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Sommario/riassunto Complex systems have long been an integral part of modern life and can be encountered everywhere. Undertaking a comprehensive study of such systems is a challenging problem, one which is impossible to solve without the use of contemporary mathematical modeling techniques. Mathematical models form the basis for the optimal design and control of complex systems. The present reprint contains all the articles accepted and published in the Special Issue of Mathematics entitled "Control, Optimization, and Mathematical Modeling of Complex Systems". This Special Issue is focused on recent theoretical and computational studies of complex systems modeling, control, and optimization. The topics addressed in this Special Issue cover a wide range of areas, including numerical simulation in physical, social, and life sciences; the modeling and analysis of complex systems based on mathematical methods and AI/ML approaches; control problems in robotics; design optimization of complex systems, modeling in economics and social sciences; stochastic models in physics and engineering; mathematical models in material science; and high-performance computing for mathematical modeling. It is our hope that the scientific results presented in this reprint will serve as valuable sources of documentation and inspiration to those seeking to delve into complex systems modeling, control, and optimization and examine their wide-ranging applications.