Laboratoire de Biochimie Théorique
Institut de Biologie Physico-Chimique
13 rue Pierre et Marie Curie
75005 Paris

# *SEMINAIRE*

Théo Leduc
CRM[2], UMR 7036 CNRS – Université de Lorraine

## MoProVirtualReality, a prototype for novel VR molecular visualization

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Electron density (ED) and electrostatic potential (ESP) are scalar fields, that both have a tremendous importance to understand molecular properties[1]. Scalar fields can be explored using topological descriptors, such as the field gradient or the Laplacian[2]. These geometric descriptors have chemical significance, for example to describe atomic bonding. Virtual reality (VR) has incredible potential to visualize multidimensional data, especially when dealing with the rich geometry of ED and ESP fields. Here, we propose a new addition to MoProSuite[3], a prototype of a molecular visualization software aimed at this purpose. The prototype includes support for protein structures and multipolar modelization of the ED[4]. VR interactions with molecular objects is still in search of its gold standards[5], so we revisited them from scratch to explore user experience.

References :
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