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Interacting fiber structures: mathematical aspects and applications

Abstract. Fiber structures resulting from a lay down of fibers have been investigated extensively. Microscopic models have been used to describe fibers in detail, whereas kinetic and macroscopic models have been used for the statistical description of the fiber distribution. We review models based on stochastic differential equations, as well as Fokker-Planck and mean field equations and their approximations. Interaction of the fibers is included in these models and a numerical and analytical investigation of the resulting equations is given. Finally an industrial example is discussed and the applicability in an industrial set-up is illustrated.

Keywords. Fiber dynamics, interacting fibers, stochastic differential equations, mean-field equations, convergence to equilibrium, production processes.

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1 - Introduction

In this review we consider the modeling and simulation of structures built from flexible fibers like, for example, non-woven materials. Such fiber structures resulting from the lay down of fibers and their production processes have been modelled on different levels of description involving different scales. Besides microscopic models to describe each single fiber, mesoscopic equations have been used for a statistical description of the fiber distributions. We refer, for example, to [52] for an overview. We note that the focus of these works has

been on the development of relatively simple surrogate fiber models suitable for large scale computations and optimization routines. Such models include basic physical features like coiling, buckling, reaction to turbulent flow in a strongly simplified way, however, the parameters appearing in these models are fitted via full physical simulations.

Simplified two- and three-dimensional stochastic models for the fiber lay-down process are introduced in [37, 43, 54]. These models describe the position of the fiber by a stochastic differential system containing parameters that characterize the process. These parameters have to be identified from a few representative fibers simulated by the detailed model. Then, the surrogate model can be used to calculate fast and efficiently the behavior of hundreds of long fibers for fleece production. The models rely on systems of stochastic differential equations in 2 or 3 spatial dimensions with a velocity space given by the unit circle or the unit sphere. We review the models in Section 2.

Moreover, important information on the processes can be gained via the corresponding Fokker-Planck (or mean field) equations. In [16, 37, 42, 45, 46, 58] an analytic investigation of the Fokker-Planck equation has been performed, asymptotic properties and ergodicity of the process have been proven and explicit rates for the convergence to the stationary solution have been obtained. To solve these kinetic problems numerically, splitting methods are used, combining a Semi-Lagrange approach for the spatial discretization with a Finite-Volume method for the velocity discretization [55, 67]. We discuss such kinetic models and their numerical treatment in Section 3.

Classically, using a diffusion scaling of the stochastic system, one derives a reduced equation for the large noise case. Starting from the associated Fokker-Planck equation the related reduced equation is the diffusion approximation. However, there are many more options to approximate the Fokker-Planck equation and, thus, the underlying stochastic process. These equations are compared for the present context, in particular, with respect to the long time behaviour, where we use the rate of convergence to equilibrium as a measure for the quality of the different approximations. This is, for example, in the context of fiber dynamics a decisive criterion for the quality of the industrial processes, see [52]. We review approximate macroscopic models in Section 4.

One more step in a hierarchy of models for fiber motion is to include the finite size of fibers and interactions between the fibers. Including fiber-fiber interaction, thereby describing the size of each fiber, on the microscopic level leads to coupled systems of stochastic differential equations. Its statistical description should also take into account the interactions and will consequently no longer be based on the classical Fokker-Planck model. The interacting fiber model makes use of a microscopic systems of retarded stochastic differential

equations, and its mesoscopic description is obtained via mean-field procedures. The mean-field limit is described by a McKean–Vlasov type equation with a delay term. We perform an analytical investigation of the mean field limit, as well as a numerical comparison of microscopic and mean field equations. The analysis of the limit is based on the work in [17, 30, 38, 39, 40, 63, 70]. For numerical methods for mean-field type equations we refer to [6, 66, 67, 69]. We review models including fiber interaction in Section 5.

Uniformity and a high quality of the web and the resulting nonwoven fabrics is related to the speed with which the solutions of these models converge to equilibrium. As mentioned, the speed of convergence is an important indicator of the quality and favorable properties of the nonwovens such as homogeneity and load capacity [42]. Since faster convergence indicates a more uniform production of the nonwovens, analysis of the speed of convergence allows the adjustment of process parameters in such a way that the optimal production process can be performed. In recent years, the trend to equilibrium for solutions of kinetic and hyperbolic equations has been widely investigated by applying entropy dissipation methods, see [29, 76] and [7, 10, 24, 27] for instance. In [31], Dolbeault et al. proposed a simplified approach to prove the trend to equilibrium for a large class of linear equations. Starting from an interacting particle model, Bolley et al. used a probabilistic approach in [12] to show convergence towards equilibrium for solutions of the Vlasov–Fokker–Planck equation in Wasserstein distance with an exponential rate. Based on these works, we consider the convergence to equilibrium for a delay mean-field model in Section 6.

As an industrial application we consider an aerodynamic web forming process. The resulting airlay fabrics range from insulation and filter materials over automotive and mattress felts to medical and hygiene products depending on the type of entering fiber material. In the airlay process the fibers leave from a rotating drum into a turbulent air flow. Suctioning onto a perforated moving conveyor belt leads to the forming of a random three-dimensional web structure, see [2]. The production of the final fabrics takes place in further post-processing steps. Simulation-based process design and management are a basis for the prediction and improvement of product properties and an objective in industry. In Section 7 we discuss a chain of mathematical models towards the simulation of such an airlay process and of the material behavior. The models cover the full simulation of dilute fiber suspension in turbulent flow, stochastic surrogates for the fiber lay-down and web formation, as well as Cosserat networks with effective material laws for tensile strength tests. They are coupled by means of parameter identification. We illustrate the applicability of the model chain for an industrial set-up, regarding computer tomography data and tensile strength

experiments of the airlay nonwoven materials.

This review is based on joint works with several people. We refer, in particular, to the papers [54], [67], [56], [15], [57] and [41].

2 - Microscopic fiber lay down models

In this section the basic two-dimensional model is described together with three-dimensional extensions. Finally, we show numerical results and state a possible strategy for parameter estimation. For further details we refer to [54].

2.1 - The basic model

Consider a slender, elastic, non-extensible and endless fiber in a lay-down regime. Let the fiber be produced with a certain spinning speed, excited into motion by a surrounding highly turbulent air flow and laid down on a conveyor belt which is for the time being assumed to be non-moving. For the case of a moving belt see Remark 1 below. Due to its slenderness, the fiber on the two-dimensional transport belt is modeled as an arc-length parametrized curve $x : \mathbb{R}_0^+ \rightarrow \mathbb{R}^2$, defined by the solution of a dynamical system for x_t with the arc-length t . This dynamical system is given by the following stochastic differential equations, see [37]

$$(2.1) \quad \begin{aligned} dx_t &= \tau(\alpha_t) dt \\ d\alpha_t &= -\nabla V(x_t) \cdot \tau^\perp(\alpha_t) dt + A dB_t, \end{aligned}$$

equipped with appropriate initial conditions x_0, α_0 . The normalized tangent is $\tau(\alpha) = (\cos \alpha, \sin \alpha)^T$, $\alpha \in [0, 2\pi)$. Introducing the corresponding orthonormal polar unit vector $\tau^\perp(\alpha) = (-\sin \alpha, \cos \alpha)^T$, the deterministic drift term in the second equation ensures that the fiber tends back to the origin as a consequence of the coiling behavior of the fiber. The throwing ranges of the fiber can be controlled with help of the potential V . One may, for example, choose $V(x) = V((x_1, x_2)) = (x_1^2/\sigma_1^2 + x_2^2/\sigma_2^2)/2$ with the throwing ranges σ_1 and σ_2 . All stochastic effects occurring in the production process are summarized in the one-dimensional Wiener process $(B_t)_{t \geq 0}$ with diffusion constant A . Defining $\tau_t := \tau(\alpha_t)$ and using $\tau'(\alpha) = \tau^\perp(\alpha)$ we rewrite (2.1) in a coordinate free form.

Ito's formula applied to $\tau(\alpha_t)$ gives

$$\begin{aligned}
 d\tau_t &= \frac{1}{2}A^2\tau''(\alpha_t)dt + \tau'(\alpha_t)d\alpha_t \\
 &= -\frac{1}{2}A^2\tau(\alpha_t)dt + \tau^\perp(\alpha_t) \left[-\nabla V(x_t) \cdot \tau^\perp(\alpha_t)dt + AdB_t \right] \\
 &= -\frac{1}{2}A^2\tau(\alpha_t)dt - \tau^\perp(\alpha_t) \otimes \tau^\perp(\alpha_t)V(x_t)dt + A\tau^\perp(\alpha_t) \otimes \tau^\perp(\alpha_t)dW_t \\
 &= -\frac{1}{2}A^2\tau(\alpha_t)dt + \left(I - \tau(\alpha_t) \otimes \tau(\alpha_t) \right) \left[-V(x_t)dt + AdW_t \right] \\
 &= -\frac{1}{2}A^2\tau_t dt + \left(I - \tau_t \otimes \tau_t \right) \left[-V(x_t)dt + AdW_t \right],
 \end{aligned}$$

where the one-dimensional Wiener process dB_t is rewritten as $dB_t = \tau^\perp(\alpha_t) \cdot dW_t$ with a two-dimensional Wiener process $(W_t)_{t \geq 0}$. I denotes the identity matrix. As a consequence

$$\begin{aligned}
 dx_t &= \tau_t dt \\
 (2.2) \quad d\tau_t &= (I - \tau_t \otimes \tau_t) \circ (-\nabla V(x_t)dt + AdW_t) \\
 \|\tau_t\| &= 1
 \end{aligned}$$

is the coordinate free formulation in Stratonovich form, where $\circ$ denotes the usage of Stratonovich integrals. The algebraic constraint takes into account the arc-length parametrization for the inextensible fibers. Thus, the appropriate state space is $\mathbb{R}^2 \times \mathbb{S}^1 = \{(x, \tau) \in \mathbb{R}^2 \times \mathbb{R}^2 \mid \|\tau\| = 1\}$.

Remark 1. *Let the fiber be produced with the spinning speed v_{spin} and laid down on a conveyor belt moving with the velocity v_{belt} . The fiber curve is now denoted as $\eta : \mathbb{R}_0^+ \rightarrow \mathbb{R}^2$. The arc-length parametrization and in-extensibility gives again*

$$d\eta_t = \begin{pmatrix} \cos \alpha_t \\ \sin \alpha_t \end{pmatrix} dt,$$

where α denotes the angle of the fiber relative to the direction of motion e_1 of the transport belt. The reference point of the spinning process determined by the position of the nozzle moves in the coordinate system of the transport belt in the direction $-e_1$. Thus,

$$x(t) = \eta(t) - (-\kappa t e_1)$$

describes the deviation of the fiber from the reference point as a function of the arc-length parameter t , where $\kappa = v_{belt}/v_{spin} \in [0, 1]$ is the ratio between

the belt and spinning speeds. Following [37], we model (x, α) by the stochastic differential system

$$(2.3) \quad \begin{aligned} dx_t &= \tau(\alpha_t) dt + \kappa e_1 dt \\ d\alpha_t &= -\nabla V(x_t) \cdot \tau_t^\perp dt + A dB_t . \end{aligned}$$

We might generalize the last model with help of the concept of reference curves allowing the consideration of further specific production processes, see [52]. Introducing a reference curve γ the generalized model reads

$$(2.4) \quad \begin{aligned} dx_t &= \tau(\alpha_t) dt + d\gamma_t \\ d\alpha_t &= -\nabla V(x_t) \cdot \tau_t^\perp dt + A dB_t . \end{aligned}$$

Remark 2. For a related model for self-driven particles we refer to [28].

2.2 - The Isotropic 3D Model

In this and the following section the above described two-dimensional model will be extended to three dimensions. Again, we model the motion of the fiber as an arc-length parametrized curve $x : \mathbb{R}_0^+ \rightarrow \mathbb{R}^3$ with normalized tangent τ , which is in spherical coordinates given by

$$\tau(\alpha, \theta) = \begin{pmatrix} \cos \alpha \sin \theta \\ \sin \alpha \sin \theta \\ \cos \theta \end{pmatrix} .$$

We introduce the orthonormal spherical unit vectors

$$n_1(\alpha) = \begin{pmatrix} -\sin \alpha \\ \cos \alpha \\ 0 \end{pmatrix}, \quad n_2(\alpha, \theta) = \begin{pmatrix} \cos \alpha \cos \theta \\ \sin \alpha \cos \theta \\ -\sin \theta \end{pmatrix} .$$

We consider the dimension invariant form (2.2), but now with state space $\mathbb{R}^3 \times \mathbb{S}^2$. Moreover, we introduce an additional factor $\frac{1}{2}$. One obtains

$$(2.5) \quad \begin{aligned} dx_t &= \tau_t dt \\ d\tau_t &= (I - \tau_t \otimes \tau_t) \circ \left(-\frac{1}{2} \nabla V(x_t) dt + A dW_t \right) \\ \|\tau_t\| &= 1 . \end{aligned}$$

with state space $\mathbb{R}^3 \times \mathbb{S}^2$ and $(W_t)_{t \geq 0}$ denotes accordingly a Brownian motion in $\mathbb{R}^3$. Next, we want to rewrite (2.5) in local coordinates. We note that the space orthogonal to the tangent τ in local coordinates is spanned by $n_1(\alpha)$ and $n_2(\alpha, \theta)$. With the identity

$$\tau \otimes \tau + n_1 \otimes n_1 + n_2 \otimes n_2 = I$$

we obtain in Ito's formulation (with $\tau_t := \tau(\alpha_t, \theta_t)$)

$$\begin{aligned} d\tau_t &= -\frac{1}{2} \left(n_1(\alpha_t) \otimes n_1(\alpha_t) + n_2(\alpha_t, \theta_t) \otimes n_2(\alpha_t, \theta_t) \right) \nabla V(x_t) dt \\ &\quad - A^2 \tau(\alpha_t, \theta_t) dt + A \left(n_1(\alpha_t) \otimes n_1(\alpha_t) + n_2(\alpha_t, \theta_t) \otimes n_2(\alpha_t, \theta_t) \right) dW_t \\ &= -A^2 \tau_t dt + n_1(\alpha_t) \left[-\frac{1}{2} n_1(\alpha_t) \cdot \nabla V(x_t) dt + A dB_t^{(1)} \right] \\ &\quad + n_2(\alpha_t, \theta_t) \left[-\frac{1}{2} n_2(\alpha_t, \theta_t) \cdot \nabla V(x_t) dt + A dB_t^{(2)} \right], \end{aligned}$$

where $(B_t^{(1)})_{t \geq 0}$ and $(B_t^{(2)})_{t \geq 0}$ are independent one-dimensional Wiener processes as projections of the three-dimensional Wiener process $(W_t)_{t \geq 0}$ onto the unit vectors n_1 and n_2 , respectively. Ito's formula applied to

$$\alpha_t := \alpha(\tau_t) = \arctan \frac{\tau_{2t}}{\tau_{1t}}, \quad \theta_t := \theta(\tau_t) = \arccos \frac{\tau_{3t}}{\sqrt{\tau_{1t}^2 + \tau_{2t}^2 + \tau_{3t}^2}}$$

yields the equations in spherical polar coordinates as

$$\begin{aligned} dx_t &= \tau(\alpha_t, \theta_t) dt \\ (2.6) \quad \sin \theta_t d\alpha_t &= -\frac{1}{2} \nabla V(x_t) \cdot n_1(\alpha_t) dt + A dB_t^{(1)} \\ d\theta_t &= -\frac{1}{2} \nabla V(x_t) \cdot n_2(\alpha_t, \theta_t) dt + \frac{1}{2} A^2 \cot \theta_t dt + A dB_t^{(2)}. \end{aligned}$$

We note, that the stochastic part

$$d\tau_t = (I - \tau_t \otimes \tau_t) \circ dW_t$$

is a 3-D Brownian motion projected on the unit sphere, see [64] or [72]. Choosing a symmetric potential $V = V(\|x\|)$ the model is invariant under rotations.

Representative fiber scenarios for varying noise amplitude A are illustrated in Figure 1 computed by (2.6) after nondimensionalization using an isotropic potential $V(x) = \|x\|^2/2$.

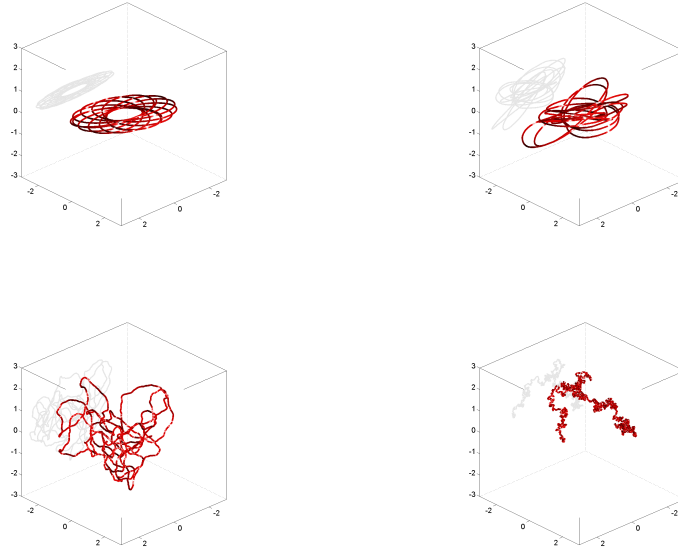


Fig. 1. Influence of noise on fiber trajectories. From left to right, top to bottom $A = 0; 0.1; 1; 5$.

However, in typical fiber lay-down processes the resulting nonwoven have usually an anisotropic orientation of the fibers as consequence of physical properties and limitations given for instance by the impenetrable conveyor belt. For example, the orientation of most of the fibers will concentrate in a direction parallel to the belt. Thus, it is necessary to modify the model such that the orientation of the fibers can be controlled and adapted to measurements. This will be done in the next section.

2.3 - The Modified 3D Model

The idea of the modified model is that by introducing an additional parameter B we obtain a 3D model, which can be adapted to the distributions of the θ -angle in a realistic fleece. With the help of this parameter we are able to weight the directions of the spherical unit-vectors n_1 and n_2 differently, such that it is possible to capture the anisotropic orientation of the fibers. Using the notation e_1, e_2 and e_3 for the Cartesian unit vectors, we suppose that the belt lies in the (e_1, e_2) -plane and that the spherical coordinates are determined in a standard way, that means θ is the angle between the direction e_3 and the

tangent τ on the fiber, whereas α is the angle between the direction e_1 and the projection of τ on the reference plane. Let $B \in [0, 1]$. We replace the equations by

$$(2.7) \quad \begin{aligned} dx_t &= \tau_t dt \\ d\tau_t &= -\frac{1}{B+1}(n_{1,t} \otimes n_{1,t} + Bn_{2,t} \otimes n_{2,t})\nabla V(x_t) dt \\ &\quad + A(n_{1,t} \otimes n_{1,t} + \sqrt{B}n_{2,t} \otimes n_{2,t}) \circ dW_t. \end{aligned}$$

This ensures, that for $B = 0$ we are back to the 2D case and for $B = 1$ to the isotropic 3D case. The modified 3D model ranges between the isotropic 3D model and the 2D model describing fibers with an orientation ranging between a random orientation and an orientation in the (e_1, e_2) -plane. Using Ito's formula, we obtain the modified 3D model in local coordinates

$$(2.8) \quad \begin{aligned} dx_t &= \tau(\alpha_t, \theta_t) dt \\ \sin \theta_t d\alpha_t &= -\frac{1}{B+1}\nabla V(x_t) \cdot n_1(\alpha_t) dt + A dB_t^{(1)} \\ d\theta_t &= -\frac{B}{B+1}\nabla V(x_t) \cdot n_2(\alpha_t, \theta_t) dt \\ &\quad + \frac{1}{2}A^2 \cot \theta_t dt + \sqrt{BA} dB_t^{(2)}. \end{aligned}$$

The effect of varying parameter B in (2.8) for an isotropic potential $V(x) = \|x\|^2/2$ is shown in Figure 2. The noise amplitude is chosen as $A = 1$. One observes that for decreasing B the orientation of the fibers is getting more anisotropic. This corresponds to a distribution of the angle θ concentrating around $\theta = \pi/2$.

2.4 - Numerical Simulations and Identification of the Parameters

In the 2D case the parameter A and the shape of the potential V have been estimated in [52] for different production processes. There, full simulations of a single representative fiber have been performed with the software tool FIDYST¹, see [48, 61] for a description of the algorithms. The noise amplitude A and the potential V in the 2D model (2.4) have been identified on the basis of the full simulation. Figure 3 shows as an example the fiber trajectories computed by the calibrated 2D model and, in comparison, an underlying full FIDYST simulation. The fiber mass distribution is captured qualitatively well

¹FIDYST:Fiber Dynamics Simulation Tool developed at Fraunhofer ITWM, Kaiserslautern

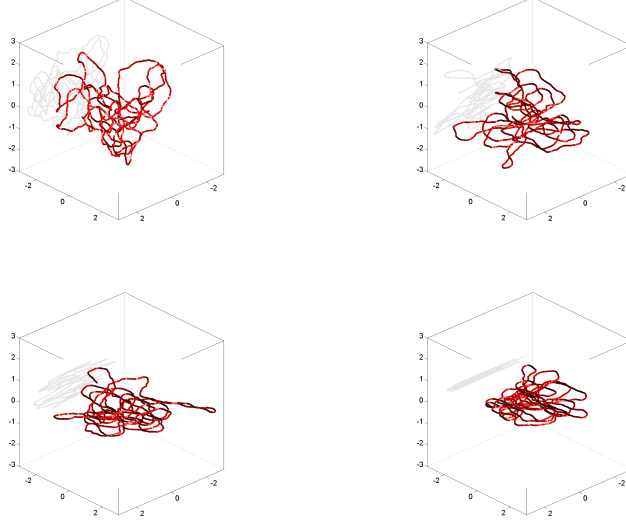


Fig. 2. Influence of the parameter B on fiber trajectories. From left to right, top to bottom $B = 1; 0.1; 0.01; 0.0001$.

in the surrogate model. The potential in x_3 might be assumed as confining potential which models the impenetrable conveyor belt. It remains to determine the distribution of the θ -angle in a real material and translate this into the corresponding parameter B . Therefore we assume that the measurement of the θ -angle in a real nonwoven leads to an axisymmetric distribution in θ with mean $m_\theta = \pi/2$ and variance $var_\theta = \sigma_\theta^2$. Observing that the θ -dependence of the stationary distribution of the process given by (2.7) is given by $P_B(\theta) = C \sin \theta^{\frac{1}{B}}$, one choses B such that the variance of this distribution coincides with var_θ .

3 - The associated Fokker-Planck equation

In this section we discuss the Fokker-Planck equations corresponding to the systems of SDE's discussed in the last section. For the numerical discretization a Finite-Volume methodology is applied for the velocity discretization of the equations. The spatial discretization is treated via a Semi-Lagrange scheme. Numerical results for several test cases are shown and the convergence to equilibrium is investigated numerically. For further details we refer to [67]. We reconsider the system of stochastic differential equations given in the last sec-

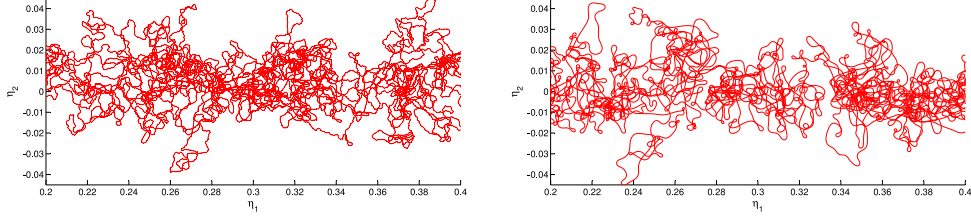


Fig. 3. Comparison of fiber path associated to the adapted 2D surrogate model (left) and the FIDYST simulation (right).

tion. As before, for $x \in \mathbb{R}^3$ $\alpha \in [0, 2\pi)$, $\theta \in [0, \pi)$ we define $\tau, n_1, n_2 \in \mathbb{S}^2$ as

$$\tau = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{pmatrix} = \begin{pmatrix} \cos \alpha \sin \theta \\ \sin \alpha \sin \theta \\ \cos \theta \end{pmatrix}$$

and

$$n_1 = \frac{1}{\sqrt{\tau_1^2 + \tau_2^2}} \begin{pmatrix} -\tau_2 \\ \tau_1 \\ 0 \end{pmatrix} = \begin{pmatrix} -\sin \alpha \\ \cos \alpha \\ 0 \end{pmatrix},$$

$$n_2 = \frac{1}{\sqrt{\tau_1^2 + \tau_2^2}} \begin{pmatrix} \tau_1 \tau_3 \\ \tau_2 \tau_3 \\ -(1 - \tau_3^2) \end{pmatrix} = \begin{pmatrix} \cos \alpha \cos \theta \\ \sin \alpha \cos \theta \\ -\sin \theta \end{pmatrix}.$$

The system of equations under consideration is given by (2.7). The associated equations in spherical coordinates α_t, θ_t are given by equations (2.8).

3.1 - The associated PDE's

Let $f = f(x, \tau, t) = f(x, \theta, \alpha, t)$ denote the probability density for the stochastic process (x_t, τ_t) . It describes the probability, that some fiber mass resides in a volume element $dx d\tau = dx \sin \theta d\theta d\alpha$ at time t . The time development of this function is governed by the Fokker-Planck or Kolmogorov forward equations, see [64]. The Kolmogorov backward operator corresponding to the

SDE systems is

$$(3.9) \quad \tau \cdot \nabla_x + \hat{T}^B + \frac{A^2}{2} \hat{L}^B$$

with

$$\hat{T}^B f = \left(-\frac{1}{B+1} (n_1 \otimes n_1 + B n_2 \otimes n_2) \nabla_x V \right) \cdot \nabla_\tau f.$$

and

$$\hat{L}^B f = ((n_1 \otimes n_1 + B n_2 \otimes n_2) \nabla_\tau) \cdot \nabla_\tau f.$$

For the isotropic case $B = 1$ this is

$$\begin{aligned} \hat{T} f &= \left(-\frac{1}{2} (I - \tau \otimes \tau) \nabla_x V \right) \cdot \nabla_\tau f, \\ \hat{L} f &= \Delta_\tau f. \end{aligned}$$

Here ∇_τ is the gradient on the sphere and Δ_τ is the Laplace-Beltrami operator on the sphere. In local coordinates gradient and divergence on the unit sphere are given by

$$\nabla_\tau f = n_1 \cdot \frac{1}{\sin \theta} \partial_\alpha f + n_2 \cdot \partial_\theta f$$

and

$$\nabla_\tau \cdot v = \frac{1}{\sin \theta} \partial_\theta (\sin \theta v_\theta) + \frac{1}{\sin \theta} \partial_\alpha v_\alpha,$$

where we first have to expand the vector field v as $v = v_\alpha n_1 + v_\theta n_2$. Thus, we have in local coordinates

$$\begin{aligned} \hat{T}^B f &= -\frac{1}{\sin \theta} \frac{1}{B+1} n_1 \cdot \nabla_x V \partial_\alpha f - \frac{B}{B+1} n_2 \cdot \nabla_x V \partial_\theta f \\ \hat{L}^B f &= \cot \theta \partial_\theta p + B \partial_{\theta\theta} p + \frac{1}{\sin^2 \theta} \partial_{\alpha\alpha} f. \end{aligned}$$

The density of the stochastic processes with respect to the canonical surface measure on $\mathbb{S}^2$ i.e. $d\tau = \sin \theta d\theta d\alpha$, is given as the solution of the Fokker-Planck equation associated to the SDE. To obtain it we have to determine the adjoint operators T^B, L^B with respect to $dx d\tau$. One obtains

$$\begin{aligned} T^B f &= \nabla_\tau \cdot \left(-\frac{1}{B+1} (n_1 \otimes n_1 + B n_2 \otimes n_2) \nabla_x V f \right) \\ &= -\frac{1}{\sin \theta} \frac{1}{B+1} n_1 \cdot \nabla_x V \partial_\alpha f - \frac{B}{B+1} n_2 \cdot \nabla_x V \partial_\theta f \\ &\quad - \tau \cdot \nabla_x f - \frac{1-B}{1+B} \cot \theta n_2 \cdot \nabla_\tau f. \end{aligned}$$

The adjoint operator L^B of $\hat{L}^B$ is given by

$$\begin{aligned} L^B f &= \nabla_\tau \cdot \left(- (1 - B) \frac{n_3}{1 - n_3^2} f n_2 + (n_1 \otimes n_1 + B n_2 \otimes n_2) \nabla_\tau f \right) \\ &= (1 - B) f + (2B - 1) \cot \theta \partial_\theta f + B \partial_{\theta\theta} f + \frac{1}{\sin^2 \theta} \partial_{\alpha\alpha} f. \end{aligned}$$

The Fokker Planck equation is finally given as

$$(3.10) \quad \partial_t f = -\tau \cdot \nabla_x f - T^B f + \frac{A^2}{2} L^B f.$$

Note, that we are back in the isotropic case, if we set $B = 1$. In the isotropic case one obtains

$$\begin{aligned} T f &= \nabla_\tau \cdot \left(-\frac{1}{2} (I - \tau \otimes \tau) \nabla_x V f \right), \\ L f &= \Delta_\tau f. \end{aligned}$$

3.2 - Discretization of the equations

We use a semi-Lagrangian method to discretize the spatial part of the state space and a Finite-Volume method on a geodesic grid ([68]) to approximate the spherical part of the state space of (3.10). The numerical methods presented below is a combination of the approaches in [55] and [79].

In the isotropic case we choose an equidistant spatial grid x_i and denote the midpoints of the l -th cell of the geodesic grid on the sphere as τ_l . Moreover, we use the notation $f_{i,l}^m := f(x_i, \tau_l; t_m)$. t_m is a value from an equidistant time grid with step size Δt . We use a splitting scheme

$$(3.11) \quad \partial_t \tilde{f} + \tau \cdot \nabla_x \tilde{f} = 0 \quad \tilde{f}(t) = f(t) \quad (\text{spatial part})$$

$$(3.12) \quad \partial_t f + T^B f = \frac{A^2}{2} L^B f \quad f(t) = \tilde{f}(t + \Delta t) \quad (\text{spherical part})$$

and proceed as follows. For the spatial discretization, follow for all τ^l the characteristic curves starting from x_i at t_{m+1} in negative time direction:

$$(3.13) \quad u(t) = x_i + (t - t_{m+1}) \tau^l.$$

Then interpolate $f(u(t_m), \tau_l; t_m) = f(x_i - \Delta t \tau_l, \tau_l; t_m)$ linearly from the known values $f_{i,l}^m$ from the previous time step. The interpolated values are taken as the new values after mass conservation is assured. We refer to [33] for mass conservation in Semi-Lagrangian methods and to [55] for mass conservation in the present case.

For the spherical discretization we proceed as follows. For all points (x_i) , use a FVM on the sphere in order to solve (3.12), see [78, 79]. The geodesic grid consists of spherical triangles. We call the i -th triangle T_i . By $N(i)$, we denote the set of neighbour cell indices of cell i . So $\{T_j | j \in N(i)\}$ is the set of all neighbours of triangle i . The boundary of triangle i is called ∂T_i and decomposes into the 3 edges ∂T_{ij} , where $j \in N(i)$. Note, that the edges are in fact great circle arcs. All the lengths and surface measures are computed for spherical geometry. Furthermore, the great circle arcs, which pass through the midpoint τ_{ij} of each edge of T_i orthogonally, meet at one point in the interior of T_i . This point is chosen as the cell midpoint τ_i . So, two cell midpoints τ_i and τ_j can always be connected by one great circle arc passing through the edge midpoint orthogonally. The edge normal $e(\tau_{ij})$ is the tangent to that curve at the edge midpoint τ_{ij} . The FVM is formulated in terms of cell averages of the solution f on triangle i at time t_m . Using the notations $\langle \cdot, \cdot \rangle$ for the scalar product and $F(x, \tau) := -\frac{1}{2}(I - \tau \otimes \tau) \nabla_x V$, we have the following scheme

$$(3.14) \quad f_i^{m+1} = f_i^m - \Delta t \cdot \left[\sum_{j \in N(i)} \frac{|\partial T_{ij}|}{|T_i|} \langle F(x, \tau_{ij}), e(\tau_{ij}) \rangle f(\tau_{ij}, t_{m+\frac{1}{2}}) - \frac{|\partial T_{ij}|}{|T_i|} \frac{A^2}{2} \left\langle \nabla_\tau f(\tau_{ij}, t_{m+\frac{1}{2}}), e(\tau_{ij}) \right\rangle \right].$$

Approximations for $f(\tau_{ij}, t_{m+\frac{1}{2}})$ and $\left\langle \nabla_\tau f(\tau_{ij}, t_{m+\frac{1}{2}}), e(\tau_{ij}) \right\rangle$ are determined as follows. $f(\tau_{ij}, t_{m+\frac{1}{2}})$ can be obtained from the cell midpoints: The numerical solution is a constant function on each cell, whose value is given by the cell average. The value of f at the cell boundary at time $t_{m+\frac{1}{2}}$ can be seen as the value of the solution of the Riemann problem given by the two cell averages on cells i and j . So we set

$$(3.15) \quad f(\tau_{ij}, t_{m+\frac{1}{2}}) \sim \frac{1}{2} \left((f_i^m + f_j^m) - \text{sgn}(\langle F(x, \tau_{ij}), e(\tau_{ij}) \rangle) (f_j^m - f_i^m) \right)$$

which results in an upwind type flux function on the geodesic grid. For the approximation of $\left\langle \nabla_\tau f(\tau_{ij}, t_{m+\frac{1}{2}}), e(\tau_{ij}) \right\rangle$ we use

$$(3.16) \quad \left\langle \nabla_\tau f(\tau_{ij}, t_{m+\frac{1}{2}}), e(\tau_{ij}) \right\rangle \sim \frac{f(\tau_j, t_{m+\frac{1}{2}}) - f(\tau_i, t_{m+\frac{1}{2}})}{h_1 + h_2} = \frac{f_j^m - f_i^m}{h_1 + h_2}.$$

Denoting the vector of all cell values f_i^m as f^m and using the matrices A_T and A_D for advection coefficients and diffusion coefficients respectively, the discrete problem is written as

$$(3.17) \quad f^{m+1} = (I - \Delta t(A_T - A_D))f^m.$$

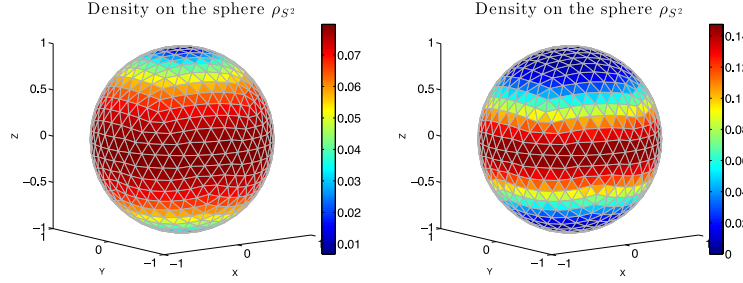


Fig. 4. Plot of ρ_{S^2} (3.19). On the left, $B = 1.0$ and on the right, $B = 0.2$.

For large diffusion coefficients A one can also apply the semi-implicit ansatz

$$(3.18) \quad (I - \Delta t A_D) f^{m+1} = (I - \Delta t A_T) f^m.$$

One may use any appropriate linear system solver for large systems in each time step. A similar procedure is used for the anisotropic case, we refer to [67]. For a second order extension, we refer to [15].

3.3 - Numerical results

For all computations we use $V(x) = \frac{\|x\|^2}{2}$. If not otherwise stated we use a grid with 25 grid points for each spatial direction (15625 spatial grid points in total) and a velocity grid with 1280 cells on the sphere. The number of realizations in the Monte-Carlo simulations is 10^6 . We note that a first order method in time is used to solve the SDE. Integrating over $\mathbb{R}^3$, we obtain the density distribution on the sphere:

$$(3.19) \quad \rho_{S^2}(\alpha, \theta, t) = \int_{\mathbb{R}^3} f(x, \alpha, \theta, t) dx.$$

Integrating this with respect to α we end up with the θ -density

$$(3.20) \quad \rho_{\Theta}(\theta, t) = \int \rho_{S^2}(\alpha, \theta, t) d\alpha.$$

To estimate the quality of the numerical solution, we compare the long time solution to the explicit stationary distribution, see [53]. This equilibrium is given by

$$f^{stat}(x, \theta, \alpha) = C \exp\left(-\frac{\|x\|^2}{2}\right) \sin \theta^{\frac{1}{B}}$$

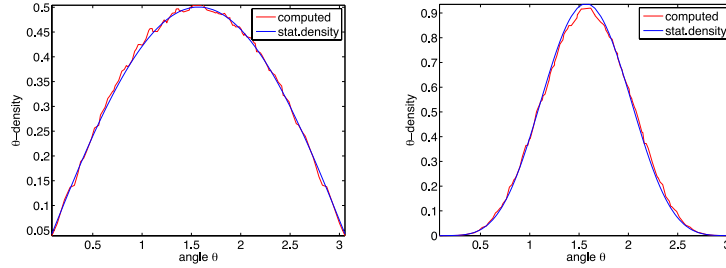


Fig. 5. Plot of stationary solution ρ_Θ (3.20) from the Fokker-Planck solution for $B = 1.0$ (left) and $B = 0.2$ (right).

which yields

$$(3.21) \quad \rho_{\mathbb{S}^2}^{stat}(\theta, \alpha) = C_{\mathbb{S}^2} \sin \theta^{\frac{1}{B}}.$$

C and $C_{\mathbb{S}^2}$ are normalisation constants. The diffusion coefficient is always chosen as $A = 0.9$.

We compute the solution up to a time where the stationary state has been reached. Figure 4 shows the numerical spherical stationary distribution (3.19) and Figure 5 shows the θ -density. The obtained density coincides well with the analytical equilibrium density $C \cdot \sin \theta^{\frac{1}{B}}$. As an example of a moving coordinate system, we solve the equation

$$(3.22) \quad \partial_t f = -(\tau + \kappa e_1) \cdot \nabla_x f - T^B f + \frac{A^2}{2} L^B f$$

with e_1 the unit vector in x-direction. See Figure 6 for the corresponding results. The fiber orientation points into opposite moving direction of the belt as the belt speed transports fiber mass in positive x direction.

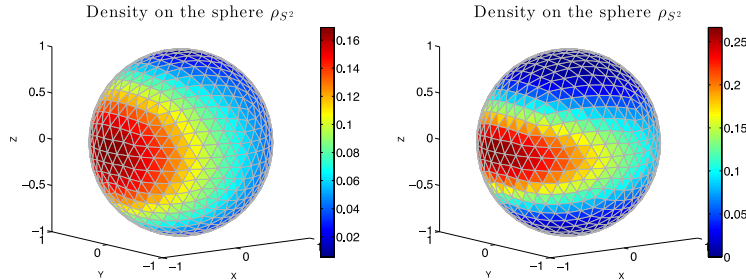


Fig. 6. Spherical density $\rho_{\mathbb{S}^2}$ (3.19) for the moving conveyor belt equation (3.22). On the left, $B = 1.0$ and on the right, $B = 0.2$.

Finally, we are interested in a quantitative comparison of deterministic Fokker-Planck solution or direct Monte-Carlo solution of the SDE. We use the distance to equilibrium as a measure for the quality of the approximation, compare [32, 42, 43, 58] for theoretical considerations. We consider $\|f(t) - f^{stat}\|_2$, that means the distance between numerical solution and equilibrium in the $\mathcal{L}^2$ -norm. On the one hand this distance is computed via the numerical solution of the Fokker-Planck equation. On the other hand, we compute it using a Monte-Carlo simulation for the SDE system. The density distribution is obtained by averaging over many realizations. The errors for different grid sizes and different numbers of Monte-Carlo realizations are plotted in Figure 7 together with the corresponding computation times. For the figures on the right the number of MC realization has been increased by a factor 5 compared to the figures on the left. Looking at Figure 7 one clearly observes that the deterministic approximation method for the Fokker-Planck equation is superior to a Monte-Carlo method, if the accuracy requirements are strict enough.

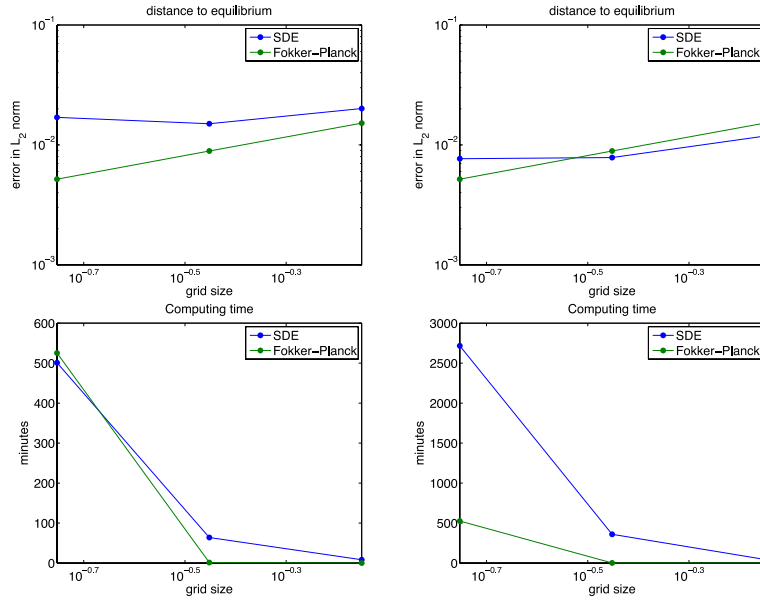


Fig. 7. Top: the deviations of the numerical equilibria of Fokker-Planck(green) and SDE (blue) from the analytical equilibrium are plotted over the density grid size. Bottom: the corresponding computing times are plotted. For the figures on the right the number of MC realizations is increased by a factor 5.

4 - Hydrodynamic approximations

In this section we discuss different procedures to obtain approximate equations for the fiber laydown models discussed above. Scalar approximations like the diffusion approximation or the flux-limited diffusion equations are stated. Moreover, linear and nonlinear two-equation models are derived from the underlying kinetic problem via a moment closure procedure. Theoretical results on the decay rates to equilibrium for the Fokker–Planck equations and the approximate equations are collected. Finally a numerical comparison of the models is presented. For further details we refer to [56].

4.1 - Basic equations

We consider the isotropic stochastic dynamic system with spherical state space in arbitrary dimensions $d \geq 2$ given by

$$(4.23) \quad \begin{aligned} dx_t &= \tau_t dt \\ d\tau_t &= (I - \tau_t \otimes \tau_t) \circ \left(-\frac{1}{d-1} \nabla_x V(x_t) dt + A dW_t \right), \\ \|\tau_t\|_2 &= 1, \end{aligned}$$

where $\circ$ denotes Stratonovich integration. The state space of the process is

$$\mathbb{M} := \mathbb{R}^d \times \mathbb{S}^{d-1} = \{(x, \tau) \in \mathbb{R}^d \times \mathbb{R}^d \mid \|\tau\|_2 = 1\},$$

where $\|\cdot\|_2$ denotes the euclidean norm in $\mathbb{R}^d$. Further, $V: \mathbb{R}^d \rightarrow \mathbb{R}$ is a given potential, A denotes the amplitude of the stochastic fluctuations and W_t is a Brownian motion in $\mathbb{R}^d$. $(I - \tau \otimes \tau)$ is a projector onto the sphere $\mathbb{S}^{d-1}$.

We denote the measure $d\nu$ to be the normalized surface measure on the sphere $\mathbb{S}^{d-1}$ and use the notation

$$\langle f \rangle = \int_{\mathbb{S}^{d-1}} f(\tau) d\nu.$$

The solution of the associated Fokker–Planck equation

$$(4.24) \quad \partial_t f + Tf = \frac{A^2}{2} Lf$$

associated to the stochastic process with respect to the measure $dx d\nu$ gives the probability density function of the process, with

$$Tf = \tau \cdot \nabla_x f - \operatorname{div}_\tau \left((I - \tau \otimes \tau) \frac{1}{d-1} \nabla_x V f \right),$$

where div_τ is the divergence on $\mathbb{S}^{d-1}$, and $L = \Delta_\tau = \operatorname{div}_\tau \circ \nabla_\tau$ is the Laplace–Beltrami operator on $\mathbb{S}^{d-1}$, where ∇_τ is the gradient on $\mathbb{S}^{d-1}$.

Using a diffusion scaling for space and time, we obtain the scaled version of (4.24) with $\epsilon > 0$, which reads

$$(4.25) \quad \epsilon \partial_t f + T f = \frac{A^2}{2\epsilon} L f.$$

In the following we consider several approximations of (4.24) based on (4.25).

The associated drift-diffusion equation is given by

$$(4.26) \quad \partial_t \rho = \frac{2}{d(d-1)A^2} \operatorname{div}_x (\nabla_x V \rho + \nabla_x \rho).$$

It may be formally derived from (4.25) using the asymptotic expansion

$$f_\epsilon = f_0 + \epsilon f_1 + \mathcal{O}(\epsilon^2).$$

Remark 3. *The stochastic differential equation associated to equation (4.26) is*

$$dx_t = -\frac{2}{d(d-1)A^2} \nabla_x V(x_t) dt + \frac{2}{\sqrt{d(d-1)}A} dW_t.$$

4.2 - Scalar and hydrodynamic flux-limited approximations

A diffusion type approximation respecting the finite speed of propagation of the kinetic problem is the so called flux-limited diffusion equations, see [26, 59]. The flux-limited diffusion equation related to the kinetic problem (4.25) is given by

$$(4.27) \quad \partial_t \rho = \frac{2}{(d-1)A^2} \operatorname{div}_x (\gamma(\|\beta\|_2) (\nabla_x \rho + \rho \nabla_x V))$$

with γ given below and

$$\beta = -\epsilon \frac{2}{(d-1)A^2} \left(\frac{\nabla_x \rho}{\rho} + \nabla_x V \right) = -\epsilon \frac{2}{(d-1)A^2} \nabla_x \log(\rho e^V).$$

To derive the equation one follows the procedure presented in [26] and uses the asymptotic expansion

$$f_\epsilon = \exp(a_0 + \epsilon a_1 + \mathcal{O}(\epsilon^2)) = \exp(a_0) + \epsilon a_1 \exp(a_0) + \mathcal{O}(\epsilon^2)$$

γ is defined by the relation

$$\gamma(\|\beta\|_2)\beta = \frac{\langle \tau \exp(\beta \cdot \tau) \rangle}{\langle \exp(\beta \cdot \tau) \rangle}.$$

The function $\gamma: \mathbb{R}^+ \rightarrow \mathbb{R}$ satisfies

$$\gamma(0) = \frac{1}{d}, \quad \text{and} \quad \gamma(b) \sim \frac{1}{b} \quad \text{for } b \rightarrow \infty.$$

We note that for ϵ tending to zero we formally obtain again the linear diffusion equation. A simple approximation of γ is given by the so called Kershaw closure (cf. [59]),

$$(4.28) \quad \gamma_{Ker}(b) = (\sqrt{1+b^2} - 1)/b^2.$$

To obtain hydrodynamic approximations of the Fokker-Planck equation, one proceeds as follows using the following notation for the moments of f . Let

$$(4.29) \quad \rho = \langle f \rangle, \quad q = \langle \tau f \rangle, \quad P = \langle \tau \otimes \tau f \rangle.$$

Integrating the scaled Fokker-Planck equation (4.25) over the sphere gives

$$\epsilon \partial_t \rho + \operatorname{div}_x \langle \tau f \rangle = \frac{A^2}{2\epsilon} \langle Lf \rangle.$$

Simple computations yield the continuity equation

$$(4.30) \quad \epsilon \partial_t \rho + \operatorname{div}_x q = 0.$$

Multiplying the Fokker-Planck equation with τ and integrating over the unit sphere one obtains the momentum balance equation

$$(4.31) \quad \epsilon \partial_t q + \operatorname{div}_x P + \frac{1}{d-1} (\rho I - P) \nabla_x V = -\frac{(d-1)A^2}{2\epsilon} q.$$

This equation may be closed by writing P as a function of ρ and q . In the following, we discuss two possibilities.

Linear closure (P_1). The so called P_1 model is given by the equations

$$(4.32) \quad \begin{aligned} \epsilon \partial_t \rho + \operatorname{div}_x q &= 0 \\ \epsilon \partial_t q + \frac{1}{d} \nabla_x \rho + \rho \frac{1}{d} \nabla_x V &= -\frac{(d-1)A^2}{2\epsilon} q. \end{aligned}$$

It is derived using the linear closure function

$$\hat{f} = a + \tau \cdot b.$$

Inserting $\hat{f}$ into (4.29) gives

$$\rho = a, \quad q = \langle \tau \otimes \tau \rangle b = \frac{1}{d}b, \quad P = \frac{1}{d}aI.$$

Therefore $P = \frac{1}{d}\rho I$, and the momentum balance system simplifies to equation (4.32). We note that for ϵ going to zero we formally obtain again the linear diffusion equation.

It is well known, that this closure has several drawbacks, see for example [26]. In particular, it might exhibit solutions with negative density ρ , which clearly does not represent solutions of the Fokker-Planck equation, due to the maximum principle. This is not the case for the following closure.

Maximum entropy closure (M_1). We refer for example to [4, 34, 59]. The flux-limited M_1 equations are given by

$$(4.33) \quad \begin{aligned} &\epsilon \partial_t \rho + \operatorname{div}_x q = 0 \\ &\epsilon \partial_t q + \operatorname{div}_x \left(\rho D\left(\frac{q}{\rho}\right) \right) + \frac{1}{d-1} \rho \left(I - D\left(\frac{q}{\rho}\right) \right) \nabla_x V = -\frac{(d-1)A^2}{2\epsilon} q \end{aligned}$$

with the nonlinear function D given below. To derive the approximation we use

$$(4.34) \quad \hat{f} = a \exp(\beta \cdot \tau)$$

with $a: \mathbb{R} \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$ and $\beta: \mathbb{R} \times \mathbb{R}^+ \rightarrow \mathbb{R}^d$. These functions are to be determined through the moment equations (4.29), which gives

$$\rho = a \langle \exp(\beta \cdot \tau) \rangle, \quad q = a \langle \tau \exp(\beta \cdot \tau) \rangle.$$

Taking the ratio of the two yields

$$(4.35) \quad \frac{q}{\rho} = \frac{q}{\rho}(\beta) = \frac{\langle \tau \exp(\beta \cdot \tau) \rangle}{\langle \exp(\beta \cdot \tau) \rangle} = \gamma(\|\beta\|_2) \beta,$$

and

$$(4.36) \quad \left\| \frac{q}{\rho} \right\|_2 = |\gamma(\|\beta\|_2)| \|\beta\|_2.$$

In general, this equation cannot be solved analytically. Nevertheless, it defines a bijection between $\|\beta\|_2$ and $\|q/\rho\|_2$, and solving this equation numerically is in general possible. However, it is necessary to evaluate the inverse of this function in every spatial point at every time step. Since the function (and its inverse) is regular it is more efficient to tabulate the solution of the nonlinear equation. Then, one proceeds as follows. Using (4.29) and the form of $\hat{f}$, one obtains $P = \rho D(\beta)$, with

$$(4.37) \quad D = D(\beta) = \frac{\langle \tau \otimes \tau \exp(\beta \cdot \tau) \rangle}{\langle \exp(\beta \cdot \tau) \rangle}.$$

Expressing β in terms of q/ρ we obtain $D = D(q/\rho)$ and $P = \rho D(q/\rho)$. Moreover, we note that, due to symmetry considerations, D can be written as a linear combination of the identity and $\beta \otimes \beta$ with weights depending on $\|\beta\|_2$. We refer to [59] for details. Finally, one obtains the maximum entropy equations (4.33). The nonlinear system is hyperbolic symmetrizable, ρ remains non-negative and the normalized flux $u = q/\rho$ is limited in absolute value by 1, compare [9].

We note that $D(0) = \frac{1}{d}I$ and $D'(0) = 0$. Therefore, linearization of (4.33) around the stationary state $(\rho, q) = (e^{-V}, 0)$ gives the P_1 equations (4.32). For ϵ going to zero we formally obtain from (4.33) again the linear diffusion equation (4.26).

4.3 - Decay rates

In this section we discuss the decay rates to equilibrium for the different models described above. We consider all models with $\epsilon = 1$ and set

$$\alpha := d(d-1)A^2/2.$$

It is known that the exponential decay for the diffusion problem is governed by a decay rate proportional to $1/\alpha$. In particular, the decay will be fast for small α and slow for large α . This is not the case for the underlying kinetic model (cf. [32]), where the decay is slow for large and small α . While the P_1 and M_1 approximations exhibit qualitatively the same decay rates as the kinetic problem, the flux-limited diffusion models give rates between the diffusion and kinetic decay rates. In this subsection we collect results on the decay via energy estimates.

The Fokker–Planck equations. For the Fokker–Planck equation

$$(4.38) \quad \partial_t f + Tf = \frac{A^2}{2}Lf,$$

one observes that e^{-V} is the unique equilibrium solution. One introduces the scalar product

$$(f, g) = \int_{\mathbb{M}} fg \, d\mu \, d\nu,$$

with $\mu(dx) = e^{V(x)}dx$, $d\nu$ the normalized surface measure on $\mathbb{S}^{d-1}$, and the associated norm $\|\cdot\|_{\mathbb{M}}$. On the space $L^2(\mathbb{M}, d\mu \, d\nu)$, the operator T is skew symmetric, and the operator L is symmetric and negative semidefinite. Convergence to the equilibrium $f_{\mathbb{M}}$ is proven in [32, 43]. This is a so-called *hypocoercivity* result, see [31]. It requires two assumptions on the potential V , besides a certain smoothness and the normalization condition $\int_{\mathbb{R}^d} e^{-V} dx = 1$, compare [31].

(H1) *Poincaré inequality*: There exists a positive constant c_P such that

$$\int_{\mathbb{R}^d} \left(u - \int_{\mathbb{R}^d} u e^{-V} dx \right)^2 e^{-V} dx \leq c_P \int_{\mathbb{R}^d} |\nabla_x u|^2 e^{-V} dx$$

for any $u \in H^1(e^{-V} dx)$.

(H2) *Pointwise condition*: There exists $C > 0$ such that

$$|\nabla_x^2 V(x)| \leq C(1 + |\nabla_x V(x)|) \quad \text{for any } x \in \mathbb{R}^d,$$

where $\nabla_x^2 V$ denotes the Hessian.

The Poincaré inequality (H1) and normalization require a sufficiently strong growth of $V(x)$ as $|x| \rightarrow \infty$, whereas condition (H2) puts a limitation on the growth behavior. This includes a large class of confining potentials such as $V(x) = (1 + |x|^2)^\beta$, $\beta \geq 1/2$.

Assume that $f_0 \in L^2(\mathbb{M}, d\mu \, d\nu)$ and (H1) and (H2) hold. Then, following [32, 43] one can prove, that the solution subject to the initial condition $f(t=0) = f_0$ satisfies

$$\|f(t) - e^{-V}(f_0, e^{-V})\|_{\mathbb{M}} \leq C \|f_0 - e^{-V}(f_0, e^{-V})\|_{\mathbb{M}} e^{-\lambda t}$$

with decay rate

$$(4.39) \quad \lambda(\alpha) = \frac{C_1 \alpha}{1 + C_2 \alpha^2},$$

where the constants $C, C_1, C_2 > 0$ depend only on n and the potential V . In particular,

$$\lambda = \mathcal{O}(\alpha) \quad \text{as } \alpha \rightarrow 0, \quad \lambda = \mathcal{O}(1/\alpha) \quad \text{as } \alpha \rightarrow \infty,$$

as mentioned above. Explicit values for the constants could be obtained depending on the potential V .

Diffusion. We consider the diffusion equation in the form

$$(4.40) \quad \partial_t \rho = \alpha^{-1} \nabla_x \cdot (e^{-V} \nabla_x (\rho e^V)).$$

We assume that the Poincaré inequality (H1) is satisfied and rewrite it with $\rho = u e^{-V}$,

$$(4.41) \quad \int (\rho - e^{-V}(\rho, e^{-V})_\mu)^2 d\mu \leq c_P \int |e^{-V} \nabla_x (\rho e^V)|^2 d\mu \quad \forall \rho \in H^1(d\mu),$$

where we denote the scalar product in $L^2(\mathbb{R}^d, d\mu)$ as

$$(f, g)_\mu = \int_{\mathbb{R}^d} f g d\mu,$$

and the associated norm with $\|\cdot\|_\mu$. Using condition (H1), the decay rate for the diffusion equation is obtained with a straightforward energy estimate. We have

$$\|\rho(t) - e^{-V}(\rho, e^{-V})_\mu\|_\mu \leq C \|\rho_0 - e^{-V}(\rho_0, e^{-V})_\mu\|_\mu e^{-\lambda t},$$

with decay rate $\lambda(\alpha) = \frac{2}{\alpha c_P}$, where c_P is the Poincaré constant in (H1).

P_1 approximation. Due to linearity, the P_1 equations may be rewritten as a second order equation. This results in a damped wave equation given by

$$(4.42) \quad \rho_{tt} + \alpha \rho_t - \operatorname{div}_x (e^{-V} \nabla_x (\rho e^V)) = 0,$$

with smooth normalized potential V satisfying the Poincaré inequality in the form (4.41), and damping coefficient α . The treatment of this equation is classical, we refer to [7] for more general cases and references. Define the following energy functionals

$$\begin{aligned} \mathbb{E}[\rho] &= \frac{1}{2} \|\rho_t\|_\mu^2 + \frac{1}{2} \|e^{-V} \nabla_x (\rho e^V)\|_\mu^2, \\ \mathcal{H}[\rho] &= \mathbb{E}[\rho] + \eta(\rho_t, \rho - e^{-V}(\rho, e^{-V})_\mu)_\mu, \end{aligned}$$

for some appropriately chosen $\eta \in (0, 1)$. We assume $\rho_0 \in L^2(\mathbb{R}^d, d\mu)$ and that (4.41) holds, and proceed similarly as in the kinetic problem. Using the functional $\mathcal{H}$ one can prove that the solution subject to the initial condition $\rho(t=0) = \rho_0$ satisfies

$$\mathbb{E}[\rho(t)] \leq C \mathbb{E}[\rho_0] e^{-\lambda t},$$

with a constant $C > 0$. The decay rate $\lambda = \lambda(\alpha)$ can be estimated by

$$\lambda(\alpha) = \frac{4 + \alpha^2 c_P}{4 + 2\alpha\sqrt{c_P} + \alpha^2 c_P} \left[\alpha - \sqrt{\frac{\alpha^4 c_P}{4 + \alpha^2 c_P}} \right].$$

This yields again an estimate of the form (4.39) for suitable constants C_1, C_2 . That means we have qualitatively the same estimate as in the Fokker–Planck case.

Remark 4. The energy estimates are in general not sharp. This can be explicitly discussed in the linear case for toy examples like the damped harmonic oscillator

$$(4.43) \quad u_{tt} + \alpha u_t + u = 0,$$

for $\alpha > 0$. Choosing

$$(4.44) \quad \mathbb{E} := \frac{1}{2}u_t^2 + \frac{1}{2}u^2, \quad \mathcal{H} := \mathbb{E} + \eta u_t u,$$

the energy estimates give as before

$$(4.45) \quad \mathbb{E}(t) \leq C\mathbb{E}(0)e^{-\lambda(\alpha)t}$$

with an approximate decay rate

$$\lambda(\alpha) = \frac{4 + \alpha^2}{4 + 2\alpha + \alpha^2} \left[\alpha - \sqrt{\frac{\alpha^4}{4 + \alpha^2}} \right].$$

In this simple case, the explicit decay rates are given by the smallest real parts of the eigenvalues of the damped oscillator. Therefore, the exact decay rate is given by

$$\lambda(\alpha) = \begin{cases} \alpha & \text{for } \alpha \leq 2 \\ \alpha - \sqrt{\alpha^2 - 4} & \text{for } \alpha \geq 2 \end{cases}.$$

In other words for α near 0 or ∞ the estimates are sharp. This is not the case for intermediate values of α , see Fig. 8.

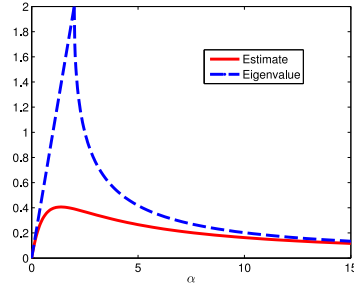


Fig. 8. Smallest real parts of eigenvalues of the damped harmonic oscillator and estimated decay rates λ for different α .

Nonlinear models. In the nonlinear case, global decay to equilibrium is a much more subtle problem.

For the flux-limited diffusion equation one can formally deduce the following. See, for example, [18] for further references and investigations of the so called relativistic heat equations. Rewriting equation (4.27) gives

$$(4.46) \quad \partial_t \rho = \frac{d}{\alpha} \operatorname{div}_x \left(\rho \gamma \left(\frac{d}{\alpha} \|\nabla_x \log(\rho e^V)\|_2 \right) \nabla_x \log(\rho e^V) \right).$$

We note that $\gamma = \gamma(\|\beta\|_2)$ satisfies $\gamma(0) = \frac{1}{d}$ and

$$(4.47) \quad \gamma = \mathcal{O}\left(\frac{1}{\|\beta\|_2}\right) \quad \text{for } \|\beta\|_2 \rightarrow \infty.$$

Thus, formally, for α going to infinity and $\|\beta\|_2$ going to zero, the problem behaves like the diffusion equation (4.26), whereas for α going to zero and $\|\beta\|_2$ going to infinity, the limit equation resembles a homogeneous relativistic heat equation (cf. [18]). Formally, using (4.47), the limit equation for α going to zero is given by

$$\partial_t \rho = \operatorname{div}_x \left(\rho \frac{\nabla_x(\rho e^V)}{\|\nabla_x(\rho e^V)\|} \right).$$

Consequently, for the flux-limited diffusion problem one expects a decay rate which converges for α going to zero to a finite positive value and not to infinity as in the case of the diffusion problem, or to zero as in case of the P_1 approximation or the Fokker–Planck equations. Analytical and numerical investigations of the decay rate and the behaviour of the solutions of the relativistic heat equation in the homogeneous relativistic heat limit can be found in [3, 18].

The nonlinear maximum entropy model is a partially dissipative hyperbolic system. The trend to approximating diffusive equations or the convergence to a stationary equations has been discussed by many authors, we refer, for example,

to [7, 10] for very general settings and to [24, 51, 60] for special applications related to the equations considered here. For example in [60] the convergence to equilibrium for the Euler–Poisson system has been proven, which is closely related to the M_1 equations with the Kershaw approximation. For explicit decay rates for a related nonlinear problem we refer to [51]. Formally, for α going to infinity the problem behaves again like the diffusion equation, and for α going to zero the convergence rate is going to zero as in the kinetic Fokker–Planck equation.

4.4 - Numerical results

The kinetic problem could either be solved by deterministic methods (see the previous section or cf. [67]), or stochastic methods via a Monte–Carlo simulation of the underlying SDE system (cf. [50]). Here, the distribution function generated from the Monte–Carlo solution of the SDE is used to determine the density and to compare the results with those of the different approximate equations. We use a standard 4-stage RK–Monte–Carlo algorithm with a large number of samples, here $3 \cdot 10^6$. For a comparison of the Monte–Carlo simulation with deterministic methods for the present equations, see [67]. The diffusion problem is solved explicitly. For flux-limited diffusion, P_1 and M_1 equations, a Discontinuous-Galerkin algorithm of order 3 is used (cf. [25]). As for the flux-limited diffusion equation, a variant described in [25] is used.

We consider dimension $d = 2$. The potential is chosen as $V(x) = \|x\|^2$. We compare the solution of the SDE system with the different approximations described above. The domain of integration is $[-7, 7]^2$. We choose a Gaussian type (in x) initial condition for the kinetic problem and the corresponding initial conditions for approximate equations. The initial conditions are normally distributed

$$f(x, v, 0) = \rho(x, 0) = C \exp\left(-\frac{\|x - x_0\|^2}{2\sigma^2}\right), \quad q(x, 0) = 0,$$

where $x_0 = (2, 2)$ and $\sigma = \sqrt{0.1}$.

First, we compare the models for short times by considering the densities obtained by solving the kinetic and the macroscopic problems for a fixed time t . In Fig. 9, we plot the densities determined by the different equations at a fixed time $t = 2.5$.

The good approximation of the SDE solution by the M_1 approximation is clearly observed in contrast to the other solutions. Diffusion and flux-limited diffusion equations give very diffusive results, whereas the P_1 solution even exhibits negative values for the density as expected.

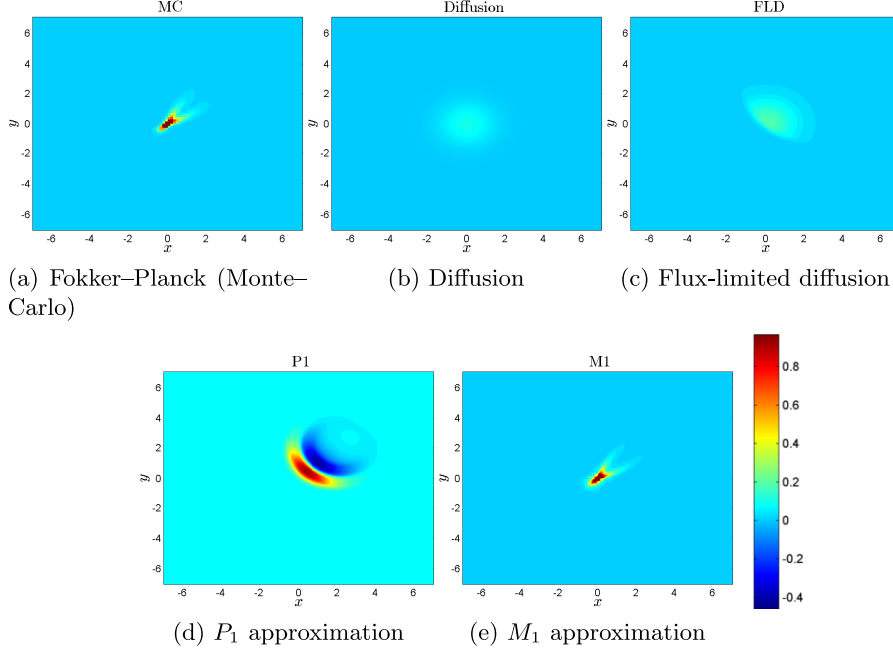


Fig. 9. Density ρ of Fokker–Planck, diffusion, flux-limited diffusion, P_1 and M_1 equations with Gaussian initial condition at $t = 2.5$.

Second, we consider the long time behaviour of the different solutions. In particular, the decay rates to equilibrium for the different approximations and the SDE system is investigated.

In Fig. 10 (a) and (b), the time development of the L^2 distance to equilibrium is shown in a logarithmic plot. For the moment models we plot the difference between the stationary distribution and the closure function $\hat{f}$ depending on the corresponding moments. We consider small $A = 0.1$ and an intermediate value $A = 0.9$. Again, it is observed that the SDE system and the M_1 approximation have very similar decay behaviour, whereas the other approximations differ strongly. Using these decay curves we determine the decay rates with an exponential least square fit of the decay curves. The numerically obtained decay rates λ are plotted in Fig. 10 (c) for a large range of values A . For large values of A all rates coincide, since we are in the diffusive limit. Even for small values of A one observes a very good fit of the SDE or kinetic rates and the M_1 decay rates. Both tend to zero with nearly the same rate as A goes to zero. The decay rate of the P_1 solution also goes to zero as A goes to zero, as predicted by the energy estimate. However, the P_1 -rates are much smaller than the original rates of the SDE problem. As expected, the flux-limited dif-

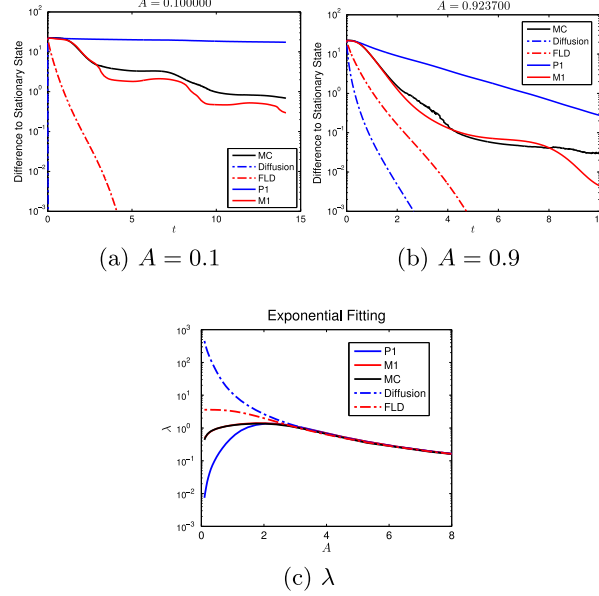


Fig. 10. Decay to equilibrium for Fokker–Planck, diffusion, flux-limited diffusion, P_1 and M_1 equations. Plot of L^2 -norm of the solutions and decay rate λ for different A using exponential fitting of decay curves.

fusion equation has a constant rate as A approaches zero, whereas the diffusion equation has a rate going to infinity.

The results clearly show the good approximation quality of the M_1 approximation for short and long times compared to the other approximate equations in the present situation. Comparing the computation times, one observes that the Monte–Carlo approximation of the kinetic problem takes roughly an order of magnitude more time than the determination of the M_1 solution. See [67] for a detailed numerical investigation of deterministic methods for the kinetic problems in 2 and 3 dimensions, and a comparison to Monte–Carlo methods.

5 - Interacting fiber models

In this section a model for interacting fibers is presented, which takes into account the finite size of the fibers and prevents intersection of the fibers. The model is based on a system of retarded stochastic differential equations with suitable interaction potentials. The mean-field limit for the corresponding deterministic system is considered and numerical results are presented. For details we refer to [15].

5.1 - Interacting isotropic fiber models

The fiber models discussed in the previous sections only describe the evolution of the center line of the fiber and do not capture the effects of the finite size of the fibers. Hence, self-intersection and intersection among fibers are not prevented in the model. A fiber model taking these points into account and including interactions between the fibers is developed in the following.

Consider $N \in \mathbb{N}$ fibers with position and velocity $(x^i, \tau^i) \in \mathbb{M} = \mathbb{R}^d \times \mathbb{S}^{d-1}$, for each $i \in \{1, \dots, N\}$. The interacting fiber model reads

$$(5.48) \quad \begin{aligned} dx_t^i &= \tau_t^i dt \\ d\tau_t^i &= (I - \tau_t^i \otimes \tau_t^i) \circ \left(-\frac{1}{d-1} \nabla_x V(x_t^i) dt \right. \\ &\quad \left. - \frac{1}{d-1} \left[\sum_{j=1}^N \int_0^t \nabla_x U(x_t^i - x_s^j) ds \right] dt + A dW_t^i \right), \end{aligned}$$

with independent Brownian motions W_t^i . In comparison to the previous fiber model, we include a nonlocal interaction term

$$\int_0^t \nabla_x U(x_t^i - x_s^j) ds,$$

where U is an interaction potential, which is repulsive in our case, so as to avoid contact among the fibers. Note that a 'non-retarded' version of this system would be similar to a model for swarming with roosting potential (cf. [19, 20]). In addition to the interaction term, our new model includes a delay term, i.e., an integration with respect to time, to describe the fact that fibers interact with each other and with itself on the whole fiber length.

There is some freedom in the choice of the interaction potential. As a simple example, one can use a mollifier type potential

$$U(x) = U(|x|) = C \exp \left(-\frac{(2R)^2}{(2R)^2 - |x|^2} \right), \quad \text{for } |x| < 2R,$$

where R is a nonnegative parameter representing the fiber radius and $C > 0$ is a fixed constant describing the strength of the interaction. Alternatively, a potential could be described by a smoothed version of Heaviside type potential

$$U(x) = U(|x|) = C\Theta(2R - |x|),$$

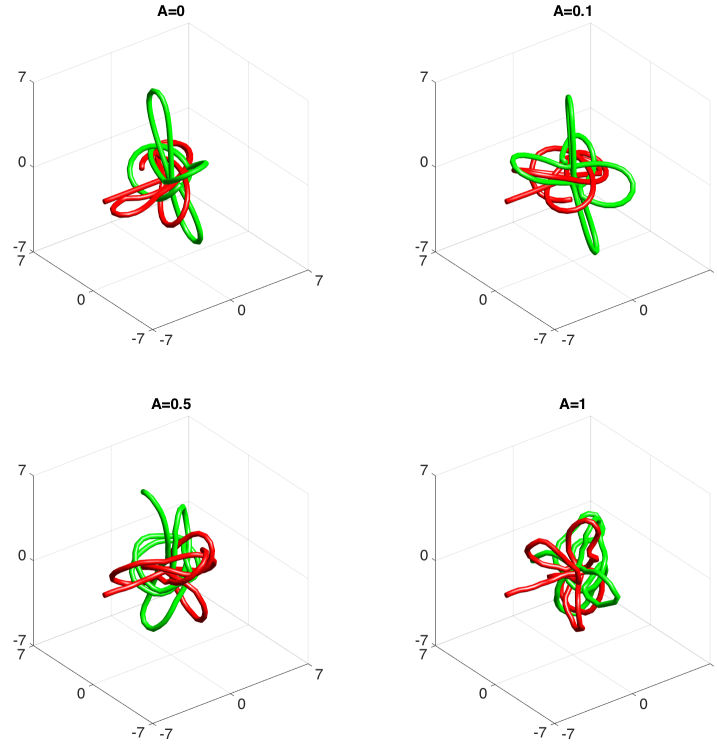


Fig. 11. Comparison of the influence of the noise A for two interacting fibers.

with Heaviside function Θ . It should be noted, that with smooth potential U intersections cannot be strictly prevented. The choices of U discussed here describe 'soft fibers'. In Figure 11 we compare the fiber curves for different noise amplitudes A .

Remark 5. To consider inelastic interactions, one could include damping terms depending on the velocity in the interaction potential. This would lead to equations where a dissipative force is included in the interaction term.

In the following, we formulate a slightly more general model than (5.48). Since, in reality, the fiber material is transported away by the belt, interaction will not take place for the full history of the fibers. Thus, it is reasonable to consider a cut-off with a cut-off size $H > 0$ depending potentially on the speed of the belt. Define

$$h(t) = \begin{cases} t & \text{for } t \leq H \\ H & \text{for } t > H \end{cases}, \quad H \in (0, \infty).$$

Then the interacting fiber model with cut-off is given by

$$\begin{aligned}
 dx_t^i &= \tau_t^i dt \\
 d\tau_t^i &= (I - \tau_t^i \otimes \tau_t^i) \circ \left(-\frac{1}{d-1} \nabla_x V(x_t^i) dt \right. \\
 (5.49) \quad &\quad \left. - \frac{1}{d-1} \left[\sum_{j=1}^N \int_{t-h(t)}^t \nabla_x U(x_t^i - x_s^j) ds \right] dt + A dW_t^i \right).
 \end{aligned}$$

5.2 - Mean-field equation, stationary solutions and large diffusion limit

For the following investigations we consider a scaled version of the equation, i.e.

$$\begin{aligned}
 dx_t^i &= \tau_t^i dt \\
 d\tau_t^i &= (I - \tau_t^i \otimes \tau_t^i) \circ \left(-\frac{1}{d-1} \nabla_x V(x_t^i) dt \right. \\
 (5.50) \quad &\quad \left. - \frac{1}{d-1} \left[\frac{1}{N} \sum_{j=1}^N \frac{1}{h(t)} \int_{t-h(t)}^t \nabla_x U(x_t^i - x_s^j) ds \right] dt + A dW_t^i \right).
 \end{aligned}$$

The factor $1/N$ leads to the so called 'weak coupling scaling' (cf. [17, 63]). Similarly, the scaling $1/t$ is a normalization of the potential with respect to the integration over t . Also note that the summation does not exclude $i = j$, which accounts for self-interaction of a fiber with itself.

We note that in this case we obtain for $H \rightarrow 0$ a non-retarded interacting particle model with constant speed, whereas, in the limit $H \rightarrow \infty$, we obtain a scaled version of (5.48) with factors $1/N$ and $1/t$ in front of the delay term.

Remark 6. *The scalings $\frac{1}{t}$ and $\frac{1}{N}$ are a normalization of the total amount of fiber material in the system. The equations with such a scaling could be viewed as a model for a textile composed of a large number of fibers with a given area weight and fiber density. The unscaled version would result in a fabric increasing to infinity with fiber length and fiber number.*

The associated mean-field equation for the distribution function $f = f(t, x, \tau)$ may be formally derived from the microscopic equations following the procedure described, for example, in [39, 40] for the classical case, in [11] for the case with stochastic forcing or [11, 39, 40] for an equation with delay terms. The equation reads

$$(5.51) \quad \partial_t f + \tau \cdot \nabla_x f + S f = L f$$

with deterministic force term $Sf = S^V f + S^U f$, given by

$$(5.52) \quad \begin{aligned} S^V f &= -\nabla_\tau \cdot \left(f (I - \tau \otimes \tau) \frac{1}{d-1} \nabla_x V \right), \\ S^U f &= -\nabla_\tau \cdot \left(f (I - \tau \otimes \tau) \frac{1}{d-1} \frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{R}^d} \nabla_x U(x-y) \rho(s, y) dy ds \right), \end{aligned}$$

where ∇_τ is the gradient on $\mathbb{S}^{d-1}$ and diffusion operator

$$(5.53) \quad Lf = \frac{A^2}{2} \Delta_\tau f,$$

where Δ_τ denotes the Laplace–Beltrami operator on $\mathbb{S}^{d-1}$. In addition, we have the normalization $\int_{\mathbb{R}^d} \rho dx = 1$, where ρ denotes the zeroth-moment $\rho = \int_{\mathbb{S}^{d-1}} f d\nu$. We refer to [15] for a proof of the mean-field limit for the deterministic interacting fiber model

$$(5.54) \quad \begin{aligned} \frac{dx_t^i}{dt} &= \tau_t^i \\ \frac{d\tau_t^i}{dt} &= (I - \tau_t^i \otimes \tau_t^i) \circ \left(-\frac{1}{d-1} \nabla_x V(x_t^i) \right. \\ &\quad \left. - \frac{1}{d-1} \frac{1}{N} \sum_{j=1}^N \frac{1}{h(t)} \int_{t-h(t)}^t \nabla_x U(x_t^i - x_s^j) ds \right), \end{aligned}$$

towards the Vlasov type equation

$$(5.55) \quad \partial_t f + \tau \cdot \nabla_x f + Sf = 0,$$

where $S = S^V + S^U$ is as given in (5.52).

Now, we formally investigate situations with large values for the noise amplitude on a diffusive time scale, i.e., we change $\tilde{L} = \epsilon L$ and $\tilde{t} = \epsilon t$ (cf. [8, 48]). Replacing the scaled operators in (5.51) and omitting the tilde lead to the scaled equation

$$(5.56) \quad \epsilon \partial_t f + \tau \cdot \nabla_x f + Sf = \frac{1}{\epsilon} Lf.$$

We use a *Hilbert expansion* of the form $f = f_0 + \epsilon f_1 + \dots$ for (5.56). To order 1, we simply get $f_0 = f_0(x) = \rho(x)$. To order ϵ , one obtains

$$\tau \cdot \nabla_x f_0 + S f_0 = \frac{A^2}{2} \Delta_\tau f_1,$$

which, due to the Fredholm alternative, gives

$$f_1 = -\frac{2}{A^2(d-1)}\tau \cdot f_0 \nabla_x \left(\ln f_0 + V + \frac{1}{h(t)} \int_{t-h(t)}^t (U \star f_0)(s, \cdot) ds \right).$$

Integrating (5.56) with respect to $d\nu$ gives

$$\epsilon \partial_t \int_{\mathbb{S}^{d-1}} f d\nu + \nabla_x \cdot \int_{\mathbb{S}^{d-1}} \tau f d\nu = 0.$$

Considering terms up to order ϵ , we obtain

$$\partial_t f_0 + \nabla_x \cdot \int_{\mathbb{S}^{d-1}} \tau f_1 d\nu = 0.$$

Therefore, inserting f_1 and computing the integral over the tensor product yields

$$\partial_t \rho = \frac{2}{d(d-1)A^2} \nabla_x \cdot \left[\rho \nabla_x \left(\ln \rho + V + \frac{1}{h(t)} \int_{t-h(t)}^t (U \star \rho)(s, \cdot) ds \right) \right].$$

This equation is similar to the diffusion approximation derived in the previous section for the case without interaction. However, additionally it contains a delay term. The stationary equation reads

$$\rho \nabla_x \left(\ln \rho + V + U \star \rho \right) = 0, \quad \int_{\mathbb{R}^d} \rho dx = 1,$$

which leads to the integral equation

$$(5.57) \quad \ln \rho + V + U \star \rho = c,$$

where the constant c is fixed by the normalization $\int_{\mathbb{R}^d} \rho dx = 1$. We note that it may be written in the equivalent fixed-point form

$$(5.58) \quad \rho = \frac{e^{-V-U \star \rho}}{\int_{\mathbb{R}^d} e^{-V-U \star \rho} dx}.$$

5.3 - Numerical method and results

In the following, we describe the extension of the numerical solver presented in Section 2 or in [21, 67] to the case with interactions and investigate the qualitative behavior of solutions corresponding to the interacting fiber model numerically. More specifically, we consider the case of isotropic fibers in three spatial dimensions.

The numerical procedure follows the semi-Lagrangian finite volume discretization discussed above or in (cf. [67, 68]). To obtain a second order scheme, we apply a Strang splitting [22] to (5.51) and second order discretizations of the resulting subproblems, see [15].

Additionally, we have to approximate the convolution $U \star \rho$. This is done using the midpoint rule on each grid cell. For the computation of the convolution, one has to compute the matrix of distances between the grid points, which consumes a lot of computing time and memory. However, one advantage compared to the solution of the microscopic system, is, that the grid points are fixed in contrast to the fiber positions in the microscopic context. Therefore, the distance matrix and the evaluation of U , $\nabla_x U$ for every entry of the distance matrix can be precomputed.

In the pre-processing, for every spatial grid point, we compute the pairwise occurring force terms exerted by the potential for all other grid points. For every grid point, we do not store all pairwise force terms $\nabla_x U(|x - y|)$, but only the ones with a relevant influence. For a given grid point, we store only force terms with absolute value that is at least 0.1 percent of the maximum occurring force term for that grid point. All other influences from other points with smaller force terms are neglected in the computation. The time integration in (5.52) for $h(t) = t$ does not increase the effort in the mean-field context, because it can be realized by summing up the interaction forces from different time steps.

We show numerical results for the microscopic model (5.49) and the mean-field equation (5.51) in three spatial dimensions. In particular, we investigate the convergence of the microscopic and mean-field solutions to the corresponding stationary state. The stationary states obtained from microscopic and mean-field computations are compared to the solution of (5.58). For a more detailed investigation of the convergence to equilibrium for different values of the delay H , we investigate the time decay of the distance to equilibrium for microscopic and mean-field equations and compare it to the one obtained for the case without interaction. For all computations we consider the three dimensional case for (5.49). For a comparison of the numerical results for the mean-field equation and the microscopic stochastic model we consider different noise coefficients A .

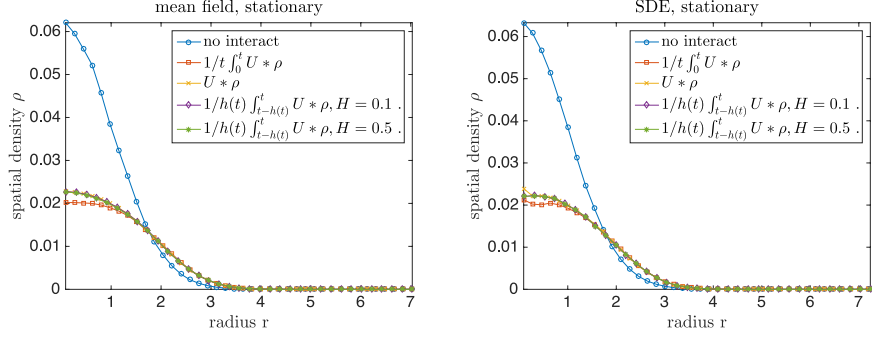


Fig. 12. Numerical stationary distributions for different cases of interaction.

In Figure 12, we consider the stationary distributions obtained from the microscopic and mean-field equations for different values of the delay H . The stationary solutions are obtained again by running either simulation until the solution does not change any more over time. We show radial plots of the radially symmetric density function. The case without interaction is compared to the case with interaction, with delay given by $H \in \{0, 0.1, 0.5, \infty\}$. The grid resolutions simulated for the mean-field equations were $n_x = 40$ points in each spatial direction with a grid size of $h_x = 0.205$. In all cases, the sphere is discretized by 320 geodesic triangles, which leads to an average cell midpoint distance of 0.175. These grid sizes are matched by the histograms generated from the microscopic fiber positions and velocities.

To achieve smooth data, the total number of simulated fibers for the microscopic simulations has to be chosen sufficiently large. In the case without interaction, the microscopic density is generated from $4.8 \cdot 10^6$ simulated fiber positions. For the cases with interaction, we have computed 800 realizations of a system of 600 interacting fibers and generated the histogram from the fiber positions of all the realizations, which means that the histogram is based on $4.8 \cdot 10^5$ microscopic fiber positions. As mentioned earlier, the interaction computation in the microscopic context is quite costly. Computing times for the mean-field solver lie in the range of 3 to 24 hours on the given hardware, which was an Intel XEON E5 2670 with 8 cores at 3.3GHz.

As expected, the stationary distribution does not change with different values of H . However the stationary distribution for the case with interaction is significantly wider than the distribution for the case without interaction. We note that the solutions obtained by the microscopic and by the mean-field equation are in very good agreement for the cases considered here.

In Figures 13 and 14, we investigate the behavior (in time) of the L^2 -norm of the distance to equilibrium for the spatial density ρ . Again, the case without

interaction is compared to the case with interaction with cut-off given by $H \in \{0, 0.1, 0.5, \infty\}$. In Figure 13, the case $A = 1.0$ is considered, while Figure 14 shows the case $A = 0.5$. The stationary solution is as before given by the end state of the numerical simulation either for the SDE system or the mean field equation. We compute the deviation of the solutions at several time steps to this stationary state in L^2 and show these values over time.

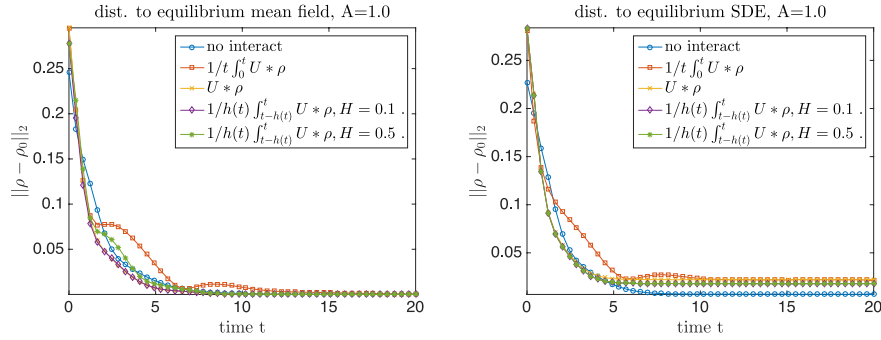


Fig. 13. Decay of the deviation between numerical solution and stationary solution over time, for different cases of interaction and noise/diffusion parameter $A = 1.0$.

The figures provide a strong indication that all cases with interaction converge to the same stationary distribution. Furthermore, the graph with the square marker shows the case with a strongly retarded potential ($\frac{1}{t} \int_0^t U \star \rho$, $H = \infty$). The decay is no longer strictly monotone and it takes more time to achieve the stationary state, in comparison to the cases without significant delay. In this case significant differences between the case with delay and interaction, the case with interaction and without delay and the case without interaction can be observed. In all cases very good coincidence between the mean-field and the solution of the microscopic SDE system is observed.

6 - Convergence to equilibrium for interacting fiber models

In this section a proof of convergence to equilibrium for the interacting fiber model in the previous section is given. Results on the long-time behavior of the mean-field model for the case of finite and infinite delay are proven, and the dependence of the rate of convergence on the different parameters is discussed. For more details we refer to [57].

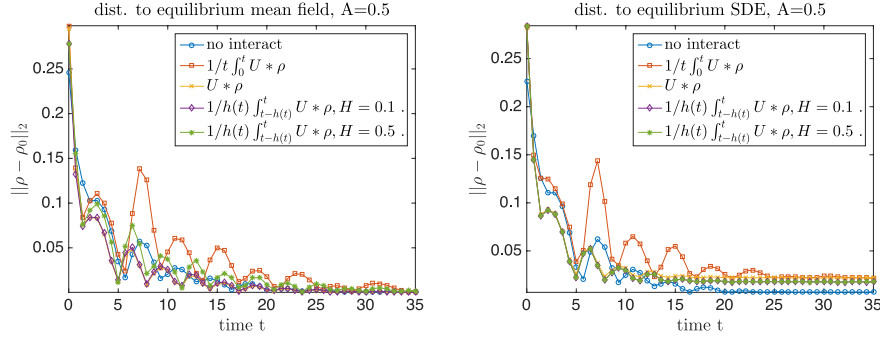


Fig. 14. Decay of the deviation between numerical solution and stationary solution over time, for different cases of interaction and noise/diffusion parameter $A = 0.5$.

6.1 - Microscopic and mean-field delay models

We reconsider the interacting fiber model (5.48) presented in the last section. The state space of this delay differential equation has been $\mathbb{R}^d \times \mathbb{S}^{d-1}$. In the subsequent analysis we concentrate on the effect of the delay term and consider a classical interacting particle model with state space $\mathbb{M} = \mathbb{R}^{2d}$ as in [12, 19] and include a delay term. To describe the models we are interested in, we introduce a notation based on the notation in [39] that will be used in the sequel. Let $d \geq 2$ denote the number of dimensions. We consider a microscopic delay model with $2N$ equations for $x_t^i \in \mathbb{R}^d$ and $v_t^i \in \mathbb{R}^d$ at time $t \geq 0$ for $i = 1, \dots, N$. The model is formulated as a stochastic delay differential equation with state space $(x_t^i, v_t^i) \in \mathbb{M}$, given by

$$(6.59a) \quad dx_t^i = v_t^i dt$$

$$(6.59b) \quad dv_t^i = -\nabla_x V(x_t^i) dt - \left(\frac{1}{N} \sum_j \frac{1}{t} \int_0^t \nabla_x U(x_t^i - x_s^j) ds \right) dt - \gamma v_t^i dt + \sqrt{2\sigma} dW_t^i,$$

subjected to the initial conditions $(x_0^i, v_0^i) \in \mathbb{M}$. Here, W_t^i for $i = 1, \dots, N$, denote independent standard Brownian motions on $\mathbb{R}^d$, $\gamma > 0$ is the friction coefficient and $\sigma > 0$ is the diffusion coefficient. The vectors $(x_0^i, v_0^i) \in \mathbb{M}$ for $i = 1, \dots, N$ are typically taken to be independent and identically distributed random variables with a given law $\mu_0 \in \mathcal{P}_2(\mathbb{M})$, where $\mathcal{P}_2(\mathbb{M})$ denotes the space of Borel probability measures with finite second moment. To simplify the considerations we assume the exterior potential V to be confining. Moreover, ∇V and ∇U are required to be globally Lipschitz continuous (cf. Assumption 1).

Note that the non-retarded version of (6.59), i.e., without the delay term, is similar to models for swarming as discussed, for example, in [19, 20].

As in the last section we introduce a cut-off

$$(6.60) \quad h(t) = \begin{cases} t & t \leq H \\ H & t > H \end{cases},$$

with the cut-off size $0 \leq H \leq \infty$. In this case, the interacting fiber model becomes

$$(6.61a) \quad dx_t^i = v_t^i dt$$

$$(6.61b) \quad dv_t^i = -\nabla_x V(x_t^i) dt - \left(\frac{1}{N} \sum_j \frac{1}{h(t)} \int_{t-h(t)}^t \nabla_x U(x_t^i - x_s^j) ds \right) dt \\ - \gamma v_t^i dt + \sqrt{2\sigma} dW_t^i.$$

The associated mean-field equation corresponding to (6.61) is formally derived replacing the pairwise interaction term for each fiber $i = 1, \dots, N$ with

$$\frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{M}} \nabla_x U(x_t^i - \hat{x}) d\mu_s^{(N)}(d\hat{x}, d\hat{v}) ds,$$

where $\mu_t^{(N)}$ is the stochastic empirical measure defined by

$$\mu_t^{(N)}(d\hat{x}, d\hat{v}) = \frac{1}{N} \sum_{i=1}^N \delta_{(x_t^i, v_t^i)}(d\hat{x}, d\hat{v}).$$

As $N \rightarrow \infty$, one would naturally postulate (not investigated here) that the sequence of stochastic empirical measures $\{\mu^{(N)}\}_{N \in \mathbb{N}} \subset \mathcal{P}(\mathcal{C}([0, T], \mathcal{P}_2(\mathbb{M})))$ converges in law towards a deterministic limit $\mu \in \mathcal{C}([0, T], \mathcal{P}_2(\mathbb{M}))$, which satisfies the retarded Vlasov–Fokker–Planck equation

$$(6.62) \quad \partial_t \mu_t + v \cdot \nabla_x \mu_t + S[\mu_t] = \nabla_v \cdot (\sigma \nabla_v \mu_t + \gamma v \mu_t)$$

in the distribution sense, where the deterministic force term $S[\mu_t]$ is given by

$$(6.63) \quad S[\mu_t] = -\nabla_x V \cdot \nabla_v \mu_t - \nabla_v \cdot \left[\left(\frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{R}^d} \nabla U(\cdot - \hat{x}) \rho_s(d\hat{x}) ds \right) \mu_t \right].$$

Here, the spatial density ρ_t denotes the first marginal of μ_t , i.e.,

$$\rho_t(B) = \mu_t(B, \mathbb{R}^d) \quad \text{for any Borel set } B \in \mathcal{B}(\mathbb{R}^d).$$

Furthermore, if a stochastic process $\{z_t = (x_t, v_t), t \geq 0\}$ is the strong solution of the so-called nonlinear Mc-Kean problem

$$(6.64a) \quad dx_t = v_t dt$$

$$(6.64b) \quad dv_t = -\nabla_x V(x_t) dt - \left(\frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{R}^d} \nabla_x U(x_t - \hat{x}) \rho_s(d\hat{x}) ds \right) dt \\ - \gamma v_t dt + \sqrt{2\sigma} dW_t,$$

with the initial condition $\mu_0 = \text{law}(z_0) \in \mathcal{P}_2(\mathbb{M})$, then $\mu = \text{law}(z)$ satisfies (6.62) in the distributional sense and the existence of a nonlinear Mc-Kean process $\{z_t\}$ corresponding to (6.64) provides the existence of a distributional solution to (6.62).

The well-posedness of the nonlinear process (6.64) can be proven under specific regularity assumptions on the potentials V and U (cf. Assumption 1). See Section 6.3 for a statement of a theorem.

6.2 - Generalized Wasserstein distances and delay inequalities

To define a generalized Wasserstein distance we consider the set of Borel probability measures on the state space $\mathbb{M}$. It is denoted by $\mathcal{P}(\mathbb{M})$. Further, we denote by

$$\mathcal{P}_2(\mathbb{M}) := \left\{ \mu \in \mathcal{P}(\mathbb{M}) \quad \text{such that} \quad \int_{\mathbb{M}} |z|^2 \mu(dz) < \infty \right\}$$

the set of Borel probability measures on $\mathbb{M}$ with finite second moment. This space may be equipped with the Wasserstein distance dist_2 defined by

$$\text{dist}_2(\mu, \hat{\mu})^2 = \inf_{\pi \in \Pi(\mu, \hat{\mu})} \left(\int_{\mathbb{M} \times \mathbb{M}} |z - \hat{z}|^2 \pi(dz, d\hat{z}) \right), \quad \mu, \hat{\mu} \in \mathcal{P}_2(\mathbb{M}),$$

where $\Pi(\mu, \hat{\mu})$ denotes the collection of all Borel probability measures on $\mathbb{M} \times \mathbb{M}$ with marginals μ and $\hat{\mu}$ on the first and second factors respectively. The set

$\Pi(\mu, \hat{\mu})$ is also known as the set of all couplings of μ and $\hat{\mu}$. Equivalently, the Wasserstein distance may be defined by

$$\text{dist}_2(\mu, \hat{\mu})^2 = \inf \mathbb{E} [|z - \hat{z}|^2],$$

where the infimum is taken over all joint distributions of the random variables z and $\hat{z}$ with marginals μ and $\hat{\mu}$ respectively.

Moreover, for a given positive quadratic form $Q: \mathbb{M} \rightarrow \mathbb{R}$, we define the distance, compare [12]

$$\text{dist}_Q(\mu, \hat{\mu})^2 = \inf_{\pi \in \Pi(\mu, \hat{\mu})} \left(\int_{\mathbb{M} \times \mathbb{M}} Q(z - \hat{z}) \pi(dz, d\hat{z}) \right) = \inf_{\pi \in \Pi(\mu, \hat{\mu})} \mathbb{E} [Q(z - \hat{z})]$$

for any two probability measures $\mu, \hat{\mu} \in \mathcal{P}_2(\mathbb{M})$.

Remark 7. *We note that*

1. *dist_2 metricizes the weak convergence in the Wasserstein space $\mathcal{P}_2(\mathbb{M})$, as well as the convergence of the first two moments. One can also show that $(\mathcal{P}_2(\mathbb{M}), \text{dist}_2)$ is a complete metric space [13, 77].*
2. *For $Q(z) = |z|^2$, we have that $\text{dist}_Q = \text{dist}_2$.*
3. *For any $z \in \mathbb{M}$, let $z = (z_1, z_2)$ with $z_i \in \mathbb{R}^d$, $i \in \{1, 2\}$. We define the quadratic form*

$$Q(z) = a|z_1|^2 + 2\langle z_1, z_2 \rangle + b|z_2|^2,$$

with positive constants $a, b > 0$, where $\langle \cdot, \cdot \rangle$ denotes the euclidean scalar product in $\mathbb{R}^d$. If the constants a, b satisfy, additionally, the inequality $ab > 1$, then there exists $p, q > 0$ such that dist_2 and dist_Q are equivalent. More specifically, since

$$p|z|^2 \leq Q(z) \leq q|z|^2,$$

holds for all $z \in \mathbb{M}$, with

$$p = \frac{(a+b) - \sqrt{4 + (b-a)^2}}{2}, \quad q = \frac{(a+b) + \sqrt{4 + (b-a)^2}}{2},$$

integrating over $\pi \in \Pi(\mu, \hat{\mu})$ and minimizing over all couplings yields the required assertion.

Lemma 6.1. *Let Q be a positive quadratic form on $\mathbb{M}$ as in Remark 7(3), i.e.,*

$$Q(z) = a|z_1|^2 + 2\langle z_1, z_2 \rangle + b|z_2|^2, \quad a, b > 0.$$

If further $ab > 1$, then Q may be represented as

$$Q(z) = \langle\langle z, M_Q z \rangle\rangle = \langle\langle Sz, Sz \rangle\rangle,$$

where M_Q and $S \in \text{Mat}(\mathbb{M})$ are invertible block matrices of the form

$$M_Q = \begin{bmatrix} a\mathbb{I}_d & \mathbb{I}_d \\ \mathbb{I}_d & b\mathbb{I}_d \end{bmatrix}, \quad S = \frac{1}{\sqrt{a}} \begin{bmatrix} a\mathbb{I}_d & \mathbb{I}_d \\ 0 & \sqrt{ab-1}\mathbb{I}_d \end{bmatrix},$$

with $\mathbb{I}_d$ being the identity matrix on $\mathbb{R}^d$ and $\langle\langle \cdot, \cdot \rangle\rangle$ denotes the euclidean scalar product in $\mathbb{R}^{2d}$.

Moreover, we state an inequality for delay differential equations, see [47], Section 4.5.

Proposition 6.1. *Let $H > 0$ and y a nonnegative function satisfying*

$$\frac{dy}{dt}(t) \leq -ay(t) + b \sup_{s \in [t-H, t]} y(s) \quad \text{for } t > t_0,$$

with initial data $y(s) = y(t_0)$, $s \in [t_0 - H, t_0]$, where a and b are nonnegative constants satisfying $a > b \geq 0$. Then, y may be estimated from above by

$$y(t) \leq y(t_0) \exp(-\lambda(t - t_0)) \quad \text{for all } t \geq t_0,$$

with the decay rate $\lambda = a - b \exp(\lambda H)$.

Remark 8. *The decay rate can be written explicitly as*

$$\lambda = a - \frac{1}{H} W(bH \exp(aH)) > 0,$$

where W is the product logarithm function, which satisfies $z = W(z) \exp(W(z))$ for any $z \in \mathbb{R}$. Indeed, we have with the above expression for λ

$$\begin{aligned} \lambda &= a - \frac{1}{H} W(bH \exp(aH)) = a - b \exp(aH) \frac{W(bH \exp(aH))}{bH \exp(aH)} \\ &= a - b \exp(aH) \exp((-W(bH \exp(aH)))) \\ &= a - b \exp\left(\left(a - \frac{1}{H} W(bH \exp(aH))\right) H\right) = a - b \exp(\lambda H) \end{aligned}$$

where we used the definition of W .

Remark 9. Let h denote a nonnegative, continuous and bounded function defined for $t \geq 0$ and $H = \sup_{t \geq 0} h(t) > 0$. Further, let y be a nonnegative function satisfying

$$\frac{dy}{dt}(t) \leq -ay(t) + b \sup_{s \in [t-h(t), t]} y(s) \quad \text{for } t > t_0.$$

Then, the estimate

$$\sup_{s \in [t-h(t), t]} y(s) \leq \sup_{s \in [t-H, t]} y(s),$$

and Proposition 6.1 leads to

$$y(t) \leq y(t_0) \exp(-\lambda(t - t_0)) \quad \text{for all } t \geq t_0.$$

The proposition will be used in this form to prove Proposition 6.3.

6.3 - Well-posedness of the delay mean-field equation

In the following, we will make use of the fact that an underlying stochastic process $\{z_t = (x_t, v_t)\}$ exists for μ_t satisfying (6.64). In fact, we will consider a more general form of our mean-field equation, namely the problem, compare again [12],

$$(6.65a) \quad dx_t = v_t dt$$

$$(6.65b) \quad dv_t = A(x_t) dt + \left(\frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{R}^d} B(x_t, \hat{x}) \rho_s(d\hat{x}) ds \right) dt - \gamma v_t dt + \sqrt{2\sigma} dW_t,$$

where A and B satisfies the following assumptions:

Assumption 1. 1. We assume that $A: \mathbb{R}^d \rightarrow \mathbb{R}^d$ is of the form

$$A(x) = -x + g(x),$$

where g is Lipschitz continuous with Lipschitz constant $c_g > 0$.

2. The function $B: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ satisfies

$$|B(x, \hat{x}) - B(y, \hat{x})| + |B(x, \hat{x}) - B(x, \hat{y})| \leq c_B(|x - y| + |\hat{x} - \hat{y}|),$$

for some constant $c_B > 0$, independent of $x, \hat{x}, y, \hat{y} \in \mathbb{R}^d$.

Following the arguments in [38] one proves

Proposition 6.2. *Under Assumption 1, there exists a unique solution $\mu \in \mathcal{C}([0, \infty), \mathcal{P}_2(\mathbb{M}))$ of the mean-field equation*

$$(6.66) \quad \partial_t \mu_t + v \cdot \nabla_x \mu_t + S[\mu_t] = \nabla_v \cdot (\sigma \nabla_v \mu_t + \gamma v \mu_t)$$

with

$$\lim_{t \searrow 0} \mu_t = \mu_0 \in \mathcal{P}_2(\mathbb{M}),$$

where the deterministic force term $S[\mu_t]$ is given by

$$S[\mu_t] = A \cdot \nabla_v \mu_t + \nabla_v \cdot \left[\left(\frac{1}{h(t)} \int_{t-h(t)}^t \int_{\mathbb{R}^d} B(\cdot, \hat{x}) \rho_s(d\hat{x}) ds \right) \mu_t \right].$$

More specifically, there exists a pathwise unique nonlinear process $\{z_t = (x_t, v_t)\}$ satisfying (6.65) with initial data $\mu_0 = \text{law}(z_0) \in \mathcal{P}_2(\mathbb{M})$ and $\mu_t = \text{law}(z_t)$ for all $t \in [0, \infty)$.

In order to obtain convergence of the solutions to (6.66) towards a stationary solution, a smallness condition for the Lipschitz constants c_g and c_B is necessary. This smallness condition is made explicit in the following section.

6.4 - Large time behavior of the delay Vlasov–Fokker–Planck equation

In this section, we prove a quantitative exponential convergence result for all solutions of (6.64) with a finite cut-off $0 \leq H < \infty$ associated to the microscopic system (6.61). The proof is based on the idea of perturbing the Euclidean metric on $\mathbb{M}$ in such a way that (6.66) is completely dissipative with respect to the new metric, compare [12, 74, 76].

The key estimate for proving the exponential convergence of all solutions to a unique equilibrium is given in the following proposition.

Proposition 6.3. *Under Assumption 1, for any $\gamma > 0$, there exist constants $\lambda > 0$ and $\bar{\eta} = \bar{\eta}(\gamma) > 0$ such that for any $c_g, c_B \geq 0$ with $\eta := c_g + 2c_B \leq \bar{\eta}$, the decay estimate*

$$(6.67) \quad \text{dist}_Q(\mu_t, \hat{\mu}_t) \leq \exp(-\lambda t) \text{dist}_Q(\mu_0, \hat{\mu}_0) \quad t \geq 0,$$

holds true for any solution $(\mu_t)_{t \geq 0}, (\hat{\mu}_t)_{t \geq 0}$ of (6.66) with corresponding initial data $\mu_0, \hat{\mu}_0 \in \mathcal{P}_2(\mathbb{M})$, where Q is a positive quadratic form on $\mathbb{M}$ of the form

$$Q(x, v) = a|x|^2 + 2\langle x, v \rangle + b|v|^2, \quad a, b > 0.$$

Furthermore, the decay rate λ is explicitly given by

$$(6.68) \quad \lambda = \lambda_1 - \frac{1}{H} W(\lambda_2 H \exp(\lambda_1 H)),$$

where λ_i , $i = 1, 2$ are given in (6.74) and $W > 0$ is the Lambert- W function, i.e., the inverse to the function $f(x) = x \exp(x)$, $x > 0$.

The idea of the proof is to find an appropriate positive quadratic form Q , such that a differential inequality appears. Applying the Halanay inequality (cf. Proposition 6.1) onto this differential inequality would then yield the required decay estimate (6.67).

Proof. Let $\{z_t, t \geq 0\}$ and $\{\hat{z}_t, t \geq 0\}$ be two solutions of (6.65) corresponding to the distributions μ and $\hat{\mu} \in \mathcal{C}([0, \infty), \mathcal{P}_2(\mathbb{M}))$ respectively. Supposing that both of these solutions satisfy the equations with the same Brownian motion W_t in $\mathbb{R}^d$ and denoting the difference of the solutions by $\bar{x}_t = x_t - \hat{x}_t$, $\bar{v}_t = v_t - \hat{v}_t$, we have that $\bar{z}_t = (\bar{x}_t, \bar{v}_t) \in \mathbb{M}$ satisfies

$$(6.69a) \quad d\bar{x}_t = \bar{v}_t dt$$

$$(6.69b) \quad d\bar{v}_t = (A(x_t) - A(\hat{x}_t))dt - \frac{1}{h(t)} \int_{t-h(t)}^t (\mathcal{K}[\mu_s](x_t) - \mathcal{K}[\hat{\mu}_s](\hat{x}_t)) ds dt - \gamma \bar{v}_t dt,$$

where for ease of notation, we define the operator $\mathcal{K}$ acting on probability measures as

$$\mathcal{K}[\mu_t](x) := \int_{\mathbb{R}^d} B(x, y) \rho_t(dy).$$

Computing the evolution of $|\bar{x}_t|^2$, $|\bar{v}_t|^2$ and $\langle \bar{x}_t, \bar{v}_t \rangle$ and defining the functional

$$\mathcal{J}_t := \mathbb{E}[Q(\bar{z}_t)] = \mathbb{E}[a|\bar{x}_t|^2 + 2\langle \bar{x}_t, \bar{v}_t \rangle + b|\bar{v}_t|^2],$$

where $a, b > 0$ are appropriately chosen later, one obtains

$$\begin{aligned} \frac{d}{dt} \mathcal{J}_t &= -2 \mathbb{E}[|\bar{x}_t|^2 - (a - b - \gamma)\langle \bar{x}_t, \bar{v}_t \rangle + (b\gamma - 1)|\bar{v}_t|^2] \\ &\quad + 2 \mathbb{E}[\langle \bar{x}_t, g(x_t) - g(\hat{x}_t) \rangle + b\langle \bar{v}_t, g(x_t) - g(\hat{x}_t) \rangle] \\ &\quad - \frac{1}{h(t)} \int_{t-h(t)}^t 2 \mathbb{E}[\langle \bar{x}_t + b\bar{v}_t, \mathcal{K}[\mu_s](x_t) - \mathcal{K}[\hat{\mu}_s](\hat{x}_t) \rangle] ds. \end{aligned}$$

Setting $\pi_t = \rho_t \otimes \hat{\rho}_t$, we estimate the terms separately to obtain

$$\langle \bar{x}_t, g(x_t) - g(\hat{x}_t) \rangle \leq c_g |\bar{x}_t|^2, \quad \langle \bar{v}_t, g(x_t) - g(\hat{x}_t) \rangle \leq c_g \left[\frac{\delta_1}{2} |\bar{x}_t|^2 + \frac{1}{2\delta_1} |\bar{v}_t|^2 \right],$$

$$\begin{aligned} \langle \bar{x}_t, \mathcal{K}[\mu_s](x_t) - \mathcal{K}[\hat{\mu}_s](\hat{x}_t) \rangle &= \iint_{\mathbb{R}^d \times \mathbb{R}^d} \langle \bar{x}_t, B(x_t, y) - B(\hat{x}_t, \hat{y}) \rangle \pi_s(dy, d\hat{y}) \\ &\leq c_B \left[\left(1 + \frac{\delta_2}{2}\right) |\bar{x}_t|^2 + \frac{1}{2\delta_2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |y - \hat{y}|^2 \pi_s(dy, d\hat{y}) \right], \end{aligned}$$

$$\begin{aligned} \langle \bar{v}_t, \mathcal{K}[\mu_s](x_t) - \mathcal{K}[\hat{\mu}_s](\hat{x}_t) \rangle &= \iint_{\mathbb{R}^d \times \mathbb{R}^d} \langle \bar{v}_t, B(x_t, y) - B(\hat{x}_t, \hat{y}) \rangle \pi_s(dy, d\hat{y}) \\ &\leq c_B \left[\frac{\delta_3}{2} |\bar{x}_t|^2 + \frac{1}{2} \left(\frac{1}{\delta_3} + \delta_4 \right) |\bar{v}_t|^2 + \frac{1}{2\delta_4} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |y - \hat{y}|^2 \pi_s(dy, d\hat{y}) \right]. \end{aligned}$$

Putting all these terms together yields

$$\begin{aligned} \frac{d}{dt} \mathcal{J}_t &\leq -2 \left(1 - \left(c_g + c_B + \frac{b}{2} (c_g \delta_1 + c_B \delta_3) + c_B \frac{\delta_2}{2} \right) \right) \mathbb{E} [|\bar{x}_t|^2] \\ &\quad - 2(a - b - \gamma) \mathbb{E} [\langle \bar{x}_t, \bar{v}_t \rangle] \\ &\quad - 2 \left(b\gamma - 1 - \frac{b}{2} \left(\frac{c_g}{\delta_1} + \left(\frac{1}{\delta_3} + \delta_4 \right) c_B \right) \right) \mathbb{E} [|\bar{v}_t|^2] \\ &\quad + c_B \left(\frac{1}{\delta_2} + b \frac{1}{\delta_4} \right) \frac{1}{h(t)} \int_{t-h(t)}^t \mathbb{E} [|\bar{x}_s|^2] ds. \end{aligned}$$

Choosing $a = b + \gamma$, $\delta_1 = \delta_3 = \delta_4 = 1$ and $\delta_2 = 2 + b$, we obtain

$$\begin{aligned} \frac{d}{dt} \mathcal{J}_t &\leq - (2 - (2 + b) \eta) \mathbb{E} [|\bar{x}_t|^2] - (2b\gamma - 2 - b\eta) \mathbb{E} [|\bar{v}_t|^2] \\ &\quad + \frac{\eta}{2} \left(b + \frac{1}{2 + b} \right) \frac{1}{h(t)} \int_{t-h(t)}^t \mathbb{E} [|\bar{x}_s|^2] ds. \end{aligned}$$

where $\eta = c_g + 2c_B$ and we used the fact that $c_B \leq \eta/2$ in the last term.

Recall from Lemma 6.1 that the quadratic form Q may be represented as

$$Q(z) = \langle Sz, Sz \rangle =: \langle \xi, \xi \rangle, \quad S = \frac{1}{\sqrt{b+\gamma}} \begin{bmatrix} (b+\gamma) \mathbb{I}_d & \mathbb{I}_d \\ 0 & \sqrt{b(b+\gamma)-1} \mathbb{I}_d \end{bmatrix}.$$

Furthermore, the first two terms on the right hand side may be equivalently written as

$$(2 - (2+b)\eta) \mathbb{E} [|\bar{x}_t|^2] + (2b\gamma - 2 - b\eta) \mathbb{E} [|\bar{v}_t|^2] = \mathbb{E} [\langle \xi_t, D_1 \xi_t \rangle],$$

with the matrix

$$D_1 = d_1 \begin{bmatrix} \mathbb{I}_d & -d_2 \mathbb{I}_d \\ -d_2 \mathbb{I}_d & d_2^2 (1 + d_3) \mathbb{I}_d \end{bmatrix},$$

where $d_i > 0$, $i = 1, 2, 3$, are given explicitly by

$$d_1 = \frac{2 - (2+b)\eta}{b+\gamma}, \quad d_2 = \frac{1}{\sqrt{b(b+\gamma)-1}}, \quad d_3 = \frac{b+\gamma}{d_1} (2b\gamma - 2 - b\eta).$$

Similarly, the last term may be reformulated to read

$$\frac{\eta}{2} \left(b + \frac{1}{2+b} \right) \frac{1}{h(t)} \int_{t-h(t)}^t \mathbb{E} [|\bar{x}_s|^2] ds = \frac{1}{h(t)} \int_{t-h(t)}^t \mathbb{E} [\langle \xi_t, D_2 \xi_t \rangle] ds,$$

with

$$D_2 = d_4 \begin{bmatrix} \mathbb{I}_d & -d_2 \mathbb{I}_d \\ -d_2 \mathbb{I}_d & d_2^2 \mathbb{I}_d \end{bmatrix}, \quad d_4 = \frac{(1+b)^2}{(2+b)(b+\gamma)} \frac{\eta}{2}.$$

At this point, we clearly see the conditions on the parameters b, γ and η , such that Q becomes a positive quadratic form. More concretely, we require that

$$(6.70) \quad b(b+\gamma) > 1, \quad 2 > (2+b)\eta, \quad 2b\gamma > 2 + b\eta,$$

which guarantees that $d_i > 0$. Reformulating the inequalities for η and b provides the conditions

$$0 < \eta < 1 + \gamma - \sqrt{1 + \gamma^2}, \quad \frac{1}{2\gamma - \eta} < \frac{b}{2} < \frac{1 - \eta}{\eta}.$$

Continuing where we left off, we reformulate the inequality for $\mathcal{J}_t$ in terms of

ξ_t to obtain

$$\begin{aligned}
\frac{d}{dt} \mathcal{J}_t &\leq -d_1 \left(\mathbb{E} [|\xi_{1,t}|^2] - 2d_2 \mathbb{E} [\langle \xi_{1,t}, \xi_{2,t} \rangle] + d_2^2 (1 + d_3) \mathbb{E} [|\xi_{2,t}|^2] \right) \\
&\quad + \frac{1}{h(t)} \int_{t-h(t)}^t d_4 \left(\mathbb{E} [|\xi_{1,s}|^2] - 2d_2 \mathbb{E} [\langle \xi_{1,s}, \xi_{2,s} \rangle] + d_2^2 \mathbb{E} [|\xi_{2,s}|^2] \right) ds \\
&\leq -d_1 \left((1 - \epsilon) \mathbb{E} [|\xi_{1,t}|^2] + d_2^2 (1 + d_3 - 1/\epsilon) \mathbb{E} [|\xi_{2,t}|^2] \right) \\
&\quad + \frac{1}{h(t)} \int_{t-h(t)}^t d_4 (1 + d_2^2) \mathbb{E} [|\xi_s|^2] ds.
\end{aligned}$$

We now choose $\epsilon > 0$ such that $(1 - \epsilon) = (1 - d_3 - 1/\epsilon)d_2^2$, which gives

$$\epsilon = \frac{1}{2} \left(1 - (1 + d_3)d_2^2 + \sqrt{4d_2^2 + (1 - (1 + d_3)d_2^2)^2} \right).$$

Consequently, we obtain

$$(6.71) \quad \frac{d}{dt} \mathcal{J}_t \leq -\lambda_1 \mathcal{J}_t + \lambda_2 \frac{1}{h(t)} \int_{t-h(t)}^t \mathcal{J}_s ds,$$

with

$$\lambda_1 = \frac{d_1}{2} \left(1 + (1 + d_3)d_2^2 - \sqrt{4d_2^2 + (1 - (1 + d_3)d_2^2)^2} \right), \quad \lambda_2 = d_4(1 + d_2^2).$$

This gives the differential inequality

$$(6.72) \quad \frac{d}{dt} \mathcal{J}_t \leq -\lambda_1 \mathcal{J}_t + \lambda_2 \sup_{s \in [t-h(t), t]} \mathcal{J}_s,$$

The goal, now, is to find $b > 0$, such that λ_1 is maximized. To do so, we begin by setting $\eta \equiv 0$. In this case, we have that

$$d_1 = 2/(b + \gamma), \quad d_3 = (b + \gamma)^2(b\gamma - 1), \quad \lambda_2 \equiv 0,$$

which consequently yields,

$$\lambda_1 = \gamma - \frac{1}{b + \gamma} \sqrt{4d_2^2 + (2 - \gamma(b + \gamma))^2} = \gamma - \sqrt{\frac{(2 - b\gamma)^2 + (b\gamma - 1)\gamma^2}{b(b + \gamma) - 1}},$$

Therefore, maximizing in b for λ_1 gives

$$(6.73) \quad b = \frac{2}{\gamma}, \quad \lambda_1 = \gamma \left(1 - \sqrt{\frac{\gamma^2}{4 + \gamma^2}} \right).$$

This particular choice of $b > 0$ clearly satisfies the inequalities (6.70). We now proceed to find conditions on $\eta > 0$ such that $\lambda_1 > \lambda_2$ is satisfied. Assuming that

$$(\gamma(1 - \eta) - \eta) > 0 \quad \Longleftrightarrow \quad 0 < \eta < \gamma/(1 + \gamma),$$

we have that $\lambda_i > 0$, where λ_i for $i = 1, 2$ are given by

$$(6.74) \quad \lambda_1 = \gamma - \left(1 + \frac{2\gamma}{4 + \gamma^2} \right) \eta - \frac{\gamma}{4 + \gamma^2} \sqrt{4\eta^2 + (4 + \gamma^2)(\gamma - \eta)^2},$$

$$(6.75) \quad \lambda_2 = \frac{(2 + \gamma)^2}{(1 + \gamma)(4 + \gamma^2)} \frac{\eta}{2}.$$

To further ensure that $\lambda_1 > \lambda_2$, we choose η satisfying such that

$$0 < \eta \leq \frac{2\gamma}{3(1 + \gamma)} =: \bar{\eta}.$$

Finally, we apply Proposition 6.1 (cf. Remark 8) onto (6.72) to obtain

$$(6.76) \quad \text{dist}_Q(\mu_t, \hat{\mu}_t) \leq \mathbb{E}[Q(z_t - \hat{z}_t)] \leq \mathbb{E}[Q(z_0 - \hat{z}_0)] \exp(-\lambda t) \quad \text{for } t \geq 0,$$

with

$$\lambda = \lambda_1 - \frac{1}{H} W(\lambda_2 H \exp(\lambda_1 H)).$$

Optimizing (6.76) over all joint distributions of the random variables z_0 and $\hat{z}_0$ with marginals μ_0 and $\hat{\mu}_0$ respectively provides the required estimate (6.67), thereby concluding the assertion. $\square$

In the case without delay [12], one recovers the equilibrium measure μ_∞ by (formally) passing to the limit $t \rightarrow \infty$. In this case, μ_∞ is required to satisfy the stationary equation

$$v \cdot \nabla_x \mu_\infty + S[\mu_\infty] = \nabla_v \cdot (\sigma \nabla_v \mu_\infty + \gamma v \mu_\infty),$$

where the operator S , defined in (6.63), reduces to the form

$$S[\mu_\infty] = -\nabla_x V \cdot \nabla_v \mu_\infty - \nabla_v \cdot \left[\left(\int_{\mathbb{M}} \nabla U(\cdot - \hat{x}) \mu_\infty(d\hat{x}, d\hat{v}) \right) \mu_\infty \right].$$

Evidently, an equilibrium measure of the non-retarded case is also an equilibrium measure of the retarded one and thus, also a solution of (6.66). Using Proposition 6.3, we can now prove the exponential convergence of any solution of (6.66) towards the equilibrium measure μ_∞ under Assumption 1 and for sufficiently small c_g and c_B .

Theorem 10. *Under the assumptions of Proposition 6.3, there exists a constant $c > 0$ such that*

$$(6.77) \quad \text{dist}_2(\mu_t, \hat{\mu}_t) \leq c \exp(-\lambda t) \text{dist}_2(\mu_0, \hat{\mu}_0) \quad \text{for } t \geq 0,$$

for all solutions $(\mu_t)_{t \geq 0}$ and $(\hat{\mu}_t)_{t \geq 0}$ to (6.66) with initial data $\mu_0, \hat{\mu}_0 \in \mathcal{P}_2(\mathbb{M})$, respectively.

Moreover, (6.66) has an equilibrium measure $\mu_\infty \in \mathcal{P}_2(\mathbb{M})$ such that

$$(6.78) \quad \text{dist}_2(\mu_t, \mu_\infty) \leq c \exp(-\lambda t) \text{dist}_2(\mu_0, \mu_\infty) \quad \text{for } t \geq 0,$$

for any solution $(\mu_t)_{t \geq 0}$ of (6.66), where the decay rate λ is as given in Proposition 6.3.

We conclude the subsection with a discussion of the decay rates. We begin by rewriting the decay rate (6.68) as

$$\lambda(\hat{H}) = \lambda_1(1 - W(\hat{\lambda}\hat{H} \exp(\hat{H}))/\hat{H}),$$

with $\hat{H} = \lambda_1 H$ and $\hat{\lambda} = \lambda_2/\lambda_1$ with $0 < \hat{\lambda} < 1$. Using the facts that $W(0) = 0$, $W'(0) = 1$ and $W(x) \sim \ln(x)$ as $x \rightarrow \infty$, we observe that

$$\lambda(0) = \lambda_1(1 - \hat{\lambda}) = \lambda_1 - \lambda_2, \quad \lim_{\hat{H} \rightarrow \infty} \lambda(\hat{H}) = 0.$$

Moreover, a simple computation gives that $\lambda = \lambda(\hat{H})$ is strictly monotonically decreasing with respect to $\hat{H}$ for $\hat{H} > 0$.

In Figure 15 we plot the region of those values which η can attain for given values of γ . More precisely, we plot the domain $0 \leq \eta \leq \bar{\eta}(\gamma)$ with $\bar{\eta}(\gamma) = 2\gamma/(3 + 3\gamma)$ as in the proof of Proposition 6.3. Moreover, the line $\eta = \gamma/(2 + 2\gamma)$ is plotted. This relation is used in the following for comparison, where we discuss the influence of the parameters η, γ and H on the decay rate λ in more detail.

The non-retarded case $H = 0$. For $\eta = 0$, the system reduces to a non-interacting system and we recover known results with the explicit decay rate

$$\lambda(\gamma) = \gamma \left(1 - \sqrt{\frac{\gamma^2}{4 + \gamma^2}} \right),$$

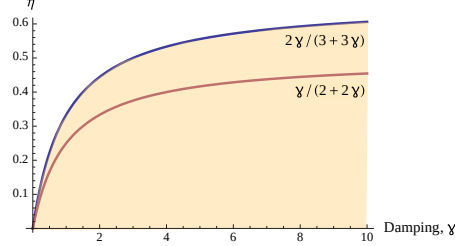


Fig. 15. Region of validity $\eta \in [0, \bar{\eta}(\gamma)]$ and typical relations of η to γ .

depicted in Figure 16 on the left. See for example [32] for more details on the investigation of such systems. The decay rate is maximal when $\gamma = (2(\sqrt{5} - 1))^{1/2}$. The case $\eta > 0$ recovers the estimates shown in [12], however, here we obtain the explicit form of $\lambda = \lambda(\gamma)$. In order to guarantee convergence towards the unique equilibrium state μ_∞ , the Lipschitz constants c_g and c_B of the potentials are required to satisfy $\eta = c_g + 2c_B \leq \bar{\eta}(\gamma)$. To illustrate, we assume for simplicity that the relation between η and γ is either $\eta = 2\gamma/(3+3\gamma)$ or $\eta = \gamma/(2+2\gamma)$, which both satisfy $\eta \leq \bar{\eta}(\gamma)$ (cf. Figure 15). This leads to the decay rates shown in Figure 16 on the right.

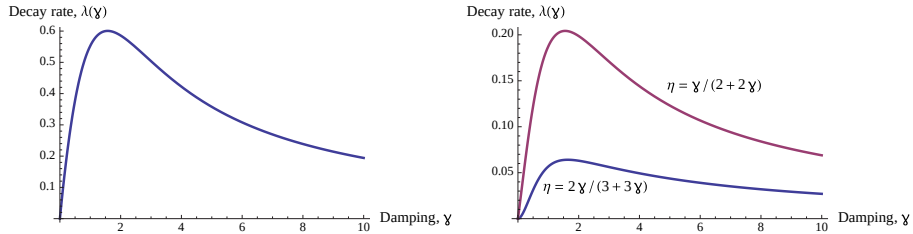


Fig. 16. Decay rates for $H = 0$ without interaction $\eta \equiv 0$ and for various $\eta = \eta(\gamma)$.

The retarded case $H \in (0, \infty)$. As mentioned before, the decay rate decreases monotonically with increasing H . This can be also seen in Figure 17 on the left. Here, we choose $\gamma = 1$, $\eta = \gamma/(2+2\gamma)$ and vary $H \in (0, \infty)$. Similarly, Figure 17 on the right shows the decay rates for different delays H , with varying γ , where for each γ , we observe a qualitative behavior of the decay rates as for the non-retarded case.

The retarded case $H = \infty$. In this part, we provide a quantitative convergence result for all solutions of the delay Vlasov–Fokker–Planck equation

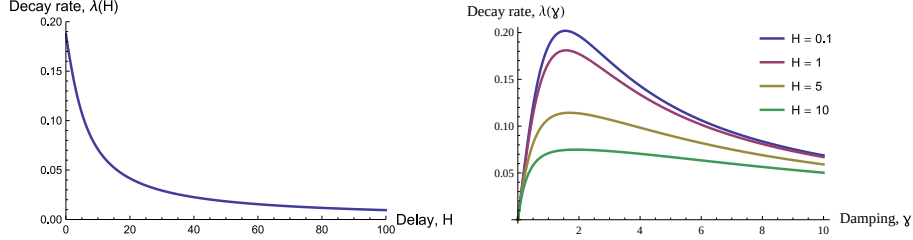


Fig. 17. Dependence of decay rate on delay H and decay rates for various delays H . With delay $H > 0$ and interaction $\eta(\gamma) = \gamma/(2 + 2\gamma)$.

(6.66) with an infinite cut-off, i.e., $h(t) = t$, associated to the microscopic system (6.59). As discussed at the beginning of the subsection and observed in Figure 17A, an increase in H reduces the decay rate. In particular, we have that $\lambda \rightarrow 0$ as $H \rightarrow \infty$. In this case, our estimates do not yield an exponential convergence rate. Fortunately, in the present case we are still able to prove an algebraic (in time) convergence result, which we elucidate in the following discussion.

Our starting point is the differential inequality (6.71). In the present situation, this reads

$$(6.79) \quad \frac{d}{dt} \mathcal{J}_t \leq -\lambda_1 \mathcal{J}_t + \lambda_2 \frac{1}{t} \int_0^t \mathcal{J}_s ds.$$

Consider some function $\phi = \phi(t)$ satisfying the equality

$$(6.80) \quad \frac{d\phi}{dt}(t) = -\lambda_1 \phi + \lambda_2 \frac{1}{t} \int_0^t \phi(s) ds.$$

This leads to

$$\mathcal{J}_t \leq \phi(t) \quad \text{for all } t \geq 0.$$

Therefore, investigating the asymptotic behavior of equation (6.80) gives us the desired decay property for the retarded mean-field equation (6.66) with an infinite cut-off.

Reformulating equation (6.80), we obtain

$$(6.81) \quad \frac{d}{dt} \left(t \frac{d\phi}{dt} \right) = -\lambda_1 \frac{d}{dt} (t\phi) + \lambda_2 \phi,$$

or equivalently

$$(6.82) \quad t \frac{d^2 \phi}{dt^2} + (1 + \lambda_1 t) \frac{d\phi}{dt} + (\lambda_1 - \lambda_2) \phi = 0.$$

Rescaling time $\tau = \lambda_1 t$ and substituting $u(\tau) = e^\tau \phi(\tau)$ leads to Kummer's equation

$$(6.83) \quad \tau \frac{d^2 u}{d\tau^2} + (1 - \tau) \frac{du}{d\tau} - \hat{\lambda} u = 0,$$

where $\hat{\lambda} = \lambda_2/\lambda_1 \in [0, 1)$.

For the present parameters, we obtain an asymptotic behavior of the form [1]

$$u(\tau) = \frac{1}{\Gamma(\hat{\lambda})} \tau^{\hat{\lambda}-1} e^\tau + \frac{(-1)^{-\hat{\lambda}}}{\Gamma(1-\hat{\lambda})} \tau^{-\hat{\lambda}} + \mathcal{O}(\tau) \quad \text{as } \tau \rightarrow \infty.$$

This gives

$$\phi(\tau) = \frac{1}{\Gamma(\hat{\lambda})} \tau^{\hat{\lambda}-1} + \mathcal{O}(\exp(-\tau)) \quad \text{as } \tau \rightarrow \infty.$$

Transforming back to the t variable, we obtain an asymptotic behavior for $\phi = \phi(t)$

$$\phi(t) - \frac{\lambda_1^{\hat{\lambda}-1}}{\Gamma(\hat{\lambda})} \frac{1}{t^{1-\hat{\lambda}}} = \mathcal{O}(\exp(-\lambda_1 t)) \quad \text{as } t \rightarrow \infty.$$

In this way we obtain an algebraic decay, in contrast to the exponential decay for finite cut-off, which we summarize in the following statement.

Theorem 11. *Under Assumption 1, for any $\gamma > 0$, there exist constants $c > 0$ and $\bar{\eta} = \bar{\eta}(\gamma) > 0$ such that for any $c_g, c_B \geq 0$ with $\eta := c_g + 2c_B \leq \bar{\eta}$, the decay estimate*

$$(6.84) \quad \text{dist}_Q(\mu_t, \hat{\mu}_t) \leq \frac{c}{t^{1-\hat{\lambda}}} \text{dist}_Q(\mu_0, \hat{\mu}_0) \quad \text{for } t \gg 1 \text{ sufficiently large,}$$

with $0 < \hat{\lambda} = \lambda_2/\lambda_1 < 1$ holds true for any solution $(\mu_t)_{t \geq 0}$, $(\hat{\mu}_t)_{t \geq 0}$ of (6.66) with $h(t) = t$ and corresponding initial data $\mu_0, \hat{\mu}_0 \in \mathcal{P}_2(\mathbb{M})$. Here λ_i , $i = 1, 2$ are given in (6.74).

7 - Applications

In this section we consider a special application, a so called airlay process. In airlay processes the fibers leave from a rotating drum into a turbulent air flow. Suctioning onto a perforated moving conveyor belt leads to the forming of a random three-dimensional fiber web structure. Additionally to the microstructure generation (Sec. 7.3) where models discussed in the previous sections are used, we consider a fiber-loaded turbulent flow simulation (Sec. 7.2) and the effective material description and investigation (Sec. 7.4). The models are applied to the industrial airlay process scenario that is specified in Sec. 7.1 as reference case. For details we refer to [41].

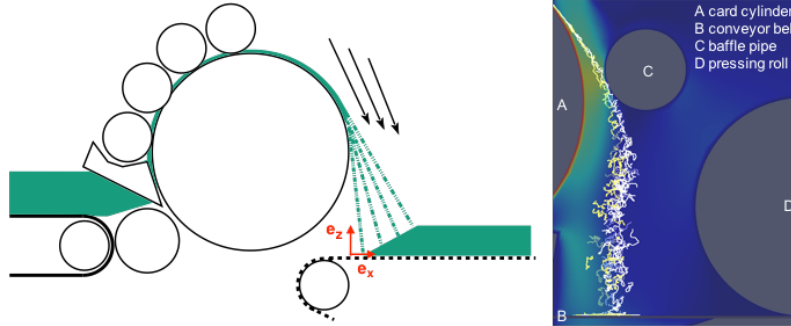


Fig. 18. *Left*: Sketch of the airlay process. *Right*: Illustration of the aerodynamic web forming zone with fiber-loaded flow. The air flow is colored by the mean velocity magnitude.

7.1 - Industrial airlay process, reference scenario

A typical airlay process with the rotating card cylinder, the aerodynamic web forming zone and the conveyor belt is sketched in Fig. 18. For the process description we introduce a fixed Cartesian coordinate system $\{e_1, e_2, e_3\}$ in $\mathbb{R}^3$ with respect to the machinery, whose origin is centered on the conveyor belt below the fibers' dropping. We refer to the machine direction (MD) e_1 and its cross direction (CD) e_2 , where the conveyor belt lies in the MD-CD plane ($z = 0$). The associated MD and CD cut planes are given by $y = \text{const}$ and $x = \text{const}$, respectively. Apart from boundary effects the process properties are homogeneous in CD. For details on the machine manufacturer we refer again to [41]. As entering fiber material a mixture of 70% solid fibers and 30% so called bicomponent fibers made from two different materials. is considered. The mixing ratios refer to the mass. The fibers are homogeneous with circular cross-sections, their properties as well as the machine properties can be found in [41]. In post-processing the nonwoven material is reinforced by thermobonding where the bicomponent fibers have an adhesive effect.

7.2 - Process simulation

The core of the aerodynamic web forming is the dilute suspension behavior of flexible fibers in the turbulent flow. The random microstructure is essentially determined by the fibers' deposition, i.e., the distribution of the fibers on the conveyor belt as well as their characteristic geometrical lay-down properties. The fiber-loaded turbulent flow is a multi-scale two-phase problem in a complex geometry. Direct numerical simulation based on first principles model as well

as approaches like immersed boundary or fictitious boundary/domain are well investigated for fluid-structure problems, but their applicability is practically limited to laminar flows and a small number of suspended solids due to the required high computational demands (from the broad existing literature see, e.g., [36, 49, 65, 71, 73, 75]). For flows with a high particle load kinetic modeling approaches have been established, leading to coupled Navier-Stokes Fokker-Planck systems (see [6] and reference therein). However, these approaches do not cover flexible fibers with infinitely many degrees of freedom. In [62] a fiber is modeled asymptotically as elastic Kirchhoff beam that is capable of large, geometrically nonlinear deformations and driven by a stochastic aerodynamic drag force due to the surrounding turbulent flow field. The flow is specified by a statistic k - ϵ turbulence model. To simplify the situation we neglect here fiber-fiber interactions as well as the fibers' impact on the turbulent flow.

According to the Cosserat theory [5] a slender fiber can be asymptotically represented by a time-dependent curve (e.g., its center-line) $r : \mathcal{I} \times \mathbb{R}_0^+ \rightarrow \mathbb{R}^3$ with material parameter $s \in \mathcal{I} = [0, \ell]$ and time $t \in \mathbb{R}_0^+$. Its dynamics due to inertia and bending, driven by turbulence can be described for fiber curve, velocity and tangential traction (r, v, N) by the following constrained partial differential equations with multiplicative Gaussian space-time noise [52, 62]

$$(7.85) \quad \begin{aligned} \partial_t r &= v, & \|\partial_s r\| &= 1 \\ (\rho A) \partial_t v &= \partial_s (N \partial_s r - \partial_s ((EI) \partial_{ss} r)) + f(r, v, \partial_s r; u) \\ &+ A(r, v, \partial_s r; u, k, \epsilon) \cdot \partial_{st} W, \end{aligned}$$

supplemented with appropriate initial and boundary conditions, where (ρA) and (EI) denote the fiber line density (titer) and bending stiffness. The unknown traction $N : \mathcal{I} \times \mathbb{R}_0^+ \rightarrow \mathbb{R}$ is the Lagrange multiplier to the pointwise inextensibility constraint $\|\partial_s r\| = 1$. The corresponding deterministic system is known as Kirchhoff beam (or Kirchhoff-Love equations), it results from the Cosserat rod model in the asymptotic limit when the slenderness parameter and the typical Mach number vanish. Crucial for the dynamic fiber behavior are the aerodynamic drag forces that depend locally on the angle of attack (fiber tangent) and the relative velocity between fluid flow and fiber. Applying the stochastic force model by [62], we presuppose an underlying statistic k - ϵ turbulence description that provides the mean flow velocity $u : \mathbb{R}^3 \times \mathbb{R}_0^+ \rightarrow \mathbb{R}^3$. Additionally, it characterizes the turbulent flow fluctuations by the kinetic turbulent energy k and the dissipation rate ϵ , i.e., $k, \epsilon : \mathbb{R}^3 \times \mathbb{R}_0^+ \rightarrow \mathbb{R}$. The drag forces are composed of the mean f in a parametric dependence on the mean flow velocity u and of a fluctuating part. The fluctuations are modeled as Gaussian space-time white noise with the vector-valued Wiener process

($W : \mathcal{I} \times \mathbb{R}_0^+ \rightarrow \mathbb{R}^3$) and the tensor-valued amplitude A that carries the correlation structure of the turbulence via a parametric dependence on the flow quantities u , k and ϵ . For details we refer to [62].

Fiber-flow computations at industrial scale require a highly efficient numerical performance. We use the commercial CFD software² ANSYS Fluent for the flow and the licensable research software³ FIDYST for the fiber simulations. For the numerics of the constrained stochastic fiber system we refer to [41].

The fibers leave the rotating card cylinder continuously over time according to the machine's mass rate (Fig. 18). They are suctioned onto the conveyor belt by the downwards directed turbulent air flow. The turbulent flow fluctuations cause the fibers to swirl and to form a random web. We are interested in the fibers' distribution on the conveyor belt and their characteristic geometrical lay-down properties as starting point for generating the resulting nonwoven material by means of a stochastic surrogate lay-down model. We note that the airlay process parameters are constant over time and all characteristic (statistic) properties are homogeneous in CD, apart from negligible boundary effects.

Consider the fixed Cartesian coordinate system $\{e_1, e_2, e_3\}$ of the machinery, whose origin is located in the middle of the conveyor belt below the fiber dropping (cf. Sec. 7.1) and let g denote the probability density function for the lay-down MD positions.

To obtain a representative deposition behavior of the two different fiber types used in the airlay process, we compute the turbulence-driven three-dimensional dynamics of bicomponent and solid fibers. Each fiber enters the flow domain from the release center at time $t = 0$ as straight stress-free body that is oriented tangentially to the machine geometry and has the effective speed of the card cylinder. The fiber ends are treated as stress-free over time, i.e., $\partial_{ss}r(s, t) = \partial_{sss}r(s, t) = 0$, $N(s, t) = 0$ for $s \in \{0, \ell\}$, $t \geq 0$, until the fiber reaches the conveyor belt. To account for the deposition of many fibers within a short time period we realize the laying down by a modification of the boundary conditions instead of using Coulomb friction: as soon as the fiber comes in contact with the conveyor belt, the fiber point is fixed and transported with the belt speed. Figure 19 shows the different dynamic behavior of the bicomponent and solid fibers. The solid fibers are less affected by the turbulent flow. Their deposition range is smaller, more pronounced and further away from the card cylinder. In contrast, the dynamics of the lighter bicomponent fibers is more diffused. The lay-down distributions of the two fiber types on the conveyor belt are presented in Fig. 20. The figure particularly shows the distribution

²www.ansys.com

³www.itwm.fraunhofer.de. FIDYST is a software tool for fiber dynamics simulations, developed by the Fraunhofer ITWM, Germany.

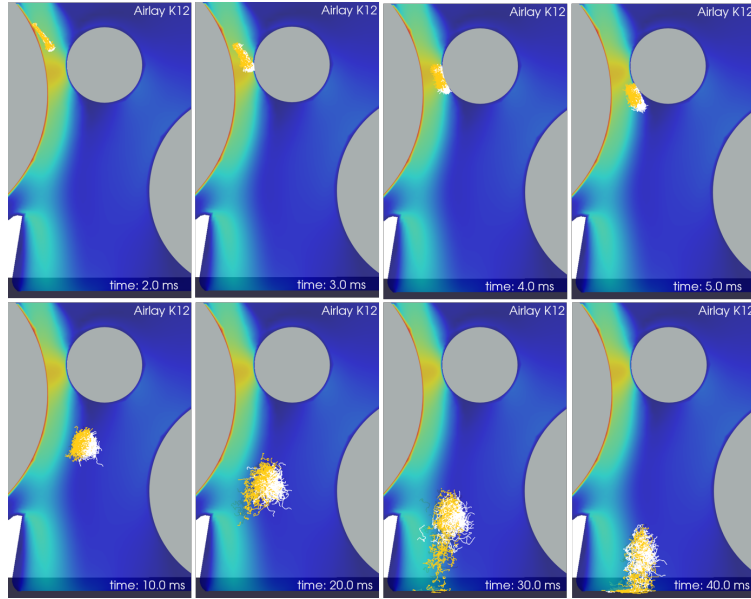


Fig. 19. Typical fiber dynamics. Visualization of 100 bicomponent fibers (orange) and 100 solid fibers (white) that enter simultaneously the aerodynamic web forming zone and move over time. In the background the air flow is colored with the velocity magnitude.

for the MD position of the fiber point that entered the flow domain at first in time, the distribution function is approximated by the superposition of the point measures.

7.3 - Virtual microstructure generation

The produced nonwoven consists of millions of fibers. We are interested in its material properties that are determined by the microstructure (Fig. 21). Since the described simulations of single elastic fibers in the turbulent air flow are computationally expensive and very time-demanding due to the huge amount of physical details, we introduce a surrogate model for the efficient virtual three-dimensional web generation. We describe the random topology of the microstructure by help of a stochastic lay-down model in the spirit of the previous sections, see also [44, 54], whose parameters are calibrated using the representative process simulation described in the previous subsection and computer tomography data.

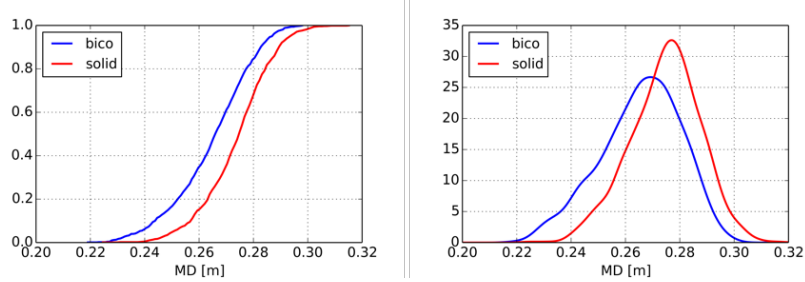


Fig. 20. Probability distribution function G (left) and density g (right) of the lay-down MD position for the two fiber types, $G(x) = \int_{-\infty}^x g(x') dx'$. The MD position is given in the fixed coordinate system of the machinery.

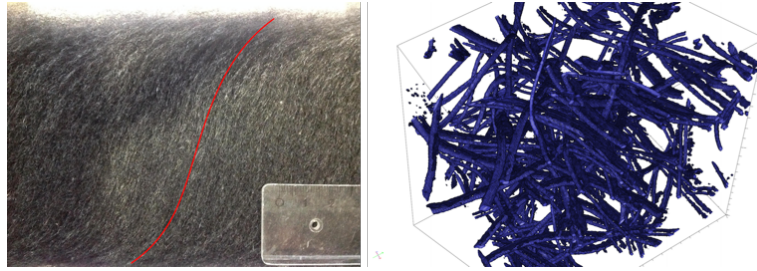


Fig. 21. Nonwoven material sample after thermobonding. *Left*: Photo (MD cut plane), ramp-like contour line in microstructure. *Right*: Computer tomography scan of a sample section, visualization by Fraunhofer ITWM, Department Image Processing.

Random fiber web. The nonwoven is the deposition image of the fibers. A striking characteristic in the microstructure is a ramp-like contour surface, see Fig. 21 for a photo of a nonwoven sample. After the aerodynamic web forming the nonwoven material is thermobonded in a post-processing step. As result of heating the bicomponent fibers melt and glue the random individual fibers together to a solid fiber network which is then explored in material testing. Our strategy is to use the contour surface that results from the lay-down probability densities as basis for a stochastic modeling of the three-dimensional deposition image. Then, we identify the contact points of the fibers in the random web, specify the adhesive joints and generate the net topology by help of a graph where the adhesive joints are interpreted as nodes and the fibers as edges.

We describe the contour line of the fiber material on the conveyor belt in MD by the graph of $R : \mathbb{R} \rightarrow [0, H]$,

$$(7.86) \quad R(x) = H \int_{-\infty}^x r(x') dx'$$

with

$$r(x) = \beta_1 g_1(x) + \beta_2 g_2(x), \quad \beta_1 + \beta_2 = 1,$$

where $H > 0$ denotes the height of the nonwoven and r is the joined probability density of the deposited material, $\text{supp}(r) = [x_{\min}, x_{\max}]$. In particular, g_1 and g_2 are the MD lay-down density functions of the two different fiber types that are obtained from the process simulation (cf. Fig. 20). The weights β_j can be determined either with respect to the number ratio or the mass ratio of the fiber types. Since the nonwoven is homogeneous in CD in $\mathcal{H}$, the contour line R implies a contour surface in the microstructure (Fig. 21).

Aiming for the three-dimensional nonwoven microstructure to investigate the material properties, we consider a cubic sample volume $[-d/2, d/2]^2 \times [0, H]$ over the nonwoven of height H with base area d^2 . The microstructure is formed by the fibers' falling onto the conveyor belt according to the contour surface (graph of R) and the given process mass rate, while the belt moves with speed v_B . To account for the belt motion we introduce a coordinate $x_B = x_B(t)$ moving with the belt velocity v_B .

We identify a deposited fiber with the lay-down time t and MD-/CD-coordinates (X, Y) of its end point, i.e., (X, Y, t) with X being g_j -distributed and Y uniformly distributed in $[-d/2, d/2]$. If especially $X - x_B(t) \in [-d/2, d/2]$ is satisfied, the deposited fiber contributes to the sample. We model the fiber in the three-dimensional web as stochastic process in terms of the curve (e.g., its centerline) $\eta^{(X, Y, t)}$ with

$$(7.87) \quad \eta_s^{(X, Y, t)} = \mathcal{R}(X) \cdot x_s + (X - x_B(t))e_1 + Y e_2 + R(X)e_3$$

with $\mathcal{R}(X) \in \text{SO}(3)$ defined such that it takes the local orientation of the tangential surface of the structure into account. Neglecting interactions, x_s is defined by the the stochastic Stratonovich differential system

$$(7.88) \quad dx_s = \tau_s ds$$

$$(7.89) \quad d\tau_s = -\frac{1}{B+1} \left((n_{1,s} \otimes n_{1,s} + B n_{2,s} \otimes n_{2,s}) \nabla V(x_s) ds \right. \\ \left. + A(n_{1,s} \otimes n_{1,s} + \sqrt{B} n_{2,s} \otimes n_{2,s}) \circ dW_s \right)$$

with $x_0 = 0$ and τ_0 uniformly distributed in the unit circle spanned by e_1 and e_2 . By construction, a fiber end point lies on the contour surface and the main fiber orientation is aligned to it. The underlying stochastic process $((x, \tau) : \mathcal{I} \rightarrow \mathbb{R}^3 \times \mathbb{S}^2)$ in (7.88) is the three-dimensional anisotropic lay-down model for fiber position and orientation around the MD-CD plane discussed in

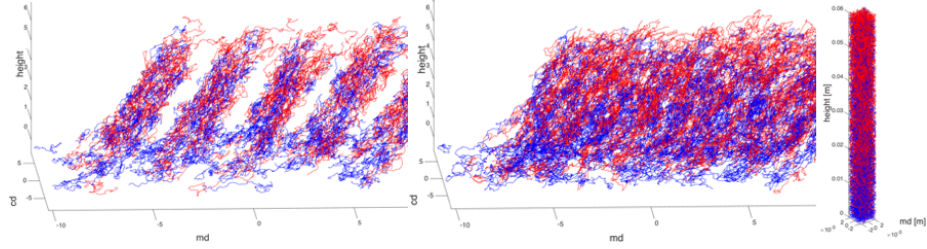


Fig. 22. Virtual deposition image with contour surface according to MD lay-down distributions (7.86) and calibrated surrogate fiber models (7.88). The numbers of bicomponent fibers (blue) and solid fibers (red) are scaled down for visualization issues. Axes units in $[10^{-2}\text{m}]$.

the first section, see also [44, 54]. It presents the path of a deposited fiber as image of an arc-length parameterized curve that is influenced by various (airlay) process parameters. The drift term with the potential V describes the typical coiling behavior of the fibers, i.e., $V(x) = x \cdot C^{-1} \cdot x / 2$ with $C = \text{diag}(\sigma_1^2, \sigma_2^2, \sigma_3^2)$ regarding the machinery coordinates. In particular, $\sigma_1, \sigma_2 \geq 0$ denote the standard deviations of the fiber throwing onto the conveyor belt in MD and CD, and $\sigma_3 > 0$ assures a height constraint. Accounting for the fluctuations in the airlay process, the drift is superposed by a white noise with a vector-valued Wiener process (W) and the scalar amplitude A . The parameter $B \in [0, 1]$ indicates the anisotropic behavior with the local orthonormal right-handed director triad $\{\tau, n_1, n_2\}$ where $n_1 \in \text{span}(e_1, e_2)$, i.e., isotropy for $B = 1$, asymptotic reduction to two-dimensional planar lay-down [14, 37] for $B = 0$.

We note that on microscale the fibers are also characterized by a crimp with a crimp number $C \in \mathbb{N}_0$ (bows per unit length). The crimp can be incorporated in the surrogate lay-down model, see [41].

Superposing bicomponent and solid fibers according to their MD lay-down distributions, number ratio and calibrated model parameters results in a virtual fiber web. To obtain the thermobonded nonwoven, the adhesive joints in the web are detected by help of a contact threshold $a \geq 0$ and the net topology is set up in terms of a graph. Details to the strategies and algorithms are given in the following subsections. For the identification of the parameters of the surrogate model (7.88) we refer again to [41].

Using such a calibrated model Figure 22 shows the fiber deposition image associated to the reference scenario.

Detection of adhesive joints. The microstructure of the thermobonded nonwoven is the random web of the deposited fibers that is glued together by the bicomponent fibers. In terms of graph theory the random net topology

can be represented by a graph, where the adhesive joints are considered as the nodes and the fiber curves as the edges.

For the identification of adhesive joints in the web (Fig. 22, right), we restrict our search to the fiber points that are associated to the spatial discretization of the individual fibers (in the lay-down model) as possible contact points. As we deal with plenty of fibers, a direct pointwise comparison would be computationally too expensive. The bounding box method that is well-known from computer graphics meets our demands on efficiency. For details and more sophisticated methods we refer to [23, 35] and references therein. We embed each fiber in a box aligned to the coordinate axes and check pairwise if the boxes intersect or not. If the intersection is empty, there are obviously no contact points. Otherwise, we restrict on the fiber parts in the intersection box and iterate the procedure. Finally, two cases can occur: either the intersection of the bounding boxes keeps unchanged or the number of fiber points in the intersection is sufficiently small. In both cases the naive pairwise computation of distances between the sets of fiber points belonging to two different fibers is used to detect possible contact points. Two fibers are considered to be in contact, if their distance is smaller than some contact threshold $a \geq 0$ which has to be chosen appropriately. In case that a bicomponent fiber is involved in the contact, we refer to the contact as adhesive joint. The adhesive joints act as nodes in the resulting fiber network. Figure 23 shows the fiber net topology before and after contact detection.

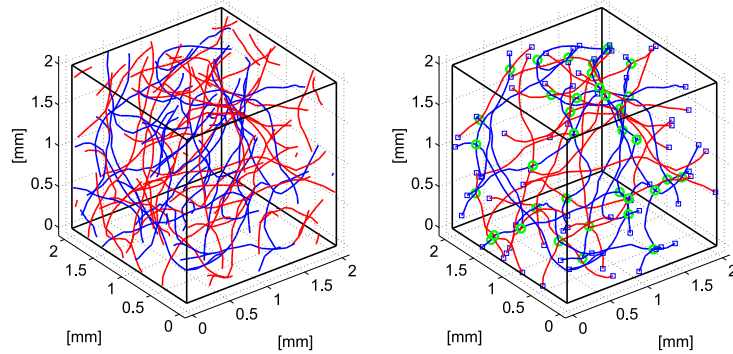


Fig. 23. Fiber net topology before (*left*) and after (*right*) contact detection with $a = 10^{-5}$ [m]. Bicomponent fibers are colored in blue, solid fibers in red. The adhesive joints are marked by the green circles, the fibers' end points by the squares.

7.4 - *Elastic fiber net and effective nonwoven material behavior*

On top of the above we model the fiber associated material properties using again a Cosserat model. The resulting Cosserat network provides the basis for our virtual material investigations. We refer again to [41] for details.

This Cosserat network is finally used to simulate stress-strain relations for the resulting non-woven material. In the experimental tensile strength test the measured stress-strain curves for the thermobonded nonwoven material samples show a large volatility, in particular for increasing strains. The simulated stress-strain relations—that are computed on basis of the process model chain—match the experimental ones in principle. However, the simulation results are obviously affected by the model parameters for the fiber net like the topological contact threshold a or the material stiffness. Investigating, for example, the impact of the contact threshold a reveals a robust tensile behavior whereas changes of the net stiffness are very sensitive. A larger contact threshold a causes an increasing number of adhesive joints and hence a more connected net topology. This implies a stiffer material behavior which is seen in slightly steeper stress-strain curves. However, this effect is mainly restricted to small strains, the further behavior (shape) of the curves is unchanged. In the airlay process the contact threshold of the net is related to the post-processing step of thermobonding. Depending on process parameters, such as adhesive properties of the used fiber material, temperature and duration of the thermobonding, the threshold a could be calibrated from experimental data. To get a general understanding of the airlay process parameters a sensitivity analysis in combination with a broader experimental study is necessary. At last, the simulated stress-strain curves indicate generally a stiffer material behavior for higher strains than the measured curves. The reason might be that the net topology, in particular the adhesive joints, is kept in the simulation—even under large tensile forces, whereas the fiber web rips and undergoes plastic changes in the experiment. This discrepancy might be overcome by introducing an additional parameter, a damage threshold, in the elastic net model. Its calibration requires certainly information about the nature of the adhesive joints and hence a deeper investigation of the post-processing step of thermobonding.

8 - Conclusion and Outlook

In this review we did discuss mathematical aspects of fiber dynamics in fiber lay down processes for virtual technical textile production. After discussing the basic models based on stochastic differential equations and the corresponding kinetic or Fokker-Planck equations, we have presented a semi-Lagrangian

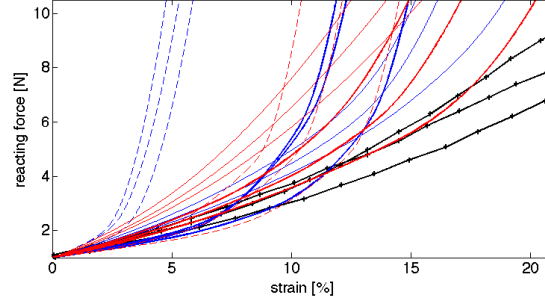


Fig. 24. Stress-strain results provided by measurements (black lines) and simulations for varying model parameters. For example, for higher contact threshold a the slopes of the curves are steeper.

scheme for the Fokker-Planck equations associated to the stochastic dynamical systems. Next, several approximate equations based on asymptotic expansions and moment expansions of the Fokker-Planck equation are presented and numerically investigated. Further we have extended the above models to a model, which captures the interaction between the fibers by using a system of retarded stochastic differential equations and their corresponding mean-field approximations. A theoretical investigation of the mean-field equation is included giving a systematic approach to determining explicit decay rates. In the last section, we did discuss a chain of mathematical models that enabled the simulation of a fiber airway process and the investigation of the material properties of the resulting nonwoven textile structures by virtual tensile strength tests. Proceeding from an process simulation with a highly turbulent dilute fiber suspension flow, we used the process parameters and the numerically obtained deposition results to set up the stochastic surrogate model for the microstructure generation.

Further research work from a mathematical point of view should include for example extension of the results on convergence to equilibrium for the interacting fiber case to spherical state space. For the long-term industrial objective, the simulation-based process design towards the prediction and improvement of product properties, the mathematical mapping between the parameters of process and material is essential. This requires in particular refined parameter identification strategies.

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