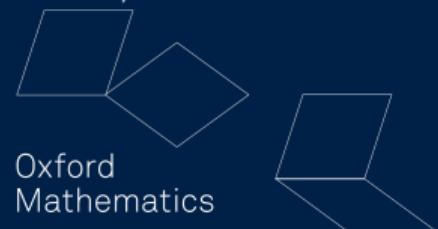


Direct Simulation Monte Carlo for Ordered Fluids

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

**Mathematical Institute – University of Oxford*

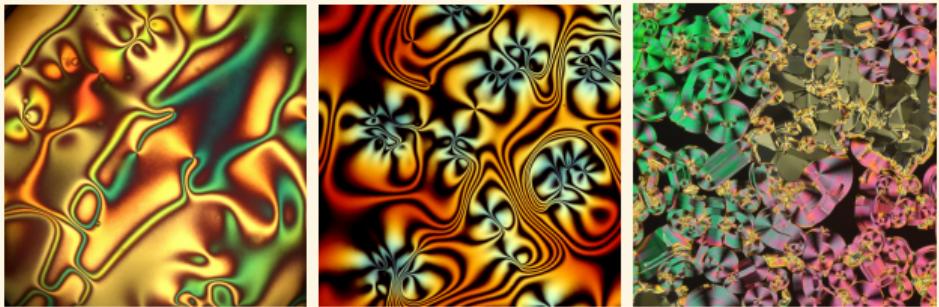
ETNA, 28th November 2025



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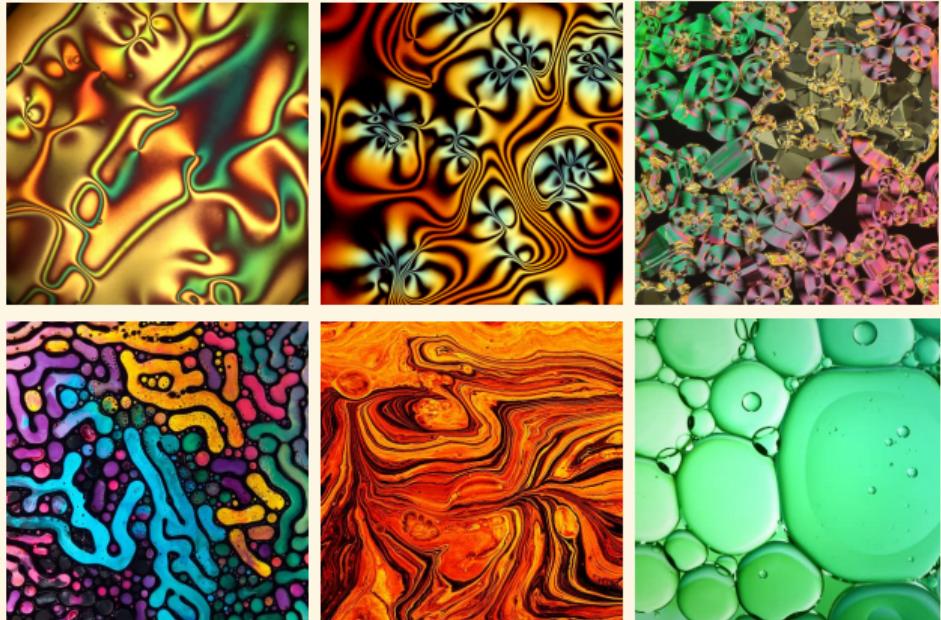
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- ▶ **Gas saturated magma melts** and other fluids with non-diffusive bubbles.

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 $\text{SO}(d)$ on \mathcal{M} , i.e. the map \mathcal{A} is smooth enough to be differentiable.



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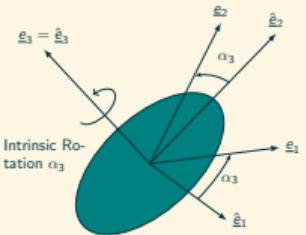
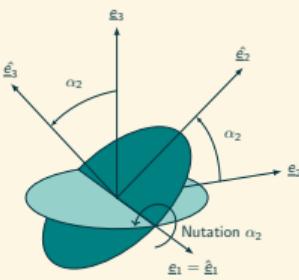
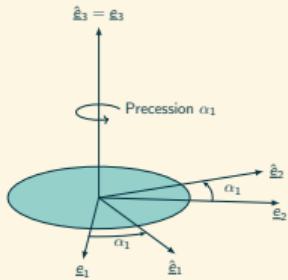
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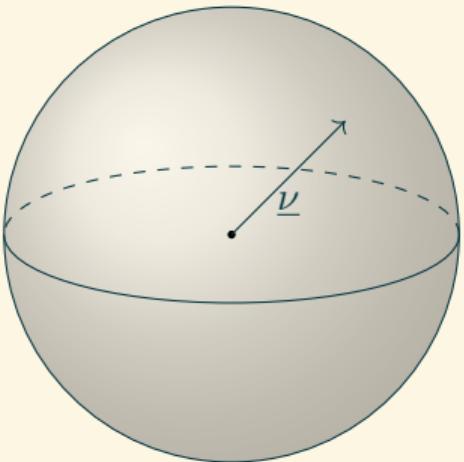
AN EXAMPLE: NEMATIC LIQUID CRYSTALS



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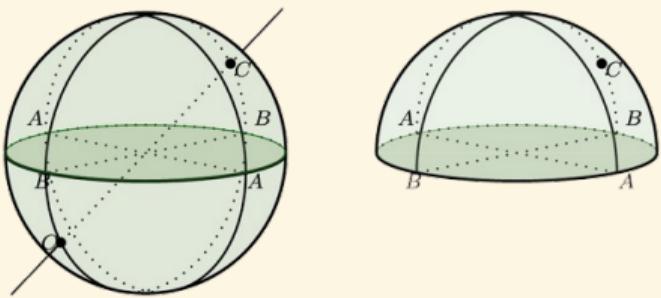
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- ▶ We can also represent the state of a calamitic molecule using a director field $\underline{\nu} \in \mathbb{S}^2$.
- ▶ For head-tail symmetric calamitic molecules, we can use \mathbb{RP}^2 .

EMBEDDING RESULTS

Embedding theorems

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



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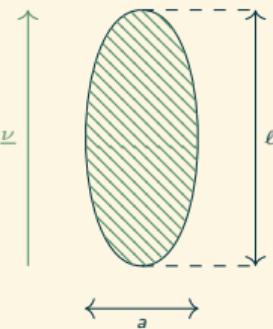
\$\$ We can embed the real projective space \mathbb{RP}^2 in \mathbb{R}^4 and work with a vector space structure.

THE MICROSCOPIC WORLD

2

LAGRANGIAN MECHANICS OF THE CONSTITUENTS

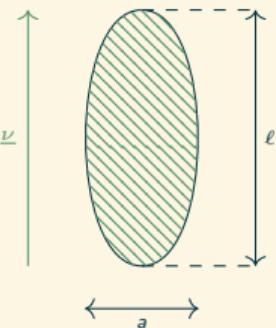
We will here assume that the fluid is composed of a set of constituents, each of which is described by a position \mathbf{x}_i , a velocity \underline{v}_i , the order parameter ν_i and its total time derivative $\dot{\nu}_i$.



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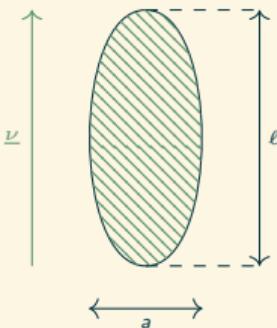
$$\mathcal{L}_i := \frac{1}{2} m_i (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2} \dot{\underline{\nu}}_i \cdot \underline{\Omega}_i(\nu_i) \dot{\underline{\nu}}_i.$$



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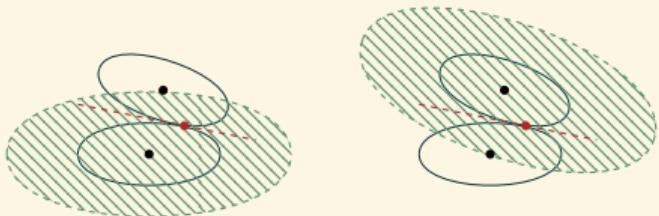
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i) + \frac{1}{2} \dot{\underline{v}}_i \cdot \underline{\Omega}_i(\nu_i) \dot{\underline{v}}_i.$$



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



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

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

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

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

is differentiable at the identity.

We will denote by $A_\nu : \mathrm{SO}(3) \rightarrow T_\nu \mathcal{M}$ the differential of \mathcal{A}_ν at the identity.

Composing the canonical isomorphism $\mathbb{R}^3 \rightarrow \mathrm{SO}(3)$ with the differential of the orbit map we obtain a map $A_\nu : \mathbb{R}^3 \rightarrow T_\nu \mathcal{M}$.



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

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

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

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

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 $\dot{\underline{\nu}}_i = \underline{\omega} \times \underline{\nu}_i$ we can rewrite one term of the previous expression as

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

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.

$$\underline{p}_i := \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i} = m\dot{\mathbf{x}}_i, \quad \underline{\varsigma}_i := \frac{\partial \mathcal{L}}{\partial \dot{\nu}_i} = \underline{\Omega}(\nu) \dot{\nu}_i.$$

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

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

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The Legendre transform of the Lagrangian \mathcal{L} is always well-defined, assuming $\underline{\Omega}(\nu)$ 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,

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

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

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

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

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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.

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

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

$$\begin{aligned} & \frac{\partial f_2}{\partial t} + \frac{1}{2} \frac{p_2 + p_1}{m} \cdot \frac{\partial f_2}{\partial \underline{X}} + \underline{\Omega}(\nu_1)^{-1} \underline{\zeta}_1 \cdot \frac{\partial f_2}{\partial \nu_1} + \underline{\Omega}(\nu_2)^{-1} \underline{\zeta}_2 \cdot \frac{\partial f_2}{\partial \nu_2} + \boxed{\frac{p_2 - p_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}}} \\ & - \boxed{- \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \cdot \left(\frac{\partial f_2}{\partial p_1} - \frac{\partial f_2}{\partial p_2} \right) - \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \cdot \frac{\partial f_2}{\partial \underline{\zeta}_1}} = 0 \end{aligned}$$

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.

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

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

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

VLASOV-TYPE EQUATION

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

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

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

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

WEAK-ORDER INTERACTIONS

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

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

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,

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

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

$$\begin{aligned} C[f_1, f_1] = & \int d\Xi'_1 d\Xi'_2 d\Xi_2 \int_0^{\frac{\pi}{2}} \int_0^{2\pi} W(\Xi'_1, \Xi'_2 \mapsto \Xi_1, \Xi_2) f_1(\Gamma'_1, t) f_1(\Gamma'_2, t) \\ & - W(\Xi_1, \Xi_2 \mapsto \Xi'_1, \Xi'_2) f_1(\Gamma_1, t) f_1(\Gamma_2, t) d\theta_2 d\varphi_2. \end{aligned}$$

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

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

SPACE HOMOGENEOUS VLASOV-TYPE EQUATION

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

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

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

$$\mathcal{C}[f, f] = \int d\underline{\nu}_2 d\underline{v}_2 d\nu_2 f' f'_* - \int d\underline{\nu}_2 d\underline{v}_2 d\nu_2 f f_*, \quad (1)$$

complemented with initial conditions $f(\underline{v}, \nu, \underline{\nu}, 0) = f_0(\underline{v}, \nu, \underline{\nu})$ and where we will denote $f_* = f(\underline{v}_2, \nu_2, \underline{\nu}_2, t)$, 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 $f^n(\underline{v}, \nu, \underline{\zeta})$ we denote an approximation of $f(\underline{v}, \nu, \underline{\zeta}, t^n)$ 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 $\hat{f} = \mathcal{T}_{\Delta t}(f^n)$

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

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

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

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

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

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-continuous) ODEs

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

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)

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

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

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

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 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

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

with

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

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

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

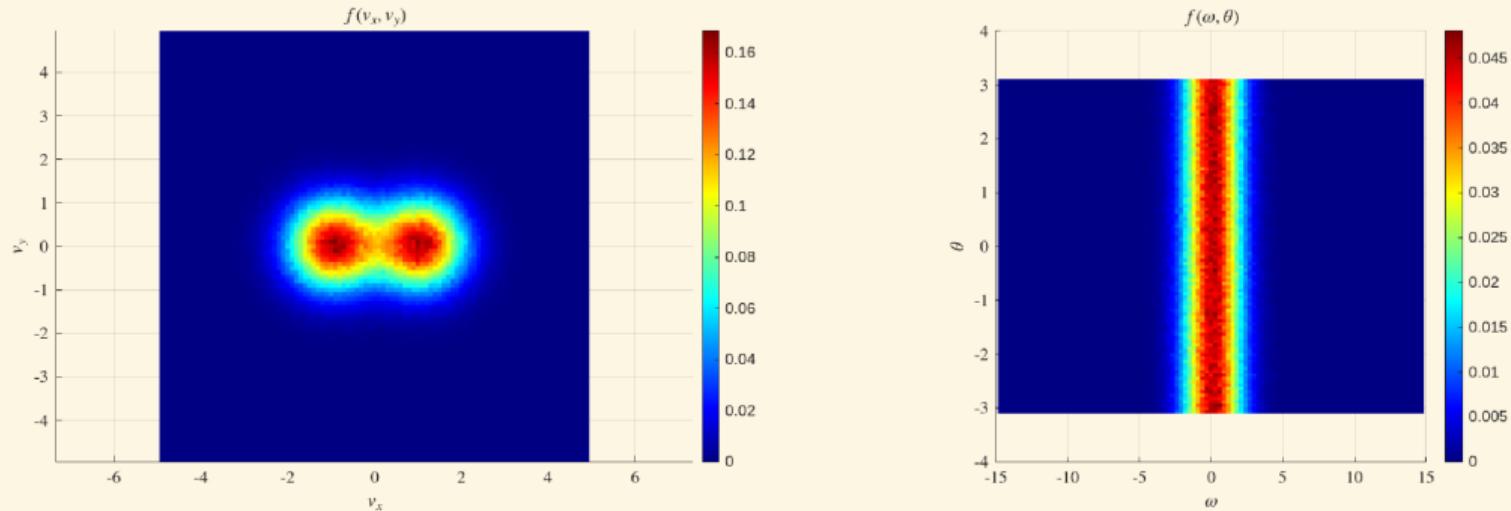


Figure: Test 1 - Zero Potential. The initial distribution function for the zero potential case. We consider a two bump initial velocity distribution (left) and a Gaussian distribution for the angular velocity with uniform distribution for the angle (right).

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

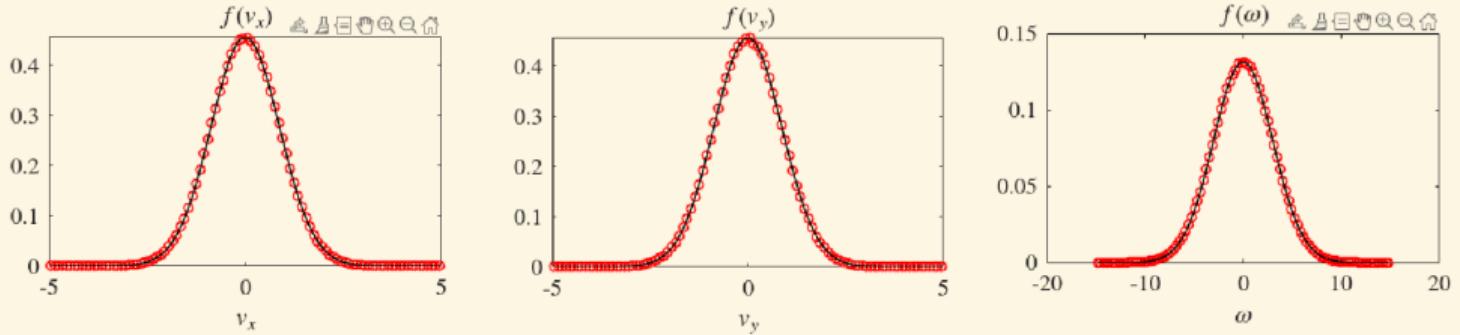


Figure: Test 1 - Zero Potential. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the exact steady state. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution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

Let us consider the mean-field potential is given by

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

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

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

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

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

We can immediately see that the fixed points of the system is unique and it is given by $\underline{\nu} = \hat{\underline{\nu}}$ 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

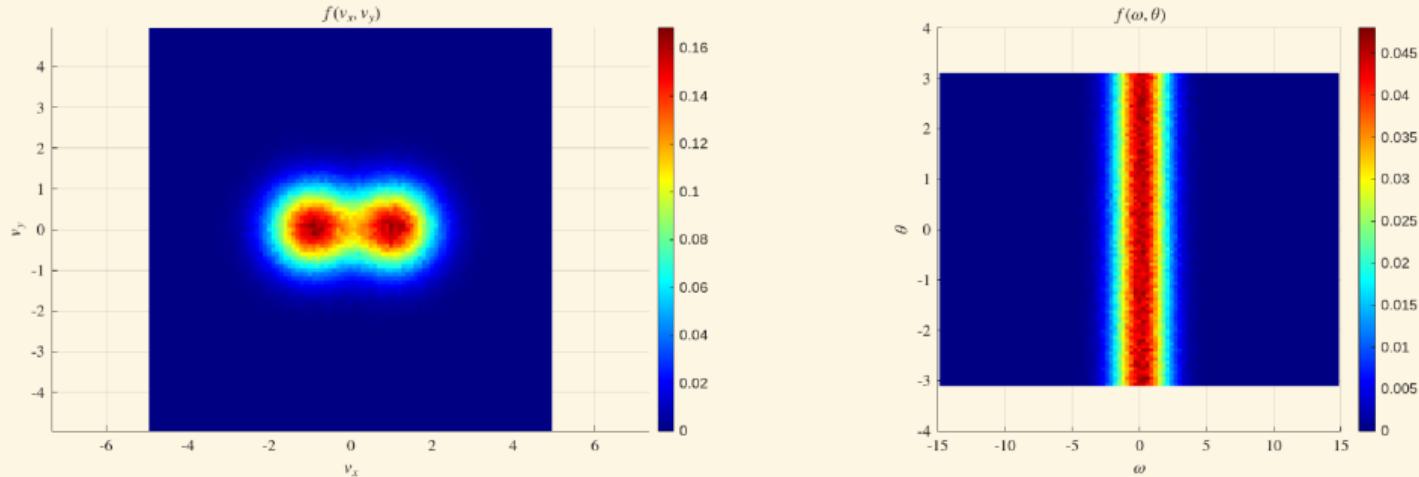


Figure: Test 2 - Quadratic potential for $\beta = 0$ and $\alpha = 1$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

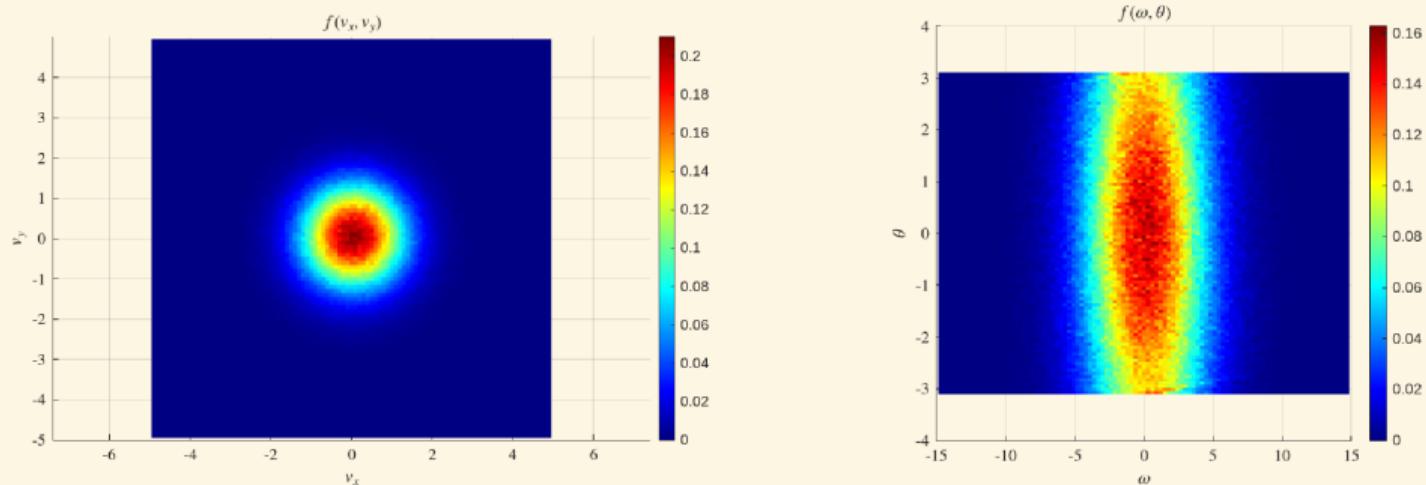


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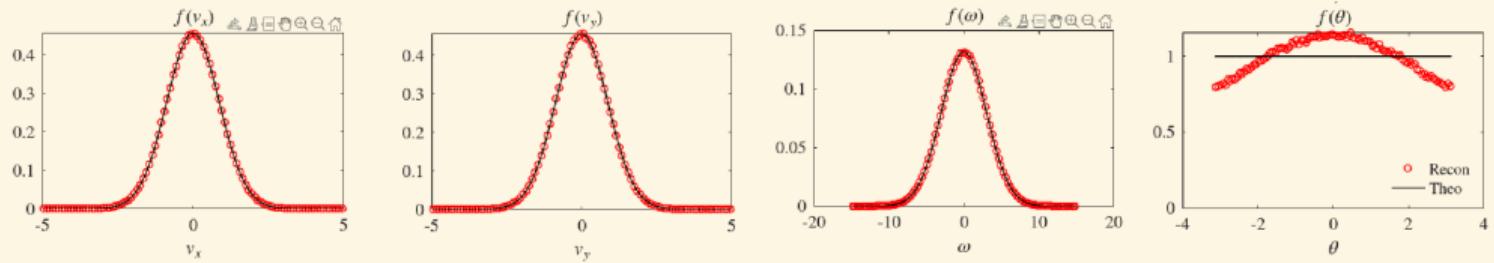


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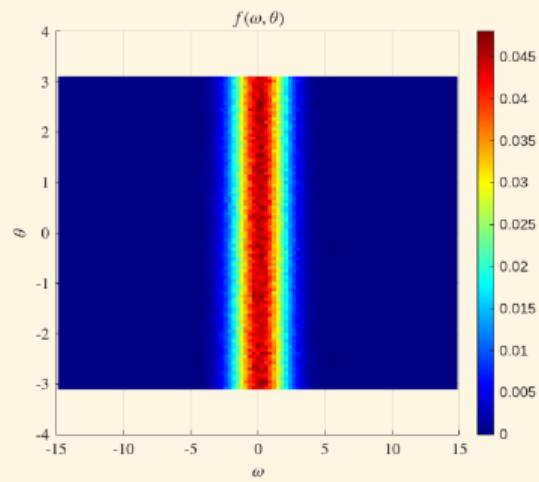
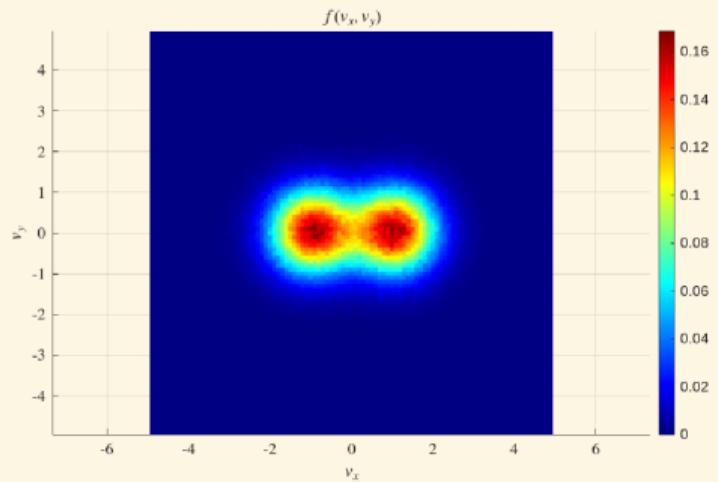


Figure: Test 3 - Non-linear potential for $\mathcal{W}(\nu) = \alpha \sin(\nu - \hat{\nu})$. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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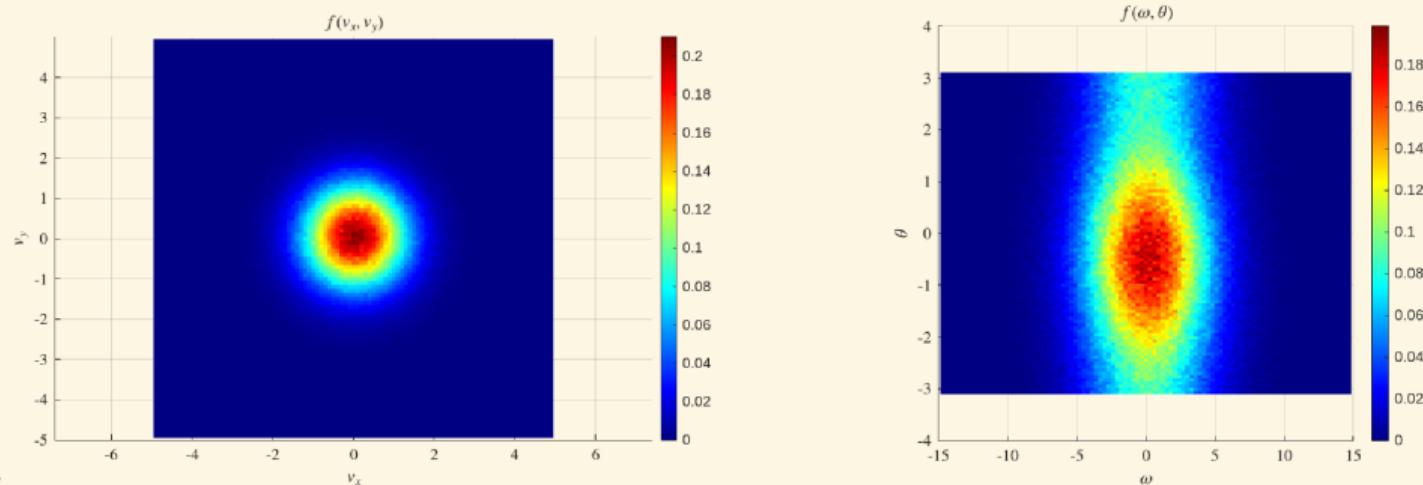


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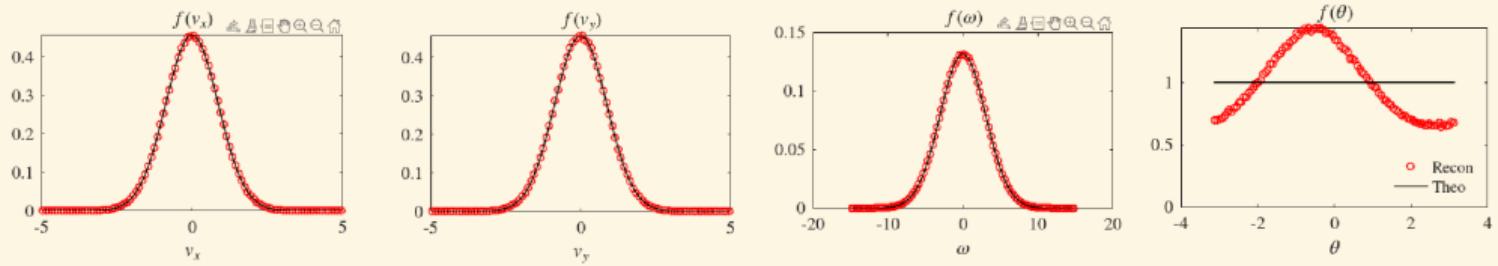


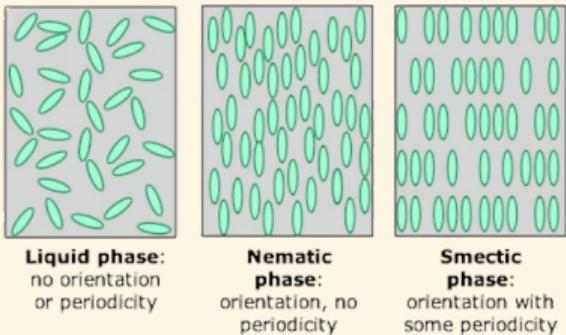
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ONSAGER STERIC POTENTIAL

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.



→ T
 Decreasing temperature

AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

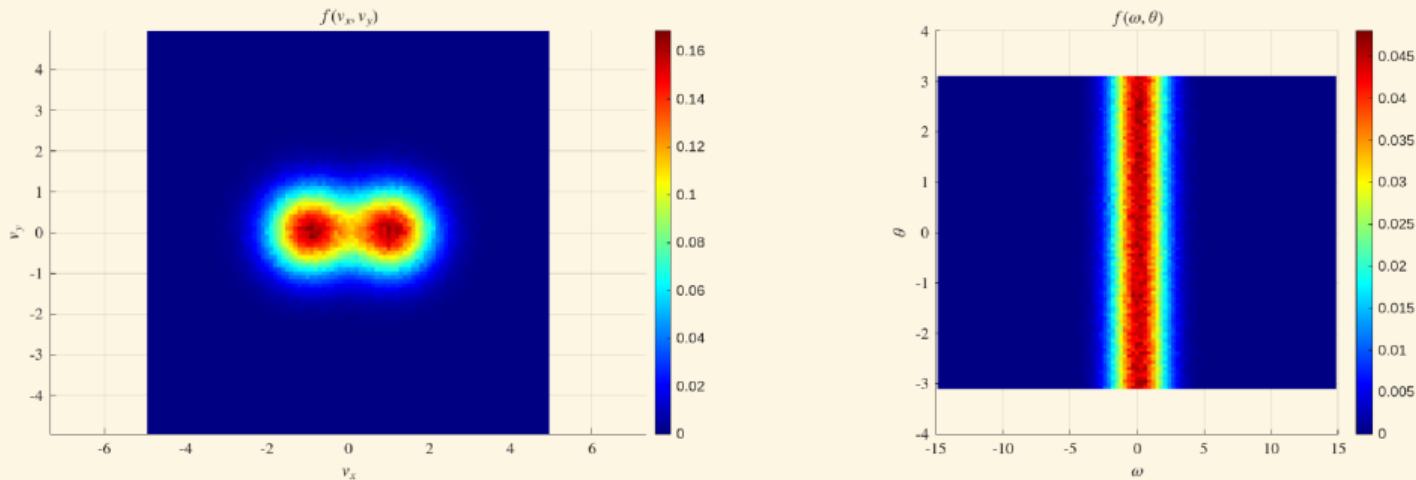


Figure: Test 4 - The Onsager potential for rod-like molecules. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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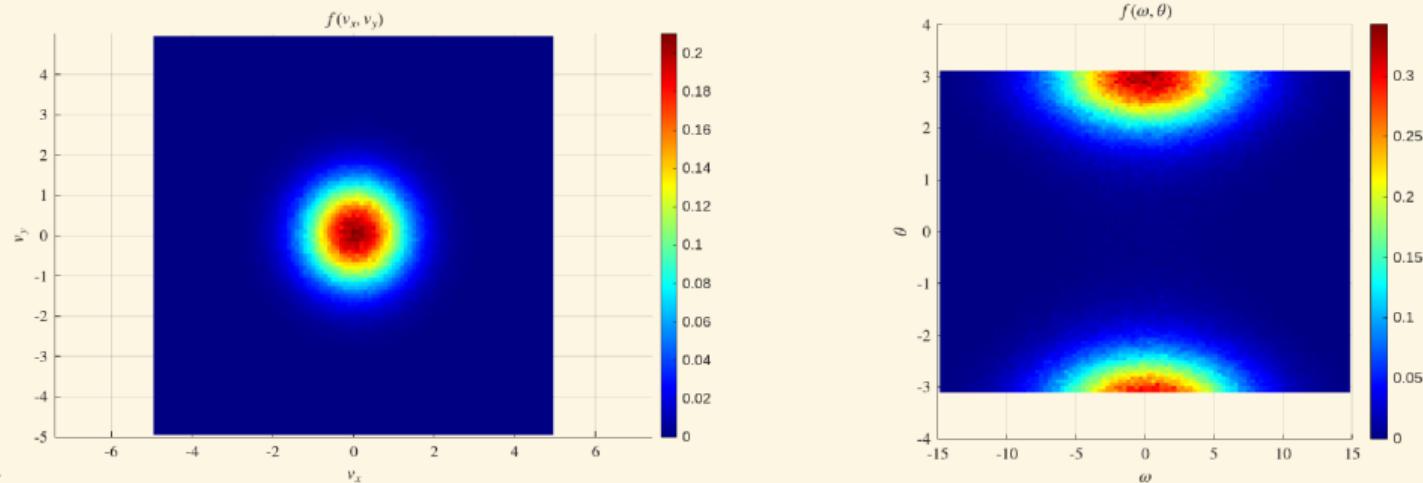


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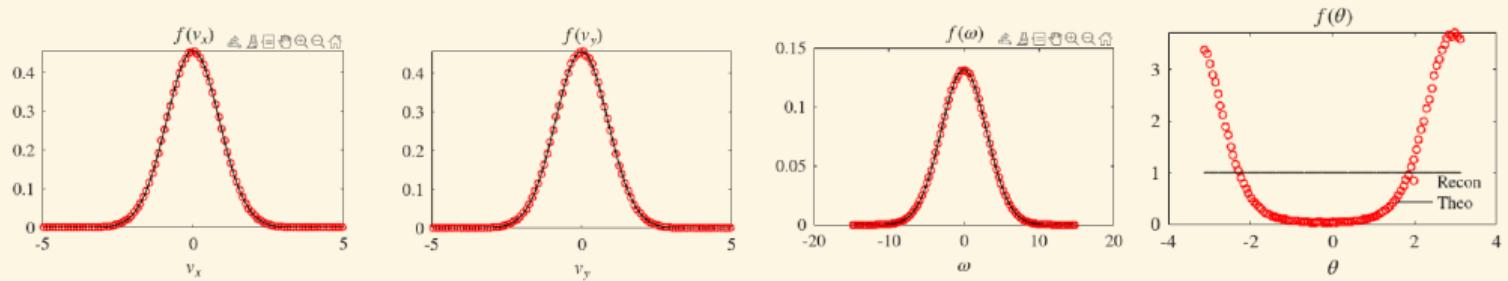


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THANK YOU!

Direct Simulation Monte Carlo for Ordered Fluids

UMBERTO ZERBINATI*, JOINT WORK WITH: J. A. CARILLO*, P. E. FARRELL*,
A. MEDAGLIA*.