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The main purpose of this short period of cooperation (21st-25th of June, 2010) with Dr. Julien Tailleur at the Department of Physics and Astronomy of the University of Edinburgh (U.K.) was to conclude the research work "Probability current sampling to investigate structural transitions in Lennard-Jones 38 cluster", whose scientific relevance was explained in the Proposed Project Work, and write up an article describing the most important results that have been attained, in order to publicize further applications of this method.

Research on this topic was in fact started some months ago in CEA Saclay, France, by M. Picciani, following ideas developed in previous articles by J. Tailleur and J. Kurchan [1, 2] for simple models, and applying - under their supervision - those ideas to more complex systems, whose dynamics are closer to challenging problems such as protein folding or condensed matter physics. In order to analyze the consistency of the obtained simulation results and establish coherent conclusions of the performed work, a direct intervention of J. Tailleur was then crucial.

During the visit, our activity has been organized in several steps. The first one was a complete screening of the results obtained in CEA Saclay, checking whether they fit with studies that were previously performed on the analyzed system, and already reported in literature. The 38-atoms Lennard-Jones cluster (LJ-38) is indeed a very deeply investigated model because of its temperature-induced phase transitions between metastable configurations, making it an optimal benchmark to check the performances of any optimization method (see for general reference [3]). It was then necessary to control that results arising from our "probability current sampling" method were able to match with such phase changes at different temperatures, i.e. that the obtained simulations really reflected the underlying physics of the system, and were not just numerical artefacts. Moreover, this first stage was definitely necessary to have a precise idea of the state of the art of transition sampling performed on LJ-38, and gave us some fundamental reference points to whom compare our achievements.

Secondly, an analysis concerning quantities related both to the physical system itself and the simulation algorithm was carried: it consisted in studying the simulations behaviour depending on some algorithm parameters (e.g., the value of the friction in the Langevin Molecular Dynamics algorithm, the total number of replicas of the system necessary to perform an appropriate Lyapunov weighted sampling, or the equilibration time needed to adequately thermalize the system) in order to individuate the optimal values of these tuning parameters.

Once achieved these preliminary studies, we than focused on writing up

an article reporting theory, numerical algorithms and simulation results of our research. For this purpose, the theoretical part has been completely reformulated compared to the first presentation given by Tailleur and Kurchan in their papers, with the aim of presenting it in a simple and straightforward way, as well as the simulation algorithm, that is now presented in details in order to be easily exploitable in current numerical sampling experiences. Finally, the large amount of simulation results was pruned in order to select the most meaningful examples that were useful to stress the main aftermaths, reported in the article and duly commented. As all this work will appear soon in scientific press, we do not report here much more informations.

The overall issue of this study, as presented in our article, was indeed really satisfying and encouraging. First, we were able to reproduce numerically the known structural transitions for our Lennard-Jones cluster in a much shorter computation time (at least of the order of a factor ten) than reported in previous works one finds in literature [6].

Moreover, our algorithm has also been able to simulate transitions between metastable states that are usually not seen at all with currently used algorithms, thus overcoming the main obstacle one often has to face in such many-body systems simulations, that is broken ergodicity [4, 5]. In other words, if usual sampling algorithms are not able to find reaction paths between the two main equilibrium configurations of the Lennard-Jones cluster below a given threshold temperature, the "probability current sampling" is able to simulate also low temperature transitions. This allows a deeper understanding of the system, and permits to find with a certain precision intermediate configurations between the two main equilibrium structures that were not seen with other sampling methods.

Finally, the proposed "probability current sampling" has given as well a powerful insight on unknown physical features of the system, such as the accurate position in the configuration space of free energy barriers between equilibrium basins, and the possibility - using the "committors" method - not only of tracing out reaction paths, but also calculating reaction constants between equilibrium basins. This last point can be said to be the proof of the validity of the method, and our most important achievement.

As this work can be definitely said to have been completed successfully, future cooperation with J. Tailleur and the Departement of Physics of the University of Edinburgh are envisaged; in particular, the possibility of applying the "probability current sampling" to the analysis of protein folding makes it a very appealing method to be used in the field of biophysics, where the host institution, specially with the group of condensed matter physics in the University of Edinburgh, is very active.

As it has just been said, an article summarizing our work is supposed to be submitted as soon as possible to specialized physics journals or reviews, in order to present it as a valid alternative to nowadays path sampling methods. The grant that has been accorded resulted then to be absolutely indispensable to the conclusion of such a promising work, allowing us to give a crucial contribution – we hope – to advances in the transition sampling research field.

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