Mathematical modeling of DNA lesions as a consequence of ionizing radiation

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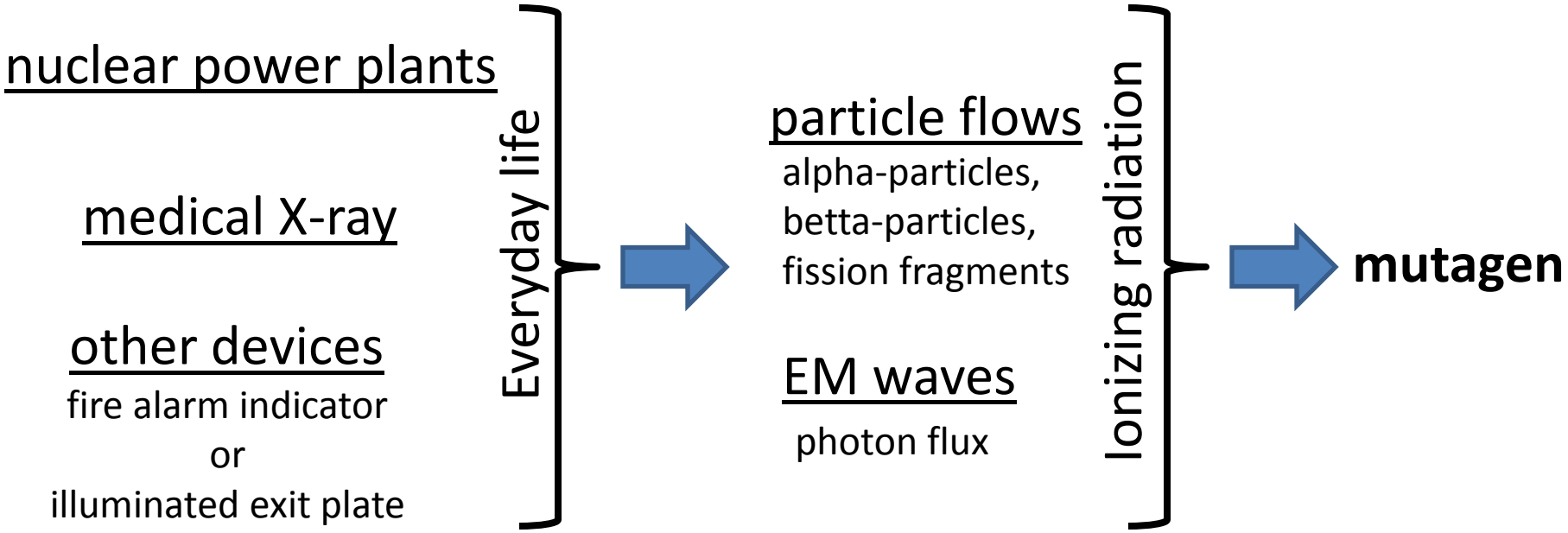
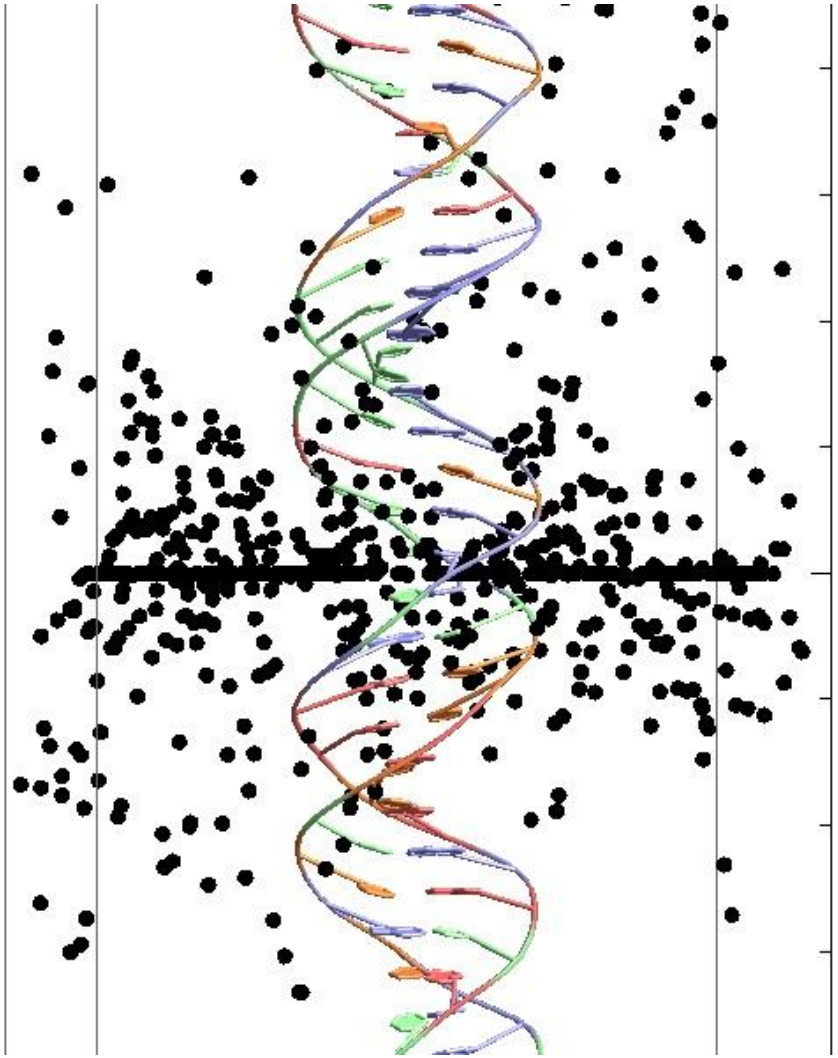
Ionizing radiation

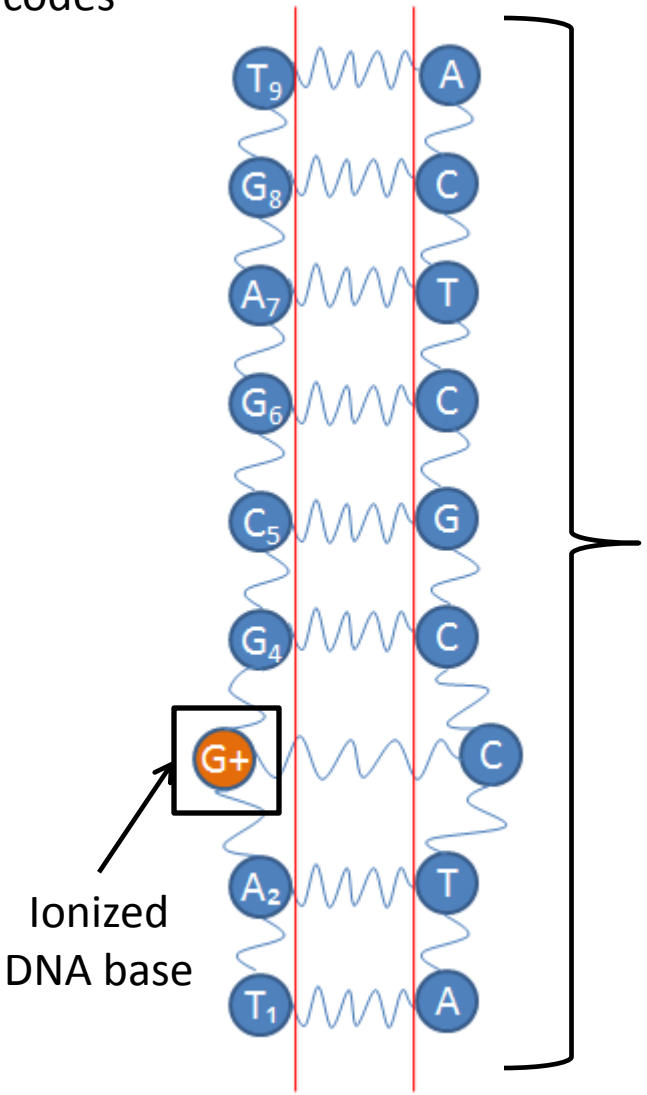
In modern world the contact between people and ionizing radiation may be very often. Thus it is important to understand the ionizing radiation risk.



Tracks of charged particles

TRIOL and GEANT4 codes

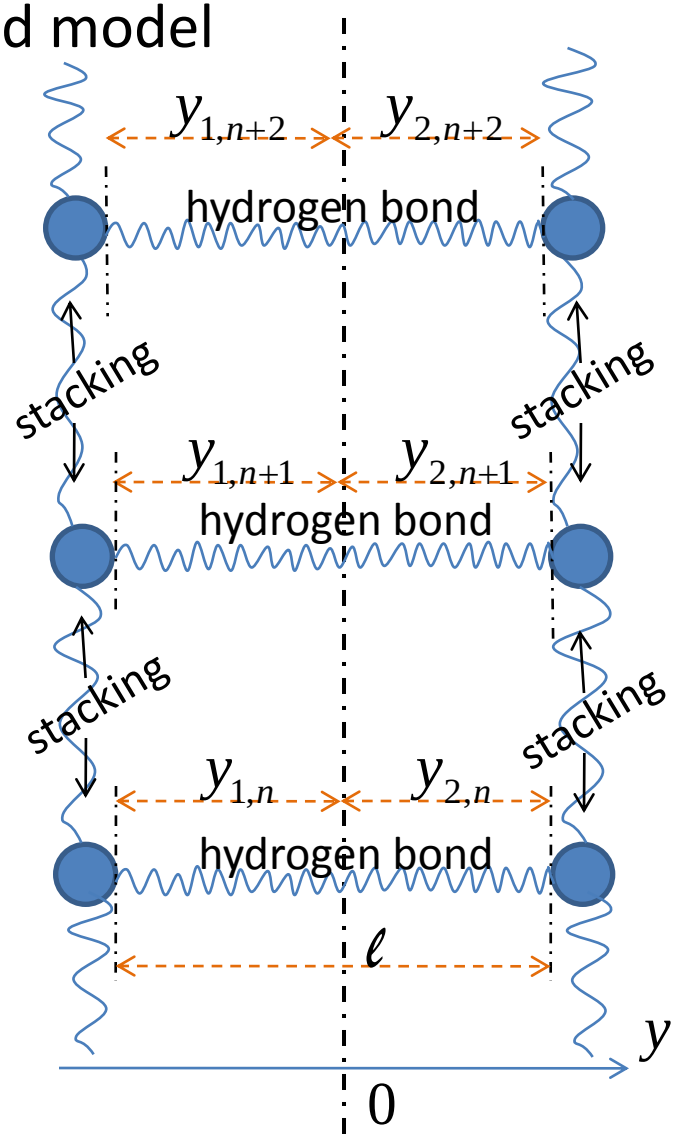




Migration of charge in DNA sequence

quasi-classical double stranded model

$$H = H_{Cl} + < \psi \mid H_Q \mid \psi >$$



$y_{1,n} < 0$ and $y_{2,n} > 0$ - base coordinates

$$shift = (y_{1,n} - y_{2,n} + l)$$

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$$H_{Cl} = \sum_n^N \left(\underbrace{M\frac{\dot{y}_{1,n}^2 + \dot{y}_{2,n}^2}{2}}_{\text{kinetic term}} + \underbrace{k_v \frac{(y_{1,n} - y_{1,n-1})^2}{2} + k_v \frac{(y_{2,n} - y_{2,n-1})^2}{2}}_{\text{stacking interaction}} + \underbrace{k_h \frac{(y_{1,n} - y_{2,n} + l)^2}{2}}_{\text{hydrogen bond}} \right)$$

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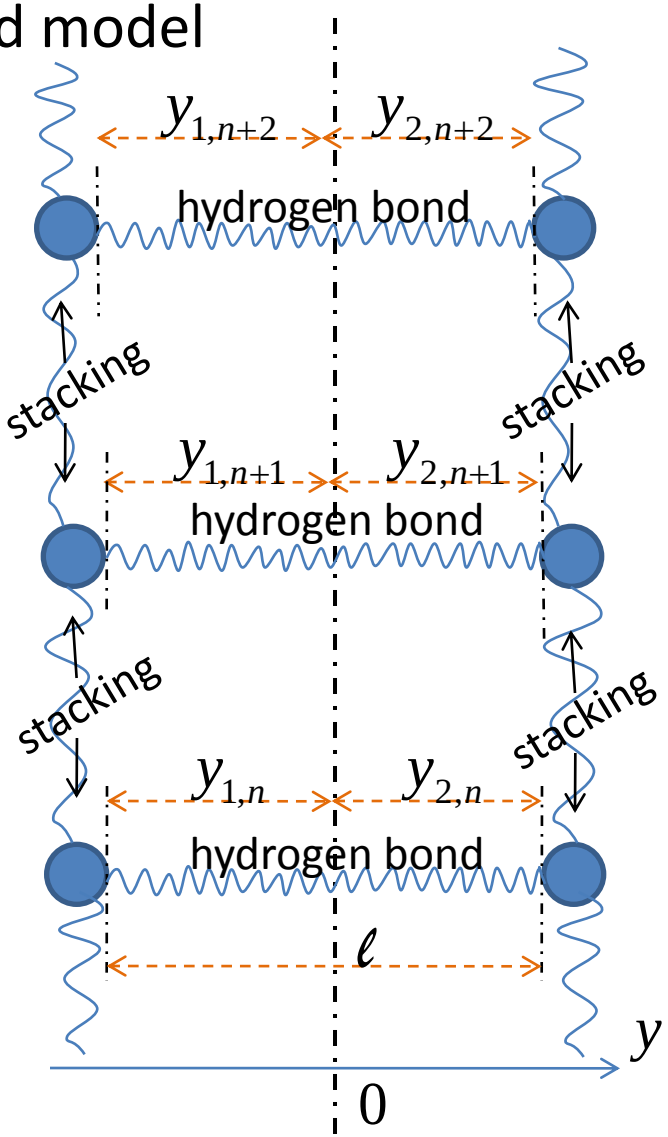

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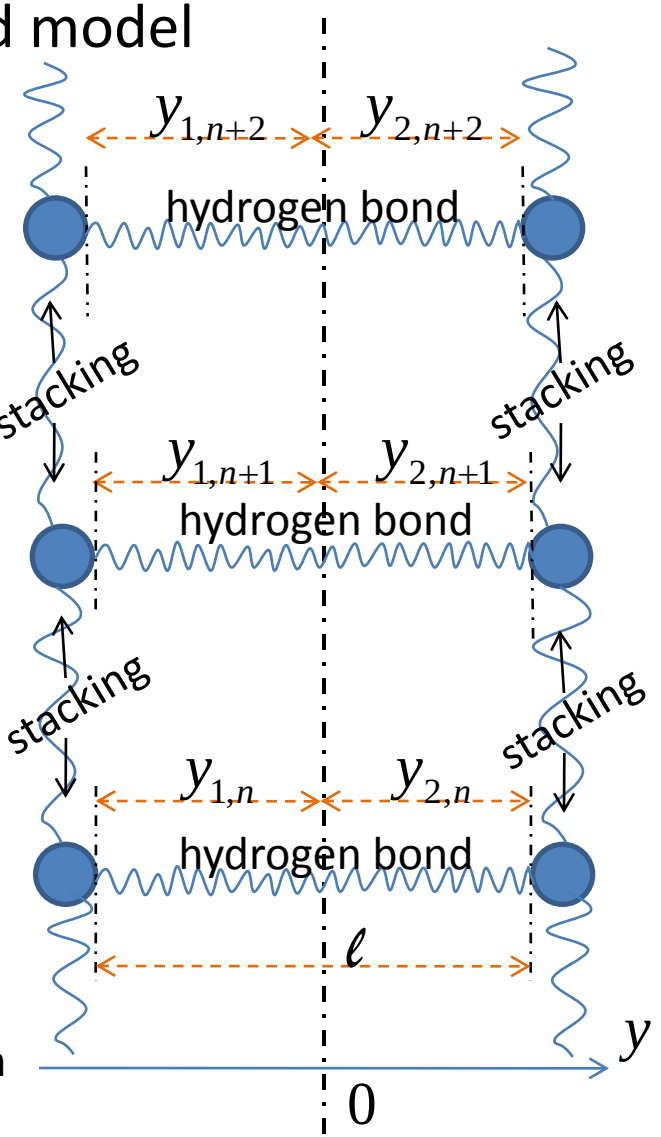
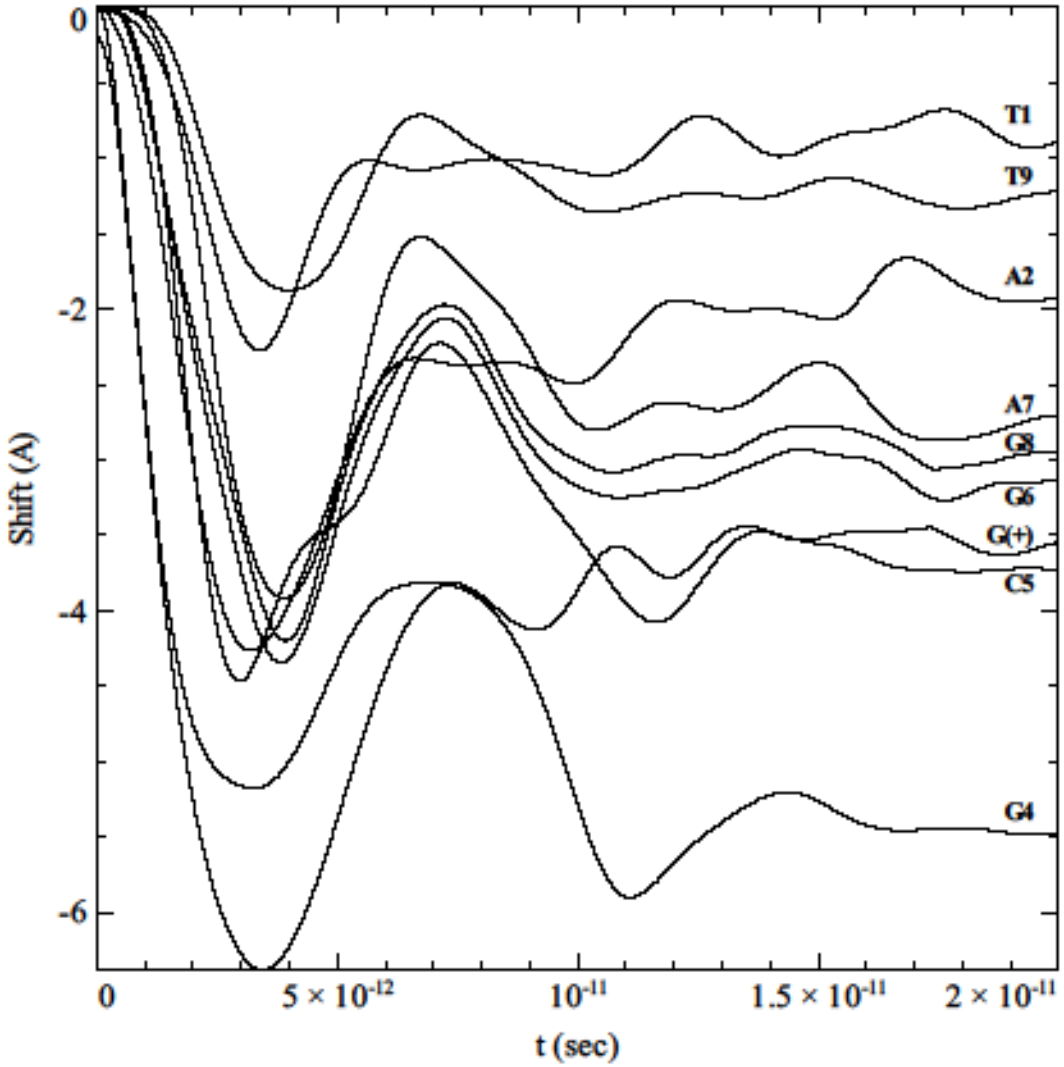
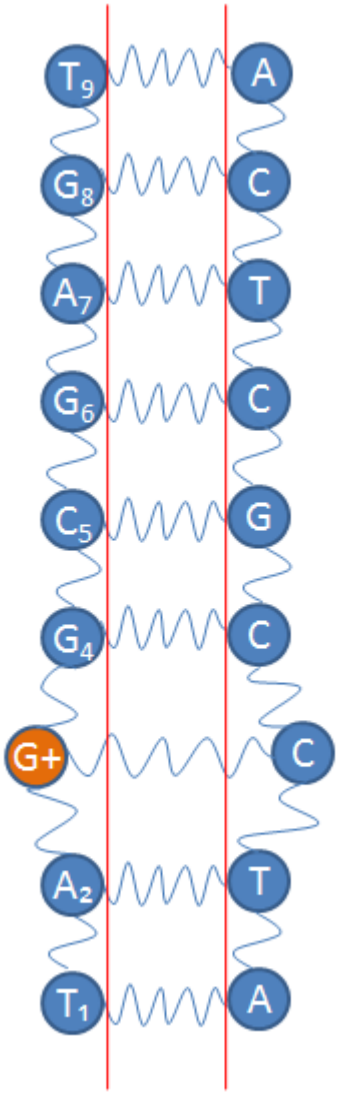
$$H_Q = \underbrace{\sum_{n=1}^N \alpha_n \mid n><n \mid}_{\text{n-base charge energy}} + \underbrace{\sum_{n=1}^N \alpha'_n (y_{1,n} - y_{2,n} + l) \mid n><n \mid}_{\text{deformation energy}} + \underbrace{\sum_{n \neq m}^N \nu_{nm} \mid n><m \mid}_{\text{energy of the transition between n, m bases}}$$

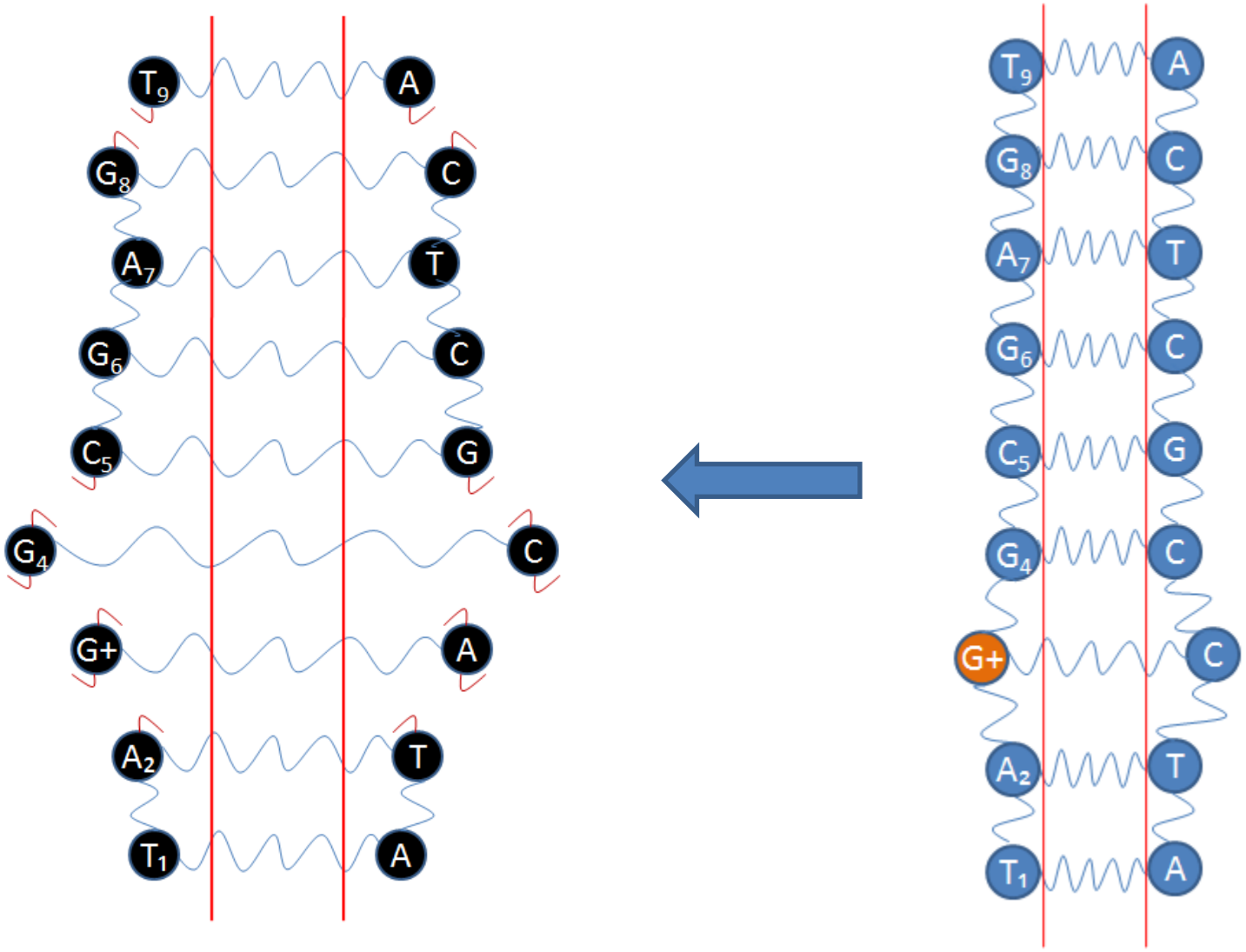


Calculation: stretching of base pairs



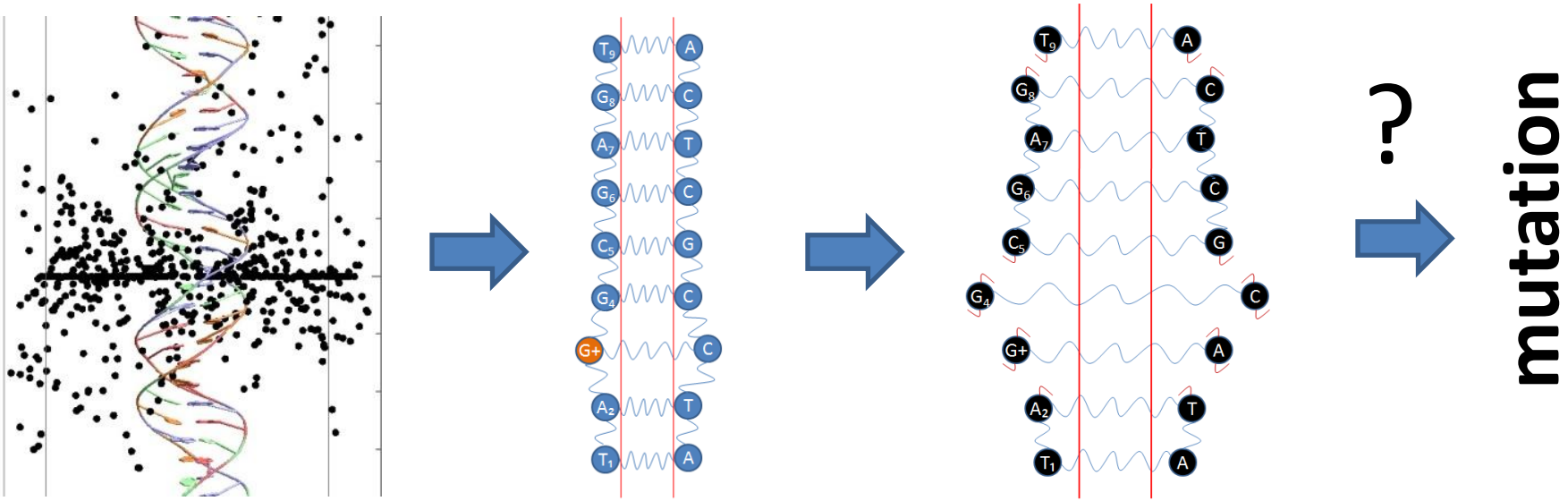


Breaks of DNA sequence



Conclusion

The following process was modeled: charged particle passes through DNA molecule , it leads to ionized of DNA bases; than charge migrates in DNA sequence and results in two strand-breaks of DNA



Thank you for attention