Forces in vertex models

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I. CELL POTENTIAL ENERGY

We introduce for each cell i a reference perimeter P_i^0 and a reference area A_i^0 , and for each of its cell corner $\mu \in \Omega_i$ a force whose effect is to bring the cell's perimeter P_i and area A_i to their reference quantities. A possible force derives from the following potential energy [1–4]

$$E_{\text{VM}} = \sum_{\text{cells } i} \left[\frac{1}{2} K_i (A_i - A_i^0)^2 + \frac{1}{2} \Gamma_i (P_i - P_i^0)^2 \right], \tag{1}$$

where K_i and Γ_i are respectively area and perimeter elastic constants. We denote r_{μ} , r_i the position of vertices μ , i (see Fig. 1). The cell's perimeter can be written

$$P_i = \sum_{\mu \in \Omega_i} |\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}|, \tag{2}$$

and the cell's area can be computed with the shoelace formula

$$A_i = \sum_{\mu \in \Omega_i} \frac{1}{2} [(\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_i) \times (\boldsymbol{r}_{\mu} - \boldsymbol{r}_i)] \cdot \hat{\boldsymbol{e}}_z.$$
(3)

Note that, by convention of ordering of cell corners, each term in this sum must be positive. With these notations, we thus write the force acting on vertex μ

$$\mathbf{F}_{\mathrm{VM},\mu} = -\nabla_{\mu} E_{\mathrm{VM}},\tag{4}$$

where $\nabla_{\mu} \equiv \partial/\partial \boldsymbol{r}_{\mu}$. We compute

$$\nabla_{\mu} \left(|\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}| \right) = \frac{\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}}{|\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}|},\tag{5}$$

as well as

$$\nabla_{\mu} \left(\left[\left(\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_i \right) \times \left(\boldsymbol{r}_{\mu} - \boldsymbol{r}_i \right) \right] \cdot \hat{\boldsymbol{e}}_z \right) = \hat{\boldsymbol{e}}_z \times \left(\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_i \right) \tag{6}$$

to write (4) in its full form

$$F_{\text{VM},\mu} = -\sum_{\text{cells i}, \mu \in \Omega_{i}} \left[\frac{1}{2} K_{i} (A_{i} - A_{i}^{0}) \left[\hat{\boldsymbol{e}}_{z} \times (\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_{i}) - \hat{\boldsymbol{e}}_{z} \times (\boldsymbol{r}_{\mu+1} - \boldsymbol{r}_{i}) \right] + \Gamma_{i} (P_{i} - P_{i}^{0}) \left[\frac{\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}}{|\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}|} + \frac{\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}}{|\boldsymbol{r}_{\mu} - \boldsymbol{r}_{\mu-1}|} \right] \right]$$

$$= \sum_{\text{cells i}, \mu \in \Omega_{i}} \left[\frac{1}{2} K_{i} (A_{i} - A_{i}^{0}) \underbrace{(\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_{\mu+1}) \times \hat{\boldsymbol{e}}_{z}}_{\text{towards cell interior}} + \Gamma_{i} (P_{i} - P_{i}^{0}) \left[\underbrace{\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_{\mu}}_{|\boldsymbol{r}_{\mu-1} - \boldsymbol{r}_{\mu}|} + \underbrace{\boldsymbol{r}_{\mu+1} - \boldsymbol{r}_{\mu}}_{|\boldsymbol{r}_{\mu+1} - \boldsymbol{r}_{\mu}|} \right] \right],$$

$$\text{towards cell interior}$$

where underbraced vectors are represented in Fig. 1. It is noteworthy that, with potential (1), the force acting on each cell centre is zero

$$\mathbf{F}_{\text{VM},i} = -\nabla_i E_{\text{VM}} = -\frac{1}{2} K_i (A_i - A_i^0) \sum_{\mu \in \Omega_i} (\mathbf{r}_{\mu-1} - \mathbf{r}_{\mu}) \times \hat{\mathbf{e}}_z = 0.$$
 (8)

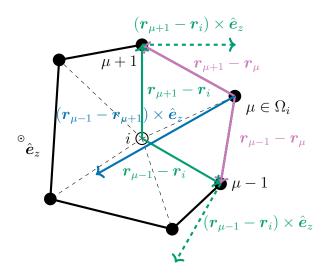


FIG. 1. Vertex representation of a single cell. By convention, cell centres are denoted by latin indices, and cell corners are denotes by greek indices. We denote Ω_i the ensemble of cell corners μ of the cell whose centre is i. By convention, $\mu+1$ (respectively $\mu-1$) denotes the next cell corner of i after μ in anticlockwise (respectively clockwise) order.

II. PRESSURE FORCE

We define a stress tensor σ such that, in 2D, the force per unit length exerted on a line orthogonal to \hat{n} is

$$f_{\hat{\boldsymbol{n}},\beta} = \sum_{\alpha} \sigma_{\alpha\beta} \hat{n}_{\alpha}. \tag{9}$$

We consider the case where

$$\sigma_{\alpha\beta} = p \, \delta_{\alpha\beta},\tag{10}$$

such that p defines the two-dimensional pressure, whose dimension is a force per unit length.

Given a closed loop of vertices μ (e.g. a cell as in Fig. 1), the edge $\mu(\mu+1)$ feels a pressure force

$$\mathbf{F}_{\mu(\mu+1)} = p \, \boldsymbol{\ell}_{\mu \to \mu+1} \times \hat{\mathbf{e}}_z,\tag{11}$$

where we have ordered vertex indices in anticlockwise order. Consequently, the sum of the forces cancels and the sum of their norms depends only on the pressure and the perimeter of the enclosed region

$$\sum_{\mu} \mathbf{F}_{\mu(\mu+1)} = p \left(\sum_{\mu} \ell_{\mu \to \mu+1} \right) \times \hat{\mathbf{e}}_z = 0, \tag{12a}$$

$$F = \sum_{\mu} |\mathbf{F}_{\mu(\mu+1)}| = p \sum_{\mu} |\mathbf{l}_{\mu \to \mu+1}| = p P.$$
 (12b)

We define pressure forces on *vertices* such that each is proportional to the sum of the pressure forces applied on the edges on each side

$$\mathbf{F}_{\mu} = C \, p \, \left(\boldsymbol{\ell}_{\mu-1 \to \mu} + \boldsymbol{\ell}_{\mu \to \mu+1} \right) \times \hat{\mathbf{e}}_{z}, \tag{13}$$

and the sum of their norms is equal to the sum of the forces exerted on the edges, therefore

$$C = P/\sum_{\mu} |\ell_{\mu-1\to\mu} + \ell_{\mu\to\mu+1}|.$$
 (14)

We eliminate the perimeter with (12b) to finally write

$$\boldsymbol{F}_{\mu} = \frac{F}{\sum_{\mu} |\boldsymbol{\ell}_{\mu-1 \to \mu} + \boldsymbol{\ell}_{\mu \to \mu+1}|} \left(\boldsymbol{\ell}_{\mu-1 \to \mu} + \boldsymbol{\ell}_{\mu \to \mu+1}\right) \times \hat{\boldsymbol{e}}_{z}. \tag{15}$$

It is noteworthy that the average norm of this force decreases with the number of vertices N

$$\frac{1}{N}\sum_{\mu}|\boldsymbol{F}_{\mu}| = \frac{1}{N}F.\tag{16}$$

We propose alternatively a force with average norm F

$$\boldsymbol{F}_{\mu}^{\prime} = N \boldsymbol{F}_{\mu}. \tag{17}$$

^[1] Reza Farhadifar, Jens-Christian Röper, Benoit Aigouy, Suzanne Eaton, and Frank Jülicher, "The Influence of Cell Mechanics, Cell-Cell Interactions, and Proliferation on Epithelial Packing," Current Biology 17, 2095–2104 (2007).

^[2] Alexander G. Fletcher, Miriam Osterfield, Ruth E. Baker, and Stanislav Y. Shvartsman, "Vertex Models of Epithelial Morphogenesis," Biophysical Journal 106, 2291–2304 (2014).

^[3] Dapeng Bi, Xingbo Yang, M. Cristina Marchetti, and M. Lisa Manning, "Motility-Driven Glass and Jamming Transitions in Biological Tissues," Physical Review X 6, 021011 (2016).

^[4] Rastko Sknepnek, Ilyas Djafer-Cherif, Manli Chuai, Cornelis Weijer, and Silke Henkes, "Generating active T1 transitions through mechanochemical feedback," eLife 12, e79862 (2023).