

Abstract Submitted
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Biomolecular Structure Determination with Divide and Concur

YOAV KALLUS, VEIT ELSER, Cornell University — Divide and concur ($D - C$) is a general computational approach, designed for the solution of highly frustrated problems. Recently applied to the problems of disk packing, the kissing number problem, and 3-SAT, it was competitive or outperformed special-purpose methods.¹ We present a method for applying the $D - C$ framework to the problem of biomolecular structure determination. From a list of geometric constraints on groups of atoms in the molecule, we construct a deterministic iterative map that efficiently searches for structures simultaneously satisfying all constraints. As our method eschews an energy function and its minimization to focus on geometric constraints, it can very naturally integrate with the geometric constraints due to chemistry and physics, experimental constraints due to NMR data or many other experimental or biological hints. We present some results of our method.

¹S. Gravel and V. Elser, Phys. Rev. E 78, 036706 (2008)

Yoav Kallus
Cornell University

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