*"Introduction to Molecular Mechanics Treatment of Protein Folding" –*
– prof. Harold A. Scheraga, Cornell University

## ABSTRACT

Beginning with an all-atom force field, extended by a coarse-grained approach, I will discuss the physical basis to compute the folded native structures of proteins (from a knowledge of their amino acid sequences) and of the dynamics in the folding pathways that lead from the unfolded form to the final native structure. The coarse-grained approach helps to access the long experimental timescale of the molecular dynamics method used to compute the folding process.