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molecular dynamics (MD) simulations (Herzberg & Moulton, 1991), or using NMR perturbation methods (Palmer, 2014). NMR studies provide insight into the conformational dynamics of proteins over a wide-range of timescales.

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'Understanding Molecular Simulation' by Daan Frenkel, Berend Smit is considered

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as a best start for beginners, as it clarifies both, the MD theory and its applications as well with simple codes.

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The simulation uses a fairly simple lattice-Boltzmann algorithm, which you can see by viewing the JavaScript source code (use your browser's View Source or Page Source menu command). As of 2019, it runs at pleasing speeds on most personal computers in the Chrome, Firefox, and Opera browsers.

Fluid Dynamics Simulation - Weber State University

The `regula_falsi()` function is the heart of a dynamic event function. It's job is to: monitor the simulation state produced by each integration step, detect when the state crosses a specified event boundary, and; guide Trick's integration scheduler to find that event. Progress toward finding the event state is recorded in a `REGULA_FALSI` variable.

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