Equilibrium configurations in Korteweg fluids

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joint work with F. Oliveri[a], A. Ricciardello[b] & P. Rogolino[a]

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Balance equations

Let $\mathcal{B}$ be a fluid occupying a compact and simply connected region $\mathcal{C}$ of a Euclidean point space E^3; at a continuum level, its evolution is ruled by the field equations (neglecting heat sources):

$$\mathcal{E}^{(1)} \equiv \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$
$$\mathcal{E}^{(2)} \equiv \rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right) - \nabla \cdot \mathrm{T} = \rho \mathbf{f},$$
$$\mathcal{E}^{(3)} \equiv \rho \left(\frac{\partial \varepsilon}{\partial t} + \mathbf{v} \cdot \nabla \varepsilon \right) - \mathrm{T} \cdot \nabla \mathbf{v} + \nabla \cdot \mathbf{q} = \rho \mathbf{f} \cdot \mathbf{v},$$

where ρ is the mass density, $\mathbf{v} \equiv (v_1, v_2, v_3)$ the velocity, ε the internal energy per unit mass, T the symmetric Cauchy stress tensor, $\mathbf{q}$ the heat flux, and $\mathbf{f}$ the external body forces per unit mass.
This system is underdetermined and must be closed by constitutive equations for T and $\mathbf{q}$ in such a way the local entropy production

$$\sigma_s = \rho \left(\frac{\partial s}{\partial t} + \mathbf{v} \cdot \nabla s \right) + \nabla \cdot \mathbf{J} \geq 0$$

along any admissible thermodynamic process, s being the specific entropy, and $\mathbf{J}$ the entropy flux; s and $\mathbf{J}$ are constitutive quantities, too. The second law of thermodynamics restricts the form of the constitutive equations!

Korteweg, 1901

D. J. Korteweg[a] introduced a constitutive relation for the stress tensor T involving, in its elastic part, the first and second order gradients of the mass density, in order to describe the cohesive forces due to long–range interactions:

$$\mathrm{T} = \left(-p + \alpha_1 \Delta\rho + \alpha_2 |\nabla\rho|^2\right) \mathbb{I} + \alpha_3 \nabla\rho \otimes \nabla\rho + \alpha_4 \nabla\nabla\rho,$$

wher p is the pressure, ρ the mass density, $\mathbb{I}$ the identity matrix and α_i $(i = 1, \dots, 4)$ are material coefficients depending on ρ.

[a] D. J. Korteweg, *Sur la forme qui prennent les équations du mouvement des fluids si l'on tient compte des forces capillaires par des variations de densité considérables mais continues et sur la théorie de la capillarité dans l'hypothèse d'une variation continue de la densité*, Archives Néerlandaises des sciences exactes et naturelles **6** Ser. II, 1–24, 1901.

A constitutive theory requires the choice of the state space variables, that can be the basic fields (local constitutive laws) or the basic fields together with some of their gradients (non–local constitutive laws). Here, we analyze the class of Korteweg–type materials described by the set of constitutive equations

$$\mathcal{F} = \mathcal{F}^*(\rho, \varepsilon, \nabla\rho, \mathbf{L}, \nabla\varepsilon, \nabla\nabla\rho),$$

where $\mathcal{F}$ is an element of the set $\{\mathrm{T}, \mathbf{q}, s, \mathbf{J}\}$, and $\mathbf{L} = \mathrm{sym}\,(\nabla\mathbf{v})$.

Exploitation of entropy–like inequality

The restrictions imposed by the second law of thermodynamics on constitutive equations can be derived by means of the procedures:

1. Coleman[1] and Noll, 1963;
2. Liu[2], 1972;
3. Extended[3] Liu, 2007.

For Korteweg fluids, the compatibility of non–local constitutive equations with the entropy principle has been investigated by means of the Extended Liu procedure.[a]

[a] M. Gorgone and P. Rogolino, *On the characterization of constitutive equations for third–grade viscous Korteweg fluids*, Phys. Fluids **33**, 043107, 2021.

[1] B. D. Coleman and W. Noll, *The thermodynamics of elastic materials with heat conduction and viscosity*, Arch. Ration. Mech. Anal. **13**, 167–178, 1963.

[2] I–Shih Liu, *Method of Lagrange multipliers for exploitation of the entropy principle*, Arch. Ration. Mech. Anal. **46**, 131–148, 1972.

[3] V. A. Cimmelli, *An extension of Liu procedure in weakly nonlocal thermodynamics*, J. Math. Phys. **48**, 113510, 2007.

Extended Liu procedure for a viscous Korteweg fluid

Let us assume the state space spanned by

$$\mathcal{Z} \equiv \{\rho, \varepsilon, \nabla\rho, \mathbf{L}, \nabla\varepsilon, \nabla\nabla\rho\}.$$

By introducing Lagrange multipliers depending on the state space variables, the entropy inequality reads

$$\rho\left(\frac{\partial s}{\partial t} + \mathbf{v}\cdot\nabla s\right) + \nabla\cdot\mathbf{J} - \lambda^{(1)}\mathcal{E}^{(1)} - \boldsymbol{\lambda}^{(2)}\cdot\mathcal{E}^{(2)} - \lambda^{(3)}\mathcal{E}^{(3)}$$
$$-\boldsymbol{\Lambda}^{(1)}\cdot\nabla\mathcal{E}^{(1)} - \boldsymbol{\Lambda}^{(2)}\cdot\nabla\mathcal{E}^{(2)} - \boldsymbol{\Lambda}^{(3)}\cdot\nabla\mathcal{E}^{(3)} - \boldsymbol{\Theta}^{(1)}\cdot\nabla\nabla\mathcal{E}^{(1)} \geq 0.$$

By expanding derivatives with the chain rule, we identify

$$\mathbf{X} \equiv \left\{\rho_{,t}, v_{i,t}, \varepsilon_{,t}, \rho_{,it}, v_{i,jt}, \varepsilon_{,it}, \rho_{,ijt}, , v_{i,jk\ell}, \varepsilon_{,ijk}, \rho_{,ijk\ell}\right\}, \qquad \text{highest derivatives,}$$
$$\mathbf{Y} \equiv \left\{v_{i,jk}, \varepsilon_{,ij}, \rho_{,ijk}\right\}, \qquad \text{higher derivatives,}$$

and the entropy inequality can be written in compact form as

$$\mathbf{A}\cdot\mathbf{X} + \mathbf{Y}^T B\mathbf{Y} + \mathbf{C}\cdot\mathbf{Y} + D \geq 0,$$

where **A** and **C** are vectors, B is a symmetric matrix, D is a scalar, all depending at most on field and state space variables.

Constitutive equations for viscous Korteweg fluids: assumptions

$$
\begin{aligned}
\mathrm{T} &= \left(-p+\alpha_1\Delta\rho+\alpha_2|\nabla\rho|^2\right)\mathbb{I}+\alpha_3\nabla\rho\otimes\nabla\rho+\alpha_4\nabla\nabla\rho+\alpha_5(\nabla\cdot\mathbf{v})\mathbb{I}+\alpha_6\mathbf{L},\\
\mathbf{q} &= q^{(1)}\nabla\varepsilon+q^{(2)}\nabla\rho,\\
s &= s_0+s_1|\nabla\rho|^2+s_2\nabla\rho\cdot\nabla\varepsilon+s_3|\nabla\varepsilon|^2+s_4\nabla\cdot\mathbf{v}+s_5\Delta\rho,
\end{aligned}
$$

where p, α_i $(i=1,\dots,6)$, $q^{(j)}$ $(j=1,2)$ and s_k $(k=0,\dots,5)$ depend on (ρ,ε).

Constitutive equations for viscous Korteweg fluids: assumptions

$$\mathrm{T} = \left(-p+\alpha_1\Delta\rho + \alpha_2|\nabla\rho|^2\right)\mathbb{I}+\alpha_3\nabla\rho\otimes\nabla\rho + \alpha_4\nabla\nabla\rho + \alpha_5(\nabla\cdot\mathbf{v})\mathbb{I} + \alpha_6\mathbf{L},$$
$$\mathbf{q} = q^{(1)}\nabla\varepsilon + q^{(2)}\nabla\rho,$$
$$s = s_0 + s_1|\nabla\rho|^2 + s_2\nabla\rho\cdot\nabla\varepsilon + s_3|\nabla\varepsilon|^2 + s_4\nabla\cdot\mathbf{v} + s_5\Delta\rho,$$

where p, α_i $(i=1,\dots,6)$, $q^{(j)}$ $(j=1,2)$ and s_k $(k=0,\dots,5)$ depend on (ρ,ε).

Constitutive equations for viscous Korteweg fluids: results and restrictions

$$\mathrm{T} = \left(\frac{\partial s_0}{\partial\varepsilon}\right)^{-1}\left(\rho^2\frac{\partial s_0}{\partial\rho} - 2\rho^2 s_1\Delta\rho - \frac{d(\rho^2 s_1)}{d\rho}|\nabla\rho|^2\right)\mathbb{I} + 2\rho s_1\left(\frac{\partial s_0}{\partial\varepsilon}\right)^{-1}\nabla\rho\otimes\nabla\rho + \alpha_5(\nabla\cdot\mathbf{v})\mathbb{I} + \alpha_6\mathbf{L},$$
$$\mathbf{q} = q^{(1)}\frac{\partial\varepsilon}{\partial\theta}\nabla\theta,$$
$$s = s_0(\rho,\varepsilon) + s_1(\rho)|\nabla\rho|^2, \qquad s_1(\rho)\leq 0,$$
$$\mathbf{J} = \frac{\mathbf{q}}{\theta} + 2\rho^2 s_1(\nabla\cdot\mathbf{v})\nabla\rho, \qquad \text{with} \qquad \frac{1}{\theta} = \frac{\partial s_0(\rho,\varepsilon)}{\partial\varepsilon},$$
$$q^{(1)}\frac{\partial^2 s_0}{\partial\rho\partial\varepsilon} - q^{(2)}\frac{\partial^2 s_0}{\partial\varepsilon^2} = 0, \qquad q^{(1)}\leq 0, \qquad q^{(2)}\geq 0, \qquad \alpha_5\geq 0, \qquad \alpha_6\geq 0.$$

Phase boundaries at the equilibrium

The problem

The search for equilibrium configurations ($\theta = \theta_0$ and $\mathbf{v} = \mathbf{0}$) of a Korteweg fluid requires to solve the conditions

$$\nabla \cdot \left(\left(-p + \alpha_1 \Delta\rho + \alpha_2 |\nabla\rho|^2\right) \mathbb{I} + \alpha_3 \nabla\rho \otimes \nabla\rho + \alpha_4 \nabla\nabla\rho\right) + \rho\mathbf{g} = \mathbf{0},$$

where $\mathbf{g}$ is the gravity acceleration, $p \equiv p(\rho)$ and $\alpha_i \equiv \alpha_i(\rho)$ ($i = 1, \dots, 4$) need to be evaluated at constant temperature.
In our case, the equilibrium conditions read

$$\nabla \cdot \left(\theta_0 \left(\rho^2 \frac{\partial s_0}{\partial \rho} - 2\rho^2 s_1 \Delta\rho - \frac{d(\rho^2 s_1)}{d\rho} |\nabla\rho|^2\right) \mathbb{I} + 2\theta_0 \rho s_1 \nabla\rho \otimes \nabla\rho\right) + \rho\mathbf{g} = \mathbf{0},$$

where θ_0 is the constant absolute temperature at the equilibrium.
This system is made by three PDEs where the only unkwnown is the mass density $\rho(x, y, z)$, *i.e.*, it is overdetermined!

Serrin, 1983

Using a general theorem proved in [Pucci[a], 1983], J. Serrin[b] established that, unless rather special conditions on the coefficients entering the Cauchy stress tensor are satisfied, the only geometric phase boundaries which are consistent with this system are either spherical, cylindrical, or planar!
In fact, in order to have the possibility to have more general geometric phase boundaries at equilibrium, it is necessary that the constitutive quantities involved in the Cauchy stress tensor satisfy the following condition:

$$\alpha_3^2 - \alpha_1 \frac{\partial \alpha_3}{\partial \rho} + 2\alpha_2\alpha_3 = 0.$$

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[a] P. Pucci, *An overdetermined system*, Quart. Appl. Math. **41**, 365–367, 1983.

[b] J. Serrin, *The form of interfacial surfaces in Korteweg's theory of phase equilibria*, Quart. Appl. Math. **41**, 357–364, 1983.

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[a] P. Pucci, *An overdetermined system*, Quart. Appl. Math. **41**, 365–367, 1983.

[b] J. Serrin, *The form of interfacial surfaces in Korteweg's theory of phase equilibria*, Quart. Appl. Math. **41**, 357–364, 1983.

Solution to Serrin condition

The recovered constitutive relations satisfy the Serrin condition, provided that

$$s_0(\rho, \varepsilon) = s_{01}(\rho) + s_{02}(\varepsilon).$$

Also, from the thermodynamical restrictions, this result implies that $\varepsilon = \varepsilon(\theta)$, and the heat flux becomes

$$\mathbf{q} = q^{(1)} \frac{d\varepsilon}{d\theta} \nabla\theta.$$

Reduction of equilibrium conditions

Let the Korteweg fluid be in the coordinate system xyz with z axis directed along the ascending vertical. The equilibrium condition reads:

$$
\begin{aligned}
&\left(\rho^2\frac{ds_{01}}{d\rho}-2\rho^2 s_1(\rho_{xx}+\rho_{yy}+\rho_{zz})-\frac{d(\rho^2 s_1)}{d\rho}(\rho_x^2+\rho_y^2+\rho_z^2)+2\rho s_1\rho_x^2\right)_x\\
&\qquad+2\left(\rho s_1\rho_x\rho_y\right)_y+2\left(\rho s_1\rho_x\rho_z\right)_z=0,\\
&2\left(\rho s_1\rho_x\rho_y\right)_x+\left(\rho^2\frac{ds_{01}}{d\rho}-2\rho^2 s_1(\rho_{xx}+\rho_{yy}+\rho_{zz})-\frac{d(\rho^2 s_1)}{d\rho}(\rho_x^2+\rho_y^2+\rho_z^2)+2\rho s_1\rho_y^2\right)_y\\
&\qquad+2\left(\rho s_1\rho_y\rho_z\right)_z=0,\\
&2\left(\rho s_1\rho_x\rho_z\right)_x+2\left(\rho s_1\rho_y\rho_z\right)_y\\
&\qquad+\left(\rho^2\frac{ds_{01}}{d\rho}-2\rho^2 s_1(\rho_{xx}+\rho_{yy}+\rho_{zz})-\frac{d(\rho^2 s_1)}{d\rho}(\rho_x^2+\rho_y^2+\rho_z^2)+2\rho s_1\rho_z^2\right)_z-\frac{g}{\theta_0}\rho=0.
\end{aligned}
$$

The idea is to reduce this overdetermined third order nonlinear system into a single equation!

Reduction of equilibrium conditions

By solving the first equation with respect to $\dfrac{d^2 s_{01}}{d\rho^2}$, we have

$$\frac{d^2 s_{01}}{d\rho^2} = \frac{\dfrac{d^2 s_1}{d\rho^2}\rho\rho_x\left(\rho_x^2+\rho_y^2+\rho_z^2\right)+2\dfrac{ds_1}{d\rho}\left(\rho_x\left(\rho(2\rho_{xx}+\rho_{yy}+\rho_{zz})+\rho_y^2+\rho_z^2\right)+\rho(\rho_{xy}\rho_y+\rho_{xz}\rho_z)+\rho_x^3\right)}{\rho\rho_x}$$

$$+\frac{2s_1(\rho(\rho_{xxx}+\rho_{xyy}+\rho_{xzz})+\rho_x(2\rho_{xx}+\rho_{yy}+\rho_{zz})+\rho_{xy}\rho_y+\rho_{xz}\rho_z)}{\rho\rho_x}-\frac{2}{\rho}\frac{ds_{01}}{d\rho}. \qquad (*)$$

Since $\dfrac{d^2 s_{01}}{d\rho^2}$ depend only on ρ, we need that the red quantity is a function depending on ρ.
This implies that

$$\text{numerator of red quantity} = \frac{\partial f(\rho)}{\partial x},$$

where $f(\rho)$ has to be determined.
By integrating with respect to x, we have

$$2\rho s_1(\rho_{xx}+\rho_{yy}+\rho_{zz})+\frac{d(\rho s_1)}{d\rho}(\rho_x^2+\rho_y^2+\rho_z^2)=f(\rho)+h(y,z), \qquad (**)$$

where $h(y,z)$ is an arbitrary integration function.

Reduction of equilibrium conditions

It follows that

$$\frac{d^2 s_{01}}{d\rho^2} + \frac{2}{\rho}\frac{ds_{01}}{d\rho} - \frac{1}{\rho}\frac{df}{d\rho} = 0,$$

providing

$$f(\rho) = \frac{d(\rho s_{01})}{d\rho} + \kappa_1, \qquad \text{with} \quad \kappa_1 \ \text{constant.}$$

Then, inserting into the equilibrium conditions the above relation, the constraints $(*)$ and $(**)$, and differentiating $(**)$ in order to eliminate the third order partial derivatives, we obtain

$$\frac{\partial h}{\partial y} = 0, \qquad \frac{\partial h}{\partial z} + \frac{g}{\theta_0} = 0,$$

i.e.,

$$h(y, z) = -\frac{g}{\theta_0} z + \kappa_2.$$

3D Phase boundaries at the equilibrium

Solving equation for equilibrium conditions

Finally, we obtain the following condition

$$2\rho s_1 \Delta\rho + \frac{d(\rho s_1)}{d\rho}|\nabla\rho|^2 - \frac{d(\rho s_{01})}{d\rho} + \frac{g}{\theta_0}z - \kappa = 0,$$

where $s_{01} \equiv s_{01}(\rho)$, $s_1 \equiv s_1(\rho)$, and κ is an arbitrary integration constant.
It represents the only second order scalar PDE to be solved in order to identically satisfy the equilibrium conditions and so find the equilibrium configurations.
The obtained solving equation is analyzed distinguishing the following cases:

1. it reduces to a linear elliptic equation;
2. it reduces to a nonlinear elliptic equation, and a suitable boundary value problem of Dirichlet type is investigated.

2D Phase boundaries at the equilibrium

Assume that

$$s_{01} = \kappa_1 \rho^m, \qquad s_1 = -\kappa_2 \rho^n,$$

with $\kappa_i \in \mathbb{R}^+$ $(i = 1, 2)$, and $m, n \in \mathbb{R}$; then, the solving equation becomes

$$2\kappa_2 \rho^{n+1} (\rho_{xx} + \rho_{yy}) + \kappa_2 (n+1)\rho^n \left(\rho_x^2 + \rho_y^2\right) + \kappa_1 (m+1)\rho^m - \frac{g}{\theta_0} y + \kappa = 0.$$

Fixing in the plane xy the rectangular domain $[0, \ell_1] \times [0, \ell_2]$ $(\ell_1, \ell_2 > 0)$, and introducing dimensionless variables by the substitutions

$$x \to \ell_1 x, \qquad y \to \ell_1 y, \qquad \rho \to R_0 \rho,$$

R_0 being a reference density, we obtain

$$\rho^{n+1} (\rho_{xx} + \rho_{yy}) + \frac{n+1}{2} \rho^n \left(\rho_x^2 + \rho_y^2\right) + \alpha (m+1) \rho^m + \beta y + \gamma = 0,$$

where

$$\alpha = \frac{\kappa_1}{2\kappa_2} \ell_1^2 R_0^{m-n-2}, \qquad \beta = -\frac{g}{2\kappa_2 \theta_0} \ell_1^3 R_0^{-n-2}, \qquad \gamma = \frac{\kappa}{2\kappa_2} \ell_1^2 R_0^{-n-2}.$$

This is a nonlinear elliptic PDE that we study, with Dirichlet boundary conditions, in the domain

$$\Omega = [0, 1] \times [0, d], \qquad d = \frac{\ell_2}{\ell_1}.$$

2D Phase boundaries at the equilibrium: linear case

- If $m = 1$ and $n = -1$, the condition for equilibrium reads

  $$\rho_{xx} + \rho_{yy} + 2\alpha\rho + \beta y + \gamma = 0,$$

  that, using the transformation

  $$\rho = \overline{\rho} - \frac{\beta y + \gamma}{2\alpha},$$

  becomes

  $$\overline{\rho}_{xx} + \overline{\rho}_{yy} + 2\alpha\overline{\rho} = 0,$$

  that is a Poisson equation for which many analytical solutions can be found, for instance in separable form.
- If $m = -1$ and $n = -1$, condition for equilibrium becomes

  $$\rho_{xx} + \rho_{yy} + \beta y + \gamma = 0,$$

  that, through the transformation

  $$\rho = \overline{\rho} - \frac{\beta}{6} y^3 - \frac{\gamma}{2} y^2,$$

  reduces to the Laplace equation

  $$\overline{\rho}_{xx} + \overline{\rho}_{yy} = 0.$$

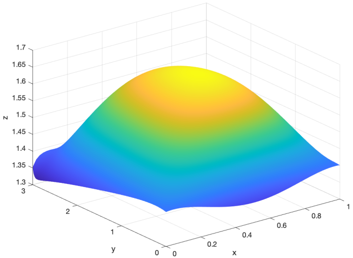
2D Phase boundaries at the equilibrium: nonlinear case

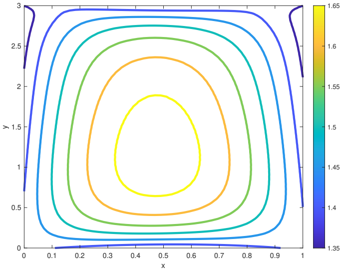
Let us now consider the following boundary value problem:

$$\begin{cases} \rho^{n+1}\left(\rho_{xx}+\rho_{yy}\right)+\dfrac{n+1}{2}\rho^{n}\left(\rho_x^2+\rho_y^2\right)+\alpha(m+1)\rho^m+\beta y+\gamma=0, \\ (x,y)\in[0,1]\times[0,d], \\ \rho(x,0)=\rho(x,d)=\rho_0-x^2(1-x)^2, \\ \rho(0,y)=\rho(1,y)=\dfrac{\rho_1-\rho_0}{d}y+\rho_0, \end{cases}$$

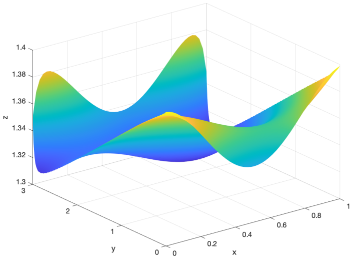
where $\rho_0 > \rho_1$ are suitable constants, that is numerically solved approximating first and second derivatives by means of second–order and fourth–order finite difference formulas, respectively.

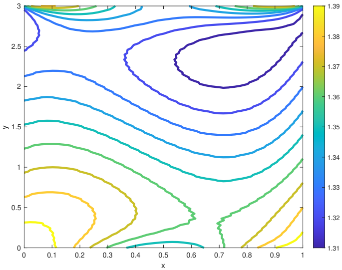
Numerical solutions: linear case, $n = -1$ and $m = 1$





$\gamma = 1$

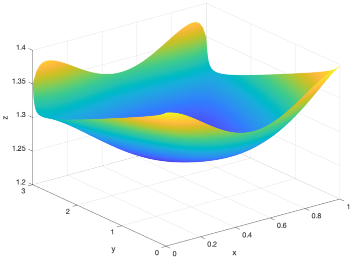


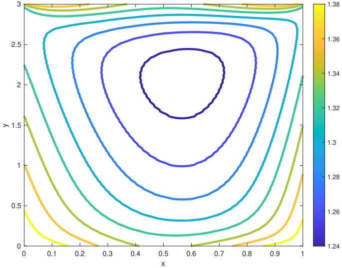


$\gamma = -1$

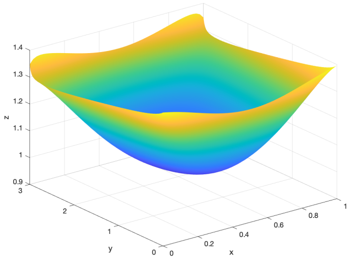
Plot of the density ρ (left) and contour plot (right), with $\alpha = 1.0$, $\beta = -1.2$, $\rho_0 = 1.4$, $\rho_1 = 1.3$, $d = 3$.

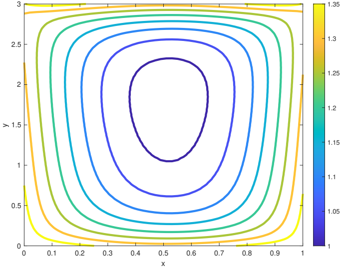
Numerical solutions: linear case, $n = -1$ and $m = -1$





$\gamma = 1$





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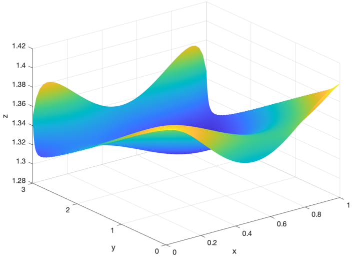
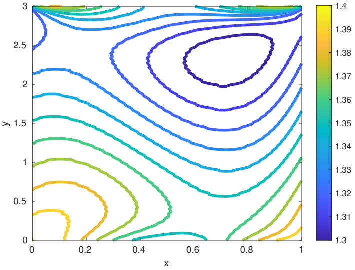
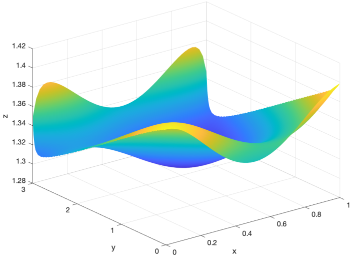
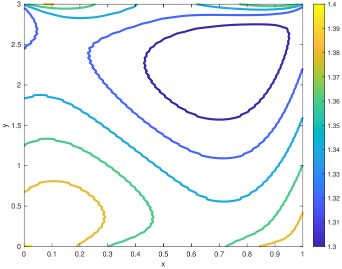
Numerical solutions: nonlinear case





$m = 1,$
$n = -2$

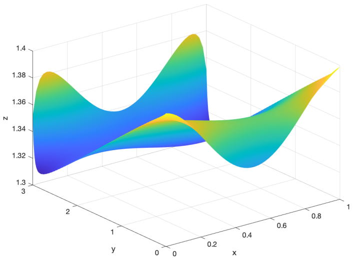


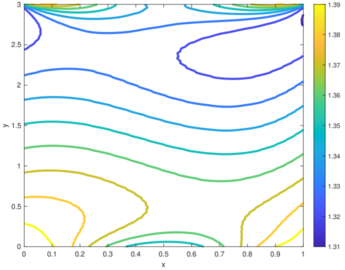


$m = 1,$
$n = -3$

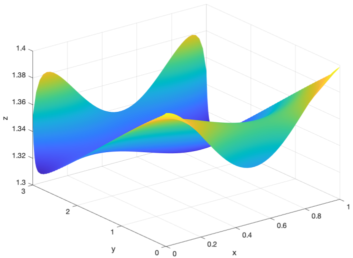
Plot of the density ρ and contour plot, with $\alpha = 1.0$, $\beta = -1.2$, $\gamma = -1$, $\rho_0 = 1.4$, $\rho_1 = 1.3$, $d = 3$.

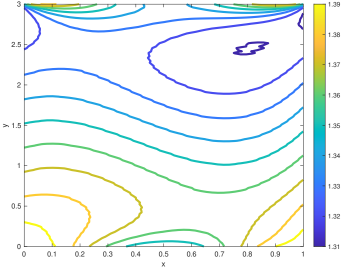
Numerical solutions: nonlinear case





$m = 1,$
$n = 1$





$m = 1,$
$n = 0$

Plot of the density ρ and contour plot, with $\alpha = 1.0$, $\beta = -1.2$, $\gamma = -1$, $\rho_0 = 1.4$, $\rho_1 = 1.3$, $d = 3$.

Conclusions

- We recovered a single equation for the equilibrium!
- The theoretical results contain some degrees of freedom and may serve as a basis for experimental and/or numerical investigations.
- We plan to investigate the equilibrium configurations of Korteweg fluids in three space dimensions and using boundary conditions and parameters suggested by experiments.

Reference

M. Gorgone, F. Oliveri, A. Ricciardello and P. Rogolino, *Two–dimensional equilibrium configurations in Korteweg fluids*, Theoretical and Applied Mechanics, **49**, 111–122, 2022.

THANKS


NOT SURE IF THEY'RE CLAPPING FOR MY PRESENTATION
OR BECAUSE ITS FINISHED