Transition paths in protein folding

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Present position

- Physicist at **the Institut de Physique Théorique**, Commissariat `a l'Energie Atomique, Saclay, since 1981. Present rank: Professor (Exceptional Class).
- Directeur de Recherches at **the Institut de Physique Théorique**, Commissariat `a l'Energie Atomique, Saclay
- From 2004 to 2011: Head of **the Institut de Physique Théorique**, Commissariat `a l'Energie Atomique, Saclay.

Positions in International Organizations

since 2005: Member of the C3 Commission of the International Union of Pure and Applied Physics (IUPAP, Statistical Physics)
since 2008: Vice-President of the IUPAP
since 2008: Chairman of the C3 Commission of the IUPAP (Statistical Physics)

Abstract : Protein folding can be described in terms of Langevin dynamics. This dynamics can in turn be represented by a "path integral" (analogous to a Feynmann path integral in quantum mechanics), which is a weighted sum over all paths joining the denatured state to the native state of the protein. In the first part of the talk, we show how one can compute the dominant paths (paths with largest weight) and how one can calculate dynamical quantities (such as rates or transition path times) from these paths. The method and its limitations are illustrated on some simple examples. In a second part of the talk, we show how the Langevin dynamics can be modified to obtain a stochastic equation which samples directly and efficiently the transition paths. This new method, called Langevin bridges.

The talk will run at **4pm** on **April 22(Tuesday)**, in **the Auditorium on the third floor of the Physics Building** of Tsinghua University,