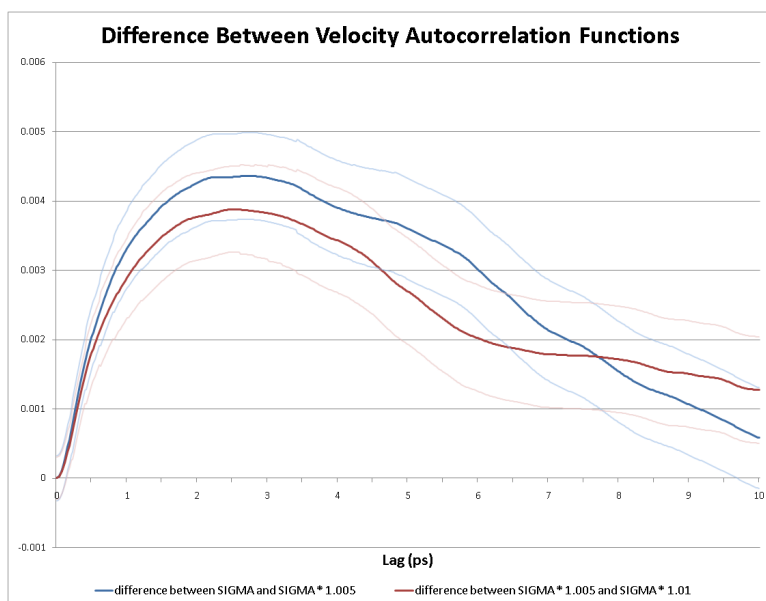


Supplement to “What Makes Molecular Dynamics Work?”

Robert D. Skeel

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The plot below is produced with the same parameters as those of Figure 1 of [1]. The blue graph is the difference between the original velocity autocorrelation function and that for σ increased by 1.05; the red graph is the difference between that with σ increased by 1.05 and that with σ increased by 1.1. A step size of 20 fs is used.



A linear relationship between perturbation and effect would require that these two graphs be the same.

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References

- [1] R. D. Skeel. What makes molecular dynamics work?, 2008. Submitted.