Simulation of the Doi–Edwards model in complex flow

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Synopsis

The Doi–Edwards model is simulated in startup of two-dimensional complex flow. The flow geometry is that of a cylinder confined between two parallel plates. Two different, new simulation methods are used. The first is based on the configuration field approach. The second method is a new method which is introduced in this paper. We refer to this approach as the deformation field method. Theoretically the methods are equivalent. It will be shown that the deformation field approach is very efficient. Furthermore, the method opens up possibilities of studying extensions of the Doi–Edwards model which include tube-stretch and convected constraint release. © 1999 The Society of Rheology.

I. INTRODUCTION

The description of the rheological properties of polymer melts remains a great scientific challenge. In contrast to dilute polymer solutions, where there is no direct interaction between polymer molecules, in a melt, the polymer dynamics is in fact dictated by the presence of the surrounding polymers. It is of course impossible to describe the extremely complicated, mutual interactions between the molecules in detail. Therefore the challenge is to present a tractable theory for these systems and to include only the key concepts in the description. This is exactly the route that Doi and Edwards (1978a,b,c) navigated. The central idea of their Doi–Edwards model for a polymer melt, is that the motion of a polymer molecule perpendicular to its backbone is strongly reduced by the neighboring polymers. That is, the surrounding chains effectively constitute a cage, called a tube in the Doi–Edwards description, and thus reduce the possible displacements of the polymer to motions along its own contour. A similar problem had already been studied by de Gennes (1971), who considered the diffusion of a polymer chain in an environment of fixed obstacles. Inspired by the snake-like motion of the chain, de Gennes referred to this motion as ‘‘reptation,’’ and because of the common underlying picture, the Doi–Edwards model is often called the reptation model.

In spite of the coarse graining in the Doi–Edwards description, the central result, a diffusion equation for the motion of a reptating polymer, is still quite complicated. This is essentially due to the coupling of the motion of different parts of the polymer. Analytical tractability therefore prompted Doi and Edwards to invoke a further simplification, the so-called independent alignment approximation. This approximation decouples the motion of different parts of the polymer. In this way the resulting model reduces to a single segment description. The Fokker–Planck equation obtained within the independent

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alignment approximation is suited for analytical investigation of simple flows such as inception of homogeneous shear flow.

The key quantity in any rheological model is of course the stress tensor. From a microscopic point of view the stress tensor is determined by the configuration of the polymers. Within the traditional framework of flow simulations, the stress is calculated from the so-called constitutive equation, a differential or integral equation for the stress. It is then crucial that this constitutive equation is of closed form, which means that the configuration distribution function of the polymers, which is not available at this macroscopic level of description, does not appear in the constitutive equation. It is well known, however, that many rheological models, that start from a microscopic description of the polymer dynamics, do not lead to a closed-form constitutive equation. And this, unfortunately, turns out to be the case for the Doi–Edwards model too.

In 1992 Öttinger and Laso initiated the simulation of complex polymer flow fields by merging the conventional methods for solving the mass and momentum balances (e.g., finite elements), with microscopic polymer simulations from which the polymer stress is determined [Öttinger and Laso (1992) and Laso and Ottinger (1993)]. The essential idea of their approach is to include ensembles of polymers in the simulation. These polymers are convected and deformed by the flow, and the stress tensor is obtained directly from their configuration distribution. Laso and Öttinger refer to this approach as the CONNFFESSIT approach. Inspired by their approach, Hulsen et al. (1997) developed a method in which the configuration distribution of the polymers is represented by a set of so-called configuration fields. Similar to real polymers, these configuration fields are convected and deformed by the flow. An important difference between the configuration field method and the original CONNFFESSIT approach is that the configuration fields define the polymer configuration distribution at every position in the flow domain, whereas in the CONNFFESSIT approach polymers are present only at a finite number of points.

To our knowledge, so far there have appeared only two papers in which the Doi–Edwards model was simulated in complex flow fields, viz. the paper by Öttinger and Laso (1994) and the paper by Hua and Schieber (1998). In their paper, Öttinger and Laso used the CONNFFESSIT method to simulate the startup of plane Couette flow for the Doi–Edwards model. Hua and Schieber, who also used the CONNFFESSIT approach, calculated the steady flow of the Doi–Edwards model in a periodic array of square-arranged cylinders. In this paper we consider the Doi–Edwards model in a two-dimensional complex flow, in this case the inception of flow past a cylinder which is confined between two parallel plates. We will solve the problem along two different lines: first we use the configuration field approach, and next we apply a new method, which we refer to as the deformation field method. Our approach is closely related to the method recently introduced by Peters et al. (1999). The essential idea of our deformation field method is to determine the stress from the initial polymer configuration and from the deformation they experienced thereafter. Although we focus on the Doi–Edwards model in this paper, we want to point out that the approach followed here may be considered as the starting point for the simulation of extensions of the model which include tube-stretch [see e.g., Marrucci and Grizzuti (1988), Pearson et al. (1989) and Pearson et al. (1991)] and convected constraint release [see Marrucci (1996), Ianniruberto and Marrucci (1996), and Mead et al. (1998)].

The paper is organized as follows: in the first sections we explain the concept of configuration fields and we discuss the simulation algorithm. Then we introduce our new method, the deformation field approach. After evaluating the methods in parallel we will present the simulation results. Our findings are commented on the conclusions.
II. GOVERNING EQUATIONS

The flow of an incompressible and isothermal polymer melt is governed by the continuity and momentum equations

\[ \nabla \cdot \mathbf{v} = 0, \]  
\[ \rho \frac{D \mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \mathbf{\tau}. \]  

In these equations \( \mathbf{v} \) is the velocity, \( \rho \) is the melt density, \( p \) denotes the pressure and \( \mathbf{\tau} \) is the polymer stress. In this paper we focus our attention on a polymer melt which can be described by the Doi–Edwards model within the independent alignment approximation. The Doi–Edwards model, however, does not lead to a closed-form constitutive equation for the polymer stress \( \mathbf{\tau} \). Therefore the stress tensor \( \mathbf{\tau} \) at a certain position must be calculated directly from the microstructure of the melt, i.e., the polymer configuration, at that position. This implies that in addition to solving for the velocity and pressure fields, in our simulation we also have to calculate the evolution of the polymer configurations.

In the Doi–Edwards model the polymer configuration changes by reptation. It can be shown that the Fokker–Planck equation derived by Doi and Edwards, describing the reptational motion of a polymer within the independent alignment approximation, can be translated into a stochastic description \cite{Oettinger89}. By virtue of the relation between stochastic differential equations and Fokker–Planck equations, this stochastic description is completely equivalent to the classical approach using diffusion equations \cite{Oettinger96}. In the stochastic framework, reptational motion of a polymer is described by the combination of two evolution equations, one for a unit vector \( \mathbf{u} \) and another for a stochastic process \( S \). The unit vector \( \mathbf{u} \) represents the orientation of a tube segment. It rotates affinely without stretching, hence

\[ \frac{D \mathbf{u}}{Dt} = \kappa \mathbf{u} - \kappa : \mathbf{uuu}. \]  

Because this equation is evaluated while following the fluid particle in which the tube segment is embedded, the time derivative in this equation is the material derivative. The first term on the right hand side (RHS), in which \( \kappa \) is the transpose of the velocity gradient, corresponds to affine deformation. The second term subtracts the projection of the first term in the direction of the momentary tube segment orientation, in order to keep the tube segment length constant. In addition to the unit vector \( \mathbf{u} \), a stochastic process \( S \) is introduced which describes a random walker, the Brownian motion of which is restricted to the interval \([0,1]\). The parameter \( S \) specifies which part of the polymer chain is currently in the tube segment \( \mathbf{u} \). For instance, the head and tail of the polymer chain are labeled by \( S = 0 \) and \( S = 1 \), respectively. The concept of reptation, in which the polymer chain gradually escapes from its original tube, is realized through the coupling between \( S \) and \( \mathbf{u} \). For, when the random walker \( S \) reaches one of the boundaries (i.e., when the polymer chain escapes from the tube segment), it is reflected at that boundary and simultaneously the associated tube segment \( \mathbf{u} \) is reset to a new random orientation. This mimics the change in orientation of a real polymer performing reptational motion \cite{Oettinger96}.

The evolution equation describing the Brownian motion of the random walker is given by the following stochastic differential equation
In this equation \( dW(t) \) denotes the increment of a Wiener process: it is a Gaussian random number with average 0 and variance \( dt \). The quantity \( \lambda \) is related to the so-called reptation or disengagement time \( \tau_d \). This reptation time is the characteristic time for a polymer chain to escape from its initial tube and is given by \( \lambda = \pi^2 \tau_d \).

The Doi–Edwards model does not lead to a closed-form equation for the stress tensor. Instead, the stress tensor is calculated directly from the microstructure of the melt, i.e., the tube segment orientation tensor, and is given by

\[
\tau(t) = G \langle uu \rangle(t).
\]

In this equation the constant \( G \) has the dimension of a modulus of rigidity, and the brackets denote ensemble averaging, i.e., an average taken over all tube segments present at time \( t \).

III. CONFIGURATION FIELDS

In order to introduce the configuration field method, we will first describe the method in the spirit of the original CONNFFESSIT approach [Oettinger and Laso (1992) and Laso and Oettinger (1993)]. In this CONNFFESSIT approach, and also in the configuration field method and in the deformation field method, which will be introduced below, the mass and momentum equations governing the flow are solved using the finite element method, but the polymer stress is determined from a microscopic model.

Consider the part of a simple finite element mesh shown in Fig. 1, which is divided into several elements. Although in a real simulation each element contains a few thousand tube segments, for illustrative purposes we consider the special case that each element contains two tube segments only. In each element initially tube segment 1 is aligned vertically, and tube segment 2 is aligned horizontally. Each tube segment is convected by the flow and its orientation changes according to Eq. (3). If the influence of the associated random walkers would not be taken into account, then, because the flow field changes smoothly from element to element, the configurations of ensembles in neighboring elements would remain highly correlated throughout the simulation. However, because each of the tube segments has an individual random walker \( S \), not only are the tube segment orientations reset at uncorrelated random times (when its associated random walker \( S \) is reflected), they are also reset to new uncorrelated random orientations. Therefore in the course of time the initial order will disappear completely (see Fig. 1.) Because the stress in an element is calculated from the configuration of the tube segments it contains, the stress will exhibit wild fluctuations when going from one ele-
ment to another. The numerical approximation for the divergence of the stress (needed in the momentum equation) is calculated from the difference of the stresses in neighboring elements. Since these stresses are obtained from independent polymer configurations, the fluctuations in the divergence of the stress are even more severe. Of course, the noise would go down by increasing the number of tube segments, but we look for a more powerful form of noise reduction.

The problem caused by the fluctuations can be avoided in a very simple way which leads to the concept of variance reduced CONNFFESSIT [see Hulsen et al. (1997) and Ottinger et al. (1997)]. Suppose that instead of assigning an individual random walker $S$ to each tube segment, we associate only one random walker $S_1$ with all tube segments that were initially aligned vertically. Similarly, we associate one random walker $S_2$ with all tube segments that were initially aligned horizontally. The random walkers $S_1$ and $S_2$ evolve completely independently. When $S_1$ is reflected at a boundary, all tube segments associated with $S_1$, in this example the ones that were initially aligned vertically, are reset to a new random orientation. Instead of giving them individual random orientations, we assign one and the same random unit vector to all of them. Thus, immediately after the reflection of a random walker, the corresponding tube segments are perfectly aligned again.

Although tube segments in different elements experience different deformations because the velocity field varies in space, since the velocity field is smoothly varying, they will remain more or less aligned. Therefore, the tube segment configuration and consequently the polymer stress will vary smoothly when going from one element to another. By construction the wild spatial variations in the stress are avoided now, and the number of tube segments required to obtain accurate averages is reduced tremendously.

An actual simulation of the approach proposed above is quite involved. This is because the tube segment configuration is defined only at the particular fluid particles that contain tube segments, i.e., at discrete positions. These fluid particles are convected by the flow and their trajectories have to be determined. Second, to calculate the stress in a certain mesh element, each time step one must determine which fluid particles it contains. Furthermore, because the statistical accuracy is determined by the number of tube segments in a mesh element, one has to ensure that each element contains a sufficiently large number of tube segments. Therefore, to maintain a given statistical error upon mesh refinement, one is forced to use more fluid particles, and one has to make sure that all mesh elements contain a sufficient number of tube segments. Recently Gallez et al. (1999) introduced a new method which adaptively adds or destructs particles where needed.

The problems associated with the tracking of fluid particles and mesh refinement are not present in the configuration field approach. Within this framework, the polymer configuration distribution is represented by a set of $N$ configuration fields. A configuration field defines a polymer configuration at every point of the flow domain. Loosely speaking, it is a kind of continuous interpolation between the tube segment configuration at the positions of the discrete fluid particles discussed above.

The $N$ configuration fields $\{u_k(x,t)\}_{k=1}^N$ are position and time dependent vector fields. These constitute a finite representation for the orientation distribution function of the tube segments. For instance, the tube segment distribution at position $\mathbf{r}$ at time $t$ is given by the set of vectors $\{u_k(\mathbf{r},t)\}_{k=1}^N$. In a typical simulation $N$ is on the order of a few thousand. The evolution equation for a configuration field is derived from that of a single tube segment, Eq. (3)
\[
\frac{D}{Dt} \mathbf{u}_k(x,t) = \mathbf{\kappa}(x,t) \cdot \mathbf{u}_k(x,t) - \mathbf{\kappa}(x,t) : \mathbf{u}_k(x,t) \mathbf{u}_k(x,t) \mathbf{u}_k(x,t),
\]

where \( k = 1, \ldots, N \). These evolution equations are to be interpreted in a Lagrangian sense, because the RHS is evaluated at the position of a fluid particle, while following that particle along its trajectory. Each configuration field has associated with it a single random walker \( S_k \), the evolution of which is governed by a stochastic differential equation, Eq. (4). This random walker is a function of time only, it is not a function of position. Whenever a random walker is reflected, the entire associated configuration field is removed from the simulation, and is immediately reset to a new, and initially spatially uniform, random configuration. Rewriting the material derivative, we obtain the evolution equation for a configuration field in Eulerian form

\[
\partial_t \mathbf{u}(x,t) + \mathbf{v}(x,t) \cdot \nabla \mathbf{u}(x,t) = \mathbf{\kappa}(x,t) \cdot \mathbf{u}(x,t) - \mathbf{\kappa}(x,t) : \mathbf{u}(x,t) \mathbf{u}(x,t) \mathbf{u}(x,t).
\]

The simulation of the tube segment configuration fields is detailed in Sec. IV.

**IV. SIMULATION ALGORITHM**

At the start of a simulation, the configuration fields are initialized as follows:

\[
\mathbf{u}_k(x,0) = \mathbf{u}_k^0,
\]

where \( k = 1, \ldots, N \). Thus, initially the tube segment configuration within each field is spatially uniform. The vector \( \mathbf{u}_k^0 \) at the RHS is a unit random vector, which is drawn from the isotropic distribution on the surface of the unit sphere. Of course, the initial orientation of the fields is uncorrelated. The associated random walkers \( \{S_k\}_k^N \) are set equal to independent random numbers between 0 and 1. In the course of the simulation the configuration fields are updated according to Eq. (7), while the random walkers perform Brownian motion given by Eq. (4). When the random walker \( S_k \) is reflected, the associated configuration field \( \mathbf{u}_k(x) \) is completely removed from the simulation, and is immediately replaced by a new, spatially uniform, random unit vector field. Because the random walkers of the fields evolve independently, the configuration fields disappear at uncorrelated random times. Of course, the new configuration to which the fields are reset are also independent.

It is clear that the random walkers \( S_k \) play an important dynamical role in the simulation. Therefore, the stochastic differential equations governing their motion should accurately be integrated. Indeed, as was shown by Öttinger (1989), a straightforward Euler discretization of the stochastic differential equation, Eq. (4), is not sufficiently accurate, unless extremely small time steps are used in the simulation. This is because while in a continuous description of Brownian motion, a random walker may have been reflected during a time step, this reflection may not be noticed in the discrete implementation. The probability of occurrence of such unobserved reflections can be calculated analytically [see Öttinger (1989)]. In our simulations we use the higher order integration scheme proposed by Öttinger (1989), in which the effect of the unobserved reflections is taken into account. The results of the configuration field calculations are presented at the end of this paper, where they are contrasted to those obtained with a new approach, the deformation field method. This latter approach will be introduced in Sec. V.
V. DEFORMATION GRADIENT FIELDS

In this section we introduce a new approach to simulations of the Doi–Edwards model in complex flow. It provides an alternative to the configuration field approach discussed in Sec. IV. Again, the description is based on the dynamics of the tube segments, but here we will look upon the process from a different point of view.

Our ultimate goal is to obtain an expression for the stress at time \( t \). Therefore, since the stress is completely determined by the tube segment orientation, we have to determine the tube segment distribution at time \( t \). Let us first concentrate on those tube segments which were created in the small time interval \( t' \rightarrow t' + dt' \) in the past (this means that in that time interval their associated random walker was reflected). Since the tube segments are reset to random unit vectors, immediately after their moment of creation, they are distributed isotropically.

Now, after their ‘‘reincarnation’’ two processes commence, operating in parallel. On the one hand the orientation of the tube segments changes because of the action of the flow field. On the other hand, and simultaneously, the associated random walkers keep performing Brownian motion, and whenever a random walker is reflected, its associated tube segment is reset to a new random orientation (this is just the approach followed in the configuration field method outlined above). Thus in the course of time, the number of tube segments created in the time interval \( t' \rightarrow t' + dt' \) which have not yet been reset will gradually decrease. However, the fact that the number of original (i.e., not yet reset) tube segments decreases, can also be taken into account in a probabilistic way. That is, at any time \( t \), to calculate the contribution to the stress of this set of tube segments, we calculate their orientation tensor \( \langle uu \rangle \rangle_t \), as if all original tube segments were still present, and subsequently multiply (i.e., weigh) this tensor by the fraction of the original tube segments that is still present. In this way we find that the contribution of the set of tube segments created in the interval \( t' \rightarrow t' + dt' \) to the momentary stress is given by

\[
d\tau(t) = G\mu(t; t')dt'Q(t; t').
\] (9)

In this expression, the tensor \( Q(t; t') \) denotes the actual orientation tensor of the tube segments

\[
Q(t; t') = \langle uu(t)u(t)\rangle_{t'}.
\] (10)

As was explained above, the brackets denote the average only over those tube segments which were created in the time interval \( t' \rightarrow t' + dt' \); this is underlined explicitly by the subscript \( t' \). The factor \( \mu(t; t')dt' \) in Eq. (9) denotes the number of the original tube segments created in the time interval \( t' \rightarrow t' + dt' \) which have survived to the current time \( t \), relative to the total number of tube segments present. Hence we have

\[
\int_{-\infty}^{t} dt' \mu(t; t') = 1.
\] (11)

For the Doi–Edwards model \( \mu(t; t') \) can be calculated analytically. The result, which is detailed in the Appendix, reads

\[
\mu(t; t') = \frac{8}{\lambda} \sum_{k=0}^{\infty} \exp\left(-\frac{(2k+1)^2\pi^2(t-t')}{\lambda}\right).
\] (12)

The disengagement time \( \tau_d \) is given by the longest relaxation time in this spectrum, so \( \tau_d = \lambda/\pi^2 \). In the present paper we will profitably make use of the available analytical expression for \( \mu(t; t') \). For more advanced reptation models, in which the relaxation
process becomes dependent on the flow history, and for which no analytical solution for 
\( \mu(t; t') \) is at hand, it will be necessary to calculate \( \mu(t; t') \) numerically.

The total stress at time \( t \) is just the sum of the contributions of the tube segments 
which were created in a small interval of time \( dt' \), somewhere in the past,

\[
\tau(t) = G \int_{-\infty}^{t} dt' \, \mu(t; t') \mathbf{Q}(t; t').
\]  

(13)

Let us consider the meaning of this expression. The total ensemble of tube segments 
present at time \( t \) is a collection of subensembles that were created at different times in the 
past. Each of these subensembles can therefore be labeled by the time \( t' \) at which it was 
created. According to Eq. (11), we can interpret the factor \( dt' \mu(t; t') \) as a weight factor.

It specifies the relative importance of the actual orientation tensor \( \mathbf{Q}(t; t') \) of the suben-
semble created between \( t' \) and \( t' + dt' \) to the momentary stress.

In order to evaluate Eq. (13), we have to know the actual orientation \( \mathbf{u}(t) \) for each tube 
segment. Consider a tube segment which at reference time \( t' \) has orientation \( \mathbf{u}(t') \). 
Integrating Eq. (3), the orientation of this tube segment at a later time \( t \), is found to be

\[
\mathbf{u}(t) = \frac{\mathbf{F}(t; t') \cdot \mathbf{u}(t')}{|\mathbf{F}(t; t') \cdot \mathbf{u}(t')|}.
\]  

(14)

In this equation \( \mathbf{F}(t; t') \) is the deformation gradient that describes the cumulative de-
formation of the tube segment between reference time \( t' \) and \( t \). The evolution equation for 
\( \mathbf{F}(t; t') \) is given by

\[
\frac{D}{Dt} \mathbf{F}(t; t') = \mathbf{\kappa}(t) \cdot \mathbf{F}(t; t'),
\]  

(15)

where \( \mathbf{\kappa} \) is the velocity gradient transposed, \( \mathbf{\kappa}(t) = (\nabla \mathbf{v})^T \). Because we consider the 
deformation of a fluid particle while following this particle along its trajectory, the time 
derivative on the left hand side (LHS) is the material derivative.

For the following discussion, Eq. (14) is of crucial importance. It implies that the 
actual orientation of a tube segment can be obtained knowing only its original orientation 
at its moment of creation and the accumulated deformation contained in \( \mathbf{F}(t; t') \). Therefore, 
instead of calculating the evolution of the tube segment orientation itself directly, we can equivalently 
keep track of the deformation gradient tensor. The concept is explained graphically in Fig. 2.

Now, imagine a polymer melt under flow and consider an infinitesimal fluid particle in 
this melt. Of all tube segments contained in this fluid particle, consider the \( N \) segments 
which were created at time \( t' \). Then, at \( t' \) the collection of tube segments \( \{\mathbf{u}_k(t')\}_{k=1}^{N} \) 
is distributed isotropically on the surface of the unit sphere. As mentioned above, at a 
later time \( t \), the new orientation of tube segment \( k \) is given by

\[
\mathbf{u}_k(t) = \frac{\mathbf{F}(t; t') \cdot \mathbf{u}_k(t')}{|\mathbf{F}(t; t') \cdot \mathbf{u}_k(t')|}.
\]  

(16)

This expression defines the mapping that transforms the initial tube segment distribution 
\( \{\mathbf{u}_k(t')\}_{k=1}^{N} \) to the tube segment distribution at time \( t \). The deformation gradient 
\( \mathbf{F}(t; t') \) has to be evaluated over the trajectory that the fluid particle has traversed. Note 
that the deformation gradient \( \mathbf{F}(t; t') \) is the same for the \( N \) tube segments, because they 
are always contained in the same fluid particle.
Obviously, a way to obtain $F(t; t')$ is to keep track of the fluid particle trajectories and to integrate Eq. (15) along these trajectories. However, since the fluid is a continuum, fluid particles are present everywhere, and therefore, instead of keeping track of individual unconnected particle trajectories along which $F(t; t')$ is evaluated, we introduce deformation gradient fields $F(x, t; t')$. That is, we define the deformation gradient at any position in the flow domain. This is underlined by the explicit presence of $x$ in the notation $F(x, t; t')$. The evolution equation for the deformation gradient fields follows from Eq. (15)

$$\frac{D}{Dt} F(x, t; t') = \kappa(x, t) \cdot F(x, t; t').$$

In passing we remark that in this equation $t'$ is a fixed, but arbitrary, reference time. Exactly in the same way as in the case of the configuration fields, the Eulerian equivalent of this equation reads

$$\partial_t F(x, t; t') + v(x, t) \cdot \nabla F(x, t; t') = \kappa(x, t) \cdot F(x, t; t').$$

In order to complete the evolution equation of a deformation gradient field, we have to specify the appropriate initial condition at time $t'$. This is easy: immediately after time $t'$ the fluid has not yet been deformed with respect its shape at $t'$, so at that time, at any position, the deformation gradient is just equal to the unit tensor

$$F(x, t'; t') = \delta.$$

Let us now return to the stress tensor and investigate how it can be expressed in terms of deformation gradient fields. The polymer stress at position $x$ is given by

$$\tau(x, t) = G \int_{-\infty}^{t} dt' \mu(t; t') Q(x, t; t'),$$

where the orientation tensor $Q(x, t; t')$ is given by

\[Q(x, t; t') = \text{orientation tensor value}\]
\[ Q(x,t{:}t') = \langle u(x,t)u(x,t) \rangle_{t'}. \]  

Using Eq. (16), the orientation tensor \( Q(x,t{:}t') \) can be expressed in terms of the tube segment orientation of the subensemble at the moment of creation \( t' \) and deformation gradient field

\[ Q(x,t{:}t') = \left( \frac{(F(x,t{:}t') \cdot u(t'))(F(x,t{:}t') \cdot u(t'))}{|F(x,t{:}t') \cdot u(t')|^2} \right)_{t'}. \]  

In principle, since the distribution of the tube segments immediately after their creation is isotropic, we could drop the \( t' \) dependence of the brackets. However, we deliberately included it; as we will soon see, this is a key ingredient to efficient calculations using our new simulation method.

VI. SIMULATION ALGORITHM

In the numerical implementation, the integral in the expression for the stress, Eq. (20), is of course replaced by a sum. Suppose we use a numerical time step \( \Delta t' \), in the simulation. This means that the reference times \( t' \) at which subensembles are created now constitute a set of discrete times \( t'_k = t - k \Delta t' \), where \( k = 0,1,2,\ldots,\infty \). Consequently also the values of the orientation tensors \( Q(x,t{:}t') \) are known at these discrete times only. To calculate the integral Eq. (20), however, we approximate the value of \( Q(x,t{:}s) \) for times \( s \) intermediate to two discrete times by linear interpolation. That is, we introduce linear top-hat base functions \( \phi_k(t) \), ubiquitous in finite element analysis, and for any time \( s \leq t \), the value of \( Q(x,t{:}s) \) is approximated as follows:

\[ Q(x,t{:}s) = \sum_{k=0}^{\infty} Q_k(x,t{:}t'_k) \phi_k(s). \]  

In this equation, the base function \( \phi_k \) is piecewise linear and nonzero only on the interval \([t'_{k-1},t'_{k+1}]\). It is completely determined by its values at \( t'_{k-1}, t'_k \) and \( t'_{k+1} \): \( \phi_k(t'_{k-1}) = 0, \phi_k(t'_k) = 1 \) and \( \phi_k(t'_{k+1}) = 0 \). Note that the intervals on which the base functions are defined need not be of equal width. As we will see at the end of this section this is of crucial importance for efficient simulations. Inserting this approximation in Eq. (20) and performing the integration, we obtain

\[ \tau(x,t) = G \sum_{k=0}^{\infty} W_k Q_k(x,t{:}t'_k). \]  

Because the base functions \( \phi_k(t) \) are piecewise linear, the error in Eq. (24) is of second order. This equation defines the quantity \( W_k \)

\[ W_k = \int_{-\infty}^{t} dt' \mu(t{:}t') \phi_k(t'). \]  

In fact, \( W_k \) specifies the relative importance of the actual orientation tensor associated with the \( k^{th} \) subensemble, \( Q_k(x,t{:}t'_k) \), in the summation. Because the relative importance of the subensembles decreases with increasing age, the infinite sum in Eq. (24) is naturally truncated, and
This truncation also limits the number of deformation fields used in the simulation to $N$. Note that the weights $W_k$ are constants; they are calculated only once, at the start of the simulation.

The orientation tensors $Q_k(\mathbf{x}, t; t'_k)$, in Eq. (26) are given by

$$Q_k(\mathbf{x}, t; t'_k) = \langle \mathbf{u}(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \rangle_{t'}.$$

i.e., they denote the orientation tensors, calculated from the actual orientation distribution of the subensemble of tube segments which were created at $t'_k$. In the simulation we replace the integral over the actual tube segment distribution function (as implied by the brackets) by an average over a finite ensemble of tube segments. That is, in the simulation each subensemble consists of $T$ tube segments and the actual orientation tensor of each subensemble is approximated as follows:

$$Q_k(\mathbf{x}, t; t'_k) \approx \frac{1}{T} \sum_{j=1}^{T} \mathbf{u}_j(\mathbf{x}, t) \mathbf{u}_j(\mathbf{x}, t).$$

Since at their moment of creation $t'_k$ the tube segments should be distributed isotropically, in the simulations we take care that the $T$ tube segments are initially distributed evenly over the surface of the unit sphere. How this is done exactly will be discussed in Sec. VII.

At any time, the actual orientation $\mathbf{u}_j(\mathbf{x}, t)$ of each tube segment can be calculated from its initial orientation and the accumulated deformation gradient field

$$\mathbf{u}_j(\mathbf{x}, t) = \frac{\mathbf{F}(\mathbf{x}, t; t'_k) \cdot \mathbf{u}_j(t'_k)}{\left| \mathbf{F}(\mathbf{x}, t; t'_k) \cdot \mathbf{u}_j(t'_k) \right|}.$$

We parenthetically remark that it is only the deformation gradient fields $\mathbf{F}(\mathbf{x}, t; t'_k)$ that evolve in time, the initial tube segment orientations are time independent, of course.

To explain the steps in the deformation field algorithm, we consider the most straightforward implementation in which the integral, Eq. (20), is discretized using a constant time step $\Delta t$. Suppose that the Doi–Edwards fluid has been at rest and that starting at $t = 0$ an external flow is enforced. This means that until $t = 0$ the subensembles have not been deformed, so

$$\mathbf{F}(\mathbf{x}, 0; t'_k) = \delta.$$
deformation of the flow field, this newly added deformation field starts its life as a unit tensor throughout the flow domain, and its initial weight is $W_0$.

An important disadvantage of this straightforward approach is that it requires a large number of deformation fields to be used in the simulation. This is because the discretization of the integral, Eq. (20), should meet two requirements. On the one hand, the time step used in the discretisation should be small enough to capture the steep decay of $\mu(t; t')$ for $t' \approx t$. On the other hand, the integral should only be truncated after a sufficient number of longest relaxation times; this in order to ensure that also the influence of deformations that occurred some relaxation times ago, is taken into account. Thus, if we discretize the integral using a constant time step $\Delta t$, then if we use $N$ deformation fields, only the behavior of $\mu(t; t')$ in the interval $[0, N\Delta t']$ is taken into account. This means that the fluid only remembers deformations that occurred no longer than a time $N\Delta t'$ ago. Therefore, in order for the product $N\Delta t'$ to be sufficiently large, the number of deformation fields, $N$, would have to be large.

A way to overcome this difficulty was proposed by Peters et al. (1999). The key idea of this method is to approximate the integral Eq. (20) using a partitioning in which the intervals of the base functions $\phi_k$ gradually increase in size. That is, in the region where $t' = t$, i.e., the region where $\mu(t; t')$ shows a steep decrease, a fine partitioning is used, equal to the time step $\Delta t$ used in the integration of the momentum equation. For times $t'$ more in the past, i.e., for increasing $t - t'$, the memory kernel $\mu(t; t')$ gradually approaches a slowly varying single exponential, see Eq. (12). In that region it is unnecessary to use the fine partitioning, and instead larger intervals are used here. In our simulations we used 100 deformation fields, and to approximate the integral Eq. (20), we partitioned the past in 100 intervals of gradually increasing width. Starting from the actual time $t$ and going into the direction of the past, we partitioned the time axis as follows: we use 25 intervals of $\Delta t'$, followed by 25 intervals of $2\Delta t'$, 10 intervals of size $4\Delta t'$, 10 intervals of size $8\Delta t'$, 10 intervals of size $16\Delta t'$, 10 intervals of size $32\Delta t'$ and 10 intervals of size $64\Delta t'$. This means that the integral Eq. (20) is truncated after $1315\Delta t'$. In our simulations we take $\Delta t' = \tau_d/100$, so Eq. (20) is truncated after approximately $13\tau_d$.

VII. GENERATION OF SUBENSEMBLES

From the point of view of accuracy, the ideal subensemble should resemble the isotropic distribution on the surface of the unit sphere. From the point of view of simulation time the ideal subensemble is of minimal size simply because larger subensembles result in a stress calculation that takes more time. At first sight these two requirements seem incompatible since a small statistical error is usually thought to be synonymous with a large ensemble size. However, this is not necessarily true, and indeed, in the underlying case the correct reasoning is somewhat more subtle. Essentially this is because in the deformation field approach we have decoupled the tube segment statistics from the tube segment deformation, whereas in the configuration field approach both the statistics and the deformation are ‘carried’ by individual tube segments. As was explained above, in the deformation field approach, the statistics are taken into account by means of the weights $W_k$: tube segments or subensembles are no longer destroyed and replaced individually, but these effects are now reflected by the gradually decreasing weights. The purpose of the tube segments in a certain subensemble is to store the deformation that the subensemble experienced since its moment of creation. In fact this deformation defines a mapping which assigns to each point on the surface of the initial unit sphere a new point, also on a unit sphere. Because the initial distribution is isotropic, each point on the unit
sphere is equally probable. However, due to the deformation, the points will attain a new position on the unit sphere, and gradually regions will occur with a high density of points, while other regions on the sphere surface become depleted of points. To optimally capture the deformation with a finite number of points on the sphere surface, these points should initially be distributed evenly on the surface.

A straightforward way to generate subensembles which have the desired isotropic character is to use well-known routines that produce random unit vectors. For it is then guaranteed that in the limit of infinite subensemble size $T \to \infty$, these unit vectors are distributed isotropically on the unit-sphere surface. From our simulations, however, we found that this straightforward implementation is far from optimal. Even for subensembles of size $T = 2000$ the moments generated by such subensembles show substantial differences with respect to those generated by the exact isotropic probability distribution $p = 1/4\pi$. In other words, due to the statistical fluctuations implied by the finite size of the subensemble, the tube segments of a subensemble generated in this way are not really evenly distributed over the surface of the unit sphere. Clearly, if the initial configuration is biased, there is little hope of obtaining an accurate representation of the deformation that occurs afterwards.

This observation prompted us to use a different strategy. Suppose we fix the subensemble size $T$ to 20 only. This typically is the size we use in our simulations. Instead of picking 20 (uncorrelated) unit vectors at random, we generate subensembles of tube segments which are evenly distributed on the surface of the sphere. This allows us to measure deformations with respect to an unbiased initial distribution of tube segments. Indeed, our simulations show that the results obtained using these small, but initially evenly distributed subensembles, outperform those using subensembles consisting of 2000 unit vectors which are picked at random! The evenly distributed subensembles can be generated using standard numerical methods to distribute a given number of points evenly on a sphere. The coordinates of these points then define the desired tube segment orientations of an initial subensemble. To obtain statistically independent subensembles for different deformation fields, one can either repeat this procedure, or one can rotate the first subensemble randomly as a solid body. In our simulations we used the latter method.

VIII. COMPARISON OF THE TWO METHODS

Although from a theoretical point of view the two approaches to the Doi–Edwards model are completely equivalent, there are important differences in practical efficiency. Regarding the equivalence, Eq. (14) is the solution of the differential equation, Eq. (3). Similarly, we exploited the relationship between the stochastic differential equation, Eq. (4), and the solution of its corresponding, equivalent, Fokker–Planck equation to replace the simulation of individual random walkers by the memory kernel $\mu(t;t')$. Given the theoretical equivalence, the merit of either method is determined by its practical efficiency, and it is here that substantial differences show up.

Note that in the configuration field method we already greatly reduced the computer memory requirements in comparison to a CONNFFESSIT interpretation, in that, instead of assigning an individual random walker to each tube segment, we only have one random walker per configuration field. In a typical simulation, we need a few thousand configuration fields, so the memory requirements put forward by the random walkers are completely negligible. However, we must store the tube segment configuration (i.e., the three vector components) at four points in each element (see Sec. IX). At a typical mesh, this corresponds to memory requirements on the order of a few hundred megabytes. Therefore, the upper limit of the number of configuration fields is dictated by the com-
puter memory available. Apart from the memory requirements, each time step every configuration field is convected and deformed, which results in substantial calculation time.

Now consider the deformation field method. Since we consider two-dimensional, planar flow, a deformation field has four components. Note that only three of these components are actually independent, since for incompressible flows $\det \mathbf{F} = 1$. In our simulations, however, we did not yet take advantage of this fact. The typical number of fields needed in a simulation is 100. This means that in comparison to the configuration field approach, we gain a tremendous reduction in memory demands. Moreover, since only 100 fields are to be convected and deformed now, as opposed to 2000 configuration fields, the time spent at updating the fields is reduced by a factor of 20.

However, to positively identify the deformation field approach as the most efficient of the two methods, we still have to compare the times the two methods spend at calculating the stress. For, in the deformation field approach, in order to find the momentary stress, we first have to determine the actual tube segment orientation of a subensemble from its reference subensemble via the mapping Eq. (14). This, of course, is not necessary in the configuration field method, because there the actual tube segment orientation is the primary simulation variable. Clearly, if the size $T$ of the subensembles were on the order of the number of fields in the configuration field approach, then in the case of the deformation field method the calculation of the contribution of a field to the stress would be more expensive than that in the case of configuration fields. However, as we will see in Sec. IX, subensembles of size as small as $T = 20$ provide results that outperform those of a 2000-sized configuration field calculation. Thus, not only is the stress calculation in the case of the deformation fields much faster, but its results will turn out to be much more accurate than those obtained using random walkers.

**IX. NUMERICAL METHODS**

The flow problem is solved by means of the finite element method. The mesh elements are quadrilaterals and the velocity and pressure are approximated by continuous bi-quad-ratic and discontinuous linear polynomials, respectively. Both the configuration fields and the deformation fields are treated by the discontinuous Galerkin method, i.e., they are approximated by bilinear polynomials which are discontinuous across the elements. This implies that four storage points per element are needed to store the fields. This discontinuous Galerkin implementation is particularly suited for the calculation of the convection terms in the evolution equations.

In the deformation field method, apart from the momentum and continuity equations, we also have to integrate the evolution equations of the deformation fields, Eq. (18). In our simulations we use a simple Euler forward discretization. Thus, using a numerical time step $\Delta t$, we have

$$F(x, t_{n+1}; t') = F(x, t_n; t') + \Delta t [-\mathbf{v}(x, t_n) \cdot \nabla F(x, t_n; t') + \kappa(x, t_n) \cdot F(x, t_n; t')]$$

(31)

The continuity and momentum equations are solved using the so-called DEVSS method. This combination of the DEVSS method with the discontinuous Galerkin method was introduced by Baaijens et al. (1997), and is found to result in a remarkably stable method. Further details concerning the implementation of the method are discussed in Hulsen et al. (1997) and in Peters et al. (1999).
As a final point of interest, note that since we simulate a polymer melt system, there is no solvent viscosity present in the system. Since we will consider inertialess flow, the absence of any solvent viscosity implies that the momentum equation reads
\[ 0 = \nabla p + \nabla \cdot \tau, \]
\[ \text{Eq. 32} \]
i.e., the velocity no longer occurs in the equation. This means that we can no longer solve for the velocity in the simulation! Inspired by the approach of Viriyayuthakorn and Caswell (1980), we circumvent this problem and modify the momentum equation such that it explicitly contains the velocity to be calculated, as follows:
\[ 0 = -\nabla p + C \nabla^2 (v_{n+1} - v_n) + \nabla \cdot \tau_{n+1}. \]
\[ \text{Eq. 33} \]
In this equation \( v_{n+1} \) denotes the velocity at the next time step that we have to solve for, and \( v_n \) denotes the current velocity. Obviously, when steady state is attained \( v_{n+1} \rightarrow v_n \) and Eq. (33) reduces to the original inertialess momentum equation, Eq. (32), again. In our simulations we take the constant \( C \), which has the dimension of viscosity, to be \( C = G \Delta t \), where \( G \) is the modulus of rigidity of the Doi–Edwards model and \( \Delta t \) is the time step used in the simulation. Therefore the term added to the original momentum equation, Eq. (32), is of order \( (\Delta t)^2 \).

**X. RESULTS**

We consider inception of two-dimensional flow past a cylinder confined between two parallel plates (see Fig. 3). The radius of the cylinder is \( R \). We take the distance \( H \) between the plates to be twice the cylinder diameter, i.e. \( H = 4R \). The length \( L \) of the simulation domain is taken to be 30 cylinder radii, \( L = 30R \). Although we are interested in the flow past a single cylinder, we use periodic boundary conditions in the flow direction. This means that we actually solve the flow past an infinite number of cylinders. An important motivation for this particular implementation is the fact that in this way we avoid the explicit specification of the configuration fields and the velocity field at the inflow boundary; note that such an explicit specification would be particularly cumbersome in the case of transient flows. In our simulations we take the length \( L \) of the simulation domain to be sufficiently large \( (L = 30R) \) to ensure that there is no interaction of our central cylinder with its periodic images and that the flow profile at the exit of the simulation domain is fully developed. Furthermore, we assume no-slip boundary conditions at the walls and at the surface of the cylinder.

In our calculations we neglect inertia, so the flow is characterized by one dimensionless group, the Weissenberg number \( We \). The Weissenberg number is the ratio of the
characteristic relaxation time of the polymer melt and the characteristic time of the flow.

The characteristic relaxation time of the melt is the reptation or disengagement time \( \tau_d \), given by \( \tau_d = \lambda / \pi^2 \) [see Eq. (12)].

We investigate the situation where, starting at a certain time, a constant flow rate \( Q \) is enforced. Thus, the characteristic velocity between the plates \( V \) is given by \( V = Q / H = Q / 4R \) and the resulting characteristic time of the flow is \( R / V \). The Weissenberg number is thus found to be \( We = \lambda Q / 4 \pi^2 R^2 \).

The results of the calculations are presented in dimensionless form. The length scales in the problem are nondimensionalized by the cylinder radius \( R \) and the velocities by \( V \). In order to present the results, we introduce a Cartesian coordinate system, the origin of which coincides with the center of the cylinder. The \( x \) axis is parallel to the two plates. In our simulations we take \( \lambda Q / R^2 = 4 \), so the Weissenberg number evaluates to \( We = 1 / \pi^2 \).

In the following, we will compare two independent configuration field calculations to the deformation field result. The configuration field calculations were performed using a collection of \( N = 2000 \) configuration fields. The result of the deformation field method was obtained using \( N = 100 \) deformation fields, each of which had associated with it a subensemble of size \( T = 20 \) tube segments. The calculations were performed on the same finite element mesh, the central part of which is shown in Fig. 4. The simulation time of a deformation field calculation (on a typical workstation) is on the order of a few hours, and this turns out to be approximately three times faster than a configuration field calculation.

An important quantity is the force per unit length \( F \) that the melt exerts on the cylinder. We define a nondimensional force per unit length \( K \) by the following relation: \( K = F / \eta_0 V \). In this equation, \( \eta_0 \) is the zero-shear-rate viscosity, and for the Doi–Edwards model \( \eta_0 = G \lambda / 60 \). In Fig. 5, we present the simulation results for \( K \). Figure 5 shows the results of the two independent configuration field calculations (i.e., starting from independent initial tube segment configurations and using other random walkers) as well as the result of the deformation field method. The results clearly demonstrate the shear-thinning behavior of the melt, for when using a Newtonian fluid, the value of \( K \) would be approximately 132, [see Hulsen et al. (1997)]. Note that the deformation field result for the drag coefficient shows a slight overshoot before reaching the steady state. In contrast, the fluctuations in the configuration field calculations completely mask this overshoot. The large fluctuations appearing in the configuration method are absent in the deformation field method. This is because in the configuration field approach a complete field is reset when its random walker is reflected. The deformation field description, however, is based on weights which are determined from the probability density for the tube segment lifetime distribution, instead of single stochastic realizations. In principle the fluctuations in the configuration results could be reduced simply by using a larger number of configuration fields. This is beyond our reach since the underlying configuration field simulations require almost 300 Mbyte of computer memory. The computer memory problem is absent in the deformation field method, because there only as few as
100 fields are used. In order to determine whether 100 deformation fields are sufficient to obtain accurate results, we also performed a simulation using 200 deformation fields, each of which also had a subensemble of 20 tube segments. The results were found to virtually superimpose, indicating that the memory of the fluid is well captured. Furthermore, to ensure that an ensemble size of 20 tube segments is sufficiently large, we also compared the results with those of a simulation using 100 fields each of which had a subensemble size of 40. In this case too, we found perfect agreement, indicating that an ensemble size of 20 is sufficiently large.

It is interesting to contrast the melt results with the results of a Newtonian fluid in the same geometry. In this respect, it is convenient to introduce a local Weissenberg number to quantify different flow regions in the domain. This local Weissenberg number $W_{e_f}$ is defined as the product of the characteristic polymer relaxation time, the disengagement time $\tau_d$, and the local shear rate $\dot{\gamma}$, so $W_{e_f} = |\tau_d \dot{\gamma}|$. From our simulations, we found that the velocity profile at the entrance of the domain is parabolic to good approximation, and the velocity gradient is nearly linear. At that position the local Weissenberg number

![Graph](image)

**FIG. 5.** Simulation results for $K$, the dimensionless force per unit length exerted on the cylinder. Shown are the results of two independent configuration field calculations, each using 2000 configuration fields; the smooth curve is the result of a deformation field calculation using 100 fields and associated subensembles of size 20. The inset figure shows that the deformation field calculation is able to reveal a slight overshoot.

![Graph](image)

**FIG. 6.** Profiles of the dimensionless velocity in the gap between the cylinder and the wall. Shown are the three results for the Doi–Edwards model: the two independent configuration field calculations (dashed lines) and the result obtained using the deformation field method (solid line). For comparison, also the velocity profile of a Newtonian fluid is shown (dotted line).
We, based on the velocity gradient at the wall, is approximately equal to $1.5/p^2$, and the melt behavior is close to Newtonian behavior.

Figure 6 shows the velocity profiles of the Doi–Edwards model and the velocity profile of a Newtonian fluid, in the gap between the cylinder and the wall. In this region the behavior of the Doi–Edwards model and that of the Newtonian fluid differ. As shown in Fig. 7, the velocity gradient at the surface of the cylinder increases more rapidly. The local Weissenberg number at the surface of the cylinder $\tilde{W}_e$ based on the velocity gradient at the surface of the cylinder evaluates to $\tilde{W}_e \approx 30/p^2$. Clearly, in this region the melt behavior is completely different from that at the entrance. At velocity gradients of this magnitude the effect of the well-known extreme shear-thinning behavior of the Doi–Edwards model shows up, and results in a velocity boundary layer at the cylinder surface.

In Fig. 8 the contour levels of the $xx$ component of the orientation tensor $\langle uu \rangle$ in steady state are shown. Apart from the constant modulus of rigidity $G$, this tensor is equal to the stress tensor [see Eq. (5)]. The upper half of the figure shows the result of a configuration field calculation, the lower half shows the same contour levels, but obtained with the deformation field method. As was already mentioned before, even in steady state the results of the configuration field method will fluctuate. Therefore, if the contour levels

FIG. 7. The component $\partial u_x/\partial y$ of the dimensionless velocity gradient in the gap between the cylinder and the wall. The three nearly superimposing curves are the results for the Doi–Edwards model: the two independent configuration field calculations (indicated by the dashed line and the dotted line) and the result obtained using the deformation field method (solid line). For comparison, also the result of a Newtonian fluid is shown (isolated dashed line).

FIG. 8. The $xx$ component of the orientation tensor $\langle uu \rangle$. The upper half shows the result of a configuration field calculation, the lower part is the result of a deformation field calculation.
in the upper half of Fig. 8 would be monitored in time, they would be found to "oscil-
late" around an average value.

In Figs. 9, 10 and 11, we compare the components of the orientation tensor obtained from the two independent configuration field simulations with those from the deformation field method. The results give information on the alignment of tube segments in the flow, and its components should be compared to those in equilibrium (i.e., in absence of flow), in which case the tube segments are distributed isotropically, and $\langle uu \rangle = \delta / 3$. From the two configuration field results, we get an impression of the statistical error due to the finite number of configuration fields used in the simulation (see Fig. 9); the relative error turns out to be approximately 3%.

**FIG. 9.** The $xx$ component of the orientation tensor $\langle uu \rangle$. The solid line shows the deformation field result, the dashed lines are the results of the two independent configuration field results. The component is evaluated along the line $y = 0$, until $x = -1$. Starting at $x = -1$, we follow the cylinder surface, until $x = 1$, and starting at $x = 1$, we follow the line $y = 0$ again.

**FIG. 10.** The $xy$ component of the orientation tensor $\langle uu \rangle$. The solid line shows the deformation field result, the dashed lines are the results of the two independent configuration field results. The component is evaluated along the line $y = 0$, until $x = -1$. Starting at $x = -1$, we follow the cylinder surface, until $x = 1$, and starting at $x = 1$, we follow the line $y = 0$ again.
XI. CONCLUSIONS

We simulated the inception of flow of the Doi–Edwards model in a complex geometry. Two different methods were used: the configuration field method and the deformation field method. This deformation field method is a new approach that we introduced in this paper. From a theoretical point of view the two methods are equivalent.

To assess the efficiency of the methods, we contrast the simulation results of the two approaches. In both approaches we consider the situation where at each point in the flow domain a total ensemble of 2000 tube segments is defined: in the configuration field calculations we use 2000 configuration fields and in the deformation field approach 100 deformation fields are used, each of which has an associated subensemble consisting of 20 tube segments. Comparing the memory requirements, the deformation field approach reduces the demands of the configuration method by a factor of 20, so within this approach there is ample room for mesh refinement. Furthermore, the time it takes to perform a time step in the deformation field method is approximately three times less than the time spent in a step of the configuration field approach. Finally, the large fluctuations present in the configuration field approach are absent in the deformation field method.

Thus, the deformation field approach introduced here is very efficient. Moreover, the method is very promising because it opens up possibilities of studying generalizations of the Doi–Edwards model which also include important mechanisms such as tube stretch and convected constraint release.

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APPENDIX A: CALCULATION OF THE MEMORY KERNEL $\mu$

Whenever a random walker is reflected, the corresponding tube segment is reset to a new random direction. Therefore, in the course of time the fraction of tube segments which has not been reset since their time of creation will gradually decrease. Using the
equivalence between the stochastic differential equation for the random walker $S$ and the corresponding Fokker–Planck equation, this fraction can be calculated analytically see Öttinger (1996). It is found that the fraction of tube segments which were created at or before time $t'$ and are still present at time $t$ is given by

$$P(t; t') = \frac{8}{\pi^2} \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2} \exp\left(-\frac{(2k+1)^2 \pi^2 (t-t')}{\lambda}\right). \quad (A1)$$

Note that this probability is equal to the fraction of all tube segments present at $t'$ and still present at $t$. Now, since the tube segments which are present at time $t'$ were born somewhere before time $t'$, we can write

$$P(t; t') = \int_{-\infty}^{t'} \chi(t; s) ds. \quad (A2)$$

From the definition of $P(t; t')$ it then follows that $\chi(t; s) ds$ is the fraction of tube segments created in the interval between $s$ and $s+ds$ which are still present at time $t$ [where it is understood that $P(t; t')$ is normalized such that $P(t; t') = 1$]. This is just the fraction that we are looking for, so $\chi(t; t') = \mu(t; t')$. From Eq. (A2) it follows that

$$\mu(t; t') = \partial_t P(t; t'). \quad (A3)$$

Substituting for $P(t; t')$ from Eq. (A1), we finally obtain

$$\mu(t; t') = \frac{8}{\pi^2} \sum_{k=0}^{\infty} \exp\left(-\frac{(2k+1)^2 \pi^2 (t-t')}{\lambda}\right). \quad (A4)$$

References


