

# BIRTH & FUTURE OF MULTISCALE MODELING OF MACROMOLECULES

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## **Abstract**

The development multiscale models for complex chemical systems began in 1967 with publications by Warshel and Levitt recently recognized by the 2013 Nobel Committee for Chemistry. The simplifications used then at the dawn of the age of computational structural biology were mandated by computers that were almost a billion times less cost-effective than those we use today. These same multiscale models have become increasingly popular in application that range from simulation of atomic protein motion, to protein folding and explanation of enzyme catalysis. In this talk I describe the origins computational structural biology and then go on to show some of the most exciting current and future applications