Formulaire de proposition de sujet de thèse

**Titre :** (en français et en Anglais)

Algorithmic challenges for biomolecular simulations and protein design

**Encadrant :** (prénom, nom, grade, mél, laboratoire)

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**Mots clés :** (en français et en Anglais)

Computational biophysics, protein structure prediction and design, Monte Carlo

**Description du sujet :** (~1 page, en français et en Anglais)

Efficient simulation strategies are needed to accurately predict the biophysical properties of proteins, and to engineer new proteins. We have developed and experimentally validated a toolbox for Monte Carlo simulations and protein design, including a unique distributed computing resource, Proteins@Home. To improve the level of physical modelling while maintaining efficiency, new algorithms are needed, which will allow the distribution of a simulation over a large number of processors. The thesis project could focus on one or both of the following aspects, depending on the student's background and interests:

- developing an adaptive Monte Carlo strategy, where information about the system is computed as needed, during the course of the simulation;

- implementing, coding and parallelizing additional terms in the energy function, corresponding to a more refined physical model of the biomolecule and its environment.

**References:**

