Abstract: The aim of this work is to design and describe a suitable coarse-grained protein model, on the basis of which protein-folding will be studied. The model will be implemented as a computer program, development of the model in time will be simulated by Hamiltonian Monte Carlo. Using computer simulations, not only the protein-folding itself will be investigated, but also the quantities that characterize the process and the similarity of the real and simulated protein's native conformation.

Keywords: protein folding, computer simulation, Hamiltonian Monte Carlo, coarse-grained model