About the buckled shape

Martin Lindén, May 18, 2017

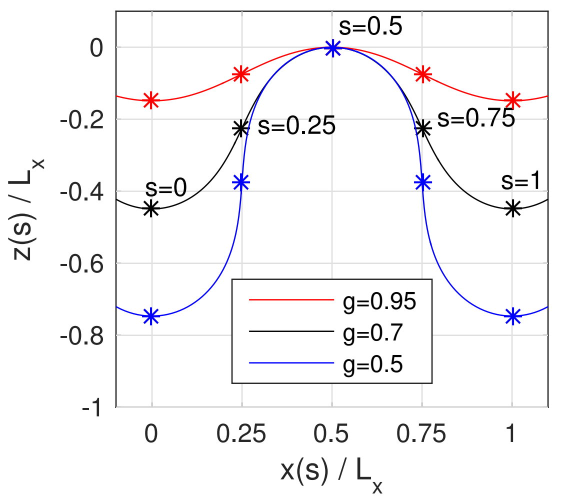

Figure 1: The buckled shape in the x, z plane for three different compression ratios $g = 0.5,\ 0.7,\ 0.95$.

Here, we describe the buckled profile used for fitting an Euler buckling profile to a set of points, with the main aim to explain the various functions and their relations.

The buckled shape is handled by the function `buckleshape_Fcoeff_lin`, which computes a parametric curve $x(s), z(s)$ (Fig. 1) and some partial derivaties. The shape is parameterized by the projected length L_x and the compression ratio g, which are related to the arc-length L through

$$g = \frac{L_x}{L}, \tag{1}$$

and related to the compression strain γ used in refs. [1, 2] via

$$\lambda = \frac{L - L_x}{L} = 1 - g. \tag{2}$$

This choice is practical when analysing buckling simulations, where L_x is kept fixed, but the arclength L (and thus the dimensionless g as well) can fluctuate slightly during a simulation. The parameter s is proportional to an arclength parameter, so

$$\int_0^1 \sqrt{\left(\frac{dX}{ds}\right)^2 + \left(\frac{dZ}{ds}\right)^2} ds = L = \frac{L_x}{g}. \tag{3}$$

Numerically, $\sqrt{\left(\frac{dX}{ds}\right)^2 + \left(\frac{dZ}{ds}\right)^2} = \frac{L_x}{g}$ holds to at least 5 decimal places when using `buckleshape_Fcoeff_lin` with a Fourier truncated after 7 terms.

The curvature along the buckled profile curve is given by

$$C(s) = -\frac{\frac{dX}{ds}\frac{d^2Z}{ds^2} - \frac{dZ}{ds}\frac{d^2z}{ds^2}}{\left(\left(\frac{dX}{ds}\right)^2 + \left(\frac{dZ}{ds}\right)^2\right)^{3/2}}, \tag{4}$$

where we use the convention that $C > 0$ when the curve curves away from the (upward-pointing) normal vector.

`buckleshape_Fcoeff_lin` uses an internal Fourier series representation, so the cuves are periodic in s, with period 1. As seen in Fig. 1, the curves are placed such that

$$x(0) = 0, \quad x(1) = L_x, \quad z(0.5) = 0, \tag{5}$$

and symmetry also dictates that $z(s)$ is symmetric, and $x(s) - s$ is antisymmetric, around $s = 0.5$:

$$z(s) = z(1-s), \quad x(s) = L_x - x(1-s). \quad (6)$$

Finally, $x(s) = sL_x$ at $s = 0, 0.25, 0.5, 0.75, 1$.

The Fourier components used by `buckleshape_Fcoeff_lin` can be recomputed using `buckleshape_Fcoeff_maketable`.

Fitting is done with the function `fit_min2D_buckle`, which solves a nonliner least squares problem. Specifically, if the positions to be fitted to are given by $x_i, z_i = 1, 2, \ldots$, the sum of squares function is given by

$$\chi = \sum_j \big(x_0 + X(s_j, g; L_x) - x_j\big)^2 + \big(z_0 + Z(s_j, g; L_x) - z_j\big)^2, \quad (7)$$

where both the translations x_0, z_0, the compression ratio g, and the projected positions s_j are fit parameters to be optimized.

Projecting: One the shape has been fitted, one might want to continue projecting down points onto the buckled curve, for example to find out the s-value of some molecule that was not used for fitting. This problem is solved by `project_min2D_buckle`.

References

[1] Jordi Gómez-Llobregat, Federico Elías-Wolff, and Martin Lindén. Anisotropic membrane curvature sensing by amphipathic peptides. *Biophys. J.*, 110(1):197–204, 2016. doi:10.1016/j.bpj.2015.11.3512.

[2] Mingyang Hu, Patrick Diggins, and Markus Deserno. Determining the bending modulus of a lipid membrane by simulating buckling. *J. Chem. Phys.*, 138(21):214110–214110–13, 2013. doi:doi:10.1063/1.4808077.