

Konrad-Zuse-Zentrum für Informationstechnik Berlin

R.Kornhuber G.Wittum

Discretization and Iterative Solution of Convection Diffusion Equations

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Discretization and Iterative Solution

of Convection Diffusion Equations

R.Kornhuber G.Wittum

Abstract. We propose an extended box method which turns out to be a variant of standard finite element methods in the case of pure diffusion and an extension of backward differencing to irregular grids if only convective transport is present. Together with the adaptive orientation proposed in a recent paper and a streamline ordering of the unknowns, this discretization leads to a highly efficient adaptive method for the approximation of internal layers in the case of large local Peclet numbers.

1. Introduction

We consider boundary value problems for the scalar, linear convection diffusion equation

$$\operatorname{div}(-\varepsilon \nabla u + \beta u) = f \tag{1.1}$$

on a bounded, polygonal domain $\Omega \subset \mathbb{R}^2$ with constant $\varepsilon > 0$ and $\beta = \beta(x) \in \mathbb{R}^2, x \in \Omega$. We assume that β has no loops, i.e. that $\beta(x) \neq \beta(y)$ if $x \neq y$. Additionally, we impose Dirichlet boundary conditions on the inflow boundary $\Gamma_{in} = \{x \in \partial \Omega | (\beta(x), n) \leq 0\}$ and natural outflow conditions on $\Gamma_{out} = \partial \Omega \setminus \Gamma_{in}$:

$$u|_{\Gamma_{\rm in}} = u_0 , \quad \frac{\partial}{\partial n} u|_{\Gamma_{\rm out}} = 0$$
 (1.2)

Though boundary layers are excluded by (1.2), internal layers still lead to severe problems both with respect to discretization and efficient resolution of the resulting linear system.

In a recent paper KORNHUBER AND ROITZSCH [5] have proposed an adaptive orientation of the underlying triangulation in streamline direction β together with local directed (blue) refinement. Compared to common adaptive strategies they obtained the same or even higher accuracy involving a much lower number of nodes. Note that no a priori information on the flux direction β is used so that the technique carries over to more general situations in fluid dynamics where β is depending on the solution.

The purpose of this paper is to exploit the local structure of the triangulation provided by adaptive orientation and directed refinement, in order to construct a monotone discretization with minimal crosswind. We introduce the so called extended box method which turns out to be a variant of standard Galerkin methods in the self-adjoint case and gives a permanent extension of backward differencing to irregular grids, if only convective transport is present. In the latter case optimal orientation together with streamline ordering of the unknowns leads to a lower diagonal stiffness matrix so that ILU and Gauß-Seidel iterations reduce to exact solvers. Non-vanishing physical or artificial diffusion is viewed as perturbation of this ideal case. It turns out that for large Peclet numbers the resulting linear systems are very efficiently solved by ordinary ILU or Gauß-Seidel iterations while an additional coarse grid transport becomes necessary as soon as the elliptic part of the problem becomes dominant. Note that a related approach to the anisotropic diffusion problem has been carried out successfully by WITTUM [9].

The Extended Box Method 2.

Let \mathcal{T} be a triangulation of the bounded polygonal domain $\Omega \subset \mathbb{R}^2$ with \mathcal{E} and \mathcal{P} denoting the set of edges and nodes, respectively. The subset of nodes which are not situated on the Dirichlet boundary is called \mathcal{P}^0 . We assume that \mathcal{T} is regular in the sense that the intersection of two triangles of \mathcal{T} is either containing a common edge, a common node or is empty. The finite dimensional space of continuous functions being linear on each $t \in \mathcal{T}$ is called $\mathcal{S}(\mathcal{T})$. We provide $\mathcal{S}(\mathcal{T})$ with basis functions $\lambda_p \in \mathcal{S}(\mathcal{T}), p \in \mathcal{P}$ defined by $\lambda_p(q) = \delta_{p,q}$ (Kronecker symbol). For a given triangulation \mathcal{T} we choose a partition $\mathcal{B} = \{\mathcal{B}_p, p \in \mathcal{P}\}$ with the properties

- (B1)
- $\bigcup_{p \in \mathcal{P}} \mathcal{B}_p = \overline{\Omega}$ $\mathcal{B}_p \subset \{t \in \mathcal{T} | p \text{ is vertex of } t\}$ (B2)
- $\mathcal{B}_p \cap \mathcal{B}_q \subset \partial \mathcal{B}_p, \ p,q \in \mathcal{P}.$ (B3)

Now integrate the differential equation (1.1) on \mathcal{B}_q , $q \in \mathcal{P}^0$, apply Greens formula and use the piecewise linear ansatz

$$U^{\mathcal{B}} = \sum_{p \in \mathcal{P}} U_p \lambda_p \in \mathcal{S}(\mathcal{T})$$
(2.1)

to obtain the well-known box method

$$\sum_{p \in \mathcal{P}} \left\{ \int_{\partial \mathcal{B}_q} -\varepsilon \frac{\partial}{\partial n_q} \lambda_p + (\beta, n_q) \lambda_p \, d\sigma \right\} U_p = \int_{\mathcal{B}_q} f \, dx \, , \ q \in \mathcal{P}^0, \tag{2.2}$$

where we used the outward normal n_q to $\partial \mathcal{B}_q$ and the Euclidean scalarproduct (\cdot, \cdot) in \mathbb{R}^2 . To avoid instabilities in case of dominating convection, we use a piecewise constant approximation of the first order terms, taking the values $U^{B}|_{\partial B_{q}}$ from upstream. The resulting upwind discretization reads

$$\sum_{p \in \mathcal{P}} \left\{ \int_{\partial \mathcal{B}_{q}} -\varepsilon \frac{\partial}{\partial n_{q}} \lambda_{p} \, d\sigma \right\} U_{p} + \left\{ \int_{\partial \mathcal{B}_{q}} (\beta, n_{q})_{+} \, d\sigma \right\} U_{q} + \sum_{p \neq q \in \mathcal{P}} \left\{ \int_{\partial \mathcal{B}_{q} \cap \partial \mathcal{B}_{p}} (\beta, n_{q})_{-} \, d\sigma \right\} U_{p} = \qquad (2.3)$$
$$= \int_{\mathcal{B}_{q}} f \, dx \, , \ q \in \mathcal{P}^{0}.$$

with $r_{+} = \max(0, r)$ and $r_{-} = \min(0, r)$, $r \in \mathbb{R}$, respectively.

It is well-known from the pioneering work of BANK/ROSE [1] and HACK-BUSCH [3] that for self-adjoint problems the box method and traditional Ritz-Galerkin scheme are closely related. In fact, if the regularity condition $\partial \mathcal{B}_p \cap e \subset \{ \text{ midpoint of } e \}, \ p \in \mathcal{P}, e \in \mathcal{E}.$ (B4)

is satisfied, the resulting stiffness matrices coincide and the difference of the approximations U^B and U^G can be estimated by

$$||U^B - U^G||_1 \le \frac{h}{\varepsilon\sqrt{2}}||f||_0 \tag{2.4}$$

with h denoting the minimal size of $e \in \mathcal{E}$ and $||\cdot||_1, ||\cdot||_0$ the usual norms in H^1 and L_2 , respectively. Moreover, if f is smooth enough and \mathcal{B} satisfies an additional symmetry condition, related second order estimates are available. We refer to [3] for details.

Obviously the construction of special box-schemes amounts to a special choice of the box-mesh \mathcal{B} . In our case this choice is preceded by a suitable extension of the underlying triangulation \mathcal{T} . More precisely, from a given \mathcal{T} we construct an extended triangulation $\overline{\mathcal{T}}$ by adding the barycenter s of each triangle $t \in \mathcal{T}$ to the set of nodes and joining it to the vertices as shown in Figure 2.1. Now the corresponding extended box-mesh $\overline{\mathcal{B}}$ is obtained from the subdivision of t in four similar subtriangles, where the inner triangle forms the box \mathcal{B}_s and the others contribute to the boxes related to the remaining vertices.



Figure 2.1 Extended triangulation \overline{T} and box mesh $\overline{\mathcal{B}}$

Note that the additional unknowns U_s are coupled only with U_p, U_q and U_r . Now the extended box method reads as follows.

- Use the upwind box scheme with respect to the extended triangulation \overline{T} and the related box-mesh $\overline{\mathcal{B}}$.
- Eliminate the additional unknowns U_s by local condensation to obtain the linear system

$$A\underline{U} = b \tag{2.5}$$

for the remaining unknowns $\underline{U} = (U_p)_{p \in \mathcal{P}^0}$.

We will investigate the properties of this scheme for pure diffusion and pure convection starting with the self-adjoint case $\beta \equiv 0$. Note that the pair \overline{T} , \overline{B} does not satisfy the regularity condition (B4). However, we can state the following Theorem which is closely related to the results summarized above.

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Theorem 2.1

Let $\beta \equiv 0$. Then A coincides with the stiffness matrix resulting from the standard Ritz – Galerkin Method with respect to the original triangulation T. Moreover, the difference of U and the Ritz – Galerkin approximation U^G can be estimated according to (2.4).

Proof: Let us apply the standard box method to the extended meshes $\overline{\mathcal{T}}$ and $\overline{\mathcal{B}}$. In view of (2.2), the contributions of some triangle $t \in \mathcal{T}$ to the stiffness matrix \overline{A} are given by

$$\overline{L}_{\nu,\mu} = -\int_{\partial \overline{B}_{\nu} \cap t} \varepsilon \frac{\partial}{\partial n_{\nu}} \overline{\lambda}_{\mu} \, d\sigma, \quad \nu,\mu = p,q,r,s,$$
(2.6)

with $\overline{\lambda}_{\mu}, \mu \in \overline{\mathcal{P}}$ denoting the standard basis functions in $\mathcal{S}(\overline{T})$. Note that $\overline{L}_{s,\mu}, \mu = p, q, r$, coincides with the entries of \overline{A} as $\overline{\mathcal{B}}_s$ is contained in t. Hence the local contributions $L_{\nu,\mu}$ to A can be obtained by local condensation:

$$L_{\nu,\mu} = \overline{L}_{\nu,\mu} - \frac{\overline{L}_{s,\mu}}{\overline{L}_{s,s}} \overline{L}_{\nu,s} , \quad \nu,\mu = p,q,r.$$
(2.7)

To show the desired equality of the stiffness matrices, we will prove

$$L_{\nu,\mu} = \int_t \varepsilon(\nabla \lambda_{\nu}, \nabla \lambda_{\mu}) \, dx =: L^G_{\nu,\mu} \, , \ \nu,\mu = p, q, r.$$
(2.8)

For this reason assume for the moment that

$$\frac{\overline{L}_{s,\mu}}{\overline{L}_{s,s}} = -\frac{1}{3} , \quad \mu = p, q, r.$$
 (2.9)

Then in view of

$$\overline{\lambda}_{\nu} + \frac{1}{3}\overline{\lambda}_{s} = \lambda_{\nu} \quad \text{on } t, \ \nu = p, q, r,$$
 (2.10)

the desired identity (2.8) takes the form

$$-\int_{\overline{B}_{\nu}\cap t}\varepsilon\frac{\partial}{\partial n_{\nu}}\lambda_{\mu}\ d\sigma = L^{G}_{\nu,\mu}\ ,\ \nu,\mu = p,q,r.$$
(2.11)

As $\partial \overline{B}_{\nu}$ intersects the edges of t at their midpoints, (2.11) is easily shown along the lines of [1] or [3]. We still have to prove (2.10) which can be rewritten as

$$\int_{\partial \overline{B}_s} \frac{\partial}{\partial n_s} (\overline{\lambda}_{\mu} + \frac{1}{3} \overline{\lambda}_s) \, d\sigma = 0.$$
 (2.12)

Now in view of (2.11) the assertion easily follows from Greens formula. To estimate the difference of the approximations U and U^G , observe that on each triangle $t \in \mathcal{T}$ the right hand side is approximated by

$$F_{\nu} = \int_{\overline{B}_{\nu}} f \, dx + \alpha_{\nu} \int_{\overline{B}_{s}} f \, dx , \quad \nu = p, q, r, \qquad (2.13)$$

with coefficients α_{ν} given by

$$\alpha_{\nu} := \frac{\overline{L}_{\nu,s}}{\overline{L}_{s,s}} = \frac{|e_{\nu}|}{|e_{p}| + |e_{q}| + |e_{r}|}, \quad \nu = p, q, r.$$
(2.14)

Now the proof is completed following almost literally the arguments in [3].

If \mathcal{T} satisfies the strong regularity condition |e| = const., $e \in \mathcal{E}$, then (2.13) obviously holds with $\alpha_{\nu} = \frac{1}{3}$, $\nu = p, q, r$, and the extended box method reduces to a variant of the box method proposed by HACKBUSCH[3]. In this case we have an analogue of (2.4) of second order. Note that for $\beta \neq 0$ the right hand side f is still approximated as in (2.13) but with α_{ν} replaced by a modified partition of unity α_{ν}^{β} , $\nu = p, q, r$.

Let us now consider the case of pure convection appearing as reduced problem of (1.1) in the sense of asymptotic analysis.

Theorem 2.2

Let $\varepsilon = 0$. Assume that $\beta(x) = \text{const.}, x \in \Omega$ and that \mathcal{T} is oriented in the sense that in each triangle $t \in \mathcal{T}$ one edge is parallel to β . Then the extended box method reduces to the first order upwind difference scheme.

Proof: Let $p \in \mathcal{P}^0$. Then it is easily seen from the assumptions on \mathcal{T} and the boundary conditions (1.2) that there is one and only one edge $e_0 = (p, p_0) \in \mathcal{E}$ pointing from p in upstream direction. Hence upwind differencing is feasible. Referring to the denotation introduced in Figure 2.1, we first observe that in case of pure convection the unknowns U_p, U_q , and U_r are coupled only via the intermediate unknowns U_s . Exploiting the orientation of \mathcal{T} in (2.3), it is easily checked that U_s and U_q or U_r are coupled only if $q = p_0$ or $r = p_0$.

The above Theorem makes sure that for oriented triangulations there is no unphysical coupling of different streamlines. This is not the case in usual variants of the Petrov-Galerkin method (see [4]), where certain averages of upwind differences are obtained. Of course, there is no artificial viscosity in this ideal case, while on unstructured grids we expect the usual diffusive behaviour of an upwind method.

Of course, the condition $\beta(x) \equiv \text{const.}$ can be weakened.

Having treated the ideal cases $\varepsilon = 0$ and $\beta = 0$ let us finally state that the properties of the extended box method applied to general convection diffusion equations are not obtained as the sum but as a nonlinear interpolation of these results. This is due to the local elimination of the U_s which is not additive.

3. Iterative Solution

In this chapter we consider the iterative solution of the linear system (2.5) resulting from the extended box method. We further assume that the triangulation \mathcal{T} is oriented in the sense of Theorem 2.2 and that $\varepsilon \ll |\beta|$. This allows to treat the general convection diffusion equation as perturbation of the singular case $\varepsilon = 0$.

Theorem 3.1

Let $\varepsilon = 0$. Assume that $\beta(x) \equiv \text{const.}$, $x \in \Omega$, and that \mathcal{T} is oriented in the sense that in each triangle $t \in \mathcal{T}$ one edge is parallel to β . Then the nodes \mathcal{P} can be ordered in streamlines following the flux direction β . With respect to this ordering the extended box method provides a lower triangular stiffness matrix A.

Proof: The Proof is obvious from Theorem 2.2.

Again, the assumption $\beta \equiv \text{const.}$ can be weakened.

Of course iterative schemes like the ILU or Gauß-Seidel iteration reduce to exact solvers, if the assumptions of Theorem 3.1 are fulfilled. But this ideal situation may be disturbed in several ways. First adaptive orientation of \mathcal{T} , as performed in the sequel, is supposed to be not exact. Hence a certain amount of artificial diffusion may be introduced by the discretization. On the other hand, any nonvanishing physical diffusion becomes dominant as soon as the local stepsize is chosen small enough. Both phenomena will show up in our numerical experiments. We conjecture that these problems arising from too much diffusion can be remedied by additional coarse grid correction, using the iterative scheme as smoother. This will be subject to subsequent work.

We are left with the problem to provide an efficient streamline ordering of the unknowns. This will be done in the well-known adaptive framework described for example in [2] or [5]. Starting with some initial triangulation T_0 , we assume that a sequence of triangulations T_1, T_2, \ldots, T_j is obtained from local regular (red) or directed (blue) refinement and irregular (green) closure. The enumeration of the corresponding nodes will be performed inductively with respect to the refinement levels j.

First, let us briefly discuss the additional requirements on the underlying data structures. As we do not insist on uniform refinement, the polygonals of edges following the streamlines may be disconnected and grow together on subsequent levels. Hence, the nodes belonging to different streamlines are stored in different linked lists. By a pointer on the initial node of the corresponding list, each node is located in its line. The further implementation heavily relies on the data structures provided by the underlying finite element code KASKADE. In particular we have a pointer from each refined triangle $T \in \mathcal{T}_j$, called father, to the resulting triangles $t_1, t_2, t_3, t_4 \in \mathcal{T}_{j+1}$, called sons, and vice versa. Note that t_3, t_4 are void in case of blue refinement. We refer to LEINEN[6] or ROITZSCH[7, 8] for details.

Now the initial numeration of \mathcal{P}_0 corresponding to the intentionally coarse grid \mathcal{T}_0 may be provided by the user or derived automatically from the approximation U_0 on level 0. In any case the initial grid has to be fine enough to guarantee that the detected streamline direction does not change dramatically in course of the refinement process (see [5]).

In the induction step we assume that the initial triangles $T \in \mathcal{T}_0$ are ordered according to the numeration of the nodes \mathcal{P}_0 . Based on the existing numeration of \mathcal{P}_j the new nodes $p \in \mathcal{P}_{j+1} \setminus \mathcal{P}_j$ arising from the actual refinement step are sorted by the recursive procedure NUMERATE(·) which is applied subsequently to the initial triangles $T_0, T_1, \ldots, T_{N_0} \in \mathcal{T}_0$.

procedure NUMERATE(t)

while $(t \text{ has sons } t_1, t_2, t_3, t_4)$

if $(t \in \mathcal{T}_{i+1} \setminus \mathcal{T}_i)$

file the new points into an existing line or make up a new one else

perform NUMERATE (t_i) , $i = 1, \dots, 4$, following the order induced by the existing numeration of \mathcal{P}_j (see Figure 3.1)



Figure 3.1 Local numeration of sons

The above algorithm may be viewed as a recursive search for new nodes $p \in \mathcal{P}_{j+1} \setminus \mathcal{P}_j$, taking care that they are picked up according to the existing order of \mathcal{P}_j . Note that the numeration follows the streamlines together with the corresponding polygonals of edges. Hence local orientation only leads to a local streamline ordering of the nodes.

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4. Numerical Results

In our numerical experiments we concentrate on the behaviour of the extended box method and of the ILU iteration applied to the resulting linear systems. For details on the underlying adaptive concept we refer to [5].

In our first example we chose $\beta \equiv (1, 0.5)^T$, $f \equiv 0$ on $\Omega = [0 \times 1, 0 \times 1]$ and the boundary conditions (1.2) with discontinuous u_0 defined by $u_0(x_1, x_2) = 1$ if $x_2 \leq 0.3$ and $u_0 = 0$ elsewhere on Γ_{in} . The initial triangulation \mathcal{T}_0 is depicted in Figure 4.1.



Figure 4.1 Initial triangulation T_0

We first illustrate the properities of the extended box method in the case of pure convection $\varepsilon = 0$. The next Figure 4.2 shows the approximation \tilde{U}_9 together with the corresponding triangulation $\tilde{\mathcal{T}}_9$, resulting from 9 isotropic refinement steps without orientation. As expected, we observe the monotone but diffusive behaviour of usual upwind schemes. Using adaptive orientation and directed (blue) refinement, we end up with the anisotropic triangulation \mathcal{T}_9 depicted in Figure 4.3. In this case, the extended box method leads to the approximation U_9 , introducing almost no unphysical crosswind but preserving the good stability properties. Note that \mathcal{T}_9 is involving a much smaller number of nodes than $\tilde{\mathcal{T}}_9$. The next Figure 4.4 shows the convergence properties of the ILU iteration applied to the linear systems (2.5), arising from the extended box method for the choice $\varepsilon = 10^{-4}, 10^{-5}, 0$. We depict the number of iterations depending on the refinement levels which are taken as a measure for the local stepsize h. We always started with $U^{(0)} = 0$ and required the unrealistic accuracy

$$|U^{(\nu+1)} - U^{(\nu)}|_{\ell_2} < 10.^{-12}$$

to amplify the effects of various physical diffusion. Note that only the adaptively oriented triangulations are considered. Obviously the method performs excellent for large local Peclet numbers $\rho = \frac{h|\beta|}{\epsilon}$ and deteriorates as soon as the local mesh size h is small enough to resolve the internal layer. Note that the small increase of the line corresponding to $\epsilon = 0$ is due to nonoptimal orientation. It should be mentioned that the Gauß – Seidel method shows a very similar behaviour but appears to be less robust with respect to perturbing diffusion.



Figure 4.2 Standard triangulation $\tilde{\mathcal{T}}_9$ (2716 nodes) and approximation $\tilde{\mathcal{U}}_9$



Figure 4.3 Oriented triangulation T_9 (121 nodes) and approximation U_9



Figure 4.4 ILU iteration for a linear layer

In the second example we produce a curved layer by the choice $\beta(x_1, x_2) = (x_2, -x_1)^T$ and a corresponding modification of u_0 . The other data including the initial triangulation remain unchanged. Of course we cannot expect that the non-linear layer is approximated by linear edges as good as the linear layer considered above. Indeed, the effect of less accurate orientation is visible both in the diffusivity of the approximate solution (see Figure 4.5) and the behaviour of the iterative solver (see Figure 4.6). But compared to the solution produced by a standard triangulation and illustrated in Figure 4.4, this approach still provides a considerable advantage both with respect to accuracy and efficiency.

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Figure 4.5 Standard triangulation \tilde{T}_9 (3106 nodes) and approximation \tilde{U}_9



Figure 4.6 Oriented triangulation T_9 (243 nodes) and approximation U_9





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