Homogenization methods for multi-phase mixtures with phase transition

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joint work with
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General setting

- Fluid carrier phase C,
  compressible continuum, inviscid, isentropic/isothermal, possibly irrotational

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- Examples: Spray droplets, bubbles, fluidized beds
- Aim: Well-posed systems of equations
  Two aspects of modeling:
  Mixture theories and averaging methods

Mixture balance laws

Continuum mixture theory

Direct modeling of phases with conservation laws,
volume fraction,
conservation laws of overall mixture
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Averaging methods

Drew 1983, Drew/Passman 1998

- Ensemble averaging   Saurel 1998, Saurel/Abgrall 1999

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- Time averaging   Ishii 1975

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Averaging methods

Drew 1983, Drew/Passman 1998

- Ensemble averaging Saurel 1998, Saurel/Abgrall 1999
- Time averaging Ishii 1975
- Volume averaging
  Nigmatulin 1979, Stewart/Wendroff 1984
  seems to be most popular approach,
  justified by homogeneity and ergodicity assumptions
  Nemat-Nasser/Hori 1999, Torquato 2002

Window function

Voinov/Petrov 1975, Rydzewski 1985

ball $B_a(x) = \{x' \in \mathbb{R}^3 \mid \; |x' - x| < a\}$,

radius $a > 0$, volume $V_a = \frac{4\pi}{3} a^3$

Window function

$$\chi_a(x) = \begin{cases} \frac{1}{V_a} & x \in B_a(0) \\ 0 & \text{otherwise} \end{cases}$$

alternatively: smoothing by Friedrichs mollifier

Disperse phase

Any bounded subset of $\mathbb{R}^3$ intersects at most finitely many balls

$$B_\alpha(t) = \{x \in \mathbb{R}^3 \mid \ |x - \mathbf{q}_\alpha(t)| < r_\alpha(t)\}$$

containing solely the dispersed phase D.

Radius $r_\alpha(t) > 0$ with $r_\alpha(t) \ll a$

midpoints $\mathbf{q}_\alpha(t) \in \mathbb{R}^3$, volume $V_\alpha(t) = \frac{4\pi}{3} r_\alpha(t)^3$

Complement

$$\Omega_C(t) = \mathbb{R}^3 \backslash \bigcup_\alpha B_\alpha(t)$$

filled completely with only the carrier fluid C.

Disperse phase cont'd

surface points $\mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t)$

mass $m_\alpha(t)$,

mass density $\rho_\alpha(t) = m_\alpha(t)/V_\alpha(t)$

midpoint velocity $\mathbf{v}_\alpha(t) = \dot{\mathbf{q}}_\alpha(t)$

boundary velocity $\mathbf{w}_\alpha(t) = \dot{\mathbf{q}}_\alpha(t) + \dot{\mathbf{R}}_\alpha(t)$

Volume fraction of disperse phase

$$c(t,x) = \sum_\alpha \chi_a(x - \mathbf{q}_\alpha(t)) V_\alpha(t)$$

Specific volume averaging

Ψ carrier fluid variable (no subscript!)

Ψ_α dispersed phase variable

Spatial carrier fluid average

$$(1-c)\overline{\Psi}(t,x) = \int_{\Omega_C(t)} \Psi(t,x')\, \chi_a(x-x')\, dx'$$

Spatial dispersed phase average

$$c\overline{\Psi_\alpha}(t,x) = \sum_\alpha \Psi_\alpha(t)\, \chi_a(x-\mathbf{q}_\alpha(t))V_\alpha(t)$$

conservative

Averaged physical variables

Mass density ρ_α, velocity $\mathbf{v}_\alpha$ of dispersed balls,

mass density ρ, velocity $\mathbf{v}$ of carrier fluid

Averaged mass densities and momenta

$$c\overline{\rho_\alpha}(t,x) = \sum_\alpha m_\alpha(t)\, \chi_a(x - \mathbf{q}_\alpha(t)),$$

$$c\overline{\rho_\alpha \mathbf{v}_\alpha}(t,x) = \sum_\alpha m_\alpha(t)\dot{\mathbf{q}}_\alpha(t)\, \chi_a(x - \mathbf{q}_\alpha(t)),$$

$$(1-c)\overline{\rho}(t,x) = \int_{\Omega_C(t)} \rho(t,x')\, \chi_a(x - x')\, dx',$$

$$(1-c)\overline{\rho\mathbf{v}}(t,x) = \int_{\Omega_C(t)} \rho(t,x')\mathbf{v}(t,x')\, \chi_a(x - x')\, dx'.$$

Macroscopic physical variables

Macroscopic mass densities and velocities

Disperse phase

$$\rho_D(t,x) = \overline{\rho_\alpha}(t,x) \qquad \text{and} \qquad \mathbf{v}_D(t,x) = \frac{\overline{\rho_\alpha \mathbf{v}_\alpha}}{\overline{\rho}_\alpha}(t,x) = \frac{\overline{\rho_\alpha \mathbf{v}_\alpha}}{\rho_D}(t,x),$$

Carrier phase

$$\rho_C(t,x) = \overline{\rho}(t,x) \qquad \text{and} \qquad \mathbf{v}_C(t,x) = \frac{\overline{\rho \mathbf{v}}}{\overline{\rho}}(t,x) = \frac{\overline{\rho \mathbf{v}}}{\rho_C}(t,x).$$

Global conservation

Globally conserved variable $\Psi(t,\cdot) \in L^1(\Omega_C(t))$ and Ψ_α for finitely many α, e.g. mass, momentum

$$\int_{\mathbb{R}^3} (1-c)\overline{\Psi}(t,x) + c\overline{\Psi_\alpha}(t,x)\,dx = \int_{\mathbb{R}^3} \Big[\int_{\Omega_C(t)} \Psi(t,x')\,\chi_a(x-x')\,dx' + \sum_\alpha \Psi_\alpha(t)\,\chi_a(x-\mathbf{q}_\alpha(t))V_\alpha(t) \Big]\,dx$$

$$= \int_{\Omega_C(t)} \Psi(t,x') \int_{\mathbb{R}^3} \chi_a(x-x')\,dx\,dx' + \sum_\alpha \Psi_\alpha(t) \int_{\mathbb{R}^3} \chi_a(x-\mathbf{q}_\alpha(t))\,dx\;V_\alpha(t)$$

$$= \int_{\Omega_C(t)} \Psi(t,x')\,dx' + \sum_\alpha \Psi_\alpha(t) V_\alpha(t)$$

Disperse phase transport

Disperse phase transport equation

For any quantity $\Psi_\alpha(t)$

averaged quantity $\overline{\Psi_\alpha}$ satisfies transport equation

$$\frac{\partial c\overline{\Psi_\alpha}}{\partial t}(t,x) + \nabla_x \cdot (c\,\overline{\Psi_\alpha \dot{\mathbf{q}}_\alpha}(t,x)) = c\,\overline{\left(\frac{(\Psi_\alpha V_\alpha)^{\cdot}}{V_\alpha}\right)}(t,x)$$

Reynolds Transport Theorem

$\Psi : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}$ continuously differentiable

$\mathbf{X}^t : \mathbb{R}^N \to \mathbb{R}^N$ continuously differentiable transformations

trajectories $y(t) = \mathbf{X}^t(y_0)$, velocity field $\mathbf{u}(t, y) = \dot{y}(t)$

$\Omega(t)$ any bounded control volume

$$\frac{d}{dt} \int_{\Omega(t)} \Psi(t, y)\, dy = \int_{\Omega(t)} \left[\frac{\partial \Psi}{\partial t}(t, y) + \nabla_y \cdot \Big(\Psi(t, y) \cdot \mathbf{u}(t, y) \Big) \right] dy$$
$$= \int_{\Omega(t)} \frac{\partial \Psi}{\partial t}(t, y)\, dy + \oint_{\partial\Omega(t)} \Big(\Psi(t, y) \mathbf{u}(t, y) \Big) \cdot \boldsymbol{\nu}(t)\, dS$$

Carrier fluid transport equation

Microscopic balance law

$$\frac{\partial}{\partial t}\Psi(t,x') + \nabla_{x'} \cdot \mathbf{F}(t,x') = G(t,x')$$

$I_\alpha(t,x) = \partial B_\alpha(t) \cap B_a(x)$, $\boldsymbol{\nu}_\alpha$ outer unit normal vector

$\mathbf{w}_\alpha(t)$ velocity of $\partial B_\alpha(t)$

$$\begin{aligned}\frac{\partial}{\partial t}(1-c)\overline{\Psi}(t,x) &+ \nabla_x \cdot (1-c)\overline{\mathbf{F}}(t,x) \\ &= \sum_\alpha \oint_{I_\alpha(t,x)} \left[\mathbf{F}(t,x') - \Psi(t,x')\mathbf{w}_\alpha\right] \cdot \boldsymbol{\nu}_\alpha \, \chi_a(x-x')\, d\alpha' \\ &\quad + (1-c)\overline{G}(t,x)\end{aligned}$$

Newton's law with mass change

Closed system: Rocket R emitting burnt gases B

m_R rocket mass, m_B burnt gas mass

burning rate $-\dot{m}_R$

v constant speed relative to rocket of gas emitted in direction of axis parallel to movement of rocket

v_R rocket speed gives $v_B = v_R - v$ burnt gas speed

Mass conservation $\dot{m}_R(t) + \dot{m}_B(t) = 0$

Total momentum of burnt gas

$$m_B v_B = -\int_{t_0}^{t} \dot{m}_R(\tau)(v_R(\tau) - v)\, d\tau$$

Momentum conservation

$$0 = \frac{d}{dt}(m_R v_R + m_B v_B) = \dot{m}_R v_R + m_R \dot{v}_R - \frac{d}{dt}\int_{t_0}^{t} \dot{m}_R(\tau)(v_R(\tau) - v)\,d\tau$$
$$= \dot{m}_R v_R + m_R \dot{v}_R - \dot{m}_R(v_R - v) = m_R \dot{v}_R + \dot{m}_R v$$

Implies

$$m_R(t)\dot{v}_R(t) = -\dot{m}_R(t)v(t)$$

thrust of rocket is $\Theta = -\dot{m}_R v$ and

$$\frac{d}{dt}(m_R v_R) = \dot{m}_R v_R + m_R \dot{v}_R = \dot{m}_R(v_R - v) = \dot{m}_R v_B$$

Newton's law of motion

Particle = rocket

Particles with mass loss or gain
$j = 1, 2, 3$

Momentum equation

$$(m_\alpha(t)\dot{q}^j_\alpha(t))^\cdot = -\oint_{I_\alpha} p\nu^j_\alpha d\alpha' + m_\alpha g^j + \frac{\dot{m}_\alpha(t)}{4\pi r_\alpha(t)^2}\oint_{I_\alpha} v^j(t, x')\, d\alpha'$$

Microscopic conservation laws, carrier phase

Compressible inviscid, ideal, polytropic, isentropic (isothermal) fluid

gravitational field

mass density ρ

pressure p

velocity field $\mathbf{v}$

Five equations: Four conservation laws and one equation of state

Conservation laws

Conservation of mass

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

Conservation of momentum

$$\frac{\partial (\rho v^j)}{\partial t} + \nabla_x \cdot (\rho v^j\, \mathbf{v}) + \frac{\partial p}{\partial x_j} = \rho g^j \qquad j = 1, 2, 3$$

$g^j = -g\delta_{3j}$ gravitational force

$p = \frac{p_0}{\rho_0^\gamma}\rho^\gamma$ with γ adiabatic constant
or $p = a^2\rho$ with local sound speed a

Balance of volume fraction

Discrete transport equation: $\Psi_\alpha = 1$

$$\frac{\partial c}{\partial t}(t,x) + \nabla_x \cdot (c\,\overline{\dot{\mathbf{q}}_\alpha}(t,x)) = c\,\overline{\left(\frac{\dot{V}_\alpha}{V_\alpha}\right)}(t,x)$$

Cold closure assumption $\mathbf{v}_C = \overline{v}$ and $\mathbf{v}_D = \overline{\dot{\mathbf{q}}}_\alpha$

$$\frac{\partial c}{\partial t}(t,x) + \nabla_x \cdot (c\,\mathbf{v}_D(t,x)) = c\,\overline{\left(\frac{\dot{V}_\alpha}{V_\alpha}\right)}(t,x)$$

Note that

$$\frac{\dot{V}_\alpha}{V_\alpha} = 3\frac{\dot{r}_\alpha}{r_\alpha}$$

Mass balances

Carrier phase: $\Psi = \rho$, $\mathbf{F} = \rho \mathbf{v}$

$$\frac{\partial}{\partial t}[(1-c)\rho_C](t,x) + \nabla_x \cdot [(1-c)\rho_C \mathbf{v}_C](t,x)$$
$$= \sum_\alpha \oint_{I_\alpha(t,x)} \rho(t,x') \left[\mathbf{v}(t,x') - \mathbf{w}_\alpha(t)\right] \cdot \boldsymbol{\nu}_\alpha \, \chi_a(x-x') \, d\alpha'$$

Disperse phase: $\Psi_\alpha(t) = m_\alpha(t)/V_\alpha(t)$

$$\frac{\partial c\rho_D}{\partial t}(t,x) + \nabla_x \cdot (c\,\rho_D \mathbf{v}_D)(t,x) = c\,\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,x)$$

Mass balance at Interface

$$2a > r_\alpha(t) \text{ for all } \alpha, \qquad x' = \mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t) \in I_\alpha(t,x)$$

$$c\,\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,x) = \sum_\alpha \dot{m}_\alpha\, \chi_a(x-(\mathbf{q}_\alpha(t)+\mathbf{R}_\alpha(t)) = \sum_\alpha \dot{m}_\alpha\, \chi_a(x-x').$$

Interface mass balance

$$\oint_{I_\alpha(t,x)} \rho(t,x')\left[\mathbf{v}(t,x') - \mathbf{w}_\alpha(t)\right]\cdot \boldsymbol{\nu}_\alpha\, \chi_a(x-x')\, d\alpha' = -\dot{m}_\alpha\, \chi_a(x-x')$$
$$= -\frac{\dot{m}_\alpha}{V_a}$$

or

$$\oint_{I_\alpha(t,x)} \rho(t,x')\left[\mathbf{v}(t,x') - \mathbf{w}_\alpha(t)\right]\cdot \boldsymbol{\nu}_\alpha\, d\alpha' = -\dot{m}_\alpha$$

Momentum carrier phase

We set

$$(1-c)p_C(t,x) = \int_{\Omega_C(t)} p(t,x')\,\chi_a(x-x')\,dx'.$$

Carrier phase $\Psi = \rho v^j$, $\mathbf{F} = \rho v^j \mathbf{v} + \mathbf{e}_j p$, $G^j = \rho g^j$ $j = 1,2,3$

$$\frac{\partial}{\partial t}[(1-c)\rho_C v_C^j](t,x) + \nabla_x \cdot [(1-c)\overline{\rho v^j \mathbf{v}}](t,x) + \frac{\partial (1-c)p_C}{\partial x_j} - (1-c)\rho_C g^j$$

$$= \sum_\alpha \Big(\oint_{I_\alpha(t,x)} \rho v^j(t,x')[\mathbf{v}(t,x') - \mathbf{w}_\alpha]\cdot \boldsymbol{\nu}_\alpha\,\chi_a(x-x')\,d\alpha' + \oint_{I_\alpha(t,x)} p(t,x')\nu_\alpha^j\,\chi_a(x-x')\,d\alpha' \Big).$$

Momentum disperse phase

Disperse phase $\Psi_\alpha(t) = \rho_\alpha(t)\dot{\mathbf{q}}_\alpha(t) = \rho_\alpha(t)\mathbf{v}_\alpha(t)$, $j = 1, 2, 3$

$$\begin{aligned}\frac{\partial c\rho_D v_D^j}{\partial t}(t,x) + \nabla_x \cdot (c\,\overline{\rho_\alpha(t) v_\alpha^j \mathbf{v}_\alpha})(t,x) =& c\,\overline{\left(\frac{(\rho_\alpha \dot{\mathbf{q}}_\alpha V_\alpha)^{\cdot}}{V_\alpha}\right)}(t,x)\\ =& c\,\overline{\left(\frac{(m_\alpha \dot{\mathbf{q}}_\alpha)^{\cdot}}{V_\alpha}\right)}(t,x).\end{aligned}$$

Interface balance

$$-\frac{\dot{m}_\alpha(t)}{4\pi r_\alpha(t)^2}\oint_{I_\alpha} v^j(t,x')d\alpha' = \oint_{I_\alpha} \rho v^j(t,x')[\mathbf{v}(T,x') - \mathbf{w}_\alpha]\cdot\boldsymbol{\nu}_\alpha \, d\alpha'.$$

Terms to be determined

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$$\overline{\rho_\alpha(t) v_\alpha^j \mathbf{v}_\alpha}, \qquad \overline{\rho v^j \mathbf{v}}$$

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Frequently taken

$$\overline{\rho_\alpha(t) v_\alpha^j \mathbf{v}_\alpha} = \rho_D v_D^j \mathbf{v}_D, \qquad \overline{\rho v^j \mathbf{v}} = \rho_C v_C^j \mathbf{v}_C$$

Future work and cooperations within DFG-CNRS research group

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- Numerical computations on test cases relevant to research group