Enhanced dial representation of angle evolution during molecular dynamics

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The dial representation of angular evolution during a computer simulation has been proposed by Beveridge and coworkers [1]. A dial plot traces the evolution of the angle within a circle where the radius is the simulation time axis. Thus if the angle at time step t_i is φ_i then the position of the track is described by the 2-dimensional polar coordinates (t_i,φ_i). This representation has been incorporated into the program Simulaid [2] for visualizing the variation various angles during simulation: torsion angles, proline kink-related angles [3], and helix-analysis related angles [4]. This note presents several enhancements that resulted in the enrichment of information than can be gleaned from the plots.

The following features have been added to the original dial plot:

1. The number of dials drawn in a row, thus the size of each dial, can be controlled by the user
2. When drawing the track, the two states are connected by an arc (instead of a straight line).
3. Optionally, the track can be omitted and just a small disk plotted for every angle value.
4. The initial value is shown as a green bar inside a small disk at the center of the dial.
5. The final value is shown as a blue bar outside the dial.
6. The average value is shown as a red line between the inside disk and the outer circle. The average angle is calculated by first averaging the sin and cosine of each angle followed by normalizing the averages to ensure that the square sum is one, giving the sine and cosine of the average angle.
7. The circular variance [5] (CV) of the angles, a measure of the spread of the angles, is shown as a vertical bar on the *y*-axis inside the dial. For a set of *n* angles $\{\varphi_i\}$ CV is defined as

$$CV = 1 - \sqrt{\left(\sum_{i=1}^{n} \sin\varphi_i\right)^2 + \left(\sum_{i=1}^{n} \cos\varphi_i\right)^2} \Big/ n$$

8. Optionally, the probability distribution of the angles is mapped on the outer circle of the dial. To be specific, for the probability distribution ρ_i the program draws the graph using points whose coordinates are $<(R+c\times\rho_i)\cos\varphi_i, (R+c\times\rho_i)\sin\varphi_i>$ where R/ is the radius of the dial's outer circle and c is just a scale factor. Note, that even when not all angles are plotted in the dial, the distributions are calculated using all angles sampled.

To illustrate the new dial plot features, a trajectory of 5000 frames from a 500 ns molecular dynamics (MD) simulation was used. Fig. 1 shows a new dial plot, using every 5th frames and also averaging every consecutive 5 angles, annotated to point out the different features.

Figure 1

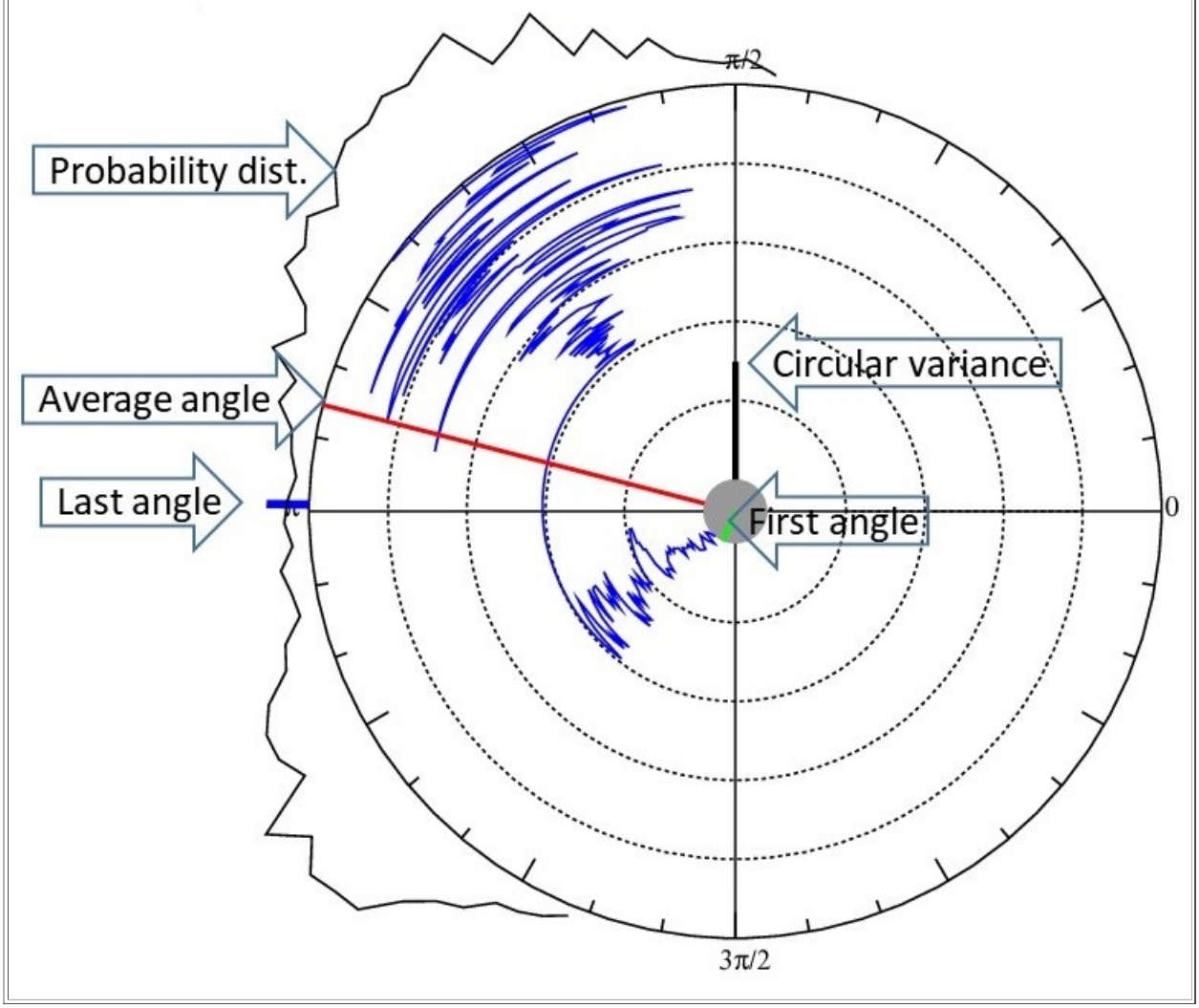
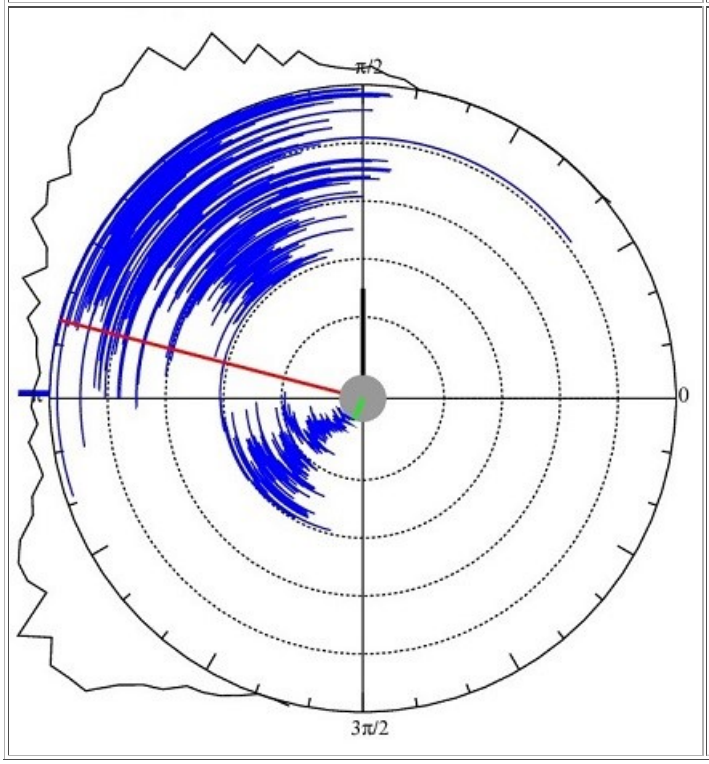
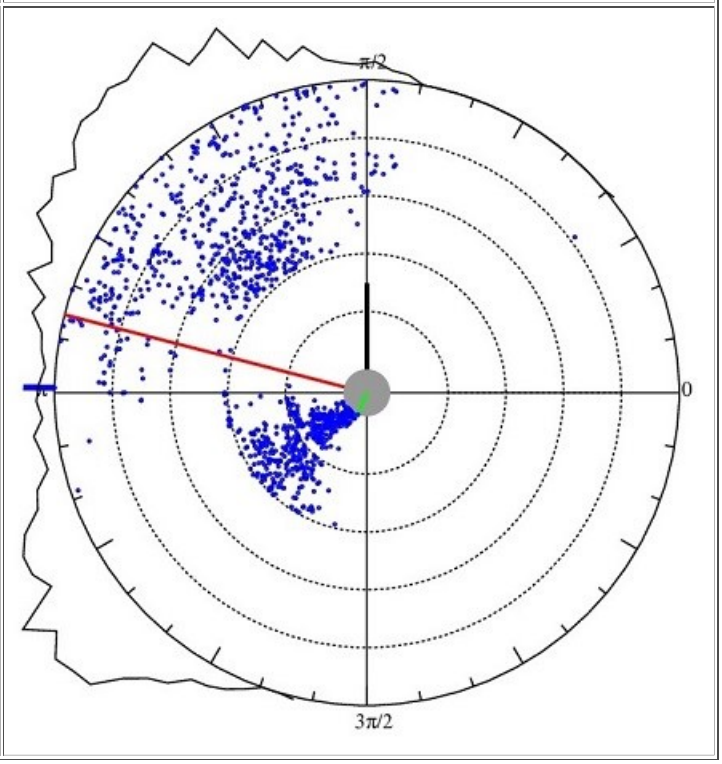


Fig. 2 shows the dial plot of the same angle, but omitting the averaging, resulting in a rather dense plot and Fig. 3 shows the dial plot of the same data as Fig. 2 but omitting the connecting arcs and just drawing small disks at the angle values. Comparison of Figs. 2 and 3 shows that omitting the arcs can significantly clarify the picture when the arcs become too dense.

Figure 2	Figure 3
	

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