Instantaneous Lyapunov vectors in DNA

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We define the notion of an Instantaneous Lyapunov Vector (ILV), a tool which we introduce for the investigation of spatiotemporal chaos. These ILVs are related to covariant Lyapunov vectors (CLVs), which are intrinsic directions in phase space along which perturbation growth rates are governed by corresponding Lyapunov exponents [1]. We show that ILVs can be computed from eigenvectors of the symmetric part of the dynamical system's Jacobian matrix, and we use these vectors to probe the spatial characteristics of chaotic dynamics at an instant in time. We compare the behaviour of ILVs to that of the long-term averaged dynamics of CLVs, which we compute using the efficient algorithm of Ginelli et al. [2, 3].

By making use of a well-known Hamiltonian model of DNA, namely the Peyrard-Bishop-Dauxois (PBD) model [4], we study the spontaneous thermal openings of base pairs in strands of DNA which are known as "bubbles" and have been linked to transcription [5]. The relationship between chaos and the appearance of bubbles in DNA has been investigated by Hillebrand et al. [6] and we use ILVs to explore this further. In particular, we show that the relationship between sensitive dependence on initial conditions at an instant in time and the presence of bubbles in DNA is significantly determined by the on-site Morse potential governing individual base pair interactions in the PBD model.

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