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Path-metadynamics: A computational study of conformational transitions in proteins

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About the author

Grisell Díaz Leines was born in Mexico City in 1983. She obtained a bachelor degree in Physics in Mexico in 2006 at the National University of Mexico (UNAM) with a grade of 9.45/10.0. During her bachelor, she got highly interested in the subject of statistical mechanics, particularly in the study of collective phenomena. Her thesis research was focused on the hydrodynamic mapping of the pattern formation in monolayers using Brewster angle microscopy, a very adventurous project, in the words of the president of her thesis committee and her supervisor. In 2007, she decided to explore a scientific area that lies between experiments and theory and she joined the international Master program in Atomic Scale Modelling (ATOSIM Erasmus Mundus Course) in Italy and The Netherlands to obtain the Master in Physics in 2008, where she was given the highest grade of the year (9.18/10.0). At the end of 2008 she joined a PhD program in Molecular Simulation in the group of Prof. Dr. Peter Bolhuis in Amsterdam, The Netherlands. Her PhD research has focused on the development of a new method (path-metadynamics) to explore high dimensional free energy landscapes of rare event transitions. This development was honoured with its publication in Physical Review Letters in 2012. In the last years of her PhD, she has done a lot of effort to apply this methodology in the study conformational transitions in proteins. In particular, she successfully applied path-metadynamics to study the unfolding process of a relevant signalling protein (the Photoactive Yellow Protein), opening up a way to study rare events in complex transitions. This work is currently closed to its submission to Proceedings of the National Academy of Sciences (PNAS). Her recent efforts are focused in the application of path-metadynamics to study a coiled coil complex transition, the Leucine Zipper domain.

Grisell has a variety of other interests. Modern art museums and painting with oil and acrylics are very good medicines for her soul. During the bachelor time, and inspired by a young impossible dream of understanding the world and save it, she studied two and a half years of a second career in Political Economics and Economical History at the National University of Mexico. In 2012, she also joined the social movement Yosoy132 in The Netherlands, a team dedicated to human rights activism for her country Mexico, where she has participated in the organization of different

cultural events and forums of information about democratization of the media and gender violence. Between 2007-2009 she participated in the Erasmus Mundus student association to promote international education. She joined the PhD council in 2012 to take actions on the interests of the PhD students at the University of Amsterdam. A beach with a lot of sun in the company of her friends or her family sounds like an ideal holiday to her!!

Publications

- Path Finding on High-Dimensional Free Energy Landscapes. Diaz Leines, G. and Ensing, B., *Phys. Rev. Letters*, **109** 020601 (2012)
- Domain Growth, Pattern Formation, and Morphology Transitions in Langmuir Monolayers, A New Growth Instability. Gutierrez-Campos, A. and Diaz-Leines, G. and Castillo, R., *J. Phys. Chem. B*, **114** 5034–5046 (2010)

To be submitted:

- Solvent exposure of Glu-46 is the rate limiting step in the light-triggered unfolding of Photoactive Yellow Protein. Diaz Leines, G., Vreede, J., Branduardi, D. and Ensing, B. In preparation.
- An assessment of Path-Metadynamics. Diaz Leines, G., Branduardi, D. and Ensing, B. In preparation.
- Predicting the mechanism of dissociation/formation of the GCN4 Leucine Zipper domain. Diaz Leines, G., Bolhuis, P. G. and Vreede, J. In preparation.