Despite established clinical use, a deep understanding of proton cancer therapy (PCT) from its underlying physicochemical processes remains elusive. This situation prevents a rational design of PCT that can maximize its therapeutic power and minimize its side effects. The poor characterization of PCT processes stems from the fact that state-of-the-art experimental techniques cannot reveal all the microscopic details of PCT, especially without putting human subjects at risk. To overcome this situation, we are performing electron nuclear dynamics (END) simulations of PCT reactions to elucidate all their microscopic details; these simulations are virtual tests harming no patients. END is a time-dependent, direct, non-adiabatic method to simulate chemical reactions. The simplest-level END (SLEND) used herein employs classical mechanics for the nuclei and a single-determinant wavefunction for the electrons. SLEND uniquely describes the numerous processes (scattering, fragmentations, and energy/electron transfers) that occur simultaneously during PCT. Our SLEND code PACE utilizes various advanced techniques in computer science: Python, FORTRAN and C++ languages, and intra- and internode parallelization. PCT healing power lies in its capacity to inflict nearly irreparable DNA damage in cancerous cells. Therefore, we simulate three types of PCT reactions leading to DNA damage: (1) Proton collisions with water clusters \((H_2O)_{1-6}\) at keV energies as prototypes of water radiolysis reactions — the initial PCT reactions in cellular water that generate the radicals, ions, and electrons that damage DNA; (2) proton collisions with DNA bases and pairs at keV energies as prototypes of DNA damage by protons; (3) single strand breaks (SSBs) in the cytosine nucleotide induced by electrons as a prototype of DNA SSBs by secondary electrons. For 1 and 2, simulations provide target-to-proton 1-electron-transfer and projectile stopping-power integral cross sections in good agreement with experimental results and predict the formation of radicals and ions involved in DNA damage. For 3, simulations provide a unique insight into electron-induced DNA SSB. The predicted properties are relevant for the simulation of mesoscopic PCT processes.