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1 Introduction 1 1 Protein structure 1 2 Structure determination 1 3 Dynamics simulation 1 4 The myth of protein folding 2 X ray crystallography computing 2 1 The phase problem 2 2 Least squares solutions 2 3 Entropy maximization 2 4 Indirect methods 3 NMR structure determination 3 1 Nuclear magnetic resonance 3 2 Distance geometry 3 3 Distance based modeling 3 4 Structural analysis 4 Potential energy minimization 4 1 Potential energy function 4 2 Local optimization 4 3 Global optimization 4 4 Energy transformation 5 Molecular dynamics simulation 5 1 Equations of motion 5 2 Initial value problem 5 3 Boundary value problem 5 4 Normal mode analysis 6 Knowledge based protein modeling 6 1 Sequence structural alignment 6 2 Fold recognition inverse folding 6 3 Knowledge based structural refinement 6 4 Structural computing and beyond

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Computing Methods in Crystallography J. S. Rollett, 2016-06-06

Computing Methods in Crystallography is a collection of lectures delivered at a Summer School held in Oxford in August 1962. The book presents the underlying mathematics and computing methods in crystallography. The text covers topics on the algebra required for the fundamental operations of transformation of coordinates, interpolation, approximation of trigonometric and exponential functions, solution of linear equations and derivation of latent roots and vectors, methods for calculation of structure factors, least squares adjustment and Fourier series evaluation, the theory and practice of intensity scaling and symmetry determination, and methods of direct phase determination. Crystallographers, physicists, and students in allied fields will find the book very useful.

[Lectures On Symmetry-assisted Computation](#) Danilo Pescia, 2023-11-29

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