Cali, Jan 10 2021

Dear Editorial Board,

We would like to submit our manuscript entitled “A fast parallel algorithm to reduce protein folding trajectories” for consideration for publication as a Software article in Algorithms for Molecular Biology.

Protein folding simulations have experienced substantial progress in recent years thanks to advances in software and hardware. At present, they can be run using diverse technologies, from low-cost general-purpose GPUs to specially designed supercomputers. Now, it is possible to simulate many more proteins, and to generate very long trajectories, reaching the microsecond timescale. However, the analysis of these trajectories is complicated, and tools are needed to simplify them in a way that both the main events and the temporal order in which they occur are preserved.

We present an algorithm to reduce long protein-folding trajectories in a fast and parallel manner. Our strategy takes advantage of the temporal order of conformations to compare them locally, avoiding an all-versus-all comparison. The algorithm reduces a trajectory by a high percentage, preserving both the patterns and the structure observed in the original trajectory. In addition, its performance is close to that of other efficient reduction techniques, and there is a significant improvement when more than one processing unit is used.

Today, long simulations with millions of protein conformations are increasingly feasible. Their handling and analysis is facilitated if the resulting trajectories are reduced without losing their most important features, while preserving their temporal order. Therefore, we believe that the algorithm presented in this manuscript will be able to support the work of the scientific community using simulations to study protein folding and interaction.

Each of the authors confirms that this manuscript has not been previously published and is not currently under consideration by any other journal. Additionally, all authors have approved the contents of this manuscript and have agreed to the journal‘s submission policies.

We are confident that our work will be of interest to your journal.

Thank you in advance for your consideration,

Best regards.

Luis Garreta
Mauricio Martinez
Néstor Díaz
Pedro A Moreno

ps. for any additional details, please contact the corresponding autor Pedro A. Moreno (pedro.moreno@correounivalle.edu.co)