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A Modular Software Approach to Intermolecular Interaction Analysis

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Computational analysis of intermolecular interaction patterns, and prediction of optimal configurations, is a frequently encountered problem arising in a wide range of subjects, such as molecular docking, conformer analysis and crystal structure prediction. While different fields may employ their own preferred models operating under specific precision and accuracy requirements, the underlying approaches often involve similar algorithms and share transferable steps, creating a niche for modular software frameworks.

As an example for a computational approach, where applying established solutions on adjacent problems is facilitated, and experimenting with novel ideas embedded into confirmed solutions would be encouraged, we have developed a set of programs for multi-molecule geometry optimization, where we implemented existing algorithms as reference solutions and added three novel ideas as experimental components.

The first among the aforementioned contributions involves a variation on the simulated annealing algorithm, which has demonstrable success in crystal structure prediction problem [1]. Our method deviates on the basis of temperature assignments, and may prove advantageous in cases where the number of interacting entities is high.

In cases where the search space has lower dimensions, as it may be the case for fewer interacting molecules, we propose a method for bisecting the search space and preemptively eliminating areas based on predicted quality limits of search results.

Finally, we offer a coarse grained, low accuracy scoring function with fast evaluation that may be used for filtering and candidate reduction steps.

[1] Demir, S., & Tekin, A. (2021). Ffcasp: A massively parallel crystal structure prediction algorithm. Journal of Chemical Theory and Computation, 17(4), 2586-2598.

Primary author(s) : Mr. DURAK, Ahmet Tuncer (Istanbul Technical University); Prof. SUNGUR, Fethiye Aylin (Istanbul Technical University)

Presenter(s) : Mr. DURAK, Ahmet Tuncer (Istanbul Technical University)