MolVA 2021

Workshop on Molecular Graphics and Visual Analysis of Molecular Data

Zurich, Switzerland (Virtual Conference)

June 14, 2021

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Sponsored by EUROGRAPHICS Association

DOI: 10.2312/molva.20212007

Published by the Eurographics Association
–Postfach 2926, 38629 Goslar, Germany–
in cooperation with
Institute of Computer Graphics & Knowledge Visualization at Graz University of Technology
and
Fraunhofer IGD (Fraunhofer Institute for Computer Graphics Research), Darmstadt

ISBN 978-3-03868-145-8

The electronic version of the proceedings is available from the Eurographics Digital Library at `https://diglib.eg.org`

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Invited Speaker

A la Carte Biomolecular Design: Algorithms and Supercomputing

Victor Guallar

Abstract

We are witnessing a significant revolution in the way science is performed. Just 20 years ago, pharmaceutical companies fired many of their computational chemists after the frustration from the (false?) high expectations that modelling had created. We should admit that most of the scientific community did not appreciate bioinformatics. My experimental faculty colleagues, at Washington University at that time, always looked over us with a fake smile. And in the last few years, all has changed. Today, there is no serious pharmaceutical effort that does not start with an exhaustive in silico study. And it is catching up in many more areas of biotechnology, such as enzyme engineering, or material science. One could even state that it is general to all science: it does first get modelled. What has happened in these 10-15 years? Clearly, we have seen an explosion of better algorithms and of the available data to test/train them; all these happening under easy and cheap access to vast supercomputing resources. We will discuss in this talk these advances, focusing on some contributions from our lab and on what we foresee for the next few years.

Short Biography

Dr. Guallar performed his PhD between the University Autonomous of Barcelona (Spain) and UC Berkeley (USA), with defense in November 1999. In 2003, after three years as a postdoctoral researcher at Columbia University (New York, USA), he was appointed assistant professor at Washington University School of Medicine (St Louis, USA). In 2006 he was awarded his current ICREA professor position at the Barcelona Supercomputing Center (BSC). Since then, his laboratory (EAPM) has grown considerably, keeping a productive international character, and developing important contributions in computational biophysics, such as the protein-ligand modeling software PELE, and biochemistry, recently centered on enzyme engineering. Prof. Guallar has been awarded several important research projects, including a prestigious advanced ERC grant (the youngest researcher to receive it in Spain). His research has produced over a 170 papers in international journals, reaching an H-index of 44 and having directed 16 PhD thesis. In addition to algorithms development (and their application), the group has recently placed importance in adding interdisciplinary fields, such as molecular visualization techniques, and data mining and software optimization through machine learning algorithms. Prof. Guallar is also a founder of the first spin off from BSC, Nostrum Biodiscovery, a young biotech enterprise created in 2015 which aims to collaborate with pharmaceutical and biotech companies dedicated to the development of drugs and molecules of biotechnological interest.

Invited Speaker

On Protein Interactions – How to Visually Communicate them?

Barbora Kozlíková

Abstract

In molecular visualization, there are several specific challenges, spanning from understanding single molecular structures, their function, and behavior, to studying their interactivity with other molecular structures. In this talk, I will focus on the latter problem, interactions of protein structures and their visual representation. We will discuss the already existing approaches, as well as the most intrinsic problems that are still waiting to be addressed.

Short Biography

Dr. Barbora Kozlíková is an Associate Professor at the Masaryk University in Brno, Czech Republic, where she established and is heading Visitlab, the research laboratory focusing on designing visualizations for different application domains. One of the core topics of her research is the visualization and visual analysis of biomolecular structures, with a specific focus on molecular dynamics simulations, molecular docking, and molecular interactions. Dr. Kozlíková is also experimenting with virtual reality and its application in molecular modeling and education.