UNIVERSITY OF
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Mathematical
Institute

A Kinetic Framework for Fluids with Ordering

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Internal Seminar, 4th April 2025

Oxford
Mathematics

ORDERED FLUIDS

Partially ordered fluids are ubiquitous in nature and have a wide range of applications.

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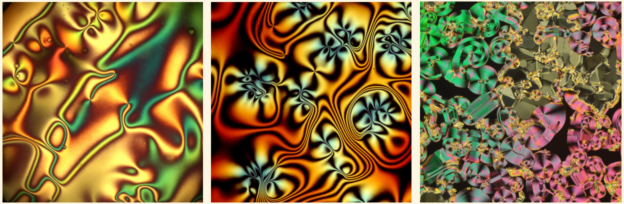

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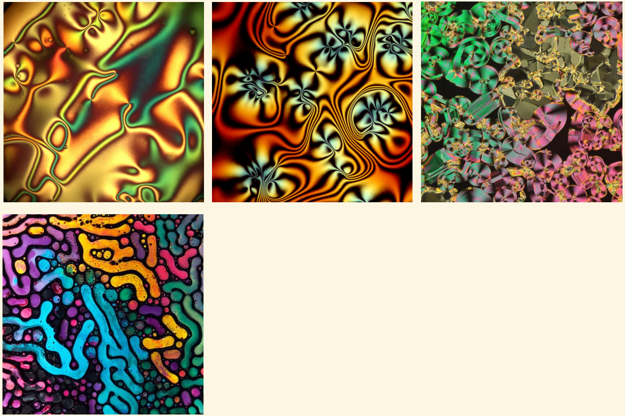

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Partially ordered fluids are ubiquitous in nature and have a wide range of applications.

- **Liquid crystals**, here depicted in nematic and smectic phases.
- **Ferrofluids**, i.e. a colloidal suspension made of nanoscale ferromagnetic or ferrimagnetic particles.
- **Gas saturated magma melts** and other fluids with non-diffusive bubbles.

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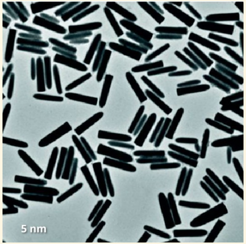

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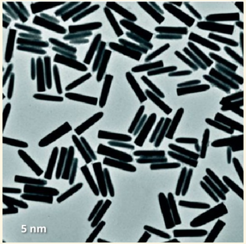

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Onsager's Approach To Liquid Crystals

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

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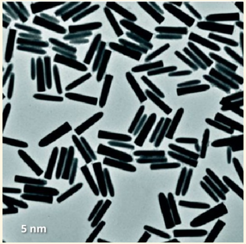

ORDER PARAMETER MANIFOLD

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Order Parameter Manifold

We say that the tuple $(\mathcal{M}, \mathcal{A})$ is an order parameter manifold if $\mathcal{M}$ is a smooth manifold with a fixed parametrization, and $\mathcal{A}$ is a Lie group action of $\mathrm{SO}(d)$ on $\mathcal{M}$, i.e. the map $\mathcal{A}$ is smooth enough to be differentiable.

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Furthermore, we say that a field $\nu : \mathbb{E}^d \to \mathcal{M}$ is an order parameter field if $\forall \underline{c} \in \mathbb{R}^d$ and $\forall \underline{\underline{Q}} \in \mathrm{SO}(d)$ we have

$$\nu(\underline{\underline{Q}}\mathbf{x} + \underline{c}) = \mathcal{A}(\underline{\underline{Q}}, \nu(\mathbf{x})), \quad \forall \mathbf{x} \in \mathbb{E}^d.$$

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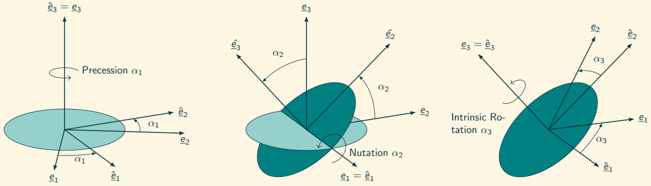
- We need to understand the action of rotations on the manifold $\mathcal{M}$.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS



Variational Theories for Liquid Crystals, (E. Virga),
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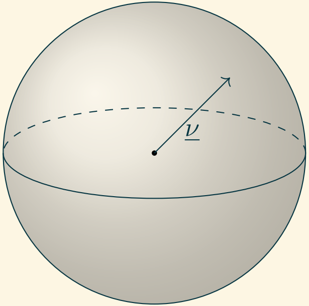

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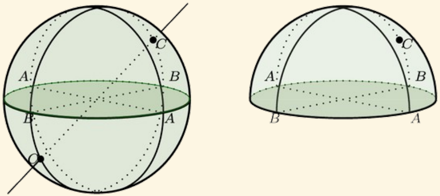

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- We can also represent the state of a calamitic molecule using a director field $\underline{\nu} \in \mathbb{S}^2$.
- For head-tail symmetric calamitic molecules, we can use $\mathbb{RP}^2$.

EMBEDDING RESULTS

Embedding theorems

- Any compact orientable 2-manifold can be embedded in $\mathbb{R}^3$.

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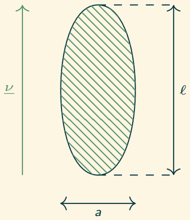
THE MICROSCOPIC WORLD

2

LAGRANGIAN MECHANICS OF THE CONSTITUENTS

We will here assume that the fluid is composed of a set of constituents, each of which is described by a position $\mathbf{x}_i$, a velocity $\underline{v}_i$, the order parameter ν_i and its total time derivative $\underline{\dot{\nu}}_i$.



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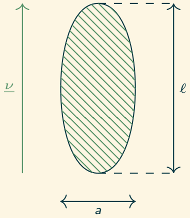
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2} \dot{\underline{\nu}}_i \cdot \underline{\underline{\Omega}}_i(\nu_i) \dot{\underline{\nu}}_i.$$



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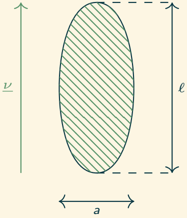
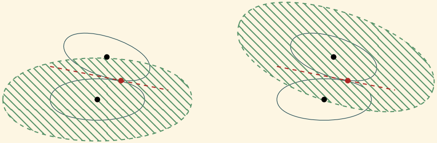


We assume the interaction between the constituents is given by a potential $\mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j)$, i.e.

$$\mathcal{L}_{i,j} = \mathcal{L}_i(\mathbf{x}_i, \Xi_i) + \mathcal{L}_j(\mathbf{x}_j, \Xi_j) + \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j),$$

where $\Xi_i := (\underline{v}_i, \nu_i, \dot{\underline{\nu}}_i)$.



NOETHER’S THEOREM: SYMMETRIES AND CONSERVATION LAWS

Oxford Mathematical Institute

Noether’s theorem

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

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_{1,2}} \cdot G\right) = 0, \qquad q_{1,2} = (\mathbf{x}_1, \mathbf{x}_2, \nu_1, \nu_2)\,.$$

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

🔖 *Analytical Mechanics: An Introduction*, (A. Fasano, S. Marmi).

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- The Lagrangian $\mathcal{L}$ is invariant under translations, i.e. the linear momentum is conserved.
- 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.

NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

Infinitesimal Generator of $\mathcal{A}$

For fixed $\nu \in \mathcal{M}$, the orbit map

$$\mathcal{A}_\nu : \mathrm{SO}(3) \to \mathrm{SO}(3)\nu, \quad \underline{\underline{Q}} \mapsto \mathcal{A}(\underline{\underline{Q}}, \nu),$$

is differentiable at the identity.

We will denote by $A_\nu : \mathrm{SO}(3) \to T_\nu\mathcal{M}$ the differential of $\mathcal{A}_\nu$ at the identity.
Composing the canonical isomorphism $\mathbb{R}^3 \to SO(3)$ with the differential of the orbit map we obtain a map $A_\nu : \mathbb{R}^3 \to T_\nu\mathcal{M}$.

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Assuming that the Lagrangian $\mathcal{L}$ is frame-indifferent, i.e. invariant under the action of SO(3), we have:

$$G = \left(\underline{r} \times \mathbf{x}, \underline{r} \times \underline{x}, A_\nu \mathbf{r}, A_\nu \underline{r}\right),$$

where $\underline{r}$ is the rotation axis. Thus, the angular momentum is conserved.

AN EXAMPLE: ANGULAR MOMENTUM NEMATIC LIQUID CRYSTALS

For segment like molecules the classical we have $\underline{\underline{\Omega}}(\underline{\nu}) = I$, where I is the Identity. Thus, Noether's theorem implies the conservation of the following quantity:

$$m_1\mathbf{x}_1 \times \underline{p}_1 + \nu \times \underline{\dot{\nu}}_1 + m_2\mathbf{x}_1 \times \underline{p}_2 + \nu \times \underline{\dot{\nu}}_2.$$

Let $\underline{\omega}$ be the angular velocity of the segment, using the triple cross product together with the well-known property of segment like rigid bodies that $\underline{\dot{\nu}}_i = \underline{\omega} \times \underline{\nu}_i$ we can rewrite one term of the previous expression as

$$\underline{\nu}_i \times \underline{\dot{\nu}}_i = \underline{\nu}_i \times \underline{\omega}_i \times \underline{\nu}_i = (\underline{\nu}_i \cdot \underline{\nu}_i)\underline{\omega} - (\underline{\nu}_i \cdot \underline{\omega}_i)\underline{\nu}_i = \underline{\omega}_i - (\underline{\nu}_i \cdot \underline{\omega}_i)\underline{\nu}_i = \mathbb{I}_i\underline{\omega},$$

where used the fact that the inertia tensor of a segment is $\mathbb{I}_i := I - \underline{\nu}_i \otimes \underline{\nu}_i$. Therefore, we retrieved the classical definition of angular momentum, i.e.

$$\mathbf{x}_1 \times \underline{p}_1 + \mathbb{I}_1\underline{\omega}_1 + \mathbf{x}_2 \times \underline{p}_2 + \mathbb{I}_2\underline{\omega}_2,$$

BBGKY HIERARCHY

3

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.

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

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

$$\mathcal{H} := \sum_{i=1}^{N} \frac{1}{2m}\underline{p_i} \cdot \underline{p_i} + \frac{1}{2}\underline{\varsigma_i} \cdot \underline{\underline{\Omega}}(\nu)^{-1}\,\underline{\varsigma_i} + \sum_{1 \leq i < j \leq N} \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j).$$

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

STATISTICAL MECHANICS APPROACH

We will also denote $\Gamma_i := (\mathbf{x}_i, \underline{p}_i, \nu_i, \underline{\varsigma}_i)$ the phase space point of the i-th constituent, and introduce

$$\pi\left(\{\Gamma_i\}_{i=1}^N\right) := \sum_{i=1}^{N} \delta\left(\Gamma_i - \Gamma_i^*(t)\right)$$

the **Klimontovich distribution function**, where $\Gamma_i^*(t)$ is the configuration of the i-th constituent at time t.

We will denote π_s the marginals of the Klimontovich distribution function, with respect to $\Gamma^{(s)} = (\Gamma_{s+1}, \dots, \Gamma_N)$, i.e.

$$\pi_s\left(\{\Gamma_i\}_{i=1}^s\right) := \int \pi\left(\{\Gamma_i\}_{i=1}^N\right) d\Gamma^{(s)}.$$

The distribution function π_s is called the ***s*-particle distribution function**, and represents the probability of finding s particles in the phase space point $\Gamma_1, \dots, \Gamma_s$.

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).

Let f_s denote the normalised π_s. We obtain the following expression for the BBGKY hierarchy,

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

where $\mathcal{H}_s = \left(\sum_{i=1}^{s} \frac{|\underline{p}_i|^2}{2m} + \frac{1}{2}\underline{\varsigma_i} \cdot \underline{\underline{\Omega}}(\nu)^{-1}\underline{\varsigma_i}\right) + \sum_{1\leq i<j\leq s} \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j)$.

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

The first two terms of the BBGKY hierarchy, under the assumption that there are no three-body interactions, amount to

$$
\begin{aligned}
&\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1} \underline{\varsigma}_1 \frac{\partial f_1}{\partial \nu_1} = \\
&+ \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \Big(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \Big) \\
&+ \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \Big(\frac{\partial f_2}{\partial \underline{\varsigma}_1} - {\color{red}\frac{\partial f_2}{\partial \underline{\varsigma}_2}} \Big)
\end{aligned}
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&\frac{\partial f_2}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1} \underline{\varsigma}_1 \cdot \frac{\partial f_2}{\partial \nu_1} \\
&+ \frac{\underline{p}_2}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}_2} + \underline{\underline{\Omega}}(\nu_2)^{-1} \underline{\varsigma}_2 \cdot \frac{\partial f_2}{\partial \nu_2} \\
&- \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \Big(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \Big) \\
&- \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0
\end{aligned}
$$

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

To highlight the same timescale separation in the second term of the hierarchy we introduce fast and slow varying coordinates, i.e.

$$\mathbf{x} = \mathbf{x}_2 - \mathbf{x}_1, \qquad \mathbf{X} = \frac{1}{2}\left(\mathbf{x}_2 + \mathbf{x}_1\right).$$

We then boxed the terms that are quickly varying in the second equation of the BBGKY hierarchy, i.e.

$$\frac{\partial f_2}{\partial t} + \frac{1}{2}\frac{\underline{p}_2 + \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \underline{X}} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \cdot \frac{\partial f_2}{\partial \nu_1} + \underline{\underline{\Omega}}(\nu_2)^{-1}\underline{\varsigma}_2 \cdot \frac{\partial f_2}{\partial \nu_2} + \boxed{\frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}}}$$
$$- \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \cdot \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right)} - \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \cdot \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0$$

EMBEDDED BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

Using the embedding results previously discussed, we can use the fast and slow varying coordinates also for the order parameters, i.e.

$$\underline{n} = \underline{\nu}_2 - \underline{\nu}_1, \qquad \underline{N} = \frac{1}{2}\left(\underline{\nu}_2 + \underline{\nu}_1\right).$$

We then introduce $\underline{A} = \frac{1}{2}\left(\underline{\underline{\Omega}}_2(\underline{\nu} a_1)^{-1}\underline{\varsigma}_1 + \underline{\underline{\Omega}}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2\right)$, $\underline{B} = \left(\underline{\underline{\Omega}}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2 - \Omega_1(\underline{\nu}_1)^{-1}\underline{\varsigma}_1\right)$, i.e.

$$\frac{\partial f_2}{\partial t} + \frac{1}{2}\frac{\underline{p}_2 + \underline{p}_1}{m}\cdot\frac{\partial f_2}{\partial \underline{X}} + \underline{A}\cdot\frac{\partial f_2}{\partial \underline{N}} + \boxed{\underline{B}\cdot\frac{\partial f_2}{\partial n}} + \boxed{\frac{\underline{p}_2 - \underline{p}_1}{m}\cdot\frac{\partial f_2}{\partial \mathbf{x}}}$$
$$- \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1}\cdot\left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right)} - \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1}\cdot\left(\frac{\partial f_2}{\partial \underline{\varsigma}_1} - \frac{\partial f_2}{\partial \underline{\varsigma}_2}\right)} = 0.$$

BOLTZMANN–CURTISS EQUATION

4

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

We can obtain from the embedded BBGKY hierarchy the following **Boltzmann** type equation,

$$\partial_t f + \nabla_{\mathbf{x}} \cdot (\underline{v} f) + \nabla_{\underline{\alpha}} \cdot (\dot{\underline{\alpha}} f) = C[f, f] \tag{1}$$

where $f(\mathbf{x}, \underline{v}, \underline{\alpha}, \underline{\varsigma})$ is the probability of having a particle at $(\mathbf{x}, \underline{v}, \underline{\alpha}, \underline{\varsigma})$ in configuration space, normalised by $\frac{1}{n}$.

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$$C[f,f] = \iiiint (f_1^{'} f^{'} - f_1 f)(\underline{k} \cdot \underline{g}) S(\underline{k}) d\underline{k} d\underline{v}_1 d\underline{\alpha}_1 d\underline{\varsigma}_1$$

with $S(\underline{k})d\underline{k}$ being the surface element of the excluded volume and $\underline{g} = \underline{v}_1 - \underline{v} + \underline{\omega}_1 \times \mathbf{x}_1 - \underline{\omega} \times \mathbf{x}$.

COLLISION INVARIANTS

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It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\underline{v}_1 d\underline{\varsigma}_1 d\underline{\alpha}_1 = 0.$$

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- $\psi^{(4)} = \frac{1}{2} m\underline{v} \cdot \underline{v} + \frac{1}{2}\underline{\omega} \cdot \mathbb{I} \cdot \underline{\omega}$, the **kinetic energy of the system**.

THE HYDRODYNAMIC EQUATIONS – NOTATION

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

$$n(\mathbf{x}) = \iiint f(\mathbf{x}, \underline{v}, \underline{\alpha}, \underline{\varsigma}) d\underline{v} d\underline{\alpha} d\underline{\varsigma}.$$

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

$$\langle\!\langle \cdot \rangle\!\rangle(\mathbf{x}) := \frac{1}{n(\mathbf{x})} \iiint \cdot\, f(\mathbf{x}, \underline{v}, \underline{\alpha}, \underline{\varsigma}) d\underline{v} d\underline{\alpha} d\underline{\varsigma}.$$

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Using this notation we can define **macroscopic stream velocity** and **macroscopic stream angular velocity** respectively as:

$$\underline{v}_0 := \langle\!\langle \underline{v} \rangle\!\rangle, \qquad \underline{\omega}_0 := \langle\!\langle \underline{\omega} \rangle\!\rangle.$$

THE HYDRODYNAMIC EQUATIONS – CURTISS BALANCE LAWS

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Testing (1) against the first two **collision invariants** and integrating, Curtiss obtained the following **balance laws**:

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

$$\rho \Big[\partial_t \underline{v}_0 + (\nabla_{\mathbf{x}} \underline{v}_0) \underline{v}_0 \Big] + \nabla_{\mathbf{x}} \cdot (\rho \mathbb{P}) = 0,$$

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

THE HYDRODYNAMIC EQUATIONS – SURPRISE BALANCE LAWS

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

$$\rho\Big[\partial_t \underline{\eta} + (\nabla_{\mathbf{x}}\underline{\eta})\underline{v}_0\Big] + \nabla_{\mathbf{x}} \cdot (\rho\mathbb{N}) = \underline{\xi},$$

where $\underline{\eta}$ is the **macroscopic intrinsic angular momentum** defined as $\underline{\eta}(\mathbf{x}) := \langle\!\langle \mathbb{I} \cdot \omega \rangle\!\rangle$ and $\mathbb{N}$ is the **couple tensor** defined as $\mathbb{N} := \langle\!\langle \underline{V} \otimes (\mathbb{I}\underline{\omega}) \rangle\!\rangle$. 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.

MAXWELL–BOLTZMANN DISTRIBUTION

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

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

where the **peculiar angular velocity** defined as $\underline{\Omega} := \underline{\omega} - \underline{\omega}_0$, $\Gamma = \prod_{i=1}^{3}\Gamma_i$, Γ_i are the moments of inertia of the spherocylinder 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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Notice in particular that we assumed $\underline{\omega}_0$ is the kinetic temperature of the system measured in energy units.

MOMENTUM CLOSURE AROUND THE EQUILIBRIUM

Now we can use the Maxwell–Boltzmann distribution to compute an approximation of the **pressure tensor** near the equilibrium, i.e.

$$\mathbb{P}^{(0)} = \frac{\Gamma}{3m}\langle\!\langle \theta \rangle\!\rangle \underline{Id}.$$

$$\left[\partial_t \underline{v}_0 + (\nabla_{\mathbf{x}} \underline{v}_0)\underline{v}_0\right] = -\frac{1}{\rho}\nabla p,$$

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Unfortunately the same procedure results in a **vanishing** $\mathbb{N}^{(0)}$.

NOETHER'S THEOREM AND MOMENTUM COUPLING

Let us consider the equation for the angular momentum, and observe that under the assumption $\mathbb{N}^{(0)} = 0$ it reads

$$\underline{\dot{\eta}} = \underline{\xi} = 0.$$

In particular, this is a consequence of Noether's theorem since when $\mathbb{N}^{(0)} = 0$ we have a **rotationally invariant** Lagrangian.

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Near the thermal equilibrium is the fluid isotropic? No!

THE NEMATIC ORDERING AND THE INERTIA TENSOR

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

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

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, U. Z.),

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:

$$\dot{\psi}_0 + \nabla_{\mathbf{x}} \underline{v}_0 : (\rho \mathbb{P}) + \nabla_{\mathbf{x}} \underline{\omega}_0 : (\rho \mathbb{N}) - \nabla \cdot \left[\mathbb{P}^T \underline{v}_0 + \mathbb{N}^T \underline{\omega}_0 \right] + \nabla_{\mathbf{x}} \cdot Q = 0$$

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

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$$\theta = \frac{m}{2} \underline{V} \cdot \underline{V} + \frac{1}{2} \underline{\Omega} \cdot \mathbb{I} \cdot \underline{\Omega}.$$

This is a **kinetic derivation** of **Leslie's rate of work hypothesis**.

THE OSEEN-FRANK STORED ENERGY

🔖 *Multiscale Model. Simul.* 2024, accepted (P. E. Farrell, G. Russo, U. Z.),

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

$$\psi_{OF}(\underline{\nu}, \nabla \underline{\nu}) = \frac{1}{2} \underline{\Omega} \cdot \mathbb{I} \underline{\Omega} = \frac{\lambda_1}{2} tr \left[\nabla \underline{\nu}^T \mathbb{P}^{(0)} \nabla \underline{\nu} \right].$$

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

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

NOLL–COLEMAN PROCEDURE

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

Since we are happy with our **pressure tensor**, we make the following **ansatz**

$$\psi = \psi(\nu, \nabla\nu)$$

where ν is the **nematic director**. Expanding the total derivative and using the Ericksen identity we get the following expression in tensor notation

$$\begin{aligned}\dot{\psi} = \varepsilon_{iqp}\Big[\big(\nu_q \frac{\partial\psi}{\partial(\nu_p)} + \partial_k(\nu_q)\frac{\partial\psi}{\partial(\partial_k\nu_p)}\big)\omega_i^0 + \nu_q \frac{\partial\psi}{\partial(\partial_k\nu_p)}\partial_k\omega_i^0\Big] \\ - \frac{\partial\psi}{\partial(\partial_k\nu_p)}\partial_q(\nu_p)\partial(v_q^0)\end{aligned}$$

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Substituting this expression in the Theorem of Power Expended and considering thermodynamic processes for which the exact divergences disappear, we get:

$$\left[\mathbb{P}_{ij} + \frac{\partial\psi}{\partial(\partial_j\nu_p)}\partial_i(\nu_p)\right]\partial_j(\nu_i) + \left[N_{ij} - \varepsilon_{iqp}\nu_q\frac{\partial\psi}{\partial(\partial_j\nu_p)}\right]\partial_j(\omega_i^0)$$

$$\left[P_{pq} - \frac{\partial\psi}{\partial(\partial_p\nu_k)\partial_q(\nu_k)}\right]\varepsilon_{iqp}\omega_i^0 \geq 0.$$

Since the above expression must hold for all thermodynamic processes for which the exact divergences disappear, we get the following **constitutive relations**:

$$\mathbb{P} = \nabla\underline{\nu}^T\frac{\partial\psi}{\partial(\nabla\underline{\nu})} + \mathbb{P}^{(0)}, \qquad \mathbb{N}_{ij} = \varepsilon_{iqp}\nu_q\frac{\partial\psi}{\partial(\partial_j\nu_p)} = \underline{\nu}\times\frac{\partial\psi}{\partial(\nabla\underline{\nu})}.$$

COMPRESSIBLE LESLIE–ERICKSEN EQUATIONS

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&\rho\Big[\partial_t \underline{\nu} + (\nabla_{\mathbf{x}} \underline{\nu})\underline{v}_0\Big] + \nabla_{\mathbf{x}} \cdot \Big(p_K \frac{\lambda_1}{2} \nabla_{\mathbf{x}} \underline{\nu}\Big) = \tau \underline{\nu},
\end{aligned}$$

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This leads to the following set of equations, which can be seen as an inviscid compressible generalisation of the Leslie–Ericksen equations:

$$\begin{aligned}
&\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \underline{v}_0) = 0,\\
&\rho\Big[\partial_t \underline{v}_0 + (\nabla_{\mathbf{x}} \underline{v}_0)\underline{v}_0\Big] + \nabla_{\mathbf{x}} \cdot \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\mathbf{x}} \underline{\nu}^T \nabla_{\mathbf{x}} \underline{\nu}\Big) = 0,\\
&\rho\Big[\partial_t \underline{\nu} + (\nabla_{\mathbf{x}} \underline{\nu})\underline{v}_0\Big] + \nabla_{\mathbf{x}} \cdot \Big(p_K \frac{\lambda_1}{2} \nabla_{\mathbf{x}} \underline{\nu}\Big) = \tau \underline{\nu},\\
&\rho\Big[\partial_t \psi_0 + \nabla_{\mathbf{x}} \psi_0 \cdot \underline{v}_0\Big] + \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\mathbf{x}} \underline{\nu}^T \nabla_{\mathbf{x}} \underline{\nu}\Big) : \nabla_{\mathbf{x}} \underline{v}_0 = 0.
\end{aligned}$$

A VLASOV–TYPE EQUATION

5

VLASOV–TYPE EQUATION

From the separation of timescales in the BBGKY hierarchy we obtain the following identity,

$$\frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}} = \frac{\partial \mathcal{W}}{\partial \mathbf{x}_1}\left(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2\right) \cdot \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right).$$

Substituting this identity in the second equation of the BBGKY hierarchy we obtain the following equation,

$$\begin{aligned}\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \cdot \frac{\partial f_1}{\partial \nu_1} &= \int \frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}} \, d\Gamma_2 \\ &+ \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \cdot \frac{\partial f_2}{\partial \underline{\varsigma}_1} \, d\Gamma_2.\end{aligned}$$

WEAK-ORDER INTERACTIONS

We might be tempted to assume interactions are **weak**,

$$f_2(\Gamma_1, \Gamma_2, t) = f_1(\Gamma_1, t) f_1(\Gamma_2, t).$$

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Weak-order Interactions

We will say that a kinetic equation is governed by **weak-order interactions** if the derivative of the two-particle distribution function factorises as,

$$\partial_{\nu_i} f_2(\Gamma_1,\Gamma_2,t) = f_1(\Gamma_i,t)\partial_{\nu_i} f_1(\Gamma_j,t),$$
$$\partial_{\varsigma_i} f_2(\Gamma_1,\Gamma_2,t) = f_1(\Gamma_j,t)\partial_{\varsigma_i} f_1(\Gamma_i,t),$$

for $i \neq j$ and $i,j = 1,2$.

VLASOV–TYPE EQUATION

Under the assumption of weak-order interactions we can rewrite the first equation of the BBGKY hierarchy as,

$$\frac{\partial f}{\partial t} + \underline{\dot{x}} \cdot \nabla_{\mathbf{x}} f + \underline{\dot{\nu}} \cdot \nabla_{\nu} f + \mathcal{V} \cdot \nabla_{\varsigma} f = C[f, f],$$

where the collision operator $C[f, f]$ can be written using the transition "probability" W as,

$$\begin{aligned} C[f_1, f_1] = \int d\Xi_1'\, d\Xi_2' d\Xi_2 \int_0^{\frac{\pi}{2}} \int_0^{2\pi} & W\left(\Xi_1', \Xi_2' \mapsto \Xi_1, \Xi_2\right) f_1(\Gamma_1', t) f_1(\Gamma_2', t) \\ & - W\left(\Xi_1, \Xi_2 \mapsto \Xi_1', \Xi_2'\right) f_1(\Gamma_1, t) f_1(\Gamma_2, t)\, d\theta_2\, d\varphi_2. \end{aligned}$$

BOLTZMANN INEQUALITY AND THERMALISATION

J. Stat. Phys. Volume 26, 795–801 (C. Cercignani, M. Lampis).

As we said before the collision operator $C[f,f]$ considered here guarantees that the system thermalises to a Maxwellian distribution. In particular, we can prove

$$\int d\Xi \, \log(f(\Gamma,t))C[f,f] \leq 0,$$

which is a generalisation of the **Boltzmann inequality** for Boltzmann's equation with internal degrees of freedom. Following the classical calculus of variation approach we can prove that the unique Maxwellian with prescribed collision invariants is

$$\bar{f}(\Gamma,t) = \exp\left(a + \underline{b}\cdot\underline{p} + c(\underline{p}\times\mathbf{x} + \underline{w}_{\nu}\times\underline{\varsigma}) + d(m^{-1}\underline{p}\cdot\underline{p} + \varsigma\cdot\underline{\underline{\Omega}}(\nu)^{-1}\varsigma)\right).$$

SPACE HOMOGENEOUS VLASOV-TYPE EQUATION

We are interested in the time evolution of the distribution $f(\underline{v}, \nu, \underline{\dot{\nu}}, t)$, $v \in \mathbb{R}^2$, $\nu \in \mathcal{M}$, $\underline{\varsigma} \in T_\nu \mathcal{M}$, and $t \geq 0$, solution to the space-homogeneous equation

$$\frac{\partial f}{\partial t} + \underline{\underline{\Omega}}(\nu)^{-1}\underline{\varsigma} \cdot \nabla_\nu f + \mathcal{V} \cdot \nabla_{\underline{\varsigma}} f = \frac{1}{\tau}\mathcal{C}[f, f],$$

where τ has been obtained rescaling the collision frequency, and as collision operator we consider the one associated with Maxwellian molecules, i.e.

$$C[f, f] = \int d\underline{\varsigma}_2 \, d\underline{v}_2 \, d\nu_2 f' f'_* - \int d\underline{\varsigma}_2 \, d\underline{v}_2 \, d\nu_2 f f_*, \tag{1}$$

complemented with initial conditions $f(\underline{v}, \nu, \underline{\varsigma}, 0) = f_0(\underline{v}, \nu, \underline{\varsigma})$ and where we will denote $f_* = f(\underline{v}_2, \nu_2, \underline{\varsigma}_2, t)$, and f', f'_* are the distributions depending on the post interaction coordinates.

DIRECT SIMULATIONS MONTE CARLO (DSMC)

We consider discretization of the time interval $[0, T_f]$, with $T_f > 0$ final simulation time, of step $\Delta t > 0$ such that $t^n = n\Delta t$. By $f^n(\underline{v}, \nu, \underline{\varsigma})$ we denote an approximation of $f(\underline{v}, \nu, \underline{\varsigma}, t^n)$ at the n-th time step and we apply a splitting method between the Vlasov-type transport operator and the collisional operator.

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Transport $\mathcal{T}_{\Delta t}(\cdot)$

We solve the Vlasov-type step $\hat{f} = \mathcal{T}_{\Delta t}(f^n)$

$$\begin{cases} \dfrac{\partial \hat{f}}{\partial t} + \Omega(\nu)^{-1}\underline{\varsigma} \cdot \nabla_\nu \hat{f} + \mathcal{V} \cdot \nabla_{\underline{\varsigma}} \hat{f} = 0 \\ \hat{f}(\underline{v}, \nu, \underline{\varsigma}, 0) = f^n(\underline{v}, \nu, \underline{\varsigma}) \end{cases}$$

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We then solve the collision step $\hat{\hat{f}} = \mathcal{Q}_{\Delta t}(\hat{f})$ with initial data given by the solution of the previous step

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The first order in time splitting finally reads $f^{n+1}(\underline{v}, \nu, \underline{\varsigma}) = \mathcal{Q}_{\Delta t}(\mathcal{T}_{\Delta t}(f^n)(\underline{v}, \nu, \underline{\varsigma}))$.

DSMC: TRANSPORT $\mathcal{T}_{\Delta t}(\cdot)$

We introduce an approximation of the distribution function with a sample of N particles identified by their velocities $\underline{v}_i^n$, order parameter ν_i^n, and conjugate momentum $\underline{\varsigma}_i^n$ at the time t^n, for $i = 1, 2, \dots, N$,

$$f^n(\underline{v}, \nu, \underline{\varsigma}) \approx f^{n,N}(\nu, \underline{\varsigma}) = \sum_{i=1}^{N} \delta(\nu - \nu_i(t^n)) \otimes \delta(\underline{\varsigma} - \underline{\varsigma}_i(t^n)).$$

The Vlasov-type transport step $\mathcal{T}_{\Delta t}(\cdot)$ is solved by considering the characteristic equations associated to the operator, which as discussed in the previous section, result in a system of (time-continuos) ODEs

$$\frac{d\underline{\nu}_i}{dt} = \underline{\varsigma}_i, \qquad \frac{d\underline{\varsigma}_i}{dt} = \mathcal{V}(\nu_i, \underline{\varsigma}_i).$$

This system is solved, at the time discrete level, with a classical first order Euler scheme for the time derivative.

DSMC: COLLISION $\mathcal{Q}_{\Delta t}(\cdot)$

The collisional step $\mathcal{Q}_{\Delta t}(\cdot)$ is solved with a classical Nanbu-Babovsky DSMC approach. First, we rewrite the collisional operator to highlight the gain and loss part integrating the second term in (1)

$$G - L = \int d\underline{\varsigma}_2 \, d\underline{v}_2 \, d\nu_2 f' f'_* - f,$$

and then we discretize the time derivative with a first order in time Euler scheme to obtain

$$f^{n+1} = \left(1 - \frac{\Delta t}{\tau}\right) f^n + \frac{\Delta t}{\tau} \int d\underline{\varsigma}_2 \, d\underline{v}_2 \, d\nu_2 f' f'_*.$$

We have thus rewritten f^{n+1} as a convex combination of f^n and the gain term, i.e. we will consider all the particles in the system with probability $\frac{\Delta t}{\tau}$ we will update the velocity, order parameter and conjugate momentum according to the binary law relating the pre and post interaction velocities, order parameters and conjugate momenta.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS

In the context of of rod-like molecules, with vanishing girth, we can explicitly compute the Vlasov-type force $\mathcal{V}$ and the transport term to obtain the following equation

$$\frac{\partial f}{\partial t} + \omega \nabla_\theta f + \mathcal{V} \cdot \nabla_\omega f = \iiint \left(f' f'_* - f f_* \right) dv_* d\theta_* d\omega_*,$$

where $f = f(\underline{v}, \theta, \omega, t)$, $f_* = f(\underline{v}_*, \theta_*, \omega_*, t)$, and f', f'_* are the distributions depending on the post interaction coordinates given by

$$\begin{aligned} \underline{v}' &= \underline{v} - (1+e_v)\frac{J}{m}\underline{n}, & \underline{v}'_* &= \underline{v}_* + (1+e_v)\frac{J}{m}\underline{n}, \\ \omega' &= \omega - (1+e_\omega) J \mathbb{I}^{-1}(r \times \underline{n}), & \omega'_* &= \omega_* + (1+e_\omega) J \mathbb{I}_*^{-1}(r_* \times \underline{n}), \end{aligned}$$

with

$$J = -\frac{V \cdot \underline{n}}{\frac{2}{m} + \left[\mathbb{I}^{-1}(r \times \underline{n}) \times r + \mathbb{I}_*^{-1}(r_* \times \underline{n}) \times r_* \right] \cdot \underline{n}}.$$

Notice that $\theta' = \theta$ and $\theta'_* = \theta_*$ since the angles are not changed by the collisional operator.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

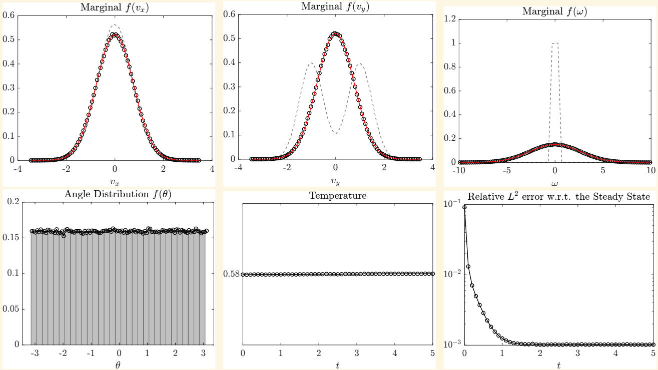

Figure: Test 1 - Zero Potential. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the exact steady state. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution remain a uniform, so we don't have aggregation.

Let us consider the mean-field potential is given by

$$\mathcal{W}(\nu, \underline{\varsigma}) = \frac{1}{2}\alpha\,(\underline{\nu} - \underline{\hat{\nu}}) \cdot (\underline{\nu} - \underline{\hat{\nu}}) + \beta\,\underline{\nu} \cdot \underline{\varsigma}.$$

Under this hypothesis the Vlasov-type force can be computed to be

$$\mathcal{V}(\nu, \underline{\varsigma}) = -\alpha\,(\underline{\nu} - \underline{\hat{\nu}}) - \beta\underline{\varsigma}.$$

This system of ODEs can be recasted as linear system of ODEs, i.e.

$$\begin{bmatrix} \frac{d\underline{\nu}_i}{dt} \\ \frac{d\underline{\varsigma}_i}{dt} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\alpha & -\beta \end{bmatrix} \begin{bmatrix} \underline{\nu}_i \\ \underline{\varsigma}_i \end{bmatrix} + \alpha \begin{bmatrix} 0 \\ \underline{\hat{\nu}} \end{bmatrix}.$$

We can immediately see that the fixed points of the system is unique and it is given by $\underline{\nu} = \underline{\hat{\nu}}$ and $\underline{\varsigma} = 0$. It remains to study the stability of the fixed point, which can be done by studying the eigenvalues of the Jacobian of the system which are given by

$$\lambda_{1,2} = \frac{-\beta \pm \sqrt{\beta^2 - 4\alpha}}{2}.$$

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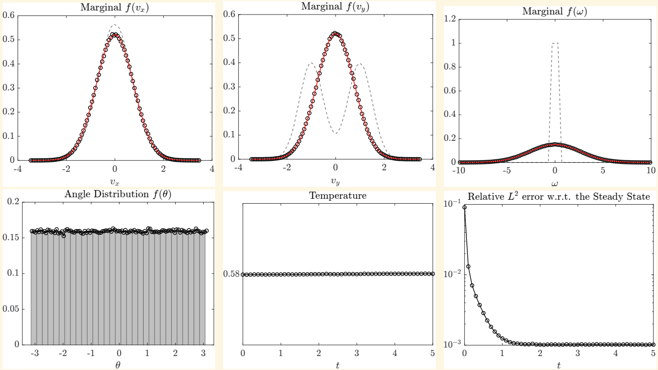

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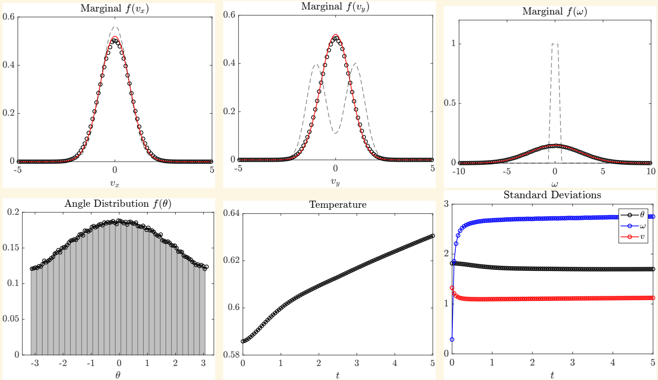

Figure: Test 2 - Quadratic potential for $\beta = 0$ and $\alpha = 1$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution remain a uniform, so we don't have aggregation.

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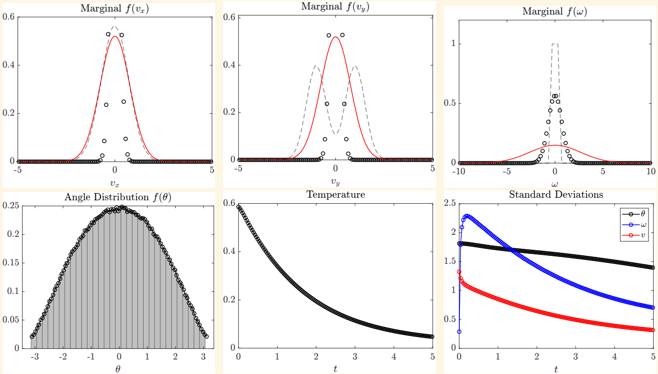

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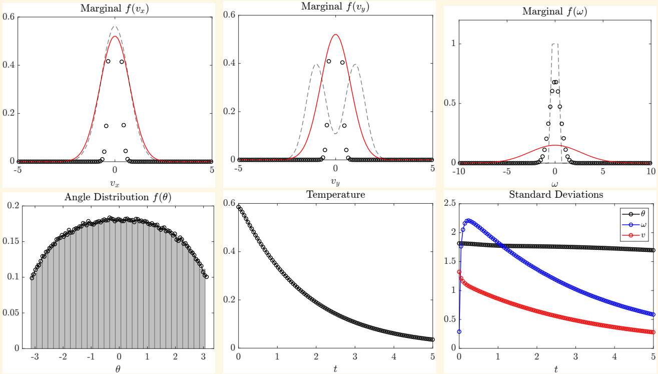

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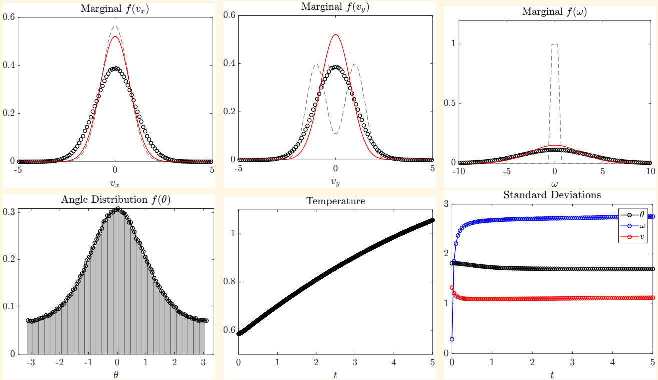

Figure: Test 3 - The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution remain a uniform, so we don't have aggregation.

CONCLUSION

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THANK YOU!

A Kinetic Framework for Fluids with Ordering

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A. Medaglia*, G. Russo[†].