CompBioMed
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e-Seminar Series

e-Seminar #17
Machine Learning Coarse-Grained Models with Graph Neural Networks

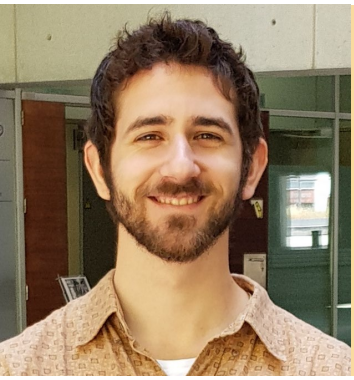
8 September 2021 1pm CEST / 12pm BST (1h duration)

Register for free here: https://register.gotowebinar.com/register/5159085993874550798

Atomistic or *ab initio* molecular dynamics simulations are widely used to predict thermodynamics and kinetics and relate them to molecular structure. A common approach to go beyond the time- and length-scales accessible with such computationally expensive simulations is the definition of coarse-grained molecular models. Recent advances in machine learning allow us to design optimal coarse-grained models for reproducing the equilibrium thermodynamics of a macromolecule.

In this seminar, we will learn how to prepare, train and simulate coarse-grained models with graph neural networks using TorchMD, a deep learning framework for molecular simulations. We will build a coarse-grained model of the fast-folding protein chignolin in order to simulate it and reproduce its folding process.

This is the 17th in a series of online e-Seminars organised by CompBioMed. Watch the full series at www.compbiomed.eu/training!



Adrià Pérez is a Research Fellow at Computational Science group, GRIB, UPF. He holds a Biochemistry degree from Universitat Autònoma de Barcelona and a Master's degree in Bioinformatics from Universitat Pompeu Fabra (UPF). The Computational science research group led by Gianni de Fabritiis is dedicated to computational science in biomedicine and machine learning. The group research interests are rooted in application of computation to solve real world problems. Specifically, we develop new methods and algorithms and we apply them to computational chemistry, drug design, protein folding, etc. The group and the spin-off company Acellera, founded in 2006, has collaborated with major industries worldwide like Sony, Nvidia, HTC mobile, UCB and Pfizer.

Moderated by Tim Weaving, **UCL**

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