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STUDY OF MICROMECHANICAL NUMERICAL MODEL APPROACH OF THE BROWNIAN DYNAMICS FORBIPOLYMER NETWORK

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ABSTRACT

A detailed understanding of biopolymer networks can be considered a corner stone for future developments in many fields of modern science and engineering ranging from biophysics and biochemistry to bioengineering, biomedical engineering and material science.Biopolymer networks consist of three essential components: filaments, crosslinker molecules connecting them by chemical bonds, and a viscous fluid into which filaments and crosslinker molecules are embedded. These three components are modelled as continua. On the level of single filaments, the laws of statistical mechanics have significant impact to the equations of motion.In so far proposed micromechanical models, those based on bead-spring discretizations, this is accounted for only in a purely heuristic manner. In opposition to that, filament dynamics is discretized in a stringent mathematical way starting from first principles of Newtonian and statistical mechanics. The numerical model's capacity to re-produce the viscoelastic moduli of biopolymer networks on biologically relevant length and time scales is demonstrated.

Keywords: biopolymer networks, Brownian dynamics, crosslinker, linkers, filaments.

I. INTRODUCTION

Biopolymer networks are formed by three main constituents: polymer filaments, crosslinker molecules (referred to also as 'linkers' in the following which connect these filaments by transient chemical bonds, and a background fluid into which filaments and linkers are embedded. The background fluid is typically an aqueous solution and therefore nearly transparent. The size of the linkers on the other hand ranges on the nanometer scale. The variety of completely different network architectures which can be formed by one and the same kind of filament just by the application of different linkers is remarkable.

It is pointed out in detail how the Brownian dynamics of rod-like continua such as filaments in biopolymer networks can be modeled numerically. In general, motion and deformation of filaments in biopolymer networks in vivo occur in three dimensions. However, in certain experiments filament motion is confined to two dimensions either by a thin gap between two plates [1] or by certain proteins fixing the filaments to a plate [2]. The reason for this is that several experiments could be conducted in planar settings only so far. Moreover, also

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for certain processes in vivo such as the formation of lamellipodia, two dimensional deformation is assumed to play an important role. Although two dimensional filament dynamics can be simulated also by means of three dimensional computer models with suitable boundary conditions, genuinely two dimensional numerical models may be preferred in these cases due to their simplicity and much higher efficiency.

II. NUMERICAL MODEL OF THE BROWNIAN DYNAMICS OF ROD-LIKE CONTINUA

2.1 Equation of Motion

A rod-like structure (referred to below simply as 'rod') of length L in $m_t \in \{2;3\}$dimensions can be modeled as a one-dimensional Cosserat continuum embedded into R^{m_t}. To this end, we assume that the geometry of the structure can be modeled at a certain point in time by some curve in space, the neutral line, to each point of which some plain cross section is assigned. For simplicity, we assume in the following that the cross sections at all points of the neutral line are congruent. Let $\xi \in [0;L]$ be the curve parameter of the neutral line. Then this line can be described in the time interval $[0;t_{max}]$ by the function:

$$x : [0; L] \times [0; t_{max}] \rightarrow R^{m_t}(\xi, t) \rightarrow x(\xi, t) \qquad (1.1)$$

To uniquely characterize the orientation of the cross section at each curve point, we define the rotation field

$$\theta : [0; L] \times [0; t_{max}] \rightarrow R^{m_r}(\xi, t) \rightarrow \theta(\xi, t) \qquad (1.2)$$

with $m_r = \binom{m_t}{2}$ for $m_t \in \{2;3\}$. The rotation $\theta(\xi,t)$is only for $m_t = 2$ a vector, whereas for $m_t = 3$ it is just a pseudo-vector. In either case, it corresponds to a spin matrix $S(\theta(\xi,t))$ and an orthonormal triad $R(\theta(\xi,t))$ whose columns $R_i(\theta(\xi,t))$ represent the principal axes of the cross section at $x(\xi,t)$.

Thus, (1.1) and (1.2) together uniquely characterize the cross section position and orientation in space. As a consequence, the motion and deformation of the polymer in time is completely.

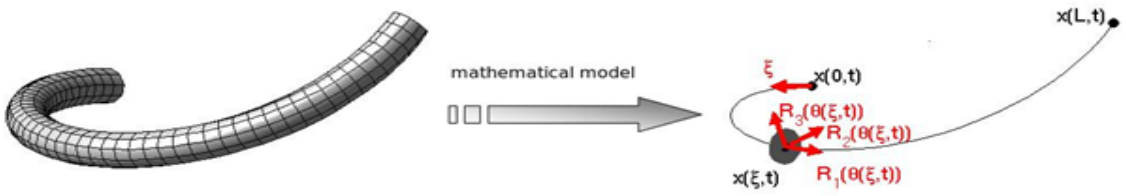

Figure1.1: Tomodelthemechanicsofarod-likecontinuumoflengthLattimetmathematically, a curve $x(\xi,t)$ with curve parameter $\xi \in [0;L]$ is defined, the neutral line. To each point $x(\xi,t)$ of the neutral line a cross section (illustrated by a circular disc) is assigned whose orientation in space is given by the column vectors $R_i(\theta(\xi,t))$ of a triad $R(\theta(\xi,t))$.

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Described by the two functions x and θ. Let the stress-free initial configuration of the polymer at time t = 0 be given by:

$$x^0 : [0, L] \rightarrow R^{m_t},\ \xi \rightarrow x^0(\xi) = x(\xi) \qquad (1.3)$$

$$\theta^0 : [0; L] \rightarrow R^{m_r},\ \xi \rightarrow \theta^0(\xi) = \theta(\xi) \qquad (1.4)$$

Then with proper boundary conditions at ξ = 0 and ξ = L the functions x and θ can be computed from the balance of linear and angular momentum, i.e. from:

$$f_{el}(x, \theta, \xi, t) + f_{visc}(x, \theta, \xi, t) = f_{ext}(x, \xi, t) + f_{stoch}(x, \theta, \xi, t) \qquad (1.5a)$$

$$m_{el}(x, \theta, \xi, t) + m_{visc}(x, \theta, \xi, t) = m_{ext}(x, \theta, \xi, t) + m_{stoch}(x, \theta, \xi, t) + x^0(\xi, t) \times f_s(x, \theta, \xi, t) \qquad (1.5b)$$

Here f_{visc}, m_{visc}, f_{stoch}, m_{stoch}, f_{ext}, m_{ext} are the viscous, stochastic and deterministic external force and moment loads per unit length. The tangent of the neutral line is denoted by $x'(\xi,t) := \partial x(\xi,t)/\partial\xi$. The elastic section force f_s and the elastic section moment m_s are, as usual for one-dimensional continua, defined as the integral and resulting moment of the internal stresses. The derivatives of the section force and moment with respect to ξ are f_{el} and m_{el} respectively.

2.2 Elastic forces and moments

Single-molecule experiments have successfully demonstrated that on a micrometer scale rods can still be modeled as continua with stretching, bending and torsion stiffness employing the linear strain measures common for beams in structural engineering. Thus the elastic forces and moments in these structures can be determined similarly as in macroscopic structural mechanics. In principle, they can be calculated on the basis of any nonlinear beam theory, especially on the basis of the Euler-Bernoulli and Reissner theory. In the following, we will denote by E and G the beams Young's and shear modulus. In BD simulations, special attention has to be payed to the definition of the geometric quantities J_r, J_i, A, and A_i. These quantities are defined in BD simulations not only as polar moment of inertia, momentofinertiaofareawith respect ttothei-thprincipalaxis,crosssectionandshearcorrected cross section with respect to the i-th principal axis, but rather as these quantities multiplied by some 'ionic correction factor'. The reason for this is that the mechanical structures considered in BD simulations are typically charged and therefore coated by a cloud of ions.

The precise way these ionic effects are to be accounted for depends on the geometry of the structures and the solvent they are embedded in. Indeed there may be cases where the ionic motion has to be factored into the external load vectors f_{ext} and m_{ext} in some way or where it has even to be accounted for by some additional simulation. However, a series of experiments has shown (e.g. [3,4] that in many cases of practical relevance the ionic effects are small and can be accounted for similarly to the shear correction factor by 'ionic correction factors' changing the effective bending, torsion, stretching and shear stiffness compared to the values one would get from a classical continuum mechanical calculation. These ionic correction factors may be determined for a

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certain combination of mechanical structure and fluid either experimentally or by some additional computer simulation.

2.2.1 Reissner beam equations in three dimensions

According to [5, 6, 7], the Reissner beam equations read in three dimensions:

$$f_{el} = \frac{\partial}{\partial \xi}\{R(\theta)k_t[R(\theta)^T x' - R(\theta^0)^T x'^0] \quad (1.6)$$

$$k_t = \begin{pmatrix} EA & 0 & 0 \\ 0 & GA_2 & 0 \\ 0 & 0 & GA_3 \end{pmatrix} \quad (1.7) \qquad m_{el} = \frac{\delta}{\delta \xi}\{R(\theta)\, k_r[k_{loc} - k_{loc}^0]\}$$

(1.8)

$$S(k_{loc}) = R(\theta)^T R'(\theta) \quad (1.9a)$$

$$S(k_{loc}^0) = R(\theta^0)^T R'(\theta^0) \quad (1.9b)$$

$$k_r = \begin{pmatrix} GJ_r & 0 & 0 \\ 0 & EJ_2 & 0 \\ 0 & 0 & EJ_3 \end{pmatrix} \quad (1.10)$$

where k_{loc} and k_{loc}^0 arethecurvaturevectorsinthelocalcoordinatesystemattachedtothecross section triad in the current and reference configuration, respectively. They are defined implicitly by their spin matrices S (k_{loc}) and S (k_{loc}^0) in (1.9). The local curvature vectors can be imagined geometrically as follows: their i-th component is the angle increment per increment in the parameter space by which the triad R rotates around its i-th axis when proceeding along the continuum. Thus the first component of the local curvature vector corresponds to the mechanical torsion, its second and third component to the bending curvature around the second and third principal axis of the cross section, respectively.

Applying the above equations to BD simulations of biopolymer networks assumes that torsion of polymers on micrometer length scale can be dealt with similarly as in macroscopic problems of structural engineering. This reveals a favorable property of the application of nonlinear finite beam elements in BD simulations: they naturally account for torsion in a proper way, whereas classical BD simulation methods such as bead-spring- and bead-rod-models do not capture torsion at all by default and do so only at the cost of intricate extensions [4, 16, 17]. Such extensions are often not only used for the sake of torsion, but also to capture anisotropic bending stiffness's.

2.2.2 Reissner beam equations in two dimensions

In two dimensions the rotation θ becomes an additive scalar, which enables significant simplifications as compared to the three dimensional case. According to [8], the elastic forces and moments in a two dimensional Reissner beam are given by:

$$f_{el} = \frac{\partial}{\partial \xi}\{R(\theta)k_t[R(\theta)^T x' - R(\theta^0)^T x'^0] \quad (1.11)$$

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$$k_t = \begin{pmatrix} EA & 0 \\ 0 & GA_2 \end{pmatrix} \quad (1.12)$$

$$m_{el} = \frac{\delta}{\delta\xi}\{k_r(\theta' - \theta'^0)\} \quad (1.13)$$

$$k_r = EJ_2 \quad (1.14)$$

2.3 Viscous forces and moments

A linear relationship between the viscous forces and moments on the one hand and the velocity of the filaments relative to the background fluid on the other hand can be assumed. Thus, the viscous damping force and moment are given in general by:

$$f_{visc} = c_t\,[\dot{x} - \vartheta(x)] \quad (1.15a)$$

$$m_{visc} = c_r[\dot{\theta} - \omega(x)] \quad (1.15b)$$

Here v and ω are the translational and rotational velocity field of the background fluid, and c_t and c_r are matrix-valued functions depending in general on ξ and t as well as on x and θ and their derivatives. The damping coefficients forming the elements of c_t andc_r can be computed in various ways. In practice, the curvatures of filaments in biopolymer networks and their velocities relative to the background fluid often remain moderate so that their damping coefficients can be set in good approximation equal to the ones of straight cylindrical rods of length L and diameter d moving through a resting fluid.

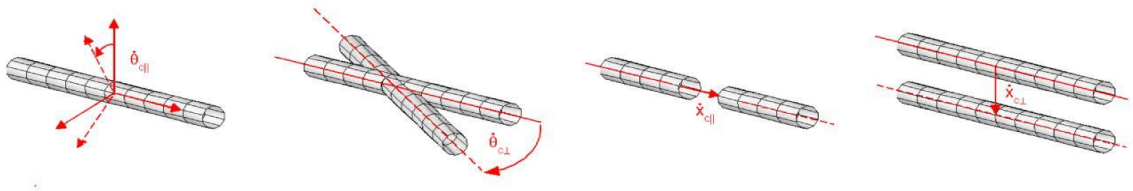

Figure 1.2: Different velocity components for motion of a rigid rod in R^3

2.3.1 Damping matrices for rigid, straight rods

In R^3, any motion of a rigid straight rod can be described uniquely by four different velocity components at the rod center as illustrated in Fig. 3.2: translation velocity $\dot{x}_{c\perp}$ perpendicular to the rod axis, translation velocity $\dot{x}_{c\parallel}$ parallel to the rod axis, rotation velocity $\dot{\theta}_{c\perp}$ perpendicular to the rod axis, and rotation velocity $\dot{\theta}_{c\parallel}$around the rod axis. In a Newtonian fluid, these four velocities cause resulting damping forces and moments directly proportional to the velocities and pointing in the opposite direction. The proportionality factors between the velocities and these damping forces and moments are denoted by, $\zeta_{t\perp}$, $\zeta_{t\parallel}$, $\zeta_{r\perp}$, and $\zeta_{r\parallel}$, respectively. On the

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other hand, the resulting damping forces and moments on a rod with the above described velocities can be expressed also in terms of the viscous forces f_{visc} and moments m_{visc} per unit length, which gives:

$$\zeta_{t\perp}\dot{x}_{c\perp} = [\int_0^L f_{visc}\, d\xi\,]_{\theta=0,\dot{x}=\dot{x}_{c\perp}} \quad (1.16a)$$

$$\zeta_{t\parallel}\dot{x}_{c\parallel} = [\int_0^L f_{visc}\, d\xi\,]_{\dot{\theta}=0,\dot{x}=\dot{x}_{c\parallel}} \quad (1.16b)$$

$$\zeta_{t\perp}\dot{\theta}_{c\perp} = [\int_0^L (m_{visc} + (x(\xi) - x_c) \times f_{visc})d\xi]_{\dot{\theta}=\dot{\theta}_{c\perp},\dot{x}=(x(\xi)-x_c)\times\dot{\theta}_\perp} \quad (1.16c)$$

$$\zeta_{t\parallel}\dot{\theta}_{c\parallel} = [\int_0^L m_{visc}\, d\xi\,]_{\dot{\theta}=\dot{\theta}_{c\parallel},\dot{x}=0} \quad (1.16d)$$

Integrands in (1.16a) and (1.16b) are constant over ξ, these two equations can be rewritten as:

$$\zeta_{t\perp}\dot{x}_{c\perp} = Lc_t\dot{x}_{c\perp} \quad (1.17a)$$

$$\zeta_{t\parallel}\dot{x}_{c\parallel} = Lc_t\dot{x}_{c\parallel} \quad (1.17b)$$

Noting that $\dot{x}_{c\perp}$ and $\dot{x}_{c\parallel}$point parallel or orthogonal to the rod axis, it is obvious that the eigenvectors of c_t are the three columns of the material triad R attached to the rod and the related eigenvalues are $\zeta_{t\parallel}$/L and $\zeta_{t\perp}$/L, which immediately provides the unique solution forc_t. Together with this result the same argumentation leads to the solution also forc_r, and one has in three dimensions:

$$c_t = R(\theta)\begin{pmatrix}\gamma_{t\parallel} & 0 & 0\\ 0 & \gamma_{t\perp} & 0\\ 0 & 0 & \gamma_{t\perp}\end{pmatrix} R(\theta)^T =: R(\theta)\, c_{t,loc} R(\theta)^T \quad (1.18a)$$

$$c_r = R(\theta)\begin{pmatrix}\gamma_{r\parallel} & 0 & 0\\ 0 & \gamma_{r\perp} & 0\\ 0 & 0 & \gamma_{r\perp}\end{pmatrix} R(\theta)^T =: R(\theta)\, c_{r,loc} R(\theta)^T \quad (1.18b)$$

and in two dimensions:

$$c_t := R(\theta)\, c_{r,loc} R(\theta)^T = R(\theta)\begin{pmatrix}\gamma_{t\parallel} & 0\\ 0 & \gamma_{t\perp}\end{pmatrix} R(\theta)^T \quad (1.19a)$$

$$c_r := \gamma_{r\perp} \quad (1.19b)$$

With:

$$\gamma_{t\perp} = \zeta_{t\perp}/L \quad (1.20a)$$

$$\gamma_{t\parallel} = \zeta_{t\parallel}/L \quad (1.20b)$$

$$\gamma_{r\perp} = \zeta_{r\perp}/L - \zeta_{t\perp}L/12 \quad (1.20c)$$

$$\gamma_{r\parallel} = \zeta_{r\parallel}/L \quad (1.20d)$$

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It is underlined that ζ denotes here effective friction coefficients for the whole rod, whereas γ denotes friction coefficients per unit length. For a rigid straight rod, the first column of the rotation matrix is equivalent to the unit tangent vector of the rod, i.e., $R^1 = x'$. Elementary calculus reveals that therefore c_t can be written both in two and three dimensions equivalently as:

$$c_t = 1\gamma_{t\parallel} + (\gamma_{t\parallel} - \gamma_{t\perp})x' \otimes x' \qquad (1.21)$$

It is underlined that (1.18a) and (1.19a) are equivalent to (1.21) only for the rigid rod considered in this section. In case of shear deformation, both ways of expressing the friction tensor distinguish in general. However, for biopolymers shear is not expected to play a major role owing to their high slenderness ratio.

2.3.2 Computation of damping coefficients

With (1.15), (1.18), (1.19), (1.20) and (1.21), the viscous quantities in (1.5) can be computed immediately once one knows the damping constants. In the following, we will discuss three of the numerous possible ways to determine them.

Computation by means of formulae: In the literature formulae for the computation of the friction coefficients of stiff rods can be looked up:

$$\zeta_{t\perp} = \frac{4\pi\eta L}{\ln(L/d) + 0.84'} \qquad (1.22a)$$

$$\zeta_{t\parallel} = \frac{2\pi\eta L}{\ln(L/d) + 0.2'} \qquad (1.22b)$$

$$\zeta_{t\perp} = \frac{\pi\eta L/3}{\ln(L/d) + 0.66'} \qquad (1.22c)$$

$$\zeta_{t\parallel} = \pi\eta d^2 L \qquad (1.22d)$$

These formulae can be applied if the viscosity η of the surrounding fluid as well as the length L and diameter d of the rods are known.

Computation by means of diffusion coefficients: Sometimes, only diffusion coefficients are known, e.g., from experiments, and the damping matrices have to be computed in accordance with them. Typically, three diffusion coefficients are known for a certain structure, the translational diffusion coefficientD_t, the orthogonal rotational diffusion coefficient $D_{r\perp}$and the axial rotational diffusion coefficient $D_{r\parallel}$. which provide three equations for the computation of the four damping coefficients. A fourth equation follows from a consideration of the relation between $\zeta_{r\perp}$and$\zeta_{r\parallel}$. To this end, one assumes that there is no difference between the hydrodynamic interactions caused by a rotation and translation orthogonal to the rod axis. Then $\zeta_{t\perp}$/L should be the friction coefficient per unit length for any length segment of the rod moving through the fluid perpendicularly to the rod axis. Therefore it is possible to express the resulting damping moment by:

$$\zeta_{r\perp}\dot{\theta}_\perp = \int_0^L \frac{\zeta_{t\perp}}{L\dot{\theta}_\perp\left(\xi - \frac{L}{2}\right)} d\xi = \frac{L^2\zeta_{t\perp}\dot{\theta}_\perp}{12} \qquad (1.23)$$

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Which immediately gives

$$\zeta_{r\perp} = \frac{L^2 \zeta_{t\perp}}{12} \tag{1.24}$$

This relation, which was gained just by neglecting the difference between the hydrodynamic interactions caused by translations and rotations perpendicular to the rod axis, provides an additional equation, enabling finally the computation of the damping coefficients from the diffusion coefficients dimensions by:

$$\zeta_{t\perp} = \frac{12 k_B T}{L^2 D_{r\perp}} \tag{1.25a}$$

$$\zeta_{t\parallel} = \frac{k_B T}{m_t D_t - L^2 (m_t - 1) D_{r\perp}/12'} \tag{1.25b}$$

$$\zeta_{t\perp} = \frac{k_B T}{D_{r\perp}} \tag{1.25c}$$

$$\zeta_{t\parallel} = \frac{k_B T}{D_{r\parallel}} \tag{1.25d}$$

Computation by means of simplified formulae: The formulae (1.22) require detailed information about length and diameter of the structure. Sometimes such information is not available (especially for the diameter), but yet at least a rough estimate for the damping coefficients is necessary to run simulations. In this case, often a simplified version of (1.22) is employed [9, 10] where the correction terms for different hydrodynamic phenomena are omitted, which gives:

$$\zeta_{t\perp} = 4\pi\eta L \tag{1.26a}$$

$$\zeta_{t\parallel} = 2\pi\eta L \tag{1.26b}$$

$$\zeta_{t\perp} = \pi\eta L^3/3 \tag{1.26c}$$

$$\zeta_{t\parallel} = \pi\eta d^2 L \tag{1.26d}$$

Using (1.26), perceptible deviations between simulated and real filament dynamics may arise. However, for the simulation of a variety of static quantities and probability distributions important in polymer physics, this deficiency does not matter at all, and using (1.26) usually allows for computer simulations on the basis of very limited knowledge, but yet with parameters close enough to the real ones in order not to miss important key phenomena.

2.4 External forces and moments

Only little can be state din general about the external forces and moments, as these functions may vary from application to application. Usually, they depend only on the position x(ξ,t) and the tangent x'(ξ,t) and do not entail any significant mathematical or practical problems so that we will skip any further discussion of these terms and assume that they can be handled by standard techniques. In practice, external loads may be for

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example electrostatic forces or contact forces owing to interactions of a filament with other filaments, linkers or also itself.

2.5 Stochastic forces and moments

The stochastic forces and moments acting on the rod originate from interactions such as collisions with particles in the surrounding fluid. Owing to the stochastic nature of these particles' motion, they can be modeled as stochastic loads per unit length summing up the excitation exerted by all surrounding particles. As the motion of these particles has no preferred direction, the mean value of the stochastic load is zero. Since it is furthermore assumed to happen on much a faster time and much a smaller length scale than relevant for the dynamics of the rod, the correlation length of the stochastic loads both in space and time is assumed to be zero.

The stochastic excitation results from the superposition of interactions with numerous particles. The set of all particles can be subdivided into subsets of identical particles. For each of these subsets, the way its particles interact with the rod follows the same probability distribution. As a consequence of the law of large numbers, the stochastic loads are therefore Gaussian random variables. Gaussian random variables are uniquely characterized by their first and second moment. Since the mean value of the stochastic loads is known to be zero, only their variance remains to be determined. To this end, one has to recall that the laws of statistical mechanic simply that each degree of freedom of a system immersed into a thermal bath of temperature T has the average energy $k_BT/2$, where k_B is the Boltzmann constant. Thus the mean absolute value of the stochastic loads (and thereby their variance) can be calculated from the requirement that they have to deform the rod so that the average elastic energy stored in each Eigen mode is $k_BT/2$. Lengthy derivations [11] reveal the so-called fluctuation-dissipation theorem, which characterizes the stochastic forces and moments by:

$$\langle f_{stoch} \rangle = 0 \qquad (1.27a)$$

$$\langle f_{stoch}(t,\xi) \otimes f_{stoch}(t^*,\xi^*) \rangle = 2k_BT c_t \delta_{tt^*} \delta_{\xi\xi^*} \qquad (1.27b)$$

$$\langle m_{stoch} \rangle = 0 \qquad (1.27c)$$

$$\langle m_{stoch}(t,\xi) \otimes m_{stoch}(t^*,\xi^*) \rangle = 2k_BT c_r \delta_{tt^*} \delta_{\xi\xi^*} \qquad (1.27d)$$

Where t, t^* and ξ, ξ^* represent in general different points in time and space, respectively, and δ_{tt^*} is the Dirac-function with argument $t-t^*$. Mean values are denoted by $\langle . \rangle$. As can be seen in the above equations, the fluctuation-dissipation theorem states a relation between the damping tensors governing the friction and the mean amplitudes of the stochastic loads. This aspect underlines the common origin of both quantities in the interactions of the rod with surrounding particles. Due to the δ-correlation, a Fourier transform of f_{stoch} and m_{stoch} in space and time is a constant function, i.e., all frequencies are equally represented. Therefore, f_{stoch} and m_{stoch} are so-called white-noise excitationsand can thus be expressed in terms of generalized derivatives of the multidimensional standard Wiener processes $W_t(\xi,t)$, $W_r(\xi,t)$ by:

$$f_{stoch} = \sqrt{2k_BTs_t} \frac{\delta^2 W_t(\xi,t)}{\delta\xi\delta t} \qquad (1.29a)$$

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$$m_{stoch} = \sqrt{2k_B T}\, s_r \frac{\delta^2 w_r(\xi,t)}{\delta\xi\delta t} \qquad (1.29b)$$

Here, s_t and s_r are some matrices satisfying $s_t s_t^T = c_t$ and $s_r s_r^T = c_r$.

2.6 Weak form of the equation of motion

For the derivation of numerical methods, it is useful writing (1.5) in the weighted-residual form. To this end, we multiply the linear and angular momentum balance in (1.5) with weighting functions W_t and W_r and integrate in space, which gives:

$$\int_0^L W_t f_{el}\, d\xi + \int_0^L W_t f_{visc}\, d\xi = \int_0^L W_t f_{ext}\, d\xi + \int_0^L W_t f_{stoch}\, d\xi \qquad (1.30a)$$

$$\int_0^L W_r m_{el} d\xi + \int_0^L W_r m_{visc}\, d\xi = \int_0^L W_r m_{ext} d\xi + \int_0^L W_r m_{stoch}\, d\xi + \int_0^L W_r x' \times f_s d\xi \qquad (1.30b)$$

The application of Gauss' divergence theorem to (1.30) leads to the weak form:

$$\int_0^L (-W_t' f_s + W_t f_{visc}) d\xi = \int_0^L (W_t f_{stoch} + W_t f_{ext}) d\xi + [W_t f_{bd}]_0^L \qquad (1.31a)$$

$$\int_0^L (-W_r' m_s + W_r m_{visc}) d\xi = \int_0^L (W_r m_{stoch} + W_r x' \times f_s + W_r m_{ext}) d\xi + [W_r m_{bd}]_0^L \qquad (1.31b)$$

Where $[\ldots]_0^L$ denotes the difference between the function in brackets evaluated at ξ = L and at ξ = 0, respectively, and $f_{bd}(\xi)$ and $m_{bd}(\xi)$ the external boundary forces and moments at ξ = 0 and ξ = L. For deterministic partial differential equations, it is well-known that the strong form is satisfied if and only if the weak form is satisfied for all weightings functions out of a sufficiently large function space. It is underlined that the situation here is different as (1.5) is an SPDE owing to the space-time white noise in (1.29), and mathematical statements for deterministic partial differential equations are not necessarily true also for SPDEs. However, the equivalence of strong and weak form can be proven also for SPDEs under fairly general conditions [12] so that for the development of a finite element approach to the BD of rod-like continua we can take the weak form (1.31) as a convenient basis.

III. CONCLUSION

In a finite element approach to the BD of polymers, polymer elasticity can be dealt with in almost the same way as the elasticity of macroscopic beams and rods in structural engineering; the only difference is in fact that stiffness parameters such as bending stiffness should be modified in BD simulations by some ionic correction factor.

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