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# MBN Explorer and MBN Studio Tutorials

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# Preface

This book describes the practical exercises with MesoBioNano (MBN) Explorer and MBN Studio software packages introducing and illustrating a broad range of applications of the software in various fields. The standard and unique algorithms for molecular and Monte Carlo dynamics and for optimisation of complex molecular systems are introduced and explained in details invoking illustrative case studies.

MBN Explorer is a multi-purpose 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 broad variety of algorithms and interatomic potentials implemented in the program allow simulations of structure and dynamics of a broad range of systems with the sizes from the atomic up to the mesoscopic scales. MBN Explorer is available for Windows, Linux, and macOS. It is fully parallelised and can be exploited on computer clusters and supercomputers.

MBN Studio is a special multi-task software toolkit with a graphical user interface for MBN Explorer. It helps setting up calculations with MBN Explorer, monitoring their progress and examining the calculation results. The graphical utility enables to visualise selected inputs and outputs. A number of built-in tools allow for the calculation and analysis of specific systems' characteristics. A special modelling plug-in allows constructing a large variety of molecular systems built 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 for the software, user's workshops and conferences.

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- MBN Explorer and MBN Studio user's workshops.

Special packages including education, dedicated hands-on training and helpdesk are also available. Contact us or visit our website www.mbnresearch.com for more details.

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