Coordinated motion of molecular motors on DNA chains with branch topology

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To understand the macroscopic mechanical behaviors of responsive DNA hydrogels integrated with DNA motors, we constructed a state map for the translocation process of a single FtsKc on a single DNA chain at the molecular level and then investigated the movement of single or multiple FtsKc motors on DNA chains with varied branch topologies. Our studies indicate that multiple FtsKc motors can have coordinated motion, which is mainly due to the force-responsive behavior of individual FtsKc motors. We further suggest the potential application of motors of FtsKc, together with DNA chains of specific branch topology, to serve as strain sensors in hydrogels.

DNA, Molecular motor, Coordinated motion, Branch topology, Strain sensor

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1. Introduction

With the carried genetic information for the synthesis of RNA and proteins, DNA molecules are known as biological macromolecules for the development and normal functions of organisms. DNA molecules are also superb components for constructing new hydrogels [1-3] due to their modularity, programmability, biocompatibility, etc. In the past two decades, DNA has become a popular building unit for new functional DNA nanostructures, nanomotors, and DNA hydrogel materials, which provide necessary mechanical support and realize specific biological functions [4-15].

Predefined secondary structures of DNA were constructed in manufacturing new DNA hydrogels. By adjusting the length, concentration, and ratio of sticky ends of Y-shaped DNA and adaptor DNA, Xing et al. [16] managed to control the mechanical strength and thermal reaction reversibility of DNA hydrogels. The pH value of the solutions strongly affected the shear modulus of DNA hydrogels, and the controlled release of drugs encapsulated in the hydrogel was realized by changing the pH value of the solution. Zhou et al. [17] integrated DNA molecular motors based on the i-motif in DNA hydrogels. By changing the DNA molecular structure at the molecular scale with the pH value, the mechanical strength of the DNA hydrogel changed from 250 Pa to 1000 Pa. Lee et al. [18] synthesized DNA hydrogels with metamaterial properties through the design of a bird’s nest structure at the molecular scale, which showed solid characteristics in water but liquid characteristics when the surrounding water was removed. Qi et al. [19] constructed DNA chains with specific sequences and controlled shapes. The side length of the units varied from 30 μm to 1 mm and spanned multiple scales. These units could be further assembled into specific macroscopic structures through self-assembly.

Bertrand et al. [20] prepared responsive hydrogels by integrating DNA motors of FtsKc. FtsK is a membrane-bound DNA translocase that localizes to the division septum in bacteria and is essential for unlinking chromosome dimers [21]. It comprises an N-terminal integral membrane domain that localizes FtsK to the septum early in cell division, a long linker of unknown function, and a C-terminal translocase

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domain (FtsKC). FtsKC was shown in single molecule assays to translocate to DNA chains up to a speed of ~5 kb/s and be stalled at a force of ~70 pN [22-26]. It was observed that the addition of these molecular motors created random contractile events and stiffened the DNA hydrogels [20].

The mechanical behaviors of responsive DNA hydrogels integrated with FtsKC are fascinating, and we are interested in developing a constitutive model of such materials. Toward this goal, one needs to understand the translocation mechanism of FtsKC motors on DNA chains at the molecular scale first. With this motivation in mind, we constructed a state map for the translocation process of motor FtsKC on a single DNA chain and then simulated the translocation of the motor on a single DNA chain, with results in excellent agreement with the experimental results. Next, we investigated the movement of multiple FtsKC motors on DNA chains with varied branch topologies. Interestingly, our studies indicate that multiple FtsKC motors on DNA chains exhibit coordinated motion, which is mainly due to the force responsive capability of a single FtsKC motor. We further suggest the potential application of motor FtsKC as strain sensors in hydrogels at the end of this work.

2. Kinetic model for a DNA-FtsKC cycle

FtsK is a DNA motor existing within *E. coli* that helps segregate chromosomes by translocating to DNAs during cell division. FtsK is the fastest known DNA pump [27]. Its N-terminal domain is used to locate the protein to the division septum, while the C-terminal domain, denoted as FtsKC, forms a translocation motor involved in chromosome segregation. The recently solved crystal structure of FtsKC revealed that six FtsK$_{50}$C domains oligomerize to form a ring that can accommodate DNA, as illustrated in Fig. 1c [28,29].

Based on previous studies in the literature, the kinetic model of FtsKC translocation to DNA is schematically shown in Fig. 1. In Fig. 1a-b, five 1st level states of FtsKC are assigned, denoted as State I, State II, State III, State IV, and State V. In State I, FtsKC exists as a monomer (blue circle), which is free in the vicinity of the DNA chain. In State II, a complete motor hexamer structure of FtsKC (blue ring) is formed, and then the hexamer is combined with the initial binding site of KOPS on the DNA chain [22]. Then, it begins to translocate to the DNA chain, and the translocation process is shown at State IV in Fig. 1d. The translocation direction of the motor in State IV is not fixed, and motor randomly switches the translocation direction and translocates either forward or backward. In State V, FtsKC stops specifically at a specific DNA sequence of XerCD-dif [30].

As illustrated in Fig. 1c, five 2nd level states exist between State I and II, which are denoted as State 1, State 2, State 3, State 4, and State 5. In Fig. 1c, black balls represent a DNA chain, and blue balls represent FtsKC monomers. State 1 is when only a single free FtsKC monomer is bound to the DNA chain. When additional free FtsKC monomers are bound to the DNA chain, the motor would, in turn, reach States 2, 3, 4, and 5. Note that once a complete motor hexamer structure is formed, the motor is in State II.

All nontrivial transition rates are displayed in Fig. 1b. In this kinetic model, transition rates among different states can be regarded as governing equations. Some transition rates

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**Figure 1** Kinetic model of FtsKC translocation to a single DNA chain. **a** Illustration of five 1st level kinetic states (I-V) within a DNA-FtsKC interaction cycle. **b** Five 1st level kinetic states (I-V) are assigned to a FtsKC motor within a DNA-FtsKC interaction cycle. **c** Five 2nd level states (1-5) exist between states I and state II. **d** When the motor is in state IV, it randomly switches the translocating direction, which can be either forward or backward.
between different states of an FtsKC have already been provided in the literature. For example, \( k_{\text{bind1}} = k_{\text{bind2}} = k_{\text{bind3}} = 1.2 \times 10^7 \text{ M}^{-1} \text{s}^{-1} \) and \( k_{\text{off1}} = k_{\text{off2}} = k_{\text{off3}} = k_{\text{off4}} = 2.8 \times 10^{-6} \text{ s}^{-1} \), which are force-independent [22]. With 100 nM FtsKC, \( k_{\text{bind1}} = k_{\text{bind2}} = k_{\text{bind3}} = 1.2 \text{ s}^{-1} \) and \( k_{\text{off1}} = k_{\text{off2}} = k_{\text{off3}} = k_{\text{off4}} = 2.8 \text{ s}^{-1} \). In addition, \( k_{\text{off5}} = k_{\text{off6}} = 7.2 \text{ s}^{-1} \), which are also force-independent [22]. From State II to State III, FtsKC goes through a single-step initiation phase with \( K_{\text{II,III}} = 28 \text{ s}^{-1} [22] \). Since the motor would immediately translocate after combining with the DNA chain when the concentration of ATP was above 2 mM [22], as considered in the current work, \( K_{\text{III,IV}} \) was set to be a very large value in the analysis.

\( K_{\text{IV,V}} \) represents the translocation rate of FtsKC on a DNA chain, which was regarded to be independent of the translocation direction but affected by environmental temperature, ATP concentration, and the load force on the DNA chain [31]. When the load force on the DNA chain was 10-15 pN, the speed of motor translocation was approximately \( (5.0 \pm 0.9) \text{ kb/s} \) [31]. This indicates that with the increase in the force applied to the DNA chain, the rate of motor translocation to the DNA chain would decrease. Mimicking the linearized Hill’s law [32], \( K_{\text{IV,V}} \) can be described by

\[
K_{\text{IV,V}} = \frac{V_0}{a} \left( 1 - \frac{F}{f_b} \right),
\]

where \( F \) is the load force on the DNA chain, \( f_b \) is the stall force, \( V_0 \) is the load-free stepping speed of the motor, and \( a \) is the fixed step length. For simplicity, here, we let \( d \) be the size of 1 bp, i.e., 0.34 nm [33]. Based on data fitting with Eq. (1), we take \( V_0 = 2080 \text{ nm/s} \) and \( f_b = 69 \text{ pN} \) in the analysis.

In the model, the motor in State IV can either translocate in the direction of DNA chain contraction (forward direction) or the opposite direction (backward direction). Denote the time duration of each forward translocation as \( T_f \) and that of each backward translocation as \( T_r \), both of which are assumed to satisfy a uniform distribution. With reported values in the experiment [31], \( T_f \) is assumed to be uniformly distributed within 0.1-0.334 s and \( T_r \) within 0-0.234 s in the analysis.

The motor stops translocating when it meets either side of the XerCD-dif. The cessation of this translocation does not significantly cause the motor to fall off the DNA chain [30], so we let \( K_{\text{V,I}} = 0 \text{ s}^{-1} \) in the analysis.

3. Simulated results of a single FtsKC translocation on a single DNA chain

The translocation process of a single motor on a single DNA chain [31] is simulated with the Monte Carlo method to validate the kinetic model for a DNA-FtsKC interaction cycle. In the reported experiment [31], a single DNA chain was tethered between two beads, as illustrated in Fig. 2a. The DNA chain was then extended under constant tension, \( \sim 10 \text{ pN} \), using a flowing buffer solution. With the introduction of 100 nM FtsKC, the DNA chain was rapidly shortened against the applied force.

In the simulation, \( K_{\text{II,III}} \) is first obtained by calculating the inverse of the average time required for the formation of an FtsKC hexamer. The lowest concentration of motor monomer was 75 nM in the experiment [31], so the decrease in concentration caused by the FtsKC hexamer formed by monomers can be ignored in the simulation. The calculated results of \( K_{\text{II,I}} \) are shown in Table 1.

Table 1 shows that the higher the motor monomer concentration is, the shorter the time required for the motor to form a hexamer from the monomer, and the greater the \( K_{\text{II,I}} \), which is reasonable. Note that the motor would not translocate to the DNA chain before the motor formed a hexamer so that the extension of the DNA chain would not change. Indeed, the motor did not work in the first 5.5 s, as observed in the experiment [31].

When a motor translocates on DNA chains in the solution, the friction force is given by

\[
F = \eta \nu a,
\]

where \( \eta \) is the viscosity of the aqueous phase of the cellular cytoplasm, \( \nu \) is the translocation speed, and \( a \) is the diameter of the motor. \( \eta \approx 10 \text{ cP} [34] \), \( \nu \approx 1000 \text{ nm/s} \), and \( a \approx 10 \text{ nm} [29] \). According to Eq. (2), the friction force is estimated to be \( \sim 1 \times 10^{-15} \text{ N} \), which is very small and can be neglected.

When a motor translocates along the DNA chain, an expanding DNA loop will be formed [31], as shown in Fig. 2a. When the motor translocates in the forward direction, the loop expands, and when the motor translocates in the backward direction, the loop shrinks. The time waiting for hexamer formation of the motor from the monomer is ignored in the analysis better to compare the simulations with the experiment [31]. The simulation results fit well with the experiment, as seen in Fig. 2a. We also carry out correlation analysis [35] on both experiments [31] and simulations, with the calculated correlation coefficients shown in Table 2. The correlation coefficients of the simulations are very close to the correlation coefficient of the experiment [31], and all their absolute values are larger than 0.75, which indicates a strong linear correlation between the contour length of the DNA strand and time in Fig. 2b. The good correlation confirms the conclusion made from the experiment [31] that the motor would apparently translocate unidirectionally on DNA chains at a large timescale, although the motor randomly translocates bi-directionally at a much lower timescale with a large difference in the time duration of forward and back-
ward translocation. Taken together, we conclude that the established kinetic model for a DNA-FtsKC cycle can well simulate the translocation of an FtsKC on the DNA chain.

4. Coordinated motion of motors on DNA chains with branch topology

Three branch topologies made of DNA chains are considered, as shown in Fig. 3. In Fig. 3a, the angle between the DNA chains with a linear topology is 180°, and both ends are fixed. Figure 3b shows DNA chains with a Y-shaped topology, where angles among three chains are all 120° and three ends are all fixed. Figure 3c shows DNA chains with an X-shaped topology, where angles between four chains are 60° or 120°, and four ends are all fixed. All DNA chains are connected by hinges in our consideration, and the initial length of each DNA chain is set to be the same, which is 1043 nm in the simulation. The relationship between the force and the extension of a DNA chain is illustrated in Fig. 3e. When the force is less than 60 pN, it can be described by a “twistable worm-like chain” model (WLC) [33], given by

$$x = L_c \left(1 - \frac{1}{2} \frac{k_B T}{F - L_p} + \frac{C}{g^2(F) + SC} \cdot F \right),$$

where $x$ is the chain extension, $F$ is the force on the chain, $L_c$ is the contour length, $C = 440$ pN nm$^2$ is the twist rigidity, $S = 1500$ pN is the stretching modulus, $L_p$ is the persistence length, and $g(F)$ is the twist-stretch coupling, given by [33]

$$g(F) = \begin{cases} 
  g_0 + g_1 F, & F < F_c, \\
  g_0 + g_1 F_c, & F \geq F_c 
\end{cases},$$

where $g_0 = -637$ pN nm, $g_1 = 17$ nm, and $F_c = 30.6$ pN is a critical force. When the force on the chain is above 60 pN, the force extension curve appears as a plateau [36], as shown in Fig. 3e.

Note that DNA chains are represented as straight lines in our figures for simplicity. However, DNA chains are not necessarily straight in our theoretical development. For example, the force stretch relation of a DNA chain described by Eqs. (3) and (4) works with local curvatures due to thermal fluctuation. It is possible that the local curvature of a DNA chain might affect the local translocation rate of motors on a DNA chain. However, the averaging effect of force on the translocation rate as described by Eq. (1) is expected to still be valid at a relatively large time scale since our model prediction is consistent with the experiment, as seen from Fig. 2b.

We then simulated the movement of multiple motors on DNA chains with varied branch topologies, where one motor was translocated to each DNA chain. Consider that the time needed for the system to achieve elastic equilibrium can be much smaller than that for a random motor event to take place [37]. Due to this separation of time scales in the system, we employ a two-level hierarchical numerical scheme in our simulation, as illustrated in Fig. 4. Take DNA chains with a Y-shaped topology in Fig. 3d as an example. The initial length of the three chains is the same, and the stretch of
the three chains is initially zero. Three motors are then combined with designated symmetric binding sites, KOPS [22], on DNA chains. Force will be generated when the contour lengths of the three chains change due to the translocation of the motor. Together with Eq. (3), forces on three DNA chains are calculated through

\[
\begin{align*}
F_1 \sin \theta_A + F_2 \sin \theta_B + F_3 \sin \theta_C &= 0, \\
F_1 \cos \theta_A + F_2 \cos \theta_B + F_3 \cos \theta_C &= 0,
\end{align*}
\]

where \( F_1, F_2, \) and \( F_3 \) are chain forces, and \( \theta_A, \theta_B, \theta_C \) are given by

\[
\begin{align*}
\sin \theta_A &= \frac{X_A - X_O}{\sqrt{(X_A - X_O)^2 + (Y_A - Y_O)^2}}, \\
\sin \theta_B &= \frac{X_B - X_O}{\sqrt{(X_B - X_O)^2 + (Y_B - Y_O)^2}}, \\
\sin \theta_C &= \frac{X_C - X_O}{\sqrt{(X_C - X_O)^2 + (Y_C - Y_O)^2}},
\end{align*}
\]

respectively, with \( X_A, X_B, X_C, \) and \( X_O \) being horizontal coordinates of \( A, B, C, \) and \( O \), displayed in Fig. 3d.

The simulation results for DNA chains with a linear topology are shown in Fig. 5a-c, where we can see that as the contour length of the two chains in the linear structure gradually decreases due to the translocation of two motors of FtsK\(_C\) on them, their respective chain force gradually increases, and the hinge connecting the two chains fluctuates in the vicinity of the initial equilibrium position. The simulation results for DNA chains with a Y-shaped topology and those for DNA chains with an X-shaped topology are displayed in Fig. 5d-f and Fig. 5g-i, respectively. These results are generally very similar to those of DNA chains with a linear topology, where the contour length of DNA chains generally decreases, the respective chain force increases, and the position of the hinge fluctuates in the vicinity of the initial equilibrium position as time evolves. The relatively small difference in the chain contour length and the chain force and the relatively small fluctuation of the hinge in the vicinity of the initial equilibrium position within chains with varied chain topology clearly indicate that motion coordination exists among multiple motors translocating on different chains with varied topology.

5. Discussion

We must clarify that individual DNA chains forming varied branch topologies in the current work are generally not straight. Indeed, due to thermal fluctuation, the configuration of long DNA chains could be similar to a random coil.
Pulling on DNA chains would reduce configuration entropy, which costs energy. Such an effect of thermal fluctuation on the relationship between the force and the extension of a DNA chain was already included in the twistable worm-like chain model, given by Eqs. (3) and (4), which would still be applicable in the current work. If, for example, the Y-shaped topology is prestressed with tensile forces, the application of Eqs. (3) and (4) would yield the prestretch on individual chains. Such tensile forces would affect the translocation rate of the motors, as indicated by Eq. (1).

In our approach, motors randomly transit among different states, which can be their combination with the DNA chain, its forward or backward translocation on the DNA chain, etc., and is simulated with the Monte Carlo method. In this approach, the exact mechanical interactions are ignored. As seen from Eq. (1), the translocation rate of the FtsK$_C$ motor, $K_{IV,V}$, decreases with increasing force on the DNA chain so that the behavior of individual FtsK$_C$ motors is force responsive. Such a force-responsive behavior of individual motors mainly leads to the coordinated motions of multiple motors on DNA chains with varied topology observed in the simulations, in our opinion. Let us take the Y-shaped DNA chain as an example. In the simulations, the three chains are initially the same. The forces on the three chains will be the same if the shortened contour lengths of the three chains due to the translocation of FtsK$_C$ are always equal. However, if the contour length of any one chain temporarily becomes larger or smaller than those of others, its chain force would become temporarily smaller or larger so that its translocation rate would temporarily become larger or smaller. In this way, the change in contour lengths of three chains would be modulated toward being the same, as indicated in Fig. 5c, f, i. In other words, the movement of three motors on the Y-shaped DNA chain would be coordinated.

In some applications of smart hydrogels, it may be desirable to obtain local forces or stretches. For example, cellular behaviors in tissue engineering may be strongly influenced by the mechanical properties of the local environment. Based on the above simulations, we propose to harness the force-responsive capability of motor FtsK$_C$ to measure local forces within these smart materials. In this method, the motor FtsK$_C$ may be labeled with a quantum dot so that its movement can be visualized by total internal reflection fluorescence microscopy [38]. Suppose that a motor attaching to a DNA chain starts to move at time 0. As illustrated in Fig. 6a, the total displacement of the motor within a relatively short duration $\Delta t$, denoted as $X(\Delta t)$, should be given by

$$X(\Delta t) = X_1(\Delta t) + X_2(\Delta t), \quad (7)$$

where $X_1(\Delta t)$ is the displacement of the motor due to the change in the initial length when the contour length changes and $X_2(\Delta t)$ is the displacement of the motor due to the change in the elastic stretch when the contour length changes. $X_1(\Delta t)$ is given by $X_1(\Delta t) = 2L_p \cdot L_0^c$, (8) where $L_0^c$ is the contour length of the DNA chain segment between one end of the DNA chain and the motor binding site at time 0, and $L_c(\Delta t)$ is the current contour length of the DNA chain segment between one end of the DNA chain and the motor attachment site at time $\Delta t$, given by

$$L_c(\Delta t) = L_0^c - V(F) \Delta t, \quad (9)$$

where $V(F) = V_0\left(\frac{1 - F}{F_b}\right)$ with Eq. (1). With Eqs. (3), (4), (9), $X_2(\Delta t)$ is given by

$$X_2(\Delta t) = V(F) \Delta t \left(1 - \frac{1}{2} \cdot \frac{k_BT}{F \cdot L_p} + \frac{C}{g^2(F) + SC} \cdot F \right). \quad (10)$$

With the measured $X(\Delta t)$ and the known $L_0^c, F$ can then be calculated with Eqs. (7)-(10), for example, by the Newton’s method [40]. In this way, DNA chains together with FtsK$_C$, as illustrated in Fig. 6b, may be built into a hydrogel, such as a cell nucleus, which may serve as a strain sensor to report the local stretches within the hydrogel when subjected to hydrostatic pressure. By measuring the displacement of the four motors, we can obtain the force on the DNA chains and

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Figure 4: Flow chart of the simulation.

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then determine the principal stretches of the DNA hydrogel at the current state.

Responsive DNA hydrogels have attracted wide scientific attention in recent years. One way to engineer responsive DNA hydrogels is to introduce the DNA motor FtsKC into the DNA hydrogel [27]. It was observed that the motors stiffened the gel and created stochastic contractile events [27]. It will be very interesting to construct a multiscale constitutive model of this kind of responsive DNA hydrogel.

6. Conclusion

In summary, we employed a kinetic model for an FtsKC-
DNA interaction cycle to simulate a single FtsK$_C$ motor translocation on a single DNA chain or multiple FtsK$_C$ motor translocations on multiple DNA chains with specific topology. By simulating motor translocation on a single DNA chain, we show that the prediction of the kinetic model is in excellent agreement with the reported experimental results. By simulating motor translocation on multiple DNA chains with specific topologies, we reveal that the movement of these motors on DNA chains will be well coordinated, which is mainly due to the force-responsive capability of individual FtsK$_C$ motors. We suggest that the force-responsive movement of motors, such as FtsK$_C$, may be harnessed in developing strain sensors in hydrogels. This work carried out at the molecular level of biomechanics [41-44] is also expected to pave the way for multiscale studies of the mechanical behavior of responsive DNA hydrogels.

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分支拓扑DNA链上分子马达的协调运动

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摘要 为理解整合了DNA马达的响应性DNA水凝胶的宏观力学行为，文章在分子水平上构建了单个FtsKc在单个DNA链上的易位过程状态图，并进一步研究了具有不同分支拓扑的DNA链上单个或多个FtsKc马达的运动。研究表明，多个FtsKc马达可以协调运动，这主要是由于单个FtsKc马达的力响应行为。文章进一步指出FtsKc马达结合特定分支拓扑的DNA链作为水凝胶中的应变传感器的潜在应用。