A Two-Phase Micromorphic Model for Compressible Granular Materials

Samuel Paolucci, Weiming Li, Joseph M. Powers

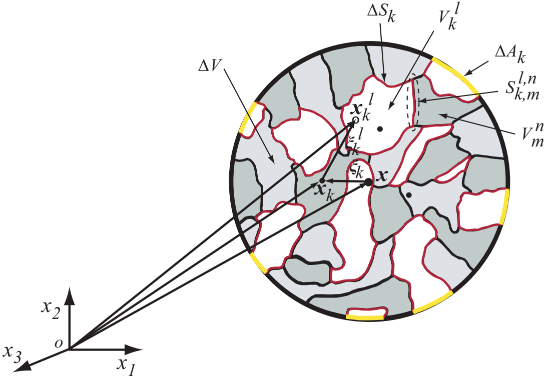
Aerospace & Mechanical Engineering
University of Notre Dame, Indiana 46556

APS-DFD, November 22, 2009
Minneapolis, Minnesota

Introduction

- Motivation:
  - study problems where internal material structure (heterogeneities) affects properties of materials: blood flows, porous media, granular materials, foams, *etc.*
  - conventional multiphase theory fails to appropriately describe the behavior of such materials.
- Microstructure theories:
  - continuum theories of materials with microstructure (*e.g.* Ericksen and Truesdell 1958, Truesdell and Toupin 1960, Mindlin 1964, Eringen 1964, *etc.*).
- Micromorphic multiphase theory:
  - we derive a closed general multiphase micromorphic theory and provide specific constitutive models;
  - obtained directly from appropriate averaging of continuum microscale equations.

Modeling of Micromorphic Multiphase Mixtures



$$\epsilon_k \equiv \frac{\Delta V_k}{\Delta V}$$

$$\gamma_k \equiv \frac{\Delta S_k}{\Delta V}$$

$$\boldsymbol{\xi}_k^l = \mathbf{x}_k^l - \mathbf{x}_k$$

$$\boldsymbol{\xi}_k = \mathbf{x}_k - \mathbf{x}$$

$$\boldsymbol{\zeta}_k^l = \mathbf{x}_k^l - \mathbf{x}$$

Figure: Illustration of a Representative Elementary Volume.

$$\langle \mathcal{F}_k^l \rangle \equiv \frac{1}{\Delta V} \sum_{l=1}^{L_k} \int_{V_k^l} \mathcal{F}_k^l dV_{\boldsymbol{\xi}}, \quad \langle\langle \mathcal{F}_k^l \mathbf{n}_k^l \rangle\rangle \equiv \frac{1}{\Delta V} \sum_{l=1}^{L_k} \int_{S_k^l} \mathcal{F}_k^l \mathbf{n}_k^l dS_{\xi}.$$

$$\langle \mathcal{F}_k^l \rangle = \epsilon_k \overline{\langle \mathcal{F}_k^l \rangle}, \qquad \langle\langle \mathcal{F}_k^l \mathbf{n}_k^l \rangle\rangle = \gamma_k \overline{\langle\langle \mathcal{F}_k^l \mathbf{n}_k^l \rangle\rangle}.$$

General Balance Laws

- In a micro element with subvolume V_k^l within the fixed REV:

$$\frac{\partial}{\partial t}\left(\rho_k^l \mathcal{F}_k^l\right) + \nabla_{\mathbf{x}_k^l} \cdot \left(\rho_k^l \mathcal{F}_k^l \mathbf{u}_k^l\right) + \nabla_{\mathbf{x}_k^l} \cdot \boldsymbol{\mathcal{J}}_k^l - \rho_k^l \mathcal{G}_k^l - \rho_k^l \mathcal{P}_k^l = 0.$$

Terms	Mass	Lin. Mom.	Ang. Mom.	Energy	Entropy
$\mathcal{F}_k^l$	1	$\mathbf{u}_k^l$	$\mathbf{x}_k^l \wedge \mathbf{u}_k^l$	$e_k^l + \frac{1}{2}\mathbf{u}_k^l \cdot \mathbf{u}_k^l$	s_k^l
$\boldsymbol{\mathcal{J}}_k^l$	$\mathbf{0}$	$-\boldsymbol{\sigma}_k^l$	$-\mathbf{x}_k^l \wedge \boldsymbol{\sigma}_k^l$	$\mathbf{q}_k^l - \mathbf{u}_k^l \cdot \boldsymbol{\sigma}_k^l$	$\mathbf{h}_k^l$
$\mathcal{G}_k^l$	0	$\mathbf{g}_k^l$	$\mathbf{x}_k^l \wedge \mathbf{g}_k^l$	$r_k^l + \mathbf{u}_k^l \cdot \mathbf{g}_k^l$	b_k^l
$\mathcal{P}_k^l$	0	$\mathbf{0}$	$\mathbf{0}$	0	Λ_k^l

- Phase equations are obtained by phase-averaging moments of the microelement balance equation:

$$\left\langle \left(\mathbf{x}_k^l\right)^n \left[\frac{\partial}{\partial t}\left(\rho_k^l \mathcal{F}_k^l\right) + \nabla_{\mathbf{x}_k^l} \cdot \left(\rho_k^l \mathcal{F}_k^l \mathbf{u}_k^l\right) + \nabla_{\mathbf{x}_k^l} \cdot \boldsymbol{\mathcal{J}}_k^l - \rho_k^l \mathcal{G}_k^l - \rho_k^l \mathcal{P}_k^l\right] \right\rangle = 0.$$

- The number of moments: 3 for mass ($n = 0, 1, 2$), 1 for linear momentum ($n = 0$), 1 for angular momentum ($n = 0$), 1 for energy balance ($n = 0$), and 1 for entropy ($n = 0$).
- The mixture balance equations are obtained by summing the phase-averaged balance equations over all phases.
- Assumed micromorphic continuum of grade one: $\grave{\boldsymbol{\xi}}_k^l = \boldsymbol{\nu}_k \cdot \boldsymbol{\xi}_k^l$, $\grave{\zeta}_k^l = \boldsymbol{\nu} \cdot \zeta_k^l$, where $\boldsymbol{\nu}_k$ and $\boldsymbol{\nu}$ are the phase and mixture microgyration tensors.

Two-Phase Model: 1-D Phase and Mixture Equations

$$\frac{\partial\left(\epsilon_k\overline{\rho}_k\right)}{\partial t}+\frac{\partial}{\partial x}\left(\epsilon_k\overline{\rho}_k u_k\right)=0,$$

$$\frac{\partial}{\partial t}\left(\epsilon_k\overline{\rho}_k i_k\right)+\frac{\partial}{\partial x}\left[\epsilon_k\overline{\rho}_k\left(i_k u_s+j_k\nu_k\right)\right]-2\epsilon_k\overline{\rho}_k i_k\nu_k=0,$$

$$\frac{\partial}{\partial t}\left(\epsilon_k\overline{\rho}_k u_k\right)+\frac{\partial}{\partial x}\left(\epsilon_k\overline{\rho}_k u_k^2-\sigma_k\right)=F_k,$$

$$\frac{\partial}{\partial t}\left(\epsilon_k\overline{\rho}_k i_k\nu_k\right)+\frac{\partial}{\partial x}\left(\epsilon_k\overline{\rho}_k i_k\nu_k u_k-m_k\right)+\epsilon_k\overline{\rho}_k u_k^2-\sigma_k=\widehat{f}_k,$$

$$\frac{\partial}{\partial t}\left[\epsilon_k\overline{\rho}_k\left(e_k+e_k^\star+\frac{1}{2}u_k^2\right)\right]+\frac{\partial}{\partial x}\left[\epsilon_k\overline{\rho}_k\left(e_k+e_k^\star+\frac{1}{2}u_k^2\right)u_k+q_k+q_k^\star-u_k\sigma_k\right]=\mathcal{E}_k,$$

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}\left(\rho u\right)=0,$$

$$\frac{\partial}{\partial t}\left(\rho i\right)+\frac{\partial}{\partial x}\left[\rho\left(iu+j\nu\right)\right]-2\sum_{k=1}^{K}\rho_k i_k\nu_k=0,$$

$$\frac{\partial}{\partial t}\left(\rho u\right)+\frac{\partial}{\partial x}\left(\rho u^2-\sigma\right)=0,$$

$$\frac{\partial}{\partial t}\left(\rho i\nu\right)+\frac{\partial}{\partial x}\left(\rho i\nu u-m\right)+\rho u^2-\sigma=\widehat{f},$$

$$\frac{\partial}{\partial t}\left[\rho\left(e+e^\star+\frac{1}{2}u^2\right)\right]+\frac{\partial}{\partial x}\left[\rho\left(e+e^\star+\frac{1}{2}u^2\right)u+q+q^\star-u\sigma\right]=\mathcal{E}.$$

Note: Assumed interfaces have no intrinsic mass but have intrinsic momentum and energy.

Two-Phase Model: 1-D Phase and Mixture Quantities

$$\rho_k i_k = \langle \rho_k^l \xi_k^l \xi_k^l \rangle,$$
$$\rho_k j_k = \langle \rho_k^l \xi_k^l \xi_k^l \xi_k^l \rangle,$$
$$\sigma_k = \langle \sigma_k^l \rangle - \rho_k i_k \nu_k^2,$$
$$F_k = \langle\langle \sigma_k^l n_k^l \rangle\rangle,$$
$$m_k = \langle \xi_k^l \sigma_k^l \rangle - \rho_k i_k \nu_k u_k - \rho_k j_k \nu_k^2,$$
$$\widehat{f}_k = \langle\langle \xi_k^l \sigma_k^l n_k^l \rangle\rangle,$$
$$\rho_k e_k = \langle \rho_k^l e_k^l \rangle,$$
$$e_k^\star = \frac{1}{2} i_k \nu_k^2,$$
$$q_k = \langle q_k^l \rangle + \nu_k \langle \rho_k^l e_k^l \xi_k^l \rangle,$$
$$q_k^\star = -\nu_k \langle \xi_k^l \sigma_k^l \rangle + \frac{1}{2} \rho_k j_k \nu_k^3,$$
$$\mathcal{E}_k = \varepsilon_k + u_k F_k + \lambda_k,$$
$$\varepsilon_k = -\langle\langle \left[\rho_k^l e_k^l \left(u_k^l - c_k^l \right) + q_k^l \right] n_k^l \rangle\rangle,$$
$$\lambda_k = \nu_k \langle\langle \xi_k^l \sigma_k^l n_k^l \rangle\rangle.$$

$$\rho i = \sum_{k=1}^{K} \langle \rho_k^l \zeta_k^l \zeta_k^l \rangle,$$
$$\rho j = \sum_{k=1}^{K} \langle \rho_k^l \zeta_k^l \zeta_k^l \zeta_k^l \rangle,$$
$$\sigma = \sum_{k=1}^{K} \langle \sigma_k^l \rangle - \rho i \nu^2,$$
$$m = \sum_{k=1}^{K} \langle \zeta_k^l \sigma_k^l \rangle - \rho i \nu u - \rho j \nu^2,$$
$$\widehat{f} = \sum_{k=1}^{K} \langle\langle \zeta_k^l \sigma_k^l n_k^l \rangle\rangle,$$
$$\rho e = \sum_{k=1}^{K} \langle \rho_k^l e_k^l \rangle,$$
$$e^\star = \frac{1}{2} i \nu^2,$$
$$q = \sum_{k=1}^{K} \langle q_k^l \rangle + \nu \sum_{k=1}^{K} \langle \rho_k^l e_k^l \zeta_k^l \rangle,$$
$$q^\star = -\nu \sum_{k=1}^{K} \langle \zeta_k^l \sigma_k^l \rangle + \frac{1}{2} \rho j \nu^3.$$

Microinertia, Microspin and Compaction Equations

Microinertia and microgyration mixture equations can be combined to give

$$\rho i \frac{d\nu}{dt} - \frac{\partial}{\partial x}\left(m + \rho j \nu^2\right) + \rho\left(u^2 + j\nu\frac{\partial \nu}{\partial x}\right) + 2\nu \sum_{k=1}^{K} \rho_k i_k \nu_k - \sigma = \widehat{f}.$$

Neglecting microinertia terms and flux terms (or assuming equilibrium), this reduces to

$$\frac{d\epsilon_s}{dt} = \frac{\epsilon_s \epsilon_g}{\overline{\mu}_c}\left(\overline{p}_s - \beta_s - \overline{p}_g\right),$$

where

$$\overline{\mu}_c = \epsilon_s[(2\overline{\mu}_s + \overline{\lambda}_s) + \alpha(2\overline{\mu}_g + \overline{\lambda}_g)] + (2\overline{\mu}_g + \overline{\lambda}_g)(1-\alpha),$$
$$\beta_s = \frac{1}{\epsilon_g}(\overline{p}_s + 2\epsilon_s \frac{\sigma_i}{a}).$$

This equation has the same form as the *compaction equation* proposed by Baer and Nunziato (*Int. J. Multiphase Flow*, 1986) and extensively used by Bdzil *et al.* (*Phys. Fluids*, 1999), Kapila *et al.* (*Phys. Fluids*, 2001), Powers (*Phys. Fluids*, 2004), Schwendeman *et al.* (*Combust. Theor. Model.*, 2008), *etc.*

Two-Phase Model: Compaction Equation

From kinematic relations, local and phase mass balance equations, we obtain

$$\frac{d\epsilon_s}{dt} = \epsilon_s \left(\nu_s - \frac{\partial u_s}{\partial x} \right)$$

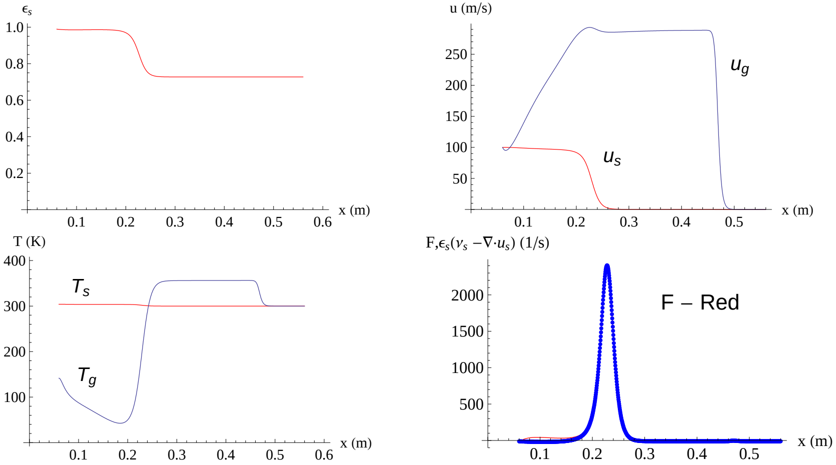
Constitutive equations:

$$\begin{aligned}
\epsilon_g &= 1 - \epsilon_s, \\
\sigma_k &= \epsilon_k \left(-\overline{p}_k + \overline{\tau}_k \right) - \epsilon_k \overline{\rho}_k i_k \nu_k^2, \\
\overline{p}_s &= \left(\gamma_s - 1 \right) c_{vs} \overline{\rho}_s T_s - \frac{1}{\gamma_s} \overline{\rho}_{s0} \varepsilon_s, \\
\overline{p}_g &= \left(\gamma_g - 1 \right) c_{vg} \overline{\rho}_g T_g \left(1 + b_g \overline{\rho}_g \right), \\
\overline{\tau}_k &= \frac{4}{3} \overline{\mu}_k \frac{\partial u_k}{\partial x}, \\
F_s &= -F_g = \overline{p}_g \frac{\partial \epsilon_s}{\partial x} - \delta \left(u_s - u_g \right), \\
m_k &= \frac{4}{3} \overline{\mu}_k \frac{\partial}{\partial x} \left(\epsilon_k i_k \nu_k \right) - \epsilon_k \overline{\rho}_k i_k \nu_k u_k, \\
\widehat{f}_k &= \begin{cases} -\epsilon_s \left(\overline{p}_{si} - \frac{4}{3} \overline{\mu}_s \nu_s \right), \\ \epsilon_s \left(\overline{p}_{gi} - \frac{4}{3} \overline{\mu}_g \nu_g \right), \end{cases}
\end{aligned}$$

$$\begin{aligned}
e_s &= c_{vs} T_s + \frac{1}{\gamma_s} \frac{\overline{\rho}_{s0}}{\overline{\rho}_s} \epsilon_s, \\
e_g &= c_{vg} T_g, \\
e_k^\star &= \frac{1}{2} i_k \nu_k^2, \\
q_k &= \epsilon_k \overline{q}_k, \\
\overline{q}_k &= -\overline{k}_k \frac{\partial T_k}{\partial x}, \\
q_k^\star &= -\frac{4}{3} \nu_k \overline{\mu}_k \frac{\partial}{\partial x} \left(\epsilon_k i_k \nu_k \right), \\
\mathcal{E}_k &= \varepsilon_k + u_k F_k + \lambda_k, \\
\varepsilon_s &= -\varepsilon_g = \mathcal{H} \left(T_g - T_s \right), \\
\lambda_s &= \nu_s \left(-\epsilon_s \overline{p}_{si} - 4 \overline{\mu}_s \nu_g \epsilon_s \right), \\
\lambda_g &= \nu_g \left(\epsilon_s \overline{p}_{gi} + 4 \overline{\mu}_g \nu_s \right).
\end{aligned}$$

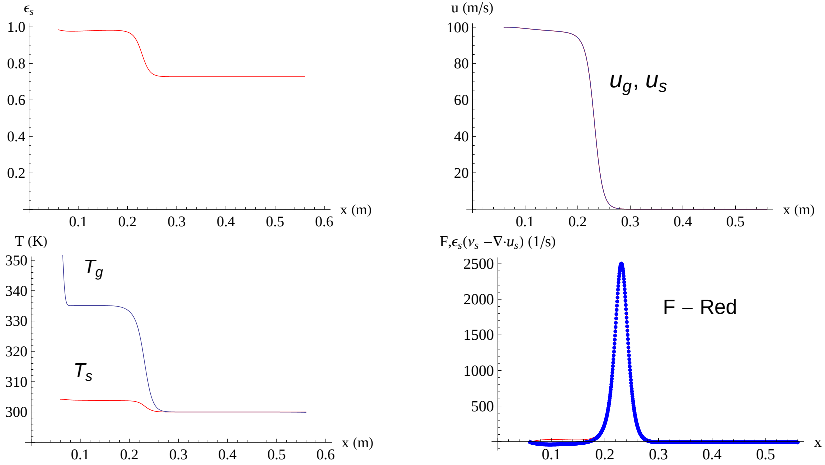
Numerical Application One

Case C of Powers (*Phys. Fluids*, 2004): Subsonic compaction with no drag or heat transfer ($\delta = 0$, $\mathcal{H} = 0$)



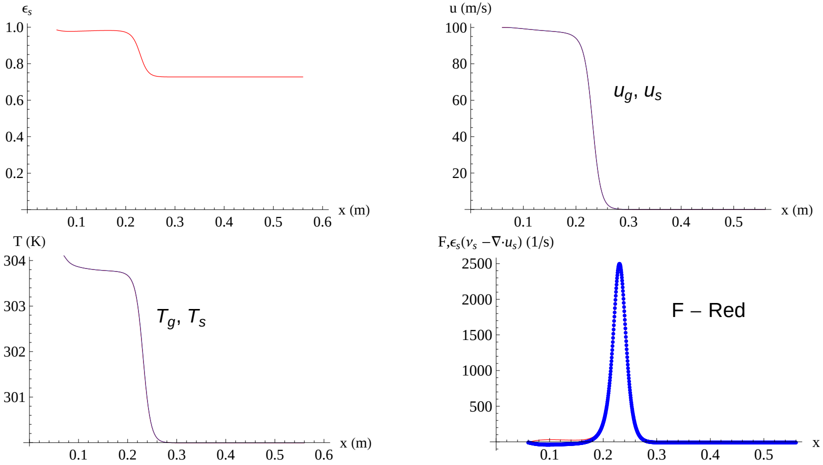
Numerical Application Two

Case D of Powers (*Phys. Fluids*, 2004): Subsonic compaction with drag but no heat transfer ($\delta \neq 0$, $\mathcal{H} = 0$)



Numerical Application Three

Case E of Powers (*Phys. Fluids*, 2004): Subsonic compaction with drag and heat transfer ($\delta \neq 0$, $\mathcal{H} \neq 0$)



Conclusions

- New balance equations for phase and mixture microinertia and microgyration tensors which describe the microstructure are derived;
- The new equations for microinertia and microgyration tensors contain the compaction equation which was previously obtained in an *ad hoc* fashion;
- Numerical results recover previous results of Powers when microinertia is negligible;
- Numerical results showing the effect of microinertia will be presented in the future — such results will need to be compared with experiments.