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The integration of graph theory into the analysis of molecular dynamics (MD) simulations offers a powerful and versatile framework for addressing complex structural identification problems[1,2]. By representing atomic or molecular interactions as nodes connected by edges within a graph, it is possible to use a vast array of well-established, highly-optimized algorithms originally developed for fields such as computer science, social networks, and transport systems, to analyze and interpret simulation data. We employ graph-based methods to investigate key structural features arising from MD simulations, including the formation and evolution of molecular aggregates and the identification of water channels within protein environments (Figure 1). These problems, often challenging to address with conventional spatial or density-based techniques, benefit significantly from the flexibility and scalability of graph approaches[3,4]. The cross-disciplinary nature of graph theory not only enhances computational performance but also allows access to new information in the study of molecular structures.

We are currently developing an open-source tool designed to make graph-theory analysis of molecular dynamics trajectories accessible and customizable for the broader scientific community. The tool will allow users to construct graphs from atomic or molecular data and to flexibly define node and edge criteria based on chemical identity of the nodes, distance thresholds, and hydrogen bonding. Leveraging the tunability of graph parameters, users can tailor the analysis to their specific system and research question, whether it involves detecting aggregating behavior, mapping solvent networks, or identifying functional pathways such as water channels in proteins. By building on widely used graph libraries, the tool aims to interface MD simulations with graph analytics in a way that is both robust and user-friendly.

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