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Exploring the low temperature thermodynamics of lattice proteins and polymers with chain lengths > 1000 THOMAS WUEST, Swiss Federal Institute for Forest, Snow and Landscape Research WSL — Coarse-grained (lattice-) models have a long tradition in aiding to decipher the physical or biological complexity of polymers and proteins. Despite their simplicity however, numerical simulations of such models are often computationally very demanding and the quest for efficient algorithms is as old as the models themselves. I present a computational method based on Wang-Landau sampling in combination with suitable trial move sets which is particularly effective to study models such as the hydrophobic-polar (HP) lattice model of protein folding or its counterpart in polymer physics, the interactive self-avoiding walk (ISAW) at low temperatures. The approach provides a versatile and powerful mean for both the ground state search and the determination of the entire energy density of states (DOS) yielding reliable estimates of thermodynamic quantities for chain lengths > 4000 (ISAW) even in the very dense collapsed phase. The appearance of multiple low temperature pseudo-transitions for ISAWs will be elucidated. Further methodological improvements will be discussed.

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