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Supporting Material

Spatial Structure and Diffusive Dynamics from Single Particle Trajectories Using Spline Analysis

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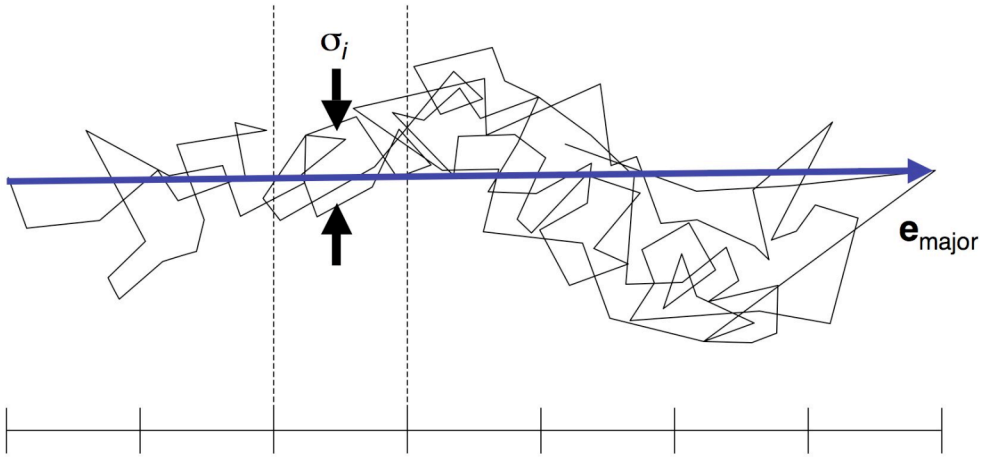
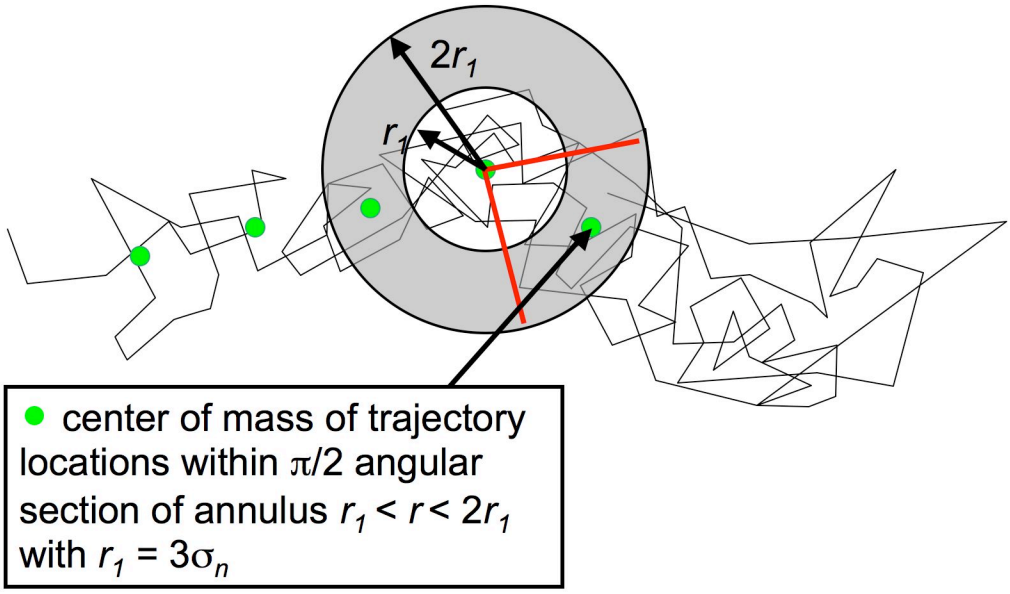
Supplemental Information

SCDA and SCSA both rely on fitting a curve to the overall shape of a curvilinear trajectory. The spline curve is constrained to pass through a series of automatically-generated points along the trajectory. The points are determined as follows:

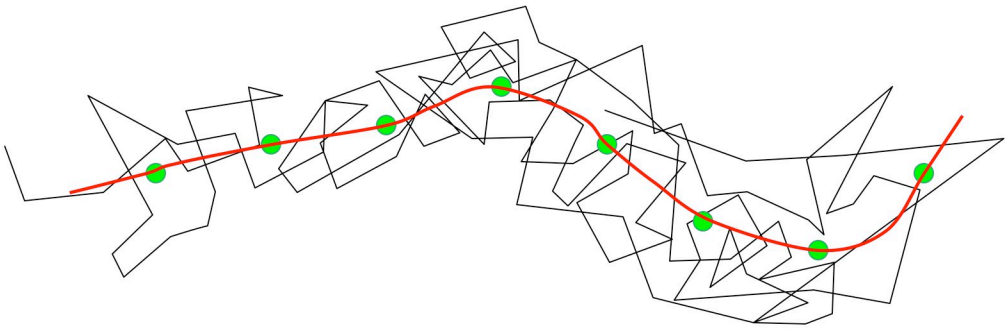


First, the width of the trajectory is approximated by dividing the trajectory into n segments along $\mathbf{e}_{major}$, the direction of maximal extent of the trajectory. The width of the distribution perpendicular to $\mathbf{e}_{major}$, σ_i, is calculated for each segment, and then the average width is calculated: $\sigma_n = (1/n)\Sigma_{i=1:n}\ \sigma_i$.



Second, the center of mass of trajectory locations within $r_1 = 3\sigma_n$ of the end of the trajectory is generated as the first point for spline fitting. Generated points for spline fitting are illustrated in green above. Then, locations within an annulus centered on this point are identified, as illustrated above. The next point characterizing the shape of the trajectory is the center of mass of trajectory points in the π /2 angular segment of the annulus in the direction of the highest density of points. To ensure that the generated points continue along curvilinear trajectory shapes, that direction is within $\theta_{max} = 0.2\pi$ of the forward direction, determined by the vector between the two previous generated points.

If a paucity of trajectory points prevents calculating the center of mass, the radius, r_1, is doubled. If trajectory points are found within the expanded radius, the iterative process continues and then r_1 is returned to its original value. If no trajectory points are found within the expanded radius, the process stops and no further points are generated.



Finally, a cubic spline curve (shown above in red) is fit through the generated points, characterizing the overall shape of the trajectory.

Here the example trajectory D (Fig. 1 *bottom right* in text) shown with the generated points used for the spline fitting.