JSSSE: An Extensible and Configurable Molecular Structure Editor for Scientific Gateways

JavaScript Sequence Structure Editor (JSSSE) has been developed to edit details obtained in data files used by researchers to improve the building of initial structures and guide user input so that the information generated is compatible with modern molecular simulation programs. SASSIE-web is a scientific gateway built using the GenApp technology (https://genapp.rocks/) that enables researchers to build structures, perform Monte Carlo and molecular dynamics simulations, calculate neutron and x-ray small-angle scattering and reflectivity data on a wide variety of soft-matter systems (https://sassie-web.chem.utk.edu/sassie2/). We have developed new user input capabilities in Javascript and HTML5 to describe and edit molecular systems visually and intuitively while still interacting with the underlying physics. These user inputs will dramatically and fundamentally improve the user experience to broaden the number of potential users of our gateway. The software will be available to all applications developed using the GenApp technology and as a stand-alone component for other scientific gateways. We believe that other scientific gateway developers with molecular simulation-based applications will be able to use JSSSE to enhance their software and improve the impact of their user communities.
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