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## Post-doc position

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**Convergence of adaptive Markov Chain Monte Carlo methods** (project ANR BigMC; Partners: TELECOM ParisTech, Univ. Dauphine, ENPC)

**Summary.** Adaptive Markov Chain Monte Carlo (MCMC) methods are currently a very active field of research. MCMC methods are sampling methods, based on Markov Chains which are ergodic with respect to the target probability measure. The principle of adaptive methods is to optimize on the fly some design parameters of the algorithm with respect to a given criterion reflecting the sampler's performance (optimize the acceptance rate, optimize an importance sampling function, etc...).

A postdoctoral position is opened to work on the numerical analysis of adaptive MCMC methods: convergence, numerical efficiency, development and analysis of new algorithms. A particular emphasis will be given to applications in statistics and molecular dynamics. *Detailed description below.*

**Position funded** by the French National Research Agency (ANR) through the 2009-2012 project ANR-08-BLAN-0218.

**Required diploma :** PhD thesis in statistics or probability, with a competitive track record.

**Required skills :** experience in MCMC methods and their mathematical analysis.

**Deadline for applications :** September 2010.

**Applications must include :**

- a detailed CV with a description of realized projects
- a motivation letter
- a summary of the thesis
- 2 or 3 recommendation letters
- preferred starting dates and duration

and must be sent to Gersende FORT ([gfort@tsi.enst.fr](mailto:gfort@tsi.enst.fr)) in pdf format; or by standard mail to Gersende FORT (LTCI, 46 rue Barrault, 75 634 Paris Cedex 13, Paris, France).

**Duration :** 12 months.

**Location :** Paris. The position will benefit from an interdisciplinary environment involving numerical analysts, statisticians and probabilists, and of strong interactions between the partners of the project ANR-08-BLAN-0218<sup>1</sup>.

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<sup>1</sup>list of the members available at <http://www.tsi.enst.fr/~gfort/BigMC/ProgramBigMC.html>

**Description.** Adaptive Monte Carlo methods i.e. self-calibrating stochastic simulation methods have proved to be efficient for small to medium scale problems. In developing adaptive methods, it became clear that a major challenge in Monte Carlo methods is to develop robust Monte Carlo sampling techniques that can handle the complexity of target distributions defined on large (and even infinite) dimensional spaces. This post-doc position will focus on a classical traditional simulation technique : Markov chain Monte Carlo (MCMC) algorithms.

The approach of most MCMC algorithms to cope with high-dimensional problem is to break the curse of dimensionality by proposing local moves. This approach does not fully answer the problem in high-dimensional simulation space. Adaptive techniques to split the state space and/or to guide the choice of the design parameters are promising directions of research.

A first family of promising MCMC samplers are the *non-linear MCMC algorithms*, which combine classical MCMC moves with interactions. The process can interact with its own past (internal adaptation procedure) or with parallel chains defined in order to target a density easier to explore (external adaptation). Non-linear MCMC provide novel perspectives to speed up the convergence but the understanding of these techniques is far from being complete and there are many open issues in this domain both from the theoretical and practical perspective. Directions to be investigated could include the study of the *equi-energy sampler*; this algorithm is general enough to provide answers for improving state partition-based MCMC algorithms and to provide answers to molecular dynamics simulations.

Another example of adaptive MCMC coming from some techniques used in molecular dynamics for the computation of free energy differences is the so-called *Adaptive Biasing method*. It is particularly well suited for the sampling of a multimodal target measure - for which regions of high probabilities are separated by regions of low probabilities - so that standard MCMC methods do not sample properly the target measure. The principle is to use an importance sampling technique, the importance function being adapted in such a way that the marginal of the sampled measure along a well chosen direction becomes uniform. Thus, the multimodal features of the original target measure along that direction are eliminated. Averages with respect to the original target measure are recovered through classical unbiasing procedures. These methods have been proven to be very useful in molecular dynamics, where there are typically used for Langevin dynamics. It may also be used within a classical Metropolis Hastings scheme, by adapting the target measure on the fly.

The following questions would be interesting to investigate:

- Analysis of the convergence: Classical methods for analyzing the longtime behaviour of partial differential equations have proven to be useful to analyze such schemes. However, it is yet unclear how to analyze the convergence of such methods using classical tools from the MCMC community, rather than entropy techniques. In particular, the optimality of the rate of convergence obtained by such approaches would be a central question.
- Discretization by particle systems and longtime properties of these interacting particle systems: Natural discretizations of these adaptive techniques involve particle systems, for which the longtime behaviour has not been studied. Such an analysis could yield a guideline to further improve the efficiency of the algorithms.

The post-doc position will benefit from an inter-disciplinary cooperation which will allow cross-fertilization among different fields of applications ((Bayesian) Statistics, mathematical finance and molecular dynamics).