On variational approaches to mixtures

Prague, 5-7 February, Mixtures: Modeling, analysis and computing

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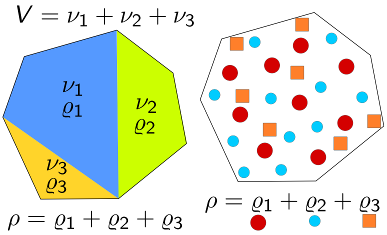
What is a mixture?

1. Classical mixtures

Mixture control volume



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2. "Immiscible" mixtures

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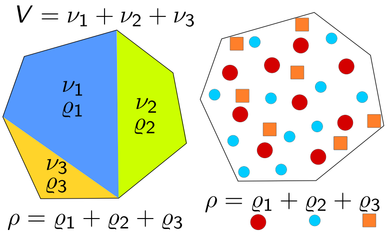

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$c_a = \frac{\varrho_a}{\rho}$ mass fraction of a-th phase

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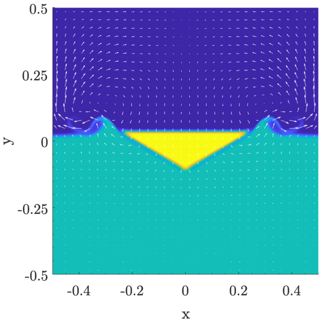

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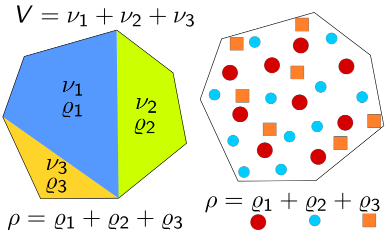

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First principle approaches to mixtures

Multiphysics problems: multispicies plasmas, poroelasticity, granular flows, surface tension, mixtures + electrodynamics, dispersive solids (metamaterials), etc.

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$$\rho_\alpha = m_\alpha \int f_\alpha \, \mathrm{d}\boldsymbol{c}_\alpha$$

$$\rho_\alpha u_i^{(\alpha)} = m_\alpha \int C_i^{(\alpha)} f_\alpha \, \mathrm{d}\boldsymbol{c}_\alpha$$

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1. **Homogenization/averaging** techniques
2. **Energetic** appoaches (Variational/Hamiltonian formulation)

$$S[\varphi] = \int L(\varphi, \dot{\varphi}, \nabla\varphi)\, d\boldsymbol{x}dt$$

$$\mathscr{H} = \mathscr{H}(\boldsymbol{p}, \boldsymbol{q}) \qquad \{A, B\} = \int A_{\boldsymbol{p}} \cdot B_{\boldsymbol{q}} - A_{\boldsymbol{q}} \cdot B_{\boldsymbol{p}} d\boldsymbol{x}$$

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$$\boxed{E = \underbrace{\varepsilon(\rho, s)}_{\text{micro}} + \ldots + \underbrace{\frac{c^2}{2}\boldsymbol{A}^2}_{\text{meso}} + \ldots + \underbrace{\frac{1}{2}\boldsymbol{v}^2}_{\text{macro}}}$$

$$+\frac{7}{5}q_i^{(\alpha)}\frac{\partial v_j}{\partial x_j}+\frac{7}{5}q_j^{(\alpha)}\frac{\partial v_i}{\partial x_j}+\frac{2}{5}q_j^{(\alpha)}\frac{\partial v_j}{\partial x_i}+\left(\sigma_{ij}^{(\alpha)}+\frac{5}{2}\rho_\alpha\theta_\alpha\delta_{ij}\right)\left(\frac{\mathrm{D}v_j}{\mathrm{D}t}-F_j^{(\alpha)}\right)=\frac{1}{2}\mathcal{P}_i^{1(\alpha)} \tag{3.7}$$

Moments method for gas mixtures (Gupta, Torrilhon, 2015, 10.1098/rspa.2014.0754)

$$\frac{\mathrm{D}m_{ijk}^{(\alpha)}}{\mathrm{D}t}+m_{ijk}^{(\alpha)}\frac{\partial v_l}{\partial x_l}+\frac{\partial u_{ijkl}^{0(\alpha)}}{\partial x_l}+\frac{3}{7}\frac{\partial u_{\langle ij}^{1(\alpha)}}{\partial x_{k\rangle}}+3m_{l\langle ij}^{(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_l}+\frac{12}{5}q_{\langle i}^{(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_j}$$
$$+3\sigma_{\langle ij}^{(\alpha)}\left(\frac{\mathrm{D}v_{k\rangle}}{\mathrm{D}t}-F_{k\rangle}^{(\alpha)}\right)=\mathcal{P}_{ijk}^{0(\alpha)}, \tag{3.8}$$

$$\frac{\mathrm{D}u_{ij}^{1(\alpha)}}{\mathrm{D}t}+u_{ij}^{1(\alpha)}\frac{\partial v_k}{\partial x_k}+\frac{\partial u_{ijk}^{1(\alpha)}}{\partial x_k}+\frac{2}{5}\frac{\partial u_{\langle i}^{2(\alpha)}}{\partial x_{j\rangle}}+2u_{ijkl}^{0(\alpha)}\frac{\partial v_k}{\partial x_l}+\frac{6}{7}u_{\langle ij}^{1(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_k}$$
$$+\frac{4}{5}u_{k\langle i}^{1(\alpha)}\frac{\partial v_k}{\partial x_{j\rangle}}+2u_{k\langle i}^{1(\alpha)}\frac{\partial v_{j\rangle}}{\partial x_k}+\frac{14}{15}\Delta_\alpha\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}+14\rho_\alpha\theta_\alpha^2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}+2m_{ijk}^{(\alpha)}\left(\frac{\mathrm{D}v_k}{\mathrm{D}t}-F_k^{(\alpha)}\right)$$
$$+\frac{28}{5}q_{\langle i}^{(\alpha)}\left(\frac{\mathrm{D}v_{j\rangle}}{\mathrm{D}t}-F_{j\rangle}^{(\alpha)}\right)=\mathcal{P}_{ij}^{1(\alpha)}, \tag{3.9}$$

and

$$\frac{\mathrm{D}\Delta_\alpha}{\mathrm{D}t}+\frac{7}{3}\Delta_\alpha\frac{\partial v_i}{\partial x_i}+\frac{\partial u_i^{2(\alpha)}}{\partial x_i}-20\theta_\alpha\sigma_{ij}^{(\alpha)}\frac{\partial v_i}{\partial x_j}-20\theta_\alpha\frac{\partial q_i^{(\alpha)}}{\partial x_i}+15\rho_\alpha\theta_\alpha^2\frac{\partial u_i^{(\alpha)}}{\partial x_i}$$
$$+15\theta_\alpha^2u_i^{(\alpha)}\frac{\partial\rho_\alpha}{\partial x_i}+4u_{ij}^{1(\alpha)}\frac{\partial v_i}{\partial x_j}+8\left(q_i^{(\alpha)}-\frac{5}{2}\rho_\alpha\theta_\alpha u_i^{(\alpha)}\right)\left(\frac{\mathrm{D}v_i}{\mathrm{D}t}-F_i^{(\alpha)}\right)$$
$$=\mathcal{P}^{2(\alpha)}-10\theta_\alpha\mathcal{P}^{1(\alpha)}. \tag{3.10}$$

Variational principles for mixtures

Why variational formulation for mixtures (Stationary Action Principle)?

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1. General Relativity
2. Electrodynamics
3. Fluid and Solid mechanics

Why it's difficult?

$$S[\varphi] = \int L(\varphi, \dot{\varphi}, \nabla\varphi)\, d\boldsymbol{x}dt \longrightarrow \text{PDE:} \qquad \frac{\partial L_{\dot{\varphi}}}{\partial t} + \nabla \cdot L_{\nabla\varphi} = L_{\varphi} \text{ (Euler-Lagrange)}$$

Baer-Nunziato-type models:

$$\frac{\partial \boldsymbol{u}_a}{\partial t} + \nabla \cdot \left(\boldsymbol{u}_a \otimes \boldsymbol{v}_a + p_a \boldsymbol{I}\right) = \sum_{b=1}^{N} p_{I,ab} \nabla \alpha_b$$

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Naive idea:

$$\boldsymbol{X}_1 = \hat{\boldsymbol{X}}_1(\boldsymbol{x}), \qquad \boldsymbol{X}_2 = \hat{\boldsymbol{X}}_2(\boldsymbol{x}) \qquad S[\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2] = \int L(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, \partial_t \boldsymbol{X}_1, \partial_t \boldsymbol{X}_2, \nabla\hat{\boldsymbol{X}}_1, \nabla\hat{\boldsymbol{X}}_2)\, d\boldsymbol{x} dt$$

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SHTC approach:

$$\boldsymbol{X} = \hat{\boldsymbol{X}}(\boldsymbol{x}), \qquad \varphi(\boldsymbol{x}) \qquad S[\hat{\boldsymbol{X}}, \varphi] = \int L(\hat{\boldsymbol{X}}, \varphi, \partial_t \boldsymbol{X}, \partial_t \varphi, \nabla \hat{\boldsymbol{X}}, \nabla \varphi)\, d\boldsymbol{x} dt$$

$\partial_t \varphi = \mu_1 - \mu_2$ chemical potential

$\nabla \varphi = \boldsymbol{v}_1 - \boldsymbol{v}_2$ relative velocity

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Euler-Lagrange:

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Governing equations

Variational formulation:

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0$$

$$E = E_1(\varrho_1, s_1, \ldots) + E_2(\varrho_2, s_2, \ldots) + \ldots$$

$$\partial_t (\rho \alpha_a) + \nabla \cdot (\rho \boldsymbol{v}) = -\Phi_a$$

$$\boxed{\partial_t (\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v} + p\boldsymbol{I} + \boldsymbol{A}_a E_{\boldsymbol{A}_a} + \boldsymbol{w}_a \otimes E_{\boldsymbol{w}_a}) = \rho \boldsymbol{g}}$$

$$\boldsymbol{v} = \frac{\varrho_1 \boldsymbol{v}_1 + \varrho_2 \boldsymbol{v}_2 + \ldots + \varrho_N \boldsymbol{v}_N}{\rho}$$

$$\partial_t \boldsymbol{A} + \boldsymbol{v} \cdot \nabla \boldsymbol{A} + \boldsymbol{A} \nabla \boldsymbol{v} = -\frac{1}{\tau} E_{\boldsymbol{A}}$$

$$\boxed{\partial_t \varrho_a + \nabla \cdot (\varrho_a \boldsymbol{v} + E_{\boldsymbol{w}_a}) = -\chi_a}$$

$$\partial_t \boldsymbol{w}_a + \nabla (\boldsymbol{w}_a \cdot \boldsymbol{v} + E_{\varrho_a}) + (\nabla \times \boldsymbol{w}_a) \times \boldsymbol{v} = -\lambda_a$$

$$\boldsymbol{w}_a = \boldsymbol{v}_a - \boldsymbol{v}_N$$

Ferrari *et al*, JCP, (2025)

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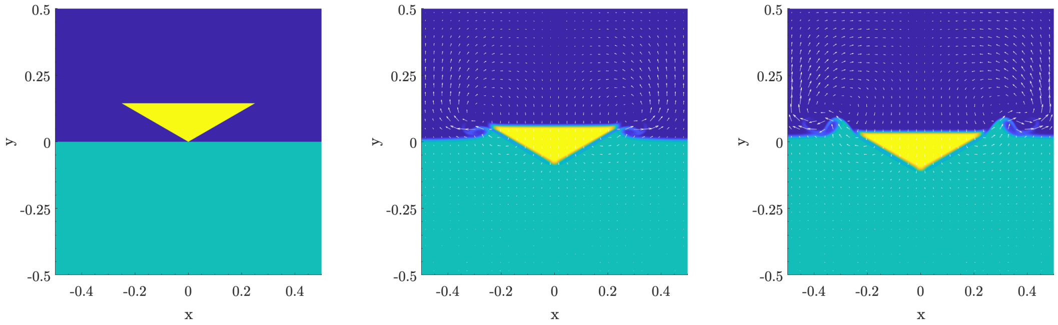
Baer-Nunziato-type formulation

$$\frac{\partial u_{a,i}}{\partial t} + \frac{\partial (u_{a,i} v_{a,k} + P_a \delta_{ki} + \sigma^{\mathrm{e}}_{a,ki} + \sigma^{\mathrm{t}}_{a,ki})}{\partial x_k} = -c_a \sum_{b=1}^{\mathrm{N}} p_b \frac{\partial \alpha_b}{\partial x_i} + p_a \frac{\partial \alpha_a}{\partial x_i}$$
$$-c_a \sum_{b=1}^{\mathrm{N}} \varrho_b \bar{w}_{b,k} \omega_{b,k,i} + \varrho_a \bar{w}_{a,k} \omega_{a,k,i}$$
$$-c_a \sum_{b=1}^{\mathrm{N}} \varrho_b s_b \frac{\partial T_b}{\partial x_i} + \varrho_a s_a \frac{\partial T_a}{\partial x_i}$$
$$-c_a \sum_{b=1}^{\mathrm{N}} \frac{\partial \sigma^{\mathrm{e}}_{b,ki}}{\partial x_k} + \frac{\partial \sigma^{\mathrm{e}}_{a,ki}}{\partial x_k}$$
$$+c_a \sum_{b=1}^{\mathrm{N}} \varrho_b \frac{\partial e^{\mathrm{e}}_b}{\partial x_i} - \varrho_a \frac{\partial e^{\mathrm{e}}_a}{\partial x_i}$$
$$-c_a \sum_{b=1}^{\mathrm{N}} \varrho_b \Lambda_{b,i} + \varrho_a \Lambda_{a,i}$$

Ferrari *et al*, JCP, (2025)

Computational examples immiscible mixtures

A three-phase flows (gas, liquid, solid)



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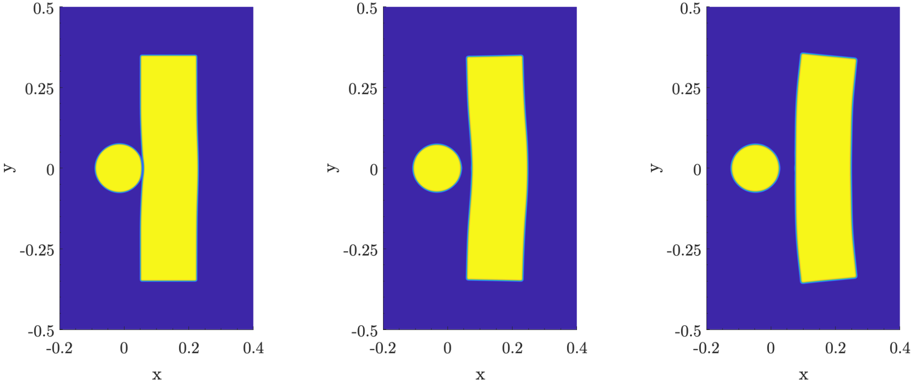
Elastic collision (gas, solid, solid)



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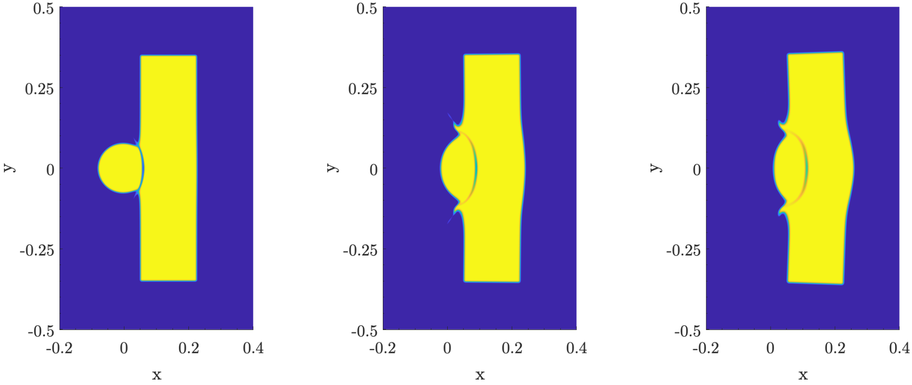

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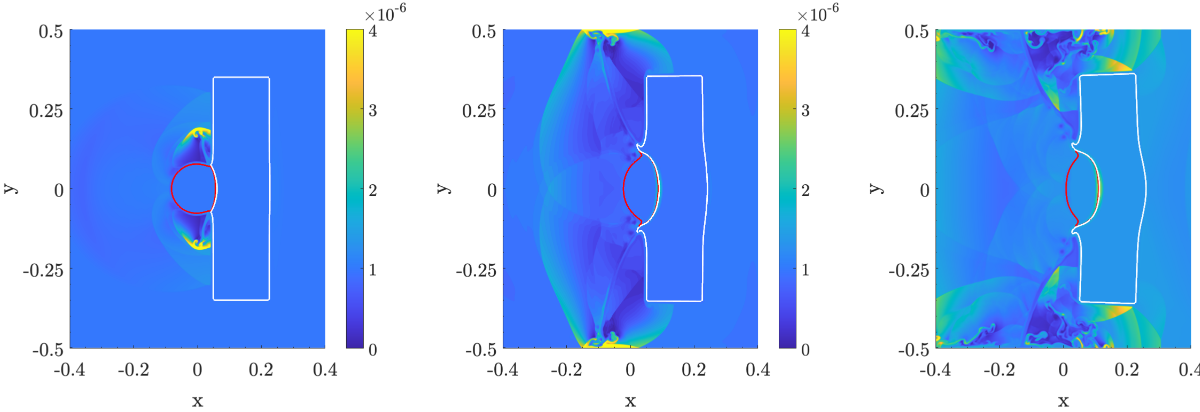

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