Training course on

Computational Methods for Complex Molecular Systems

The Open University
Milton Keynes, United Kingdom
May 4 - 5, 2017

MBN Research Center

The Open University

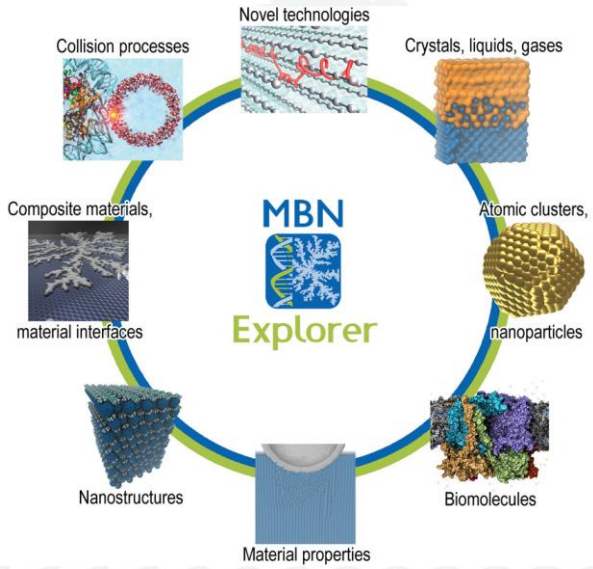
ANNOUNCEMENT

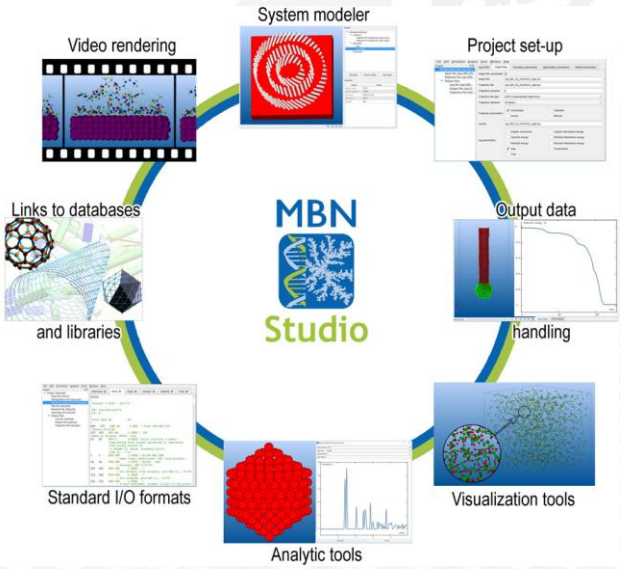
Scope

The 7th training course on Computational Methods for Complex Molecular Systems will be held at School of Physical Sciences, the Open University (Milton Keynes, United Kingdom) on May 4-5, 2017.

The hands-on tutorial will explore physical models and computational approaches used for the simulations of Meso-Bio-Nano (MBN) systems and the investigation of their structure and dynamics at the atomic level of detail. The course is based on practical exercises with the universal computational package MBN Explorer and MBN Studio - a special graphical user interface and multitask toolkit for MBN Explorer. The tutorial will be performed with the latest release 3.0 of MBN Explorer and MBN Studio to be announced officially by MBN Research Center on March 31, 2017.

Figures below illustrate the main areas of application of MBN Explorer and the key features of MBN Studio.





In particular, the case studies of atomic clusters, nanoparticles, biomolecular systems, nanomaterials, composite materials and material interfaces, crystalline, liquid and gaseous systems, thermo-mechanical properties of materials, dynamical, collision, chemical and irradiation driven multiscale phenomena will be discussed. Relevant physical concepts, mathematical techniques and computational methods will be introduced, including force fields and algorithms used in molecular modeling, molecular dynamics (MD), and Monte Carlo simulations on parallel computers.

The tutorial is designed for graduate students, postdoctoral researchers and staff in computational and/or bio/nanophysical and chemical fields, material science, radiochemistry and radiobiology who seek to extend their research skills to include computational and theoretical expertise, as well as for all other researchers interested in theoretical and computational physics and chemistry.

Important Dates

Registration deadline:	**April 16, 2017**
Acceptance of the registered participants for the tutorial:	**April 23, 2017**

Program

May 4, 10:00 - 18:30, Robert Hooke seminar room at the Hooke building

10:00 - 10:15	**Training course opening**
10:15 - 11:00	**Basics of MBN Explorer and MBN Studio** Short description of main features of MBN Explorer and MBN Studio: universality, tuneable force fields, multiscale approach, computational efficiency, etc.; areas of application of MBN Explorer and MBN Studio
11:00 - 11:20	**Coffee break**
11:20 - 11:50	**Setting up the calculation** Specification of input files and formats, and instructions on how to run MBN Explorer
11:50 - 12:50	**MBN Studio** An introduction to MBN Studio - a multipurpose toolkit for MBN Explorer - and an overview of its main features. Overview of the MBN Explorer examples library, which contains the trial case studies representing certain physical experiments and demonstrating capacities of the program
12:50 - 14:00	**Lunch**
14:00 - 15:00	**Gases, liquids, crystals** Description of setting up simulations of gaseous, liquid and crystalline media with MBN Explorer. Different types of boundary conditions. Energy and temperature control in MBN Explorer
15:00 - 16:00	**Atomic clusters and nanoparticles** Description of setting up calculations involving atomic clusters and nanoparticles. Construction of clusters and nanoparticles with MBN Studio
16:00 - 16:30	**Coffee break**
16:30 - 17:30	**Biomolecular systems** Exploration of dynamical processes with biomolecular systems. Use of the molecular mechanics potential for setting up calculations of biomolecular systems. Simulation of bond breakage processes in biomolecular systems using MBN Explorer
17:30 - 18:30	**Collision and irradiation induced processes** MD simulation of collision and irradiation-induced processes in organic and inorganic molecular systems and materials
19:30 - 22:00	**Dinner**

May 5, 09:30 - 17:45, Robert Hooke seminar room at the Hooke building

9:30 - 10:30	**Multiscale modeling: composite materials and material interfaces** Application of the kinetic Monte Carlo method for simulations of fractal structures growth and their post-growth relaxation
10:30 - 11:30	**Nanostructured materials** Application of classical MD for simulations of carbon-based nanomaterials
11:30 - 12:00	**Coffee break**
12:00 - 13:00	**Thermo-mechanical properties of materials** Investigation of thermo-mechanical properties of crystalline, nanostructured and amorphous materials by means of MD simulations of the nanoindentation process
13:00 - 14:00	**Lunch**
14:00 - 15:00	**Propagation of particles through medium** MD simulations of particles propagation through media (heterocrystalline structures, bent crystals, amorphous materials, solids, nanotubes, biological environment, etc.)
15:00 - 16:00	**Irradiation induced transformations of biomolecular systems** Exploration of dynamical processes related to the irradiation induced thermo-mechanical damage of molecular and biomolecular systems

16:00 - 16:30	**Coffee break**
16:30 - 17:30	**Modeling of focused electron beam-induced deposition** Introduction to the concept of irradiation-driven molecular dynamics; MD simulations of the focused electron-beam induced deposition process
17:30 - 17:45	**Tutorial closing and concluding remarks**

Registration and Fee

The participation in the tutorial is free of charge.

All the participants are requested to register electronically by filling in the registration form in the training course webpage:

http://mbnresearch.com/tutorial-6-registration

Since the number of tutorial participants is limited to 20 the registration for the tutorial will be closed automatically once the maximum possible number of registrations will be reached.

All the attendees of the tutorial will receive the e-book of MBN Explorer and MBN Studio Tutorials, 1 month license for running MBN Explorer and MBN Studio and a memory stick with MBN Explorer, MBN Studio and Tutorial files. Coffee and other drinks will be served during the breaks.

Attendees are assumed to cover travel and accommodation expenses themselves. The list of the recommended hotels and B&Bs in the vicinity of the tutorial venue can be found below. The travel hints are also available below. Lunch can be purchased at the Hub restaurant located next to the tutorial venue. Dinner will be arranged on Thursday, May 4th evening for all the participants.

Venue and Travel Information

The tutorial will be held at School of Physical Sciences, the Open University Campus (Milton Keynes, UK).

The tutorial venue is the Robert Hooke seminar room at the Hooke building.

The travel instructions how to reach the Open University Campus at Walton Hall are available under the following link: http://www.open.ac.uk/about/estates/travel-advice/directions-walton-hall-campus

Accommodation

The organizers recommend the tutorial attendees to book their accommodation in the following hotels and Bed & Breakfasts located on the walking distance from the tutorial venue:

Hotels:

Kents Hill Park:
http://kentshillpark.com/accommodation

Hilton Milton Keynes:
http://www3.hilton.com/en/hotels/united-kingdom/hilton-milton-keynes-MIKHNHN/index.html?WT.mc_id=zELWAKN0EMEA1HI2DMH3LocalSearch4DGGenericx6MIKHNHN

Premier Inn:
http://www.premierinn.com/gb/en/hotels/england/buckinghamshire/milton-keynes/milton-keynes-south.html?cid=GLBC_MILCAL

Bed & Breakfasts:

Apple Tree House:
https://www.4hotels.co.uk/uk/hotels/appletree2.html

Flowers House:
http://www.flowershouse.co.uk/index.html

Official Invitation and Visa

The participants of the training course are advised to check the passport and visa requirements for travel to the United Kingdom. For assistance with official invitation and the visa support please contact Mrs. Beverley Bishop, beverley.bishop@open.ac.uk

Training Course Language

The language of the training course is English.

Tutorial Organizers

Dr. Pablo de Vera and Prof. Dr. Nigel J. Mason
School of Physical Sciences
The Open University
MK7 6AA Milton Keynes, United Kingdom
E-mail: n.j.mason@open.ac.uk

Dr. Alexey Verkhovtsev and Prof. Dr. Andrey V. Solov'yov
MBN Research Center at FiZ - Frankfurt Innovation Center of Biotechnology
Altenhöferallee 3
60438 Frankfurt am Main
E-mail: solovyov@mbnresearch.com

Contact Information

For further information please visit the training course page: mbnresearch.com/tutorial-6-scope
or write an e-mail to team@mbnexplorer.com