Evolutionary Computation in Computational Structural Biology'15 Chairs' Welcome

It is our great pleasure to welcome you to the 2015 *ACM Workshop Evolutionary Computation in Computational Structural Biology*, associated with GECCO 2015, 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.

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 different countries in Europe (Luxembourg, UK, Spain), United States, Mexico and Brazil. The accepted papers in Evolutionary Computation in Computational Structural Biology 2015 cover important bioinformatics problems such as: use of multi-objective genetic search for finding active sites in proteins, hybrid solutions between differential evolution and fragment-based replacements for protein structure prediction using the Rosetta environment, the definition of NK landscape instances to mimic the properties of the protein inverse folding problem, mapping multiple minima in protein energy landscapes with evolutionary algorithms, an experimental analysis of the performance of side chain packing algorithms and the use of machine learning to explore the relevance of local and global features during decoy generation in Rosetta.

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 the 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.



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