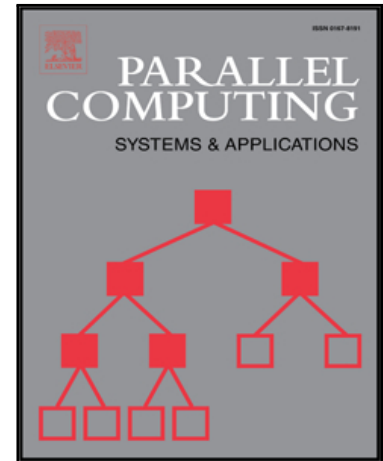


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Enabling Scalable and Accurate Clustering of Distributed Ligand Geometries on Supercomputers

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Highlights

- Scalable method to cluster molecules from docking simulations on distributed systems
- Projections and interpolations into 3-D and 6-D capture molecular geometries
- Our approach scales up to 2,048 processing cores and 2 TB input data
- Our approach is more accurate than energy-based and centralized clustering methods

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