Mathematical
Institute

Diffuse interface model for calamitic fluids

Patrick E. Farrell*†, Umberto Zerbinati*

** Mathematical Institute – University of Oxford, United Kingdom,*
† Mathematical Institute – Charles University, Czechia.

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Oxford
Mathematics

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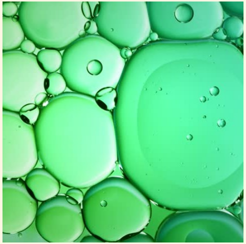

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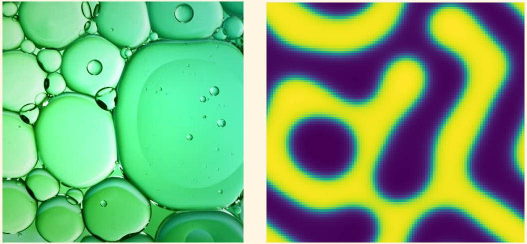

- **Liquid-Vapour Mixtures**: in this model the density ρ is the **order parameter** distinguishing the bulk of the fluid and the interface region.
- **Binary fluids**: in this model the concentration of a chemical species is the **order parameter** distinguishing the two fluids.

CALAMITIC FLUIDS

Calamitic fluids are fluids whose molecular constituents are rod-like. Calamitic fluids can be found in different states of matter. A typical state of matter for calamitic fluids is the liquid crystal state, subdivided in multiple phases:

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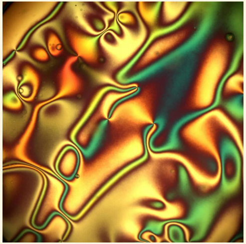

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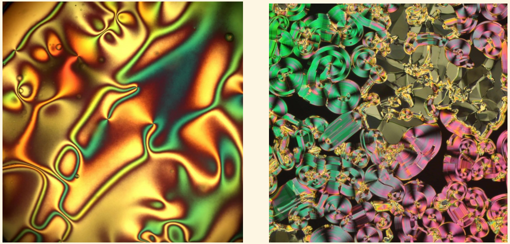

- **nematic phase**: in this phase the molecules are oriented along a common direction.
- **smectic phase**: in this phase the molecules present a layered structures with orientational order within layers.

A KINETIC THEORY APPROACH

- A kinetic theory approach seeks to describe the evolution of the fluid using a statistical description and knowledge of the microscopic interactions.

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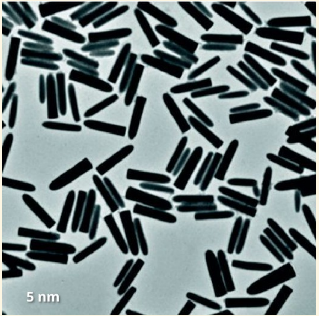
J. Am. Chem. Soc. 2011 133 (8), 2346-2349 (A. Kuijk, A. van Blaaderen, A. Imhof).



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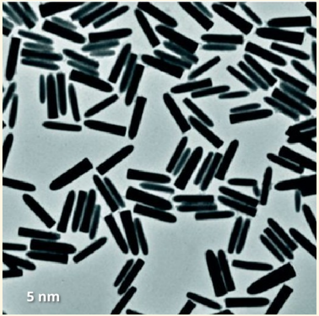

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Onsager's Approach To Liquid Crystals

Onsager first explained the emergence of nematic ordering in liquid crystals by a truncation of the Mayer cluster expansion, valid for dilute systems.

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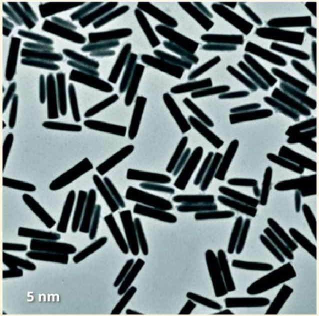
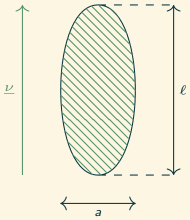


THE MICROSCOPIC WORLD

1

LAGRANGIAN MECHANICS OF THE CONSTITUENTS

We assume that the fluid is composed of a set of constituents, each of which is described by a position $\underline{q}_i$, a velocity $\underline{v}_i$, and a set of Euler angles α_i and their total time derivatives $\underline{\dot{\alpha}}_i$.



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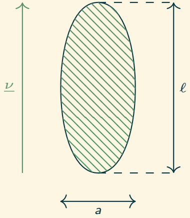
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2}\dot{\underline{\alpha}}_i \cdot \underline{\underline{\Omega}}_i(\alpha_i)\dot{\underline{\alpha}}_i, \qquad \Omega_i = \mathbb{I}\Pi(\underline{\alpha}_i).$$



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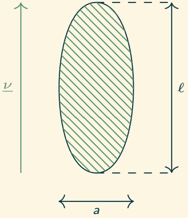

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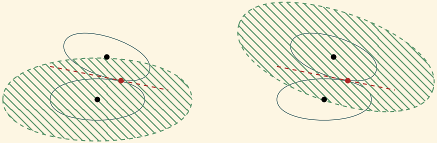
We assume the interaction between the constituents is given by a potential $\mathcal{W}(|\underline{q}|, \underline{\alpha}_i, \underline{\alpha}_j)$, i.e.

$$\mathcal{L}_{ij} = \mathcal{L}_i(\mathbf{x}_i, \Xi_i) + \mathcal{L}_j(\mathbf{x}_j, \Xi_j) + \mathcal{W}(|\underline{q}_{ij}|, \underline{\alpha}_i, \underline{\alpha}_j),$$

where $\Xi_i := (\underline{v}_i, \underline{\alpha}_i, \underline{\varsigma}_i)$, and $|\underline{q}_{ij}| = |\underline{q}_i - \underline{q}_j|$.



THE GAY–BERNE POTENTIAL

The Gay–Berne potential is an anisotropic generalization of the Lennard–Jones potential, designed to model interactions between elongated, ellipsoidal particles.

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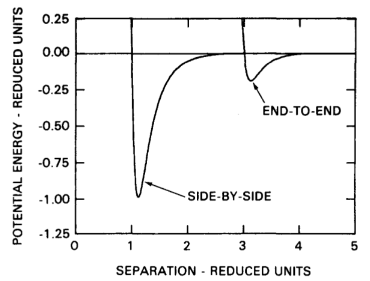

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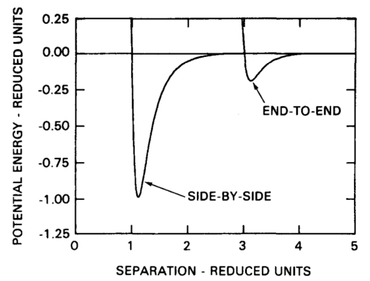
$$\mathcal{W}(\underline{\alpha}_i, \underline{\alpha}_j, \underline{q}_{ij}) = \varepsilon(\underline{\alpha}_1, \underline{\alpha}_2, \underline{q}_{ij}) \left[\left(\frac{1}{|q|_{ij} - \sigma(\underline{\alpha}_1, \underline{\alpha}_2, \underline{q}_{ij}) + \sigma_0} \right)^{12} - \left(\frac{1}{|q|_{ij} - \sigma(\underline{\alpha}_1, \underline{\alpha}_2, \underline{q}_{ij}) + \sigma_0} \right)^{6} \right]$$



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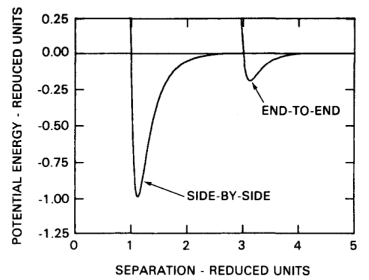

where ε and σ are respectively the strength and range of the interaction.

NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

Mathematical Institute

Noether's theorem

If a Lagrangian $\mathcal{L}$ is invariant under a group action with infinitesimal generators G then

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{X}_{1,2}} \cdot G\right) = 0, \qquad X_{1,2} = \left(\underline{q}_1, \underline{q}_2, \underline{\alpha}_1, \underline{\alpha}_2\right).$$

In other words for any physical symmetry of the system, there is a conserved quantity.

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- The Lagrangian $\mathcal{L}$ is independent of time and the kinetic energy is a homogeneous quadratic form of the conjugate moments, i.e. the energy is conserved.
- The Lagrangian $\mathcal{L}$ is invariant under rotations, i.e. the angular momentum is conserved.

ENSKOG TYPE EQUATION

2

HAMILTONIAN MECHANICS OF THE CONSTITUENTS

We introduce the Hamiltonian formalism associated to the Lagrangian $\mathcal{L}$ introduced in the previous section. As usual, we introduce the conjugate momenta to the generalised coordinates, i.e.

$$\underline{p_i} := \frac{\partial \mathcal{L}}{\partial \underline{\dot{q}}_i} = m\underline{\dot{q}}_i, \qquad \underline{\varsigma_i} := \frac{\partial \mathcal{L}}{\partial \underline{\dot{\alpha}_i}} = \underline{\underline{\Omega}}(\alpha)\, \underline{\dot{\alpha}_i}.$$

We then introduce the Hamiltonian $\mathcal{H}$ of the full system of N constituents, only interacting in pairs, as

$$\mathcal{H} := \sum_{i=1}^{N} \frac{1}{2m}\underline{p_i} \cdot \underline{p_i} + \frac{1}{2}\underline{\varsigma_i} \cdot \underline{\underline{\Omega}}(\alpha)^{-1}\, \underline{\varsigma_i} + \sum_{1 \leq i < j \leq N} \mathcal{W}(|\underline{q}_{ij}|, \underline{\alpha}_i, \underline{\alpha}_j).$$

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The Legendre transform of the Lagrangian $\mathcal{L}$ is always well-defined, assuming $\underline{\underline{\Omega}}(\alpha)$ is symmetric and positive definite for all Euler angles α.

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

An Introduction to the Theory of the Boltzmann Equation, (S. Harris),
Statistical Physics of Particles, (M. Kardar),
Statistical Mechanics, 2nd Edition (K. Huang). *Multiscale Model. Simul.* 2024, accepted
(P. E. Farrell, G. Russo, ∼),

Let f_s denote the normalised s-particle distribution function. We obtain the following expression for the BBGKY hierarchy,

$$\begin{aligned}\frac{\partial f_s}{\partial t} + \{\pi_s, \mathcal{H}_s\} &= \int \sum_{i=1}^{s} \frac{\partial f_{s+1}}{\partial \underline{p}_i} \cdot \frac{\partial \mathcal{W}(|\underline{q}_{i,s+1}|, \underline{\alpha}_i, \underline{\alpha}_{s+1})}{\partial \underline{q}_i}\, d\Gamma_{s+1} \\ &\quad + \int \sum_{i=1}^{s} \frac{\partial f_{s+1}}{\partial \underline{\varsigma}_i} \cdot \frac{\partial \mathcal{W}(|\underline{q}_{i,s+1}|, \underline{\alpha}_i, \underline{\alpha}_{s+1})}{\partial \underline{\alpha}_i}\, d\Gamma_{s+1},\end{aligned}$$

where $\mathcal{H}_s = \left(\sum_{i=1}^{s} \frac{|\underline{p}_i|^2}{2m} + \frac{1}{2}\underline{\varsigma}_i \cdot \underline{\underline{\Omega}}(\alpha)^{-1}\underline{\varsigma}_i\right) + \sum_{1\leq i<j\leq s} \mathcal{W}(|\underline{q}_{ij}|, \underline{\alpha}_i, \underline{\alpha}_j)$.

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

Multiscale Model. Simul. 2024 22 (4) 1585-1607 (P. E. Farrell, G. Russo, ∼),

$$
\begin{aligned}
&\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \underline{q}_1} + \underline{\underline{\Omega}}(\underline{\alpha}_1)^{-1} \underline{\varsigma}_1 \frac{\partial f_1}{\partial \underline{\alpha}_1} = \\
&+ \int \frac{\partial \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2)}{\partial \underline{q}_1} \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \right) \\
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\end{aligned}
$$

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\begin{aligned}
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&- \frac{\partial \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2)}{\partial \underline{q}_1} \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \right) \\
&- \frac{\partial \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2)}{\partial \underline{\alpha}_1} \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0
\end{aligned}
$$

HYDRODYNAMIC LIMIT

3

THE HYDRODYNAMIC EQUATIONS – NOTATION

J. Chem. Phys. 1956, 24, 225–241 (C. F. Curtiss),
J. Chem. Phys. 1963, 38, 2352–2363 (C. F. Curtiss, J. S. Dahler).

We first introduce the **number density**, i.e.

$$n(\underline{q}_1, t) = \int f_1(\underline{q}_1, \underline{v}_1, \underline{\alpha}_1, \underline{\varsigma}_1) d\Xi_1, \qquad n_2(\underline{q}_1, \underline{q}_2, t) = \iint f_2(\underline{\Gamma}_1, \underline{\Gamma}_2) d\Xi_1 d\Xi_2.$$

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Then we can give a meaning to the following double and triple *chevrons*, i.e.

$$\langle\!\langle \cdot \rangle\!\rangle(\underline{q}_1) := \frac{1}{n(\underline{q}_1, t)} \int \cdot \, f_1(\underline{q}_1, \underline{v}_1, \underline{\alpha}_1, \underline{\varsigma}_1) d\Xi_1,$$

$$\langle\!\langle\!\langle \cdot \rangle\!\rangle\!\rangle(\underline{q}) := \frac{1}{n_2(\underline{q_1} - (1-\mu)\underline{q}_{12}, \underline{q}_1 + \mu \underline{q}_{12}, t)} \iint \cdot \, f_2(\underline{\Gamma}_1, \underline{\Gamma}_2) d\Xi_1 d\Xi_2.$$

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Using this notation we can define **macroscopic stream velocity** and **macroscopic stream angular velocity** respectively as $\underline{v}_0 := \langle\!\langle \underline{v} \rangle\!\rangle$ and $\underline{\omega}_0 := \langle\!\langle \underline{\omega} \rangle\!\rangle$

THE HYDRODYNAMIC EQUATIONS – CURTISS BALANCE LAWS

Mathematical theory of transport processes in gases, (J. H. Ferziger, H. G. Kaper).
Phys. Rev. E 2020, 102 (1) 012110 (V. Giovangigli).

Testing the first equation in the BBGKY hierarchy against 1 and $m\underline{v}_1$ and integrating, we obtained the following **balance laws**:

$$\partial_t \rho + \nabla_{\underline{q}_1} \cdot (\rho \underline{v}_0) = 0,$$

$$\rho\Big[\partial_t \underline{v}_0 + (\nabla_{\underline{q}_1} \underline{v}_0)\underline{v}_0\Big] + \nabla_{\underline{q}_1} \cdot (\rho \underline{\underline{\mathbb{P}}} + \underline{\underline{\mathcal{P}}}) = 0$$

where ρ is the **density** defined as $\rho(\underline{q}_1) = mn(\underline{q}_1)$, $\underline{\underline{\mathbb{P}}}$ is the **pressure tensor** defined as $\mathbb{P} := \langle\langle \underline{V} \otimes \underline{V} \rangle\rangle$, with V being the **peculiar velocity** $\underline{V} := \underline{v} - \underline{v}_0$, and $\underline{\underline{\mathcal{P}}}$ is defined as

$$\underline{\underline{\mathcal{P}}} := \frac{1}{2m} \int \int_0^1 \langle\langle\langle |\underline{q}_1|^{-1} \partial_{|\underline{q}_1|} W(|\underline{q}_1|, \underline{\alpha}_1, \underline{\alpha}_2) \rangle\rangle\rangle (\underline{q}_{12} \otimes \underline{q}_{12}) \; d\mu d\underline{q}_{12}.$$

THE HYDRODYNAMIC EQUATIONS – SURPRISE BALANCE LAWS

For the third collision invariant we took a different route than Curtiss, which led to the following balance law

$$\rho\left[\partial_t \underline{\eta} + (\nabla_{\underline{q}_1} \underline{\eta})\underline{v}_0\right] + \nabla_{\underline{q}_1} \cdot (\rho \underline{\underline{\mathbb{N}}} + \underline{\underline{\mathcal{N}}}) = \underline{\xi} + \underline{\zeta},$$

where $\underline{\omega}$ is the **angular velocity**, $\underline{\eta}$ is the **macroscopic intrinsic angular momentum** defined as $\underline{\eta}(\underline{q}_1) := \langle\langle \underline{\underline{\mathbb{I}}}\,\underline{\omega} \rangle\rangle$ and $\underline{\underline{\mathbb{N}}}$ is the **couple tensor** defined as $\mathbb{N} := \langle\langle \underline{V} \otimes (\underline{\underline{\mathbb{I}}}\,\underline{\omega}) \rangle\rangle$. Here ξ_l is defined in tensor notation as $\langle\langle mn(\varepsilon_{lki} v_i v_k)\underline{e}_l \rangle\rangle$ and we proved that $\underline{\xi}$ vanishes. Furthermore, $\underline{\underline{\mathcal{N}}}$ and $\underline{\zeta}$ are defined as

$$\underline{\underline{\mathcal{N}}} := \frac{1}{2m} \iint_0^1 \langle\langle\langle |\underline{q}_{12}|^{-1} \partial_{|\underline{q}_{12}|} W(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2) \rangle\rangle\rangle \Big((\underline{q}_1 - \underline{q}_{12}) \otimes \underline{q}_{12} \Big)\, d\mu\, d\underline{q}_{12}$$

$$\underline{\zeta} := \iint \mathbb{I}\underline{\Pi}\partial_{\underline{\alpha}_1} \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2) f_2\, d\underline{\Xi}_1\, d\underline{\Gamma}_2.$$

MAXWELL–BOLTZMANN DISTRIBUTION

J. Chem. Phys. 1956, 24, 225–241 (C. F. Curtiss),
J. Chem. Phys. 1963, 38, 2352–2363 (C. F. Curtiss, J. S. Dahler),
Phys. Rev. E 2020, 102 (1) 012110 (V. Giovangigli).

Curtiss gives an expression for the Maxwell–Boltzmann distribution, i.e. the distribution $f^{(0)}$ such that $C[f^{(0)}, f^{(0)}]$ vanishes:

$$f_1^{(0)}(\underline{v},\underline{\omega}) = \frac{n\sin(\alpha_2)Q}{\int Q\sin(\alpha_2)d\underline{\alpha}}\frac{m^{\frac{3}{2}}}{(2\pi k_B T)^3}(\Gamma)^{\frac{1}{2}}\exp\left[-m\frac{|\underline{V}|}{2k_B T}-\frac{\underline{\Omega}\cdot\mathbb{I}\cdot\underline{\Omega}}{2k_B T}\right],$$

where the **peculiar angular velocity** defined as $\underline{\Omega} := \underline{\omega} - \underline{\omega}_0$, $I = \prod_{i=1}^{3} I_i$, I_i are the moments of inertia of the molecule we are considering and $Q := \exp\left[\frac{\underline{\omega}_0\cdot\mathbb{I}\cdot\underline{\omega}_0}{2\theta}\right]$.

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Furthermore, we will assume that $f_2^{(0)}$ can be written as

$$f_2^{(0)}(\underline{\Gamma}_1,\underline{\Gamma}_2) = f_1^{(0)}(\underline{v}_1,\underline{\omega}_1)f_1^{(0)}(\underline{v}_2,\underline{\omega}_2)\mathbf{g}(\underline{q}_{12},\underline{\alpha}_1,\underline{\alpha}_2),$$

where $\mathbf{g}$ is the density correction function $\mathbf{g}(\underline{q}_{12},\underline{\alpha}_1,\underline{\alpha}_2) := \exp\big[-k_B^{-1}T^{-1}\mathcal{W}(|\underline{q}_{12}|,\underline{\alpha}_1,\underline{\alpha}_2)\big]$.

MOMENTUM CLOSURE AROUND THE EQUILIBRIUM

Phys. Rev. E 2020, 102 (1) 012110 (V. Giovangigli).

Near the Maxwell–Boltzmann distribution we can approximate the **pressure tensor** as,

$$\mathbb{P}^{(0)} = I(3m)^{-1}\langle\langle\theta\rangle\rangle\underline{\underline{Id}}.$$

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The Maxwell–Boltzmann distribution for $f_2^{(0)}$ justifies the following expansion for n_2:

$$\begin{aligned} n_2(\underline{q}_1 - (1-\mu)\underline{q}_{12}, \underline{q}_1 + \mu\underline{q}_{12}, t) &= \mathbf{g}(\underline{\mathbf{q}}_{\mathbf{12}}, \underline{\alpha}_{\mathbf{1}}, \underline{\alpha}_{\mathbf{2}}) \\ &\times \left[n(\underline{q}_1, t) - (1-\mu)\nabla n(\underline{q}_1, t)\cdot \underline{q}_{12} + \frac{1}{2}(1-\mu)^2 \mathcal{H} n(\underline{q}_1, t) : (q_{12}\otimes q_{12})\right] \\ &\times \left[n(\underline{q}_1, t) + \mu\nabla n(\underline{q}_1, t)\cdot \underline{q}_{12} + \frac{1}{2}\mu^2 \mathcal{H} n(\underline{q}_1, t) : (q_{12}\otimes q_{12})\right]. \end{aligned}$$

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Using this expansion it is possible to compute some terms of $\mathcal{P}$, i.e.

$$\nabla \cdot \mathcal{P} \approx \nabla \cdot \Big[-3\chi_3\rho\Delta\rho\, \underline{\underline{Id}} + (\chi_4 - 2\chi_3)|\nabla\rho|^2 \underline{\underline{Id}} + 2(\chi_3+\chi_4)\nabla\rho\otimes\nabla\rho. \Big]$$

The spherical and transversely isotropic terms of $\mathcal{P}$ are weighted differently in a calamitic fluid. In particular, we **conjecture** $\chi_4 < 2\chi_3$.

MICROSCOPICALLY MOTIVATED ENERGY

4

PARTIAL ORDERING AND THE INERTIA TENSOR

We know that for a **slender body** the inertia tensor can be decomposed as,

$$\mathbb{I} = \lambda_1 (I - \underline{\nu} \otimes \underline{\nu}) + \mathcal{O}(\varepsilon)$$

where $\varepsilon = (\frac{r}{a})^2$. Furthermore, the macroscopic kinetic energy can be computed as

$$m\frac{1}{2}|\underline{v}_0|^2 + \frac{1}{2}\underline{\omega}_0 \cdot \mathbb{I}\underline{\omega}_0 = \frac{1}{2}m|\underline{v}_0|^2 + \frac{\lambda_1}{2}|\dot{\underline{\nu}}|^2 + \mathcal{O}(\varepsilon),$$

as $\varepsilon \to 0$ we retrieve the same energy that is the starting point for **Ericksen theory of anisotropic fluids**.

BALANCE LAWS FOR KINETIC TEMPERATURE

Multiscale Model. Simul. 2024, accepted (P. E. Farrell, G. Russo, ∼),

We need another way to formulate the **constitutive relation** for the **couple tensor**. We begin by observing that from $\psi^{(4)}$ we get the following balance law:

$$\rho\dot{\psi}_0 + \nabla_{\underline{q}_1}\underline{v}_0 : (\rho\mathbb{P} + \mathcal{P}) + \nabla_{\underline{q}_1}\underline{\omega}_0 : (\rho\mathbb{N} + \mathcal{N}) + \nabla_{\underline{q}_1}\cdot(Q + \mathcal{Q}) = 0$$

where $\psi_0 = \langle\langle\theta\rangle\rangle + \psi_K$, $Q = \frac{1}{2}\langle\langle\underline{V}(m|\underline{V}|^2 + \underline{\Omega}\cdot\mathbb{I}\underline{\Omega})\rangle\rangle$,

$$\theta = \frac{m}{2}\underline{V}\cdot\underline{V} + \frac{1}{2}\underline{\Omega}\cdot\mathbb{I}\cdot\underline{\Omega} \text{ and } \psi_K = \frac{1}{\rho}\iint\frac{1}{2}\mathcal{W}(|\underline{q}_{12}|,\underline{\alpha}_1,\underline{\alpha}_2)f_2\,d\underline{\Xi}_1\,d\underline{\Gamma}_2.$$

We have not yet managed to compute an explicit expression for $\mathcal{Q}$.

THE OSEEN–FRANK STORED ENERGY

Multiscale Model. Simul. 2024, accepted (P. E. Farrell, G. Russo, ∼),

Making use of the fact that $\dot{\underline{\nu}} = \underline{\omega} \times \underline{\nu} = \partial_t \underline{\nu}(\nabla \underline{\nu})\underline{v}$ we can rewrite part of the stored energy as

$$\psi_{OF}(\underline{\nu}, \nabla_{\underline{q}_1}\underline{\nu}) = \frac{1}{2}\underline{\Omega} \cdot \mathbb{I}\underline{\Omega} = \frac{\lambda_{\mathbf{1}}}{2} tr\left[\nabla_{\underline{q}_1}\underline{\nu}^T \mathbb{P}^{(0)} \nabla_{\underline{q}_1}\underline{\nu}\right].$$

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Using $\mathbb{P}^{(0)}$ we get a **stored energy functional** very similar to the **Oseen–Frank** energy

$$\psi_{OF} = p\frac{\lambda_1}{2} tr\left[\nabla_{\underline{q}_1}\underline{\nu}^T \nabla_{\underline{q}_1}\underline{\nu}\right].$$

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The kinetic pressure p acts the **degree of orientation parameter**. This explains the experimental observation that defects acts nanoparticles attractors.

Existence of minimizers

Let's assume that $\mathcal{S}$ is bi-Lipschitz homeomorphic to a ball. Then for any prescribed pressure field $p \in A_2(\mathcal{S}) \cap \mathcal{W}^{1,\infty}(\mathcal{S}, \mathbb{R}_{\geq 0})$ and $\underline{\nu}_0 \in L^2_{p|_{\partial \mathcal{S}}}(\partial \mathcal{S}, \mathbb{S}^2) \cap Lip(\mathcal{S}, \mathbb{R}^3)$ then

$$\exists\, \underline{\nu} \in \mathcal{A} \text{ such that } I[\underline{\nu}] = \inf_{\mu \in \mathcal{A}} I[\underline{\mu}],$$

where $\mathcal{A}$ is the admissible set defined as $\mathcal{A} \coloneqq \left\{ \underline{\nu} \in W^{1,2}_{\omega}(\mathcal{S}, \mathbb{S}^2) \mid \gamma \underline{\nu} = \underline{\nu}_0 \right\}$.

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Trace Theorem (P. .E. Farrell, $\sim$)

Let $\mathcal{S}$ be a precompact domain and fix $p \in (1, \infty)$ and $\omega \in A_p(\mathcal{S}) \cap \mathcal{W}^{1,\infty}$. Then there exists a unique **compact** bounded and linear operator $\gamma : W^{1,p}_{\omega}(\mathcal{S}, \mathbb{R}^3) \to L^p_{\omega|_{\partial\mathcal{S}}}(\partial\mathcal{S}, \mathbb{R}^3)$, such that for any $\underline{\nu} \in C^{\infty}(\overline{\mathcal{S}}, \mathbb{R}^3)$ we have $\gamma(\underline{\nu}) = \underline{\nu}|_{\partial\mathcal{S}}$, provided that $\partial\mathcal{S}$ is a C^1 manifold and the weight ω is such that

$$\frac{r^4}{R^4} \leq C \left[\frac{\omega\left(B_r(\underline{x})\right)}{\omega\left(B_R(\underline{x})\right)} \right],$$

for any $\underline{x} \in \partial\mathcal{S}$ and $r \in (0, R]$, where as before $\mathcal{S} \subset B_R(\underline{0})$.

THE KORTEWEG ENERGY TERM

Phys. Rev. E 2020, 102 (1) 012110 (V. Giovangigli).

The additional Enskog term in the definition of θ can be rewritten as

$$\frac{1}{\rho(\underline{q_1, t})} \int \langle\!\langle\!\langle \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2) \rangle\!\rangle\!\rangle \, n_2(\underline{q}_1, \underline{q}_2, t) \, d\underline{q}_2.$$

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If $\mathcal{W}(|\underline{q}_{12}|,\underline{\alpha}_1,\underline{\alpha}_2$ is isotropic expanding n_2 as we previously did we obtain a relevant term of the form,

$$\frac{1}{2}\int \langle\!\langle\!\langle \mathcal{W}(|\underline{q}_{12}|)\rangle\!\rangle\!\rangle\,\mathcal{H}_{\underline{q}_1} n(\underline{q_1},t) : (q_{12}\otimes q_{12})\,d\underline{q}_{12} = -\frac{1}{2}K_5\Delta n(\underline{q_1},t) = -\frac{1}{2}\hat{K}_5\Delta\rho(\underline{q_1},t).$$

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Modifying the heat flux term in the balance law it is possible to obtain the following expression for the **Korteweg energy**:

$$\rho\psi_K = \frac{1}{2}\hat{K}_5|\nabla\rho|^2.$$

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$$\frac{1}{2}\int \langle\!\langle\!\langle \mathcal{W}(|\underline{q}_{12}|, \underline{\alpha}_1, \underline{\alpha}_2)\rangle\!\rangle\!\rangle (\nabla_{\underline{q}_1} n \otimes \nabla_{\underline{q_1}} n) : (q_{12} \otimes q_{12}) d\underline{q}_{12}$$

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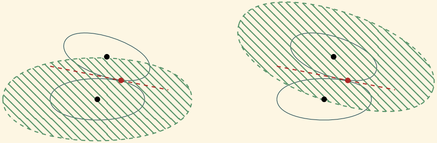

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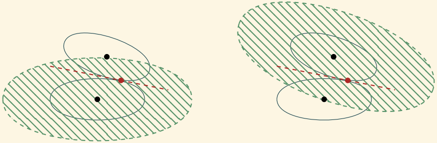

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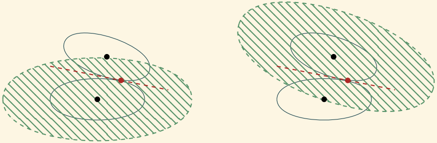

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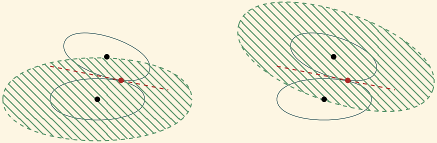

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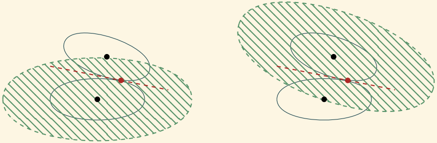

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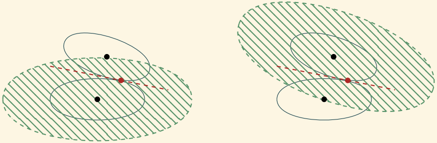

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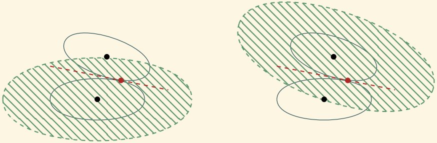

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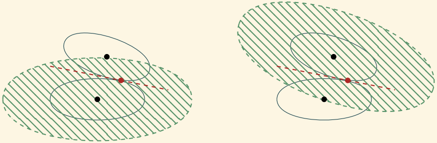

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CONCLUSIONS

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Phys. Rev. E 2009, 80 (1) 031705 (E. Virga),
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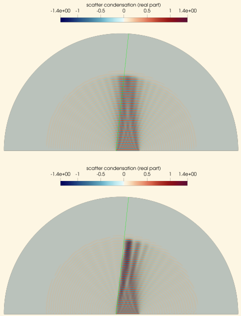
- We have used this Enskog type equation to derive a diffuse interface model for calamitic fluids, in the hydrodynamic limit.



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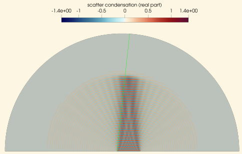

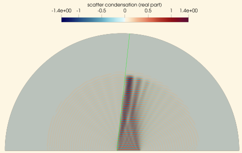

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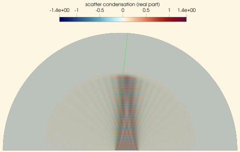

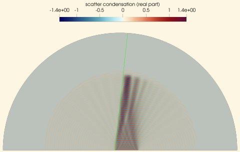

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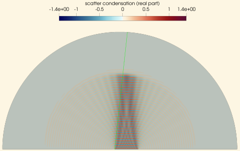
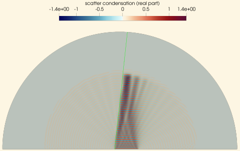
- We showed liquid crystal can be regarded as Korteweg fluids. This hypothesis is supported by nematoacoustic experiments and theories.
- We microscopically motivated an energy similar to the one by Pevnyi et al.

$$\rho\psi = \frac{a}{2}\rho^2 + \frac{b}{3}\rho^3 + \frac{c}{4}\rho^4 + B|\mathcal{H}\rho - q^2\rho\underline{nu}\otimes\underline{nu}|^2 + \frac{K}{2}|\nabla\underline{\nu}|^2.$$





THANK YOU!

Diffuse interface model for calamitic fluids

Patrick E. Farrell*†, Umberto Zerbinati*