Computational Approach to Optimal Transport Network Construction in Biomechanics

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Abstract. Long-distance liquid transport in biosystems is provided by special branching systems of tubes (arteries, veins, plant vessels). Geometry of the systems possesses similar patterns and can be investigated by computer methods of pattern recognition. Here some results on plant leaf venation investigation are presented. The lengths, diameters and branching angles are estimated for the leaves of different shape, size and venation type. The statistical distributions of the measured parameters are similar to the corresponding ones which have been obtained for arterial beds. The both correspond to the model of optimal branching pipeline which provide liquid delivering at minimum total energy consumptions. The biomechanical model of liquid motion in a system consisting of a long thin tube with permeable walls which is embedded into a biological porous medium is considered. The pressure distributions and velocity fields for different geometry of the system are obtained. The main result is when the delivering liquid is completely absorbed by the alive cells in the porous medium the relation between the diameter and the length of the tube and the total volume of the medium which correspond to the measured data is reached.

1 Introduction

Transport of liquids and dissolved substances on the distances comparable to the characteristic size of the biological system is provided by special conducting structures. In animals and higher plants the conducting systems are represented by branching networks with 5-9 branching orders in plant leaves and 20-30 branching orders in mammalian arterial and venous systems. Design principles of network geometry can be investigated on special plastic casts of blood vessels (3D-geometry), X-ray pictures of vessels filled with special substances (arteriography), cleared leaf preparations (leaves that have been bleached and stained to make their venation patterns more visible) by using computer methods of image analysis. A few general statistical relations between the diameters D_i, lengths L_i and branching angles φ_i of separate vessels (fig.1a) have been revealed in intra-and extraorgan arterial [1-4] and respiratory systems [5-6] of mammals, in fluid transport systems of sponges [1], vein branching in plant leaves [7-9], branching in trees and shoots [10-11]. Structure of arterial beds corresponds to

the model of optimal branching pipeline. The appropriate biomechanical models of development of the optimal transport system in a growing biological system are based on theoretical problem of liquid motion through a branching system of tubes with special properties [2,3,12]. Corresponding models of liquid motion in the conducting systems of plants are not investigated yet.

2 Measurements and Principles of Construction of the Networks

Geometry of the conducting systems of plant leaves of different shape, size and venation type is investigated on high-resolution digital pictures of the fresh-cutted leaves (fig.1b). A few main stages have been provided:

- Contrast enhancement of an image and edges-finding (leaf blade perimeter, leaf veins) (fig.1c)
- Allocation of separate bifurcations, measurement of the diameters and branching angles (fig.1d)
- Skeletization of the vein system, measurement the lengths of veins (fig.1e)
- Allocation of influence domains of different veins (leaf areas S_i which are supplied by liquid through separate main veins) (fig.1f)

Using the procedure more then 327 images of dicotyledonous leaves have been investigated. In spite of the complicated topology of the conducting systems a few simple principles of their organization have been found out.

Principle 1. The diameters of the parent and daughter's vessels $d_{0,1,2}$ at each bifurcation obey the relation $d_0^\gamma = d_1^\gamma + d_2^\gamma$ which is called Murray's law. For mammalian vessels $\gamma \approx 3$ ($\gamma = 2.55 - 3.02$ for arterial, $\gamma = 2.76 - 3.02$ for venous, $\gamma = 2.61 - 2.91$ for respiratory systems) [1-6]. For the large blood vessels and bronchi $\gamma \sim 2.33$. For the small vessels when rheology of the fluid should be taken into account $\gamma \sim 2.92$. For the most part of investigated images of plant leaves $\gamma \approx 3$. The correspondent dependence is presented in fig.2a for one leaf (approximately 200-250 vein bifurcations). Validity of Murray's law for arterial systems can be explained by formation of an optimal vessel with $Q \sim d^3$ due to maintaining the shear stress τ_w at the vessel wall at a constant level $\tau_w \approx const$ [12]. In plant leaves the veins with $d \geq 0.08$ mm obeys Murray's law at $\gamma = 3$ (fig2a).

Principle 2. Branching angles $\varphi_{1,2}$ are defined by the diameters $d_{0,1,2}$ by the formula:
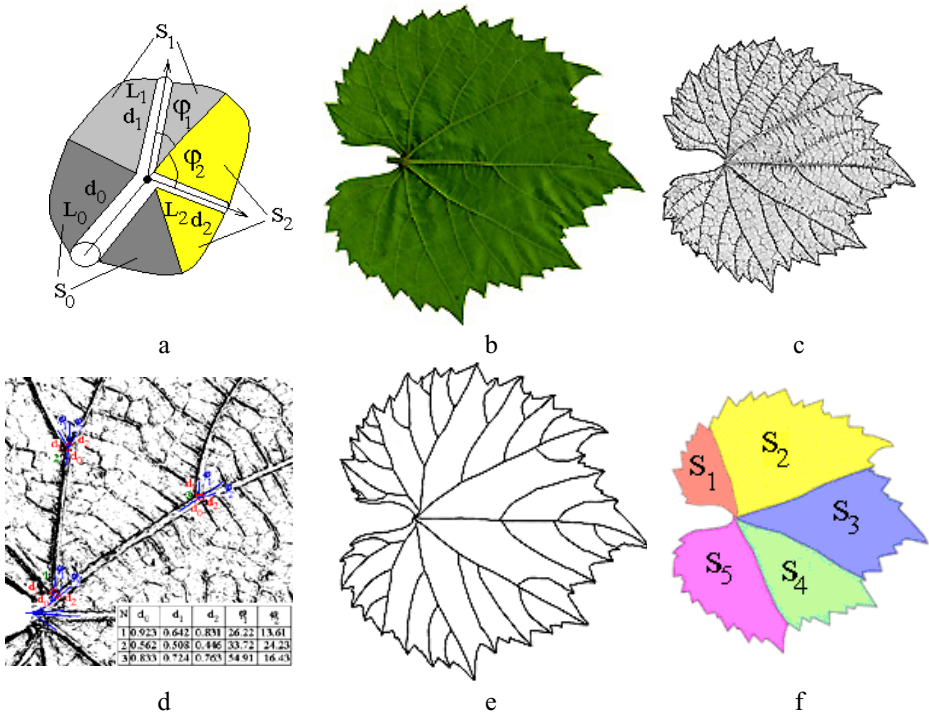
Fig. 1. Image analysis procedure: measured parameters of a bifurcation of the veins (a); digital picture of Vitis vinifera leaf (b); result of edge-finding procedure (c); measurement of the diameters $d_{0,1,2}$ and branching angles $\varphi_{1,2}$ in separate bifurcations 1-3 (d); result of the skeletization procedure, measurement the lengths of the veins (e); measurement of the areas S_{1-5} of influence domains of the first-order veins (f).

$$cos(\varphi_1) = \frac{(1+\xi^3)^{4/3}+1-\xi^4}{2(1+\xi^3)^{2/3}}, \quad cos(\varphi_j) = \frac{(1+\xi^3)^{4/3}+\xi^4-1}{2\xi^2(1+\xi^3)^{2/3}}$$

where $\xi = d_2/d_1 < 1$, $d_2 = min\{d_{1,2}\}$ is asymmetry of the bifurcation. The relation between the diameters and angels in a bifurcation is valid for mammalian arterial beds and is derived from an optimality principle [12]. Both principles 1 and 2 represent an optimal branching that minimizes the costs of delivery of the liquid, the construction and maintenance of the transport system. For plant veins optimality of the branching angles is peculiar to the bifurcations with $K \in [1.5;2]$ where $K = (d_1^2 + d_2^2)/d_0^2$ (fig.2b).
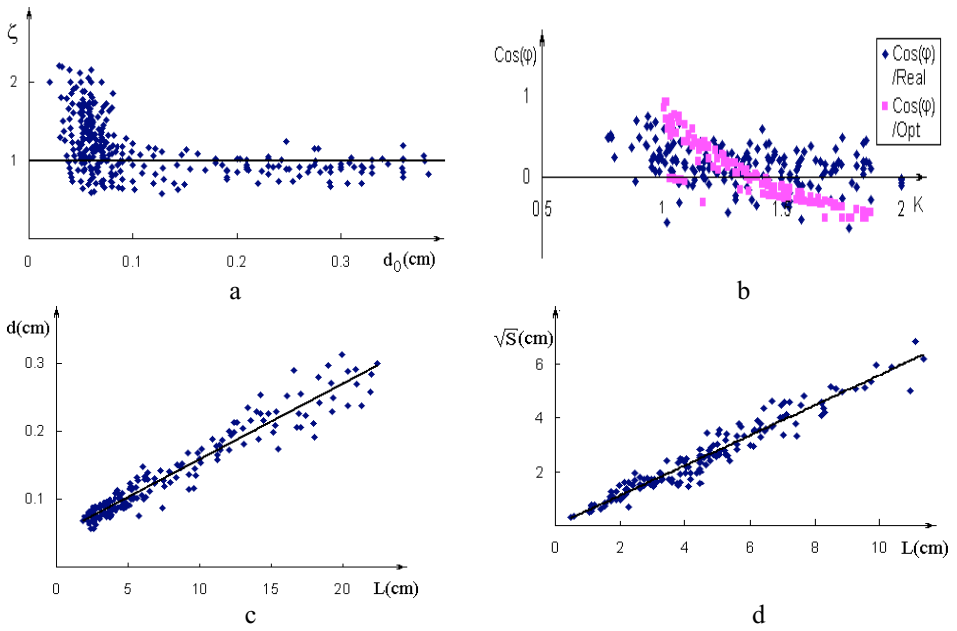
Fig. 2. Results of measurements by the image analysis procedure: a relation between the Murray's parameter $\zeta = (d_1^3 + d_2^3)\big/ d_0^3$ and the diameter d_0 of the parent vein for 200 bifurcations of a leaf (a); dependence of the optimal (theoretical) and real (measured) angles on the branching coefficient K (b); dependence $d(L)$ for one Vitis vinifera leaf (200 segments of veins) (c); dependence $\sqrt{S}(L)$ for vein segments ($n = 1-3$) and their domains of influence (d).

Principle 3. The relation $L = \alpha d^{\beta}$ has been revealed for mammalian arterial systems [13] where $\alpha \in [2.6;7.59]$, $\beta \in [0.84;1.16]$ (approximately $\beta \sim 1$). The principle can be regarded as an allometric rule as applied to different kinds of mammals with different mass of the body. The dependence between the lengths and diameters of the leaf veins with orders $n = 1-3$ is presented in fig.2c. The linear dependence $L = \alpha d$ with $\alpha \in [82;96]$ is valid to each leaf from our database.

Principle 4. The dependence $S = AL^2$ has been obtained for all leaves, $A \in [0.19;0.32]$ varies insignificantly for leaves with different sizes (1-35 cm). Shapes and sizes of the domains of influence are quite different that indicate the nonallometric character of the relation. The same relation $L \sim \sqrt{S}$ is well-known for river systems and their drainage areas in geophysics as Hack's law. The geometrical similarity of the vein (fig2d) and river systems is deep and revealed the common design principles of network construction in Nature [14].

3   A Biomechanical Model of Liquid Motion in a Plant Leaf

A 2-D steady motion of an incompressible viscous liquid in a porous medium is considered. Domain of influence is modeled as a curvilinear polygon that bounded by thin channels (leaf veins) and impermeable border (edge of the leaf blade) taking into account symmetry of the region about the x_1-axis (fig.3a). The governing equations have been taken to be the following [15-16]:

$$\rho\, div(\vec{v}) = -q \tag{1}$$

$$v_i = -\frac{\Lambda_{ik}}{\mu}\left(\frac{\partial p}{\partial x_k} - \sigma\frac{\partial \pi}{\partial x_k}\right) \tag{2}$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}(Cv_i) = D_c\frac{\partial^2 C}{\partial x_i^2} + q_c \tag{3}$$

where $\vec{v}$ is velocity vector in the porous medium and the generalized Darcy law (2) is introduced, Λ_{ik} is permeability tensor, p, π are hydraulic and osmotic pressures, ρ, μ are the fluid density and viscosity, C is concentration of an osmotically active dissolved mineral component. As fluid moves along the channels and through their permeable walls into the porous medium it is adsorbed by alive cells of the leaf and evaporate into the atmosphere. The total absorption is modeled as distributes sinks of water $q(x, y)$ and of the mineral component $q_c(x, y)$, D_c, σ are diffusion coefficient and the so-called reflection coefficient of the mineral component. It was assumed the permeability tensor is defined by the directions of the secondary veins $i = 2 - 3$ which are thought to be parallel and form two orthogonal sets of directions. The directions of the secondary veins in different domains of influence can slightly differ (fig.3b). Here a Vitis vinifera leaf (fig.1b) is modeled by a cardioid (fig.3a) or by a circle with a notch at the base of the lamina (fig.3b).

The fluid moves from the inlet $x_{1,2} = 0$ of the transport system through the tubes 1-2, then through their permeable walls into the porous media I-II. The driving forces are gradients of hydrostatic and osmotic pressures. The osmotic pressure is defined by concentration of the solute which can be maintained by the alive cells at a constant level providing the propelling force for the flux. The van't Hoff equation for osmotic pressure can be written as
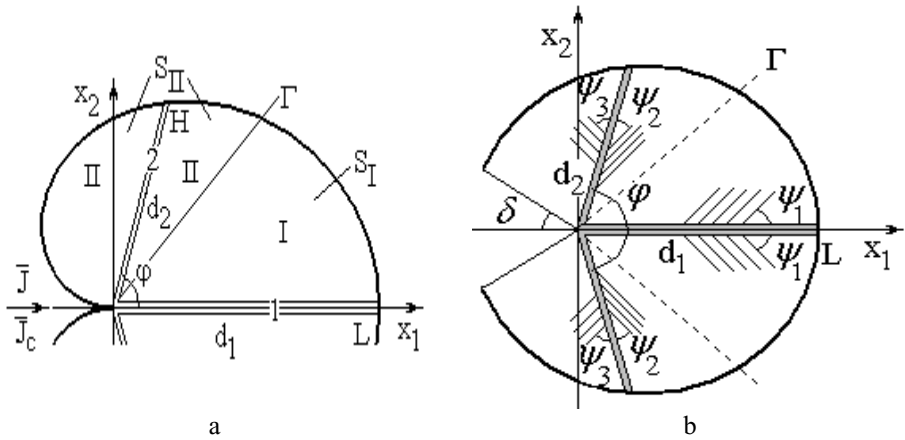
$$\pi = RTC / M_c \tag{4}$$

Fig. 3. Model of the leaf with 2 veins (1-2) and their domains of influence (I-II) (a); a round leaf with a notch at the base and venation pattern of the secondary veins (b).

where T is temperature that is taken to be constant, R is gas constant, M_c is the molar mass of the mineral component. Substituting (4) into (2) and into (1),(3) gives

$$\frac{\partial}{\partial x_i}\left(\frac{\Lambda_{ik}}{\mu}\left(\frac{\partial p}{\partial x_k} - \frac{RT\sigma}{M_c}\frac{\partial C}{\partial x_k}\right)\right) = \frac{q}{\rho} \tag{5}$$

$$\frac{\partial C}{\partial t} - \frac{\Lambda_{ik}}{\mu}\left(\frac{\partial p}{\partial x_k} - \frac{RT\sigma}{M_c}\frac{\partial C}{\partial x_k}\right)\frac{\partial C}{\partial x_i} - \frac{Cq}{\rho} = D_c\frac{\partial^2 C}{\partial x_i^2} + q_c \tag{6}$$

Numerical simulations have been used for solution of the system (5)-(6) and for illustration some key features of the water and the solute motion in regions with different geometry. Poiseulle flow in a rectangular channel is considered for the liquid motion in the veins. The pressure and flow continuity conditions at the walls of the channels and the constant water and solute fluxes $J = const$, $J_c = const$ at the inlet of the transport system $x_{1,2} = 0$ are given. The corresponding procedure of numerical calculations is described in [16]. Different distributions $q(x_1, x_2)$, $q_c(x_1, x_2)$ are introduced for simulations using the preliminary experimental data in form $q, q_c = \{const; q_0(1 - x_1/L)(1 - x_2/H); q_0\,exp(-a_1 x_1 - a_2 x_2)\}$.

The goal of the simulations was calculation an optimal branching angle φ and the asymmetry of the bifurcation $\zeta = d_2/d_1$ at given $H, L, d_1/L, q, q_c, J, J_c$ which define the optimal transport system with the optimization criterion [12]:

$$\Phi = \int_{S_I} \tau_{ik}^I v_{ik}^I dS_I + \int_{S_{II}} \tau_{ik}^{II} v_{ik}^{II} dS_{II} + \int_{S_1} \tau_{ik}^1 v_{ik}^1 dS_1 + \int_{S_2} \tau_{ik}^2 v_{ik}^2 dS_2 \to min \qquad (7)$$

$$V = \pi(d_1^2 L + d_2^2 H) + S_I + S_{II} = const \qquad (8)$$

where $\tau_{ik} = 2\mu v_{ik}$, v_{ik} is rate of deformation tensor. Total value $S = S_I + S_{II}$ are given whereas the border between S_I and S_{II} are defined after the calculations on (5)-(6) as a border Γ with $J_\Gamma = \int_\Gamma v_n d\Gamma = 0$, where $\vec{n}$ is a normal vector to Γ. After calculation the pressure and concentration by (5)-(6) the velocity field was obtained by (2),(4). As an illustration the velocity field and the corresponding domains of influence are presented in fig.4 for $q, q_c = const$, $L = H$, $d_1 = d_2$, $d_1/L = 0.1$. The border Γ has been defined after the velocity (v_1, v_2) calculation. The iterative procedure is consisted of determining the direction $\vec{n}_\Gamma$ in each point starting with $x_{1,2} = 0$ so that $\vec{v}_I \parallel \vec{v}_{II} \parallel \vec{n}_\Gamma$. After that the areas $S_{I,II}$ were calculated.
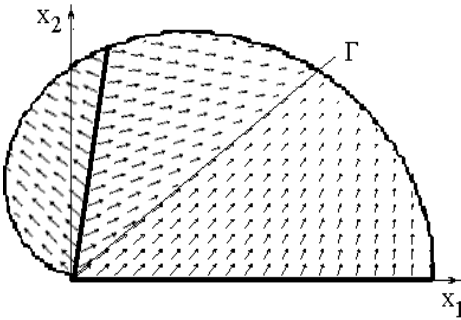

Fig. 4. Velocity field for a heart-shaped leaf with two first-order veins
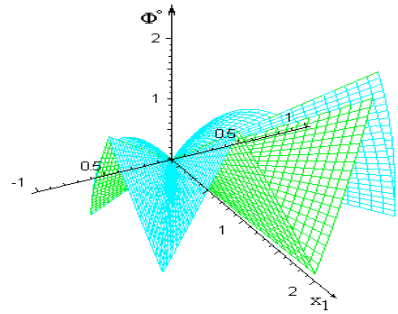
Fig. 5. Distribution $\Phi^\circ(x_1, x_2)$ for a round leaf, $L = 2$, $d_1 = d_2$, $d_1/L = 0.1$.

4   Results and Discussions

Total energy dissipation strongly depends on geometry of the leaf: its shape, number and diameters of the veins. Hydraulic conductance of the main veins is significantly higher then the conductance of the porous medium where the most part of the total energy is expended (fig.5). During the computer simulations a few simple shapes (round, elliptic, cardioid's) as well as shapes of some real leaves have been investi-

gated. All the angles of the secondary veins φ_j, ψ_j and of the notch of the blade δ, the radii r_j and lengths L_j of the veins have been obtained by measurements on the pictures of the leaves by image analysis procedure described in the previous chapter.

The optimal criterion (7)-(8) has been evaluated after the calculations on (5)-(6) and (2)-(4) by variation of separate geometrical parameters $\zeta, d_2/L, \varphi, \psi_{1-3}, \delta$ for a leaf with 3 main veins at a constant shape of the leaf blade (round with radius L, cardioid's $r = L(1 - \cos\theta)$, where (r,θ) are polar coordinates) or the parameters $\zeta_1 = d_2/d_1, \zeta_2 = d_3/d_1, d_2/L, d_3/L, \varphi_{1-2}, \psi_{1-5}, \delta$ for a leaf with 5 main veins. For real leaf blades the Lagrange function $\Theta = \Phi + \lambda V$, $\lambda = const$ has been evaluated after the calculations on (5)-(6) and (2)-(4) at small variations of the geometrical parameters of the corresponding models (figs 3a,b) at close range of the measured data. For the cases with simple geometry of the leaf blade and the veins the corresponding inverse problem (7)-(8) can be solved.

For a round leaf at a given number of the main veins the total volume of the system remains constant whereas the dimensionless function Φ° reaches its minima at certain branching angle between the main first-order veins (fig.6a). For wide variations of the branching angles ψ_{1-3} and the diameters of the veins $d_{1,2}$ at a constant L the energy dissipation decreases at increasing the conductivity of the veins. Nevertheless the optimal values of the branching angle φ vary insignificantly for all possible combinations of other geometrical parameters and close to $\varphi_{opt} = 35.1 - 35.5^\circ$ (fig.6a). The corresponding results for a symmetrical cardioid's leaf with 3 main first-order veins (fig.3a) are presented in fig.6b. Here increasing of the diameters of the veins leads to decreasing of the total energy dissipation at a constant total volume of the system. The dependence $\Phi^\circ(\varphi)$ reaches its minimum at $\varphi = 68.5 - 75.8^\circ$ for different pairs of the dimensionless geometrical parameters d_2/d_1, d_2/L of the model.

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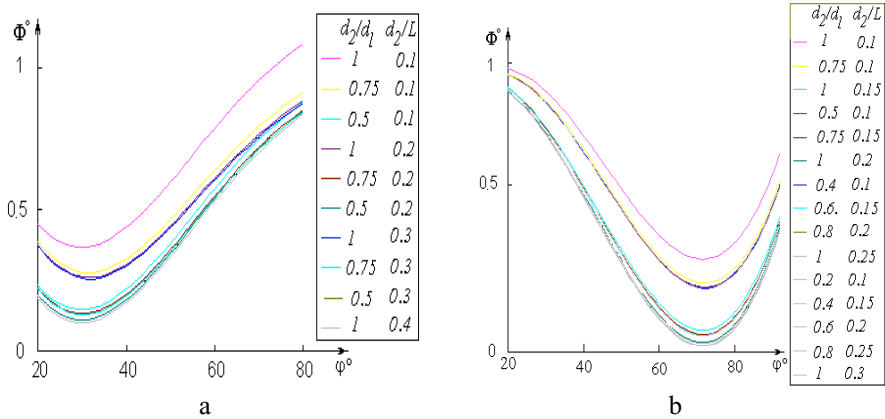
Fig. 6. Dependence $\Phi^\circ(\varphi)$ at different pairs of the parameters d_2/d_1, d_2/L for the round leaf (a) and for the cardioid's leaf (b).

The main results of the computer simulations can be summarized as a number of regularities:

- For any given shape of the leaf blade the optimal branching angle of the first-order veins exists and depend on the number and diameters of the veins. Some increase/decrease in the branching angle comparable to the optimal value leads to significant increase in the energy loss due to the viscous dissipation in the I/II domain of influence. The corresponding mechanism of the optimal branching angle formation during the leaf growth and development can be defined by the balance of the liquid delivery by the vein and its absorption by the alive cells of the corresponding domain of influence. When the branching angle increases/decreases due to some growth fluctuations the area of I/II domain of influence will increase/decrease and the cells in I/II region receive relatively less/more amount of water and dissolves mineral and organic substances. It will lead to the corresponding decrease/increase of the growth rate in I/II and to decrease/increase the area I/II and the branching angle. The feedback system can underlay the mechanism of the optimal branching angle formation during the normal growth.

- Optimal branching pattern ψ_{1-3} of the secondary veins $i = 2$ is defined by increasing all the angles up to $\psi_{1-3} \sim 90^\circ$. The result corresponds to experimental observations and the statement of evolutional biology concerning the increase the branching angle for the secondary veins during the evolutional transition from palmate to the pinnate (with $\psi \rightarrow 90^\circ$) leaf venation pattern.

- When pressure at the ends of the main veins equals to the pressure in the surrounding porous medium so that the total volumetric rate of the liquid motion through the vein equals to its total absorption by the alive cells in the corresponding domain the relation $L_j \sim \sqrt{S_j}$ is found out for the main veins and their domains of

influence of all the investigated shapes of leaves. The relation can be regarded as a relation between form and function of a leaf.

The results of the dynamic computer simulations correspond to the results of measurements on the leaves of different types and to the experimental biological observations. The balance relations of the liquid motion, redistribution and adsorption can play an important role in formation the optimal transport systems in plant leaf venation.

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