On finite volume discretization of elliptic interface problems

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ABSTRACT. *A finite volume discretization of elliptic problems with discontinuous coefficients (interface problems) is presented. This approximation ensures second order truncation error for the fluxes. It uses a minimal stencil (5 points in 2-D and 7 points in 3-D) for the case when each interface is orthogonal to one of the coordinate axes on a mesh that, in general, is not required to be aligned with the interfaces.*

KEYWORDS: *finite volume discretization, elliptic interface problems, modified harmonic averaging.*

1. Introduction

Elliptic problems with discontinuous coefficients, called often interface problems, arise naturally in mathematical modeling of heat and mass transfer processes, diffusion in composite materials, flow in porous media, etc. The governing equation in this case can be written as

$$-\nabla(K\nabla u) = f(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega \qquad [1]$$

subject to various boundary conditions. Here $\Omega \subset R^n$ is a bounded polyhedra, $K(\mathbf{x})$ is a symmetric and uniformly in Ω positive definite matrix which may have a jump discontinuity across a given surface Γ. The flux vector, $\mathbf{W}$, is defined as

$$\mathbf{W} = -K\nabla u.$$

The assumption that the solution and the normal component of the flux are continuous through the interface, is physical and is mostly used to close the mathematical problem. In our notations, this condition is written as follows:

$$[u] \ = [\mathbf{W}.\mathbf{n}] \ = 0, \quad \text{for } \mathbf{x} \in \Gamma, \qquad [2]$$

where $\mathbf{n}$ stands for the outer normal to the interface Γ, and $[\phi]$ denotes the jump of ϕ. This interface condition is often called *perfect contact* condition.

A straightforward application of the finite volume method to a generic interface problem results in a scheme which uses harmonic averaging of the coefficient (see, for example, [SAM-77, WES-91]). Inspecting this scheme, one easily sees that the normal component of the flux at the interface is discretized with a local truncation error $O(h)$. From the recent works, devoted to discretization of interface problems, we refer to [CAI-02, ARB-98, ILI-98, KNY-01, EWI-99]. Cai, Douglas, and Park [CAI-02] derive high order finite volume discretizations for interface problems, however, on a much larger stencil. Arbogast, et al. [ARB-98] introduce enhanced cell-centered discretizations, which reduce the work, required by mixed hybrid finite element method. Both, diagonal and full tensor coefficients are considered. In the case of diagonal tensor and discontinuous coefficients their scheme reproduces harmonic averaging discretization. Knyazev and Widlund [KNY-01] use Lavrentiev regularization in order to obtain uniform with respect to jump of coefficients a posteriori error estimate. Their method ensures $O(h)$ accuracy for the fluxes. Ewing, Li, and Lin [EWI-99] make an extension of immersed interface idea to finite element discretization and recreate harmonic averaging of the discontinuous coefficients.

In this paper we present a modification of the classical finite volume discretization of interface problems, so that the normal component of the flux in the derived scheme has $O(h^2)$-local truncation error. We assume that the interfaces are perpendicular to a coordinate axis, but, in general, are not aligned with cell faces. This work exploits two known approaches: (i) coupled discretization of fluxes in a cell [ILI-02, EWI-01], and (ii) use of the governing equation at the interface [ILI-98]. In the first case, the normal component of the flux is assumed to be continuously differentiable in normal direction at the interface. In the second case, the discretizations are derived for uniform grid, when the interface is aligned with a cell face. In this paper, we combine both approaches and derive a second order discretization of the flux without additional smoothness requirements. The only restriction in this case is that we assume that the diffusivity coefficient is piecewise constant.

In general, our approach can be viewed as a defect correction of the standard scheme with harmonic averaging of the coefficient, since it takes into account the next term in the Taylor expansion of the flux. This correction does preserve the standard $(2n+1)$-point overall stencil and uses data only from the neighboring 2^n cells. The elimination of the $O(h)$ term is based on some ideas from explicit jump immersed interface method (EJIIM) (see for details [LEV-95, WIE-98]). Recall, that in EJIIM the unknown jumps across the interface are new variables. Here we want to account explicitly for the jump of the normal derivative of the normal component of the flux. However, instead of introducing new variable, as done in EJIIM, we approximate this jump with $O(h)$. To get such approximation, we use the equation at the interface. Further, we derive approximation to each of the flux components, and combine them with a finite volume discretization of the continuity equation written in terms of the fluxes. That is, we discretize the mixed form of the governing equations, while IIM and EJIIM discretize directly the second order equation. The discretization of the mixed form has two advantages: (i) we obtain $O(h^2)$ local truncation error for the flux discretization, and $O(h^2)$ accuracy for the fluxes; (ii) we obtain a coefficient in front of the remainder which is bounded independently of the jump discontinuity of coefficients so that our discretization is not sensitive to the jump.

2. Modified finite volume discretization

We begin our presentation with one-dimensional problem on $(0,1)$ and in order to simplify the notations, we assume that the grid is uniform. Then, $\mathbf{W} = W$ and $\mathbf{x} = x$. Further, we use the notations $x_i = ih$, $x_{i+\frac{1}{2}} = x_i + \frac{1}{2}h$, where, h is the step-size. Integrating the differential equation over the volume $(x_{i+\frac{1}{2}}, x_{i-\frac{1}{2}})$ we get the following equation for each internal node x_i:

$$W_{i+\frac{1}{2}} - W_{i-\frac{1}{2}} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x)dx. \qquad [3]$$

Our aim is to derive $O(h^2)$-approximations to $W_{i+\frac{1}{2}}$ and $W_{i-\frac{1}{2}}$.

Suppose, there exist an interface at the point x_ξ, $x_i < x_\xi < x_{i+1}$ so that $x_\xi = x_i + \theta\ h$. For definiteness, we consider the case $0 < \theta < \frac{1}{2}$. Recall that the case when the interface is aligned with cell faces, $\theta = \frac{1}{2}$, is covered by [ILI-98]. Obviously, $x_i - x_\xi = -\theta\ h$, $x_{i+1} - x_\xi = (1-\theta)\ h$, $x_\xi - x_{i+\frac{1}{2}} = (\theta - \frac{1}{2})\ h$. The discretization of $W_{i+\frac{1}{2}}$ is done in several steps. First we expand u_i around the interface point. Next we use interface conditions in order to transform derivatives from the left of the interface into derivatives form the right of the interface. Further, these are expanded around $x_{i+\frac{1}{2}}$. The obtained expansion is combined with the expansion of u_{i+1} around $x_{i+\frac{1}{2}}$ in order to obtain a discretization for the flux at $x_{i+\frac{1}{2}}$. The obtained approximation to

$W_{i+\frac{1}{2}}$ has $O(h)$ local truncation error. In order to account explicitely for this $O(h)$ term, we use the equation at the interface as well as the approach for coupled discretization of fluxes.

Let us now explain some details of our approach. Expand u_i to get:

$$u_i = u_{\xi-} \;-\theta\; h\; \frac{\partial u_{\xi-}}{\partial x} + \;\frac{1}{2}\theta^2\; h^2\; \frac{\partial^2 u_{\xi-}}{\partial x^2} + O(h^3).$$

Here and below $u_{\xi-}$ ($u_{\xi+}$) denotes the limit of $u(x)$ when x tends to x_ξ from below (above). Further, we expand the first two terms in the right hand side around the point $x_{i+\frac{1}{2}}$ and use the fact that the solution and the normal component of the flux across the interface are continuous, i.e. $u_{\xi-} = u_{\xi+}$ and $W_{\xi-} = W_{\xi+}$.

$$\begin{aligned} u_i \;&=\; u_{i+\frac{1}{2}} \;+ (\theta - \frac{1}{2})\; h\; \frac{\partial u_{i+\frac{1}{2}}}{\partial x} \;+ \frac{1}{2}(\theta - \frac{1}{2})^2\; h^2\; \frac{\partial^2 u_{i+\frac{1}{2}}}{\partial x^2} \;+ O(h^3) \\ &\quad -\theta\; h \frac{k_{i+1}}{k_i}\; \left(\frac{\partial u_{i+\frac{1}{2}}}{\partial x} + (\theta - \frac{1}{2})\; h\; \frac{\partial^2 u_{i+\frac{1}{2}}}{\partial x^2} \right) + \frac{1}{2}\theta^2\; h^2\; \frac{\partial^2 u_{\xi-}}{\partial x^2}. \end{aligned}$$

Rearranging the terms in the equality above, we obtain

$$\begin{aligned} u_i \;&=\; u_{i+\frac{1}{2}} \;- h\; \left(\frac{\theta - \frac{1}{2}}{k_{i+1}} - \frac{\theta}{k_i} \right)\; W_{i+\frac{1}{2}} \\ &\quad -h^2\; \left(\frac{1}{2}\; \frac{(\theta - \frac{1}{2})^2}{k_{i+1}} - \frac{\theta\; (\theta - \frac{1}{2})}{k_i} \right) \frac{\partial W_{\xi+}}{\partial x} - \;\frac{1}{2}\theta^2\; h^2\; \frac{\partial W_{\xi-}}{\partial x} + O(h^3). \end{aligned}$$

Combining the above expansion of u_i with an expansion of u_{i+1} around $x_{i+\frac{1}{2}}$, and rearranging terms, we get an approximation to the flux in the form:

$$\begin{aligned} W_{i+\frac{1}{2}} &= -\; k^H_{i+\frac{1}{2}}\; \frac{u_{i+1} - u_i}{h} + \qquad [4] \\ &+ k^H_{i+\frac{1}{2}}\; \frac{h}{2}\; \left[\left(\frac{\frac{1}{4} - (\theta - \frac{1}{2})^2}{k_{i+1}} + \frac{\theta(\theta - \frac{1}{2})}{k_i} \right)\; \frac{\partial W_{\xi+}}{\partial x} - \frac{\theta^2}{k_i}\; \frac{\partial W_{\xi-}}{\partial x} \right] + O(h^2), \end{aligned}$$

where we have used the harmonic average

$$k^H_{i+\frac{1}{2}} = \left(\frac{1-\theta}{k_{i+1}} + \frac{\theta}{k_i} \right)^{-1} = \frac{k_i\; k_{i+1}}{(1-\theta)\; k_i \;+\; \theta\; k_{i+1}}. \qquad [5]$$

Neglecting the $O(h)$-term in (4), we get the standard harmonic averaging based discretization to the flux $W_{i+\frac{1}{2}}$. In order to obtain an $O(h^2)$-approximation to the flux, we have to account for the $O(h)$-term. In 1-D case it can be done, assuming that the equation is satisfied at the interface. An $O(h^2)$-approximation to the flux $W_{i+\frac{1}{2}}$ is given in this case by the expression

$$W_{i+\frac{1}{2}} = -k^H_{i+\frac{1}{2}}\; \frac{u_{i+1} - u_i}{h}$$

$$+ \, k^H_{i+\frac{1}{2}} \; \frac{h}{2} \left[\left(\frac{\frac{1}{4} - (\theta - \frac{1}{2})^2}{k_{i+1}} + \frac{\theta(\theta - \frac{1}{2})}{k_i} \right) \; f_{\xi+} - \frac{\theta^2}{k_i} \; f_{\xi-} \right]. \qquad [6]$$

In 2-D and in 3-D the situation is much more complicated. Consider, for brevity, 2-D case. Again, in order to simplify the notation, denote by $\mathbf{x} = (x, y)$, $\mathbf{W} = (W^{(1)}, W^{(2)})$ and by (x_i, y_j) the grid nodes. Further, assume that there is one interface along the line $(x_i + \theta h, y) := (x_\xi, y)$. Now we rewrite the expression for the flux in the following form

$$W^{(1)}_{i+\frac{1}{2},j} = -k^H_{i+\frac{1}{2},j} \; \frac{u_{i+1,j} - u_{i,j}}{h} + O(h^2)$$
$$+ \; \frac{h\theta}{2} \frac{\left[(1-\theta) \; k_{i,j} \; + \; 2 \; (\theta - \frac{1}{2}) \; k_{i+1,j}\right] \; \frac{\partial W^{(1)}_{\xi+,j}}{\partial x} - \theta \; k_{i+1,j} \; \frac{\partial W^{(1)}_{\xi-,j}}{\partial x}}{(1-\theta) \; k_{i,j} \; + \; \theta \; k_{i+1,j}}. \qquad [7]$$

Our aim is to express $\frac{\partial W^{(1)}_{\xi+,j}}{\partial x}$ and $\frac{\partial W^{(1)}_{\xi-,j}}{\partial x}$ by known quantities, at least as an $O(h)$ approximation. For this purpose, we will derive below two linear algebraic equations with respect to these two unknowns. First, suppose that the governing equation is satisfied on the interface and rewrite it as:

$$\frac{\partial W^{(2)}_{\xi+,j}}{\partial y} = f_{\xi+,j} - \frac{\partial W^{(1)}_{\xi+,j}}{\partial x}, \qquad \frac{\partial W^{(2)}_{\xi-,j}}{\partial y} = f_{\xi-,j} - \frac{\partial W^{(1)}_{\xi-,j}}{\partial x}. \qquad [8]$$

Further, assume the solution is twice continuously differentiable in tangential direction at the interface (x_ξ, y). The condition for continuity of the solution on the interface, $u(x_{\xi+}, y) = u(x_{\xi-}, y)$, will imply:

$$\frac{\partial}{\partial y} \left(\frac{\partial u_{\xi+,j}}{\partial y} \right) = \frac{\partial}{\partial y} \left(\frac{\partial u_{\xi-,j}}{\partial y} \right), \quad \text{i.e.} \quad k_{i,j} \frac{\partial W^{(2)}_{\xi+,j}}{\partial y} = k_{i+1,j} \frac{\partial W^{(2)}_{\xi-,j}}{\partial y}. \qquad [9]$$

Denote by $\lambda = \lambda_{i+\frac{1}{2},j} = \frac{k_{i+1,j}}{k_{i,j}}$. Substituting (8) in (9), we obtain the relation:

$$f_{\xi+,j} - \frac{\partial W^{(1)}_{\xi+,j}}{\partial x} = \lambda \left(f_{\xi-,j} - \frac{\partial W^{(1)}_{\xi-,j}}{\partial x} \right). \qquad [10]$$

We need one more relation between $\frac{\partial W^{(1)}_{\xi+,j}}{\partial x}$ and $\frac{\partial W^{(1)}_{\xi-,j}}{\partial x}$. To derive it, consider expansions of $W^{(1)}_{i+\frac{1}{2},j}$ and $W^{(1)}_{i-\frac{1}{2},j}$ around the interface point (x_ξ, y_j):

$$W^{(1)}_{i+\frac{1}{2},j} = W^{(1)}_{\xi+,j} \; + \; (-\theta + \frac{1}{2}) \; h \; \frac{\partial W^{(1)}_{\xi+,j}}{\partial x} \; + \; O(h^2),$$

$$W^{(1)}_{i-\frac{1}{2},j} = W^{(1)}_{\xi-,j} \; + \; (-\theta - \frac{1}{2}) \; h \; \frac{\partial W^{(1)}_{\xi-,j}}{\partial x} \; + \; O(h^2).$$

From these expansions we obtain

$$(-\theta+\frac{1}{2})\,\frac{\partial W^{(1)}_{\xi+,j}}{\partial x} \;+\; (\theta+\frac{1}{2})\,\frac{\partial W^{(1)}_{\xi-,j}}{\partial x} \;=\; \frac{W^{(1)}_{i+\frac{1}{2},j}-W^{(1)}_{i-\frac{1}{2},j}}{h} \;+\; O(h). \qquad [11]$$

Thus, we have a system of two equations, (11) and (10), with respect to two unknowns. We solve the system and obtain:

$$\frac{\partial W^{(1)}_{\xi+,j}}{\partial x} \;=\; \frac{r_+(\lambda,\theta,f) \;+\; \lambda\, h^{-1}(W^{(1)}_{i+\frac{1}{2},j}-W^{(1)}_{i-\frac{1}{2},j})}{p(\lambda,\theta)} \;+\; O(h), \qquad [12]$$

$$\frac{\partial W^{(1)}_{\xi-,j}}{\partial x} \;=\; \frac{r_-(\lambda,\theta,f) \;+\; h^{-1}(W^{(1)}_{i+\frac{1}{2},j}-W^{(1)}_{i-\frac{1}{2},j})}{p(\lambda,\theta)} \;+\; O(h), \qquad [13]$$

where $p(\lambda,\theta) := \theta+\frac{1}{2} \;+\; \lambda\,(-\theta+\frac{1}{2})$ and

$$r_- \equiv r_-(\lambda,\theta,f) := -(\theta-\frac{1}{2})\;(\lambda\; f_{\xi-,j} \;-\; f_{\xi+,j}),$$

$$r_+ \equiv r_+(\lambda,\theta,f) := -(\theta+\frac{1}{2})\;(\lambda\; f_{\xi-,j} \;-\; f_{\xi+,j}).$$

Recall, that we are considering now the case $0<\theta<\frac{1}{2}$, therefore all expressions are well defined. *Note*, that we can replace $f_{\xi-,j}$ and $f_{\xi+,j}$ with each their $O(h)$ approximation, for example, $f_{i,j}$ and $f_{i+1,j}$. Now we can return to the general expression for the flux given by (7). Substituting there (12) and (13), we obtain the desired approximation of the flux with $O(h^2)$.

$$W^{(1)}_{i+\frac{1}{2},j} = -\;k^H_{i+\frac{1}{2}}\;\frac{u_{i+1,j}-u_{i,j}}{h}$$

$$+\;\frac{h\theta}{2}\;\frac{\left((1-\theta)k_{i,j} \;+\; (\theta-\frac{1}{2})k_{i+1,j}\right)\left[r_+(\lambda,\theta,f)+\lambda\; h^{-1}(W^{(1)}_{i+\frac{1}{2},j}-W^{(1)}_{i-\frac{1}{2},j})\right]}{\left((1-\theta)k_{i,j} \;+\; \theta\; k_{i+1,j}\right)\left[(\theta+\frac{1}{2}) \;+\; \lambda\;(-\theta+\frac{1}{2})\right]}$$

$$-\;\frac{h\theta}{2}\;\frac{\theta k_{i+1,j}\;\left[r_-(\lambda,\theta,f) \;+\; h^{-1}(W^{(1)}_{i+\frac{1}{2},j}-W^{(1)}_{i-\frac{1}{2},j})\right]}{\left((1-\theta)k_{i,j} \;+\; \theta\; k_{i+1,j}\right)\left[(\theta+\frac{1}{2}) \;+\; \lambda\;(-\theta+\frac{1}{2})\right]} + O(h^2).$$

Note, that the obtained expression involves some linear combination of $W_{i+\frac{1}{2},j}$ and $W_{i-\frac{1}{2},j}$. It is similar to the equation used in deriving *Improved harmonic* averaging scheme in [EWI-01]. The flux components through opposite sides were discretized in a couple there, and here we can proceed in the same way. We can derive similar second order approximations for $W^{(1)}_{i-\frac{1}{2},j}$, $W^{(2)}_{i,j+\frac{1}{2}}$, $W^{(2)}_{i,j-\frac{1}{2}}$. Let us introduce notations $\phi=\phi(\theta,\lambda)$ and $\tilde{f}_{i+\frac{1}{2},j}$:

$$\phi_{i+\frac{1}{2},j}(\theta,\lambda) = \frac{\theta}{2}\frac{\left[(1-\theta)+(2\theta-1)\lambda\right]\lambda-\theta\lambda}{\left((1-\theta)+\theta\lambda\right)p(\lambda,\theta)}, \qquad [14]$$

$$\tilde{f}_{i+\frac{1}{2},j} = \frac{\theta}{2}\frac{\left((1-\theta)k_{i,j}+(2\theta-1)k_{i+1,j}\right)r_{+}-\left((1-\theta)k_{i}+\theta\; k_{i+1}\right)r_{-}}{\left((1-\theta)\; k_{i}+\theta\; k_{i+1}\right)p(\lambda,\theta)}. \qquad [15]$$

In a similar way, expressions for $\phi_{i-\frac{1}{2},j}$, $\phi_{i,j+\frac{1}{2}}$, $\phi_{i,j-\frac{1}{2}}$ and for $\tilde{f}_{i-\frac{1}{2},j}$, $\tilde{f}_{i,j+\frac{1}{2}}$, $\tilde{f}_{i,j-\frac{1}{2}}$ will be obtained, if there will exist interfaces between respective grid nodes. Note, that $\phi_{i-\frac{1}{2},j}=0$ and $\tilde{f}_{i-\frac{1}{2},j}=0$ if there is no interface beteen $x_{i-1,j}$ and $x_{i,j}$. Then the derived finite volume discretization of the interface problem (1) can be written as follows:

$$\begin{aligned}
&-\frac{(1-\phi_{i+\frac{1}{2},j}+\phi_{i-\frac{1}{2},j})^{-1}}{h_1}\left(k^H_{i+\frac{1}{2},j}\,\frac{u_{i+1,j}-u_{i,j}}{h_1}-k^H_{i-\frac{1}{2},j}\,\frac{u_{i,j}-u_{i-1,j}}{h_1}\right)\\
&-\frac{(1-\phi_{i,j+\frac{1}{2}}+\phi_{i,j-\frac{1}{2}})^{-1}}{h_2}\left(k^H_{i,j+\frac{1}{2}}\,\frac{u_{i,j+1}-u_{i,j}}{h_2}-k^H_{i,j-\frac{1}{2}}\,\frac{u_{i,j}-u_{i,j-1}}{h_2}\right)\\
&\qquad\qquad = f_{i,j}+\tilde{f}_{i+\frac{1}{2},j}+\tilde{f}_{i-\frac{1}{2},j}+\tilde{f}_{i,j+\frac{1}{2}}+\tilde{f}_{i,j-\frac{1}{2}}.
\end{aligned}$$

3. Discussion

It can be shown, that ϕ is uniformly bounded, $|\phi(\theta,\lambda)| < \frac{1}{2}$. This means, that the derived here scheme satisfies the maximum principle. We expect to provide a theoretical proof for $O(h^2)$-convergence rate of the flux.

Our numerical experiments on various model problems showed that the derived in this paper discretization is much more accurate, compare to other schemes, including the scheme with standard harmonic averaging. Some of the results can be found in [EWI-01, ILI-98].

Also we have considered the Problem I from [KNY-01]. In this example, the unit square is halved so that the diffusion coefficient $k(\mathbf{x})$ takes value 1 and $\bar{k} = \mathit{const}$ in both halves, respectively. The exact solution of the problem is given by

$$u(x,y) = \begin{cases} \bar{k}x(x-0.5)y(y-1), & 0 \le x \le 0.5,\; 0<y<1 \\ -(x-0.5)(x-1)y(y-1), & 0.5 \le x \le 1,\; 0<y<1 \end{cases} \qquad [16]$$

The reported error in [KNY-01] is of order 10^{-1} for $h = 10^{-1}$, and decreases lineraly with the decrease of h. Our scheme reproduces *exactly* the solution in the grid nodes. This can be explained by the fact, that the remainder term in our discretization depends on third order partial derivatives, which are definitely zero in this case.

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