MesoBioNano (MBN) Studio is a special multi-task software toolkit with graphical user interface developed to facilitate the practical work with MBN Explorer. It simplifies modelling of MBN systems, setting up calculations, monitoring their progress, visualising and examining the calculation results. MBN Studio can be utilised for any type of calculations supported by MBN Explorer.

MBN Studio has a number of built-in analytic tools allowing the calculation of specific characteristics that are determined by the output of simulations.
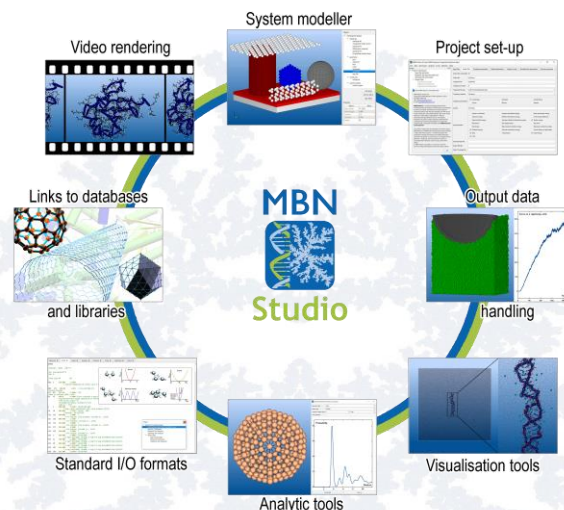
A special modelling plug-in of MBN Studio allows to easily construct a large variety of molecular systems of different geometry built of arbitrary atomic and molecular constituents.

MBN Studio allows setting up application-specific projects which involve special algorithms. Such projects are designed for the particular tasks that are linked to the applications of significant impact and importance, such as novel and emerging technologies.

MBN Studio assists in utilising libraries and databases that provide coordinates and geometries for atomic clusters, nanoparticles, biomolecules, crystals and other MBN systems.

Read more on www.mbnresearch.com

System modeller
Video rendering
Project set-up
Links to databases and libraries
MBN Studio
Output data handling
Standard I/O formats
Analytic tools
Visualisation tools

IN SUMMARY

MesoBioNano (MBN) Studio is a special multi-task software toolkit with graphical user interface developed 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 allows 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 Studio is being developed and distributed by MBN Research Center, which organises hands-on tutorials for the software, user's workshops and conferences.

MBN Studio can be utilised for any type of calculations that are supported by MBN Explorer, such as single-point energy calculations, structure optimisation, molecular dynamics (non-relativistic, relativistic, Euler, irradiation driven) and kinetic Monte Carlo simulations. MBN Studio is being continuously developed by the joint participation of world class scientists and professional IT developers. Being tested by several research groups worldwide, the MBN Studio software toolkit is described in detail in the book of MBN Explorer and MBN Studio Tutorials, and also in the book *"Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer"* published by Springer in 2017, ISBN 978-3-319-56085-4.

MBN Research Center

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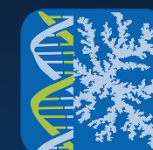
MBN Studio

MULTITASK SOFTWARE
TOOLKIT WITH GRAPHICAL
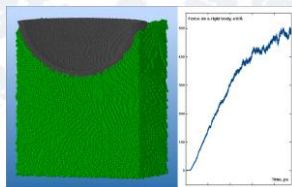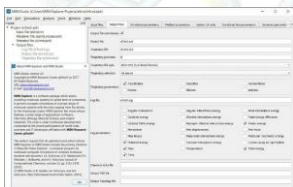USER INTERFACE FOR
MBN Explorer

www.mbnresearch.com

Meso**B**io**N**ano systems
modelling with a single software

Computational Physics at the Life Science interface: MesoBioNano Science
Computational Physics, Chemistry and Biology
Computational Material Science
High Performance Computing

VISUALISATION TOOLS
- Visualisation of input and output data
- Visualisation of simulated atomic trajectories
- Modelling, virtual manipulation and design of MBN systems
- Different representation and colour schemes

OUTPUT DATA HANDLING
- Built-in drawing tool for plotting systems' characteristics
- Graphical representation of data
- Easy handling of output data and their representation

ANALYTIC TOOLS
- Built-in tools for analysis of output data
- Calculation of diffusion coefficients of atoms and molecules, melting temperatures, heat capacities, radial distribution functions, etc.
- Applicable to any modelled system

PROJECT SET-UP
- User-friendly interface
- Support of all types of MBN Explorer calculations
- Setting-up standard and application-specific projects
- Use of MBN Explorer examples library

Longstanding development
now available for the community

STANDARD I/O FORMATS
- Working with the coordinate, trajectory, potential, topology, manipulation and chemical rules files
- Support of several popular file formats, including XYZ, DCD, PDB and PSF

ACADEMIC LICENSING
The use of MBN Explorer and MBN Studio for non-commercial purpose is granted through low price academic licenses. This licensing agreement is restricted to Universities and Research Centers aiming for scientific publication of their results. Reference to MBN Explorer and MBN Studio in reports, publications, or communication mentioning research results obtained with the use of MBN Explorer and MBN Studio is required. All details about terms and conditions are available on www.mbnresearch.com

ENTERPRISE LICENSING
Accessible individual and multi-users license agreements are offered for commercial exploitation of MBN Explorer and MBN Studio.
Purchased license rights provide access to:
- MBN Explorer and MBN Studio software and its updates
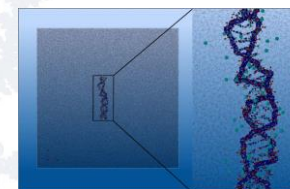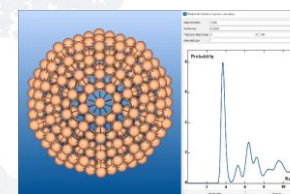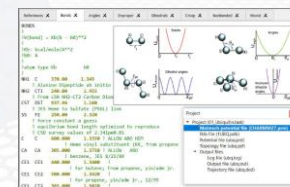- Documentation package
- User's workshops

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

LINKS TO DATABASES AND LIBRARIES
- Built-in library of illustrative examples
- Links to online resources containing coordinates and geometries of various molecular systems, as well as parameters of interaction force fields
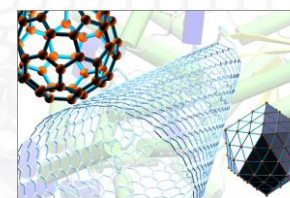
VIDEO RENDERING
- Composing and editing of image frames
- Video rendering of results of MD and MC simulations
- Encoding of sets of frames as MPEG movies

COMPATIBLE WITH
- MICROSOFT WINDOWS
- LINUX
- MAC OS X
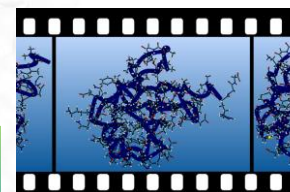
SYSTEM MODELLER
- Creating of input files for MBN Explorer
- Construction of complex molecular systems of different geometry and composition
- Built-in tools for generating 1D, 2D and 3D objects of different shapes