Training course on

Multiscale Computational Methods for Complex Molecular Systems

Cranfield University
Cranfield, United Kingdom
November 29 - December 01, 2017

MBN Research Center

Cranfield University

The Open University

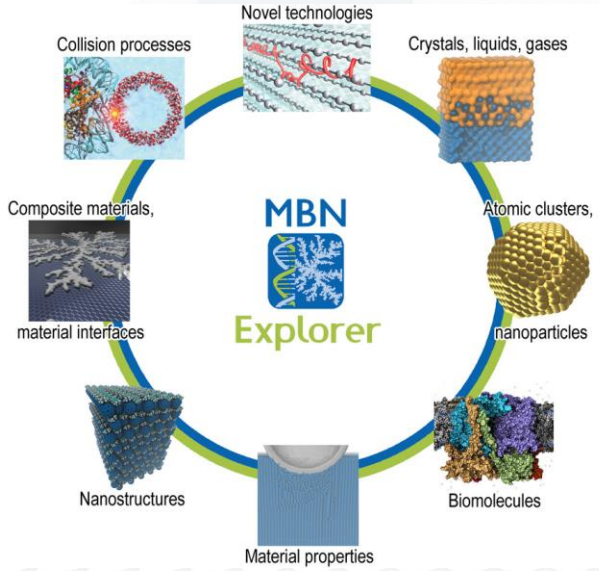
ANNOUNCEMENT

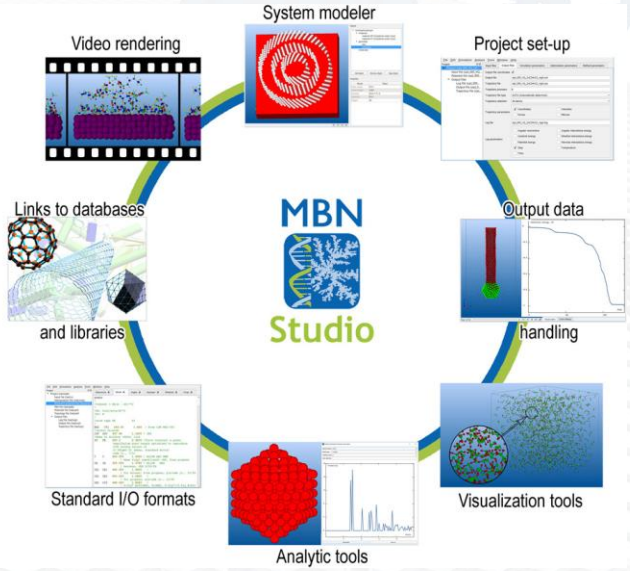
Scope

The training course on Multiscale Computational Methods for Complex Molecular Systems will be held at the Cranfield University (Cranfield, United Kingdom) on November 29 - December 01, 2017.

The hands-on tutorial aims at exploring 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 announced officially by MBN Research Center in March 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 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.

The recommended literature for the background reading:

1. I.A. Solov'yov, A.V. Korol, A.V. Solov'yov, *Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer*, Springer International Publishing AG, Switzerland (2017); Hardcover ISBN 978-3-319-56085-4; eBook ISBN 978-3-319-56087-8, DOI 10.1007/978-3-319-56087-8

2. I.A. Solov'yov, G. Sushko, A.V. Solov'yov, *MBN Explorer Users' Guide Version 3.0*, MesoBioNano Science Publishing, Frankfurt am Main, Germany; Verlag: CreateSpace Independent Publishing Platform, (2017), ISBN-10: 1975639049, ISBN-13: 978-1975639044

3. I.A. Solov'yov, G.B. Sushko, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, *MBN Explorer and MBN Studio Tutorials: Version 3.0*, MesoBioNano Science Publishing, Frankfurt am Main, Germany; Verlag: CreateSpace Independent Publishing Platform (2017), ISBN-10: 1976460921, ISBN-13: 978-1976460920

Important Dates

Registration deadline: **November 21, 2017**
Acceptance of the registered participants for the tutorial: **November 22, 2017**

Program

Wednesday, November 29
Venue: University of Cranfield, Building B83, Room B. Wallis

11^{30} - 11^{45}	**Training course opening**
11^{45} - 12^{30}	**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
12^{30} - 13^{00}	**Setting up the calculation** Specification of input files and formats, and instructions on how to run MBN Explorer
13^{00} - 14^{00}	**Lunch**
14^{00} - 15^{00}	**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
15^{00} - 16^{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
16^{00} - 16^{30}	**Coffee break**
16^{30} - 17^{30}	**Atomic clusters and nanoparticles** Description of setting up calculations involving atomic clusters and nanoparticles; construction of clusters and nanoparticles with MBN Studio

Thursday, November 30
Venue: University of Cranfield, Building B83, Room B. Wallis

09^{30} - 10^{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
10^{30} - 11^{30}	**Collision and irradiation induced processes**

	MD simulation of collision and irradiation-induced processes in organic and inorganic molecular systems and materials
11^{30} - 12^{00}	**Coffee break**
	Multiscale modelling: composite materials and material interfaces
12^{00} - 13^{00}	Application of the kinetic Monte Carlo method for simulations of fractal structures growth and their post-growth relaxation
13^{00} - 14^{30}	**Lunch**
	Nanostructured materials
14^{30} - 15^{30}	Application of classical MD for simulations of carbon-based nanomaterials
	Thermo-mechanical properties of materials
15^{30} - 16^{30}	Investigation of thermo-mechanical properties of crystalline, nanostructured and amorphous materials by means of MD simulations of the nanoindentation process

Friday, December 01
Venue: University of Cranfield, Building B83, Room B. Wallis

	Propagation of particles through medium
09^{30} - 10^{30}	MD simulations of particles propagation through media (heterocrystalline structures, bent crystals, amorphous materials, solids, nanotubes, biological environment, etc.)
	Irradiation induced transformations of biomolecular systems
10^{30} - 11^{30}	Exploration of dynamical processes related to the irradiation induced thermo-mechanical damage of molecular and biomolecular systems
11^{30} - 12^{00}	**Coffee break**
	Modelling of focused electron beam-induced deposition
12^{00} - 13^{00}	Introduction to the concept of irradiation-driven molecular dynamics; MD simulations of the focused electron-beam induced deposition process
13^{00} - 13^{15}	**Tutorial closing and concluding remarks**

Registration and Fee

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-8-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 participants are requested to bring their own laptops to the tutorial.

All the attendees of the tutorial will receive the e-book of MBN Explorer and MBN Studio Tutorials, a library of Tutorial examples, and one-month license for running MBN Explorer and MBN Studio.

Attendees are assumed to cover meals, travel and accommodation expenses themselves.

Venue and Travel Information

The Training Course will be hosted by the Cranfield University, United Kingdom. The Cranfield University Campus is located close to Milton Keynes and Bedford, in Wharley End, very close to Cranfield village, and is about 10 minutes from the M1 motorway. There is rail and road access to most major airports as well as coach and train stations. Cranfield campus also has its own airport for private executive business travel. The venue of the tutorial will be building B83, room B.Wallis.

For more information on how to get to the Cranfield University Campus and the tutorial venue see the webpage.

Accommodation

Information on the hotels close to the venue can be found here.

Official Invitation and Visa

Training course participants are advised to check the passport and visa requirements for travel to the United Kingdom well in advance.

Training Course Language

The language of the training course is English.

Tutorial Organizers

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Contact Information

For further information please visit the training course page: www.mbnresearch.com/tutorial-8-scope
or write an e-mail to team@mbnexplorer.com