Training course on
Multiscale Computational Methods for Complex Molecular Systems

Università degli Studi di Ferrara
Ferrara, Italy
October 26 - 27, 2017

MBN Research Center

**UNIVERSITÀ DEGLI STUDI DI FERRARA**
- EX LABORE FRUCTUS -

ANNOUNCEMENT

Scope

The training course on Multiscale Computational Methods for Complex Molecular Systems will be held at the Università degli Studi di Ferrara (Ferrara, Italy) on October 26-27, 2017. It will be preceded by the Workshop of the H2020-RISE-PEARL project "Periodically Bent Crystals for Crystalline Undulators", which will be held during October 23-25.

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.
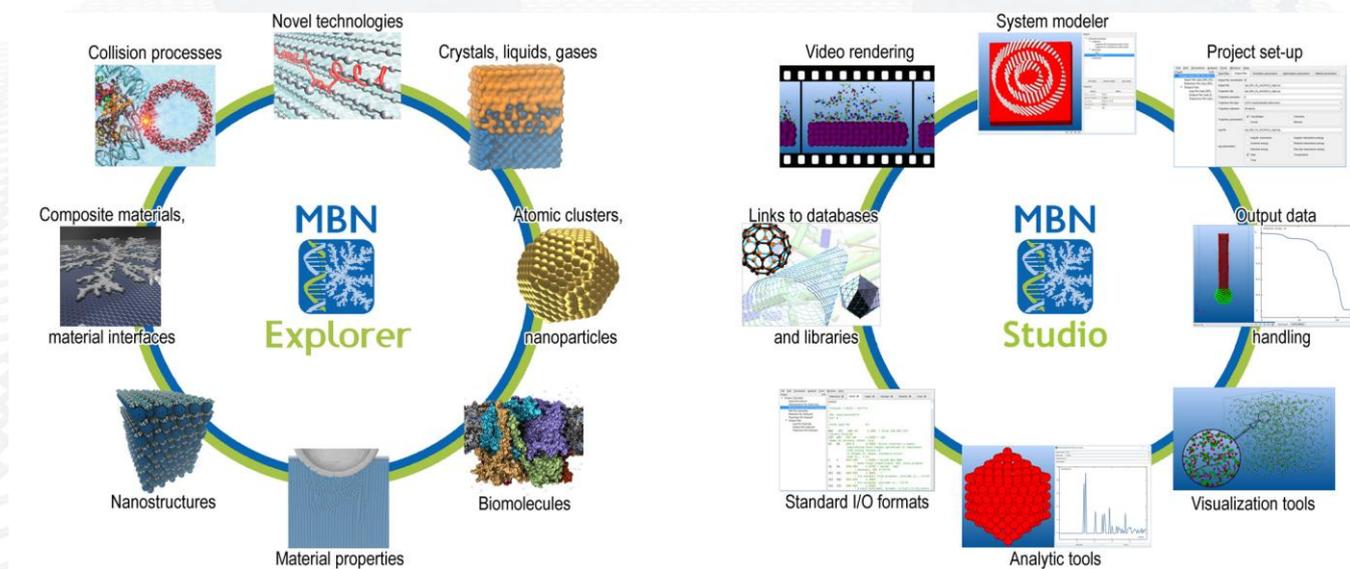
In particular, the case studies of atomic clusters, nanoparticles, biomolecular systems, nanomaterials, composite materials and material interfaces, crystalline, liquid and gaseous systems, thermo-mechanical properties of materials, dynamical, collision, chemical and irradiation driven multiscale phenomena 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. Special attention will be devoted to modeling crystalline structures, propagation of relativistic projectiles in crystals, quantitative analysis of the channeling and related phenomena.

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:	**October 17, 2017**
Acceptance of the registered participants for the tutorial:	**October 18, 2017**

Program

Thursday, October 26
Venue: Polo Scientifico Tecnologico - Università degli Studi di Ferrara, via Saragat 1, 44122 Ferrara

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

Friday, October 27,
Venue: Polo Scientifico Tecnologico - Università degli Studi di Ferrara, via Saragat 1, 44122 Ferrara

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 - 16:00	**Propagation of particles through medium**

	MD simulations of particles propagation through media (heterocrystalline structures, bent crystals, amorphous materials, solids, nanotubes, biological environment, etc.); modeling of particles' propagation in crystalline media by means of Geant4
16:00 - 16:30	**Coffee break**
16:30 - 17:30	**Irradiation induced transformations of biomolecular systems** Exploration of dynamical processes related to the irradiation induced thermo-mechanical damage of molecular and biomolecular systems
17:30 - 18:30	**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
18:30 - 18:45	**Tutorial closing and concluding remarks**

Registration and Fee

The fee for participation in the training course is 50 Euro. The payment to the order of "Training course in Ferrara" should be made **by bank transfer** to:

Bank Account Name:	MBN Research Center gGmbH
Bank Name:	Deutsche Bank
Branch Address:	Hauptstr. 5, 61462 Koenigstein, Germany
IBAN:	DE15500700240137588000
BIC:	DEUTDEDBFRA

Please quote your NAME and "MBN Training" on the transfer. Please ensure there are NO charges to us.

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

http://mbnresearch.com/tutorial-7-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, one-month license for running MBN Explorer and MBN Studio, and Tutorial files. A student cafeteria is available at the University for coffee and lunch.

Attendees are assumed to cover meals, travel and accommodation expenses themselves. The list of the recommended hotels in the vicinity of the tutorial venue can be found below.

Venue and Travel Information

The tutorial will be held at the Università degli Studi di Ferrara, via Savonarola, Ferrara, Italy. The University is located in the historical center of the World Heritage medieval city of Ferrara. You can get to Ferrara

By plane from:

- Bologna airport "Guglielmo Marconi" is located 35 km from Ferrara (about 30 minutes by car). The region has a new flybus service between Bologna airport and Ferrara called "bus&fly" (http://www.ferrarabusandfly.it/).

Ferrara/ Bologna rail line is direct (www.trenitalia.it); the airport is connected to the train station by means of a direct bus system named "aerobus" and provides direct flights to the most important Italian and European cities all year. For further information see www.bologna-airport.it.

- <u>Venice airport "Marco Polo"</u> is located 116 km from Ferrara (about 1 hour and 15 minutes by car). Ferrara/Venice rail line is direct (www.trenitalia.it); the airport is connected to the train station by means of a direct bus system named "flybus" and provides direct flight to the most important Italian and European cities all the year. For further information see www.veniceairport.it.

- <u>Verona airport "Valerio Catullo"</u> is located 106 km far from Ferrara (about 1 hour and 20 minutes). Ferrara/Verona rail line is not direct, it is necessary to change train in Padua or Bologna (www.trenitalia.it); the airport is connected to the train station by means of a direct bus system and provides direct flights to the most important Italian and European cities all year. For further information see www.aeroportoverona.it

By train:

All important information can be found at www.trenitalia.it. The train station of Ferrara is not far away from the city center.

Accommodation

The organizers recommend the tutorial attendees to book their accommodation in the following hotels located close to the tutorial venue:
- Hotel Annunziata
- Hotel Carlton
- Hotel Turing
- Hotel Europa
- Hotel De Prati

Official Invitation and Visa

Training course participants are advised to check the passport and visa requirements for travel to Italy 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: mbnresearch.com/tutorial-7-scope or write an e-mail to team@mbnexplorer.com