Cali, Oct 24 2020

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. These advances allow simulations of many more proteins that are reaching the microsecond timescale and greater, generating very long trajectories. 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 way. Our strategy grasps the temporal order of the 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 gets better when more than one core are used.

Today, it is increasingly affordable to perform long simulations with millions of protein conformations. Handling and analysis of these simulations can be facilitated if they can be reduced without losing their most important characteristics, while preserving their temporal order. Therefore, we believe that the algorithm presented in this manuscript will be of great interest to the scientific community that uses 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

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