Computational structural biology is an important, growing research area that includes diverse problems, such as protein structure prediction, computational molecular assembly, and computer-assisted drug design problems, that include protein-ligand binding, protein-protein, protein-RNA, and protein-DNA docking, as well as computer-assisted wet-laboratory structure resolving problems, like registration, reconstruction, and refinement. The focus of this special section is on the application of non-linear optimization to problems in structural biology, thus turning the spotlight on a growing area of interdisciplinary research that brings together expertise in meta-heuristic optimization and computational structural biology. The five articles included in this section provide a glimpse of the diversity of work in this area, highlighting the adaptation and use of a variety of state-of-the-art meta-heuristics for a range of problems linked to the wider area of structural biology.

The first three articles particularly illustrate the promise of integrating population-based search heuristics with problem-specific local search techniques to improve search performance on challenging optimization problems. Specifically, “A Memetic Algorithm for 3D Protein Structure Prediction Problem” by Corrêa et al. describes a memetic algorithm for the problem of de novo protein structure prediction. Structural knowledge from the Protein Data Bank is employed to constrain the space of possible protein conformations, and a simulated annealing protocol is employed as the local search protocol in the underlying evolutionary algorithm.

“A Global Network Alignment Method Using Discrete Particle Swarm Optimization” by Huang et al. describes the use of particle swarm optimization for the problem of network alignment. Particle swarm optimization is well known as a meta-heuristic for continuous optimization. In this article, a discrete version of the algorithm is developed and combined with problem-specific seeding mechanisms and a greedy search technique that builds upon these seeds.

“From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes” by Sapin et al. uses an evolutionary algorithm to explore and map the energy landscape characterizing the transitions between different structural states of dynamic proteins. Here, local search techniques are used as an efficient means of properly descending into local energy basins of the search landscape.

“Conformational Sampling of a Biomolecular Rugged Energy Landscape” by Rydzewski et al. also considers the problem of sampling full-atom biomolecular energy landscapes, but it does so with a focus on the structural refinement of protein structures. For this purpose, it employs another established type of meta-heuristic, an immune algorithm; based on the general principles of this meta-heuristic, the article describes the designated implementation of such an approach that is capable of dealing with the complex energy landscapes encountered for the problem of structural refinement.

Finally, “GPU-Based Point Cloud Superpositioning for Structural Comparisons of Protein Binding Sites” by Leinweber et al. describes the development of an evolution strategy to assist with the structural comparison of binding sites. The approach takes advantage of the capabilities of GPU to speed up computations, and the authors demonstrate possible performance gains both from the perspective of classification accuracy and computational performance.

We would like to thank all of the authors and reviewers involved in producing this special section. As a result of their diligent work, we hope that this special section provides an interesting read both for readers new to or already familiar with non-linear optimization. The selected articles cover a range of different problems in structural biology and highlight some of the design issues that are key to adapting meta-heuristics to these complex problem domains. For readers unfamiliar with meta-heuristic optimization, we are hoping that this special section provides both a flavor of both the variety of meta-heuristics available in the literature, and the breadth of problems that are amenable to the application of such techniques.

Julia Handl is with the Decision and Cognitive Sciences Research Centre, The University of Manchester, UK. E-mail: julia.handl@manchester.ac.uk.

A. Shehu is with the Department of Computer Science, George Mason University, Fairfax, VA 22030. E-mail: amarda.shehu@gmail.com.

J. Santos Reyes is with the Department of Computer Science, Universidade da Coruña, Spain. E-mail: jose.santos@udc.es.

For information on obtaining reprints of this article, please send e-mail to: reprints@ieee.org, and reference the Digital Object Identifier below.

Digital Object Identifier no. 10.1109/TCBB.2018.2817267

1. Reviews were blind and guest editor Amarda Shehu was not involved in the review process of this paper.
Julia Handl received the BS (Hons) degree in computer science from Monash University in 2001, an MS degree in computer science from the University of Erlangen-Nuremberg in 2003, and the PhD degree in bioinformatics from the University of Manchester in 2006. From 2007 to 2011, she held an MRC Special Training Fellowship at the University of Manchester, and she is now a senior lecturer in the Decision and Cognitive Sciences Group at the Manchester Business School. Her PhD work explored the use of multiobjective optimization in unsupervised and semi-supervised classification. She has developed multiobjective algorithms for clustering and feature selection tasks in these settings, and her work has highlighted some of the theoretical and empirical advantages of this approach.

Amarda Shehu received the BS degree in computer science and mathematics from Clarkson University in Potsdam, NY, in 2002 and the PhD degree in computer science from Rice University in Houston, TX, in 2008, where she was an NIH fellow of the Nanobiology Training Program of the Gulf Coast Consortia. Dr. Shehu is an associate professor in the Department of Computer Science at George Mason University. She holds affiliated appointments in the School of Systems Biology and the Department of Bioengineering. Dr. Shehu's research contributions are in computational structural biology, biophysics, and bioinformatics with a focus on issues concerning the relationship between biomolecular sequence, structure, dynamics, and function. Her research on probabilistic search and optimization algorithms for protein structure modeling is supported by various NSF programs, including Intelligent Information Systems, Computing Core Foundations, and Software Infrastructure. She is also the recipient of an NSF CAREER award in 2012.

José Santos Reyes received the MS degree in physics (specialization in electronics) from the University of Santiago de Compostela, Spain, in 1989, and the PhD degree from the same university in 1996 (specialization in artificial intelligence). He is currently an associate professor, accredited as a full professor, in the Department of Computer Science at the University of A Coruña, Spain. His research interests include artificial life, neural computation, evolutionary computation, autonomous robotics, and computational biology. In the last years, his research was focused on computational biology, applying all the knowledge acquired in the other research lines to the computational modeling of biological problems.

For more information on this or any other computing topic, please visit our Digital Library at www.computer.org/publications/dlib.