g} + \boldsymbol{\beta}^\nu, \quad \nu = s, l.
\end{aligned}
$$

A static system of 10 small and 5 large particles.



Magnitude of small and large phase stress $|\boldsymbol{\sigma}^s|$, $|\boldsymbol{\sigma}^l|$ *(left, centre) and interspecies drag* $|\boldsymbol{\beta}^l|$ *(right),* $w = d_s/8$.

Kinetic Sieving

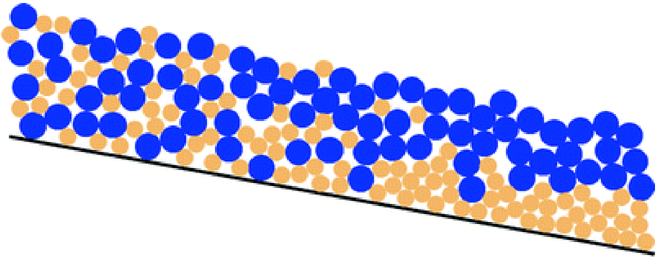


Figure from Marks, Einav, Rognon, Geomat. Proc., (2011)

- Discrete Description: small particles fall easier through holes
- Continuum description: Large particle phase supports more downward stress than small particles phase ("overstress"):

$$f^l = \frac{\sigma^l_{zz}}{\sigma_{zz}} > \phi^l = \frac{\rho^l}{\rho}$$

.

Segregation equation

We define

- large particle volume fraction $\phi^l = \frac{\rho^l}{\rho}$ and
- large particle stress fraction $f^l = \frac{\sigma^l_{zz}}{\sigma_{zz}}$,

and describe the overstress by

$$f^l = \phi^l + B\phi^s\phi^l, \quad B > 0.$$

Gray Thornton, Proc Royal Soc A (2005)

Segregation equation

We define

- large particle volume fraction $\phi^l = \frac{\rho^l}{\rho}$ and
- large particle stress fraction $f^l = \frac{\sigma^l_{zz}}{\sigma_{zz}}$,

and describe the overstress by

$$f^l = \phi^l + B\phi^s\phi^l, \quad B > 0.$$

We further assume a drag law, with drag coefficient c,

$$\boldsymbol{\beta}^\nu = \boldsymbol{\sigma}\boldsymbol{\nabla} f^\nu - \rho^\nu c(\mathbf{u}^\nu - \mathbf{u}),$$

Gray Thornton, Proc Royal Soc A (2005)

Segregation equation

We define

- large particle volume fraction $\phi^l = \frac{\rho^l}{\rho}$ and
- large particle stress fraction $f^l = \frac{\sigma^l_{zz}}{\sigma_{zz}}$,

and describe the overstress by

$$f^l = \phi^l + B\phi^s\phi^l, \quad B > 0.$$

We further assume a drag law, with drag coefficient c,

$$\boldsymbol{\beta}^\nu = \boldsymbol{\sigma}\boldsymbol{\nabla} f^\nu - \rho^\nu c(\mathbf{u}^\nu - \mathbf{u}),$$

Then momentum balance for shallow flow yields

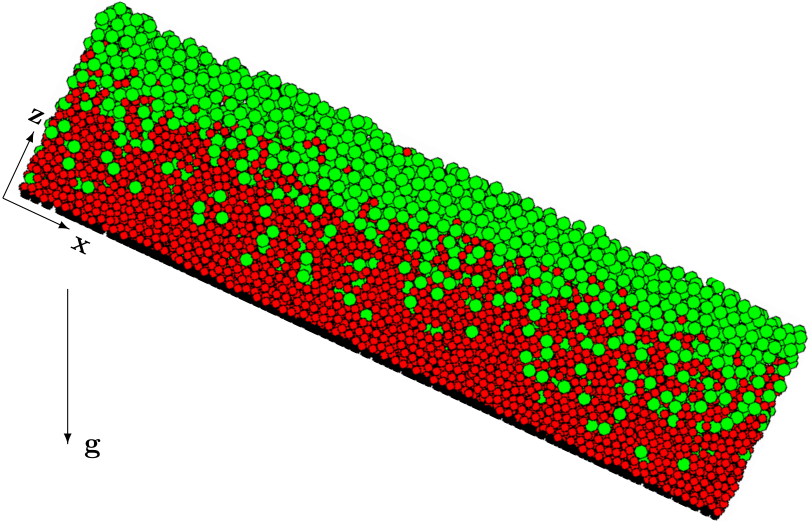
$$(w^l - w) = q\phi^s, \quad (w^s - w) = -q\phi^l,$$

with segregation velocity

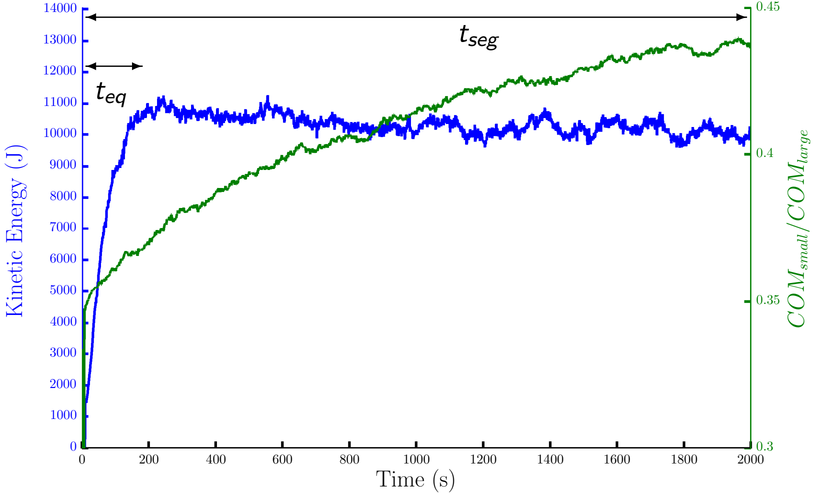
$$q = \frac{B}{c} g \cos\theta.$$

Gray Thornton, Proc Royal Soc A (2005)

Segregating flow in a periodic box



Simulation snapshot at $t = 100\,\text{s}$ for $\theta = 24^\circ$, $\phi^l = 0.5$, $d_l/d_s = 1.5$.
Colors indicate fixed (black), large (green) and small (red) particles.



Kin. energy and COM over time (initially inversely segregated)

Observation

Segregation kinetics are much slower than equilibration.

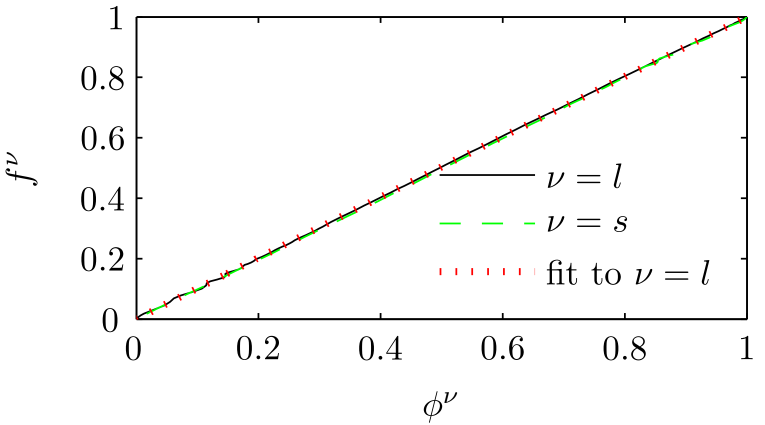


Figure : Stress fraction $f^\nu = \sigma^\nu_{zz}/\sigma_{zz}$ in steady state as a function of volume fraction $\phi^\nu = \rho^\nu/\rho$, for each constituent $\nu = s, l$ and fit $f^{l,fit}$ for $B = 0.02$, $w = d_s$.

Observation

$f^l > \phi^l$, as required for gravity-driven segregation.

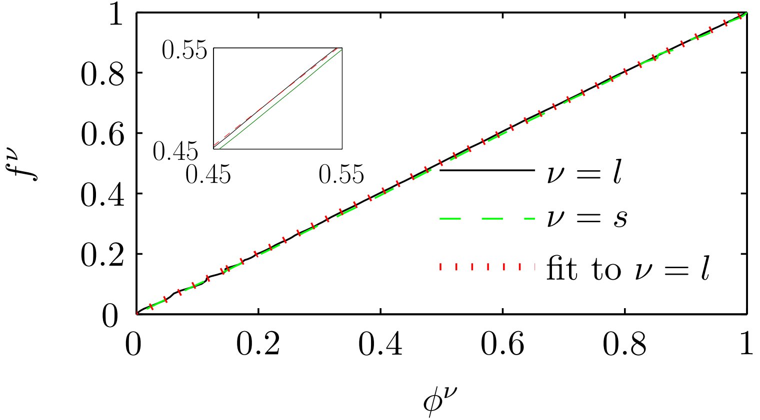


Figure : Stress fraction $f^{\nu} = \sigma^{\nu}_{zz}/\sigma_{zz}$ in steady state as a function of volume fraction $\phi^{\nu} = \rho^{\nu}/\rho$, for each constituent $\nu = s, l$ and fit $f^{l,fit}$ for $B = 0.02$, $w = d_s$.

Observation

$f^{l} > \phi^{l}$, as required for gravity-driven segregation.

Overstress B

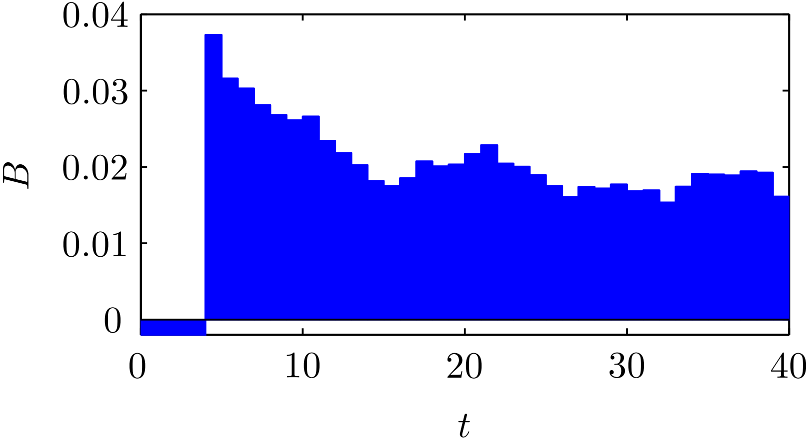
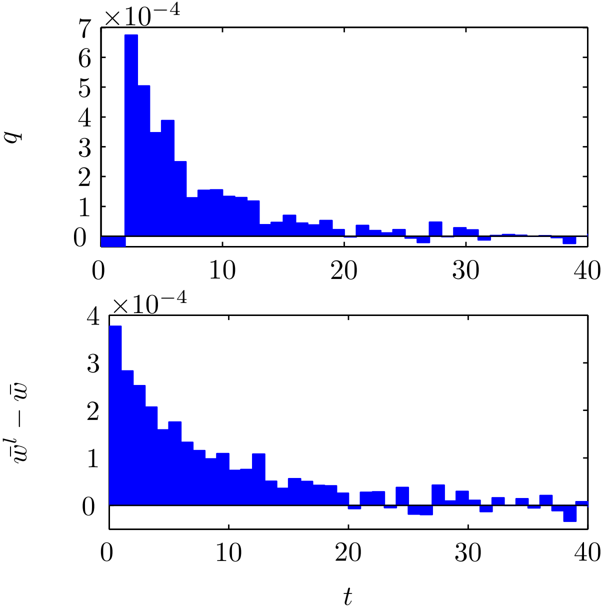


Figure : Magnitude of overstress, B, over time t.



Segregation velocity (from stress and drag), $q = (B/c)g_z$, over time t.

Mean relative velocity of large phase, $\bar{w}^l - \bar{w}$, over time t.

Observation

Segregation kinetics can be measured accurately.

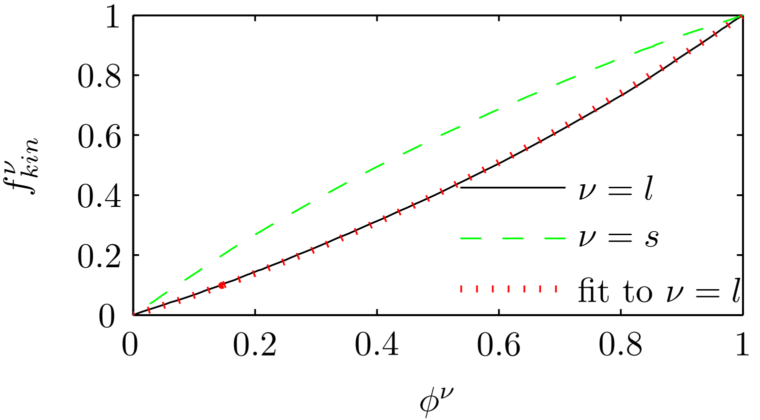


Figure : Kinetic stress fraction $f^{\nu} = \sigma^{k,\nu}_{zz}/\sigma^{k}_{zz}$ in steady state as a function of volume fraction $\phi^{\nu} = \rho^{\nu}/\rho$, for each constituent $\nu = s, l$ and fit $f^{l,fit}$ for $B = -0.38$.

Observation

$f^{l,kin} < \phi^{l}$, as required for shear-induced segreg. (Fan Hill 2011).

Conclusions

1. Coarse-graining formulation for mixtures allows measuring the species' stress fraction and the interspecies drag.
2. Segregation kinetics are much slower than equilibration.
3. Large particles support a stress fraction (slightly) higher than their volume fraction, as postulated for gravity-driven segregation. Segregation velocity roughly follows the drag law used in (Gray Thornton 2005).
4. Large particles support a fraction of the kinetic stress *much smaller* than their volume fraction, as postulated in the shear-induced segregation theory of (Fan Hill 2011).