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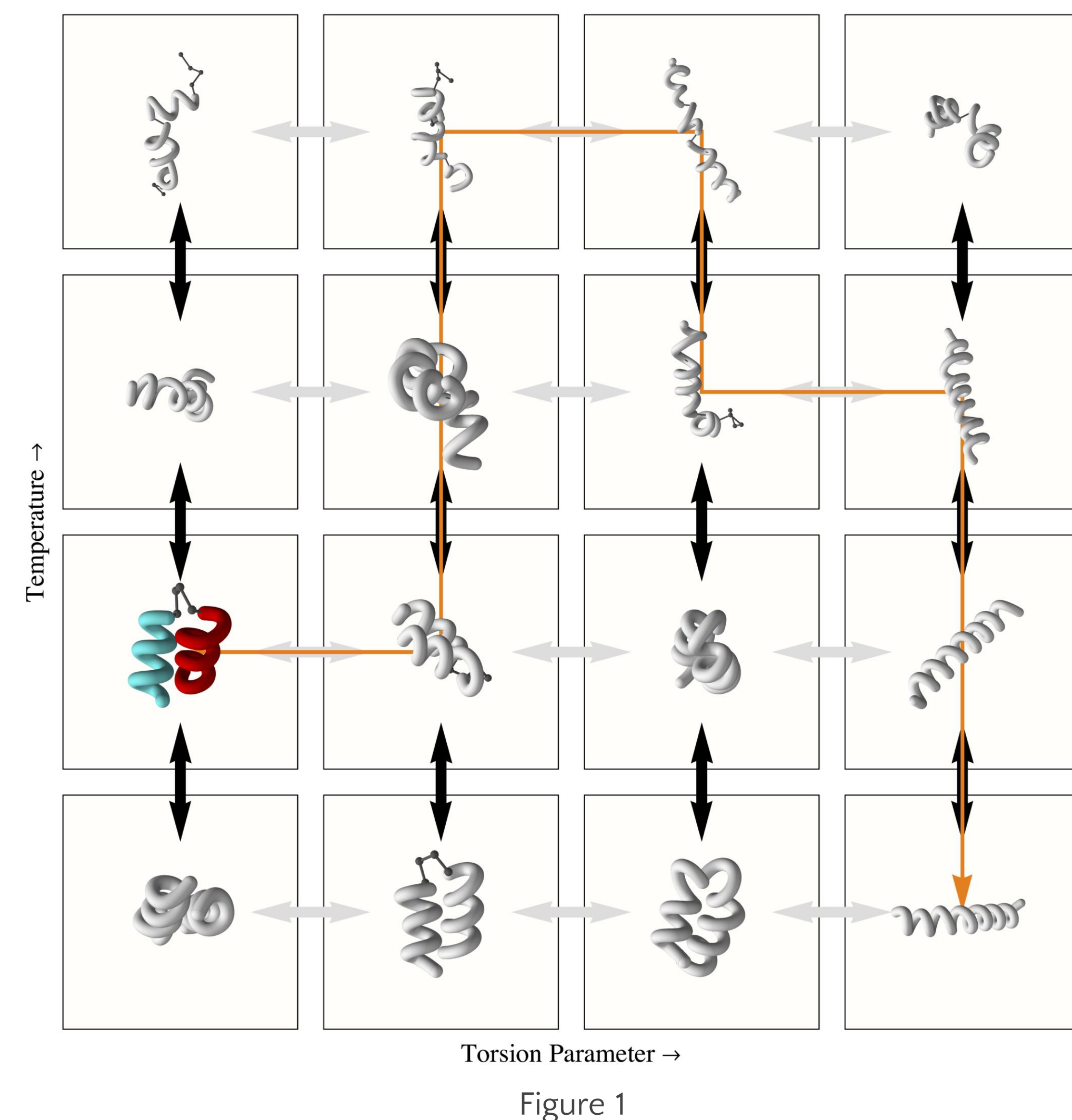


One-Dimensional and Two-Dimensional Simulations of Helical Homopolymers: A Comparative Analysis of Energy Stabilization and Efficiency

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Introduction

Polymers, long chains of similar molecules bonded together, constitute many of the materials found in living organisms as well as industrial materials. Polymer structures can evolve into nearly limitless configurations determined by their effective potentials and by the influence of their surroundings. Our research deals specifically with helical polymers modeled by a set of effective potentials described in [2]. Example configurations are shown below in Figure 1 with outcomes specified by unique torsion strength and temperature values.



- **Temperature:** cumulative random kinetic energy of each polymer
- **Torsion:** stiffness of helical polymer segments

As an example of the type of observable output from the data generated in a 2D parallel tempering simulation, a structural phase diagram is provided in Figure 3. Structural transitions are found by analyzing the specific heat curves for an array of simulations. Peaks in the specific heat are used to denote phase transitions, and these have been marked with different phases and three distinct polygons. The red region represents random coil structures, the green region represents single-helix structures, and the yellow region represents two-helix bundles. This data has been generated using both the 2D and 1D parallel tempering simulations with results agreeing within statistical error bars.

Methodology

Individual simulation threads each represent structures produced at an array of temperature and torsion strength values. Figure 2 corresponds to a specific thread with a torsion value of 11 and a temperature value of 0.2. Solid lines represent rolling averages with a window size of 250 time-series measurements. Equilibration is analytically determined by the stability algorithm and plotted as a vertical dashed line. The stability algorithm finds the lowest energy value of each data series and bisects the data at this point. Then, energy values following the minimum are averaged. Equilibration occurs when the first energy value crosses below this post-stabilization average.

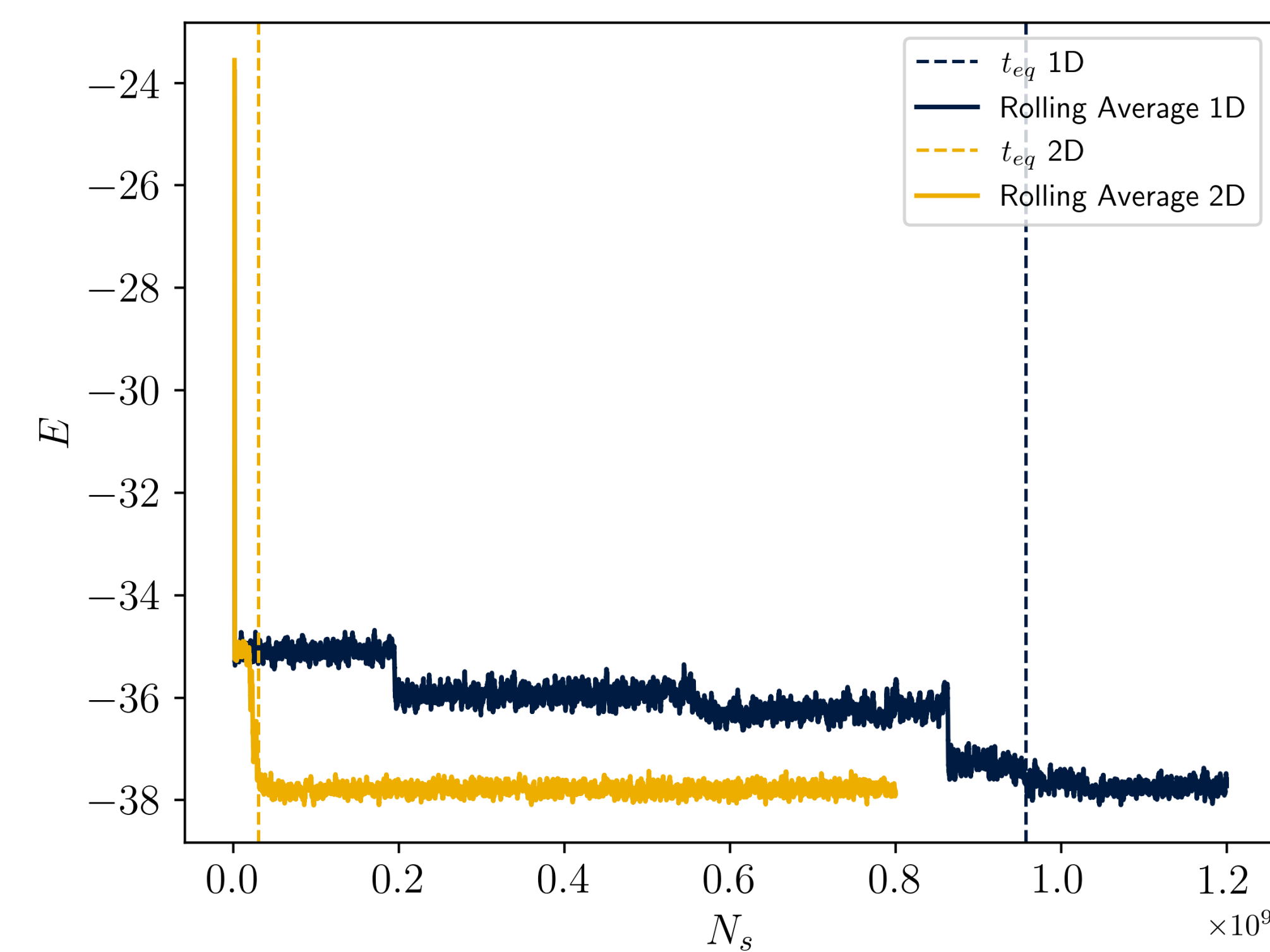


Figure 2: Energy of a one- and two-dimensional parallel tempering simulation vs. Monte Carlo time step [3]

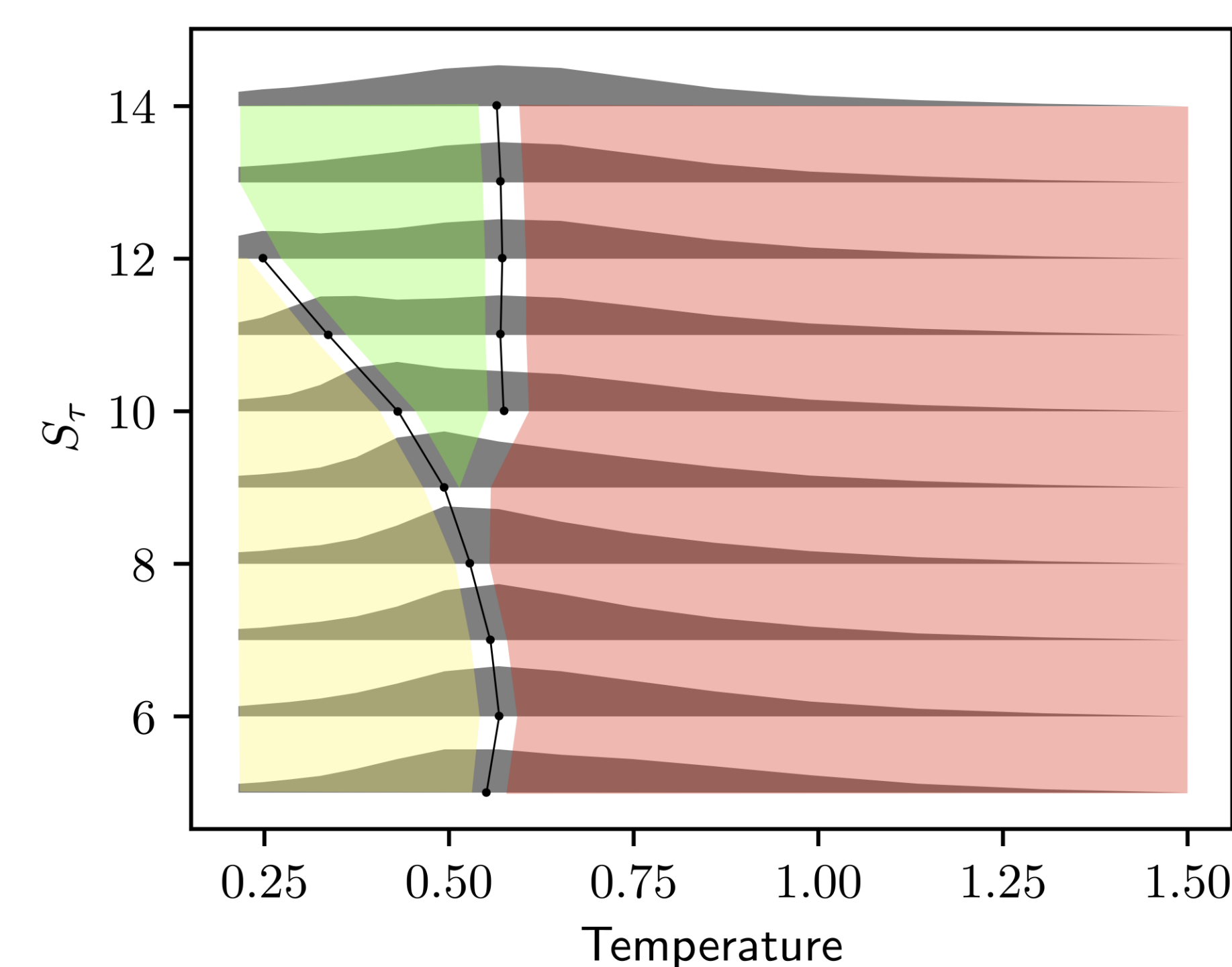


Figure 3: The specific heat is plotted against temperature for each value of torsion parameter (S_τ). This layout allows immediate visualization of the phase transitions marked in black. Phases are visualized as three distinct regions of different color to make a hyper-phase diagram.

Methodology

For each torsion value, the maximum equilibration time for all temperature values was used to compare the efficiency increase of the 1D and 2D parallel tempering.

S_τ	$t_{max1D} \times 10^6$	$t_{max2D} \times 10^6$
5	25.3	49.8
6	49.2	48.4
7	35.4	45.3
8	109	54.0
9	150	47.8
10	296	50.6
11	1020	49.4
12	559	39.7
13	1.88	1.74
14	3.42	4.64

Table 1: Equilibration Time at simulated torsion values [3]

The solid points represent the average number of time steps between the appearance of a unique replica structure. This is specifically representative of the data collected after energy equilibration at corresponding torsion values shown with sampling errors.

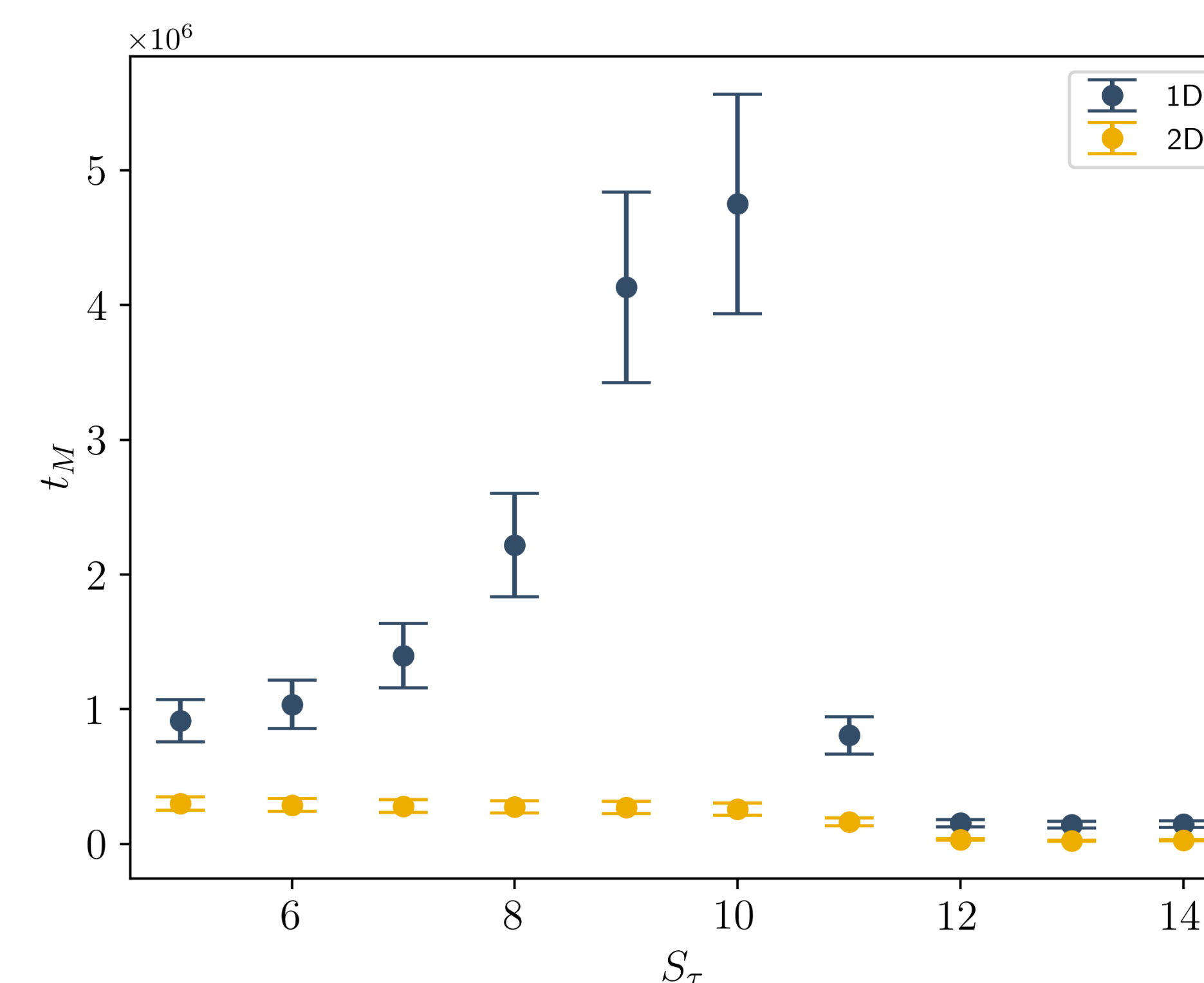


Figure 4: Average number of time steps per unique configuration measured against the torsion value of the thread for 1D and 2D parallel tempering Hamiltonian exchanges for helical homopolymers. [3]

Results

Polymer thermodynamics were simulated across a wide range of temperature and torsion values. Figure 2 shows the time to equilibration for one specific simulation thread. The equilibration time of the 2D parallel tempering exchange scheme decreased by as much as 95% as compared to the 1D simulation shown in Table 1. [3] Figure 4 generalizes these results to show the average unique configuration generation times for each torsion value. Incorporation of the Hamiltonian exchange into parallel tempering simulations leads to an average of a seven-fold increase in the rate at which new structures are generated in this model. This is most apparent at intermediate torsion values representing transitional structures.

Conclusion

Many scientists are researching ground-state structures of biological polymers. We use a coarse-grained model of a common structure type, illustrated in Figure 5, to study the thermodynamics of structural transitions of these systems. One-dimensional and two-dimensional parallel tempering simulations of polymer structures provide equivalent predictions about the thermodynamics of polymer structures, but the two-dimensional exchange scheme achieves these results quicker and provides more precise predictions. The developed equilibration determination algorithm graphically and analytically aids in discerning the stability of polymer simulations and gives insight into simulation efficiency. Stability determination proves useful in guiding the development of more efficient and realistic simulations that are applicable to biomedical and polymer sciences, among others.

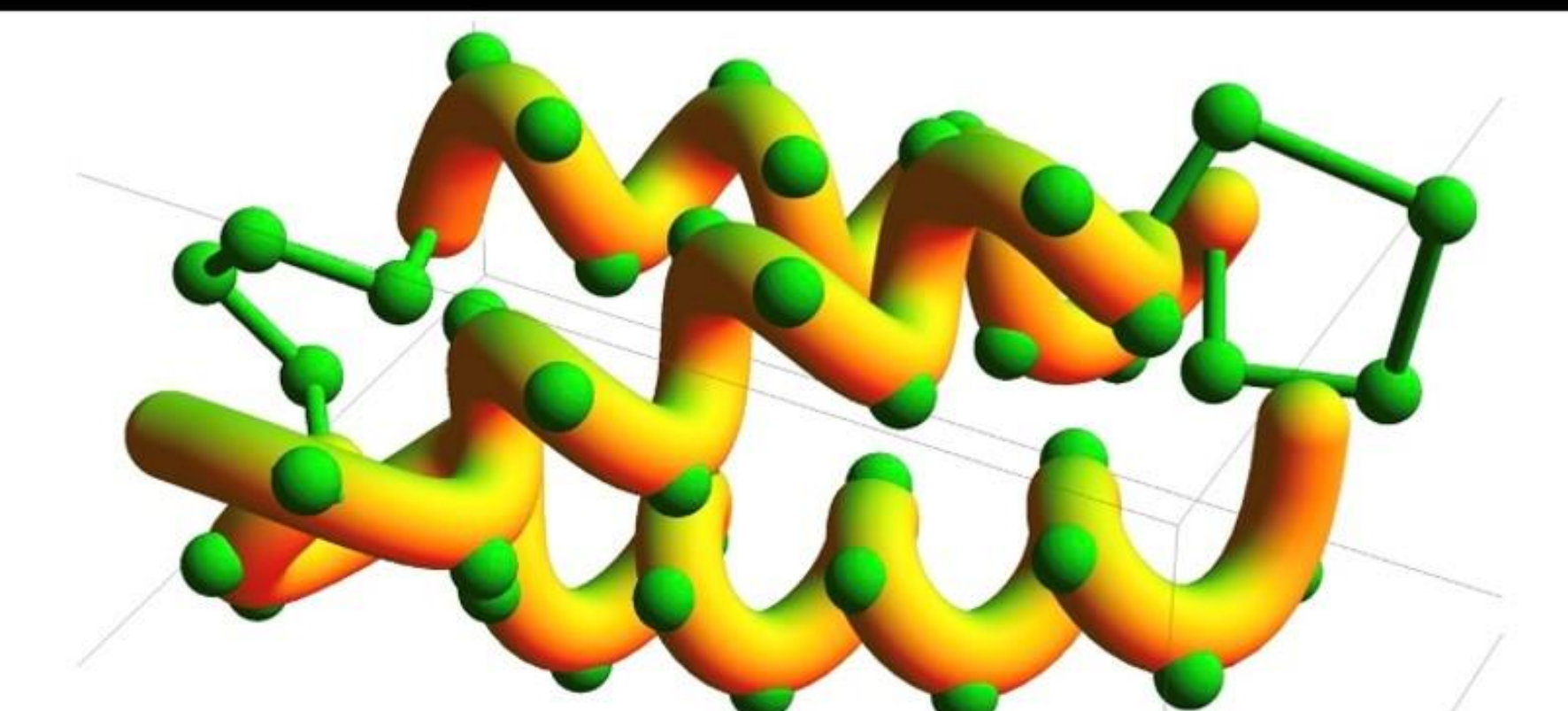
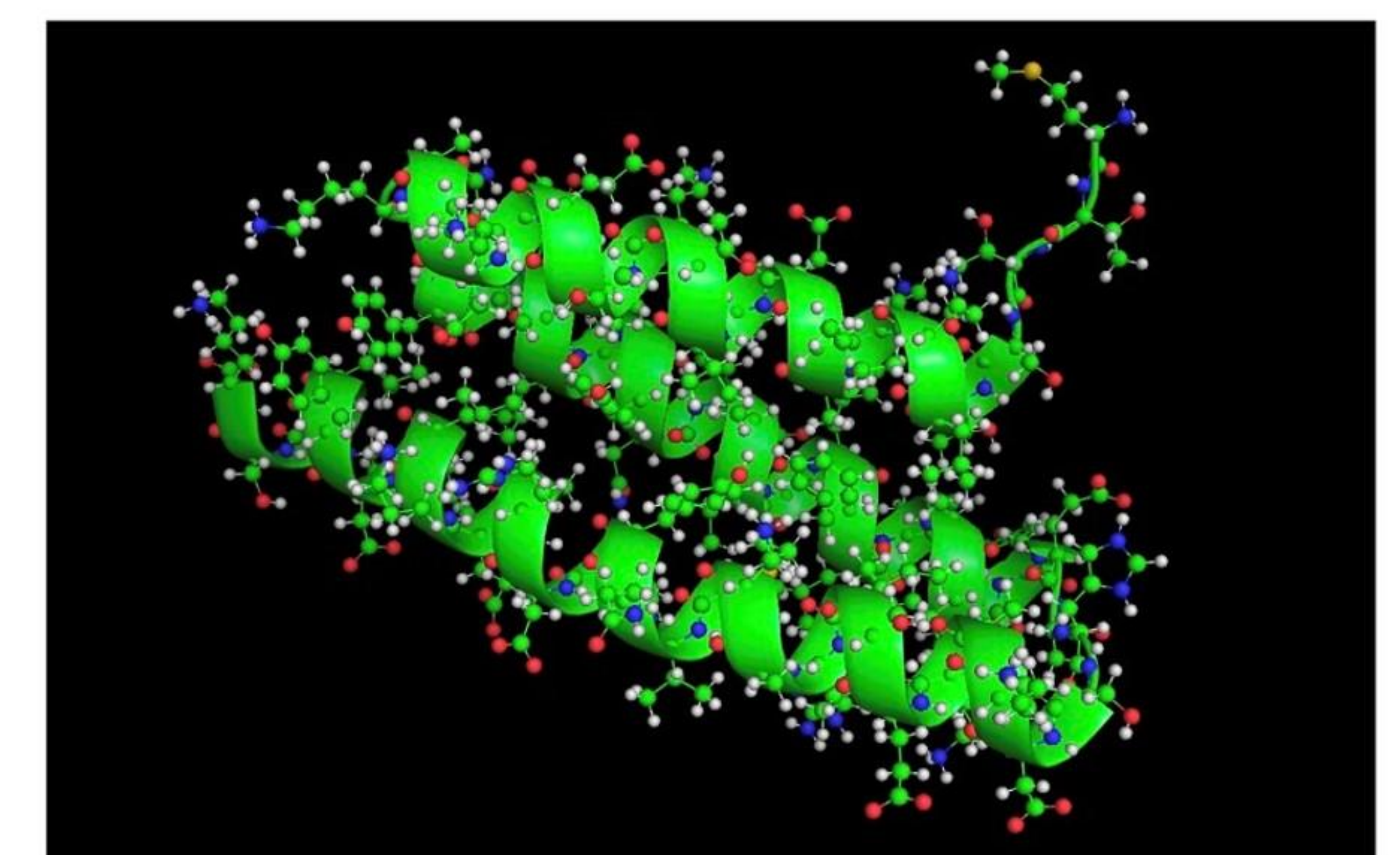


Figure 5 - Top: All atom representation of the Structure of VPS4A protein [2]. Bottom: Coarse grain representation of a similar 3-helix bundle.