0.1 The biological process

0.2 The simulation framework

0.2.1 The simulation domain

All simulation are performed in a two-dimensional open domain. The maximal z-projection values of DNA and nucleosome signals measured in experiments [REF].Our simulation framework is constructed to describes the dynamics of the chromatin post UV-C. All dynamics takes place in the local micro-environment of the UV beam.

0.2.2 The polymer model

We use a cross-linked Gaussian chain [REF] of N monomers connected by harmonic springs to represent a coarse-grained model of the chromatin. Springs connecting adjacent monomers in the linear chain are assigned a spring constant $2k_BT/b^2$ and a minimal length L_0. Cross links are represented as harmonic springs having spring constant $2k_BT/b^2$ and a minimal length zero. Cross-linking measure is given by the percentage $0 \leq \alpha \leq 100$ of non-nearest-neighbor monomers connected out of the N monomers of the chain. For each realization of the polymer, cross-links are added between non nearest-neighbor pairs of monomers chosen uniformly at random. The cross-linked polymer is then simulated up to its relaxation time, set to be the slowest mode of the Gaussian chain [REF], after which the UV beam is shot.

0.2.3 UV irradiation

At the end of relaxation steps the UV beam's focal point is placed at the polymer's center-of-mass where the beam is shot. A damage region (DR) is set to be a fixed two-dimensional circular region of area A_0 and centered at laser's focal point. Damages to DNA are represented by labeling monomers as damaged. For each UV dose u, damages caused by UV are uniformly distributed between the monomers located in A_0 at the time of beam shot. With increase of UV dose, we increase the probability of damages linearly as $k_t u$, with k_t in units of $bp/msec$.

Affect of UV irradiation on the polymer, the repair stage

To simulate the affect of repair proteins crowding at sites of DNA damage, a circular exclusion region is centered at each damaged monomer. The exclusion region is represented by an elastic spring pushing force of radius r_p, originating from each damaged monomer. The elastic force applied on any monomer within the exclusion range is thus oriented outwards. In addition to the exclusion region, all cross-links from and to damaged monomers are removed.

The polymer will evolve into a new steady spatial configuration which represents the chromatin 15 minutes post UV-C. At which point, the region of interest (ROI) is defined as the circle containing 95% of the damaged monomers and centered at their center-of-mass. The ROI remains a fixed region used to track the number of damaged and undamaged monomers within it. Measurements are done off-line, such that the ROI is always centered at the center-of-mass of the monomers known to be damaged.

0.2.4   Post repair stage

As damaged monomers are repaired the exclusion region is removed from damaged monomers. Cross-links are reintroduced gradually according to the spatial distance between monomers. The amount of cross-links re-introduces is such that the initial cross-linking percentage α is restored.