Supplementary Information for *The physical basis* of mollusk shell chiral coiling

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1. Conceptual idea

Our conceptual framework consists of modelling the animal's body by two elastic rods, one representing the ventral side of the animal, and one representing the dorsal side (This terminology holds for ammonites. As it will be mentioned in Section 7, anatomically, the blue rod corresponds to the anterior side and the red rod to the posterior side as classically defined in gastropods, a difference in terminology that however has no theoretical consequence). The body is given prescribed growth rates, through which the reference shape of the body (i.e. the shape of the body if it were extracted from the shell) is determined. These are to be distinguished from secretion rates, which determine the rate of shell production. If the body growth rates exactly match the secretion rates, then the reference shape of the body is always identical to the shell in which it resides; in this case the animal is completely stress free. Our main conceptual idea is to investigate the effect of a mismatch between these rates. If the animal secretes a shell that does not exactly match its own reference shape, this will induce mechanical stress in the animal, since its body will have to deform from its natural shape in order to fit inside the shell tube that it is secreting. In such a case, some of the stress may be relieved by the animal twisting inside the shell tube. To appreciate this, consider Fig 1. The red and blue rods represent respectively the dorsal and ventral sides of the animal in the reference state. Note that both rods are curved in the shape of a logarithmic spiral, such that the ventral side is longer, reflecting a bend in the reference shape of the animal.^{*} There is also a gradient in shell secretion rate along the dorso-ventral axis: shell secretion is highest on the ventral side and lowest on the dorsal side, which produces a curved shell.

Now, suppose that there exists a mismatch between the body growth and secretion rates. In particular, if the secretion rates are lower, then the shell will not be as long as the animal, meaning that the animal is compressed when constrained to the shell. In the middle picture of Fig 1, the animal's body is compressed along its length. Some of this compressive energy can be relieved by the body twisting inside the shell. By twisting, the length of the red and blue rods is longer than in the untwisted state, so some of the compressive stress is relieved; that is, the twisting has reduced the compression energy, at the cost of bending energy. By twisting, the orientation of the ventro-dorsal axis rotates about the center line of the shell, meaning that the secretion gradient axis rotates. This will by necessity introduce a non-planarity to the shape of the shell. For instance, suppose that the animal is secreting a planar shell up to a given time, at which point it undergoes a discrete twisting rotation: the subsequent portion of shell will be secreted in a new plane, determined by the degree of rotation.

Our objective is to determine when twisting (as a continuous process) is energetically favorable, and if so what form of twisting (and thus subsequent form of shell) is the one with minimum energy. Our mathematical framework for analyzing these questions is presented below. This consists of first developing a geometric description of the body and shell, then constructing the mechanical energy of the body, and then comparing the energy between three main shell types – planar, helicospiral, and meandering – for a given mismatch between the rates of growth and secretion.

^{*} In principle, it is possible within our model to assume that the body is not bent in the reference state. Such a choice would generate a greater degree of stress when the body is in the shell. Though most evidence seems to point at a curved shape, e.g. when a *Nautilus* is removed from its shell the body remains bent.



Fig. 1. Schematic for the conceptual idea of the model. A mismatch between growth of the animal, idealized by two elastic rods on the dorsal (red) and ventral (sides), and the secretion of the shell induces stress in the animal that may lead to a twisting within the shell, thereby changing the orientation of the dorso-ventral secretion gradient and impacting the subsequent shape of the shell.

2. Geometry

To construct the geometry of the shell and the ventral and dorsal rods representing the soft body of the animal, we start from the geometry of the centerline of the shell, denoted parametrically by $\mathbf{r}(t)$ where t is its arc length, and a local Frenet basis attached to the centerline and consisting of the tangent $\boldsymbol{\tau}$, normal $\boldsymbol{\nu}$, and binormal $\boldsymbol{\beta}$ vectors that satisfy the Frenet equations

$$\dot{\boldsymbol{r}}(t) = \boldsymbol{\tau} \tag{1}$$

$$\dot{\boldsymbol{\tau}}(t) = \kappa(t)\boldsymbol{\nu} \tag{2}$$

$$\dot{\boldsymbol{\nu}}(t) = -\kappa(t)\boldsymbol{\tau} + \tau(t)\boldsymbol{\beta}$$
^[3]

$$\dot{\boldsymbol{\beta}}(t) = -\tau(t)\boldsymbol{\nu},\tag{4}$$

where an overdot denotes derivative with respect to the arc length t, and where κ and τ are, respectively, the curvature and torsion of the centerline curve. Our task is to define classes of functions for κ and τ corresponding to the possible shell and body shapes under consideration. Given such functions, the full 3D shell is given by

$$\boldsymbol{R}(t,s) = \boldsymbol{r}(t) + R(t) \left(\boldsymbol{\nu}\cos s + \boldsymbol{\beta}\sin s\right)$$
^[5]

where R(t) is the shell radius. The arguments below can be easily generalised to a non-circular aperture, though for simplicity we restrict to circular.

A. Body shape. We assume that the growth of the body is such that in its stress-free state, the centerline of the body is a logarithmic spiral, which can be expressed by the polar equation

$$r(\theta) = ae^{b\theta}.$$
 [6]

As noted, it is more convenient to work in an arc length description. The arc length satisfies

$$t(\theta) = \int_0^\theta \sqrt{r^2 + r'^2} \, d\theta = \frac{a\sqrt{1+b^2}}{b} \left(e^{b\theta} - 1\right).$$
 [7]

The integration could alternatively begin at $\theta = -\infty$, so that the spiral begins at the origin, though beginning at $\theta = 0$ will have no appreciable difference in what follows. We can also compute the curvature

via standard formulas, which expressed as a function of arc length is given by

$$\kappa(t) = \frac{1}{a\sqrt{1+b^2}+bt}.$$
[8]

Inserting κ into Eq. (1)-Eq. (4), with $\tau \equiv 0$, produces a logarithmic spiral for $\mathbf{r}(t)$.

B. Shell shape. The shell shape will be taken to be either a planispiral, a helicospiral, or meandering. A planispiral shape was worked out in the previous subsection, with a curvature given by Eq. (8). For helicospiral and meandering shells, we consider a non-vanishing torsion of the form

$$\tau = \kappa \left(d_0 + d_1 \sin(d_2\theta) \right). \tag{9}$$

A helicospiral corresponds to $d_1 = 0$, $d_0 \neq 0$, where the constant d_0 determines the rotation rate and thus the pitch of the helicospiral, while the scaling by curvature κ is needed to maintain a self-similar shape (see Section D).

A self-similar meandering shell is attained by taking $d_0 = 0$, $d_1 \neq 0 \neq d_2$. In this case there is an oscillatory rotation rate with amplitude determined by d_1 and frequency determined by d_2 . Notice that Eq. (9) is expressed in terms of the angular parameter θ ; this is so that a fixed number of oscillations occur per whorl. To express the torsion in terms of arc length, we simply invert Eq. (7), thus obtaining

$$\theta(t) = \frac{\log\left(1 + \frac{bt}{a\sqrt{1+b^2}}\right)}{b}.$$
[10]

C. Shell radius. To maintain the self-similar shape, the shell radius must follow the same exponential growth as the logarithmic spiral, i.e.

$$R(\theta) = R_0 e^{b\theta} \Rightarrow R(t) = R_0 \left(1 + \frac{bt}{a\sqrt{1+b^2}} \right)$$
[11]

where R_0 is an initial radius.

D. Secretion rates - connection to intrinsic formulation. We have developed a construction of shell for the three shell types. To formulate the mechanical energy of the body, we must view the surface as a shell secreted by the mantle at the aperture in order to describe the shell shape in terms of the location and secretion properties of the dorso-ventral axis.



Fig. 2. A. Geometric connection between the tangent-normal-binormal ($\{\tau, \nu, \beta\}$ frame attached to the centerline curve r, and the $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3\}$ frame attached to the aperture of the shell surface R. B. The dorsal (red) and ventral (blue) rods are situated along the edge of the points of the shell with shortest (dorsal) and longest (ventral) arc length, which is in the direction of the normal ν . The centerlines R_d and R_v are located at an offset φ from the centerline \mathbf{r} .

To link the geometric construction to local secretion rates, we require a map between the extrinsic formulation above – in which the shell is constructed via the properties of a (physically non-existent)

centerline curve – to the intrinsic formulation of (1), in which the shell is constructed via the local growth properties defined along the aperture.

In the intrinsic formulation, we define an orthonormal basis $\{d_i\}$ at each point on the aperture, and the shell is governed by growth velocity functions q_i such that

$$\dot{\boldsymbol{R}} = \sum_{i=1}^{3} \boldsymbol{\mathsf{q}}_i \boldsymbol{d}_i, \qquad [12]$$

where R is the position vector of the shell surface. Letting s again be a parameter denoting position around the aperture, we also have the relation

$$\mathbf{R}' = \lambda \mathbf{d}_3, \tag{13}$$

where prime denotes $\frac{\partial}{\partial s}$, λ is a stretch factor, and we have chosen d_3 to align with the tangent to the curve. It is customary in this formulation to also orient d_1 with the normal to the aperture curve, and then d_2 is the binormal direction, pointing orthogonal to the plane of the aperture. The functions \mathbf{q}_i define the growth rates in the tangent, normal, and binormal directions. Given particular forms of these functions, it is shown in (1) that the full shell may be determined parametrically in an analytical form. Here, our objective is to connect these local growth rates, which provide the information on local secretion rates, with the extrinsic formulation.

From Eq. (5), we may take a derivative with s, and compare with Eq. (13) to find

$$\boldsymbol{d}_3 = -\boldsymbol{\nu}\sin s + \boldsymbol{\beta}\cos s, \quad \boldsymbol{\lambda} = R(t).$$
^[14]

Noting that the aperture lives in the plane spanned by d_1 and d_3 , or equivalently the plane spanned by ν , and β , we have by orthonormality that

$$d_1 = -\nu\cos s - \beta\sin s \tag{15}$$

where the choice of sign aligns d_2 with τ . The relation between the two orthonormal frames, the shell surface R, and the centerline curve r, is illustrated in Fig 2 A.

Next, we take a derivative of Eq. (5) with t, and use Eq. (1)-Eq. (4) to obtain

$$\dot{\boldsymbol{R}} = (1 - R\kappa\cos s)\,\boldsymbol{\tau} + \left(\dot{R}\cos s - R\tau\sin s\right)\boldsymbol{\nu} + \left(\dot{R}\sin s + R\tau\cos s\right)\boldsymbol{\beta}.$$
[16]

By inverting the relations Eq. (14)-(15) for ν , β in terms of d_1 , d_3 , inserting in Eq. (16), and comparing with Eq. (12), we then obtain an explicit connection between the curvature κ , torsion τ , and radius R of the centerline curve in the intrinsic formulation, and the local growth rates:

$$q_1 = -\dot{R}, \quad q_2 = 1 - R\kappa \cos s, \quad q_3 = R\tau.$$
 [17]

Unsurprisingly, the expansion rate \dot{R} exactly matches the growth in the (negative) normal direction. In the self similar formulation we have provided, the radius is an exponential function of θ , while the curvature is an exponentially decaying function of θ ; the product of radius and curvature is thus constant:

$$R\kappa = \frac{R_0}{a\sqrt{1+b^2}}.$$
[18]

It is this constant that defines the gradient of secretion rates that is necessary for a coiled shell. Observe from Eq. (17) that the maximum binormal growth occurs at the point $s = \pi$, which corresponds to the direction $-\nu$ (see Eq. (5)), while the minimal growth is at s = 0, the direction ν . Therefore, assuming that the highest secretion occurs on the ventral side, with lowest secretion on the dorsal side, we conclude that the ventral side is located in the direction $-\nu$ with a secretion rate $1 + R\kappa$, and the dorsal side is located in the direction ν with a secretion rate $1 - R\kappa$. In terms of torsion, the connection $\mathbf{q}_3 = R\tau$, combined with the form Eq. (9), gives

$$\mathbf{q}_3 = \frac{R_0}{a\sqrt{1+b^2}} \left(d_0 + d_1 \sin(d_2\theta) \right).$$
 [19]

This last relation shows that a helicospiral shell $(d_1 = 0, d_0 \neq 0)$ has a constant "tangential growth rate", i.e. constant twist rate, while a meandering shell $(d_0 = 0, d_1, d_2 \neq 0)$ has oscillatory twist.

Intrinsic growth parameters. The value of the intrinsic formulation is that the parameters governing the form of the shell are more naturally linked to the growth and secretion process of the animal. Based on the above, we can rephrase the problem in terms of an expansion rate c_1 so that

$$\mathbf{q}_1 := -c_1, \tag{20}$$

and a coiling gradient c_2 such that

$$\mathbf{q}_2 := 1 - c_2 \cos s.$$
 [21]

These intrinsic parameters connect to the extrinsic parameters via

$$c_1 = \frac{R_0 b}{a\sqrt{1+b^2}}, \quad c_2 = \frac{R_0}{a\sqrt{1+b^2}},$$
[22]

In terms of c_1 , c_2 , and R_0 , the shell radius takes the simple form

$$R(t) = R_0 + c_1 t,$$
[23]

while the curvature satisfies

$$\kappa(t) = \frac{c_2}{R(t)}.$$
[24]

We can also write the torsion as

$$\tau(t) = \kappa \left(d_0 + d_1 \sin\left(\frac{d_2 c_2}{c_1} \log(1 + \frac{c_1 t}{R_0})\right) \right)$$

$$[25]$$

Note that the initial radius R_0 now lives in the expression for the curvature and torsion of the centerline curve; this is due to the fact that the intrinsic formulation is constructed on the shell itself. However, we may exploit the self-similarity and set without loss of generality $R_0 = 1$. In this way, we construct a shell by imposing values of c_1 and c_2 , plus any twist as captured in the values d_0 , d_1 , d_2 .

Eq. (25) enables us to define a "whorl" in the meandering shell by an increase in the argument of the sine function by 2π . Setting the argument to $2n\pi$, $n \in \mathbb{N}$, and solving for t gives that the arc length of a meandering shell with n whorls is

$$L_n = \frac{1}{c_1} \left(\exp\left(\frac{2\pi n c_1}{d_2 c_2} - 1\right) \right),$$
 [26]

where we have fixed $R_0 = 1$ as noted above. It should also be noted that while the parameter t above represents time and the parameters \mathbf{q}_i are growth rates, with units of length per time, in practice (e.g. in comparing with shell growth data), t need not be absolute time, as the absolute growth may vary with food availability, age, etc. The growth rates may also be scaled in different ways to account for such changes, or e.g. to maintain a self-similar secretion of shell material (1), without changing the shape. **E.** Full shell. Inserting given values of the coiling parameters $\{c_1, c_2\}$ and twist parameters $\{d_0, d_1, d_2\}$ into the torsion and curvature equations Eq. (24)-Eq. (25), the complete shell is constructed by integrating the system Eq. (1)-Eq. (4), and inserting into Eq. (5) with R given by Eq. (23). To illustrate the effect of the coiling and twisting parameters, representative examples of each shell type are shown in main text Fig 2 D, using the following sets of parameters:

- Planispiral (top): $c_1 = 0.02, c_2 = 0.25$
- Planispiral (bottom): $c_1 = 0.07, c_2 = 0.5$
- Helicospiral (top): $c_1 = 0.06, c_2 = 0.5, d_0 = 0.25$
- Helicospiral (bottom): $c_1 = 0.06, c_2 = 0.5, d_0 = 0.5$
- Meandering (top): $c_1 = 0.02, c_2 = 0.4, d_1 = 0.6, d_2 = 0.8$
- Meandering (bottom): $c_1 = 0.02, c_2 = 0.4, d_1 = 0.9, d_2 = 0.8$.

3. Mechanics

Having constructed the shell, both in terms of the properties of the centerline, and the intrinsic secretion rates, we turn to the mechanical description of the body inside the shell. As described, our modeling approach is to idealise the body as an elastic rod representing the high-secreting ventral side of the animal, and a separate elastic rod representing the low-secreting dorsal side. Before considering the mechanical energy of the idealised body, we must first consider the geometry of the ventral and dorsal "rods" when constrained to the shell.

A. Curvature and torsion of ventral and dorsal "rods". For a given body/shell shape, we require the curvature and torsion of the ventral and dorsal rods. To do this, we model the rods as seen in Fig 2B. We introduce a parameter $\varphi \in (0, 1)$ that characterises the offset from the centerline, such that the centerline of the ventral rod is given by

$$\boldsymbol{R}_{v}(t) = \boldsymbol{r}(t) - \varphi R(t)\boldsymbol{\nu}$$
^[27]

and the dorsal rod is centered at

$$\boldsymbol{R}_d(t) = \boldsymbol{r}(t) + \varphi R(t)\boldsymbol{\nu}.$$
[28]

Here and in what follows we use the subscript v for a ventral quantity and subscript d for a dorsal quantity. Notice that the lengths of the two curves $\mathbf{R}_v(t)$ and $\mathbf{R}_d(t)$ will not be the same as the length of the centerline curve \mathbf{r} (this is the critical feature for generating a twist). Thus, the variable t in Eq. (27), Eq. (28) is not arc length of the ventral and dorsal center lines. We can compute the curvature and torsion of the ventral and dorsal curves via the standard formulas:

$$\kappa_x = \frac{\left\| \dot{\boldsymbol{R}}_x \times \ddot{\boldsymbol{R}}_x \right\|}{\left\| \dot{\boldsymbol{R}}_x \right\|^3}, \quad \tau_x = \frac{\left(\dot{\boldsymbol{R}}_x \times \ddot{\boldsymbol{R}}_x \right) \cdot \ddot{\boldsymbol{R}}_x}{\left\| \dot{\boldsymbol{R}}_x \times \ddot{\boldsymbol{R}}_x \right\|^2}, \quad [29]$$

where $x \in \{v, d\}$. We may also compute a stretch factor

$$\alpha_x = \left\| \dot{\boldsymbol{R}}_x \right\|,\tag{30}$$

which gives the stretch between the arc length of the centerline and the arc length of the ventral/dorsal curves.

By using the relations Eq. (1)-Eq. (4), explicit formulas may be obtained for these in terms of the centerline curvature $\kappa(t)$ and torsion $\tau(t)$, radius $R(t) = R_0 + c_1 t$, and offset φ . These are provided in Appendix A.

B. Mechanical energy. The formulas above enable to compute the curvature and torsion of the ventral and dorsal curves, for any given configuration. The approach then is to distinguish between a *reference* configuration, denoting the unstressed *body shape*, and a *current* configuration, denoting the *shell shape*. We denote quantities in the former by overhats, e.g. the intrinsic curvature of the ventral side is $\hat{\kappa}_v$, while the latter will be denoted with no overhat. For consistency, we take the initial radius R_0 to be the same in both body and shell.

In the shell constructions we have outlined, these configurations may be defined in terms of distinct sets of parameters, one set for expansion and coiling:

$$\mathcal{S}_1 = \{c_1, c_2\},\$$

and one set for twisting/torsion:

$$\mathcal{S}_2 = \{d_0, d_1, d_2\}.$$

Since the body shape is assumed planispiral and untwisted in the first instance $(\hat{d}_0 = 0)$, the reference configuration may then be defined by

$$\hat{\mathcal{S}}_1 = \{\hat{c}_1, \hat{c}_2\}, \ \hat{\mathcal{S}}_2 = \{0, 0, 0\},\$$

while the shell shape is defined by

$$\mathcal{S}_1 = \{c_1, c_2\},\$$

and one of

$$S_{2_p} = \{0, 0, 0\}, \ S_{2_h} = \{d_0, 0, 0\}, \ S_{2_m} = \{0, d_1, d_2\}$$

for planispiral, helicospiral, and meandering, respectively.

A mismatch in secretion is described by any difference between S_1 and \hat{S}_1 , while any twist of the body is described by the parameters in S_2 . As noted in the main text, another type of mismatch between body and shell may occur: the secretion rates may not match the body growth rates, even if e.g. the expansion and binormal growth gradients match. In other words, the animal may be growing in such a way as to match the shell shape it is secreting, but at a faster or slower rate. This type of mismatch may be accounted for by a scaling of arc length between the body and shell:

$$\hat{t} = \xi t, \tag{31}$$

where \hat{t} is the arc length of the centerline corresponding to the body, t is arc length corresponding to the shell, and $\xi \neq 1$ if there is a mismatch: $\xi > 1$ means the body is growing faster than the shell it is secreting, and vice versa if $0 < \xi < 1$. Note that the parameter ξ provides a unique degree of freedom in the shell construction. To appreciate this conceptually, consider the planar shell, which is created via an expansion and a growth gradient; the latter corresponds to nonuniform growth in the direction orthogonal to the aperture (the binormal growth \mathbf{q}_2), taken as a linear function along a given axis in the plane of the aperture. A linear function really consists of two degrees of freedom, a constant and a gradient, but in our geometric formulation the constant becomes set to 1 (see Eq. (21)). It is in that constant that the extra degree of freedom lies. In terms of actual growth rates, the q_i defined in Eq. (20)-Eq. (21) have units of length per time, and are defined entirely by the c_i . Changing the ξ parameter could thus mathematically be interpreted as a rescaling of time (and thus arc length of the center line), which could be incorporated into a scaling of the c_i , except that then the constant would be shifted away from 1.

The mechanical energy is defined by the difference between the curvature and torsion in the reference and current configurations. In general, the energy of an extensible elastic rod is given by

$$\mathcal{E} = \frac{1}{2} \int_0^T C_0 (\zeta - 1)^2 + C_1 (\mathbf{u}_1 - \hat{\mathbf{u}}_1)^2 + C_2 (\mathbf{u}_2 - \hat{\mathbf{u}}_2)^2 + C_3 (\mathbf{u}_3 - \hat{\mathbf{u}}_3)^2 dt$$
[32]

where ζ is the extensional stretch from reference to current configuration,

$$\mathsf{u} = \mathsf{u}_1 \boldsymbol{d}_1 + \mathsf{u}_2 \boldsymbol{d}_2 + \mathsf{u}_3 \boldsymbol{d}_3$$

is the Darboux curvature vector, and the same quantity with overhats is the reference curvature. Note that the vectors d_i are a basis attached to the centerline of the rod. In principle we must attach a local frame to both the dorsal and ventral rods, however it suffices for these to match and be defined by $d_1 = \beta, d_2 = \nu, d_3 = \tau$. In that case, we have (2)

$$u_1 = 0, \ u_2 = \zeta \kappa, \ u_3 = \zeta \tau.$$
 [33]

and similarly for the \hat{u}_i .

The coefficients C_i , are respectively the stretching (C_0) , bending (C_1, C_2) , and torsional stiffness (C_3) . For the ventral and dorsal rods, recall that the centerline is defined by the offset parameter φ . If we treat the rods as circular, and define the radius such that the outer edge is located at the shell edge, the radius satisfies

$$\rho_x = (1 - \varphi)\hat{R}.$$

Here we use the body radius \hat{R} to define the radii, as these may differ from the shell radius due to secretion mismatch.

In Eq. (32), we must also be careful in defining the extensional stretch ζ . This is the stretch in arc length from the reference to the current configuration, however we only have access to this via a composition of maps:

$$\zeta_x = \frac{\alpha_x}{\xi \hat{\alpha}_x}, \ x \in \{v, d\}$$
[34]

where α and $\hat{\alpha}$ as defined by Eq. (30) give the stretch from centerline to offset, in reference (hatted) and current (unhatted) configurations, and ξ accounts for the centerline arc length stretch via Eq. (31). The intrinsic curvatures $\hat{\kappa}_x$ must also be scaled by $\xi \hat{\alpha}_x$, since these are not defined in an arc length parameterisation.

Combining the above, we obtain the elastic energy of the ventral and dorsal rods for centerline arc length L via

$$\mathcal{E}_x = \frac{\pi}{2} \int_0^L f_x(t) \, dt, \text{ with}$$
[35]

$$f_x(t) := K_1 \left((1-\varphi)\hat{R} \right)^2 \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} - 1 \right)^2 + K_2 \frac{\left((1-\varphi)\hat{R} \right)^4}{4} \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} \kappa_x - \frac{\hat{\kappa}_x}{\hat{\alpha}_x} \right)^2 + K_3 \frac{\left((1-\varphi)\hat{R} \right)^4}{6} \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} \tau_x \right)^2 dt, \ x \in \{v, d\}$$

$$[36]$$

Note that we have assumed transverse isotropy of the section so that a single bending stiffness coefficient remains and use the parameters K_1 , K_2 , K_3 to characterise the scaled stretching, bending, and torsional stiffness, respectively. We do not connect these effective parameters to a classical constitutive law for elastic rod to account for the fact that the animal has a more complex structure than two rods with circular cross-section; the varying stiffness coefficients may characterise the geometrical structure of the body, mechanical anisotropy, etc, and also potentially with differing constants on the ventral and dorsal sides. Rather, we will examine the energy landscape for varying stiffness ratios. We also note that the overall stretching stiffness scales with radius squared, while the bending and twisting stiffnesses scale with radius to the fourth; in this way the mechanical energy maintains a self-similar form. We note also that this elastic rod formulation only considers axial compression of the rods, as is standard in rod theory. This means that any lateral compression of the animal is not included in the energy. Such compression will naturally be present if the radius of the animal is different than the radius of the shell; such effects have previously been demonstrated to provide a mechanical motor for the formation of commarginal ribs (3). It is also worth noting that an additional degree of tension/compression may exist in ammonites due to the chamber formation cycle: septal formation in ammonites is episodic, with the mantle detaching from the previous septum, moving forward in the shell tube, and then reattaching to the shell wall to construct a new septum. We contend that this cycle is not the primary motor for the generation of twist underlying the shell morphology in heteromorph ammonites, because these discrete episodic movements characterise also the development of planispiral species, the development of planispiral stage of some heteromorph species (e.g. Nipponites, Didymoceras, Heteroceras, Colchidites...) and there is no evidence of difference in the chamber formation in chiral versus planispiral stages. Still, there remains the question of how this cycle would impact on the shape generated by the mechanism of mismatch between body growth and shell secretion that we have outlined here. In principle, an episodic movement forward of the mantle could be incorporated in our modeling framework, though this would break the self-similarity assumption that has enabled for analytical progress. A last question is whether these episodic movements affect the whole body or only the part of the body situated between the last formed septum and the posterior muscle attachment zones, and indirect evidences partly based on observations of *Nautilus* suggest that the second possibility is the right one. We leave analysis of such forces in this system as future work.

C. On self-similarity and oscillation frequency. In Fig 3, we provide an example of the total energy integrand f(t) for the 3 shell types (for two different values of the coiling frequency d_2). That is, we plot the $f_v(t) + f_d(t)$ with f defined in Eq. (36), summing the ventral and dorsal sides. Here the growth and secretion parameters are fixed as

$$\hat{c}_1 = 0.02 = c_1, \hat{c}_2 = 0.35, c_2 = 0.4, \xi = 1.05;$$

the twist parameters are

$$d_0 = 0.75, d_1 = 0.9, d_2 = 0.8$$
 (solid line), $d_2 = 1$ (dashed line);

the mechanical stiffness parameters are set at

$$K_1 = 5, K_2 = 1, K_3 = 5;$$

and the offset parameter $\varphi = 0.8$.

There are some general features of the energy that can be readily observed in this example. First, we see that the planispiral (green) and helicospiral (red) shells have simple monotonically increasing energy, due to the fact that these shell types are entirely self-similar (no portion of the shell can be differentiated from any other portion except by a scaling). The energy in the blue meandering case, on the other hand, is oscillatory, due to the oscillatory nature of the torsion. Nevertheless, the meandering energy is also self-similar, when viewed at an integer number of whorls, where one whorl is defined as in Eq. (25). This reflects the fact that each "whorl" of the meandering shell is equivalent to any other whorl up to an appropriate scaling, but any arbitrary segment cannot be scaled to match any other segment.

This feature creates a complication in determining the energy minimizer. In the example of Fig 3, while the helicospiral energy is always below the planispiral energy, the meandering energy oscillates around the helicospiral energy. A consistent approach is to compare the integrated energy computed over an integer number of meandering shell whorls. When compared this way, since the meandering shell is self-similar on integer whorls, the actual integer used in computation is irrelevant — the energy minimizing shell type will be the same for all choices. This is the approach we adopt here. However, applying this approach creates a different complication with the oscillation frequency. Recalling the relationship between centerline arc length and whorl number n in Eq. (26),

$$L_n = \frac{1}{c_1} \left(\exp\left(\frac{2\pi n c_1}{d_2 c_2} - 1\right) \right),$$



Fig. 3. Sample plot of the total energy for planispiral (green), helicospiral (red), and meandering (blue solid, $d_2 = 0.8$, blue dashed, $d_2 = 1.0$) shells. The arc length corresponding to the end of the 1st and 2nd whorl for the meandering shells, defined by a complete oscillation of the torsion, is indicated by the solid and dashed arrows.

for a given number of whorls the arc length is exponentially dependent on the oscillation frequency d_2 , diverging as $d_2 \rightarrow 0$. This implies that the energy minimization will be biased toward higher oscillation frequencies, since the energy will be integrated over a lower total arc length. Here, we solve this issue by fixing the oscillation frequency and perform energy minimization for meandering shells over the oscillation amplitude d_1 only. While this does not guarantee the lowest energy state of all meandering shells, it does provide a consistent approach for comparing shell types and captures an upper bound on the meandering shell with lowest energy: that is, if the meandering shell type is the energy minimizer with d_2 fixed, it is indeed the energy minimizer. Based on known specimens (4), the parameter d_2 only varies in a narrow range that can be all described realistically by $d_2 = 0.8$, as evidenced in main text Fig 2. We can verify this choice a posteriori, by looking at minimizers for other fixed values of d_2 and showing that there is no qualitative difference. Indeed, in Fig 4, we plot the phase space of energy minimizing shell type while sweeping over mechanical stiffness ratios (as in main text Fig 3) for 3 different values of d_2 : 0.7, 0.8, and 0.9.



Fig. 4. Phase space for three different values of coiling frequency: $d_2 = 0.7$ (left), $d_2 = 0.8$ (middle), and $d_2 = 0.9$ (right). For each value of stiffness ratios $(K_1/K_2, K_3/K_2)$, the energy minimizing shell type is indicated by color: green=planispiral, red=helicospiral, blue=meandering. Body growth and secretion values correspond to main text Fig 3 A: $\hat{c}_1 = 0.02$, $\hat{c}_2 = 0.2$, $c_1 = 0.02$, $c_2 = 0.25$, $\xi = 1.0$.

D. Energy minimizer. To determine whether twisting may occur, we consider the following flow of information:

1. We input parameters for the reference body shape: $\hat{S}_1 = \{\hat{c}_1, \hat{c}_2\}$

- 2. We input coiling and aperture expansion parameters for the shell, $S_1 = \{c_1, c_2\}$, as well as a secretion rate mismatch parameter ξ . (If $\hat{c}_1 = c_1$, $\hat{c}_2 = c_2$, and $\xi = 1$, body growth and secretion are a perfect match and no stress is developed, i.e. the energy is identically zero in the case of no twist $S_2 = \{0, 0, 0\}$; hence the problem is only interesting if there is mismatch in at least one parameter.)
- 3. Given offset φ and stiffness parameters $\{K_1, K_2, K_3\}$, the energy is a function only of the twist parameters $S_2 = \{d_0, d_1, d_2\}$ and the arc length L. As discussed above, we fix $d_2 = 0.8$, and choose (without loss of generality) the arc length to correspond to one whorl for the meandering shell, i.e. $L = L_1$ in Eq. (26). We can then write the total integrated energy $\mathcal{E} = \mathcal{E}(d_0, d_1) = \mathcal{E}_v + \mathcal{E}_d$. We then compute three energies:

$$\mathcal{E}_{\text{planispiral}} = \mathcal{E}(0,0)$$

$$\mathcal{E}_{\text{helicospiral}}(d_0) = \mathcal{E}(d_0,0)$$

$$\mathcal{E}_{\text{meandering}}(d_1) = \mathcal{E}(0,d_1)$$
[37]

4. The minimal helicospiral shape is the one for which d_0 minimizes f; similarly there is a minimal meandering shell.[†] If we assume that the actual act of the body twisting does not cost energy, then the shell we predict the creature to actually secret is the one which is the minimizer over all the shapes.

E. Energy profiles. In this section we compare the form of the three energy components (stretching, bending, twisting) for the different shell types. An example appears in Fig 5. Here we plot the energy components as functions of arc length (and scaled with radius as described above), with coiling/expansion parameters for both body and shell corresponding to the baseline meandering case, and twisting parameters set as $d_0 = d_1 = 0.7$. The only mismatch is in the parameter ξ , which is given a value $\xi = 1.05$ for the plots on the left (meaning the animal is secreting at a slower rate than the body growth rate, so the body is in compression), and a value $\xi = 0.95$ in the right column (body in tension).

Energy components are broken down into shell type – helicospiral is red, meandering is blue, planispiral is green – and ventral (solid) versus dorsal (dashed) curves. These plots thus contain a lot of information; however, several trends are apparent and worth noting. In the case of $\xi = 0.95$, all energy components are lower in the planispiral shell, and the stretching energy is almost an order of magnitude higher than the bending and torsion energies. This is not surprising: in this case the body is oversecreting and thus in tension in the planispiral configuration; twisting and secreting either a helicospiral or meandering shell only increases the ventral and dorsal arc lengths, which only serves to increase the tension. Here the planispiral shell will be the energy minimizer for any choice of stiffness parameters.

In the case of undersecreting and a compressive body, $\xi = 1.05$, the energy landscape is more interesting. Here, all energy components have comparable magnitude. The planispiral shell now has the highest stretching energy, since the increased arc length in helicospiral and meandering relieves some compression, while the stretching energy for the meandering shell is sandwiched between the helicospiral and planispiral. In terms of stretching energy alone, the helicospiral shell is the clear winner; however, the helicospiral shell has the highest bending and twisting energy components, and with significantly higher energy on the dorsal side compared to the ventral.

The specific form that these plots take depends on a wide ranging parameter space, and we have only plotted energy components for a single choice of twisting parameters, as opposed to finding the energy minimizing values. Nevertheless, further exploration of the energy landscape (not plotted) shows that the points above highlight some general trends that seem to hold when the body is in compression: (i) the stretching energy is typically lowest in the helicospiral shell, and highest in the planispiral shell, (ii) the bending and twisting energies are typically highest in the helicospiral shell and lowest in the planispiral shell, and (iii) the twisting energy is significantly higher in the helicospiral shell. Due to these differences, there may exist stiffness ratios for which any of the shell types are the overall energy minimizer. For

 $^{^\}dagger$ In some cases the energy minimizer may occur at $d_0=0$ (equivalently $d_1=0$), which correspond to the planispiral shell.



Fig. 5. Comparison of stretching, bending, and torsion energy, plotted as a functions of arc length of current shell.

instance, with high enough stretching stiffness, both the helicospiral and meandering shells will have lower total energy than the planispiral shell; then, if the twisting stiffness is low, the helicospiral shell will be the minimizer of total energy, while if it is increased, the helicospiral can be penalised sufficiently so that the meandering shell is the minimizer; however, if too high the meandering is also penalised sufficiently so that the planispiral has lowest total energy.

4. Data comparison

Shell images and best fit simulated shells appear in Figs 6 (helicospiral) and 7 (meandering). Specimen info and extracted coiling parameters are given in Tables 1 (helicospiral) and 2 (meandering). Coiling parameters were extracted by visual fit by continuously varying (c_1, c_2) and d_0 (helicospiral) or d_1 (meandering) using the Manipulate command in Mathematica. That is, the simulated shell was plotted in a GUI environment in which the shell parameters $\{c_1, c_2, d_0, d_1\}$ as well as the total arc length could be varied with immediate updating of the shell shape. The shape was compared to the images in Figs 6 (helicospiral) and 7 (meandering) until the shell shape was deemed to best capture the shell image. In some instances, a clear difference in coiling existed between the juvenile and adult stages – e.g. see Fig 6 N or P – in these cases the fitting was performed on the adult stage. See Appendix C for specimen abbreviations and collections information.





Shell	Specimen info	Extracted parameters (c_1, c_2, d_0)
A	NMNS PM7231	(0.01, 0.395, 0.372)
В	NMNS PM7234	(0.02285, 0.328, 0.662)
С	NMNS PM7251	(0.0115, 0.464, 0.32)
D	NMNS PM14970	(0.02015, 0.3265, 0.426)
E	NMNS PM14971	(0.01055, 0.292, 0.286)
F	NMNS PM14972	(0.0132, 0.278, 0.42)
G	NMNS PM14973	(0.0149, 0.337, 0.298)
н	NMNS PM14974	(0.02645, 0.573, 0.568)
1	NMNS PM16657	(0.02825, 0.547, 0.438)
J	NMNS PM16701	(0.01995, 0.428, 0.38)
K	UMUT MM1858	(0.0157, 0.506, 0.38)
L	UMUT MM18524a	(0.0122, 0.506, 0.38)
M	UMUT MM18524b	(0.00645, 0.279, 0.146)
N	UMUT MM18529	(0.0172, 0.377, 0.258)
0	NMNS PM16699	(0.0171, 0.367, 0.248)
Р	MCM A0500	(0.01545, 0.355, 0.304)
Q	GK H5853	(0.01135, 0.18, 0.142)

Table 1. Shell specimen info and extracted coiling parameters for helicospiral shells. Corresponding images in Fig 6.

Shell	Specimen info	Extracted parameters (c_1, c_2, d_1)
A	35126-pal.soc.japan	(0.005, 0.602, 0.892)
В	GK H5846	(0.0191, 0.558, 0.866)
С	HMG-1996	(0.0193, 0.646, 0.934)
D	HMG-1997	(0.0152, 0.385, 0.77)
E	INM-4-346	(0.0071, 0.508, 0.878)
F	MCM-A0435	(0.0276, 0.529, 0.8)
G	MCM-K0058	(0.0071, 0.523, 0.914)
н	NMA-606	(0.03065, 0.457, 0.852)
1	NMA-902	(0.0163, 0.402, 0.83)
J	NMNS PM14977	(0.01315, 0.492, 0.854)
ĸ	NMNS PM14990	(0.01315, 0.368, 0.884)
L	NMNS PM16654	(0.01315, 0.597, 0.884)
м	NMNS PM16655	(0.01315, 0.689, 0.915)
N	UMUT MM7560	(0.01975, 0.689, 0.933)
0	KUM unnumbered	(0.0129, 0.684, 0.905)
Р	UMUT MM18254	(0.01, 0.356, 0.847)
Q	UMUT MM18571a	(0.0204, 0.58, 0.85)
R	GK H5853	(0.01925, 0.35, 0.944)
s	20269975 MCL	(0.481, 0.01205, 0.825)

 S
 20209975 MOL
 (0.481, 0.01205, 0.825)

 Table 2. Shell specimen info and extracted coiling parameters for meandering shells. Corresponding images in Fig 7.



Fig. 7. Shell images and best visual fit simulated shells for meandering shell type.

5. Shell transitions

Fig 5 of the main text shows simulations of Didymoceras nebrascense and Nostoceras malagasyense. Theseshells were generated by varying the mismatch and/or stiffness parameters at different stages in development,Chirat et al.PNAS | December 4, 2021 | vol. XXX | no. XX | 15

and computing at each stage the energy minimizing shell type. The stages for *Didymoceras* are defined as follows:

Initial stage: In the juvenile stage, the shell is planispiral. We have simulated this with coiling parameters $c_1 = \hat{c}_1 = 0.05$, $c_2 = \hat{c}_2 = 0.6$, $\xi = 1.0$. The stiffness ratios are $K_1/K_2 = 10$, $K_3/K_2 = 1.75$. For these values there is no mismatch and the energy minimizer is the planispiral shell. This stage is plotted for center line arc length $t \in [0, 8]$.

Transition to helicospiral: Beyond the juvenile stage, the shell has helicospiral form. In our model, we increase the compression parameter to $\xi = 1.03$, for which the planispiral shell is energy minimizer with value $d_0 = 0.24$. However, for intermediate values of ξ , the energy minimizer passes through the meandering shell type. To capture this via discrete shell sections, we set $\xi = 1.015$ and compute the energy minimizing meandering shell, which has value $d_1 = 0.2$. The meandering portion is plotted for center line arc length $t \in [8, 14]$. The helicospiral portion is assumed to persist for a large part of the animal's development, plotted for center line arc length $t \in [14, 114]$. Based on visual inspection, we also decrease the expansion rate in the helicospiral stage: $\hat{c}_1 = c_1 = 0.04$.

Late stage transition: the late stage of *Didymoceras nebrascense* shells are marked by a transition back to planispiral, in a plane orthogonal to the axis of coiling of the helicospiral stage. As before, as regions of parameter space where the meandering shells are minimizers are located in between the planispiral and helicospiral regions, from the mechanical perspective a transition from helicospiral to planispiral generally requires passing through a meandering stage. Moreover, a meandering stage is necessary geometrically as well, in order to orient the plane of the final planispiral coiling stage. In the shell simulation of main text Fig 4 F, we have generated this transition by decreasing the compression parameter back to $\xi = 1.015$ (meandering stage) and then $\xi = 1.0$ (planispiral stage), while also changing the stiffness parameters to $K_1/K_2 = 5, K_3/K_2 = 5$, and decreasing the coiling gradient to $\hat{c}_2 = 0.55, c_2 = 0.6$ (meandering stage) and then to $\hat{c}_2 = 0.5, c_2 = 0.5$ (planispiral stage). The meandering stage has energy minimizing value $d_1 = 0.47$, and was plotted for $t \in [114, 140]$; the planispiral stage was plotted for $t \in [140, 165]$.

For the *Nostoceras* shell, the juvenile transition is missing due to breakage in our specimen. For simplicity, here we do not simulate an early transition, and consider that the first visible preserved stage is a helicospiral stage, as in the specimen of the photo.

Helicospiral stage: the helicospiral stage has coiling parameters $c_1 = \hat{c}_1 = 0.06$, $c_2 = \hat{c}_2 = 0.648$, and mismatch parameter $\xi = 1.028$. the stiffness ratios are $K_1/K_2 = 10$, $K_3/K_2 = 1.24$, for which the energy minimizing twisting rate is $d_0 = 0.174$. The helicospiral portion is plotted for centerline arc length $t \in [0, 131]$.

Late stage transition: the late stage of *Nostoceras* is similar to *Didymoceras*, with a transition to planispiral, but with rotated axis of coiling. In the case of *Nostoceras*, the plane of coiling for the planispiral stage is inclined with respect to the coiling axis for the helicospiral stage. Again, this rotation is achieved by a transitional meandering stage. The meandering and planispiral stages are characterized by a marked decrease in expansion rate, to almost zero. We decrease to $c_1 = \hat{c_1} = 0.001$ for these stages. Geometrically, the specimen we model has an interesting variation in coiling gradient: the meandering stage has low coiling gradient, which accounts for the significant protrusion of the shell following the helicospiral stage. The shell then completes a near hairpin turn, implying a brief but strong increase in coiling gradient; the final portion of the shell is nearly straight, with almost no coiling gradient. We simulate this morphology with coiling gradient $c_2 = 0.32$ for the meandering stage, then $c_2 = \hat{c}_2 = 0.66$ for a brief portion of the planispiral stage, followed by $c_2 = \hat{c}_2 = 0.25$ for the final portion. The stiffness ratio K_3/K_2 is increased to 7.0. For the meandering stage, the mismatch parameter is increased slightly to $\xi = 1.018$, for which the energy minimizing twist rate is $d_1 = 0.49$. For the planispiral stage, we decrease ξ to 1.0: as there is no mismatch, the planispiral shell is the energy minimizer. The meandering stage was plotted for $t \in [131, 178.4]$, the first planispiral stage for $t \in [178.4, 201.4]$, and the final portion for $t \in [201.4, 221.4]$.

For both shell simulations, in computing the energy minimizer at each stage, we have followed the same computational approach as in the rest of the paper. This is not technically correct, since the shell is not self-similar but rather composed of self-similar sections. However, as noted, computing the shape in full generality couples at each point in development the orientation and mechanical energy, which renders the problem largely intractable mathematically. Here, the energy minimization via piecewise self-similarity calculations provides a strong indication of the mechanically favorable twisting at each point.

The simulated shells were created by attaching each subsequent shell section to the end of the previous section, with continuity in position, radius, and tangent vectors. Since the meandering shell has a sinusoidal torsion, we also introduce a potential phase shift in the torsion; that is we modify the torsion Eq. (38) to

$$\mathbf{q}_{3} = \frac{R_{0}}{a\sqrt{1+b^{2}}} \left(d_{1}\sin(d_{2}\theta + \delta) \right).$$
[38]

where the phase shift δ determines at which point in the meandering oscillation cycle the shell begins the section at; this was chosen to be $\delta = 0$ for both meandering stages of the *Didymoceras* shell, and was given the value $\delta = 1.8$ for the *Nostoceras* shell. Continuity in normal and binormal vectors is also applied at each transition, with one exception: at the transition from helicospiral to meandering, we incorporated a discrete twist around the tangent. Explicitly, defining $(\boldsymbol{\nu}_P, \boldsymbol{\beta}_P)$ as the normal and binormal vectors at the end of the helicospiral section, and $(\boldsymbol{\nu}_M, \boldsymbol{\beta}_M)$ the equivalent vectors at the beginning of the meandering stage, we initialize

$$\boldsymbol{\nu}_M = \cos\psi\boldsymbol{\nu}_P - \sin\psi\boldsymbol{\beta}_P, \quad \boldsymbol{\beta}_M = \sin\psi\boldsymbol{\nu}_P + \cos\psi\boldsymbol{\beta}_P, \quad [39]$$

where we have used the value $\psi = 4.54$ for the *Didymoceras* and $\psi = 5.2$ for the *Nostoceras*. This definition implies a discrete rotation of the ventro-dorsal axis by angle ψ at the transition point, i.e. a discrete twisting of the animal inside the shell, as opposed to the continuous twisting that characterizes our model. We found that we were best able to match our simulated shell to the shell images by incorporating such a twist. Physically, such a discrete twist could occur due to a mechanical instability, possibly due to threshold effects resulting from continuous variations in developmental parameters not incorporated in our model. In ammonites, these discontinuous variations during development have been used for a long time to recognize discrete growth stages in the context of the studies of heterochronies. In many heteromorphs, the modifications in shell coiling are abrupt, whether during the early of late stage of development. The question remains however to what a threshold effect and a discontinuous twist could be linked during the last stage of development of *Didymoceras* (e.g. Allometric development of muscles? Allometric development of the external head-foot complex as in many current cephalopods, generating stresses on the part of the body situated inside the shell?).

While we leave further investigation of a discrete twist due to mechanical instability as further work, we note that the model is capable of generating a very similar morphology without incorporating any discrete twist. This is demonstrated in Fig 8 : the shells on the left are the same as the *Didymoceras* shell shown in Fig 5 of the main text, generated as described above. The shells on the right do not involve a discrete twist. In this simulation, the transition to the planispiral stage is achieved by a higher value of twisting amplitude d_1 during the meandering stage, combined with a longer meandering section. Explicitly, this shell appears via sections of energy minimizers with all parameters equivalent to those described above for the first 3 stages, and with the transition from helicospiral to meandering) and $c_2 = 0.45$, $\hat{c}_2 = 0.45$, $\xi = 1.015$ (meandering) and $c_2 = 0.45$, $\hat{c}_2 = 0.45$, $\xi = 1.0$ (planispiral), while changing the mechanical parameters to $K_1/K_2 = 5$, $K_3/K_2 = 10$. In the meandering stage, the energy minimizing value is $d_1 = 0.73$; the phase shift for this section was taken to be $\delta = 4.39$.

6. Extensive parameter sweep

In this section we support via an extensive parameter sweep the claim that the regions of parameter space for which the planispiral and helicospiral shells are mechanically favorable are separated by a region in which the meandering shell is favorable. In Figure 9 we plot an array of phase spaces – each phase space sweeps over the mechanical stiffness ratios, with energy minimizing shell type denoted by color: green=planispiral, red=helicospiral, blue=meandering. Phase spaces are computed over a range of coiling gradient parameters



Fig. 8. Simulations of *Didymoceras nebrascense*. The transition from helicospiral to meandering to planispiral is characterised by the coiling plane in the final stage orthogonal to the coiling axis of the helicospiral stage. This can be accomplished in the model by incorporating a discrete twist at the transition to meandering (left), or by a continuous twist but with a longer meandering stage and increased oscillation amplitude d_1 .

 (c_2, \hat{c}_2) , and two different values of compression parameter ξ . Plots are shown for $c_1 = \hat{c}_1 = 0.02$; a very similar diagram emerges with different values, as the expansion rate seems to have little effect on the energy minimizer.

Fig 10 shows the result of a similar computation, but with each phase plot computed as a sweep over (c_2, \hat{c}_2) , and repeated with $(K_3/K_2, K_1/K_2)$ varying over the range 0.5 to 8.0. In all cases, we find the red helicospiral regions separated from the green planispiral regions by a blue meandering region. Note that in Fig 10, some parameter values do show a red region neighboring a green region; however, upon closer inspection with a finer grid, we find that in fact a small blue region does exist. This is demonstrated by the inset, which zooms in on the boundary between green and red and confirms the presence of a meandering region.

7. Gastropod

To investigate the form of gastropod shell, we modify the model by incorporating an intrinsic twist. That is, we assume that the animal's body has a helicospiral reference shape defined by the set of parameters

$$\hat{\mathcal{S}}_1 = \{\hat{c}_1, \hat{c}_2, \hat{d}_0\},\$$

Fig. 9. An array of phase spaces is computed for varying coiling parameters (c_2, \hat{c}_2) , and two different values of compression parameter ξ . Each phase space sweeps over the stiffness ratios $(K_3/K_2, K_1/K_2)$ varying between 0.5 and 10.

Fig. 10. An array of phase spaces is computed for varying stiffness ratios $(K_3/K_2, K_1/K_2)$, and two different values of compression parameter ξ . Each phase space sweeps over the coiling parameters (c_2, \hat{c}_2) varying between 0.2 and 0.7.

where \hat{c}_1, \hat{c}_2 describe the expansion rate and coiling gradient of the body, as before, while \hat{d}_0 captures the intrinsic twist. The calculations then proceed in the same way as before, with the mechanical energy for both sides (anatomically anterior for the blue rod and posterior for the red rod in a gastropod) Eq. (36) being adapted to account for a non-zero intrinsic torsion:

$$\mathcal{E}_x = \frac{\pi}{2} \int_0^T K_1 \left((1-\varphi)\hat{R} \right)^2 \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} - 1 \right)^2 + K_2 \frac{\left((1-\varphi)\hat{R} \right)^4}{4} \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} \kappa_x - \frac{\hat{\kappa}_x}{\hat{\alpha}_x} \right)^2 + K_3 \frac{\left((1-\varphi)\hat{R} \right)^4}{6} \left(\frac{\alpha_x}{\xi \hat{\alpha}_x} \tau_x - \frac{\hat{\tau}_x}{\hat{\alpha}_x} \right)^2 dt.$$
[40]

A sample phase space is given in the main text, with the coiling parameters chosen to match a typical gastropod. In Fig 11 we provide two further examples, with coiling parameters chosen to correspond to a planispiral shell (Fig 11 (a)) and a meandering shell (Fig 11 (b) In these plots we vary both the intrinsic twist via $\hat{d}_0 \in \{0.1, 0.3\}$ and the mismatch via $\xi \in \{0.95, 1.05\}$. For each choice, we then sweep over the stiffness ratios and then color the point with the energy minimizing shell type. In the case of the body in compression, i.e. an undersecreting shell, the helicospiral shell type is the energy minimizer for every single parameter choice. These points appear in red, with the color indicating the energy minimizing twist value d_0 . For an oversecreting shell, $\xi = 0.95$, the planispiral shell appears in some cases as the energy minimizer (green points); the meandering shell never appears as the energy minimizer.

(a) Coiling parameters $c_1 = \hat{c}_1 = 0.012$, $c_2 = \hat{c}_2 = 0.2$ correspond to a planispiral (b) Coiling parameters $c_1 = \hat{c}_1 = 0.02$, $c_2 = \hat{c}_2 = 0.5$ correspond to a meandering shell.

Fig. 11. Morphological phase space in the case of an added intrinsic twist.

Appendix

A. Stretch, curvature, torsion formulas. In the absence of centerline torsion, the stretch α_v and curvature κ_v on the ventral side satisfy

$$\alpha_v = \sqrt{\varphi^2 \dot{R}^2 + \varphi^2 R^2 \kappa^2 + 2\varphi R \kappa + 1},$$
[41]

$$\kappa_{v} = \frac{\sqrt{\left(\varphi^{2}\dot{R}\left(2\kappa\dot{R}+R\dot{\kappa}\right)+\left(\varphi R\kappa+1\right)\left(-\varphi\ddot{R}+\varphi R\kappa^{2}+\kappa\right)\right)^{2}}}{\left(\varphi^{2}\dot{R}^{2}+\varphi^{2}R^{2}\kappa^{2}+2\varphi R\kappa+1\right)^{3/2}}.$$
[42]

If the centerline has non-zero torsion, these formulas are adapted to:

$$\alpha_v = \sqrt{\varphi^2 \dot{R}^2 + \varphi^2 R^2 \left(\kappa^2 + \tau^2\right) + 2\varphi R\kappa + 1},$$
[43]

$$\kappa_{v} = \left(\varphi^{2} \left(\tau(\varphi R^{2}\dot{\kappa} - 2\dot{R}) - R\dot{\tau}(\varphi R\kappa + 1)\right)^{2} + \left(\varphi^{2}\dot{R}(2\kappa\dot{R} + R\dot{\kappa}) + (\varphi R\kappa + 1)\left(\kappa - \varphi\ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2}\right)\right)^{2} + \varphi^{2} \left(R\tau(\kappa - \varphi\ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2}) + \varphi\dot{R}(2\tau\dot{R} + R\dot{\tau})\right)^{2}\right) \right/ (44)$$

$$\left(\varphi^{2}\dot{R}^{2} + \varphi^{2}R^{2}(\kappa^{2} + \tau^{2}) + 2\varphi R\kappa + 1\right)^{3/2}.$$

The ventral torsion τ_v is:

$$\begin{aligned} \tau_{v} &= \left[\left(\varphi^{2} \dot{R} \left(2\kappa \dot{R} + R\dot{\kappa} \right) + (\varphi R\kappa + 1) \right) \\ \left(-\varphi \ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2} + \kappa \right) \right) \\ \left(-3\varphi \left(\dot{R}\dot{\tau} + \tau \ddot{R} \right) + \varphi R\kappa^{2} \tau + \varphi R \left(\tau^{3} - \ddot{\tau} \right) + \kappa \tau \right) \\ &+ \varphi \left(R\tau \left(-\varphi \ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2} + \kappa \right) + \varphi \dot{R} \left(2\tau \dot{R} \right) \\ &+ R\dot{\tau} \right) \right) \left(3\varphi \dot{R}\dot{\kappa} + 3\varphi \kappa \ddot{R} + \varphi R\ddot{\kappa} - \varphi R\kappa \tau^{2} - \varphi R\kappa^{3} - \kappa^{2} \right) \\ &- \varphi \left(\tau \left(\varphi R^{2} \dot{\kappa} - 2\dot{R} \right) - R\dot{\tau} (\varphi R\kappa + 1) \right) \left(3\varphi \kappa^{2} \dot{R} + 3\varphi \tau^{2} \dot{R} \right) \\ &- \varphi R^{(3)} + 3\varphi R\kappa \dot{\kappa} + 3\varphi R\tau \dot{\tau} + \dot{\kappa} \right) \right] / \left[\varphi^{2} \left(\tau \left(\varphi R^{2} \dot{\kappa} - 2\dot{R} \right) \right) \\ &- R\dot{\tau} (\varphi R\kappa + 1) \right)^{2} + \left(\varphi^{2} \dot{R} \left(2\kappa \dot{R} + R\dot{\kappa} \right) + (\varphi R\kappa + 1) \right) \\ &\left(-\varphi \ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2} + \kappa \right) \right)^{2} \\ &+ \varphi^{2} \left(R\tau \left(-\varphi \ddot{R} + \varphi R\kappa^{2} + \varphi R\tau^{2} + \kappa \right) + \\ \varphi \dot{R} \left(2\tau \dot{R} + R\dot{\tau} \right) \right)^{2} \right]. \end{aligned}$$

In both cases, the corresponding formulas for the dorsal side are obtained by the change $\varphi \to -\varphi$.

B. Specimens number and collections of Fig. 1.. (A) *Turrilites costatus* (Cenomanian, France). UCBL-FSL 14018a, Université Lyon1, France. (B) *Colchidites breistrofferi* (Barremian, Columbia). UJF-ID 3052, Université Grenoble Alpes, France. (C) *Nipponites mirabilis* (Turonian, Japan). MCM-A0435, Mikasa City Museum, Japan. (D) *Nipponites mirabilis* (Upper Cretaceous, Japan). INM-4-346, Ibaraki Prefecture Natural Museum/Paleontological Society of Japan. (E) *Didymoceras stevensoni* (Late Cretaceous, USA). MCFO0465, Museum CosmoCaixa, Spain. (F) *Didymoceras stevensoni* (Late Cretaceous, USA). DMNH 8711, Denver Museum of Nature & Science, USA. **C.** Abbreviations and collections (Data Comparison). NMNS: National Museum of Nature and Science, Tokyo, Japan UMUT: The University Museum, The University of Tokyo, Japan (Photos: Okamoto 1989 (5)). NMA: Nakagawa Museum of Natural History, Japan (Paleontological Society of Japan) MCM: Mikasa City Museum, Japan. KUM: Kyushu University, Japan, Haruyoshi Maeda Coll. GK: Kyushu University Museum, Japan (Photos: Matsumoto 1977 (6)). INM: Ibaraki Prefecture Natural Museum, Japan (Paleontological Society of Japan). HMG: Mukawa Choritsu Hobetsu Museum, Japan (Paleontological Society of Japan). MCL: Musée des Confluence de Lyon, France.

D. Specimens number and collections of Fig 5. *Didymoceras nebrascense* : Di1084A, Upper Cretaceous, South Dakota, USA; Coll. S. Jorgensen; Photo S. Luallin. *Nostoceras malagasyense* : HC-733, Upper Cretaceous, Madagascar; Coll. H. Châtelier.

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