

Cali, Sept 8 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.

Simulations are among the most important tools for studying the mechanisms underlying protein folding. Protein folding simulations have experienced substantial progress in recent years. Diverse technologies are employed, and simulations are reaching the microsecond timescale and greater, which generate very long trajectories. However, the analysis of long trajectories is complicated, and tools are necessary to simplify them so 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. The algorithm divides a trajectory into segments to be processed in parallel and then selects from each segment the most representative conformations using a rapid clustering strategy. This strategy leverages 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 obtained by other, more complex reduction techniques. In addition, its performance is close to that of other efficient reduction techniques and is improved when executed in parallel using more than one core.

Due to increasing computing power, it is becoming increasingly affordable to perform long protein folding simulations that generate trajectories of millions of conformations, which are complex to handle and analyze. Therefore, we believe that the algorithm presented in this manuscript will be of great interest to the scientific community that uses this type of simulations to study the folding and interaction of proteins.

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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Pedro A Moreno

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