

## RECONNAISSANCE METADYNAMICS RIDES AGAIN

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In my talk I will discuss the Adaptive Topography of Landscape for Accelerated Sampling (ATLAS) method. This is a new biasing method that I recently developed with Federico Giberti and Michele Ceriotti that is capable of working with many CVs. The root idea of ATLAS is to apply a divide-and-conquer strategy where the high-dimensional CVs space is divided into basins, each of which is described by an automatically-determined, low-dimensional set of variables. A well-tempered metadynamics-like bias is constructed as a function of these local variables. Indicator functions associated with the basins switch on and off the local biases, so that the sampling is performed on a collection of low-dimensional CV spaces, that are smoothly combined to generate an effectively high-dimensional bias. The unbiased Boltzmann distribution is recovered through reweighing, making the evaluation of conformational and thermodynamic properties straightforward. The decomposition of the free-energy landscape in local basins can be updated iteratively as the simulation discovers new (meta)stable states.

In the paper, we say that new tools like ATLAS are useful because when you use more standard methods such as umbrella sampling or metadynamics you are forced to operate with a small number of collective variables. Towards the end of my talk I will discuss why I am no longer convinced this is true. My hope in doing so is to encourage conversation with the audience about this work and its potential usages. I firmly believe that we should be doing more to stimulate conversation when we give in-person talks as this justifies the expense associated with bringing everyone to one place.