Workshop Evolutionary Computation in Computational Structural Biology 2016 Chairs' Welcome

It is our great pleasure to welcome you to the 2016 *ACM Workshop Evolutionary Computation in Computational Structural Biology*, associated with GECCO 2016, the largest international conference in the field of genetic and evolutionary computation (with proceedings published by ACM Digital Library).

In the last two decades, many computer scientists in Artificial Intelligence have made significant contributions to modeling biological systems as a means of understanding the molecular basis of mechanisms in the healthy and diseased cell. In particular, the field of computational structural biology is now highly populated by researchers in evolutionary computation. Great progress is being made by these researchers on novel and powerful algorithms to solve exceptionally challenging computational structural biology problems at the heart of molecular biology, such as structure prediction, analysis, and design of biological macromolecules (proteins, RNA). These problems pose difficult search and optimization tasks on modular systems with vast, high-dimensional, continuous search spaces often underlined by non-linear multimodal energy surfaces.

The focus of this workshop is the use of nature-inspired approaches to central problems in computational structural biology, including optimization methods under the umbrella of evolutionary computation. A particular emphasis is on progress in the application of evolutionary computation to problems related to any aspects of protein structure modeling, characterization, and analysis. The workshop allows for a broader focus on all structure-related problems that necessitate the design of novel evolutionary computation approaches. These may include broader structure modeling settings beyond *de novo* structure prediction, such as mapping of protein and peptide energy landscapes, structure analysis, design, docking, and other emerging problems in computational structural biology.

Following the previous edition in GECCO 2015, one of the objectives of this workshop is to aid evolutionary computation researchers to disseminate recent findings and progress. The workshop provides a meeting point for authors and attendants of the GECCO conference who have a current or developing interest in computational biology. We believe the workshop additionally can attract computational biology researchers that will further add to the attendance and GECCO community and possibly spur novel collaborations. We hope this workshop stimulates the free exchange and discussion of novel ideas and results related to structure-central problems bridging computational biology and evolutionary computation.

Within the aims of the workshop, the call for papers attracted submissions from Spain, United States and Brazil. The accepted papers in Evolutionary Computation in Computational Structural Biology 2016 cover important bioinformatics problems such as: i) use of multi-objective (MO) genetic search for protein structure prediction (PSP) with the insertion of the crowding-distance technique in a MO evolutionary algorithm to obtain a more diversified and well distributed Pareto Set; ii) the use of evolutionary strategies to map protein energy landscapes effectively with the ultimate objective of using the maps to identify the structural paths taken by dynamic proteins during basin-to-basin switches; iii) the use of a parallel ecology-inspired algorithm to a hard problem related to PSP: the protein structure reconstruction from Contact Maps; iv) the modeling of the temporal and dynamic folding of proteins with neural cellular automata in off-lattice models. In addition, we have a keynote talk by Professor Kenneth A. De Jong, from George Mason University.

We hope that you will find this program interesting and thought-provoking, stimulating your interest in the many issues surrounding Computational Structural Biology and Evolutionary Computation. The topics covered in the papers are timely and important, and the authors have done an excellent job of presenting the material. We express our gratitude to Professor De Jong, the authors and presenters as well as the

participants for making this workshop a success. We sincerely hope that the symposium will provide you with a valuable opportunity to share ideas with other researchers and practitioners from institutions around the world.

José Santos
University of A Coruña, Spain
Workshop Chair

Julia Handl
University of Manchester, UK
Workshop Chair

Amarda Shehu
George Mason University, USA
Workshop Chair