Finite Volume Methods for Reaction–Diffusion Problems

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ABSTRACT *We derive and study cell-centered finite volume approximations of reaction-diffusion equations. For Voronoi and circumscribed volumes we obtain monotone schemes. If the volumes satisfy regularity condition then the schemes are H^1-positive definite and first order accurate. For finite volumes satisfying an additional symmetry condition the schemes are second order accurate.*

Key Words: Voronoi volumes, reaction-diffusion, stability, error estimates.

1. Introduction

We consider the model convection-reaction-diffusion equation

$$\nabla \cdot (-A\nabla u + \mathbf{b}u) + cu = f \qquad \text{in } \Omega\,, \qquad u = 0 \qquad \text{on } \partial\Omega\,, \tag{1}$$

where Ω is a bounded domain in $\mathbf{R}^d, d = 2, 3$, $A(x) = \{a_{ij}\}_{i,j=1}^d$, $c(x)$, $f(x)$, and $\mathbf{b} = (b_1(x), ..., b_d(x))$ are given sufficiently smooth functions in Ω that satisfy the following conditions: $\xi^T A(\mathrm{x})\xi \geq \alpha_0 \xi^T \xi$, $\alpha_0 > 0$, $\xi \in \mathbf{R}^d$, $\frac{1}{2}\nabla \cdot \mathbf{b}(\mathrm{x}) + c(x) \geq 0$. These assumptions guarantee that the model problem (1) has a unique solution in $H_0^1(\Omega)$. In groundwater applications A is the diffusion-dispersion tensor, u is the concentration of the contaminant, $\mathbf{b}$ is the Darcy's velocity, and c is the reaction rate, and f is the strength of the sources (sinks). For such applications inflow and outflow boundary conditions may be specified on parts of the boundary and transient regimes of flow and transport leading to parabolic problems can be considered. The technique developed in this paper is applicable for such problems as well. The solution of this model problem has various interesting properties which correspond to the properties of the physical model:

conservation of mass in each volume, monotonic solution (of the homogeneous equations), stable solution in maximum and energy norms, etc. For such applications desirable properties of the numerical method include: 1) stability in maximum and energy norms; 2) the approximation method conserves the "mass" element by element; 3) the discrete solution satisfy the maximum principle; 4) the corresponding matrix is positive definite; 5) the method works for general domains and fairly general grids.

Finite volume approximation strategy is based on the discretization over a partition of Ω into cell-centered or vertex-centered finite volume. Vertex-centered finite volume approximations have been derived in the pioneering work of Tikhonov and Samarskii [11]. It has been proven that for 1-D problems with discontinuous coefficients the discrete conservation property is a necessary condition for the convergence of the finite difference schemes. A consistent theory of vertex-centered schemes on rectangular and triangular grids has been developed in [9] and [5], respectively. Interesting results for quadrilateral finite volumes have been reported in [8]. Approximation of the balance equation over the finite volume partition with polynomial extension of grid functions over the finite elements led to finite-volume element method (see, e.g. [1, 3, 10]) and box schemes (see, e.g. [2]).

We focus our study on cell-centered uniform triangular and rectangular grids, Voronoi meshes, and Delaunay meshes. Such schemes are natural for polygonal partition of the domain. In general, a polynomial interpolation on the polygons is not available and an approach which is closer to finite difference technique has to be used. The constructed schemes are locally mass conservative and satisfy the discrete maximum principle. Two geometric conditions are formulated, and under these conditions coercivity and error estimates in the discrete H^1–norm are derived. For general grids, the constructed schemes have first order of accuracy. In special cases of grids with certain symmetry property the schemes are second order accurate.

2. Discretization schemes

We suppose that the domain Ω is covered by finite number of convex polygons (polyhedra in 3–D). We call these polygons *finite volumes*. In the interior of each finite volume one point, called *cell–center*, is chosen. The cell–centers (and the finite volumes) are numbered in a unique way, i.e., $\{\mathrm{x}_i : i = 1, \ldots, n\}$, and correspondingly $\{V_i : i = 1, \ldots, n\}$. We denote by $\overline{\omega}$ the cell–centered mesh, $\overline{\omega} = \{\mathrm{x}_i\}_{i=1}^n$, by ω the interior grid points, i.e., $\omega = \overline{\omega} \cap \Omega$, and by $\gamma = \overline{\omega} \cap \partial\Omega$. We also need the index set $\Sigma(i)$ of all neighbors of x_i in $\overline{\omega}$, i.e., $j \in \Sigma(i)$ if the finite volumes V_i and V_j have a common face γ_{ij}, $\gamma_{ij} = V_i \cap V_j$.

We require that finite volumes be chosen in a such way that there exists a circumscribed circle around each finite volume and the cell-center coincides with the center of the circumscribed circle, or cell–centered finite volumes are Voronoi regions. Voronoi regions have the property that each point in the

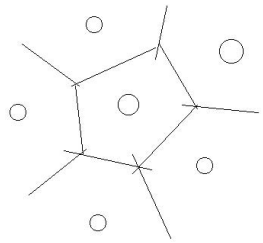

Figure 1: *Voronoi diagram*

interior of given finite volume is closer to the cell–center of that volume than to any other cell–center. We call the former one a *circumscribed cell–centered* grid and the latter one a *Voronoi cell–centered* grid. Simple examples of Voronoi and circumscribed cell–centered grids are shown on Fig. 1 and Fig. 2.

We denote by $m(S)$ the measure of the set S, and by $d(\mathrm{x},\mathrm{y})$ the Euclidean distance between the points x and y. Functions defined for $\mathrm{x} \in \omega$ are called grid functions. We use the subindex h to indicate the dependence of the grid and the value at a given point is referred by the index of the point, i.e., $u_h(\mathrm{x}_i) = u_{h,i}$. For given grid functions u_h and v_h we define the following discrete inner products and norms:

$$\begin{aligned}
(u_h, v_h) &= \sum_{x_i \in \omega} m(V_i) u_{h,i} v_{h,i}\,, \quad \|u_h\|^2_{0,\omega} = (u_h, u_h), \\
|u_h|^2_{1,\omega} &= \frac{1}{2} \sum_{x_i \in \overline{\omega}} \sum_{j \in \Sigma(i)} m(\gamma_{ij}) d(x_i, x_j) \left(\frac{u_{h,i} - u_{h,j}}{d(x_i, x_j)} \right)^2 , \\
\|u_h\|^2_{1,\omega} &= \|u_h\|^2_{0,\omega} + |u_h|^2_{1,\omega}\,,
\end{aligned}$$

For such triangulations we add an extra regularity condition.

Assumption 1 (regular triangulations) *There exist two positive constants C_1 and C_2 such that the following inequalities hold for $i = 1, \ldots, n$:*

$$\begin{aligned}
&C_1 m(\gamma_{ij}) d(x_i, x_j) \le m(V_i) \le C_2 m(\gamma_{ij}) d(x_i, x_j) \quad \forall\, j \in \Sigma(i)\,, \\
&C_1 h^d \le m(V_i) \le C_2 h^d\,,
\end{aligned}$$

where h is the characteristic size of the mesh.

Let u be a sufficiently smooth function in Ω and the grid function u_h be such that $u_{h,i} = u(\mathrm{x}_i)$. Assumption 1 guarantees that $\|u_h\|_{1,\omega} \to \|u\|_{1,\Omega}$ when $\max_i(m(V_i)) \to 0$.

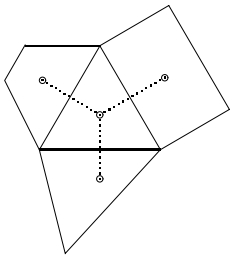

Figure 2: *Cell–centered control volume*

In general, the rate of convergence of of the approximation method depends on the geometric properties of the triangulation. For some special triangulations we will prove that higher rates of convergence can be achieved for properly designed finite volume methods. Such triangulations usually exhibit some special symmetries of the position of the point $x_{ij} = (x_i, x_j) \cap \gamma_{ij}$ with respect to the points x_i and x_j and to the face γ_{ij}. The exact conditions are formulated in the following assumption.

Assumption 2 (symmetry assumption) *The following conditions hold true:*
(i) x_{ij} is the middle point of the interval (x_i, x_j);
(ii) for triangular faces γ_{ij}, x_{ij} is the barycenter of γ_{ij}. Otherwise, we require that γ_{ij} has two perpendicular axes of symmetry and x_{ij} is their intersection point.

Now we derive the finite volume approximation of the equation (1). First, we introduce the diffusive and convective fluxes $\mathbf{W} = -A(\mathrm{x})\nabla u(\mathrm{x})$ and $\mathbf{V} = \mathbf{b}(\mathrm{x})u(\mathrm{x})$. Next, we split the boundary of each finite volume in the following way: $\partial V_i = \cup_{j\in\Sigma(i)}\gamma_{ij}$. Finally, integrating (1) over each finite volume V_i, $i = 1, \dots n$, using Green's formula, and dividing by $m(V_i)$ we get

$$\frac{1}{m(V_i)} \sum_{j\in\Sigma(i)} \int_{\gamma_{ij}} (\mathbf{W}.\mathbf{n} + \mathbf{V}.\mathbf{n})\, ds = \frac{1}{m(V_i)} \int_{V_i} (f(x) - cu)\, d\mathrm{x}\,, \qquad (2)$$

where $\mathbf{n}$ is the outer nomal unit vector to the boundary ∂V_i.

This equation, called balance equation, is the basis of our approximation. We split the approximation of the balance equation (2) in three parts

$$A_h u_h \equiv A_h^{(2)} u_h + A_h^{(1)} u_h + A_h^{(0)} u_h \equiv \sum_{j\in\Sigma(i)} w_{i,j} + \sum_{j\in\Sigma(i)} v_{i,j} + r_{h,i}, \quad x_i \in \omega, \ (3)$$

where $A_h^{(2)}$ is the approximation of the diffusive flux, $A_h^{(1)}$ comes from the approximation of the convection flux, and $A_h^{(0)}$ is an approximation of the reaction term.

In this presentation w_{ij}, v_{ij} and $z_{h,i}$ are some approximations of the corresponding integrals $\int_{\gamma_{ij}} \mathbf{W}.\mathbf{n}\, ds$, $\int_{\gamma_{ij}} \mathbf{V}.\mathbf{n}\, ds$, and $\int_{V_i} cu\, dx$. Now, in order to complete the approximation we have to express the discrete fluxes w_{ij} and v_{ij} and the reaction term through the approximate solution $u_h(x)$ at the grid points. In order to simplify our presentation we consider only the case $A(\mathrm{x}) = a(\mathrm{x})I$. For more details see [7].

We use the following approximations:

$$\begin{aligned} w_{ij}(\mathrm{x}) &= -\frac{m(\gamma_{ij})}{m(V_i)} k_{ij} \frac{[u_{h,j} - u_{h,i}]}{d(x_i, x_j)}\,, \\ v_{ij}(\mathrm{x}) &= \beta_{ij}^{+} u_{h,i} + \beta_{ij}^{-} u_{h,j}\,, \quad r_{h,i} = c_i u_{h,i}\,, \end{aligned} \tag{4}$$

where k_{ij}, β_{ij}^{+} and β_{ij}^{-} are properly chosen. Central difference, exponentially fitted and two upwind schemes on grids introduced above were derived and studied in [7]. Special case of rectangular uniform partitionings were discussed in [6]. Particularly simple is the case $\mathbf{b}(\mathrm{x}) \equiv 0$ which we shall discuss further in this paper. A possible choice for k_{ij} is:

$$k_{ij} = \left(\frac{1}{d(x_i, x_j)} \int_{x_i}^{x_j} \frac{ds}{a(s)} \right)^{-1}. \tag{5}$$

The discrete problem corresponding to (1) is defined as follows: find a grid function u_h such that

$$A_h u_h = \phi_h \qquad \text{in} \quad \omega\,, \qquad u = 0 \qquad \text{on} \quad \gamma\,, \tag{6}$$

where $\phi_{h,i} = \frac{1}{m(V_i)} \int_{V_i} f(\mathrm{x})\, d\mathrm{x}$.

Remark 1 *It is easy to check that*

(i) the difference scheme defined by (4), (5) satisfies the discrete maximum principle and the corresponding matrix A_h is an $\mathbf{M}$–matrix;

(ii) If the Assumption 1 is satisfied, then the matrix A_h is positive definite in the discrete H^1–norm, i.e.,

$$(A_h y, y) \geq C \|y\|_{1,\omega}^2 \ \text{, for all } y \in D^0 = \{y,\, y_{|\gamma} = 0\}.$$

3. Stability and error estimates

The stability of problem (6) is a simple consequence of the positive definiteness of the matrix A_h. Namely, we prove the following lemma.

Lemma 1 *Let the Assumptions 1 be satisfied. Then for the solution u_h of (6) the following estimate holds:*

$$\|u_h\|_{1,\omega} \leq C \sup_{v_h \neq 0} \frac{|(\phi_h, v_h)|}{\|v_h\|_{1,\omega}}\,,$$

with a constant C independent of h and u_h.

The error analysis presented here is done in the general framework of the methods developed in [9] and [4]. To demonstrate our idea we consider the case $a(x) \equiv 1$. Let

$$z(x) = u_h(x) - u(x)\,,\ x \in \omega$$

be the error of the finite difference method. Substituting $u_h = z + u$ in (6) we obtain

$$A_h z = \phi - A_h u \equiv \psi = \psi_2 + \psi_0\,. \tag{7}$$

Then using (2)–(6) we transform ψ in the following form

$$\sum_{j\in\Sigma(i)} \left[\frac{1}{m(V_i)}\int_{\gamma_{ij}} \mathbf{W}.\mathbf{n}\,ds - w_{i,j}\right] + \left[\frac{1}{m(V_i)}\int_{V_i} cu\,d\mathrm{x} - c_i u_{h,i}\right] \equiv \psi_i\,.$$

We define the local truncation error in the following way:

$$\begin{aligned} \eta_{i,j} &= \frac{1}{m(\gamma_{ij})}\int_{\gamma_{ij}} \mathbf{W}.\mathbf{n}\,ds - \frac{m(V_i)}{m(\gamma_{ij})} w_{i,j}\,, \\ \mu_{i,j} &= \frac{1}{m(V_i)}\left[\int_{\Delta_{ij}} cu\,d\mathrm{x} - m(\Delta_{ij})c_i u_{h,i}\right]\,. \end{aligned} \tag{8}$$

Here Δ_{ij} is the triangle (pyramid) with base γ_{ij} and node x_i. First we consider the term (ψ_2, z). By the definition of the discrete inner product and $\psi_{2,i}$ we have

$$(\psi_2, z) = \sum_{x_i\in\omega}\sum_{j\in\Sigma(i)} \left[\int_{\gamma_{ij}} \mathbf{W}.\mathbf{n}\,ds + m(\gamma_{ij})k_{ij}\frac{[u_j - u_i]}{d(x_i,x_j)}\right] z_i\,.$$

We can regroup the terms (we call this nonuniform summation by parts) to get

$$(\psi_2, z) = -\frac{1}{2}\sum_{x_i\in\omega}\sum_{j\in\Sigma(i)} d(x_i,x_j)m(\gamma_{ij})\eta_{i,j}\frac{[z_j - z_i]}{d(x_i,x_j)}\,.$$

By the regularity of the grid and Cauchy–Schwartz inequality follows

$$(\psi_2, z) \le \left(\sum_{x_i\in\omega}\sum_{j\in\Sigma(i)} m(V_i)\eta_{i,j}^2\right)^{1/2} \|z\|_{1,\omega} \equiv \|\eta\|_{*,\omega}\|z\|_{1,\omega}\,.$$

Here for convenience we denote with $\|\eta\|_{*,\omega}$ the first sum above.

Likewise

$$\begin{aligned} (\psi_0, z) &= \frac{1}{2}\sum_{x_i\in\omega} m(V_i)\sum_{j\in\Sigma(i)}[\mu_{i,j} + \mu_{j,i}]z_i + \frac{1}{2}\sum_{x_i\in\omega}\sum_{j\in\Sigma(i)} m(V_i)\mu_{i,j}[z_i - z_j] \\ &\le C\left[\left(\sum_{i,j} m(V_i)[\mu_{i,j} + \mu_{j,i}]^2\right)^{\frac{1}{2}} + \left(\sum_{i,J} m(V_i)[d_{i,j}\mu_{i,j}]^2\right)^{\frac{1}{2}}\right]\|z\|_{1,\omega} \\ &\equiv C(\|\mu'\|_{*,\omega} + \|\mu''\|_{*,\omega})\|z\|_{1,\omega}\,. \end{aligned}$$

Here we used abbreviations for the double sums and the distance $d(x_i, x_j)$. Summarizing these results and using the coercivity of the operator A_h we obtain the following main result.

Lemma 2 *Let the Assumption 1 be satisfied. The error* $z(x) = u_h(x) - u(x)$, $x \in \omega$ *of the considered finite difference scheme satisfies the a priori estimate*

$$\|z\|_{1,\omega} \le C \left(\|\eta\|_{*,\omega} + \|\mu'\|_{*,\omega} + \|\mu''\|_{*,\omega} \right) . \tag{9}$$

In order to use the estimate (9) we have to bound the corresponding norms of the local truncation error components. These estimates are provided in the lemma given below. Theorem 1 follows from Lemmas 1 and 2.

Lemma 3 *Let the solution of the problem (1) be* H^s*-regular,* $\frac{3}{2} < s$*. Then*

$$\begin{aligned} |\eta_{i,j}| &\le Ch^{s-d/2-1} |u|_{s,e_{ij}} , \ \frac{3}{2} < s \le 2 + sym , \\ |d_{ij}\mu_{i,j}| \, , \, |\mu_{i,j} + \mu_{j,i}| &\le Ch^{1+sym-d/2} |c|_{1,\infty,e} |u|_{1+sym,e} . \end{aligned}$$

where $sym = 1$ *if the Assumption 2 is satisfied, and zero otherwise.*

Theorem 1 *If the solution* $u(x)$ *of the problem (1) is* H^s*-regular, then*

$$\|u_h - u\|_{1,\omega} \le Ch^{s-1} \|u\|_{s,\Omega}$$

with

(i) $\frac{3}{2} < s \le 2$ *for meshes satisfying Assumption 1;*
(ii) $\frac{3}{2} < s \le 3$ *for meshes satisfying Assumptions 1 and 2.*

4. Remarks and conclusion The discussed schemes were tested on various model and applied problems. The predicted by the theory convergence rates have been fully confirmed by the computations. For such experiments we refer to [6, 7].

Although our theory does not cover singularly perturbed problems, i.e. problems in which $A(x)$ is small relatively to $c(x)$ and $\mathbf{b}(x)$, our computer experiments show that the predicted convergence rates are asymptotically correct for small step-size and give meaningful results for practical grids.

Important and interesting direction is application of the finite volume method to time-dependent linear and nonlinear problems. This is a subject of current research of one of the authors.

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