Voronoi-based finite volume method for transport problems

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Summary
Transport problems, as, for instance, the transport of sediment in hydraulic engineering and the transport of harmful substances through porous media, play an important role in many fields of civil engineering. Other examples include the dissipation of heat or sound as well as the simulation of traffic with macroscopic models.

The contribution explains the analysis of the applicability of Voronoi-based finite volume methods for the approximation of solutions of transport problems. A special concern is the discretisation of the transport equation. Current limitations of the method as well as ideas for stabilisation are explained with examples.

1 Introduction
Finite volume methods base on the integration of a differential equation over a set of control volumes. In order to solve a problem numerically, representative vertices are chosen in each control volume. There are several problem-adopted specialisations of this general idea, for example the cell-vertex finite volume method, where a center of a volume is chosen. The distinction between the various methods lies in the positioning of the vertices.

Transport problems concern conservation quantities and their transport through a problem area. The conservation quantities like mass, momentum or energy are transported by moving media or molecular movement along concentration gradients. The mathematical expression for the Eularian form of the transport equation can be derived from the Eularian description of motion, where variations of quantities are considered with respect to a fixed control volume V. The computational domain for the unsteady transport problem is the union of all control volumes. The solution is a scalar conservation quantity, for example the density or the concentration.

$$\frac{d}{dt}\int_V c(\vec{x},t)dV + \int_V \nabla\cdot\vec{\Phi}^c dV + \int_V q_c dV = 0 \tag{1}$$

The variation of the considered quantity c per unit time is

$$\frac{d}{dt}\int_V c(\vec{x},t)dV\ . \tag{2}$$

Incoming flux, advective as well as diffusive flux, can be described as

$$\int_V \nabla\cdot\vec{\Phi}^c dV \ \text{ with } \Phi^c = \vec{u}c - k\nabla c\ . \tag{3}$$

$\vec{u} := u(\vec{x},t)$ is a given velocity field. k is a coefficient of molecular diffusivity. The increase of c due to sources is

$$\int_V q_c dV\ . \tag{4}$$

This all together leads to an integral form of the transport equation:

$$\frac{d}{dt}\int_V c(\vec{x},t)dV + \int_V \nabla(\vec{u}c)dV - \int_V \nabla(k\nabla c)d\Omega + \int_V q_c dV = 0\,. \tag{5}$$

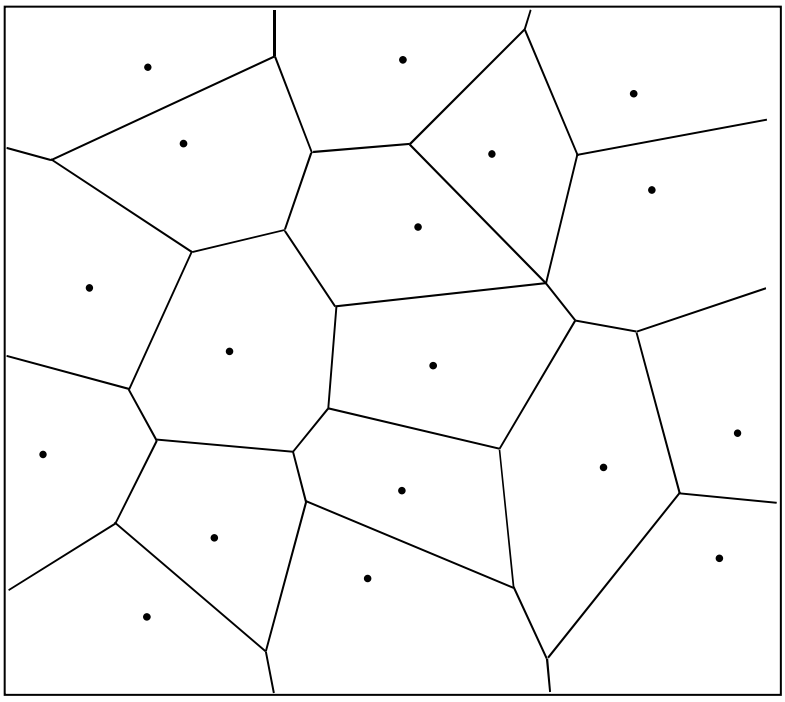
As the conservation laws have to be fulfilled for the whole domain as well as for each subdomain, the finite volume method applies exactly this affiliated integral form to control volumes. The next step is to decompose the domain in control volumes.

2 Finite volume decomposition with Voronoi cells

For a given finite set of nodes $P \subset \mathbb{R}^n$, the plane is partitioned into Voronoi cells of the form

$$V_{p\in P} = \left\{ x \in \mathbb{R}^n : \|x-p\| \le \|x-y\|, y \in P\backslash\{p\} \right\} \subset \mathbb{R}^n\,. \tag{6}$$

A Voronoi cell can either be bounded or unbounded. All unbounded cells of a decomposition build a border-section to the boundary of the domain. For our two dimensional examples all unbounded cells are bounded by intersecting the regions with a boundary line, which limits a rectangular domain. Those cells are no Voronoi cells anymore.



Voronoi diagram of the node set *P*

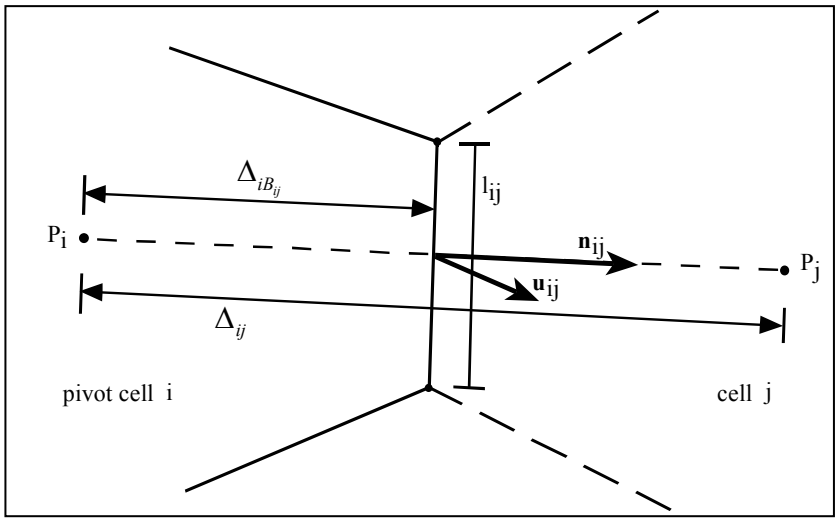
Each bounded Voronoi cell V_p is a convex polytope containing all points of the plane that are nearer to its so called center p than to any other point in P. The figure above shows an example.

3 Descretisation of the transport equation

Let the equation be transformed with the Gauss divergence theorem in order to introduce the fluxes through the cell boundaries:

$$\frac{d}{dt}\int_V c(\vec{x},t)dV = -\int_S c\vec{u}\vec{n}\ dS + \int_S (k(\nabla c)\vec{n})\ dS - \int_V q_c dV\ . \tag{7}$$

To approximate the solution, the transport equation (7) is discretised. To derive the discretised form of the transport equation, the flux terms at a border of two neighboured cells are considered.



Metrics between two neighboured Voronoi cells

The advection term can be approximated by

$$\int_S c\vec{u}\vec{n}\ dS \approx \sum_j \left[\left(c_i + \frac{c_j - c_i}{\Delta_{ij}} \Delta_{iB_{ij}} \right) \vec{u}_{ij}\vec{n}_{ij}l_{ij} \right], \tag{8}$$

with i and j as the indices of two adjacent cells. c_i and c_j denote the values of the conservative quantity at the respective centers. $\vec{u}_{ij}$ denotes the velocity vector in the midpoint of the bisector of the cells induced by c_i and c_j, $\vec{n}_{ij}$ means the normal vector on the bisector. Note that the positive direction of $\vec{n}_{ij}$ is always chosen in the direction from inside to outside of the cell i.

Because c and the advective flux $c_{ij}\vec{u}_{ij}\vec{n}_{ij}$ are scalar quantities it is possible to linearly interpolate them on the connecting line between the two centers P_i and P_j at the midpoint of the bisector. In the most decompositions the connecting line between any two centers will probably not intersect the bisector in the midpoint. In some cases it might even not intersect with the bisector, because another cell interferes. The influence of these special constellations has to be the issue of further examinations.

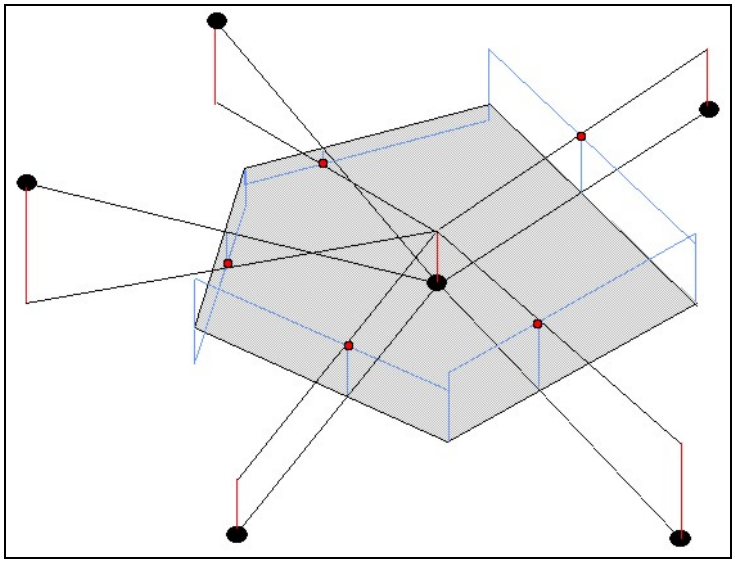
To compute the diffusive flux, the concentration gradient is supposed to be the increase of c between the two centers P_i and P_j:

$$\int_S k(\nabla c)\vec{n}\, dS \approx k\sum_j \left[\frac{c_j - c_i}{\Delta_{ij}} l_{ij}\right]. \tag{9}$$

Assuming that the conservative quantity is evenly distributed in the control volume, the integration over the control volume is often approximated by the product of the integrant with the size of the volume. Hence, the source term is discretised by

$$\int_V q^c dV \approx q_{c,i} V_i, \tag{10}$$

where V_i means the volume of the cell i. It must be noted that the assumption of an evenly distributed quantity is inconsistent to the linear interpolation between cell centers. The following figure shows the linear gradients between a cell and its neighbours as well as the value on the edges taken for the integration. There are discontinuities at the edges of the cell. This might lead to numerical difficulties.



Constant run of c on each edge

Finally in the discretisation, the time derivative can be approximated by

$$\frac{d}{dt}\int_V c\, dV \approx \frac{c_i^{n+1} - c_i^n}{\Delta t} V_i. \tag{11}$$

The discrete form of the complete transport equation is

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} V = -\sum_{j=0}^{n}\left[\left(c_i + \frac{c_j - c_i}{\Delta_{ij}} \Delta_{iB_{ij}}\right)\vec{u}_{ij}\vec{n}_{ij} l_{ij}\right] + k\sum_j \left[\frac{c_j - c_i}{\Delta_{ij}} l_{ij}\right] - q_{c,i} V_i. \tag{12}$$

For explicit computing schemes the quantity c is evaluated at time level n, for implicit schemes at time level $n+1$. Analog to Crank-Nicolson, known for the finite difference method, a mixture of time levels is possible. To get a linear equation system the transport equation is sorted by the different time levels of c:

$$c_i^{n+1}\left[\frac{A_i}{\Delta t}-\theta_1\sum_j(1-\frac{\Delta_{iB_{ij}}}{\Delta_{ij}})\alpha_{ij}^{n+1}+\theta_2\sum_j\beta_{ij}\right]-\sum_j\left[c_j^{n+1}\left(\theta_1\frac{\Delta_{iB_{ij}}}{\Delta_{ij}}\right)\alpha_{ij}^{n+1}+\theta_2\beta_{ij}\right]=$$
$$c_i^{n}\left[\frac{A_i}{\Delta t}+(1-\theta_1)\sum_j(1-\frac{\Delta_{iB_{ij}}}{\Delta_{ij}})\alpha_{ij}^{n}-(1-\theta_2)\sum_j\beta_{ij}\right]+\sum_j\left[c_j^{n}\left((1-\theta_1)\frac{\Delta_{iB_{ij}}}{\Delta_{ij}}\right)\alpha_{ij}^{n}+(1-\theta_2)\beta_{ij}\right] \tag{13}$$

with $\alpha_{ij}^n=\vec{u}_{ij}^n\vec{n}_{ij}l_{ij}$, $\beta_{ij}^n=l_{ij}/\Delta_{ij}$. θ_1 and θ_2 declare the time level for advection and diffusion ($0\le\theta\le1$, where 0 is fully explicit and 1 is fully implicit). The source term was omitted for simplification. The implicit schemes lead to an equation system with a symmetrical sparse matrix. Actual research work is dealing with sparse matrix algorithms, e.g. (Pick 2004).

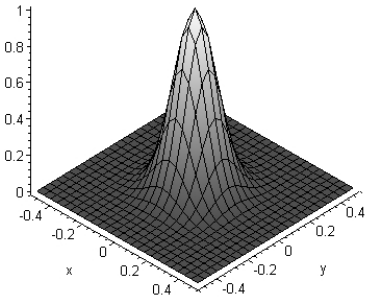
4 Numerical tests

The propagation of a concentration in a closed system is considered. We distinguish between purely diffusive transport and advection-dominated transport. We use two different initial conditions for the two cases.

At first, points for the node set P are determined. The rectangular area, $-10.0\le x,y\le10.0$, is subdivided in 20 x 20 rectangular subareas. One x- and one y-coordinate are randomly chosen in each subarea, yielding 400 points inside the whole domain.

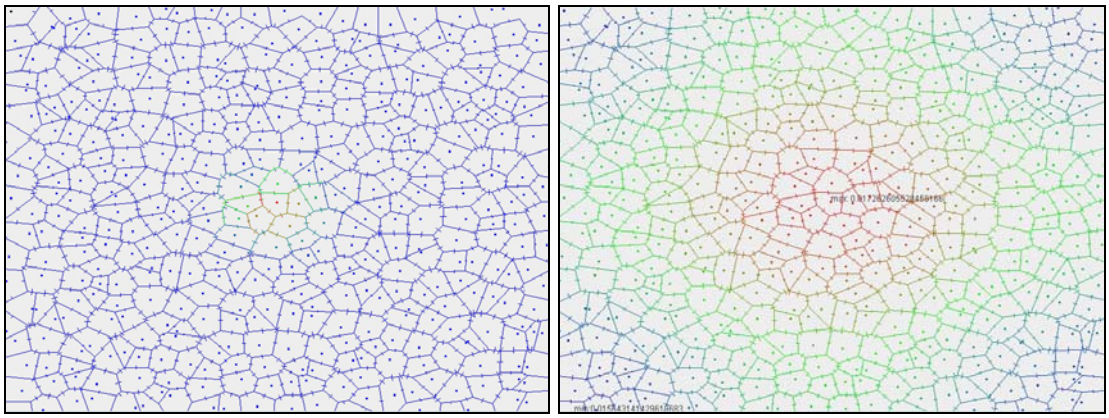
4.1 Diffusive transport

In the first test case the velocity field is set to zero at each node. So, only diffusive terms can contribute to the change of the concentration. The following function is evaluated at each node as initial condition.



$$f(x,y)=e^{-50x^2}e^{-50y^2} \tag{14}$$

For the semi-implicit Crank-Nicolson scheme and for a diffusivity coefficient of 1.0 this test case delivers the expected distribution of the concentration. The figure below shows the state after 11 seconds, where the initial peak in the center has decreased from 1.0 to about 0.017. All nodes of the domain converge to the same value.



As an indicator for mass conservation, the mass in the domain is calculated by accumulating the mass in each cell. This is approximated by the product of the center value and the cell volume. For the diffusion test case the mass is nearly constant over the time.

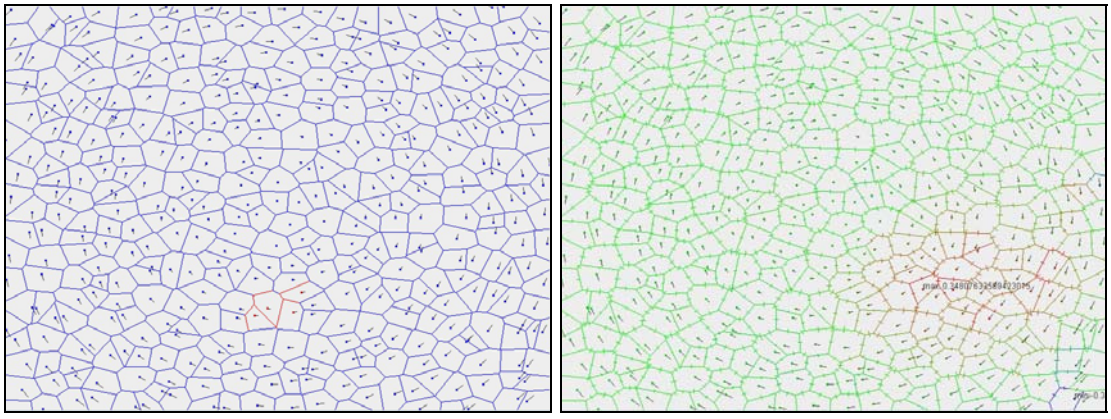
4.2 Advection-dominated transport

In the second test case the components of the velocity vector at a point (x,y) are given as:

$$u_{x[y]} = \frac{\overline{u}}{\overline{r}}\left(\sqrt{x^2+y^2}\right)\cos\left(\frac{[-]\pi}{2} - \arcsin\left(\frac{y[x]}{\sqrt{x^2+y^2}}\right)\right), \tag{15}$$

where $\overline{u}$ is the maximum velocity and $\overline{r}$ the distance from the center to a corner of the domain. The initial boundaries introduce a spot of concentration:

$$c(x,y) = \begin{cases} 1 & \text{if } -1 \le x \le 1,\ 4 \le y \le 6 \\ 0 & \text{otherwise} \end{cases} \tag{16}$$



The length of the time step is controlled with the Courant number criteria

$$u\frac{dt}{dx} \le 1, \tag{17}$$

where dx is the smallest distance between two neighboured cell centers. The coefficient for diffusivity, k, is set to 0.10.The Peclet criteria is fulfilled as well.

However, the concentration peak (marked with red) is transported along the velocity field for a few time steps only before the system becomes instable. The mass in the domain seems to oscillate around the initial value with a low frequency.

5 Ideas for stabilisation

Several ways of stabilisation are known for traditional methods like the finite difference method or the finite element method. The implementation of artificial diffusion in the transport equation is the historically oldest possibility to improve the stability. In our case the artificial diffusion is set to the projection of the velocity vector on the normal of the bisector, scaled with cell dimension.

$$k = \left|\vec{u}_{ij}\vec{n}_{ij}\right| \cdot \frac{\Delta_{ij}}{2} \tag{18}$$

Although this term yields a high damping of the concentration peaks, it stabilises the procedure, as we observed the expected movement of the concentration peak in the circulating mass.

According to the stabilised finite element method, mentioned in (Milbradt 2002), another promising approach is the correction of the rate of change with a residual. The residual results from one dimensional considerations on the connecting line between the cell centers of two neighboured cells.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial s} - k\frac{\partial^2 c}{\partial s^2} + q_c = \varepsilon \tag{19}$$

In (19) the rate of change of c as well as the values c_i and c_j are known from the above-mentioned solution procedure. The spatial differential term is discretised by

$$u_{ij}\frac{c_j - c_i}{\Delta x} \tag{20}$$

and the second order derivation vanishes due to the disability of the linear interpolation. The velocity u_{ij} is determined at the midpoint of the connecting line, respectively at the intersection point with the bisector in the two dimensional case. From evaluating (19) follows a residual ε at each center. Now, the timestep is recalculated. But this time the interpolation of c on the bisector is corrected by the arithmetic mean of the epsilons at the respective centers.

Drawing a parallel to the finite difference method, a third way of stabilisation can be found. As the refinement of the spatial discretisation might not be enough to stabilise the method, using upstream variants is a common way to achieve stability. Upstream methods give up-stream nodes a higher weight and increase the influence of those nodes on the calculation of the new time level. Considering the Voronoi cells as control volumes, like we did, this shifting of weight might be achieved by a displacement of control volumes in the direction of the flow. This can be only be done consistently, preserving the properties of Voronoi cells, if a distance function can be found, which represents this shift.

6 Conclusions

The Voronoi-based finite volume method might be understood as generalisation of the finite diffence method for unstructured domains. One advantage should be the simple possibility to refine the cells at interesting locations. Unfortunately the resolution of the spatial discretisation seems not to be the main problem, so we could not benefit from this property yet. The method works for diffusive transport but lacks of stability when advection is added. The presented ideas for stabilisation are promising and are worth doing more research on the Voronoi-based finite volume method.

7 References

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