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Modeling the diffusion of CO_2 inside leaves

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Abstract

Propagation of fluids or gasses in closed compartments, like CO_2 in green plants, is described by diffusion equation. This partial differential equation is usually solved iteratively and, especially in higher dimensions, tends to be computationally intensive.

In this work, we propose to cast the n-dimensional problem to 1D diffusion. First, we apply a constrained distance transform to compute, for every voxel, its distance to the closest stoma. Second, we cast the iterative computation of CO_2 concentration to the evaluation of closed-form, polynomial functions. This in turn allows us to restrict the computation of CO_2 concentration to places of interest, e.g., to the close vicinity of the epidermis or cell walls where photosynthesis takes place.

1. Introduction

To study gas exchanges, the diffusion equation is widely used [2, 7, 8]. The diffusion equation we choose is the heat equation, described in 1D by the following formula:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (1)$$

where $u(x,t)$ is the concentration at position x in time t and α is the diffusion coefficient.

1.1. Iterative Solution in 1D

The majority of solutions use an iterative method using a finite difference scheme [4,5]. This method in 1D is defined as follows:

$$u(x,t+1) = u(x,t) + \alpha \sum_{n \in \Gamma(x)} \left(u(n,t) - u(x,t)\right) / |\Gamma(x)| \quad (2)$$

where $\Gamma(x)$ is the set of neighbors of pixel x.

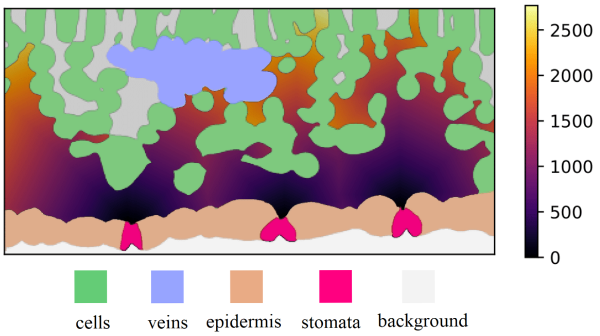

Figure 1. Constrained distance transform in air seeded at 3 stomata from 2D cross-section of a poplar leaf.

This formulation implicitly includes Neumann boundary condition [3] with a flow of 0. This condition assumes that the total gas volumes does not change by the diffusion, *e.g.* for all iterations t the total gas volume is constant Eq. (3).

$$\sum_x u(x,t) = \sum_x u(x,0) \quad (3)$$

1.2. Constrained Distance Transform

To see the distance between two areas of interest in an image, we can use the constrained distance transform [9]. It is initialized by setting all elements of the constrained region R [1] to ∞ and setting some seed points (stomata) to zero. Then the elements of the region repeatedly recompute their values with Eq. (4) until convergence. This algorithm can be performed with a logarithmic comlexity [1].

$$d(x) = \min\{d(x), \min_{n \in \Gamma(x)} d(n) + 1\} \quad (4)$$

where $\Gamma(x)$ is the set of neighbors of pixel x.

In Fig. 1, the distance transform assigned *every* air-pixel its distance from the closest stoma. Of uttermost interest,

[1] CO_2 diffuses in R

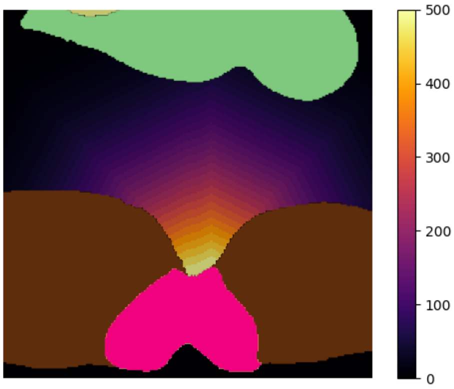

Figure 2. Eq. (5) used to describe the diffusion of CO_2 from the central stoma of Fig. 1.

however, are pixels next to cells (green), where photosynthesis takes place. In the following, we aim to show how to skip the calculation in areas that are of lesser interest.

2. Polynomial Basis Function

Consider one 1D sequence of 4-connected pixels without self-intersection. The out-of leaf half ($x \leq 0$) is initialized with high concentration of CO_2, H, and the inner-leaf ($x > 0$) with low concentration of CO_2, L, the situation before the stomata open. Iterating with Eq. (2) we can see that the diffusion can be described by a polynomial in the diffusion coefficient α of degree t with coefficients $c(t, k, x)$:

$$u(x,t) = H - (H - L) \sum_{k=0}^{t} c(t,k,x)\, \alpha^k \qquad (5)$$

Deriving the coefficients of the polynomial (Tab. 1 shows the coefficients for the first 5 time steps), we arrived at the following closed-form involving binomial coefficients for negative arguments[2] [6].

$$c(t,k,x) = (-1)^{1+k+x} \binom{t}{k} \binom{2k-1}{k+x-1} \qquad (6)$$

3. Results

To study the diffusion of CO_2 in the leaf from stomata to the leaf cells, we first compute the distance transform $d(x)$ of each pixel $x \in R$ in the airspace R. Afterward, we compute the coefficients $c(t, k, x)$ with $t = \max_{x \in R} d(x)$. Once we have the coefficients, we can compute the concentration $u(x, t)$ by Eq. (6). The result is identical to the iterative solution and is visualized in Fig. 2.

Another point of interest is to compute only the diffusion values for the pixels corresponding to the leaf cells border. Indeed, to know the concentration of the leaf cells, we don't need to compute the diffusion values for the other parts of the leaf.

[2]Explaining the colored entries in Tab. 1

4. Further Work

This method can be extended to higher dimensions. Computation using Eq. (5) can be further optimized. Approximately half of the coefficients are equal to zero. With the symmetry of coefficients, only the upper half of the coefficients (for $x > 0$) needs to be numerically (pre)computed. To sum the coefficients efficiently, we can use logarithmic coefficients $log(c(t, k, x)\alpha^k)$ and then make an exponentiation of the sum.

5. Conclusions

The paper presented a new approach to apply 1D diffusion on a pre-computed constrained distance transform. The method is based on polynomials and can be used to compute the concentration levels at specific times or for a specific pixel. One of the purposes is to study the CO_2 concentrations at locations that contribute to the photosynthesis. With this method, we can restrict the computations only to those parts of the leaf where the photosynthesis is likely to happen.

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Table 1. Coefficients $c(t, k, x)$ for the very first time steps ($t = 0 \dots 5$).

t	0	1		2			3				4					5					
x \ k	0	0	1	0	1	2	0	1	2	3	0	1	2	3	4	0	1	2	3	4	5
4	1	1	0	1	0	0	1	0	0	0	1	0	0	0	-1	1	0	0	0	-5	9
3	1	1	0	1	0	0	1	0	0	-1	1	0	0	-4	7	1	0	0	-10	35	-36
2	1	1	0	1	0	-1	1	0	-3	5	1	0	-6	20	-21	1	0	-10	50	-105	84
1	1	1	-1	1	-2	3	1	-3	9	-10	1	-4	18	-40	35	1	-5	30	-100	175	-126
0	0	0	1	0	2	-3	0	3	-9	10	0	4	-18	40	-35	0	5	-30	100	-175	126
-1	0	0	0	0	0	1	0	0	3	-5	0	0	6	-20	21	0	0	10	-50	105	-84
-2	0	0	0	0	0	0	0	0	0	1	0	0	0	4	-7	0	0	0	10	-35	36
-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	5	-9

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