Supplementary text

The following text describes 3D nonlinear finite element method implementation of the expanding beam model for pavement cells lobe formation. The formation and growth of pavement cells undulation pattern were modeled using 3D nonlinear elastic finite element model using an 8-node brick element with 24 degrees of freedom. The model was implemented in Matlab with the isotropic hyperelastic material model using total Lagrangian approach, where the strain energy density function was given by three-parameter compressible Money-Rivlin material:

$$W(J_1, J_2, J_3) = A_{10} \cdot (J_1 - 3) + A_{01} \cdot (J_2 - 3) + A_{11} \cdot (J_3 - 3)^2 \qquad (1)$$

Where the J_1, J_2, J_3 are reduced invariants of right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}\mathbf{F}^T$ and $\mathbf{F}$ is a deformation gradient. The invariants of Green-Cauchy tensor are: $I_1 = tr(\mathbf{C})$, $I_2 = [tr(\mathbf{C})^2 - tr(\mathbf{C}^2)]$, $I_3 = det\mathbf{C}$ and the reduced invariants: $J_1 = I_1 I_3^{-1/3}$, $J_2 = I_2 I_3^{-2/3}$, $J_3 = I_3^{1/2}$ The total deformation gradient was multiplicatively decomposed into a growth deformation tensor and an elastic deformation tensor: $\mathbf{F} = \mathbf{F}_g\mathbf{F}_e$, see Figure 1. The growth of pavement cells presented here is nonuniform. At i_{th} growth step each solid element in the body is grown independently according to the law described in the section below. Such incompatible growth state $\mathbf{B_{t_1}}$ may lead to discontinuities and overlaps between the parts of a body. In order to bring all grown parts together, the elastic deformation is introduced, which assembles all the elements into compatible grown body (29) his, in turn, may create residual stress. It is assumed, that the accommodating elastic deformation is instantaneous to growth deformation so that the later can be considered a virtual state, a convenient mathematical construct to solve the growth problem. Furthermore, the growth process occurs at much slower time-scale compared to elastic equilibrium, hence it can be assumed, that at each growth step, the body is in equilibrium. The incompatible growth state is, by definition, stress-free so that all the stresses arise due to accommodating elastic deformation and external forces. Here we assume, that stresses due to accommodating elastic deformation are relaxed between successive growth step, by the processed of a cell wall remodeling, which is not explicitly modeled. This allows for the assumption that at the start of each growth iteration, the stresses due to internal body forces are negligible, so that evolving initial grown state is a compatible growth state without external loads applied. In the presence of external load, e.g. turgor pressure or atmospheric pressure, the elastic deformation gradient can be further decomposed into elastic deformation due to loading and the growth accommodating

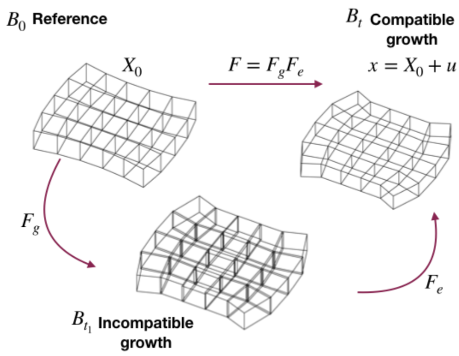

Figure 1: Schematic representation of a FE model of growth. At each growth iteartion deformation gradient $\mathbf{F}$ transforms the initial body $\mathbf{B_0}$ with the nodal position vector $\mathbf{X_0}$ into $\mathbf{B_t}$ state with the nodal position vector $\mathbf{x}$, were $\mathbf{u}$ is a nodal dispalcement vector. Vector $\mathbf{u}$ includes nodal dispalcement due to a known growth deformation gradient $\mathbf{F_g}$ and the unknown accomodating elastic deformation gradient $\mathbf{F_e}$

elastic deformation $\mathbf{F_e} = \mathbf{F_{el}}\mathbf{F_{eg}}$. Given the growth deformation gradient, the unknown at each iteration is the nodal displacement vector $\mathbf{u}$ due to total elastic deformation. The solution of nonlinear problem consists of solving a variational equation with respect to unknown nodal displacements $\mathbf{u}$, derived from equating virtual work performed by internal body forces $a(\mathbf{u}, \bar{\mathbf{u}})$ and a virtual work performed by external loads $l(\mathbf{u}, \bar{\mathbf{u}})$:

$$a(\mathbf{u}, \bar{\mathbf{u}}) \equiv \int\limits_{\Omega_0} \frac{\partial W}{\partial \mathbf{E}} : \bar{\mathbf{E}} \, \mathrm{d}\Omega = \int\limits_{\Omega_0} \bar{u}^T f^b \, \mathrm{d}\Omega - \int\limits_{\Gamma} \bar{u}^T t \, \mathrm{d}\Gamma \equiv l(\mathbf{u}, \bar{\mathbf{u}}) \qquad (2)$$

Where $\mathbf{E}$ is a Lagrangian strain and $\bar{\mathbf{E}}$ is a variation of Lagrangian strain with respect to nodal displacements, f^b is a body force and t surface traction, Ω and Γ denote volume and surface integrals. The first term correspond to internal energy and can be rewritten as $\int\limits_{\Omega_0} S(\mathbf{u}) : \bar{\mathbf{E}}(\mathbf{u}, \bar{\mathbf{u}}) \, \mathrm{d}\Omega$, where $S(\mathbf{u})$ is Second Piola-Kirchoff stress.

The detailed procedure of solving system of nonlinear equation using Newton-Rapson method and the procedure for solving nonlinear FEM problems we adopted is described in (19) The solution consist of residual linearization through tangent stiffnes matrix calculation, where the residual is defined as $R = a(\mathbf{u}, \bar{\mathbf{u}}) - l(\mathbf{u}, \bar{\mathbf{u}})$. It is important to note, that the system is solved for an elastic deformation gradient given by $\mathbf{F}_e = \mathbf{F}/\mathbf{F}_g$, given the known growth deformation gradient $\mathbf{F}_g$. Since the load does not depend on dispalcement, only internal energy needs to be linearised: $a^*(\mathbf{u}; \Delta\mathbf{u}, \bar{\mathbf{u}}) = \int\limits_{\Omega_0} [\Delta S(\mathbf{u}) : \bar{E}(\mathbf{u}, \bar{\mathbf{u}}) + S(\mathbf{u}) : \bar{\Delta} E(\mathbf{u}, \bar{\mathbf{u}})] \, \mathrm{d}\Omega$

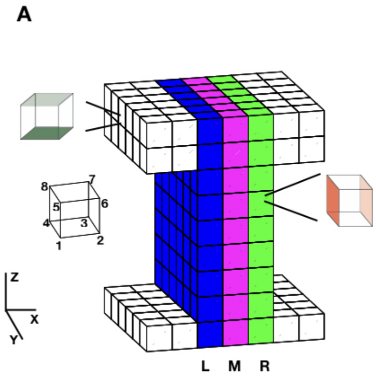

Figure 2: (A) Miniaturised mesh used for the FE model. The anticlinal wall has three element thickness: left (L), right (R), and middle (M). Bottom and top periclinal wall have a thickness of one and two elements respectively.

The growth laws

At the start of a simulation the width of an anticlinal wall is along X direction, its length along Y direction and hight along Z. The periclinal wall is perpendicular to the anticlinal wall and its width and length span XY plane. The anticlinal wall was modeled with a three-element width, Figure 2.

The growth laws for the anticlinal wall

At each growth iteration, the nodal displacements due to local growth of an anticlinal wall element are given by:

$$G_{A_x}(x,y) = D_{exo}(W_p + D^{L,R}_{dmet}(x,y)E_{XY})/2 \tag{3}$$

$$G_{A_y}(x,y) = D_{exo}D^{L,R}_{dmet}(x,y)E_{XY}L_{ij}/2 \tag{4}$$

$$G_{A_z}(x,y) = D_{exo}D^{L,R}_{dmet}(x,y)E_{Z}L_{ij}/2 \tag{5}$$

Where $D_{exo}/D^{L,R}_{dmet}$ is the exocytosis/dymethylation rate respectivelly for left (L) or right (R) element. $D_{exo} = 0.05$, unless stated otherwise. $E_{XY} = 0.348$ nm is pectin expansion perpendicular to the axis of the pectin filament and $E_Z = -0.013$ nm is a contraction along the axis of pectin filament. The L_{ij} is a relaxed edge length connecting node of interest with its neighbor, e.g., for the displacement of nodes 1 or 2 in x direction it will be the edge L_{12}. $W_p = 0.838$ nm is the width of a single pectin polymer. For the middle (M) anticlinal wall nodes 2, 3, 6, 7 (see Figure 2) follow the equations for the right (R) anticlinal wall and the nodes 1, 4, 5, 8 the equations for the left (L) anticlinal wall.

The expanding beam growth model has one parameter, which is not determined experimentally, exocytosis rate. The local methylation asymmetry, here presented as local demethylation rate was obtained from immunolocalization with dSTORM. HG expansion rates due to demethylation were calculated using the parameters published in (18) and were obtained as follow. Methylated HG forms a hexagonal latice with a step 0.837 nm in X and Y plane and a helical repeating unit of 1.34 nm in the Z direction. Upon demethylation HG form a rectangular lattice with steps 0.99 nm and 1.23 nm in two lateral dimensions and a helical repeating unit of 1.327 nm in the Z direction. Then the average (assuming rotational symmetry of pectins in the cell wall) HG expansion in lateral dimensions E_{XY} was obtained as $\sqrt(A_{rec}/A_{rom})W_p - W_p)$ where A_{rec} is an area of the rectangular unit cell (with the dimensions as described above) and $A_{rom} = 0.837^2\sqrt(3)/2$ is an area of the rhomboidal unit cell. The contraction in Z direction (along the HG polymer) due to demethylation was calculated as follows: $E_Z = 1.327 - 1.34$.

The growth laws for the periclinal wall

The periclinal walls were modeled with the width of one and two elements for the bottom and the top wall, respectively. The bottom periclinal wall element had 16 degrees of freedom, and the displacement along the Z direction was preset to 0.

$$G_{P_x} = D_{exo} D^P_{dmet} E_{XYZ} L_{ij}/2 \tag{6}$$

$$G_{P_y} = D_{exo} D^P_{dmet} E_{XYZ} L_{ij}/2 \tag{7}$$

$$G_{P_z} = D_{exo}(W_p + D^P_{dmet} E_{XYZ})/2 \tag{8}$$

Where D^P_{dmet} is the dimethylation rate for the periclinal wall. $E_{XYZ} = 0.22$ nm is an average pectin expansion in three dimensions.