## **Reconnaissance Metadynamics**

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Metadynamics has proven to be a very effective method for sampling complex configurational space and overcoming in a relative short time large free energy barriers. Metadynamics relies however on the identification of a small set of collective coordinates able to describe the system at hand. Here we propose a new method, reconnaissance metadynamics, that using machine learning techniques is able to identify a manifold of local coordinates. These local coordinates push the system out of the local minima in which it is trapped and forces it to explore complex energetic landscapes. In a second step we perform a dimensional reduction, which reduces this complex manifold to a low dimensional one. For technical reason these collective coordinates cannot be used with standard metadynamics. This led us to develop a new variant of the method field metadynamics, which allows calculating free energy surfaces for complex systems. We apply these set of new methods to the exploration complex non linear optimization problems, to the folding of small peptides and to ligand -protein binding.