

# Direct Simulation Monte Carlo for Ordered Fluids

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

*\*Mathematical Institute – University of Oxford*

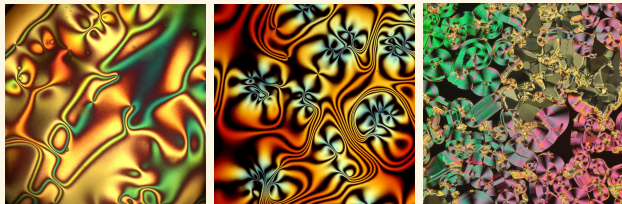
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Oxford  
Mathematics



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- ▶ **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

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Furthermore, we say that a field  $\nu : \mathbb{E}^d \rightarrow \mathcal{M}$  is an order parameter field if  $\forall \underline{c} \in \mathbb{R}^d$  and  $\forall \underline{\underline{Q}} \in SO(d)$  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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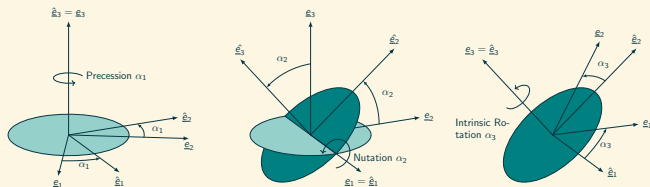
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- ▶ We need to understand what manifold  $\mathcal{M}$  captures the nature of the order parameters.
- ▶ We need to understand the action of rotations on the manifold  $\mathcal{M}$ .

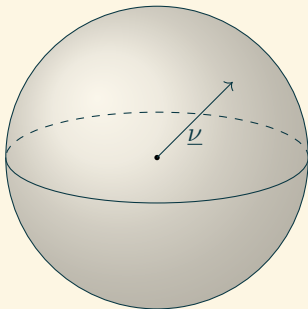
# AN EXAMPLE: NEMATIC LIQUID CRYSTALS



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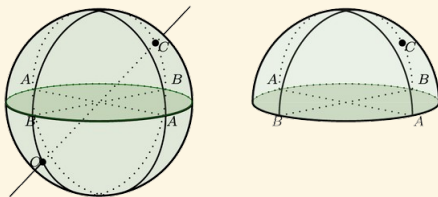
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- ▶ For head-tail symmetric calamitic molecules, we can use  $\mathbb{RP}^2$ .

# EMBEDDING RESULTS

## Embedding theorems

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



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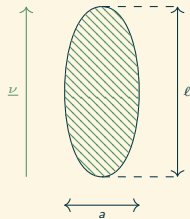
# THE MICROSCOPIC WORLD

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## LAGRANGIAN MECHANICS OF THE CONSTITUENTS

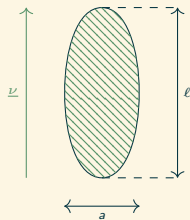
We will here assume that the fluid is composed of a set of constituents, each of which is described by a position  $\mathbf{x}_i$ , a velocity  $\underline{v}_i$ , the order parameter  $\nu_i$  and its total time derivative  $\dot{\nu}_i$ .



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



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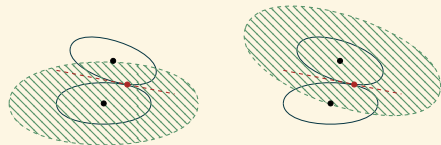
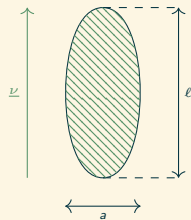
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We assume the interaction between the constituents is given by a potential  $\mathcal{W}(\mathbf{x}_i - \mathbf{x}_j, \nu_i, \nu_j)$ , i.e.

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

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

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

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

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

is differentiable at the identity.

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

Composing the canonical isomorphism  $\mathbb{R}^3 \rightarrow SO(3)$  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  $\text{SO}(3)$ , 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  $\underline{\underline{\Omega}}(\underline{\nu}) = I$ , where  $I$  is the Identity. Thus, Noether's theorem implies the conservation of the following quantity:

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

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

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# 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.

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

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

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

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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,

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

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



# 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

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

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

# BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

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

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

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

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

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

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

## 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,

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

## 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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Thus, we have no guarantee that the system described thermalises to a Maxwellian distribution.

### 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,

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

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

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

# 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

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



## SPACE HOMOGENEOUS VLASOV-TYPE EQUATION

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

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

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

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

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  $\hat{f} = \mathcal{T}_{\Delta t}(f^n)$

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

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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

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

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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  $\nu_i^n$ , 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

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

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)

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

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

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

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

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

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



# AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

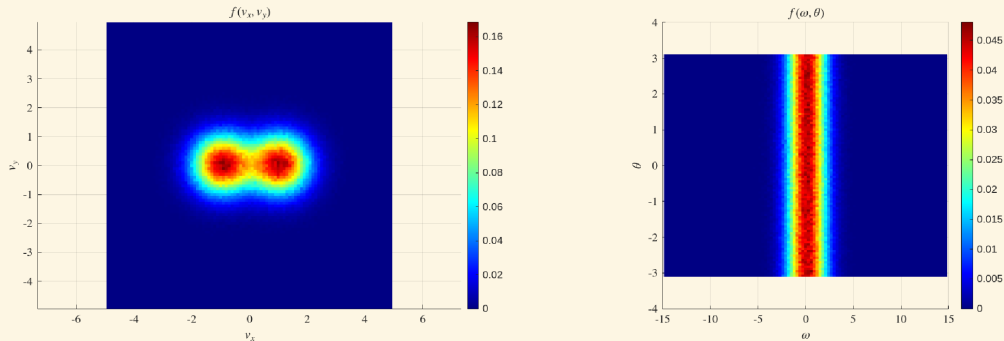


Figure: Test 1 - Zero Potential. The initial distribution function for the zero potential case. We consider a two bump initial velocity distribution (left) and a Gaussian distribution for the angular velocity with uniform distribution for the angle (right).

## AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

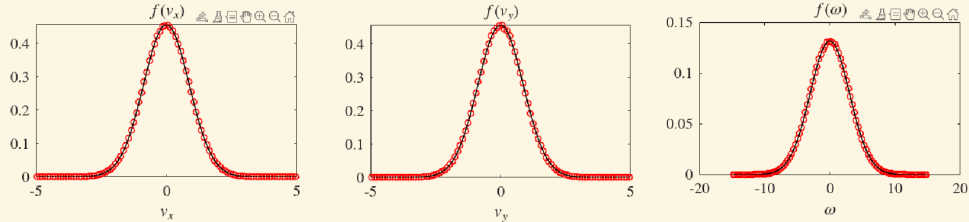


Figure: Test 1 - Zero Potential. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the exact steady state. We observe a good accordance between numerical and exact results, the temperature (and energy) is conserved exactly, and the angle distribution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

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

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

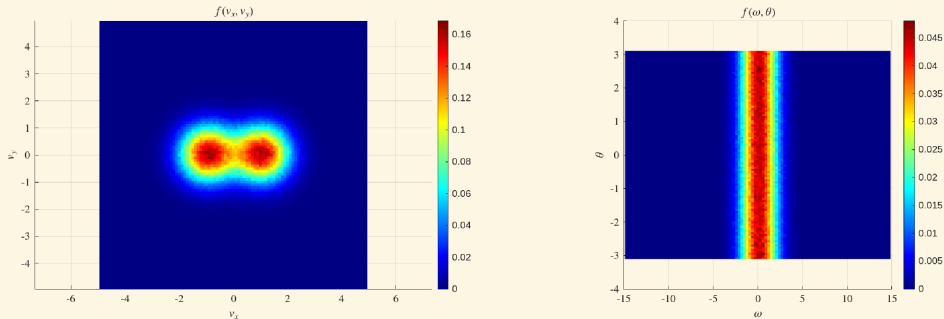


Figure: Test 2 - Quadratic potential for  $\beta = 0$  and  $\alpha = 1$ . The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

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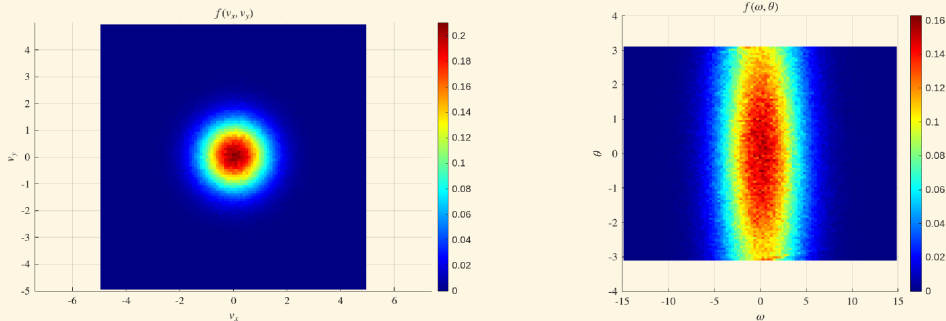


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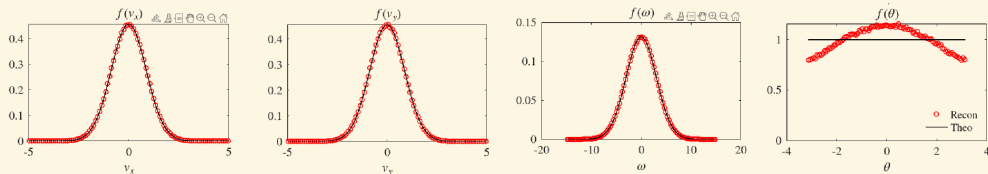


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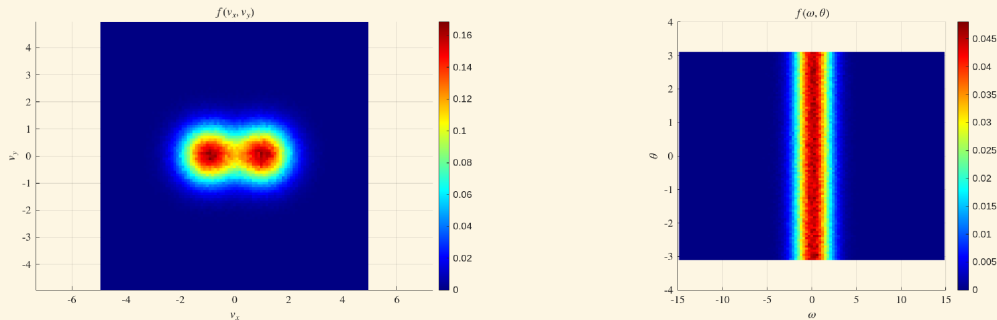


Figure: Test 3 - Non-linear potential for  $\mathcal{W}(\underline{\nu}) = \alpha \sin(\underline{\nu} - \hat{\underline{\nu}})$ . The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between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

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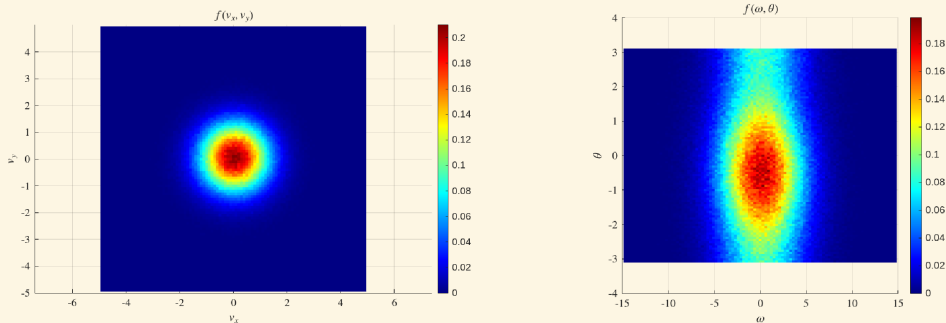


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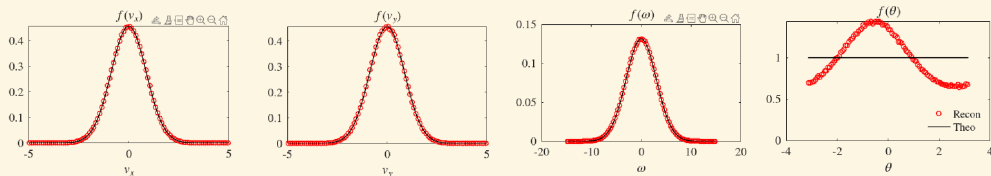


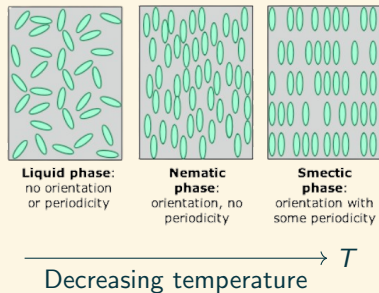
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## ONSAGER STERIC POTENTIAL

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.



# AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

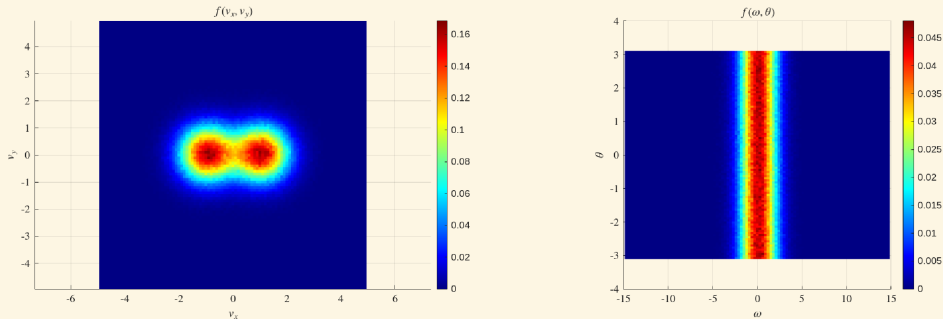


Figure: Test 4 - The Onsager potential for rod-like molecules. The grey dashed lines are the initial data, the black circles the numerical results, the solid red lines the steady state from Test 1. We observe a good accordance between numerical and exact results.

# AN EXAMPLE: NEMATIC LIQUID CRYSTALS DSMC SIMULATIONS

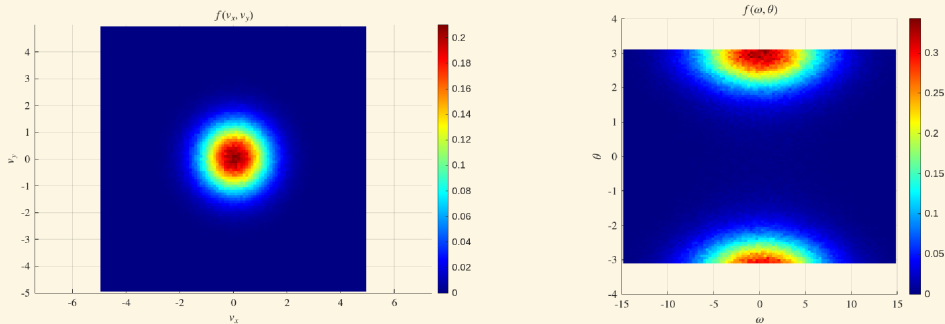


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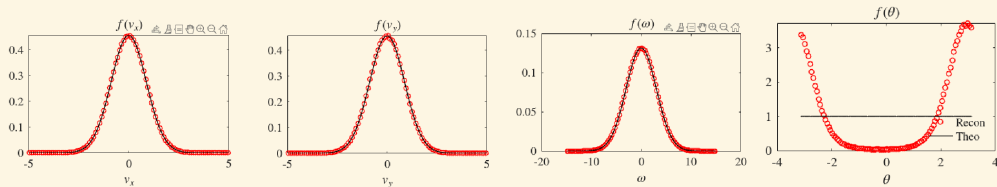


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# THANK YOU!

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Direct Simulation Monte Carlo for Ordered Fluids

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