Transforming the Accuracy and Numerical Stability of ReaxFF Reactive Force Fields

David Furman*,†,‡ and David J. Wales*,†

E-mail: df398@cam.ac.uk; dw34@cam.ac.uk

Supporting Information

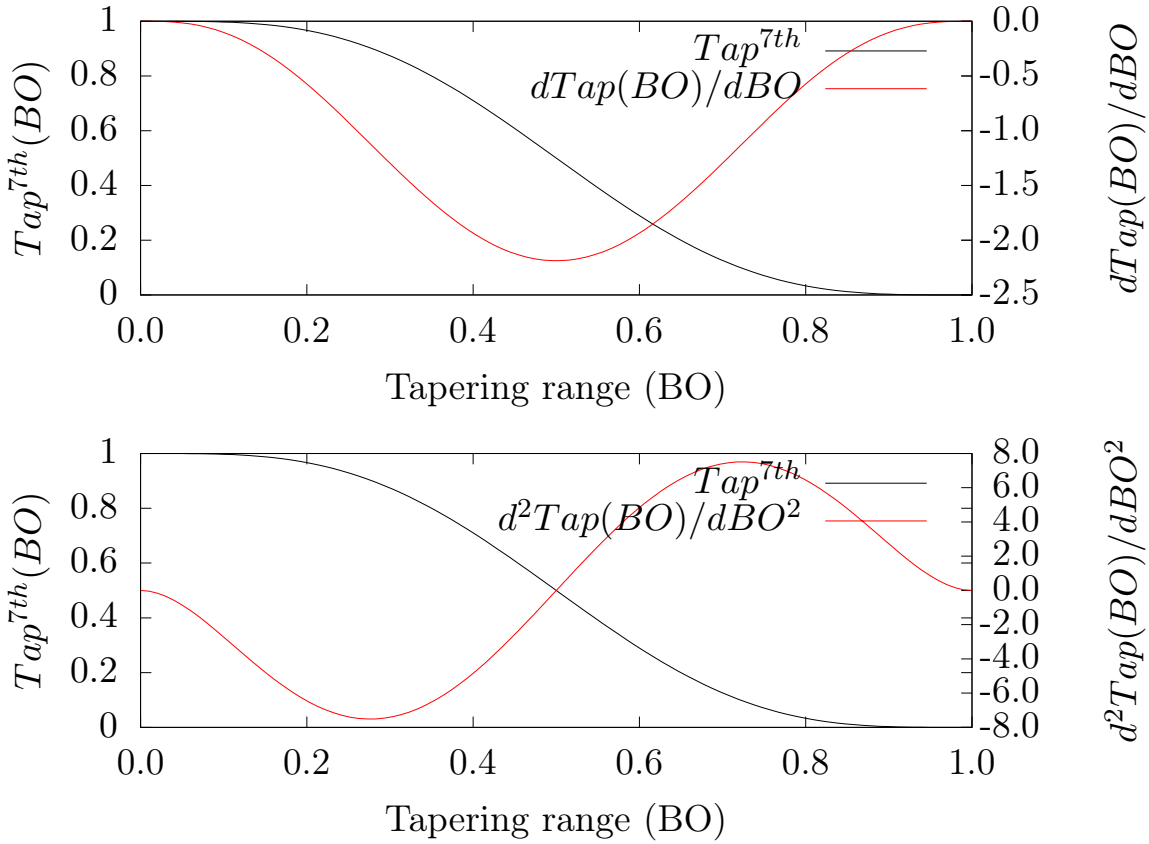

Figure S1. 7^{th} degree tapering polynomial and its 1^{st} (top panel) and 2^{nd} (bottom panel) derivatives. The tapering range is arbitrarily chosen as $x_r = x_{max}$ - x_{min}=1.0, where x_{max} and x_{min} are the upper and lower bond order cutoffs, respectively.

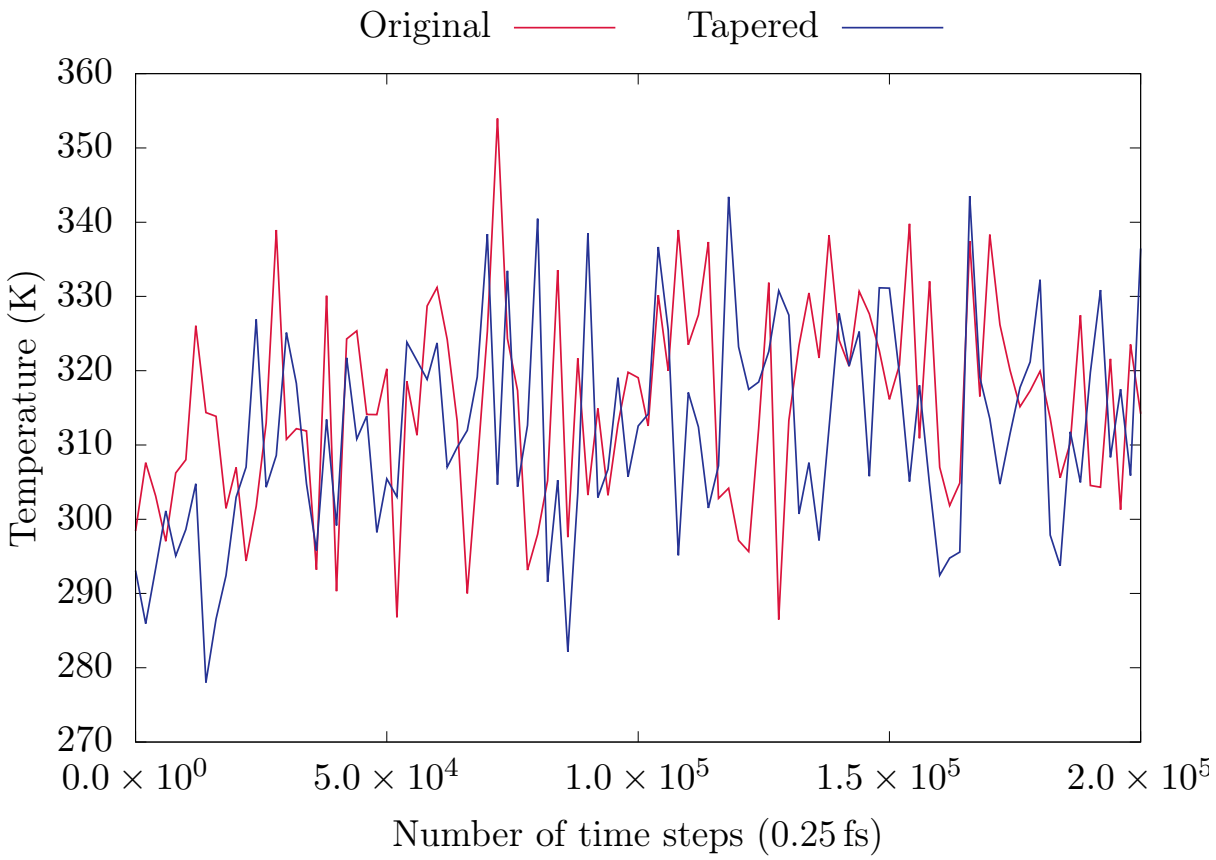

Figure S2. Evolution of temperature for the trpzip2 peptide in the NVE ensemble of a pre-equilibrated system (300 K) for the original and tapered ReaxFF formulations.

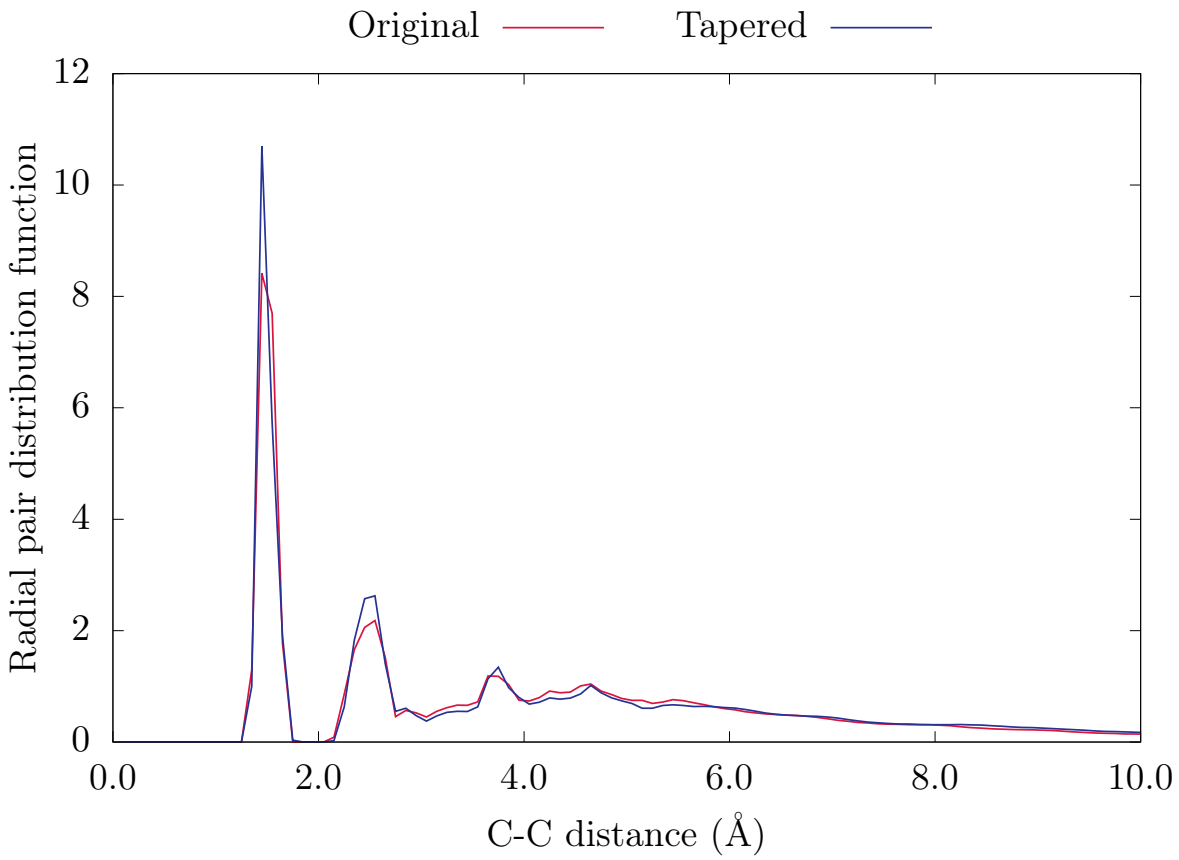

Figure S3. Radial pair distribution function of carbon atoms in the trpzip2 peptide (calculated in the NVE trajectory) for the original and tapered ReaxFF formulations.

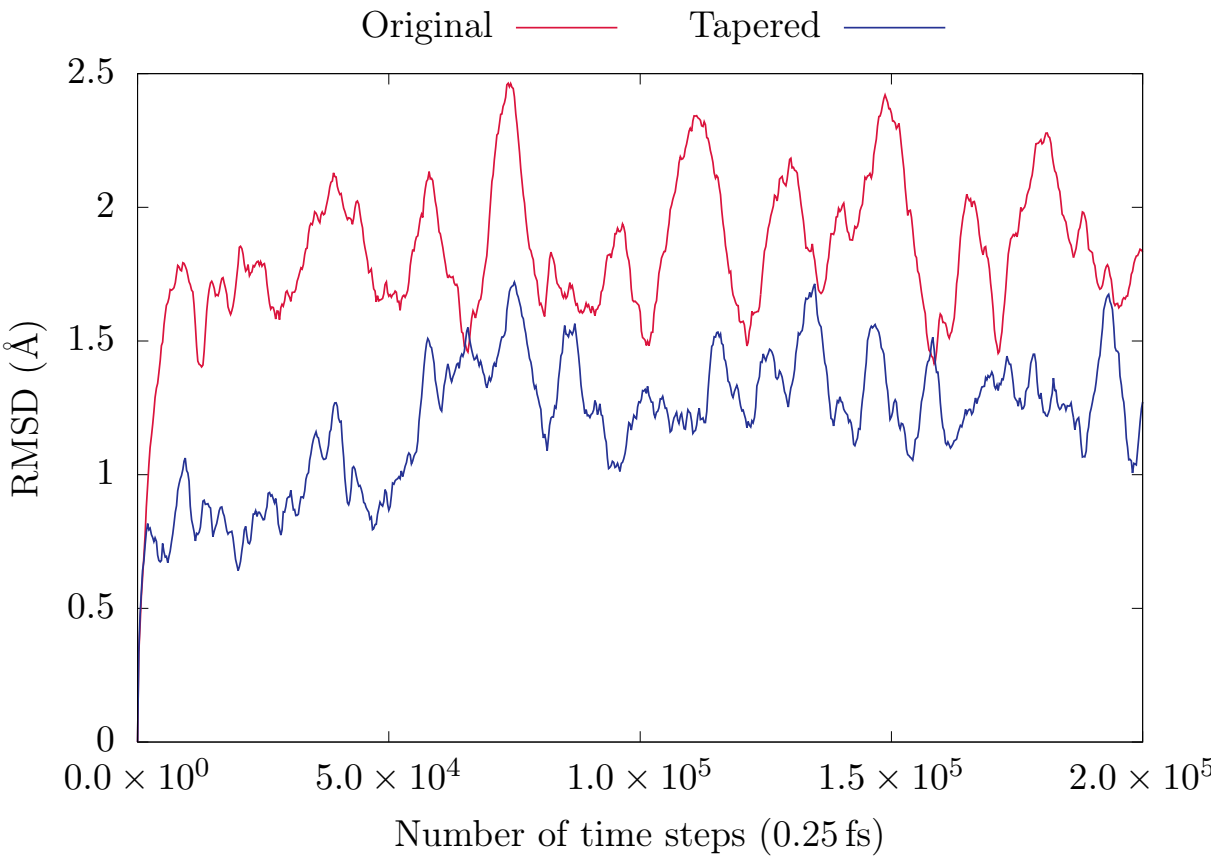

Figure S4. Root mean square displacement (RMSD) for all atoms in the trpzip2 peptide (calculated in the NVE trajectory) for the original and tapered ReaxFF formulations.

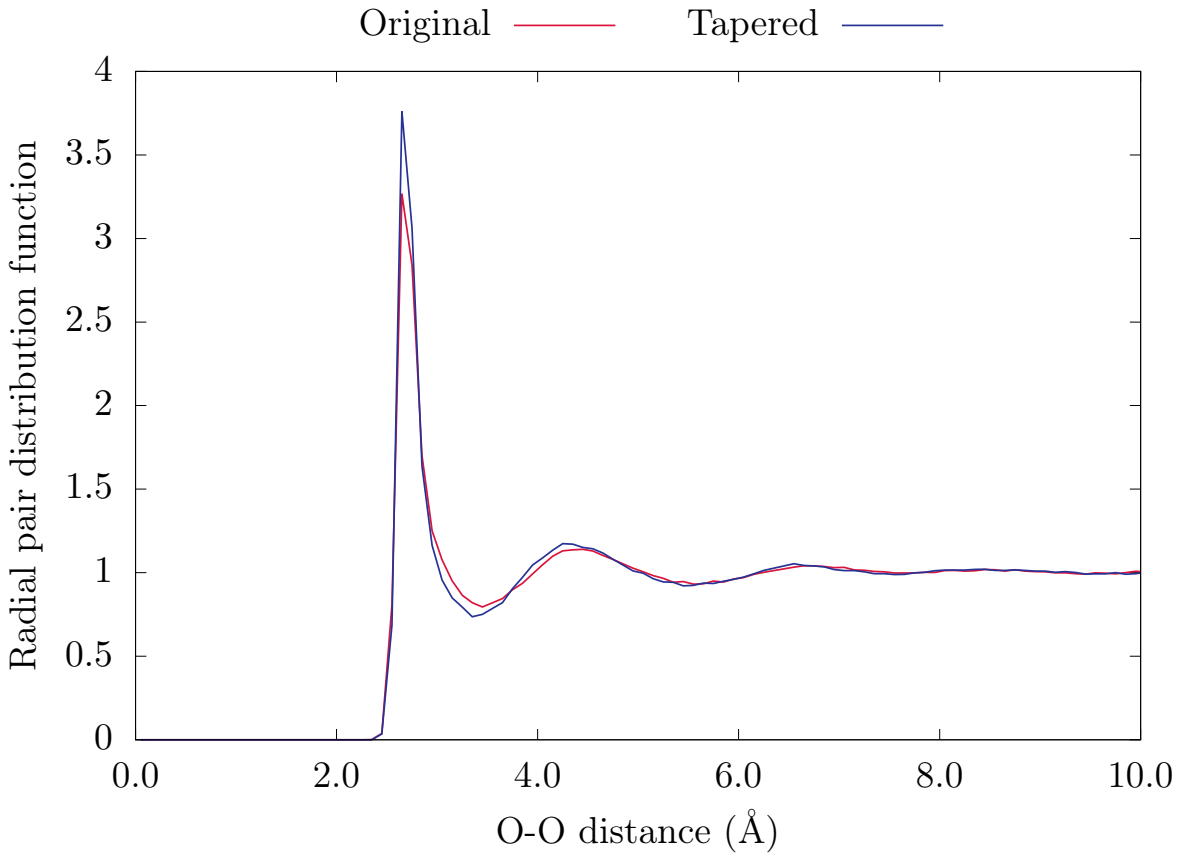

Figure S5. Radial pair distribution function of oxygen atoms in the bulk liquid water system (calculated in the NVE trajectory) for the original and tapered ReaxFF formulations.