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Modelling Transcription Factors Search and Polymerase Recruitment Dynamics within a complex chromatin structure

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The diffusion of transcription factors within the nucleus plays a crucial role in the dynamics of transcriptional regulation. Transient TF-DNA interaction events in specific binding sites within regulatory regions lead to the recruitment of Polymerase and the activation of transcription. More recently, it has been shown that weak protein-protein interactions lead to condensates of TFs and Polymerase which may have an important implication for transcription. However, how the 3D structure of chromatin influences these processes is not well understood yet. Here, we propose a mathematical model with high-resolution information on chromatin structure as well as DNA-protein interactions. The dynamics of transcription factors were modeled as a slide plus jump-diffusion process on a chromatin network based on pair-wise contact maps obtained from high-resolution Hi-C experiments. Our model allows us to uncover the effects of chromatin structure on transcription factor diffusion and polymerase recruitment dynamics. Stochastic simulations on different chromatin structures reveal the connection between structure and transcriptional bursting.