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SolvationAnalysis: A Python toolkit for understanding liquid solvation structure in classical molecular dynamics simulations

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Summary

The macroscopic behavior of matter is determined by the microscopic arrangement of atoms, but this arrangement is often difficult or impossible to observe experimentally. Instead, researchers use simulation techniques like molecular dynamics to probe the microscopic structure and dynamics of everything from proteins to battery electrolytes. SolvationAnalysis extracts solvation information from completed molecular dynamics simulations, letting researchers access key solvation structure statistics with minimal effort and accelerating scientific research.

Statement of need

Molecular dynamics studies of liquid solvation structures often replicate established analyses on novel systems. In electrolyte systems, it is common to calculate coordination numbers, radial distribution functions, solute dissociation, and cluster speciation (Hou et al., 2019). In principle, these analyses are highly similar across a diversity of systems. In practice, many specialized bespoke tools have sprung up to address the same underlying problem. Enter `SolvationAnalysis`, an easy-to-use Python package with an interactive interface for computing a wide variety of solvation properties. Building on `MDAnalysis` and pandas (Michaud-Agrawal et al., 2011) (Gowers et al., 2016) (DevTeam, 2020), it efficiently processes output from a wide variety of Molecular Dynamics simulation packages.

`SolvationAnalysis` was designed to free researchers from laboriously implementing and validating common analyses. In addition to routine properties like coordination numbers, solute-solvent pairing, and solute speciation, SolvationAnalysis uses tools from the SciPy ecosystem (Harris et al., 2020) (Virtanen et al., 2020) to implement analyses of network formation (Xie et al., 2023) and residence times (Self et al., 2019), summarized in Figure 1. To make visualization fast, the package includes a robust set of plotting tools built on top of `Matplotlib` and `Plotly` (Hunter, 2007) (Plotly, 2015). Paired with nglview (Nguyen et al., 2017), both exploration and 3d visualization can be done in a Jupyter notebook. A full set of tutorials based on state-of-the-art battery electrolytes (Hou et al., 2019) (Yoo et al., 2022) are also included to familiarize new researchers with solvation structure analysis. Together, these features allow for rapid interactive or programmatic calculation of solvation properties.

Figures

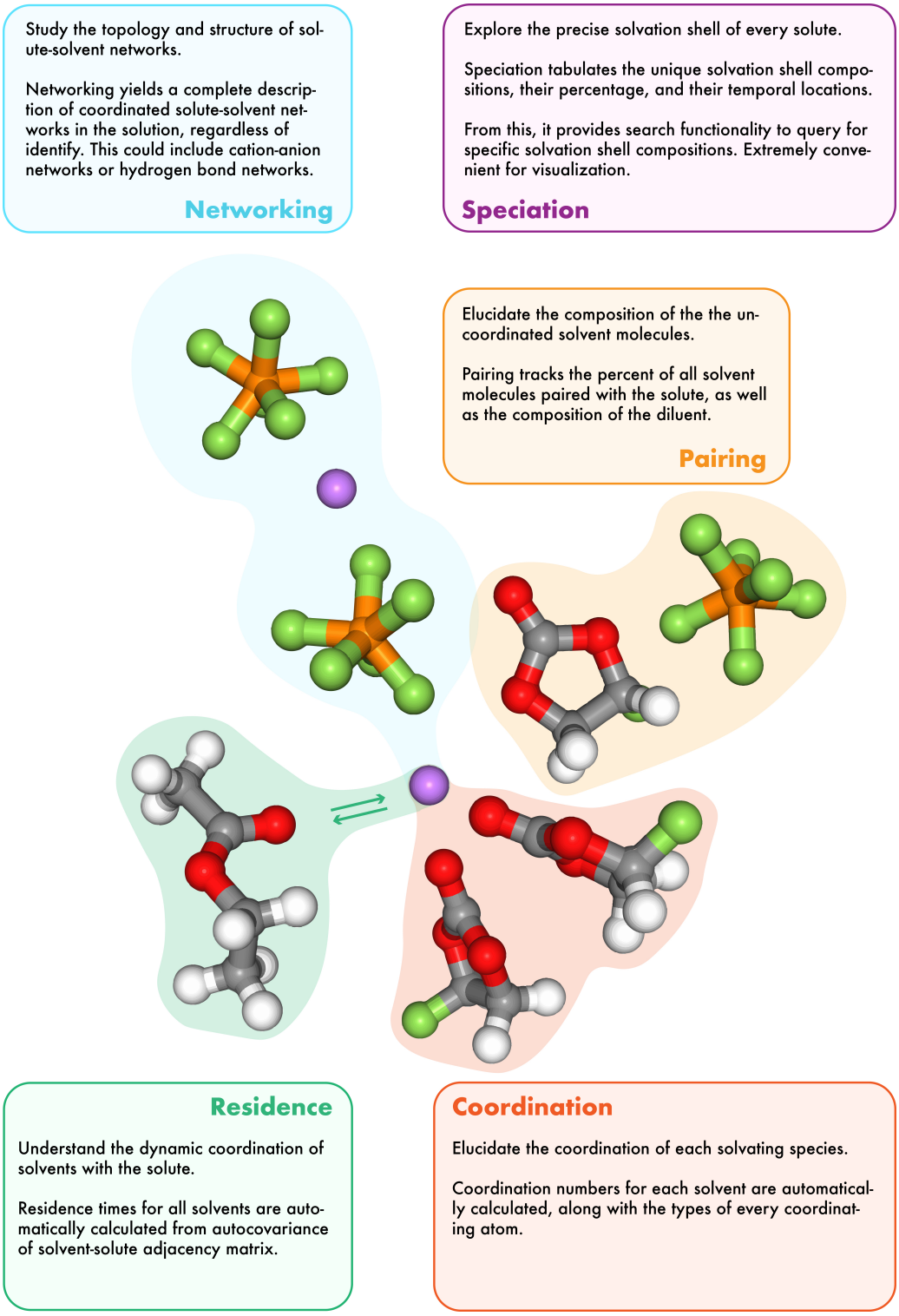

Figure 1: A visual summary of SolvationAnalysis capabilities.

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