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Comparative Study of Cubic and B-Spline Interpolation Methods

Numerical methods are essential in many scientific applications for their ability to make discrete data sets continuous. Interpolation is one commonly used method, which helps one to predict the value of any point between two adjacent data points of a data set. Cubic spline interpolation is highly regarded as the most useful method for its ability to interpolate between data points in a piece-wise fashion. However, this advantageous method comes with the price of high computation time, especially in cases such as molecular dynamics (MD) simulations where it must be applied repetitively. An alternative representation of a cubic spline was proposed in previous research, where each spline could be described as the linear combination of basis set functions, thus naming the method B-spline interpolation [1]. It was proposed that implementing this new formulation can accelerate many scientific computing operations which involve interpolation.

In this study, the performance of B-spline method was evaluated and compared to cubic spline interpolation using a series of analytic functions. The effects were also evaluated in a Free Energies from Adaptive Reaction Coordinates (FEARCF) [2] reaction sampling of protonation of ammonia into ammonium [2]. Significant CPU speed up was observed at four-dimensional B-spline up to 10^5. It provided identical results regarding the accuracy. Furthermore, the speed up of the splining method led to a 4-fold overall increase of the CPU speed of reaction sampling.

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