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S E M I N A I R E

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« **Adaptive techniques for molecular dynamics computations** »

I will present how adaptive techniques can be used for efficient sampling by focusing on two algorithms: free energy adaptive biasing methods and the adaptive multilevel splitting algorithm. The first class of algorithm is used to compute thermodynamic quantities, and in particular free energy differences. The second algorithm has been recently introduced in order to estimate dynamical quantities and sample reactive trajectories. We will in particular present the mathematical foundations for these two numerical methods.

Mercredi 23 mars 2016
14h30

SALLE DE CONFERENCE