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Foreword on special issue on robotics methods for structural and dynamic modeling of molecular systems

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Molecular biological systems can be seen as extremely complex mobile systems. The development of methods for modeling the structure and the motion of such systems is essential to better understand their physiochemical properties and biological functions. In recent years, many computer scientists in robotics and artificial intelligence have made significant contributions to modeling biological systems. Research expertise in planning, search, learning, evolutionary computation, constraint programming, and data mining is being used to make great progress on molecular motion, structure prediction, and design.

This special issue is associated with the Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems that took place on July 12th, 2014 in Berkeley California as part of the Robotics Science and Systems (RSS) Conference. The workshop, and subsequently this special issue, highlights many connections between robotics and molecular modeling and features research that crosses the boundaries of robotics, learning, and computational structural biology. Authors from the workshop were invited to submit extended papers to this special issue. Also, submission was open to the wider community. The review process of the *Robotica* Journal was applied to select and refine the papers.

This issue highlights molecular biology systems of varied scale from peptides¹ to proteins^{2,3} to multiple interacting molecules^{4,5} to cells⁶. The problems addressed cover structural prediction^{1,3}, molecule or cell motion^{2,6}, and molecular packing^{4,5}. Despite this diversity, each presented methodology draws inspiration from, parallels, or directly applies solutions from robotics.

The Guest Editors would like to also thank *Robotica* Editor, Greg Chirikjian, who not only was a keynote speaker at the original workshop but also encouraged and supported this special issue. As a result of the significant efforts by Authors, Reviewers, Editors, and *Robotica*, we are pleased to share with you this selection of papers that we hope you will find valuable and will promote further research into and understanding of the ties between molecular systems and robotics.

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