PRACE Winter School 2018 - Computational Chemistry, Biochemistry and Medicinal chemistry– Methods and Tools

Monday, 26 November 2018 - Thursday, 29 November 2018

National Centre for Supercomputing Applications, Bulgaria

Scientific Programme

Programme committee:
Prof. Toni Spassov
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The program is designed to demonstrate and encourage the application of computational methods and tools in solving numerous problems in Chemistry, Materials science and related fields and to introduce young researchers to the ideology and potential of this modern approach in solving scientific problems at atomic and molecular level. The advantages of the High Performance Computing (HPC) in the above fields will be also a focus of the school, discussing the methodologies, numerical methods and their implementation used by the state-of-the-art codes in the HPC environment.

Keynote lectures by scientists with different research profile in the field of chemistry and materials science will present the benefits gained by using the HPC facilities. Predictive models of the relationships between molecular structure and useful properties, chemistry and thermodynamics of molecules in gas phase and condensed matter will be part of the topics presented.

The attendants will learn the different techniques and their implementation in various codes, as well as will acquire the results that can be attained on the most recent HPC architectures. A particular focus will be the next technological developments and the possibilities that will be opened to chemists, biochemists and material scientists. Conditions for discussion and interaction with lecturers will be provided.

The experiences the UK's Hartree Centre has had in this direction over the last couple of years will be exchanged. To showcase a number of studies of academic interest and their relation to molecular modeling and HPC. To encourage industrial and academic establishments **to jointly seek and provide funding schemes for working together and expose students and** researchers to industrial modes of modeling work. To provide information and training of HPC applications relevant for the materials modeling studies, developed at STFC Daresbury Laboratory.