CHEM279
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HW1

In this first homework assignment, part two, we can see the comparison between the true analytical force, the approximated force through central differences, and the approximated force through forward differences. These approximations are calculated with varying stepsizes: h = 0.1, 0.01, 0.001, and 0.0001.

The total error, the truncation error, is calculated by subtracting the true value (assumed to be the calculated analytical force) and the approximated force values. The truncation error is named so because the approximation 'truncates' the Taylor series approximation at the first order derivative.

The error values were collected by calculating the total potential energy of the system with the aforementioned varying step sizes, then element-wise subtracting the 'true' value from the approximated values, and averaging the subsequent matrix to yield an overall error value. These four values were plotted against their respective stepsizes to generate the graph seen in the subdirectory /*output*.

The graph depicts that the forward differences error decreases as h increases, while the central differences error increases as h increases. This makes sense, since the truncation error in forward difference is proportional to h while the truncation error in central differences in proportional to h^2.