UNIVERSITY OF OXFORD
Mathematical Institute

Direct Simulation Monte Carlo for Ordered Fluids

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**Mathematical Institute – University of Oxford*

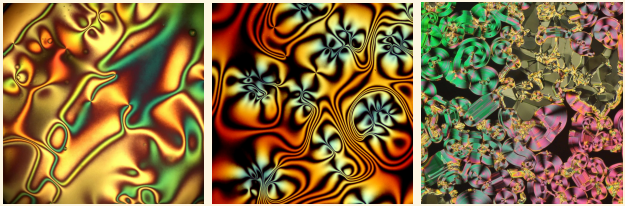
ETNA, 28th November 2025

Oxford Mathematics

ORDERED FLUIDS

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

ORDERED FLUIDS



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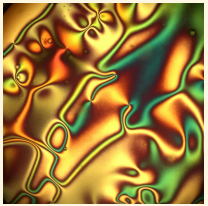
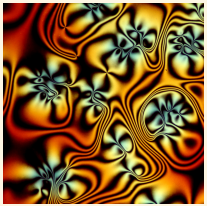
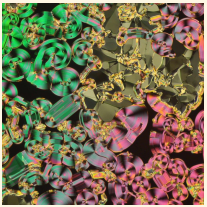


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- **Liquid crystals**, here depicted in nematic and smectic phases.
- **Ferrofluids**, i.e. a colloidal suspension made of nanoscale ferromagnetic or ferrimagnetic particles.

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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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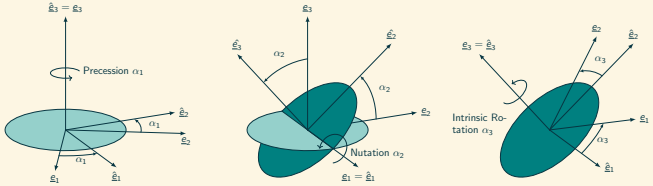
- We need to understand what manifold $\mathcal{M}$ captures the nature of the order parameters.
- We need to understand the action of rotations on the manifold $\mathcal{M}$.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS



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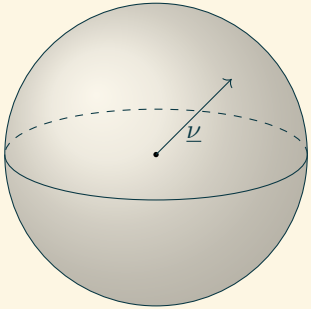

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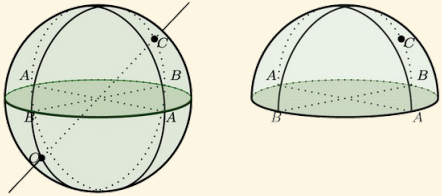

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- We can also represent the state of a calamitic molecule using a director field $\underline{\nu} \in \mathbb{S}^2$.
- For head-tail symmetric calamitic molecules, we can use $\mathbb{RP}^2$.

EMBEDDING RESULTS

Embedding theorems

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

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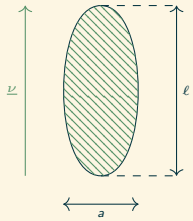
THE MICROSCOPIC WORLD

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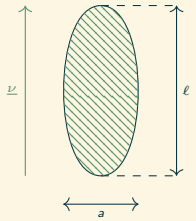
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2} \dot{\underline{\nu}}_i \cdot \underline{\underline{\Omega}}_i(\nu_i) \dot{\underline{\nu}}_i.$$



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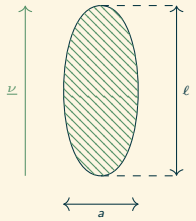
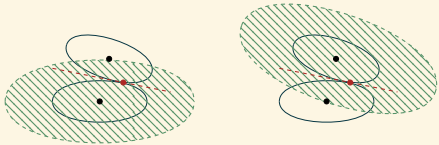
We assume the interaction between the constituents is given by a potential $\mathcal{W}(\mathbf{x}_i - \mathbf{x}_j, \nu_i, \nu_j)$, i.e.

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

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**,

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

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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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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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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

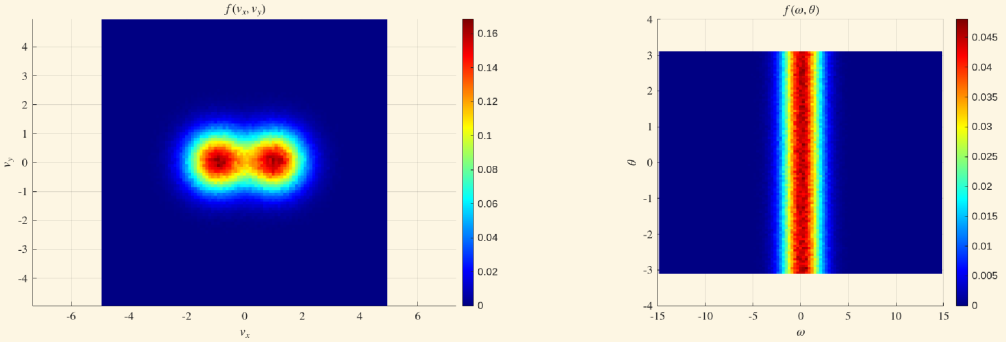

Figure: Test 1 - Zero Potential. The initial distribution function for the zero potential case. We consider a two bump initial velocity distribution (left) and a Gaussian distribution for the angular velocity with uniform distribution for the angle (right).

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

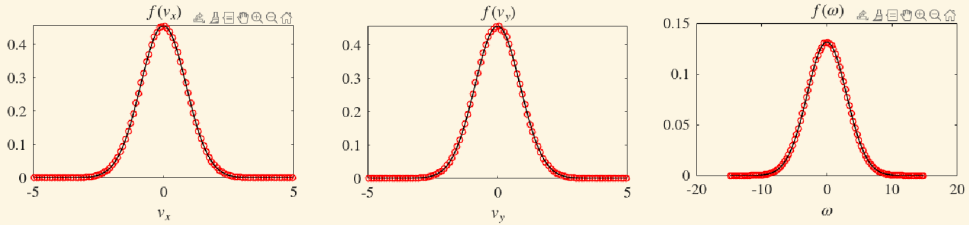

Figure: Test 1 - Zero Potential. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the exact steady state. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution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

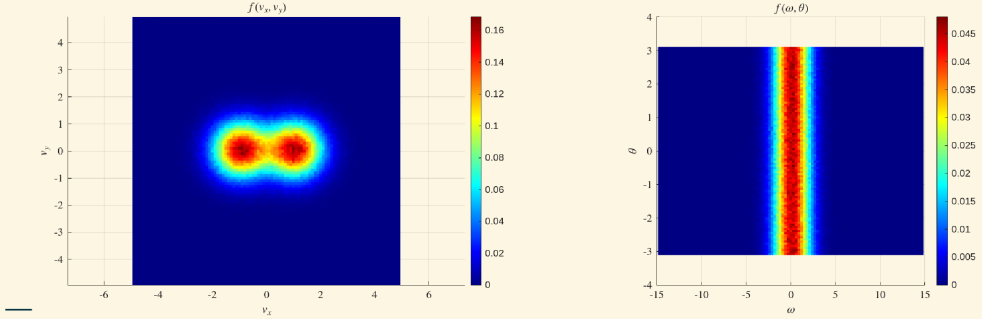

Figure: Test 2 - Quadratic potential for $\beta = 0$ and $\alpha = 1$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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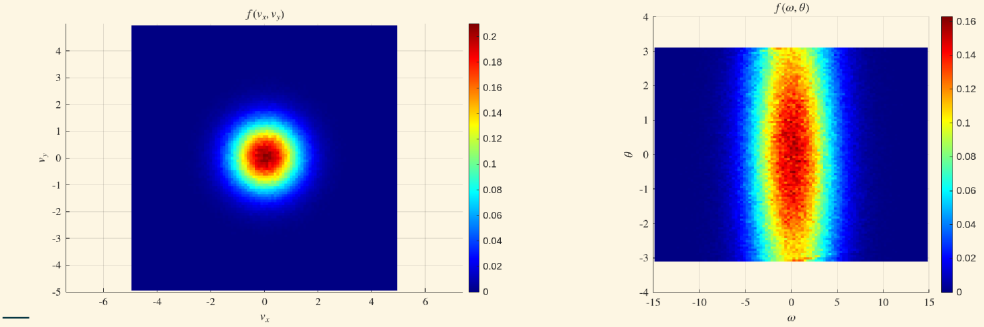

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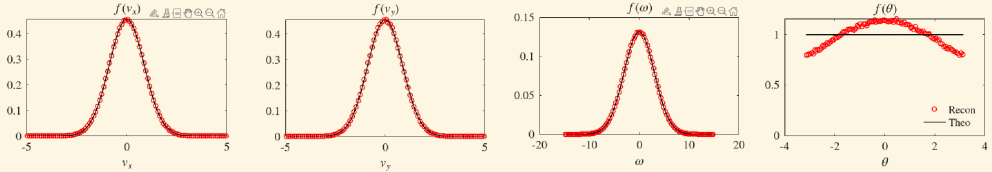

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AN EXAMPLE: NEMATIC LIQUID CRYSTALS

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.

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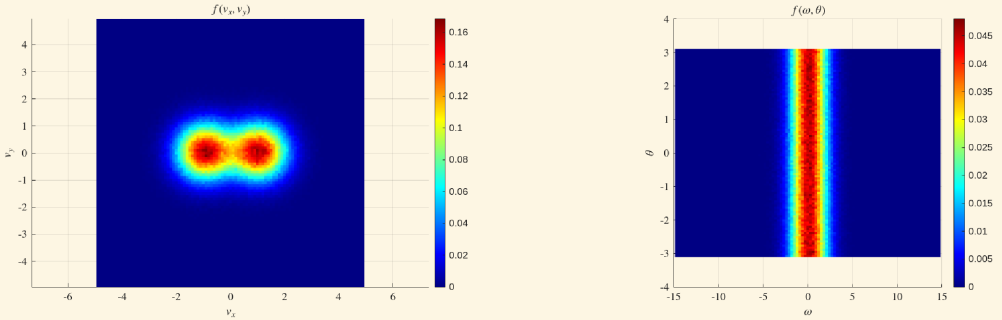

Figure: Test 3 - Non-linear potential for $\mathcal{W}(\nu) = \alpha \sin(\underline{\nu} - \hat{\underline{\nu}})$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and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

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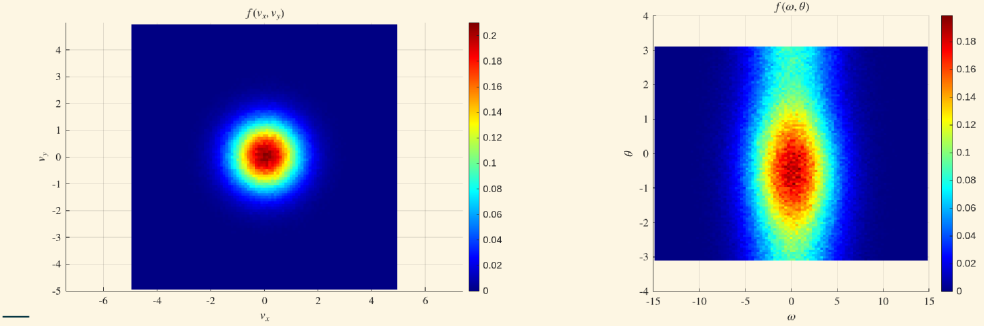

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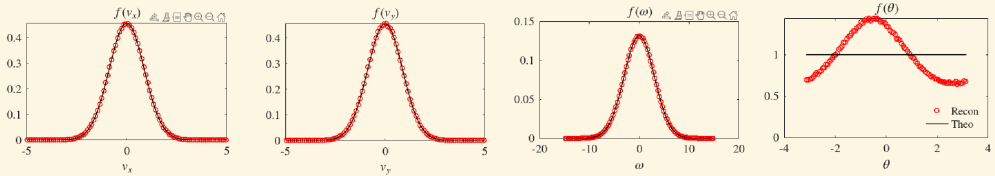

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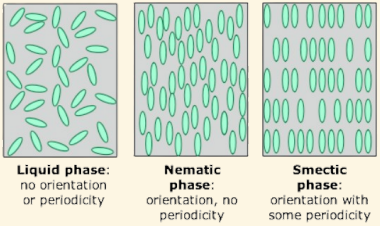
ONSAGER STERIC POTENTIAL

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.



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

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

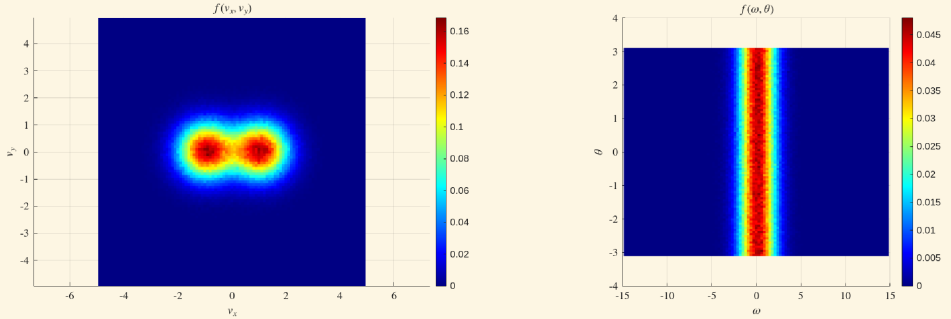


Figure: Test 4 - The Onsager potential for rod-like molecules. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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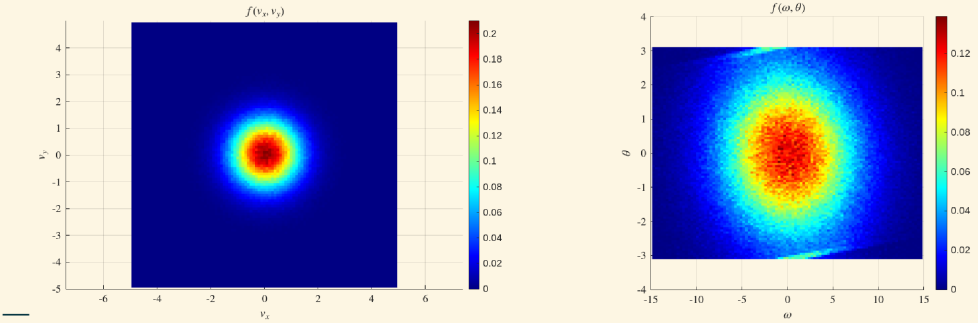

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AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

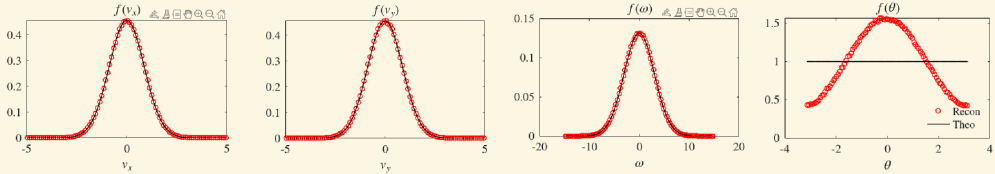

Figure: Test 4 - The Onsager potential for rod-like molecules. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

THANK YOU!

Direct Simulation Monte Carlo for Ordered Fluids

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