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Creating Metaphase DNA Model with Loop Extrusion BRYAN DINH, YOUFANG LAI, YUJIE CHI, None — The structure of DNA at different phases is critical in determining radiobiological responses to ionizing radiation. Yet, due to its complexity, metaphase DNA has never been studied in radiobiological simulations. In this work, we report our recent progress in applying the loop-extrusion method to construct a metaphase DNA model for this purpose. We modeled a section of chromosome of a human cell containing 12 million DNA base pairs (bp) with polymer physics, with each monomer representing a nucleotide (˜200 bp). A series of loop extrusion factors (LEFs) arranged in a helical structure were applied to divide polymer chain into distinct loops. Four forces in harmonic, repulsive, stiffness, and cylindrical confinement formats among monomers and a harmonic force among LEFs were applied to obtain the desired structure until reaching equilibrium amongst monomers. The contact frequency of monomers were computed after each set of parameters tuning. The contact frequency map is consistent with the empirical measurements in the regions of DNA separations between 0.1 and 1 Mbp. This model is promising to represent metaphase DNA for radiobiological study.

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None

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