UNIVERSITY OF OXFORD
Mathematical Institute

Direct Simulation Monte Carlo for Ordered Fluids

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**Mathematical Institute – University of Oxford*

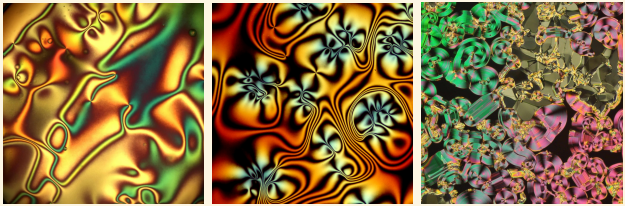
ETNA, 28th November 2025

Oxford Mathematics

ORDERED FLUIDS

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

ORDERED FLUIDS



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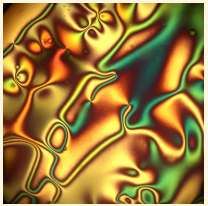
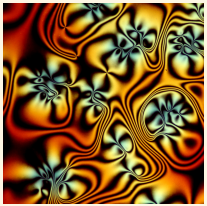
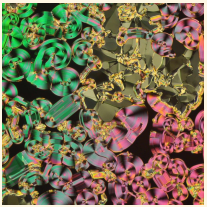


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- **Liquid crystals**, here depicted in nematic and smectic phases.
- **Ferrofluids**, i.e. a colloidal suspension made of nanoscale ferromagnetic or ferrimagnetic particles.

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- **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.

ORDER PARAMETER MANIFOLD

1

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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.

Continua with microstructure, (G. Capriz),
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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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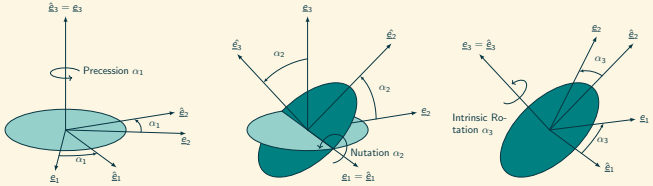
- We need to understand what manifold $\mathcal{M}$ captures the nature of the order parameters.
- We need to understand the action of rotations on the manifold $\mathcal{M}$.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS



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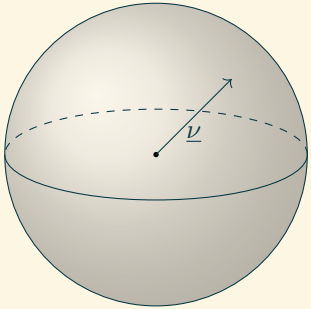

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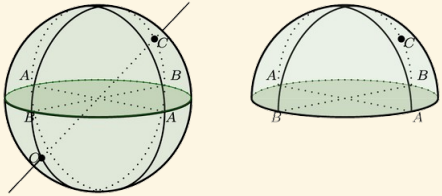

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- We can also represent the state of a calamitic molecule using a director field $\underline{\nu} \in \mathbb{S}^2$.
- For head-tail symmetric calamitic molecules, we can use $\mathbb{RP}^2$.

EMBEDDING RESULTS

Embedding theorems

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

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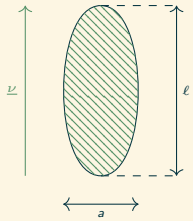
THE MICROSCOPIC WORLD

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 $\underline{\nu}_i$, the order parameter ν_i and its total time derivative $\dot{\underline{\nu}}_i$.



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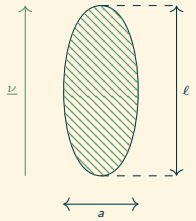
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2} \dot{\underline{\nu}}_i \cdot \underline{\underline{\Omega}}_i(\nu_i) \dot{\underline{\nu}}_i.$$



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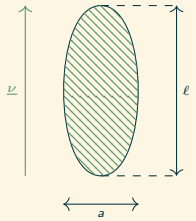
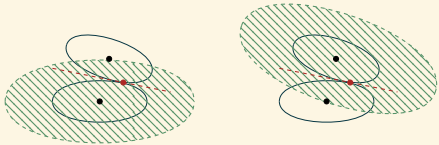
We assume the interaction between the constituents is given by a potential $\mathcal{W}(\mathbf{x}_i - \mathbf{x}_j, \nu_i, \nu_j)$, i.e.

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

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





NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

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.

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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:

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

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 $\underline{\underline{\Omega}}(\nu) = I$, 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

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

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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 $\nu \in \mathcal{M}$.

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 s-particle distribution function. We obtain the following expression for the BBGKY hierarchy,

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

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

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

$$\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \frac{\partial f_1}{\partial \nu_1} =$$
$$+ \int \frac{\partial \mathcal{W}(\mathbf{x}_1 - \mathbf{x}_2, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \right)$$
$$+ \int \frac{\partial \mathcal{W}(\mathbf{x}_1 - \mathbf{x}_2, \nu_1, \nu_2)}{\partial \nu_1} \left(\frac{\partial f_2}{\partial \underline{\varsigma}_1} - \frac{\partial f_2}{\partial \underline{\varsigma}_2} \right)$$

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$$- \frac{\partial \mathcal{W}(\mathbf{x}_1 - \mathbf{x}_2, \nu_1, \nu_2)}{\partial \nu_1} \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0$$

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

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

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,

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

WEAK-ORDER INTERACTIONS

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

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

This leads to equations of a **reversible nature**, compatible with **Loschmidt's paradox**.
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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,

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

$$\mathcal{V}(\mathbf{x}_1, \nu_1, t) = \iiint \frac{\partial \mathcal{W}(\mathbf{x}_1 - \mathbf{x}_2, \nu_1, \nu_2)}{\partial \nu_1} f(\mathbf{x_2}, \nu_2, \varsigma_2, t) \, d\mathbf{x}_2 \, d\nu_2 \, d\varsigma_2.$$

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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Collision $\mathcal{Q}_{\Delta t}(\cdot)$

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

$$\begin{cases} \tau \dfrac{\partial \hat{\hat{f}}}{\partial t} = \mathcal{C}[\hat{\hat{f}}, \hat{\hat{f}}] \\ \hat{\hat{f}}(\underline{v}, \nu, \underline{\varsigma}, 0) = \hat{f}(\underline{v}, \nu, \underline{\varsigma}, \Delta t). \end{cases}$$

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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 $i = 1, 2, \ldots, N$,

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

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 semi-implicit 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

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

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

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

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

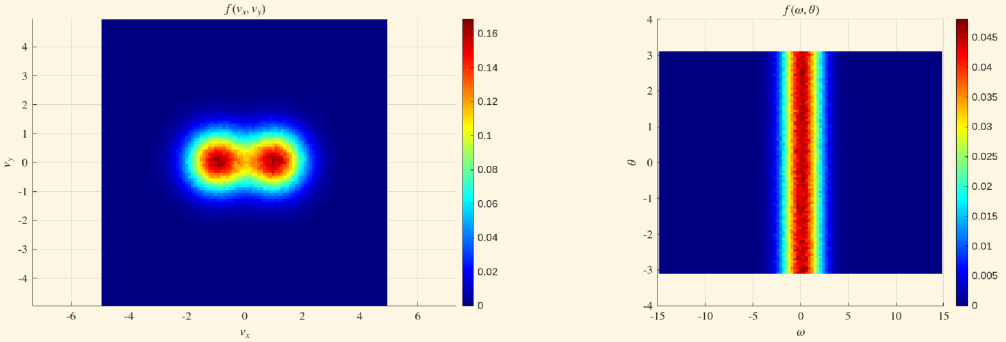

Figure: Test 1 - Zero Potential. The initial distribution function for the zero potential case. We consider a two bump initial velocity distribution (left) and a Gaussian distribution for the angular velocity with uniform distribution for the angle (right).

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

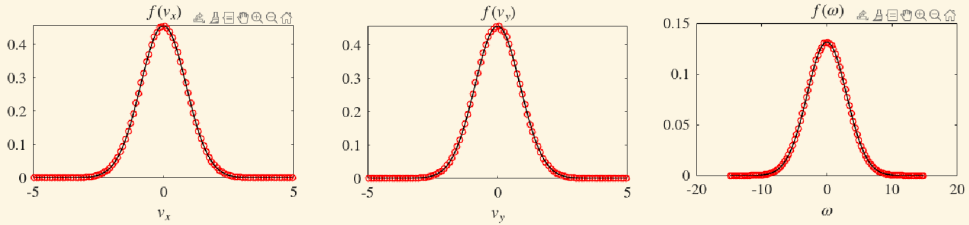

Figure: Test 1 - Zero Potential. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the exact steady state. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution 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

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

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

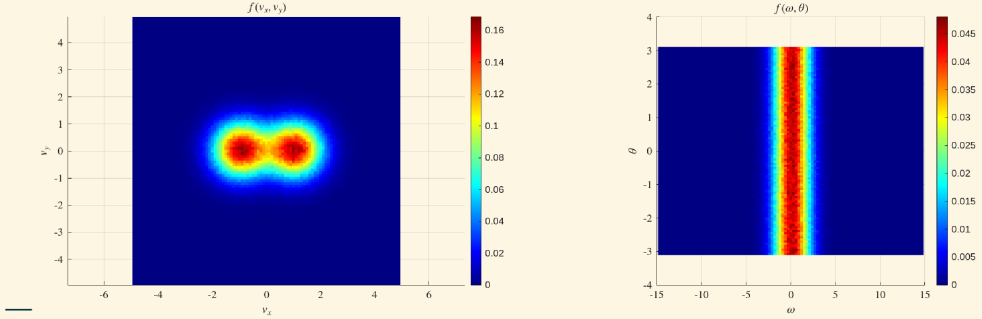

Figure: Test 2 - Quadratic potential for $\beta = 0$ and $\alpha = 1$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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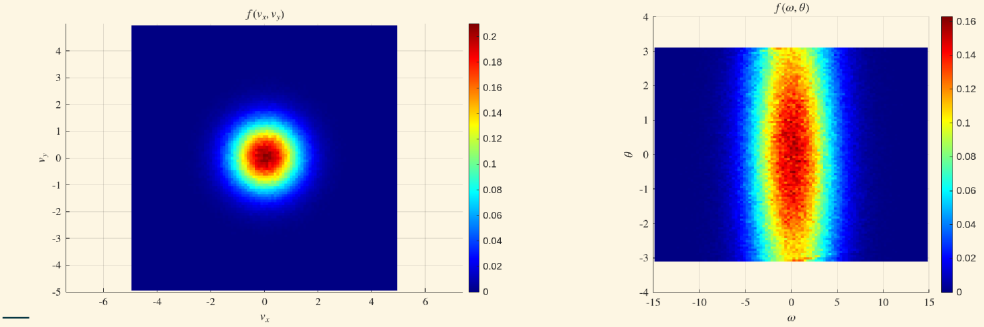

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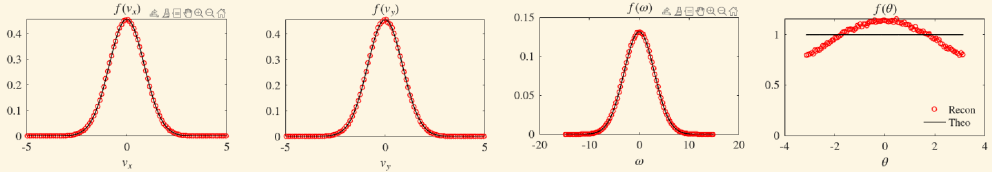

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AN EXAMPLE: NEMATIC LIQUID CRYSTALS

We now consider a non-linear potential inspired by the moment of an electric dipole in an external field, i.e.

$$\mathcal{W}(\nu) = \alpha \sin(\theta - \hat{\theta}), \qquad \theta = \arctan(\nu_x, \nu_y), \qquad \hat{\theta} = \arctan(\hat{\nu}_x, \hat{\nu}_y),$$

where $\alpha > 0$ is a constant measuring the strength of the potential, and $\underline{\hat{\nu}}$ is the communal alignment direction.

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where $\alpha > 0$ is a constant measuring the strength of the potential, and $\underline{\hat{\nu}}$ is the communal alignment direction.

With this potential we see the alignment around random orientations resulting from the competition between the potential and the thermal agitation induced by the collisions.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

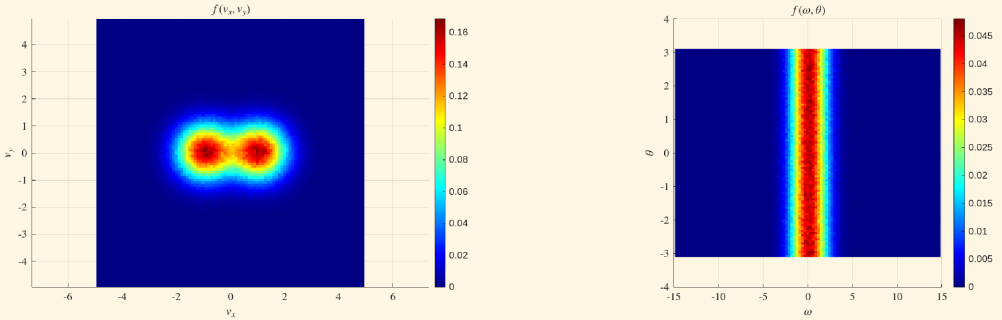

Figure: Test 3 - Non-linear potential for $\mathcal{W}(\nu) = \alpha \sin(\underline{\nu} - \hat{\underline{\nu}})$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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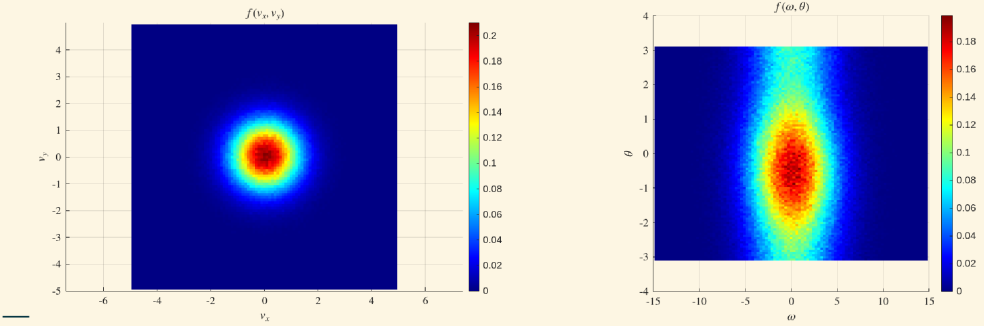

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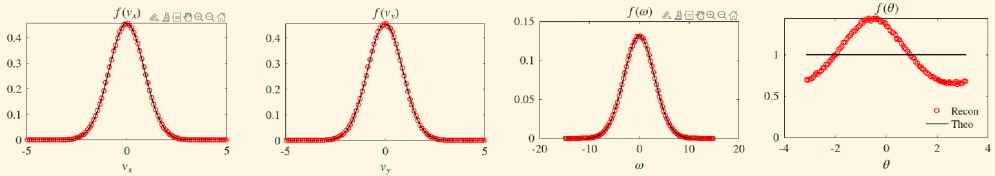

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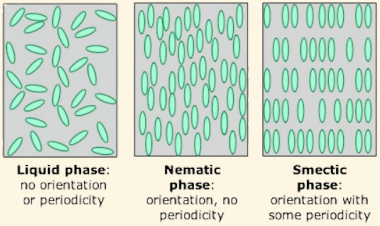
ONSAGER STERIC POTENTIAL

Lastly we consider the Onsager potential for rod-like molecules, i.e.

$$\mathcal{W}(\theta_1, \theta_2) = L^2 |\sin(\theta_1 - \theta_2)|$$

where L is the length of the molecule. This potential can be derived considering purely steric interactions between two rod-like molecules, and has been used by Onsager in his seminal work on liquid crystals. In fact, this potential favours alignment between molecules via a purely entropic driven mechanism.



$$\mathcal{V}(\theta) = L^2 \int_0^{2\pi} \int_{-\infty}^{\infty} \partial_{\theta_1} \left(|\sin(\theta - \theta_2)| \right) f(v_2, \theta_2, \omega_2, t) \, dv_2 \, d\theta_2 \, d\omega_2,$$

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

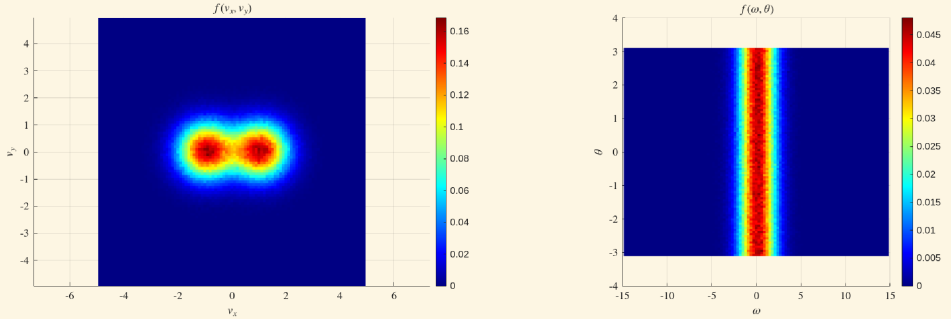


Figure: Test 4 - The Onsager potential for rod-like molecules. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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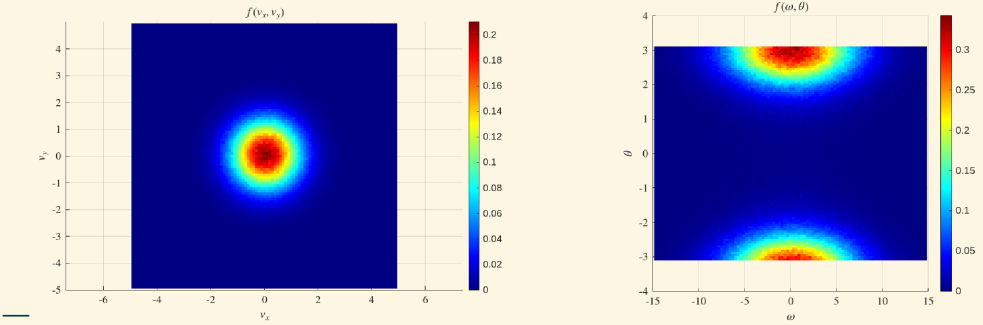

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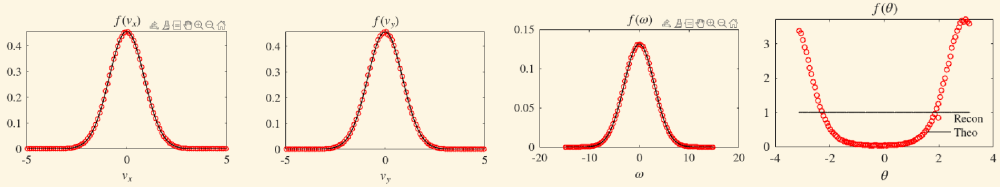

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THANK YOU!

Direct Simulation Monte Carlo for Ordered Fluids

Umberto Zerbinati*, joint work with: J. A. Carillo* ,P. E. Farrell*, A. Medaglia*.