Hydrodynamic interactions between two semi-flexible in-extensible filaments in Stokes flow

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Hydrodynamic interactions between two semi-flexible in-extensible filaments are shown to have a significant impact on filament buckling and their subsequent motion in Stokesian fluids. In linear shear flow, hydrodynamic interactions lead to filament shear dispersion that depends on the filament slenderness and the initial filament separation. In linear extensional flow, hydrodynamic interactions lead to complex filament dynamics around the stagnation point. These results suggest that hydrodynamic interactions need to be taken into account to determine the self-diffusion of non-Brownian semi-flexible filaments in a cellular flow [1].

I. INTRODUCTION

Hydrodynamic interactions between rigid particles have significant effects on the macroscopic mechanical properties of their suspension. For example, hydrodynamic interactions between rigid fibers are crucial to the concentration instability observed in sedimenting fiber suspensions [2]. For suspension of rigid active fibers such as actuated swimmers, hydrodynamic interactions are found to help order the swimmers over short length scales, and have a significant impact on the mean swimming speed [3–5]. Recently hydrodynamic interactions between rigid spheres in a thin channel are found to lead to novel nonlinear patterns formation and dynamics [6].

When combined with particle deformability, hydrodynamic interactions affect both the individual particle dynamics and the macroscopic properties of the suspension. An example is the non-Brownian viscous drop suspensions in shear flow. Loewenberg and Hinch [7] use the boundary integral formulation to numerically investigate the effects of hydrodynamic interactions on dilute suspension of viscous drops in shear flow, and conclude that the hydrodynamic interaction and drop deformation conspire to suppress drop breakup during the collision process. The self-diffusion coefficients of the non-Brownian drops in a dilute sheared emulsion are obtained from trajectories of different collision processes between a pair of viscous drops, and are found to be anisotropic and dependent on the viscosity ratio and the shear rate. As a result, the mixing efficiency of drop suspensions is affected by the hydrodynamic interactions between deformable drops. Another example of hydrodynamic interactions effects on macroscopic properties of soft particle suspension is the semi-dilute vesicles suspension in a shear flow: Hydrodynamic interactions between vesicles give rise to strong fluctuations of vesicle shape and inclination angle [8]. The macroscopic viscosity of vesicle suspension is found to depend non-monotonically on the viscosity ratio between the inner and outer fluids of the vesicles.

The hydrodynamics of semi-flexible in-extensible filaments in viscous fluids has gained interest due to their close relevance in bio-fluids and micro-fluidics: Many semi-flexible biopolymers, such as DNA, cilia and flagella, are virtually in-extensible, and their dynamics in viscous fluids plays a central role in their motion [9–12]. New advances in micro-fabrication and micro-manipulation enable direct interaction with semi-flexible biopolymers in simplified in vitro environments, and stimulate more interest to investigate the dynamics of flexible bio-filaments. For example, optical tweezers are employed to periodically oscillate actin filaments connected to micron-sized beads, in order to devise an artificial
“one-armed swimmer.” [13]. Polymer-linked magnetic beads are used to design artificial swimmers that can be controlled in a magnetic field [14]. This novel design enables an easier control of the filaments through magnetic fields and has allowed quantitative measurements of the physical properties of the chains, such as their bending stiffness. Similar methodologies are applied to induce properties of the linker molecules [15] or the affinity of chemical contacts between polymer and particle coating from video microscopy [16]. Semi-flexible actin filaments are now used as nano-cargos in micro-fluidic devices for directed transport on chemically patterned surfaces [17]. Fabrication of synthetic ciliary arrays and technological applications of artificial swimmers are also new possibilities to be explored.

The aspect ratio (radius to length) of most semi-flexible in-extensible bio-polymers ranges from $10^{-5}$ to $10^{-1}$. The extreme filament slenderness justifies the slender-body formulation in Stokes flow, a very viscous flow with essentially zero Reynolds number. A significant amount of work has been devoted to the studies of a single elastic in-extensible filament in slender-body formulation [9, 18–20]. Recently the hydrodynamics of multiple filaments in Stokes flow has been investigated: Tornberg and Shelley [21] use the non-local slender-body model to numerically simulate dynamics of multiple (up to 25) interacting filaments in a background oscillating shear flow. Llopis et al. [22] investigate the effects of hydrodynamic interactions on the sedimentation of a pair of in-extensible filaments using the bead model. Dillon et al. [11] examine multiciliary interaction in a mucus layer using the immersed boundary method.

While sufficient progress has been made to understand the complex hydrodynamics of elastic filaments, quantitative detail of interacting semi-flexible filament dynamics remains incomplete. For example, how does a semi-flexible filament buckle under hydrodynamic interactions with other filaments in the neighborhood? Do the hydrodynamic interactions between two buckling filaments in shear flow cause filament self-diffusion as in the case of viscous drop suspension? How will HIs between non-Brownian elastic filaments in cellular flow affect the diffusive transport due to filament buckling around the stagnation points [1]? To gain fundamental insights into the complex interplay between filament self-diffusion, filament deformation and hydrodynamic interactions, it is useful to consider the dynamics of a pair of semi-flexible filaments in simple flows.

We will examine the effects of hydrodynamic interactions (HIs) between a pair of filaments in configurations where a single elastic in-extensible filament is known to exhibit buckling instability [1, 21]. We will examine how HIs induce differences in the buckling dynamics and the subsequent filament motion. For a single semi-flexible filament subject to a body force, different filament shape and dynamics are found as a result of both the non-local HIs and elasticity [23]. For a pair of sedimenting filaments, filament elasticity and non-local HIs conspire to cause interesting filament shapes and cooperative filament motion under gravity [22]. Our goal is to elucidate how such combination affects buckling of a pair of semi-flexible filaments in simple flows.

In particular, we will focus on the buckling dynamics of a pair of interacting filaments in two prototypical linear flows: planar shear flow and planar extensional flow. (1) Filaments in the plane of shear flow (in the $x$-direction) experience compressive stress only when rotating toward the cross-shear axis ($y$-axis). Special arrangements of filaments are chosen as initial conditions in the simulations for elucidating HI effects on buckling dynamics in shear flow. (2) Filaments in linear extensional flow experience compression when they move toward the stagnation point. Two filaments parallel to the compressional axis are initially placed on the opposite sides of the stagnation point. We will focus on how HIs affect filament buckling as they move toward the stagnation point in extensional flow. These
initial configurations allow us to gain quantitative insights into the roles of HIs in buckling of two interacting filaments.

The rest of the paper is organized as follows. In § II the slender-body formulation for interacting in-extensible elastic filaments immersed in Stokes flow is presented. The Hasimoto transformation is utilized to convert the integro-differential slender-body equations to a system of equations for the complex curvature of the filament centerlines [24]. The resultant system is numerically integrated using the numerical scheme summarized in § II A. We quantify HIs effects on the buckling dynamics of two filaments in time-independent, two-dimensional linear flows: In § III we summarize results from simulating a pair of semi-flexible filaments immersed in the plane of linear shear flow. In particular we focus on how HIs induce different buckling dynamics and cause filament dispersion in shear flow. In § IV we summarize results from simulating a pair of semi-flexible filaments moving toward each other around the stagnation point in extensional flow. HIs lead to novel dynamics of filaments in straining flow, and simulation data provide quantitative description of different filament dynamics. We also discuss how the non-local slender-body formulation needs to be modified to enforce the non-contact, non-crossing conditions for two filaments undergoing buckling instability. Finally in § V we present conclusions and discuss ongoing work.

II. FORMULATION

We consider interacting semi-flexible, in-extensible slender filaments immersed in a viscous fluid. Ignoring external forcing (such as gravity) and focusing on low-Reynolds number flows (no inertia effects), the Stokes equations are appropriate to describe the dynamics of the system sketched in FIG. 1. For very slender filaments the governing Stokes equations can be reduced to a system of nonlinear, non-local integro-differential equations as in [21]. Immersed in a background flow with a characteristic time \( \gamma^{-1} \), all filaments are assumed to be of equal length \( L \) with the same bending rigidity \( E \) and filament aspect ratio \( \epsilon \) (hence the same coefficient \( c \equiv \log(\epsilon^2) \)). The equations are rendered dimensionless by using \( L \) for length unit, \( \gamma^{-1} \) for time unit and \( E/L^2 \) for force unit. In the slender-body formulation, the \( l \)-th filament is described by its centerline position \( x_l \) parameterized by arclength \( s \in [0,1] \). Throughout the paper the subscript \( s \) denotes the derivative with respect to arclength. The dynamics of the \( l \)-th filament interacting with other filaments in a background flow \( U_0 \) is given by the following dimensionless equations [21]

\[
\frac{8\pi \mu \gamma L^4}{E} \left( \frac{\partial x_l}{\partial t} - U_0(x_l) \right) = \left[ (-c + 2) \mathbf{I} + (-2 - c)x_{ls}x_{ls} \right] f_l - K_l - \sum_{k \neq l}^M V_{lk},
\]

with \( \mu \) the fluid viscosity and \( \mathbf{I} \) the identity tensor, and \( x_{ls}x_{ls} \) a dyadic product. The force-free boundary conditions give \( x_{lss} = x_{lsss} = 0 \) at filament end points. The line force density \( f_l \) consists of a bending force and a tensile force that enforces filament in-extensibility

\[
f_l(s) = -(T_l(s)x_{ls}) + x_{lsss}.
\]

The self hydrodynamic interaction \( K_l \) is given by the finite-part integral

\[
K_l = \int_0^1 \left( \frac{\mathbf{I} + \hat{R}_l(s,s') \hat{R}_l(s,s')}{|\hat{R}_l(s,s')|} f_l(s') - \frac{\mathbf{I} + x_{ls}(s)x_{ls}(s)}{|s - s'|} f_l(s) \right) ds',
\]
FIG. 1: Illustration of two filaments in a planar shear flow $U_0$. $x_l(s)$ (left filament, thick solid line) and $x_k(s)$ (right filament, thick dashed line) are the filament center-line positions, and $\theta$ is the filament angle with respect to the $x$-axis.

and the hydrodynamic interaction between the $l$-th and $k$-th filaments are

$$V_{lk} = \int_0^1 \frac{1 + \hat{R}_{lk}(s, s') \hat{R}_{lk}(s, s')}{|\hat{R}_{lk}(s, s')|} f_k(s') ds'.$$

In the above integrals $R_l(s, s') = x_l(s) - x_l(s')$ and $R_{lk}(s, s') = x_l(s) - x_k(s')$ as sketched in FIG. 1, and $\hat{R}_l(s, s') = R_l(s, s')/|R_l(s, s')|$, $\hat{R}_{lk}(s, s') = R_{lk}(s, s')/|R_{lk}(s, s')|$.

The in-extensibility condition of the $l$-th filament $x_{ls} \cdot x_{ls} = 1$ gives the following equation for the line tension

$$2cT_{ls} + (2 - c)(x_{lss} \cdot x_{lss}) T_l = x_{ls} \cdot \frac{\partial}{\partial s} \left( \frac{8\pi \mu \gamma L^4}{E} U_0(x_l) - K_l - \sum_{k \neq l} V_{lk} \right) +$$

$$(2 - 7c)(x_{lsss} \cdot x_{lsss}) - 6c(x_{lsss} \cdot x_{lsss}),$$

subject to the force-free boundary condition $T_l(s = 0, 1) = 0$. The above slender-body equations for interacting filaments in Stokes flow have been numerically investigated by Tornberg and Shelley [21]. The authors regularize the finite-part interaction integral and construct a numerical method to successfully avoid severe stability constraint due to the bending force. Using this numerical method, the authors are able to simulate the collective dynamics of 25 interacting elastic filaments in a shear flow.

In the present work we apply the Hasimoto transformation [19, 24, 25] to the above slender-body equations with hydrodynamic interactions. Instead of the center-line position for the $l$-th filament, the filament complex curvature $\psi_l \equiv \kappa_l e^{i\phi_l}$ is the main dynamical variable, and $\tau_l \equiv \partial \phi_l / \partial s$ is the corresponding torsion. In this formulation the natural coordinate system is the unit tangent ($\hat{t}_l$), normal ($\hat{n}_l$), and binormal ($\hat{b}_l$) vectors along the filament centerline. The slender-body equations are recast in terms of complex curvature $\psi_l$ and the three unit vectors

$$\frac{8\pi \mu \gamma L^4}{E} \frac{\partial \psi_l}{\partial t} = (\partial_s + |\psi_l|^2) \Gamma_l + G_l,$$

$$\Gamma_l \equiv (U_l + iV_l)e^{i\phi_l},$$

$$G_l \equiv \psi_l \text{Im} \int ds' \psi_{ls'} \Gamma_{l,'} + \psi_{ls} \psi_{ls},$$
where $U_l$, $V_l$ and $W_l$ are projections of the filament centerline velocity onto $\mathbf{n}_l$, $\mathbf{b}_l$, and $\mathbf{t}_l$, respectively:

\[
\frac{8\pi \mu \gamma L^4}{E} \frac{\partial \mathbf{x}_l}{\partial t} = U_l \mathbf{n}_l + V_l \mathbf{b}_l + W_l \mathbf{t}_l, 
\]

\[
U_l = \mathbf{n}_l \cdot \left\{ \frac{8\pi \mu \gamma L^4}{E} \mathbf{U}_0 + \mathbf{u}_l' + \left[ (-c + 2) \mathbf{I} + (-2 - c) \mathbf{x}_{ls} \mathbf{x}_{ls} \right] \mathbf{f}_l \right\}, \tag{10}
\]

\[
V_l = \mathbf{b}_l \cdot \left\{ \frac{8\pi \mu \gamma L^4}{E} \mathbf{U}_0 + \mathbf{u}_l' + \left[ (-c + 2) \mathbf{I} + (-2 - c) \mathbf{x}_{ls} \mathbf{x}_{ls} \right] \mathbf{f}_l \right\}, \tag{11}
\]

\[
W_l = \mathbf{t}_l \cdot \left\{ \frac{8\pi \mu \gamma L^4}{E} \mathbf{U}_0 + \mathbf{u}_l' + \left[ (-c + 2) \mathbf{I} + (-2 - c) \mathbf{x}_{ls} \mathbf{x}_{ls} \right] \mathbf{f}_l \right\}. \tag{12}
\]

The disturbance velocity $\mathbf{u}_l'$ due to hydrodynamic interactions (including both self and mutual interactions among $M$ filaments) is defined as

\[
\mathbf{u}_l' = -K_l - \sum_{k \neq l} V_{lk}. \tag{13}
\]

Instead of using equation 12 for $W_l$, we compute $W_l$ from the normal projection $U_l$ based on the in-extensibility condition (Hou, Shelley and Lowengrub [26]) as

\[
W_l = \int_0^s U_l ds' + W_l(s = 0), \tag{14}
\]

where $W_l(s = 0)$ is the tangential velocity at $s = 0$. From the complex curvature $\psi_l$, the filament centerline position can be reconstructed from the Frenet geometric identities as follows. Given a complex curvature $\psi_l$, the complex vector

\[
\omega_l = (\mathbf{n}_l + i\mathbf{b}_l) \exp(i\psi_l) \tag{15}
\]

satisfies the following equations along the filament centerline

\[
\omega_{ls} = -\psi_l \mathbf{t}_l, \tag{16}
\]

\[
\mathbf{t}_{ls} = \frac{\mathbf{t}_l^* \omega_l + \psi_l \omega_l^*}{2}. \tag{17}
\]

$\omega_l$ and $\mathbf{t}_l$ are obtained from integrating equations 16-17, and the centerline position is obtained by integrating the tangent vector

\[
\mathbf{x}_l = \int_0^s \mathbf{t}_l ds' + \mathbf{x}_l(s = 0). \tag{18}
\]

Substituting equations 10, 11 and 12 into equation 6 gives a fourth-order nonlinear integro-differential equation for $\psi_l$

\[
\eta \frac{\partial \psi_l}{\partial t} = (1 + 2\delta) \left( \partial_{ss} + |\psi_l|^2 \right) \left\{ \left[ -\psi_{lss} + (|\psi_l|^2 + T_l) \psi_l \right] + \omega_l \cdot \left( \eta \mathbf{U}_0 + \mathbf{u}_l' \right) \right\} + G_l, \tag{19}
\]

with effective viscosity $\eta$ and filament slenderness $\delta$ defined as

\[
\eta \equiv \frac{8\pi \mu \gamma L^4}{-c E} = \frac{8\pi \mu \gamma L^4}{-\ln(\epsilon^2) E}, \quad \delta \equiv \frac{1}{-c} = \frac{1}{-\ln(\epsilon^2)}. \]
The force-free boundary conditions expressed in terms of \( \psi_l \) are \( \psi_l(s = 0, 1) = \psi_{ls}(s = 0, 1) = 0 \). Equation 5 for the line tension can be recast in terms of the complex curvature \( \psi_l \) as

\[
2T_{lss} - |\psi_l|^2 (1 + 2\delta) T_l = -\left( \int_0^s ds' \frac{\psi_l^* \omega_l + \psi_l \omega_l^*}{2} + \hat{t}_l(0) \right) \cdot (\eta U_0 - \delta u'_l) + (7 - 2\delta) (\hat{t}_{ls} \cdot \hat{t}_{lss}) - 6 (\hat{t}_{lss} \cdot \hat{t}_{ls}).
\]  

(20)

The advantage of the above formulation is that the filament in-extensibility condition is exactly satisfied when the filament centerline is re-constructed from the tangent vector. Numerically this means that the filament in-extensibility condition is obeyed up to the round-off errors without the need of penalty function in the numerical scheme. The end-point tangent vector \( \hat{t}_l(s = 0) \) and the filament centerline position \( x_l(s = 0) \) are required for constructing the filament centerline. This information is obtained by computing the tangent vector and the filament end point from markers that are convected by the filament velocity from equation 9. In the following we outline the implementation of this formulation.

### A. Summary of Numerical Methods

The integral in equation 3 is regularized using the high-order regularization scheme in [21] to achieve consistent asymptotic accuracy of the slender-body formulation of filament dynamics. Equations 19-20 are discretized using a second-order time-stepping scheme, and second-order divided differences to discretize the spatial derivatives. An explicit treatment of all terms in equation 19 yields a very strict fourth-order stability limit for the time-step size, arising from the high derivatives of \( \psi_l \). Consequently the term \( \psi_{lssss} \) is treated implicitly for stability of larger time-step size. Schematically, we write

\[
\frac{\partial \psi_l}{\partial t} = F(\psi_l, \psi_{lssss}) + G(\psi_l),
\]  

(21)

where the dependence on \( \psi_{lssss} \) is to be treated implicitly, and all other terms are to be treated explicitly using a second-order backward differentiation formula. Thus the approximate decomposition reads

\[
\frac{1}{2\Delta t} \left( 3\psi_l^{n+1} - 4\psi_l^n + \psi_l^{n-1} \right) = F \left( 2\psi_l^n - \psi_l^{n-1}, \psi_{lssss}^{n+1} \right) + 2G(\psi_l^n) - G(\psi_l^{n-1}),
\]  

(22)

where \( \Delta t \) is the time step, and the time at the \( n \)th level \( t^n = n\Delta t \). For the first time step, before any previous time levels are available, we replace the time discretization above by a first-order Euler step. The spatial discretization in the arclength \( s \) is uniform with \( N \) intervals of grid space size \( h = 1/N \). Second-order divided differences are used to approximate spatial derivatives. The corresponding line tension is then computed by solving equation 20 using the same second-order divided differences for spatial discretization. More detail on the spatial discretization is provided in [21]. Combining both the temporal and spatial discretizations, we find that this time discretization yields only a first-order constraint for the time-step size, i.e., \( \Delta t \) can be chosen proportional to the spatial grid size.

At every time level, the complex vector \( \omega_l \) and tangent vector \( \hat{t}_l \) are obtained by integrating equations 16-17 with moving boundary conditions \( \hat{t}_l(s = 0, t) \). As the filament evolves, the boundary condition \( \hat{t}_l(s = 0) \) also varies with time. To update \( \hat{t}_l(s = 0) \) at the \( n + 1 \)st level, we use markers
that are independent of the filament centerline. The marker velocity is given by equation 9 with \( U^n \) and \( V^n \) from equations 10-11 and \( W^n \) from equation 14, all computed from \( \psi^n(s) \) and \( \omega^n(s) \) at the \( n \)th time level. The same explicit second-order time-stepping scheme is used to advance the marker positions. Re-initialization of markers is performed if the distance between marker is stretched too much by the velocity field.

The filament shape reconstructed from integrating \( \hat{\ell} \) along the center-line is always of the same length up to the numerical errors in the integration. No penalty function is needed for enforcing the in-extensible condition in the above formulation. The numerical code has been validated against analytic results for a single elastic fiber in prototypical flows such as a linear shear flow and a straining flow. The numerical integrals for hydrodynamic interactions have been validated by checking against analytical results for straight rods in various flow configurations [27].

III. TWO FILAMENTS IN LINEAR SHEAR FLOW

In this section we investigate effects of HIs between two elastic filaments immersed in linear shear flow. In particular, we focus on HI-induced change in their buckling dynamics and the filament dispersion in shear flow.

To minimize the effects of initial conditions, all the simulation results presented in this section start with a configuration where both filaments have exactly the same shape and angle. Initial locations of the two identical filaments in a linear shear flow \( U_0 = (y, 0, 0) \) are in the \( xy \)-plane with one centered at \((0, 0, 0)\) and the other centered at \((d, 0, 0)\).

The buckling of a single straight filament in the plane of shear flow has been well studied [21]: Initially placed at the center of the flow \((y = 0)\) with an angle \( \theta \) to the \( x \)-axis, the filament slowly rotates to align with the shear flow. The filament experiences compression as it rotates toward the \( y \)-axis and decompression as it rotates past the \( y \)-axis. For a stiff filament the effective viscosity \( \eta \) is essentially zero, and the filament simply rotates to align with the shear flow. For a floppy filament, buckling occurs when sufficient stress is exerted from the fluid during the compression. The filament keeps rotating as it buckles, and eventually straightens out and gradually aligns with the \( x \)-axis.

At the beginning of the simulations, the angle \( \theta \) (with respect to the \( x \)-axis, see FIG. 2(a)) is set to \( \theta = 0.9936\pi \) for both filaments; this value is chosen so that a single straight filament will become vertical at \( t = 49.664 \) [21]. The initial filament shape is the same slightly perturbed line for both filaments. Simulations show that hydrodynamic interaction is negligible when the filament separation is much larger than five times the filament length.

A. Effect of filament slenderness \( \delta \) in shear flow

For the first set of simulations, the initial filament separation is fixed at five times the filament length \((d = 5)\) with the effective viscosity \( \eta = 15000 \). The filament slenderness varies from \( \delta = 0.01 \) to \( \delta = 0.1 \), or filament aspect ratio from \( \epsilon = 10^{-22} \) to \( \epsilon = 4 \times 10^{-3} \). HIs are expected to be more important to filament dynamics for larger filament slenderness.
FIG. 2: Buckling instability of two interacting filaments at a distance $d = 5$ in a planar shear flow. Effective viscosity $\eta = 15000$ and filament slenderness $\delta = 0.1$. Both filaments have exactly the same initial shape and angle $\theta(0) = 0.9936\pi$. At the center of each panel the two filaments are superimposed for comparison.

FIG. 2 shows buckling of two interacting semi-flexible filaments in the plane of the shear flow with the initial filament separation $d = 5$ and filament slenderness $\delta = 0.1$. For direct comparison, the two filaments are superimposed at the center of each panel. With the initial angle slightly smaller than $\pi$, both filaments rotate clockwise in synchrony at this separation. The filament is under compressive stress from the shear flow before it rotates past the $y$-axis. For $\eta = 15000$ the fluid exerts sufficiently strong compressive stress to induce buckling as filaments rotate past $\theta = 3\pi/4$ ($t \sim 48.5$). When both filaments are under compression, HIs also induce the most significant difference in the filament shape around $t = 49.75$, when the elastic energy $\kappa^2 \equiv \int_0^1 |\psi|^2 ds$ reaches maximum for both filaments, see FIG. 2(c) and FIG. 3(a). The dotted line in the figure is the elastic energy of the non-interacting filament, which is exactly the average of the elastic energy for two interacting filaments. This is
FIG. 3: (a) Elastic energy versus time for interacting filaments in shear flow: Solid line for left filament and dashed line for right filament in FIG. 2. The dotted line is for a non-interacting filament with the same initial conditions. (b) Elastic energy of the right filament at $x = 5$ (ordinate) versus elastic energy of the left filament at $x = 0$ (abscissa). The evolution of the buckling instability follows the arrow. The dashed line is for reference to the evolution of the non-interacting case.

because the initial conditions are exactly the same for the two interacting filaments, and two filaments rotate and buckle at the same time with the right filament reaching higher curvature than the left. If the sign of perturbation is reversed for both filaments, the left filament will reach higher maximum curvature.

FIG. 3(b) plots the elastic energy of the right filament (ordinate) against that of the left filament (abscissa). The arrows indicate the direction of evolution in terms of the elastic energy of two filaments. The same trend is observed for other values of filament slenderness as shown in FIG. 4(a). At this distance the two filaments still rotate in synchrony under HIs. Stronger HIs (larger $\delta$) lead to more asymmetric filament shape at the time of buckling ($t \sim 49.75$ for these simulations). After the two filaments buckle and rotate past the vertical axis, they quickly straighten out in FIG. 2(e)-(f).

Another significant consequence of HIs is the filament dispersion in shear flow, which depends on the transverse filament displacement (in the cross-stream direction) defined as $\Delta_y \equiv y_{1c} - y_{2c}$, where $y_{lc}$ is the vertical coordinate of the $l$-th filament center. The transverse displacement $\Delta_y$ reaches a constant value after the buckling instability subsides and both filaments align with the shear flow. In the absence of HIs the two filaments slowly align with the $x$-axis without any shear dispersion: the transverse filament displacement remains zero, and the filament separation remains constant before and after the buckling. From the simulation data it is found that for $d = 5$, larger HIs lead to larger transverse filament displacement. FIG. 4(b) shows dependence of $\Delta_y$ on filament slenderness via the buckling instability mediated by HIs. The transverse displacement between two filaments is proportional (identical) to the difference in filament translational velocity in shear flow (after non-dimensionalization). The difference in translational velocity gives rise to a horizontal filament displacement $\Delta_x = \Delta_y t$, which in turn leads to the filament shear dispersion

$$\Delta(t) \equiv \sqrt{\Delta_x^2 + \Delta_y^2} = \Delta_y \sqrt{t^2 + 1} \to \Delta_y t \quad \text{as} \quad t \to \infty.$$  

Therefore, results in FIG. 4(b) suggests that for a fixed initial filament separation, large filament
dispersion correlates to large hydrodynamic interaction in the planar shear flow.

B. Effect of initial filament separation in shear flow

For force-free filaments their mutual HIs (integral $V_{lk}$ in equation 4) vary as $1/|R_{lk}|^2$ [21], and more substantial HIs are expected for smaller filament separation. In this subsection we conduct the following set of simulations to examine how the previous results for $d = 5$ may vary with initial filament separation. For the following simulation data, filament slenderness $\delta$ is fixed at 0.07, which corresponds to a filament aspect ratio of $\epsilon \sim 5 \times 10^{-4}$. The initial filament shapes and angles from the previous set of simulations are used while the initial filament separation $d$ is varied from $d = 5$ to $d = 1.5$.

FIG. 5 shows an example of different HIs-induced buckling dynamics for two filaments at a distance $d = 2.5$. At this separation HIs cause the filament to lose synchrony in their rotation; as illustrated in FIG. 6(a) the right filament rotates faster than the left filament until $t > 51$, when the left filament catches up with the right filament (see inset in FIG. 6(a)). Furthermore, the filament deformation is almost anti-symmetric due to HIs, as shown at the center of FIG. 5(b)-(d). The corresponding evolution of elastic energy for the two filaments is shown in FIG. 6(b). The right filament (dashed line) reaches maximum earlier than the left (solid line). On the other hand, contrary to the $d = 5$ case (also shown in FIG. 6(b)), the left filament deforms more than the right filament which attains a higher maximum elastic energy at a later time.

For smaller filament separation ($d = 1.5$), HIs induce the buckling instability as early as $t \sim 46$. The evolution of filament buckling is demonstrated in FIG. 7. At $t = 48.12$ the filaments already undergo significant deformation. After $t = 49.37$, half of the filament already straightens out while the other half is still bent. Both filaments straighten out around $t = 52.37$, after when they rotate to gradually align with the shear. The corresponding evolution of the elastic energy is shown as the dash-dotted line in FIG. 8(a). The elastic energy evolution for $d = 2.5$ (dotted line) and $d = 5$ (solid line) are also
FIG. 5: Buckling instability of two interacting filaments at a distance $d = 2.5$ in a planar shear flow. Effective viscosity $\eta = 15000$ and filament slenderness $\delta = 0.07$. The same initial conditions are used for both filaments with $\theta(0) = 0.9936\pi$. At the center of each panel the two filaments are superimposed for comparison.

plotted in the figure. For all three curves in FIG. 8(a), the evolution is in the clockwise direction. From these figures we conclude that the asymmetry between the two filaments is most prominent when the filament separation is $d = 2.5$. This is also reflected in the transverse filament displacement $\Delta_y$ in FIG. 8(b), where $\Delta_y$ reaches maximum at $d = 2.5$.

The above findings can be understood as follows. When two filaments are far from each other (at a distance greater than five times the filament length), hydrodynamic interaction is negligible and the two filaments rotate in synchrony given the same initial filament shape and angle. When two
filaments are in close range of each other, the hydrodynamic interaction causes both filaments to start to rotate early. In particular if the initial filament separation is comparable to their length, strong hydrodynamic interaction acts to synchronize the filament rotation. In addition, the shapes of the buckling filaments are (almost) mirror images of each other as clearly demonstrated in FIG. 7. This mirror symmetry (invariant under transformation $x \rightarrow -x$) is inherent from the linear shear flow. As a result, even though the initial perturbed filament shape (identical for both filaments) does not have the mirror symmetry, strong hydrodynamic interaction enforces this symmetry in the subsequent dynamics. For initial filament separation between the two extreme limits, hydrodynamic interaction is strong enough to induce faster rotation and larger filament deformation than the non-interacting filament, but not enough to enforce the mirror symmetry. Therefore, the buckling dynamics of two filaments at $d = 2.5$ shows the most asymmetry, and consequently the largest transverse displacement (FIG. 8(b)).

In summary, HIs between two elastic filaments induce novel buckling dynamics and filament dispersion (transport) in linear shear flow. Simulation results suggest that filament dispersion is small when the initial filament separation is either too large or too small, and maximum filament dispersion is found for filament separation $d = 2.5$ (or two and a half the filament length). The buckling of filament pair at this distance is found to be most asymmetric, in terms of both average filament curvature evolution and filament rotation.

### IV. TWO FILAMENTs IN LINEAR STRAINING FLOW

In this section we elucidate the effects of HIs between two elastic filaments immersed in the plane of a linear straining flow, see FIG. 9(a). The initial configuration is two filaments parallel to the $x$-axis with one on the left (thick solid line) and the other on the right (thick dashed line) of the stagnation

![FIG. 6: (a) Evolution of averaged filament angle ($\theta$): Right filament (ordinate) versus left filament (abscissa) for initial filament separation $d = 5$, $d = 2.5$ and $d = 1.5$. The arrow indicates the direction of evolution. The inset shows the angle of the left filament versus time. (b) Elastic energy versus time for pairs of filaments at different initial separations with effective viscosity $\eta = 15000$ and slenderness $\delta = 0.07$. Solid lines are for the left filaments, and dashed lines are for the right filaments.](image-url)
FIG. 7: Buckling instability of two interacting filaments at a distance $d = 1.5$ in a planar shear flow with effective viscosity $\eta = 15000$ and slenderness $\delta = 0.07$. The same initial conditions are used for both filaments with $\theta(0) = 0.9936\pi$. At the center of each panel the two filaments are superimposed for comparison.

point, located at the center of FIG. 9(a). The left filament is centered at $(-0.5, -0.03, 0)$ and the right is centered at $(0.5, 0.03, 0)$ to avoid direct collision as they move toward the stagnation point. The converging flow advects both filaments toward the stagnation point. The initial filaments shapes are a slightly perturbed curve that is invariant under $\mathbf{x} \rightarrow -\mathbf{x}$. The filament dynamics is expected to be symmetric under the transformation $\mathbf{x}_1 \rightarrow -\mathbf{x}_2, \mathbf{x}_2 \rightarrow -\mathbf{x}_1$ as they are advected by the extensional flow and move along the arrows in FIG. 9(a). This is because both the initial conditions and the straining flow are invariant under this transformation. In the simulations this mirror symmetry is obeyed up to the numerical discretization errors: For unit filament length with 200 grid points for each filament, the filament shapes and trajectories satisfy the mirror symmetry up to errors of the order $\sim 10^{-5}$.

Starting from the initial configuration described in FIG. 9(a), two filaments experience compression on their way toward the center and experience maximum compressive stress when they are closest to the stagnation point. In this configuration the dynamics of two filaments is always synchronous and spatially invariant under the mirror symmetry. Buckling instability occurs if the effective viscosity is sufficiently large, as in the case of a single filament [1].

For a single horizontal filament ($\theta = 0$) lying on the compressional ($x$) axis, the critical viscosity for buckling instability is $\eta_c = 328$. If $\eta < \eta_c$ the filament does not buckle nor rotate. If $\eta > \eta_c$ the filament
FIG. 8: (a) Elastic energy of the right filament (ordinate) versus elastic energy of the left filament (abscissa) for three initial filament separations. The evolution of the buckling instability follows the clockwise direction. The dashed line is for reference to the evolution of the non-interacting case. (b) Dependence of transverse filament displacement $\Delta y$ versus initial filament separation $d$.

FIG. 9: (a) Illustration of two filaments (thick solid line and thick dashed line) inserted in a linear straining flow $U_0 = (-x, y, 0)$. The arrows indicate the flow directions, and the contour lines are the streamlines. (b) Critical value of $\eta$ for buckling instability of two filaments (parallel to the $x$-axis) around the stagnation point. One filament is moving toward the center from the left at a distance of $0.03$ above the $x$-axis and the other at $0.03$ below. The inset at the lower left corner is the trajectories of two filaments (with $\eta = 200$ and $\delta = 0.01$) and their shapes. The inset at the upper right corner is an example of the elastic energy versus time for $\eta = 300$ and $\delta = 0.1$.

buckles, rotates and aligns with the extensional axis. Once aligned, the filament moves away from the stagnation point along the extensional axis [1]: The complete dynamics of a single filament with supercritical $\eta$ is the sequence of buckling, rotation and translation. For a single horizontal filament at a distance from the compressional axis (at a distance $0.03$, for example), the critical viscosity is higher than 328, and the filament buckles without rotation as it moves away from the stagnation point.
Different filament dynamics is found from simulations of a pair of interacting filaments approaching the stagnation point. Firstly, HIs cause filaments to buckle at a lower critical effective viscosity, which is now a function of filament slenderness $\delta$ as shown in FIG. 9(b). For $\eta$ below the critical value, filaments with small $\delta$ approach the stagnation point without buckling or rotation, and move away from the stagnation point as shown in the lower left inset of FIG. 9(b) (for $\delta = 0.01$ and $\eta = 190$). For filaments with larger $\delta$ (and $\eta$ still below the critical value), however, the straight filaments rotate under HIs as shown in FIG. 10(a) (for $\delta = 0.1$ and $\eta = 100$).

Secondly, for supercritical effective viscosity $\eta > \eta_c$, the two filaments buckle and their elastic energy reaches a maximum (upper right inset of FIG. 9(b)). The buckling of two interacting filaments around the stagnation point is more complicated than the buckling dynamics of a single filament: The sequence of dynamics for a single filament is found for a pair of interacting filaments only for $\eta$ slightly above the critical value, as shown in FIG. 10(b) for $\eta = 300$ and $\delta = 0.1$. FIG. 11(a) summarizes the trajectories of filament center from simulations with small to moderate values of $\eta$ such that filaments rotate to align with the extensional axis.

For $\eta$ much larger than the critical value, HIs induce significant shape deformation, and the deformed filaments move along the extensional axis without rotation as shown in FIG. 12(a) with $\eta = 1000$ and $\delta = 0.1$. Without HIs, buckling is followed by rotation for a horizontal filament lying on the compressional axis with $\eta = 1000$ and $\delta = 0.1$. FIG. 11(b) summarizes the trajectories of filament center with sufficiently large $\eta$ such that filaments buckle without rotating around the stagnation point. The corresponding elastic energy for buckling filaments with different values of $\eta$ is plotted versus time in FIG. 12(b).
FIG. 11: Trajectories of the center of left filament with $\delta = 0.1$ for different values of $\eta$. The right filament trajectories are mirror images with respect to the origin. (a) Moderate $\eta$ where the filament buckles mildly for $\eta > \eta_c$ and rotates as it leaves the stagnation point (FIG. 10). (b) Large $\eta$ where the filament deforms significantly and does not rotate as it leaves the stagnation point (FIG. 12(a)).

FIG. 12: (a) Trajectories (dash-dotted lines) and shapes of filaments with $\delta = 0.1$ and $\eta = 1000$ at six different times. The initial configuration is two filaments parallel to the $x$-axis located at ($0.5$, $-0.03$, $0$) and ($0.5$, $0.03$, $0$). (b) Elastic energy versus time for $\eta$ from 300 to 1000.

A. Effect of filament slenderness $\delta$ in extensional flow

Next we examine the $\delta$-dependence of buckling dynamics of two filaments as we vary slenderness from 0.01 to 0.1. $\eta = 1000$ is chosen so that filaments buckle for all values of $\delta$. The evolution of the elastic energy versus time is plotted in FIG. 13(a). Detailed buckling dynamics for $\eta = 0.01$, 0.02 and 0.03
is illustrated in FIG. 13(b). For all three values of $\delta$ filaments start to buckle around $t = 2.04$, and the early filament deformation is proportional to $\delta$. For $\delta = 0.03$ the filament is more deformed and moves faster than the other two filaments. The filament with $\delta = 0.01$ has the least deformation before $t = 3.24$. As the $\delta = 0.01$ filament moves away from the stagnation point in the $V$-shape, it reaches maximum deformation much later than the other two filaments. The corresponding filament center trajectories also demonstrate the non-monotonic dependence on slenderness, and the $\delta = 0.01$ filament eventually catches up with the $\delta = 0.02$ filament after $t \sim 3.24$. HIs between $\delta = 0.01$ filaments induce buckling at a slower rate, and the filament pair reaches maximum curvature farther away from the stagnation point.

B. Buckling filaments in near contact

If filament are too close to the compressional axis of the extensional flow, their buckling dynamics and rotation around the stagnation point may cause them to be in near contact with each other. An example is shown in FIG. 14(a), where two horizontal filaments are initially centered at $(-0.5, -0.02, 0)$ and $(0.5, 0.02, 0)$. With $\eta = 300$ and $\delta = 0.1$, two filaments first buckle and then rotate. Around $t = 3.64$ the two filaments come into near contact of each other.

Special treatment is required to avoid physical contact and crossing between slender bodies in the slender-body formulation [28]. A strong and very short-range repulsive force often used in the dynamic simulations of rigid fiber suspension is sometimes used as an alternative to prevent fiber crossing [29–
FIG. 14: (a) Buckling filaments with $\eta = 300$, $\delta = 0.1$ and $d = 0.02$. The two filaments come in to near contact around $t = 3.64$. Repulsive force is needed to prevent filament crossing in the simulation. (b) Elastic energy for different initial displacement from the compressional ($x$) axis: solid line is for a displacement of 0.03 and dashed line is for a displacement of 0.02. $\eta = 300$ and $\delta = 0.1$ for both cases.

This repulsive force can be modified for semi-flexible filaments as follows

$$ F_l^R(s) = \pm a_0 \frac{\tau e^{-\tau h_{lk}(s)}}{1 - e^{-\tau h_{lk}(s)}} \hat{n}_l, $$

where $h_{lk}(s)$ is the shorted distance between two filaments at a given point on the $l$th filament, and proper signs are chosen to denote the repulsive direction.

Without the short-range repulsive force, the two filaments in FIG. 14(a) come into physical contact and the slender-body formulation breaks down right after $t = 3.64$. Adding the repulsive force with $a_0 = 10^{-4}$ and $\tau = 10^3$ in the simulation, the two filaments slide next to each other after $t = 3.64$, rotate and align with the extensional axis and diverge from the stagnation point after $t = 4.28$. FIG. 14(b) shows the corresponding evolution of the elastic energy (dashed line). In comparison with the elastic energy for $d = 0.03$ (solid line), HIs suppress filament deformation when they are in close range of each other, an effect also found in the case of viscous drops [7]. Further numerical investigation on the buckling filaments in close range shows that the repulsive force in equation 23 fails to keep the buckling filaments from crossing each other in some cases.

V. CONCLUSION

The effects of HIs on the buckling dynamics of a pair of semi-flexible in-extensible filaments in two simple linear flows are reported in this work. The non-local slender-body formulation for interacting filaments immersed in Stokes flow is utilized to describe the dynamics. Specific initial conditions are used in the numerical simulations to elucidate the various aspects of HIs.
For a pair of identical filaments (same shape, angle, and bending rigidity) lying at the center of shear flow with an initial separation $d$, we find HIs change the filament rotation in nontrivial fashions. Firstly, HIs induce filaments to rotate earlier than non-interacting filaments. Secondly, simulations show that filament rotation is synchronous when the filament separation is large (with negligible HIs) or small (very strong HIs). For an intermediate filament separation $d = 2.5$ filament rotation is out of sync, with the right filament completing the rotation earlier than the left one for the given initial conditions. Thirdly, HIs also induce non-trivial filament shear dispersion in shear flow: without HIs the filament shear dispersion is zero for the given initial conditions. Filament shear dispersion first increases with decreasing filament separation, attains a maximum at $d = 2.5$ when the loss of synchrony in filament dynamics is the greatest, and decreases when the filaments are synchronized again by strong HIs at short filament separation.

We have also simulated the dynamics of a pair of filaments initially centered at $(-49.664, 1, 0)$ and $(0, 0, 0)$, both with an angle $\theta = 0.9936\pi$. The top, left filament translates horizontally toward the right at a dimensionless velocity of 1. Two filaments are closest to each other at $t = 49.664$ when the top filament center reaches $(0, 1, 0)$. As both filaments buckle around $t = 49.664$, HIs induce most differences in shape deformation. As in the previous cases, the consequence of filament buckling under HIs is an increase in filament dispersion after both filaments straighten out and align with the shear. However, for this configuration, the final transverse displacement for $\delta = 0.1$ is $\Delta y \sim 1.01$, an increase of only 0.01. Therefore we conclude that HIs have little impact on the shear dispersion of filaments moving toward each other at this vertical separation. For smaller vertical separation, two filaments may come into physical contact around $t = 49$.

For a pair of filaments in the extensional flow, a special initial condition is chosen so that (1) two filaments would approach the stagnation point from equal distance, and (2) the subsequent dynamics retains the mirror symmetry up to numerical discretization errors. HIs reduce the threshold in bending rigidity for buckling instability in this configuration. For stiff filaments converging to the stagnation point in the flow, strong HIs can induce rotation. For moderately floppy filaments, HIs induce both buckling and rotation of filaments, much similar to the buckling dynamics of a single filament around the stagnation point. For very floppy filaments, HIs induce strong filament deformation and the highly-deformed filaments diverge from the center without rotation.

We have also shown that two filaments come into near contact as they buckle around the stagnation point. The slender-body formulation breaks down if two filaments are in physical contact, which occurs when two filaments are very close to the compressional axis as suggested in FIG. 14(a). A short-range repulsive force is found to be able to keep two filaments apart only for certain ranges of effective viscosity and slenderness. More detailed investigation is required to ensure the slender-body formulation remains consistent in these cases. Once we have a better treatment of the repulsive force for buckling filaments in near contact, we will investigate how HIs affect the transport of filaments in a cellular flow.

An ongoing project is to examine how macroscopic properties of semi-flexible filament suspension correlate to HIs effects on the buckling dynamics of a pair filaments summarized in this paper. We are now working on incorporating the smooth-particle mesh Ewald (SPME) scheme for fast computation of the interaction integral $V_{lk}$ into the non-local formulation for multi-filaments in a periodic domain. We aim to simulate more than hundreds of interacting semi-flexible filaments, and these results will be useful for constructing and validating the modeling of HIs in the framework of kinetics theory for
complex filament flows in the dilute or semi-dilute limit. For example, the integral kernel of filament interaction [32] may be consistently constructed based on the findings presented in this paper.

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