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MBN Explorer and MBN Studio Tutorials

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Preface

This book describes the practical exercises with the MesoBioNano (MBN) Explorer and MBN Studio software packages introducing and illustrating a wide range of applications of the software in different fields. The standard and unique algorithms for classical, Euler, reactive, irradiation-driven, relativistic molecular dynamics and stochastic dynamics and for the structure optimisation of complex molecular systems are introduced and explained in detail using illustrative case studies.

MBN Explorer is a versatile software package for advanced multiscale simulations of complex molecular structure and dynamics. It has many unique features and a wide range of applications in physics, chemistry, biology, materials science and industry. A wide variety of algorithms and interatomic potentials implemented in the program allow simulations of the structure and dynamics of a wide range of systems from atomic up to mesoscopic scales. MBN Explorer is available for Windows, Linux, and MacOS. It is fully parallelised and can be used on computer clusters and supercomputers.

MBN Studio is a dedicated multi-tasking software toolkit with a graphical user interface for MBN Explorer. It helps to set up calculations with MBN Explorer, monitor their progress and examine the calculation results. The graphical utility allows visualisation of selected inputs and outputs. A number of built-in tools allow for the calculation and analysis of specific system characteristics. A special modelling plug-in allows the construction of a wide variety of molecular systems composed of arbitrary atomic and molecular constituents.

MBN Explorer and MBN Studio are being developed and distributed by MBN Research Center, www.mbnresearch.com, which organises hands-on tutorials, user workshops and conferences.

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Contents