Distributional equations and diffuse and sharp interfaces

Hans Wilhelm Alt

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Plan of the talk:

- Distributions in spacetime
- Examples: Surfaces, lines, points
- Objectivity (Frame indifference)
- Phase field model: Asmptotic limit towards distributions

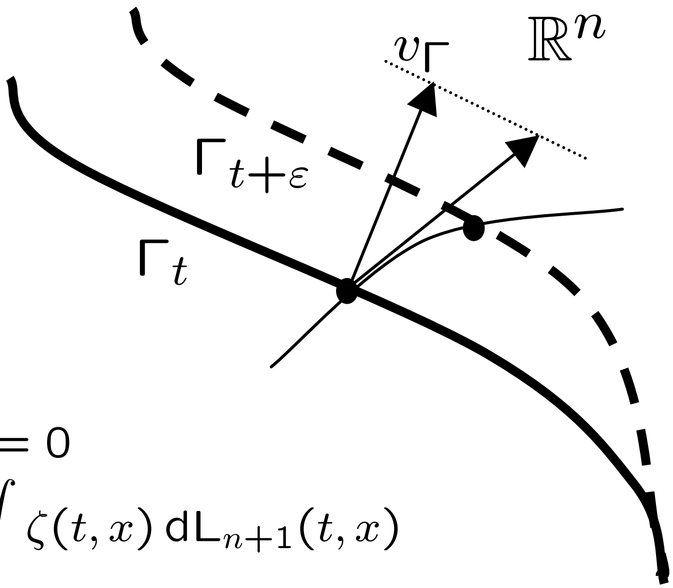
Surfaces: $(t,x) \in \Gamma \iff x \in \Gamma_t$

$$\Gamma \subset \mathbb{R} \times \mathbb{R}^n \quad (m+1)\text{-dimensional}\,, \quad T_{(t,x)}\Gamma \neq \{0\} \times \mathbb{R}^n$$

$$\Gamma_t := \{x \in \mathbb{R}^n\,;\; (t,x) \in \Gamma\} \quad m\text{-dimensional}\,, \quad 0 \le m \le n$$

$$v_\Gamma \;\text{“surface velocity”}\;, \quad T_{(t,x)}\Gamma = \text{span}\,\{(1, v_\Gamma(t,x))\} \cup \{0\} \times T_x\Gamma_t$$

Surface measures:



$$\langle\, \zeta \,,\, \boldsymbol{\mu}_\Gamma \,\rangle := \int_{\mathbb{R}} \int_{\Gamma_t} \zeta(t,x)\, \mathrm{dH}_m(x)\, \mathrm{dL}_1(t)$$

$$= \int_{\Gamma} \frac{\zeta(t,x)}{\sqrt{1+|v_\Gamma|^2}}\, \mathrm{dH}_{m+1}(t,x)$$

Extreme cases $m = n$ and $m = 0$:

Ω (Ω_t n-dimensional = open set) $\quad v_\Omega = 0$

$$\langle\, \zeta \,,\, \boldsymbol{\mu}_\Omega \,\rangle = \int_{\mathbb{R}} \int_{\Omega_t} \zeta(t,x)\, \mathrm{dH}_n(x)\, \mathrm{dL}_1(t) = \int_{\Omega} \zeta(t,x)\, \mathrm{dL}_{n+1}(t,x)$$

Γ ($\Gamma_t = \{y_t\}$ 0-dimensional = point) $\quad v_\Gamma = \dot{y}_t$

$$\langle\, \zeta \,,\, \boldsymbol{\mu}_\Gamma \,\rangle = \int_{\mathbb{R}} \int_{\{y_t\}} \zeta(t,x)\, \mathrm{dH}_0(x)\, \mathrm{dL}_1(t) = \int_{\mathbb{R}} \zeta(t,y_t)\, \mathrm{dL}_1(t)$$

Theorem (Distributional and strong version)

Let $t \mapsto \Gamma_t$ be m-dimensional, $0 \le m \le n$. The equation

$$\partial_t(e\boldsymbol{\mu}_\Gamma) + \text{div}\,(q\boldsymbol{\mu}_\Gamma) = f\boldsymbol{\mu}_\Gamma$$

is equivalent to

$q - ev_\Gamma$ tangential on Γ $\qquad (q - ev_\Gamma)(t,x) \in T_x\Gamma_t$

$\partial_t^\Gamma e - ev_\Gamma \bullet \kappa_\Gamma + \text{div}^\Gamma(q - ev_\Gamma) = f$ on Γ $\qquad \partial_t^\Gamma e + \text{div}^\Gamma q = f$

Here

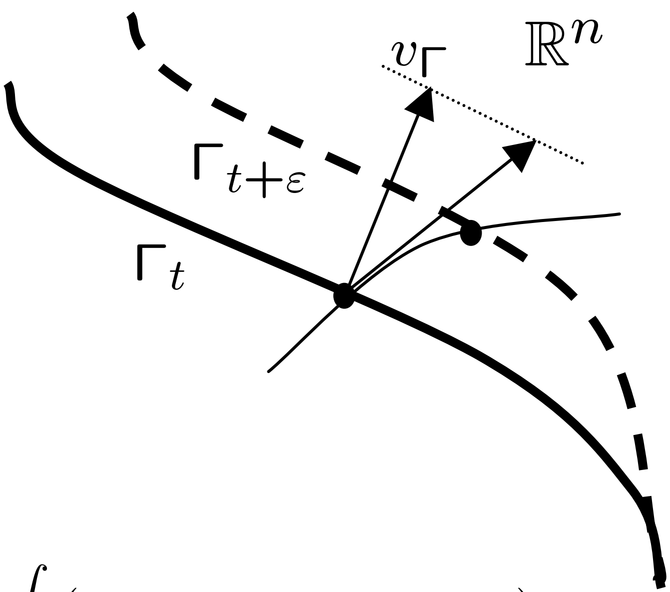
$\Gamma_t := \{x \in \mathbb{R}^n\,;\ (t,x) \in \Gamma\}$

$v_\Gamma(t,x) \in T_x\Gamma_t^\perp$ "surface velocity" of Γ_t

$\kappa_\Gamma(t,x)$ m-times mean curvature of Γ_t

$\partial_t^\Gamma := \partial_t + v_\Gamma \bullet \nabla$

$\text{div}^\Gamma := \sum_{i=1,\dots,m} \tau_k \bullet \partial_{\tau_k}$



$$\langle\, \zeta\,,\, -\partial_t(e\boldsymbol{\mu}_\Gamma) - \text{div}\,(q\boldsymbol{\mu}_\Gamma) + f\boldsymbol{\mu}_\Gamma \,\rangle$$

$$= \langle\, \partial_t\zeta\,,\, e\boldsymbol{\mu}_\Gamma \,\rangle + \langle\, \nabla\zeta\,,\, q\boldsymbol{\mu}_\Gamma \,\rangle + \langle\, \zeta\,,\, f\boldsymbol{\mu}_\Gamma \,\rangle = \int \big(\partial_t\zeta \cdot e + \nabla\zeta \bullet q + \zeta \cdot f\big)\, \mathrm{d}\boldsymbol{\mu}_\Gamma$$

Examples of distributions in $\mathcal{D}'(U)$, $U \subset \mathbb{R} \times \mathbb{R}^n$:

Body Ω with mass exchange at the boundary $\Gamma = \partial\Omega$

$$\partial_t(\varrho \boldsymbol{\mu}_\Omega) + \text{div}\,(\varrho v \boldsymbol{\mu}_\Omega) = \tau \boldsymbol{\mu}_\Gamma$$

(τ mass production at boundary)

$$\Longleftrightarrow$$

$$\partial_t \varrho + \text{div}(\varrho v) = 0 \quad \text{in } \Omega$$

$$0 = \tau + \varrho(v - v_\Gamma) \bullet \nu_\Omega \quad \text{on } \Gamma$$

PDE as distribution Body $\Omega = U$

$$\partial_t(\varrho \boldsymbol{\mu}_U) + \text{div}\,(\varrho v \boldsymbol{\mu}_U) = 0$$

$$\Longleftrightarrow$$

$$\partial_t \varrho + \text{div}(\varrho v) = 0 \quad \text{in all of } U$$

Mass balance on a membrane Γ

with mass density $\varrho^s > 0$ and "particle velocity" v^s

$$\partial_t(\varrho^s \boldsymbol{\mu}_\Gamma) + \text{div}\,(\varrho^s v^s \boldsymbol{\mu}_\Gamma) = 0$$

$\Longleftrightarrow$ on Γ:

$v^s - v_\Gamma$ tangential

$$\partial_t^\Gamma \varrho^s - \varrho^s\, \kappa_\Gamma \bullet v_\Gamma + \text{div}^\Gamma(\varrho^s(v^s - v_\Gamma)) = 0$$

κ_Γ $(n-1)$-times mean curvature vector of Γ

$\partial_t^\Gamma := \partial_t + v_\Gamma \bullet \nabla$ time derivative of Γ

Strong differential equality $\Longleftrightarrow$ $\partial_t^\Gamma \varrho^s + \text{div}^\Gamma(\varrho^s v^s) = 0$

Mass in a system of M curves Γ_t^k which meet at point P_t, everything is moving

$$\partial_t\Big(\sum_{k=1}^{M}\varrho^k\boldsymbol{\mu}_{\Gamma^k}\Big) + \mathrm{div}\,\Big(\sum_{k=1}^{M}\varrho^k v^k\boldsymbol{\mu}_{\Gamma^k}\Big) = a\,\boldsymbol{\mu}_P$$

$$\Longleftrightarrow$$

$$\left.\begin{array}{ll} v^k - v_{\Gamma^k} & \text{tangential} \\ \partial_t^{\Gamma^k}\varrho^k + \mathrm{div}^{\Gamma^k}(\varrho^k v^k) = 0 & \end{array}\right\} \quad \text{on } \Gamma^k,\ k = 1,2,3$$

$$\sum_{k=1}^{M}\varrho^k\frac{(1,v^k)\bullet\underline{n}_{\Gamma^k}}{\sqrt{1+|v_\Gamma^k|^2}} = \frac{a}{\sqrt{1+|v_P|^2}} \qquad \text{on } P$$

$\underline{n}_{\Gamma^k}$ tangent at Γ^k, normal to P

Objectivity (Frame indifference)

- The value of physical quantities depend on the observer
- The type of a physical quantity is given by a transformation rule
- The description of physical processes has to be independent of the observer

Observer transformations (classical group = Newton's physics)

$$\begin{bmatrix} t \\ x \end{bmatrix} = y = Y(y^*) = Y(t^*, x^*) = \begin{bmatrix} T(t^*, x^*) \\ X(t^*, x^*) \end{bmatrix} = \begin{bmatrix} t^* + a \\ Q(t^*)x^* + b(t^*) \end{bmatrix}$$

where $a \in \mathbb{R}$, $b : \mathbb{R} \to \mathbb{R}^n$, $Q : \mathbb{R} \to \mathbb{R}^{n\times n}$ orthogonal transformation, $\det Q = 1$

$$\underline{\mathrm{D}}Y = (Y_{k\,'l})_{k,l=0,\ldots,n} = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \dot{Q}x^* + \dot{b} & Q \end{bmatrix}$$

Examples of transformation rules:

ϱ objective scalar $\iff$ $\varrho \circ Y = \varrho^*$

that is $\varrho(t,x) = \varrho^*(t^*,x^*)$ for $(t,x) = Y(t^*,x^*)$

v velocity $\iff$ $v \circ Y = \dot{X} + Qv^*$ (Doppler effect)

that is $v(t,x) = \dot{X}(t^*,x^*) + Q(t^*)v^*(t^*,x^*)$ for $(t,x) = Y(t^*,x^*)$

$\mathbf{f}$ force $\iff$ $\mathbf{f} \circ Y = \varrho^*(\ddot{X} + 2\dot{Q}v^*) + \dot{Q}J^* + r^*\dot{X} + Q\mathbf{f}^*$

(if mass conservation is $\partial_t \varrho + \mathrm{div}\,(\varrho v + J) = r$)

They come from objectivity of balance laws

Theorem (Objectivity for certain systems of balance laws)

$$\partial_t(e^k \mu_\Gamma) + \sum_{i=1}^{n} \partial_{x_i}(q_i^k \mu_\Gamma) = f^k \mu_\Gamma \qquad \text{(k=1,...,N)}$$

Physical type given by (linear) transformation rule for test functions

$$\zeta \circ Y = Z^{-\mathsf{T}} \zeta^* \qquad (\zeta^* = Z^{\mathsf{T}} \zeta \circ Y)$$

Then this system is objective, if

$$e \circ Y = Z e^*$$

$$q_i \circ Y = \dot{X}_i Z e^* + \sum_{j=1}^{n} Q_{ij} Z q_j^* \qquad \text{for } i = 1, \ldots, n$$

$$f \circ Y = Z_{,t} e^* + \sum_{j=1}^{n} Z_{,j} q_j^* + Z f^*$$

Examples:

mass — mass-momentum — mass-momentum-energy

$$Z = 1 \qquad Z = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} = \underline{\mathsf{D}} Y \qquad Z := \begin{bmatrix} 1 & 0 & 0 \\ \dot{X} & Q & 0 \\ \frac{1}{2}|\dot{X}|^2 & \dot{X}^{\mathsf{T}} Q & 1 \end{bmatrix}$$

($Z = Z(Y)$ is a differential operator in Y)

Proof: All μ_Γ have the same transformation behaviour

Weak formulation in spacetime:

$$\partial_0 := \partial_t,\ q_0 := e,\ q_i = (q_i^k)_{k=1,\dots,N},\ f = (f^k)_{k=1,\dots,N}$$

$$\int \Big(\sum_{i=0}^{n} \partial_i\zeta\bullet q_i + \zeta\bullet f\Big)\,\mathrm{d}\mu_\Gamma = 0 \text{ for test functions } \zeta = (\zeta^k)_{k=1,\dots,N}$$

$$\zeta^* = Z^\mathsf{T}\zeta\circ Y \quad \Rightarrow \quad \partial_j\zeta^* = {Z_{'j}}^\mathsf{T}\zeta\circ Y + \sum_{i=0}^{n} Y_{i'j}Z^\mathsf{T}(\partial_i\zeta)\circ Y$$

$\Longrightarrow$

$$\int \Big(\sum_{j=0}^{n} \partial_j\zeta^*\bullet q_j^* + \zeta^*\bullet f^*\Big)\,\mathrm{d}\mu_{\Gamma^*}$$

$$= \int \Big(\sum_{i=0}^{n}(\partial_i\zeta\circ Y)\bullet(\sum_{j=0}^{n} Y_{i'j}Zq_j^*) + (\zeta\circ Y)\bullet(Zf^* + \sum_{j=0}^{n} Z_{'j}q_j^*)\Big)\,\mathrm{d}\mu_{\Gamma^*}$$

$$\overset{(\det=1)}{=} \int \Big(\sum_{i=0}^{n}\partial_i\zeta\bullet(\sum_{j=0}^{n} Y_{i'j}Zq_j^*)\circ Y^{-1} + \zeta\bullet(Zf^* + \sum_{j=0}^{n} Z_{'j}q_j^*)\circ Y^{-1}\Big)\,\mathrm{d}\mu_\Gamma$$

$$\overset{!}{=} \int \Big(\sum_{i=0}^{n}\partial_i\zeta\bullet q_i + \zeta\bullet f\Big)\,\mathrm{d}\mu_\Gamma$$

$\Longleftarrow$

$$q_i\circ Y = \sum_{j=0}^{n} Y_{i'j}Zq_j^* \text{ for } i = 0,\dots,n \qquad f\circ Y = \sum_{j=0}^{n} Z_{'j}q_j^* + Zf^*$$

Examples:

Mass-momentum system

$$\partial_t(\varrho\mu_U) + \mathrm{div}(\varrho v \mu_U) = 0$$

$$\partial_t(\varrho v \mu_U) + \mathrm{div}((\varrho v v^{\mathsf{T}} + \Pi)\mu_U) = \mathbf{f}\mu_U$$

The transformation matrix is

$$Z = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} = \underline{\mathrm{D}}Y$$

Objectivity says

$$\begin{bmatrix} \varrho & \varrho v^{\mathsf{T}} \\ \varrho v & \varrho v v^{\mathsf{T}} + \Pi \end{bmatrix} \circ Y = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} \begin{bmatrix} \varrho^* & \varrho^* v^{*\mathsf{T}} \\ \varrho^* v^* & \varrho^* v^* v^{*\mathsf{T}} + \Pi^* \end{bmatrix} \begin{bmatrix} 1 & \dot{X}^{\mathsf{T}} \\ 0 & Q \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ \mathbf{f} \end{bmatrix} \circ Y = \begin{bmatrix} 0 & 0 \\ \ddot{X} & \dot{Q} \end{bmatrix} \begin{bmatrix} \varrho^* \\ \varrho^* v^* \end{bmatrix} + \sum_{j=1}^{n} \begin{bmatrix} 0 & 0 \\ \dot{X}_{,j} & 0 \end{bmatrix} \begin{bmatrix} \varrho^* v_j^* \\ \cdots \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} \begin{bmatrix} 0 \\ \mathbf{f}^* \end{bmatrix}$$

$\Longleftrightarrow$

ϱ is an objective scalar, i.e. $\varrho \circ Y = \varrho^*$

v is a velocity, i.e. $v \circ Y = \dot{X} + Q v^*$

Π is an objective tensor, i.e. $\Pi \circ Y = Q \Pi^* Q^{\mathsf{T}}$

$\mathbf{f}$ is a force, i.e. $\mathbf{f} \circ Y = \varrho^*(\ddot{X} + 2\dot{Q} v^*) + Q\mathbf{f}^*$

Choice of Π as an objective tensor:

For fluids (Velocity v is independent variable)

$$\Pi = p\mathrm{Id} - S$$

$$p = \varrho f'_{\varrho} - f \qquad \text{free energy: } f = \widehat{f}(\varrho, v) = \frac{\varrho}{2}|v|^2 + \widehat{f}_0(\varrho)$$

$$S = \lambda_1 \mathrm{div}\, v \ \mathrm{Id} + \lambda_2\Big((\mathrm{D}v)^{\mathsf{S}} - \frac{1}{n}\mathrm{div}\, v \ \mathrm{Id}\Big)$$

$(\mathrm{D}v)^{\mathsf{S}}$ objective tensor

$\lambda_1 = \widehat{\lambda}_1(\varrho)\,, \quad \lambda_2 = \widehat{\lambda}_2(\varrho)$ objective scalars

For solids (Velocity v is dependent variable)

$$\Pi = -\sum_{i=1}^{n} \lambda_i e_i {e_i}^{\mathsf{T}}$$

$e_i = \widehat{e}_i(\underline{x})$ objective vectors

$\lambda_i = \widehat{\lambda}_i(\underline{x})$ objective scalars

Reference coordinates $\underline{x} = \xi(t,x)$ components ξ_i are objective scalars

$$(t,\underline{x}) \mapsto (t,x) = \tau(t,\underline{x}) := (t, \phi(t,\underline{x}))$$

$v(t,x) = \partial_t\phi(t,\underline{x})$ for $x = \phi(t,\underline{x})$ or $\underline{x} = \xi(t,x)$

It follows: $\underline{\varrho} = \underline{\varrho}(\underline{x})$, $\partial_t(\underline{\varrho}V) - \mathrm{div}\, P = \underline{\mathbf{f}}$

where $P = J \cdot (-\Pi\circ\tau) F^{-\mathsf{T}}$ first Piola-Kirchhoff stress tensor

$J = \det \mathrm{D}\phi$, $V = \partial_t\phi$, $F = \mathrm{D}\phi$, $\underline{\varrho} = J \cdot \varrho\circ\tau$, $\underline{\mathbf{f}} = J \cdot \varrho\mathbf{f}\tau$

Mass-momentum system for an interface problem

Let $\Gamma := \partial\Omega$

$$\partial_t(\varrho\boldsymbol{\mu}_\Omega) + \mathrm{div}(\varrho v\boldsymbol{\mu}_\Omega) = \mathbf{r}^s\boldsymbol{\mu}_\Gamma$$

$$\partial_t(\varrho v\boldsymbol{\mu}_\Omega) + \mathrm{div}((\varrho v v^\mathsf{T} + \Pi)\boldsymbol{\mu}_\Omega + \Pi^s\boldsymbol{\mu}_\Gamma) = \mathbf{f}\boldsymbol{\mu}_\Omega + \mathbf{f}^s\boldsymbol{\mu}_\Gamma$$

The transformation matrix is still

$$Z = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} = \underline{\mathsf{D}}Y$$

Objectivity says on Γ

$$\begin{bmatrix} 0 & 0 \\ 0 & \Pi^s \end{bmatrix} \circ Y = \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & \Pi^{s*} \end{bmatrix} \begin{bmatrix} 1 & \dot{X}^\mathsf{T} \\ 0 & Q \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{r}^s \\ \mathbf{f}^s \end{bmatrix} \circ Y = \begin{bmatrix} 0 & 0 \\ \ddot{X} & \dot{Q} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \sum_{j=1}^{n} \begin{bmatrix} 0 & 0 \\ \dot{X}_{,j} & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \cdots \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ \dot{X} & Q \end{bmatrix} \begin{bmatrix} \mathbf{r}^{s*} \\ \mathbf{f}^{s*} \end{bmatrix}$$

$\Longleftrightarrow$

$\mathbf{r}^s$ is an objective scalar, i.e. $\mathbf{r}^s \circ Y = \mathbf{r}^{s*}$

Π^s is an objective tensor, i.e. $\Pi^s \circ Y = Q\Pi^{s*}Q^\mathsf{T}$

$\mathbf{f}^s$ is surface force, i.e. $\mathbf{f}^s \circ Y = \mathbf{r}^{s*}\dot{X} + Q\mathbf{f}^{s*}$

Lemma A possible choice is $\mathbf{f}^s = \mathbf{r}^s v + \mathbf{f}^s_0$ with $\mathbf{f}^s_0 \circ Y = Q\mathbf{f}^{s*}_0$

Drop given by distributional conservation laws
for mass and momentum in Ω and on $\Gamma := \partial\Omega$

$$\partial_t(\varrho\boldsymbol{\mu}_\Omega) + \mathrm{div}(\varrho v\boldsymbol{\mu}_\Omega) = 0$$

$$\partial_t(\varrho v\boldsymbol{\mu}_\Omega) + \mathrm{div}\Big((\varrho v v^\top + \Pi)\boldsymbol{\mu}_\Omega + \Pi^s\boldsymbol{\mu}_\Gamma\Big) = \mathbf{f}\boldsymbol{\mu}_\Omega$$

System gives transformation rules

$\Longleftrightarrow$

mass and momentum equation in Ω

on Γ: $(v - v_\Gamma)\bullet\nu_\Omega = 0$, $\Pi^s\nu = 0$ for normal ν, $\mathrm{div}^\Gamma\Pi^s = \Pi\nu_\Omega =: \mathbf{f}^s$

Therefore it contains the

Surface tension law on Γ

$$\mathrm{div}(\Pi^s\boldsymbol{\mu}_\Gamma) = \mathbf{f}^s\boldsymbol{\mu}_\Gamma \qquad \left(\Longleftrightarrow \int (\mathrm{D}\zeta\bullet\Pi^s + \zeta\bullet\mathbf{f}^s)\,\mathrm{d}\boldsymbol{\mu}_\Gamma = 0 \text{ for } \zeta \in \mathcal{D}(U;\mathbb{R}^n)\right)$$

$\mathrm{D}\zeta = (\partial_j\zeta_i)_{i,j=1,\dots,n}$

$\Longleftrightarrow$

$\mathrm{div}^\Gamma\Pi^s = \mathbf{f}^s$,

$\Pi^s\nu = 0$ for $\nu = \pm\nu_\Omega$

Objectivity

v_Γ is "surface velocity":	$v_\Gamma\circ Y = \dot{X}\bullet(Q\nu^*)Q\nu^* + Qv_{\Gamma^*}$
Π^s objective tensor	ν_Ω objective vector
$\Pi^s\nu_\Omega = 0$ is objective	$\mathbf{f}^s = \Pi\nu_\Omega$ objective vector

Surface tension as function of normal

It is $\Pi^s \nu_\Omega = 0$, and if Π^s symmetric tensor, $n = 3$

Result: If $\Pi^s = \widehat{\Pi}^s(\nu)$ then

$$\Pi^s = -\gamma(\mathrm{Id} - \nu\nu^\mathsf{T})$$
$\gamma \in \mathbb{R}$ surface tension

Result: If Π is constant, then

$$\Pi = p\mathrm{Id}$$
$p \in \mathbb{R}$ pressure

General: Π^s (and Π) can depend also on objective scalars, like ϱ or p or θ

Laplace formula: If $\gamma : \Gamma \to \mathbb{R}$ and $\Pi^s = -\gamma(\mathrm{Id} - \nu\nu^\mathsf{T})$ then

$$\mathrm{div}^\Gamma \Pi^s = \mathrm{div}^\Gamma(-\gamma(\mathrm{Id} - \nu\nu^\mathsf{T})) = -\gamma\kappa_\Gamma - \nabla^\Gamma\gamma$$

Hence the surface law of the momentum equation is $\gamma\kappa_\Gamma + \nabla^\Gamma\gamma + \Pi\nu_\Omega = 0$

Liquid drop If $\Pi^s = -\gamma(\mathrm{Id} - \nu\nu^\mathsf{T})$ and $\Pi = p\mathrm{Id} - S$ then

mass and momentum equation in Ω

$$\left.\begin{array}{l} (v - v_\Gamma)\bullet\nu = 0 \\ \partial_\tau\gamma = \tau\bullet S\nu_\Omega \quad \text{for tangential vectors } \tau \\ \gamma\kappa_\Gamma\bullet\nu_\Omega + p = \nu\bullet S\nu \end{array}\right\} \text{ on } \Gamma$$

Further constitutive constraints $\mathrm{D}v\bullet S \geq 0$, $f^s = \gamma = \mathrm{const}$ come from free energy inequality:

Free energy inequality

$$\partial_t F + \operatorname{div}\Phi - G_0 \le 0$$

that is

$$0 \ge \partial_t\big(\underbrace{f\boldsymbol{\mu}_\Omega + f^s\boldsymbol{\mu}_\Gamma}_{F} \big) + \operatorname{div}\big(\underbrace{(fv + \Pi^\mathsf{T} v)\boldsymbol{\mu}_\Omega + (f^s v + \Pi^{s\mathsf{T}} v)\boldsymbol{\mu}_\Gamma}_{\Phi} \big) - \underbrace{v\bullet\mathbf{f}\ \boldsymbol{\mu}_\Omega}_{G_0}$$

$$=: \ g\,\boldsymbol{\mu}_\Omega + g^s\,\boldsymbol{\mu}_\Gamma$$

that is

$$g \le 0 \text{ on } \Omega \quad \text{and} \quad g^s \le 0 \text{ on } \Gamma$$

that is on Ω:

$$0 \ge g = \partial_t f + \operatorname{div}(fv + \Pi^\mathsf{T} v) - v\bullet\mathbf{f} \qquad f = f(\varrho, v) = \frac{\varrho}{2}|v|^2 + f_0(\varrho)$$

$$= \partial_t f_0 + \operatorname{div}(f_0 v) + \mathrm{D}v\bullet\Pi \qquad \Pi = p\mathrm{Id} - S$$

$$= \mathrm{D}v\bullet((f_0 - \varrho f_0{}'_\varrho)\mathrm{Id} + \Pi) = -\mathrm{D}v\bullet S \qquad p = \varrho f_0{}'_\varrho - f_0$$

and on Γ: $\quad (f^s v + \Pi^{s\mathsf{T}} v)\bullet\nu_\Omega = f^s v_\Gamma\bullet\nu_\Omega, \quad (v - v_\Gamma)\bullet\nu_\Omega = 0$

$$0 \ge g^S = \partial_t^\Gamma f^s + \operatorname{div}^\Gamma(f^s v + \Pi^{s\mathsf{T}} v) - (f(v - v_\Gamma) + \Pi^\mathsf{T} v)\bullet\nu_\Omega$$

$$= (\partial_t^\Gamma + v\bullet\nabla^\Gamma)f^s + (\mathrm{D}^\Gamma v)\bullet(f^s\mathrm{Id} + \Pi^s) + v\bullet\big(\underbrace{\operatorname{div}^\Gamma \Pi^s - \Pi\nu_\Omega}_{=0} \big)$$

$$= (\partial_t + v\bullet\nabla)f^s + (\mathrm{D}^\Gamma v)\bullet(f^s\mathrm{Id} + \Pi^s) \qquad \mathrm{D}^\Gamma v = \sum_\tau (\partial_\tau v)\otimes\tau$$

satisfied, if $\mathrm{D}v\bullet S \ge 0$, $f^s = \gamma = \text{const}$

Liquid drop It is $\gamma = \text{const}$, and it follows

$$\left.\begin{array}{l} \partial_t \varrho + \operatorname{div}(\varrho v) = 0 \\ \partial_t(\varrho v) + \operatorname{div}(\varrho v v^{\mathsf{T}} + p\mathrm{Id} - S) = \mathbf{f} \\ p = \varrho f_0{}'_\varrho - f_0, \qquad \mathrm{D}v \bullet S \geq 0 \end{array}\right\} \text{ on } \Omega$$

$$\left.\begin{array}{l} (v - v_\Gamma) \bullet \nu = 0 \\ \tau \bullet S\nu = 0 \qquad \text{for tangential vectors } \tau \\ \gamma \kappa_\Gamma \bullet \nu_\Omega + p = \nu \bullet S\nu \\ f^s = \gamma \end{array}\right\} \text{ on } \Gamma$$

Remark If $v = 0$, $v_\Gamma = 0$, $\varrho = \text{const}$, $\mathbf{f} = 0$ define ($\Gamma = \partial\Omega$)

$$E_\Gamma = \int_\Gamma \gamma \, \mathrm{dH}_{n-1} - \int_\Omega p \, \mathrm{dL}_n \quad \Big(= \int_\Gamma f^s \, \mathrm{dH}_{n-1} + \int_\Omega f \, \mathrm{dL}_n \Big)$$

and solution is "stationary point" of E_Γ

In general the solution is related to the free energy inequality

$$\partial_t(f \boldsymbol{\mu}_\Omega + f^s \boldsymbol{\mu}_\Gamma) + \operatorname{div}(\ldots) - v \bullet \mathbf{f} \, \boldsymbol{\mu}_\Omega \leq 0$$

An Allen-Cahn model for compressible fluids

Witterstein model

$$\partial_t \varrho + \mathrm{div}\,(\varrho v) = 0 \qquad f_\delta = f_\delta(\varrho, \varphi, \nabla\varphi)$$

$$\varrho(\partial_t \varphi + v \bullet \nabla\varphi) = -\mathbf{r}_\delta \qquad \mathbf{r}_\delta := c_\delta(\varrho, \varphi)\frac{\boldsymbol{\delta} f_\delta}{\boldsymbol{\delta}\varphi}$$

$$\partial_t(\varrho v) + \mathrm{div}\,(\varrho v v^{\mathsf{T}} + \Pi_\delta) = \mathbf{f}_\delta \qquad \Pi_\delta = P_\delta - S$$

with

$$P_\delta := (\varrho f_{\delta\,'\varrho} - f_\delta)\mathrm{Id} + \nabla\varphi (f_{\delta\,'\nabla\varphi})^{\mathsf{T}}$$

$$S := \lambda_1(\varrho, \varphi)\mathrm{div}\, v\ \mathrm{Id} + \lambda_2(\varrho, \varphi)\Big((\mathrm{D}v)^{\mathsf{S}} - \frac{1}{n}\mathrm{div}\, v\ \mathrm{Id}\Big)$$

$$f_\delta(\varrho, \varphi, \nabla\varphi) := \frac{1}{\delta}\varrho W(\varphi) + \delta\, h(\varrho)\frac{|\nabla\varphi|^2}{2} + U(\varrho, \varphi)$$

W has two local minima at 0 and 1, $U_{'\varphi}(\varrho, 0) = 0$, $U_{'\varphi}(\varrho, 1) = 0$

$$\frac{\boldsymbol{\delta} f_\delta}{\boldsymbol{\delta}\varphi} = \frac{1}{\delta}\varrho W_{'\varphi}(\varphi) - \delta\,\mathrm{div}\,(h(\varrho)\nabla\varphi) + U_{'\varphi}(\varrho, \varphi)$$

Free energy inequality $f = f(\varrho, \varphi, v, \nabla\varphi) = \frac{\varrho}{2}|v|^2 + f_\delta(\varrho, \varphi, \nabla\varphi)$

$$\partial_t f + \mathrm{div}\,(f v + \Pi_\delta^{\mathsf{T}} v - \dot\varphi f_{'\nabla\varphi}) - v \bullet \mathbf{f}_\delta = -\frac{1}{\varrho}\mathbf{r}_\delta \frac{\boldsymbol{\delta} f_\delta}{\boldsymbol{\delta}\varphi} - \mathrm{D}v \bullet S \le 0$$

System written for the two masses ϱ^1 and ϱ^2

$$\varrho^1_\delta = (1-\varphi)\varrho\,, \quad \varrho^2_\delta = \varphi\varrho\,, \quad \text{or} \quad \varrho = \varrho^1_\delta + \varrho^2_\delta\,, \quad \varphi = \frac{\varrho^2_\delta}{\varrho^1+\varrho^2}$$

becomes

$$\partial_t(\varrho^1_\delta \mu_U) + \operatorname{div}(\varrho^1_\delta v_\delta \mu_U) = \mathbf{r}_\delta \mu_U$$

$$\partial_t(\varrho^2_\delta \mu_U) + \operatorname{div}(\varrho^2_\delta v_\delta \mu_U) = -\mathbf{r}_\delta \mu_U$$

$$\partial_t(\varrho v \mu_U) + \operatorname{div}\big((\varrho v v^\mathsf{T} + \Pi_\delta)\mu_U\big) = \mathbf{f}\mu_U$$

Theorem In the limit $\delta \to 0$ this becomes

$$\partial_t(\varrho^1 \boldsymbol{\mu}_{\Omega^1}) + \operatorname{div}(\varrho^1 v^1 \boldsymbol{\mu}_{\Omega^1}) = \mathbf{r}\,\boldsymbol{\mu}_\Gamma$$

$$\partial_t(\varrho^2 \boldsymbol{\mu}_{\Omega^2}) + \operatorname{div}(\varrho^2 v^2 \boldsymbol{\mu}_{\Omega^2}) = -\mathbf{r}\,\boldsymbol{\mu}_\Gamma$$

$$\partial_t\Big(\sum_m \varrho^m v^m \boldsymbol{\mu}_{\Omega^m}\Big) + \operatorname{div}\Big(\sum_m(\varrho^m v^m v^{m\mathsf{T}} + \Pi^m)\boldsymbol{\mu}_{\Omega^m} + \Pi^s\boldsymbol{\mu}_\Gamma\Big) = \sum_m \mathbf{f}^m\boldsymbol{\mu}_{\Omega^m}$$

The convergence is in the sense of distributions, in particular

$$(\varrho v v^\mathsf{T} + \Pi_\delta)\boldsymbol{\mu}_U \quad \longrightarrow \quad \sum_m(\varrho^m v^m v^{m\mathsf{T}} + \Pi^m)\boldsymbol{\mu}_{\Omega^m} + \Pi^s\boldsymbol{\mu}_\Gamma$$

$$\Pi^s = -\gamma(\mathrm{Id} - \nu\nu^\mathsf{T})\,, \quad \gamma \text{ given by an integral over “local coordinates”}$$

where $U = \Omega^1 \cup \Gamma \cup \Omega^2$

For $\eta \in \mathcal{D}(U;\mathbb{R}^n \times \mathbb{R}^n)$, $U \subset \mathbb{R} \times \mathbb{R}^n$, $U = \Omega_\delta^1 \cup \Gamma_\delta \cup \Omega_\delta^2$

$$\int_U \eta \bullet (\varrho v v^{\mathsf{T}} + \Pi_\delta)\,\mathrm{dL}_{n+1} = \sum_m \int_{\Omega_\delta^m} \ldots\,\mathrm{dL}_{n+1} + \int_{\Gamma_\delta} \ldots\,\mathrm{dL}_{n+1}$$

In a small neighbourhood of Γ

$$\begin{aligned}
\Pi_\delta = \;& \mathsf{p}_U\,\mathrm{Id} + \frac{\delta}{2}\mathsf{p}_h|\nabla\varphi|^2\,\mathrm{Id} + \delta h \nabla\varphi(\nabla\varphi)^{\mathsf{T}} - (\lambda_1 - \frac{\lambda_2}{n})\mathrm{div}\,v\,\mathrm{Id} - \lambda_2(\nabla v)^{\mathsf{S}} \\
= \;& \frac{1}{\delta}\Big(\frac{1}{2}\mathsf{p}_h|\partial_r\Phi^0|^2\,\mathrm{Id} + h|\partial_r\Phi^0|^2\nu\nu^{\mathsf{T}} \\
& -(\lambda_1 - \frac{\lambda_2}{n})\nu\bullet\partial_r V^0\,\mathrm{Id} - \frac{1}{2}\lambda_2(\nu(\partial_r V^0)^{\mathsf{T}} + \partial_r V^0\nu^{\mathsf{T}})\Big) + \mathcal{O}(1)
\end{aligned}$$

$$\begin{aligned}
\delta\Pi_\delta\nu \to \;& \frac{1}{2}\mathsf{p}_h|\partial_r\Phi^0|^2\nu + h|\partial_r\Phi^0|^2\nu - (\lambda_1 - \frac{\lambda_2}{n})\nu\bullet\partial_r V^0\nu - \lambda_2\nu\bullet\partial_r V^0\nu \\
= \;& (\frac{1}{2}\mathsf{p}_h + h)|\partial_r\Phi^0|^2\nu - (\lambda_1 + \frac{(n-1)\lambda_2}{n})\partial_r V^0 \;=\; 0
\end{aligned}$$

$$\begin{aligned}
(\delta\Pi_\delta)_{\mathrm{tan}} := \;& \delta\Pi_\delta - (\delta\Pi_\delta\nu)\nu \;=\; \delta\Pi_\delta(\mathrm{Id} - \nu\nu^{\mathsf{T}}) \\
\to \;& \Big(\frac{1}{2}\mathsf{p}_h|\partial_r\Phi^0|^2 - (\lambda_1 - \frac{\lambda_2}{n})\nu\bullet\partial_r V^0\Big)(\mathrm{Id} - \nu\nu^{\mathsf{T}}) \\
= \;& \Big(\frac{1}{2}\mathsf{p}_h(R^0)|\partial_r\Phi^0|^2 - \big(\lambda_1(R^0,\Phi^0) - \frac{\lambda_2(R^0,\Phi^0)}{n}\big)\nu\bullet\partial_r V^0\Big)(\mathrm{Id} - \nu\nu^{\mathsf{T}})
\end{aligned}$$

$$\gamma = \int_{\mathbb{R}} \Big(-\frac{1}{2}\mathsf{p}_h(R^0)|\partial_r\Phi^0|^2 + \big(\lambda_1(R^0,\Phi^0) - \frac{\lambda_2(R^0,\Phi^0)}{n}\big)\nu\bullet\partial_r V^0\Big)\,\mathrm{d}r$$

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