



# Computational Approaches in Molecular Radiation Biology: Monte Carlo Methods (Basic Life Sciences)

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The Office of Health and Environmental Research (OHER) has supported and continues to support development of computational approaches in biology and medicine. OHER's Radiological and Chemical Physics Program initiated development of computational approaches to determine the effects produced by radiation of different quality (such as high energy electrons, protons, helium and other heavy ions, etc. ) in a variety of materials of biological interest-such as water, polymers and DNA; these include molecular excitations and sub-excitations and the production of ionization and their spatial and temporal distribution. In the past several years, significant advances have been made in computational methods for this purpose. In particular, codes based on Monte Carlo techniques have been developed that provide a realistic description of track-structure produced by charged particles. In addition, the codes have become sufficiently sophisticated so that it is now possible to calculate the spatial and temporal distribution of energy deposition patterns in small volumes of subnanometer and nanometer dimensions. These dimensions or resolution levels are relevant for our understanding of mechanisms at the molecular level by which radiations affect biological systems. Since the Monte Carlo track structure codes for use in radiation chemistry and radiation biology are still in the developmental stage, a number of investigators have been exploring different strategies for improving these codes.

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