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ON SPLITTING SCHEMES OF PREDICTOR-CORRECTOR TYPE IN MIXED FINITE ELEMENT METHOD

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Abstract. In this work we develop a previously proposed approach to constructing vector splitting schemes for heat transfer problem solved by mixed finite element method on rectangular meshes. As was shown numerically before, a particular flux splitting scheme based the alternating direction scheme for flux divergence has no convergence for some smooth test solutions. We provide theoretical analysis of the stability estimates for the scheme based on the eigensystem information. The main drawback of that particular flux splitting scheme is the nonzero component of the heat flux in the kernel of divergence operator.

Based on the analysis and numerical experiments we suggest, explain and verify numerically that flux splitting schemes obtained from predictor-corrector schemes for flux divergence don't have this drawback. The main conclusion is that due to the presence of simple and strong stability estimates one should prefer using predictor-corrector type of schemes for the heat flux rather than others.

Keywords: heat transfer, mixed finite element method, splitting schemes. a priori estimates, predictor-corrector.

Introduction

The presented work is a further development of other works by the authors devoted to constructing economical numerical algorithms for heat transfer problem. By economical we understand stable and easy-to-implement algorithms which allow one to exploit distributed and shared memory parallelism.

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In paper [1] a new approach was proposed for constructing splitting schemes in 2D and 3D for heat transfer problem written as a system of first-order differential equations in terms of temperature and heat flux. This setting of the problem makes it possible to obtain both temperature and heat flux by a conservative numerical algorithm. For space approximation mixed finite element method [2] is implemented with Raviart-Thomas finite elements [3] of lowest order on rectangular meshes. Using structured mesh one can develop efficient numerical algorithms without iterations at the each time level. This can be obtained by constructing splitting schemes for the vector equation on the heat flux which naturally arises in the 1st order setting of the heat transfer problem.

The main idea of the approach consists in formulating a way to recover a vector splitting scheme for the heat flux from the "underlying" scheme for heat flux divergence. As an "underlying" scheme one can use well-known splitting schemes [4], [5], [6] for scalar parabolic equation, e.g., alternating direction scheme, locally one-dimensional schemes, predictor-corrector type of schemes, etc.

In [7] a priori stability estimates with respect to initial data were obtained for vector splitting schemes based on alternating direction scheme [8] (in 2D) and Douglas-Gunn scheme [9] (in 3D). The crucial point in getting those estimates was to split the heat flux into two orthogonal components – discrete divergence-free and discrete potential vectors. It should be also noticed that this idea can be also used for other "underlying" schemes and corresponding vector splitting schemes for the flux as well. A remarkable point about the a priori estimates was that additional smoothness requirements were imposed on initial heat flux approximation. These requirements imply a certain seminorm (dependent on the "underlying" scheme) of initial heat flux error to be bounded independently of mesh parameter in order to guarantee convergence.

Numerical experiments for vector splitting scheme based on alternating direction scheme, see [10], showed that for uniform and nonuniform meshes (even with constant heat conductivity coefficient) convergence for heat flux is poor or absent for some tests when $\tau \sim h$. At the same time temperature converges with second order. A hypothesis was suggested that the observed behavior is closely connected to the additional smoothness requirements which appeared in a priori stability estimates. Namely, it seemed like an error for the heat flux exist in the kernel of discrete divergence operator and the error does not converge for $\tau \sim h$.

In this work convergence issues described above are studied more carefully. Based on the known results from [11] for generalized eigenproblem (for the mass matrix and discrete gradient and divergence matrices) the seminorm behavior from the stability estimates is studied. The obtained results show that the previously known convergence issues are in full accordance with a priori estimates. Sufficient conditions on initial temperature in terms of discrete Fourier coefficients are given that guarantee conditional convergence. In some cases, convergence can be recovered by choosing initial heat flux vector as a solution of a minimization problem with appropriately chosen quadratic functional.

The following idea is suggested to circumvent the difficulties which arise for the vector splitting scheme obtained from the alternating direction scheme. Since the error for the heat flux resides in the kernel of divergence operator, it is reasonable to consider predictor-corrector type of schemes for which the discrete Fourier law is satisfied, i.e., heat flux is orthogonal to the kernel of divergence operator all the time.

When one used locally one-dimensional pure implicit scheme as a predictor, the obtained vector splitting scheme coincides with the scheme proposed by T. Arbogast et.al. [12]. In [12] the scheme was proposed based on so-called Uzawa algorithm for non-stationary problems in the mixed form and rigorous theoretical analysis using finite element technique was provided but only under a very restricting requirement $\tau \sim h^2$.

For this scheme numerical experiments are carried out that show that no conditional convergence issues for the heat flux take place for this scheme of predictor-corrector type. With that, using the developed framework, stability results are obtained in a more simple way than in [12] and for the general case $\tau \sim h$.

Therefore, the main conclusion of the paper is that using predictor-corrector type of schemes should be preferable since they are easy to analyze and do not impose strong smoothness requirements on the initial heat flux since the heat flux has always zero component in the kernel of discrete divergence operator. The vector splitting scheme obtained from the alternating direction scheme happens to be practically inapplicable in case when one does not have the exact values of the heat flux at the initial time moment. The proposed approach provides an easy way to develop different schemes and obtain stability results in a unified manner whenever stability results can be obtained for the "underlying" scalar splitting schemes for heat flux divergence.

The paper is organized as follows. In section 1 we briefly describe the considered approach to constructing vector splitting schemes for the heat flux. Section 2 presents flux splitting schemes and a priori stability estimates that can be obtained using the approach. Analysis for the flux splitting schemes based on alternating-direction scheme for flux divergence is given in case of uniform mesh in section 3. Theoretical results presented in sections 2 and 3 are then verified by a series of numerical experiments in section 4. In subsection 4.1 we show that numerically splitting scheme based on alternating direction behaves the way it is predicted by a priori estimates. Results presented in subsection 4.2 illustrate that flux splitting scheme of predictor-corrector type don't suffer from the same drawback and do converge with second order with no additional conditions on the initial heat flux approximation. Finally, main results of the paper are summarized in the short conclusion.

1. Approach to constructing splitting schemes for the heat flux

Consider in a rectangle $\Omega \subset R^2$ the following initial boundary value problem which describes heat transfer process in Ω for $t \in [0, t_{fin}]$:

$$
\left\{
\begin{array}{c}
c_p \rho \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{w} = f, \\
\mathbf{w} = -\lambda \nabla T, \\
T|_{t=0} = T_0, \\
T|_{\mathbf{x} \in \Gamma_0} = g_0, \\
\mathbf{w} \cdot \mathbf{n}|_{\mathbf{x} \in \Gamma_1} = g_1,
\end{array}
\right.
\tag{1}
$$

where unknowns are T (temperature) and $\mathbf{w}$ (heat flux), and the coefficients and right-hand side are given: ρ (density), c_p (heat capacity), λ (heat conductivity), f (heat sources). For the sake of simplicity we assume coefficients of density and heat capacity equal to one and homogeneous boundary conditions in what follows.

The next step is implementing space approximation of (1) via mixed finite element method.

Now suppose that the domain Ω is covered by a rectangular, in general, nonuniform mesh with cells $K_{i,j} = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$ so that $\overline{\Omega} = \cup_{i,j} K_{i,j}$. For approximating temperature T piecewise-constant elements are used, i.e.

$$T_h \in Q_h = \{\, q_h \,|\, q_h(\mathbf{x}) = \sum_{i,j} q_{i,j}\chi_{i,j}(\mathbf{x})\},$$

where $\chi_{i,j}$ is a characteristic function of mesh cell $K_{i,j}$. For approximating heat flux $\mathbf{w}$ Raviart-Thomas finite elements [3] of lowest order on rectangular meshes are used:

$$\mathbf{w}_h \in \mathbf{W}_h \cap \mathbf{H}_{\mathrm{div}}(\Omega, \Gamma_1),\ \mathbf{W}_h = W_{h,x} \times W_{h,y},$$

where $W_{h,x} = \mathrm{span}\{\varphi_{x,i}\}_i$, $W_{h,y} = \mathrm{span}\{\varphi_{y,j}\}_j$, $\varphi_{x,i}$ and $\varphi_{y,j}$ are standard piecewise-linear "hat"-functions of x and y correspondingly.

Finally, in matrix-vector form the semidiscrete system can be written as

$$M\frac{dT_h}{dt} + \mathbf{B}^T\mathbf{w}_h = f_h\ , \quad \mathbf{A}\mathbf{w}_h = \mathbf{B}T_h\ , \tag{2}$$

where in natural ordering of unknowns M is diagonal mass matrix for temperature,

$$\mathbf{A} = \begin{pmatrix} A_x & 0 \\ 0 & A_y \end{pmatrix}, \qquad \mathbf{B} = \begin{pmatrix} B_x \\ B_y \end{pmatrix},$$

A_x, A_y – tridiagonal matrices (actually, block diagonal with tridiagonal blocks). It is necessary to remark that matrices $B_xM^{-1}B_x^T$ and $B_yM^{-1}B_y^T$ are also tridiagonal due to the structured rectangular mesh and low-order elements used in the considered framework. This fact implies that all splitting schemes which will be discussed further are economical since their implementation requires inverting only matrices of the form $A_x + \alpha B_xM^{-1}B_x^T$ or $A_y + \alpha B_yM^{-1}B_y^T$ with different α, and this inversion reduces to solving tridiagonal systems along mesh lines (for each mesh line independently from the other).

In paper [1] authors proposed a new approach to constructing splitting schemes for the heat flux. The main idea is to formulate a procedure how to recover a scheme for the flux from the "underlying" (chosen beforehand) scheme for flux divergence.

Obviously, there exist more than one way to do it since the divergence operator has a large kernel. However, it is suggested to fix the transformation by a certain way which allows to derive stability results from that for the "underlying" scheme. The formal procedure is sketched below.

Let us introduce the following operators

$$\Lambda = \equiv -M^{-1/2}(B_x^TA_x^{-1}B_x + B_y^TA_y^{-1}B_y)M^{-1/2} \equiv \Lambda_x + \Lambda_y. \tag{3}$$

Briefly, the transformation from a scheme for the flux divergence to a scheme for the heat flux consists of the following steps:

(1) Assume the initial scalar splitting ("underlying") scheme for flux divergence ξ is given in fractional steps with operators Λ_x and Λ_y which approximate second space derivatives.
(2) Replace ξ by $\mathbf{B}^T\mathbf{w}$ and Λ, Λ_x and Λ_y by the corresponding expressions from (3). As a result, one gets an equation of the following type for each fractional step of the "underlying" scheme:

$$B_x^TA_x^{-1}(...) + B_y^TA_y^{-1}(...) = 0$$

(3) Group terms with discrete derivative operators (B_x, B_y ...) together.
(4) Set each of the grouped terms to zero omitting the outer space derivatives. Thus, from each fractional step of the "underlying" scheme one obtains two equations which form together a fractional step of the recovered scheme for the heat flux.

Notice that as the "underlying" scheme one can take here well-known schemes like alternating direction schemes, locally one-dimensional schemes, predictor-corrector schemes and their various modifications, see, e.g. [4], [5], [6].

The inverse transformation (from scheme for the flux to the scheme for flux divergence) is much simpler and requires only to apply discrete divergence operator to an appropriate form of the initial vector scheme:

(1) Introduce (if necessary) additional fractional step variables $\mathbf{w}^{n+\beta}$ so that each equation of the scheme takes the form of

$$\frac{\mathbf{w}^{n+\frac{j}{p}} - \mathbf{w}^{n+\frac{j-1}{p}}}{\tau_p} + \sum_{k\le j} \alpha_k \mathbf{C}_k \mathbf{B}^T \mathbf{w}^{n+\frac{k}{p}} = 0$$

for some values of α_k, τ_p and matrices C_k. Matrices C_k will be of the same size as matrix $\mathbf{B}$. Apparently, any scheme can be rewritten in this form..

(2) Apply discrete divergence operator $\mathbf{B}^T$ to get the final scheme for the flux divergence in the form of

$$\frac{\xi^{n+\frac{j}{p}} - \xi^{n+\frac{j-1}{p}}}{\tau_p} + \sum_{k\le j} \alpha_k \mathbf{B}^T \mathbf{C}_k \xi^{n+\frac{k}{p}} = 0.$$

2. Splitting schemes for the heat flux and stability estimates

In this section we consider and analyze from the viewpoint of stability estimates two splitting schemes for the heat flux which were developed by the approach described above. The "underlying" scheme for the first is alternating direction scheme, for the second – predictor-corrector scheme.

First of all, to simplify notations of stability estimates, let's change notations from T and $\mathbf{w}$ (subscript h omitted) to $M^{1/2}T$ and $\mathbf{A}^{1/2}\mathbf{w}$ retaining the same names T and $\mathbf{w}$. Similarly, we replace operator $\mathbf{B}$ by $\mathbf{A}^{-1/2}\mathbf{B}M^{-1/2}$. Finally, replace f by $M^{-1/2}f$. Using new notations, the semidiscrete system (2) looks like:

$$\frac{dT}{dt} + \mathbf{B}^T\mathbf{w} = f\ , \quad \mathbf{w} = \mathbf{B}T\,. \tag{4}$$

Now let us write down the first splitting scheme for the heat flux [1] which is based on the "underlying" scheme of alternating directions proposed long ago in [8]. Obviously, this scheme approximates (4) with second order in time. In the canonical form of Samarskii [13] with zero right-hand side the scheme can be written as:

$$\left(\mathbf{E} + \frac{\tau}{2}\mathbf{B}\mathbf{B}^T + \frac{\tau^2}{4}\mathbf{D}\right)\frac{\mathbf{w}^{n+1} - \mathbf{w}^n}{\tau} + \mathbf{B}\mathbf{B}^T\mathbf{w}^n = \mathbf{0}\,. \tag{5}$$

Here, using notations (3),

$$\mathbf{D} = \begin{pmatrix} B_x\Lambda_y B_x^T & B_x\Lambda_y B_y^T \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} B_x\Lambda_y \\ 0 \end{pmatrix}\mathbf{B}^T\,, \tag{6}$$

For stability estimates we will also need finite-dimensional Hilbert space $\mathbf{H}$ with following dot product and norm

$$(\mathbf{u},\mathbf{v})_{\mathbf{H}} = (\mathbf{u},\mathbf{v})_{\mathbf{E}} + (\mathbf{B}\mathbf{B}^T\mathbf{u},\mathbf{v})_{\mathbf{E}}\,, \quad \|\mathbf{u}\|_{\mathbf{H}} = \sqrt{(\mathbf{u},\mathbf{u})_{\mathbf{H}}}\,,$$

where $(\mathbf{u},\mathbf{v})_{\mathbf{E}}$ is the standard euclidean dot product. Defined in this way, space $\mathbf{H}$ is the mesh counterpart of functional space $\mathbf{H}_{\mathrm{div}}(\Omega,\Gamma_1)$.

In paper [7] stability estimates were obtained for splitting scheme (5) with respect to initial data from the subspace $\widetilde{\mathbf{H}} \subset \mathbf{H}$ with stronger norm $\|\cdot\|_{\widetilde{\mathbf{H}}}$.

One should remark here that this norm appears due to the splitting error which perturbs mesh Fourier law in such way that the heat flux obtained by (5) has a nonzero component in the kernel of discrete divergence operator. This drawback happens to spoil convergence for scheme (5) as it is shown in the section 4 by numerical examples, but luckily does not take place for any scheme of predictor-corrector type.

The following theorems are valid for scheme (5)-(6):

Theorem 1. *Let operators Λ_x and Λ_y commute. Then the flux splitting scheme (5)-(6) is uniformly stable in $\mathbf{H}$ for initial data located in $\widetilde{\mathbf{H}}$, i.e., there exists such $c_1 > 0$ independent from τ and h such that $\forall\, \mathbf{w}^0 \in \widetilde{\mathbf{H}}$ there holds*

$$\begin{aligned} &\|\mathbf{w}^n\|_{\mathbf{H}} \le c_1\|\mathbf{w}^0\|_{\widetilde{\mathbf{H}}}\,, \quad n = 1,2,\ldots \\ &\|\mathbf{w}\|_{\widetilde{\mathbf{H}}} = \Big(\|\mathbf{w}\|^2_{\mathbf{H}} + \tau^4\|\Lambda_y\mathbf{B}^T\mathbf{w}\|^2_{\Lambda}\Big)^{1/2}. \end{aligned} \tag{7}$$

Theorem 2. *For scheme (5)-(6) there exists such $c_2 > 0$ independent from τ and h such that $\forall\, \mathbf{w}^0 \in \widetilde{\mathbf{H}}$ there holds*

$$\begin{aligned} &\|\mathbf{w}^n\|_{\mathbf{H}} \le c_2\Big(1 + \tfrac{\tau}{h}\Big)\|\mathbf{w}^0\|_{\widetilde{\mathbf{H}}}\,, \quad n = 1,2,\ldots \\ &\|\mathbf{w}\|_{\widetilde{\mathbf{H}}} = \Big(\|\mathbf{w}\|^2_{\mathbf{E}} + \|(E + \tfrac{\tau}{2}\Lambda_y)\mathbf{B}^T\mathbf{w}\|^2_2\Big)^{1/2} \end{aligned}$$

Thus, in order to guarantee convergence for splitting scheme (5) it is necessary that the initial heat flux approximates well the exact initial heat flux in the sense of the boundedness of the norm $\|\cdot\|_{\widetilde{\mathbf{H}}}$ from the corresponding theorem.

Recall that usually we have only temperature as initial data for the considered problem. Within our mixed finite element setting the initial heat flux is computed as the solution of

$$\mathbf{A}\mathbf{w}^0 = \mathbf{B}T^0.$$

Usual estimates [3] from finite element theory claim that $\mathbf{w}^0$ approximates exact initial heat flux $\mathbf{w}^0_{ex}$ with second order in space in the norm of space $\mathbf{H}$ which is the mesh counterpart of space $\mathbf{H}_{div}$. But not in the norm needed by stability results! Therefore, the question of how the norm $\|\mathbf{w}^0 - \mathbf{w}^0_{ex}\|_{\widetilde{\mathbf{H}}}$ behaves with respect to τ and h is nontrivial.

Now let us show that stability analysis is much simpler in case when the "underlying" scheme is of predictor-corrector type. It turns out that for this type of schemes the computed heat flux has always exactly zero component in the kernel of discrete divergence operator.

Indeed, assume that at each time moment discrete Fourier law is valid, i.e. $\mathbf{A}\mathbf{w}^n = \mathbf{B}T^n$, or, equivalently, $\mathbf{w}^{n,0} \equiv 0$ and, hence, component of the heat flux in the kernel is always zero. This can be also written as

$$\mathbf{A}\frac{\mathbf{w}^{n+1} - \mathbf{w}^n}{\tau} = \mathbf{B}\frac{T^{n+1} - T^n}{\tau}. \tag{8}$$

Notice that for any splitting scheme constructed via proposed approach, the temperature equation takes the form of

$$\frac{T^{n+1}-T^n}{\tau}+\mathbf{B}^T\mathbf{w}^{n+1/2}=0. \tag{9}$$

with appropriate choice of $\mathbf{w}^{n+1/2}$. Then in order to have (8) valid, it is necessary that

$$\mathbf{A}\frac{\mathbf{w}^{n+1}-\mathbf{w}^n}{\tau}+\mathbf{B}\mathbf{B}^T\mathbf{w}^{n+1/2}=0.$$

This equation can be considered as the corrector step and the only thing left to be defined is how we compute the intermediate heat flux $\mathbf{w}^{n+1/2}$.

Thus, the general form of a flux splitting scheme with zero component in the kernel of $\mathbf{B}^T$ is the following:

$$\left\{\begin{array}{ll} 1. & \text{predictor step – conputing } \mathbf{w}^{n+1/2} \\ 2. & \frac{T^{n+1}-T^n}{\tau}+\mathbf{B}^T\mathbf{w}^{n+1/2}=0 \\ 3. & \mathbf{A}\frac{\mathbf{w}^{n+1}-\mathbf{w}^n}{\tau}+\mathbf{B}\mathbf{B}^T\mathbf{w}^{n+1/2}=0 \end{array}\right. \tag{10}$$

Obviously, the "underlying" scheme for (10) is then:

$$\left\{\begin{array}{ll} 1. & \text{predictor step – computing}\xi^{n+1/2} \\ 2. & \frac{\xi^{n+1}-\xi^n}{\tau}+(\Lambda_x+\Lambda_y)\xi^{n+1/2}=0 \end{array}\right.$$

For flux splitting scheme (10) of predictor-corrector type stability analysis can be simplified whenever we have stability of the "underlying" predictor-corrector scheme for ξ.

Indeed, if predictor is stable in a norm denoted as $\|\cdot\|_T$, then $\|\xi^{n+1/2}\|\le C\|\xi^n\|\le C_{st}\|\xi^0\|$. This implies for temperature:

$$\|T^n\|_T\le\|T^0\|_T+C_{st}\|\mathbf{B}^T\mathbf{w}^0\|_T,$$

and for heat flux, since $\mathbf{w}^{n,0}\equiv 0$,

$$\|\mathbf{w}^n\|_w=\|\mathbf{w}^{n,1}\|_w\le C\|\mathbf{B}^T\mathbf{w}^{n,1}\|_T=C\|\xi^n\|_T\le C^{'}_{st}\|\xi^0\|_T\le C^{'}_{st}\|\mathbf{B}^T\mathbf{w}^0\|_T.$$

For instance, one of the possible predictors (among a variety of them) can be locally one-dimensional scheme based on the implicit scheme

$$\begin{array}{c} \frac{\xi^{n+1/4}-\xi^n}{\tau/2}+\Lambda_x\xi^{n+1/4}=0, \\ \frac{\xi^{n+1/2}-\xi^{n+1/4}}{\tau/2}+\Lambda_y\xi^{n+1/2}=0. \end{array}$$

The corresponding flux splitting scheme after fractional steps elimination takes the form of

$$\begin{array}{c} (\mathbf{A}+\frac{\tau^2}{4}\mathbf{S})\frac{\mathbf{w}^{n+1}-\mathbf{w}^n}{\tau}+\mathbf{B}M^{-1}\mathbf{B}^T\frac{\mathbf{w}^{n+1}+\mathbf{w}^n}{2}=\mathbf{B}M^{-1}\frac{f^{n+1}+f^n}{2} \\ M\frac{T^{n+1}-T^n}{\tau}+\mathbf{B}^T\frac{\mathbf{w}^{n+1}+\mathbf{w}^n}{2}+\frac{\tau^2}{4}B_x^TA_x^{-1}B_xM^{-1}B_y^T\frac{w_y^{n+1}-w_y^n}{\tau}=\frac{f^{n+1}+f^n}{2}, \end{array} \tag{11}$$

where

$$\mathbf{S}=\begin{pmatrix} 0 & B_x\Lambda_xB_y^T \\ 0 & B_y\Lambda_xB_y^T \end{pmatrix},$$

and is (after some simple change of notations) the scheme presented and studied in the work by Arbogast et. al. [12]. In [12] this scheme was proposed based on Uzawa algorithm implemented for non-stationary problem in the mixed form. Stability results were obtained in [12] using standard finite element technique. Unfortunately,

Gronwall's argument implies restriction like $\tau \sim h^2$ which seems rather impractical.
Remark. (on stability of classical predictor-corrector scheme for scalar equation)

In commutative case the scheme is another form of alternating direction scheme and, therefore, is stable in usual $\|\cdot\|_2$. In non-commutative case, as it is shown in [4],[5], the scheme is stable in a weaker norm $\|\cdot\|_{(E+\frac{\tau}{2}\Lambda_x)^{-1}}$.

3. Analysis on the uniform mesh

In this section we study the norm $\|\cdot\|_{\widetilde{\mathbf{H}}}$ from a priori stability estimate (7) using decomposition onto discrete harmonics.

Under the conditions of Theorem 1 the squared norm in the right-hand side of (7) differs from squared norm in discrete $\mathbf{H}$ by the following term:

$$\|\mathbf{v}\|^2_{\widetilde{\mathbf{H}}} - \|\mathbf{v}\|^2_{\mathbf{H}} = (\tau^2\|\mathbf{v}\|_*)^{\mathbf{2}} = \tau^{\mathbf{4}}\|\mathbf{\Lambda_y B^T v}\|^{\mathbf{2}}_{\mathbf{\Lambda}},$$

In the component-wise representation $\|\mathbf{v}\|^{\mathbf{2}}_*$ can be rewritten as

$$\|\mathbf{v}\|^2_* = \|\Lambda_y\mathbf{B}^T\mathbf{v}\|^2_\Lambda = \|\Lambda^{1/2}\Lambda_y\mathbf{B}^T\mathbf{v}\|^2_2 = ((\Lambda_x+\Lambda_y)\Lambda_y\mathbf{B}^T\mathbf{v}, \Lambda_y\mathbf{B}^T\mathbf{v})$$

or, taking into account the equation for the initial heat flux $\mathbf{w}^0$,

$$\|T\|^2_{**} = \|\mathbf{A^{-1}Bv}\|^2_* = ((\Lambda_x+\Lambda_y)\Lambda_y(\Lambda_x+\Lambda_y)T, \Lambda_y(\Lambda_x+\Lambda_y)T)$$

From this representation one may suppose that on uniform mesh (at least, far from the boundaries) the mesh operator which generates the norm, approximates 4th space derivatives of the heat flux or, equivalently, 5th derivatives of the initial temperature. The further suggestion is that if initial temperature T^0 is a mesh projection of a smooth function, then the expression $\|\mathbf{v}\|_*$ will be bounded independently from the mesh step. However, as we show below this is not true.

In case of uniform mesh additional smoothness requirements imposed in stability estimates of Theorem 1 can be analyzed through decomposition onto generalized eigenvectors which were obtained in an explicit form in [11]. In one-dimensional case the eigenvectors and eigenvalues can be written for different boundary conditions (D for Dirichlet and N for Neumann, i.e. DD means Dirichlet conditions on both sides) in the following form:

(DD):
$\gamma^k_{DD} = 2sin\frac{(k+1)\pi}{2N}, k = 0, ..., N-1$
$u^k_{DD}(i) = sin\frac{(k+1)\pi(2i+1)}{2N}, i, k = 0, ..., N-1$
$p^k_{DD}(i) = cos\frac{k\pi i}{N}, i, k = 0, ..., N$

(NN):
$\gamma^k_{NN} = 2sin\frac{k\pi}{2N}, k = 0, ..., N-1$
$\gamma^k_{NN} = cos\frac{k\pi(2i+1)}{2N}, k = 0, ..., N-1$
$\gamma^k_{NN} = sin\frac{k\pi i}{N}, i, k = 0, ..., N$

where N is the number of mesh points in one direction. With this in mind, one can then formulate the main equalities:

$$Ap^k = \frac{6-(\gamma^k)^2}{6}Mp^k, \quad Bu^k = \frac{\gamma^k}{h}Mp^k, \quad B^Tp^k = \frac{\gamma^k}{h}u^k$$

where diagonal matrix M is defined as $M = diag\{\frac{1}{2}, 1, ..., 1, \frac{1}{2}\}$. Finally, one can deduce that for one-dimensional operators Λ_x and Λ_y

$$\Lambda_{x(y)}u^k \equiv B^TA^{-1}Bu^k = \lambda^k u^k, \quad \lambda^k = \frac{6(\gamma^k)^2}{(6-(\gamma^k)^2)h^2}$$

Due to the definition of Raviart-Thomas finite elements these results on eigenvectors and eigenvalues can be easily extended to the two- and three-dimensional cases by considering tensor product of one-dimensional operators.

Using the given eigensystem one can notice that

$$\|T\|_{**}^2 = \sum_{i=1}^{N}\sum_{j=1}^{N} T_{ij}^2 (\lambda^j)^2 (\lambda^i + \lambda^j)^3 (\psi_{ij}, \psi_{ij})_{2,h}$$

where indices i, j correspond to the $x-$ and $y-$directions, basis vectors are $\psi_{ij} = u_x^i \otimes u_y^j$ and T_{ij} are the decomposition coefficients of mesh temperature T onto the basis vectors ψ_{ij}.

Now we estimate behavior of $\|T\|_{**}^2$ with respect to mesh step $h = \frac{1}{N}$. First notice that

$$(\psi_{ij}, \psi_{ij})_{2,h} \sim \int_0^1 cos(\pi i x)dx \int_0^1 sin(\pi j y)dy \sim 1.$$

Then,

$$\gamma^j = 2sin\frac{\pi j h}{2} \sim \pi j h, \quad h \to 0,$$

and the two-sided estimate of eigenvalues follows:

$$j^2 \sim \frac{(\gamma^j)^2}{h^2} \le \lambda^j \equiv \frac{6(\gamma^j)^2}{(6-(\gamma^j)^2)h^2} \le 3\frac{(\gamma^j)^2}{h^2} \sim j^2, \quad h \to 0.$$

Thus,

$$\|T\|_{**}^2 \sim \sum_{i=1}^{N}\sum_{j=1}^{N} T_{ij}^2 j^4 (i^2 + j^2)^3$$

From this it is easy to deduce sufficient conditions on asymptotic behavior of coefficients T_{ij}. For instance,

1) if $T_{ij} \sim h^2 \frac{1}{j^2(i^2+j^2}^{3/2}$ for sufficiently small h and sufficiently large i, j, then $\|T\|_{**} \sim 1$,

2) if $T_{ij} \sim h \frac{1}{j^2(i^2+j^2}^{3/2}$ for sufficiently small h and sufficiently large i, j, then $\|T\|_{**} \sim h^{-1}$.

One of the possible applications of the above analysis is modifying the initial flux computation so as to guarantee convergence of the heat flux. For instance, as the initial heat flux one can consider solution of a minimization problem for a quadratic functional of type $\|\mathbf{A}\mathbf{w} - \mathbf{B}T\|^2 + h^{2\alpha}\|\mathbf{w}\|_*^2$, where α depends on the asymptotic behavior of coefficients T_{ij} for large i, j and small h. It is also important to notice that smoothness of the initial temperature as a function does not play a part since it affects only slightly the asymptotic behavior of T_{ij}. This is illustrated by numerical experiments (tests 2 and 3) which are given in the next section.

4. Numerical experiments

For all experiments the domain was the unit square $[0, 1]^2$. If it is not mentioned it is assumed that boundary conditions are homogeneous (Dirichlet for y and Neumann for x), all coefficients equal to one. In tables below the following short notations are used:

$$\varepsilon_T^n = T^n - T_{ex}^n$$
$$\varepsilon_w^n = \mathbf{w}^n - \mathbf{w}_{ex}^n$$

If a temperature or heat flux norm does not have a time index it is assumed that maximum over all time moments t_n is chosen. In all tables but one in the last row the rate of decaying with respect to h is given for the corresponding column values.

4.1. **Flux splitting scheme based on alternating direction scheme.**

4.1.1. *Uniform mesh.* First we consider the simplest case when the mesh is uniform and coefficients are constant. The analytical test solutions were:

$$T_1(x, y) = e^{-t} \cdot cos(2\pi x) \cdot sin(2\pi y)$$
$$T_2(x, y) = e^{-t} \cdot cos(2\pi x) \cdot y \cdot sin(2\pi y)$$
$$T_3(x, y) = cos(\pi t) \cdot sin(x(1-x)y(1-y))$$

which we refer to as test 1 – test 3 correspondingly.

In table 1 errors of the heat flux are given in discrete C and L_2 norms for tests 1 – 3 are presented. Time step was chosen so that $\frac{\tau}{h} = 3.2$.

Table 1. Heat flux error, $\frac{\tau}{h} = 3.2$, tests 1 – 3.

	test 1		test 2		test 3	
h	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$
2^{-5}	3.5e-1	2.5e-1	**3.1e+2**	**6.4e+1**	**8.6e+0**	**1.8e+0**
2^{-6}	5.9e-2	4.1e-2	**3.1e+2**	**4.6e+1**	**1.1e+1**	**1.5e+0**
2^{-7}	1.3e-2	9.1e-3	**4.1e+2**	**4.3e+1**	**1.2e+1**	**1.2e+0**
	h^2	h^2	h^{0-}	$h^{1/2}$	h^{0-}	$h^{1/2}$

Results in table 1 show that only test 1 converges with second order, for test 2 and 3 there is no convergence ($\sim h^0$) in the C-norm and only a rather weak convergence ($\sim h^{1/2}$) in L_2-norm. This happens despite the fact that all tests are smooth inifinitely differentiable functions.

In table 2 error for the heat flux is presented in case when $\frac{\tau}{h^2} = 3.2$ (cf. with Table 1).

Table 2. Heat flux error, $\frac{\tau}{h^2} = 3.2$, tests 1 – 3.

	test 1		test 2		test 3	
h	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$
2^{-5}	3.5e-1	2.5e-1	3.1e+2	6.4e+2	8.6e+0	1.8e+0
2^{-6}	1.6e-2	1.0e-2	1.0e+2	1.5e+1	2.3e+0	4.2e-1
2^{-7}	1.0e-3	6.4e-4	3.4e+1	3.6e+0	8.5e-1	4.2e-2

These results show that having $\tau \sim h^2$ implies convergence with order higher than two in L_2-norms for all tests. Hence, comparing tables 1 and 2 we understand that the convergence is conditional. Obviously, restriction $\tau \sim h^2$ is of the same type as stability condition of the explicit time discretization which makes the idea of any splitting schemes completely useless in this case..

In table 3 heat flux error for test 3 is given in case of nonuniform mesh when $\tau \sim h$ but exact(!) initial heat flux values are used instead of computing it from the discrete Fourier law.

Table 3. Heat flux error for $\mathbf{w}^0 = \mathbf{w}^0_{ex}$ with nonuniform mesh, $\frac{\tau}{h} = 3.2$, test 3.

h		test 3	
h_1	h_2	$\Vert \varepsilon_w \Vert_C$	$\Vert \varepsilon_w \Vert_{L_2}$
$1/30$	$1/36$	1.3e-2	7.2e-3
$1/60$	$1/72$	3.6e-3	1.7e-3
$1/120$	$1/144$	9.3e-4	4.3e-4
		h^2	h^2

As Table 3 shows, when $\mathbf{w}^0 = \mathbf{w}^0_{ex}$ the convergence is of second order and the overall accuracy is very high even for test 3 even for nonuniform mesh. Summing up results presented in tables 1 - 3 we notice that the main difficulty for the flux splitting scheme based on alternating direction scheme hides in the initial heat flux computation (from the viewpoint of a priori stability estimate (7)).

In table 4 we analyze the behavior of the norm from a priori estimate (7) for tests 1 – 3.

Table 4. Behavior of $\|\cdot\|_{**}$ for tests 1 – 3.

	test 1		test 2		test 3	
h	$\|T^0_{ex}\|_{**}$	$\|\varepsilon^0_T\|_{**}$	$\|T^0_{ex}\|_{**}$	$\|\varepsilon^0_T\|_{**}$	$\|T^0_{ex}\|_{**}$	$\|\varepsilon^0_T\|_{**}$
2^{-5}	1.4e+4	6.7e+1	1.0e+7	4.3e+5	4.1e+4	1.7e+4
2^{-6}	1.4e+4	1.7e+1	5.6e+7	2.4e+6	2.3e+5	9.9e+4
2^{-7}	1.4e+4	4.0e+0	3.2e+8	1.4e+7	1.3e+4	5.6e+5
	h^0	h^2	$h^{\mathbf{-5/2}}$	$h^{\mathbf{-5/2}}$	$h^{\mathbf{-5/2}}$	$h^{\mathbf{-5/2}}$

Although all test solutions are smooth, for test 2 and 3 the norm $\|T^0_{ex}\|_{**}$ is increasing when $h \to 0$ as $h^{-5/2}$. The difference between test 1 and test 2 – 3 is the behavior of coefficients T_{ij} of decomposition onto discrete harmonics. Spectrum of test 1 contains only one harmonic whereas test 2 and 3 have a bunch of them in the spectrum due to the presence of polynomials in y.

For tests 2 and 3 the error is localized near the domain boundary with Dirichlet boundary conditions ($y = 0, y = 1$). Below we check the suggestion that the convergence issues occur due to the Dirichlet boundary conditions which are implicitly included in the mesh operators and the norm $\|\cdot\|_{**}$. Consider another test which satisfies both Neumann and Dirichlet boundary conditions for $y = 0$ and $y = 1$.

$$T_4(x, y) = e^{-t} \cdot cos(2\pi x) \cdot y^2(1 - y)^2$$

In table 5 behavior of $\|\varepsilon^0_T\|_{**}$ is studied for Dirichlet and Neumann boundary conditions.

Table 5. Comparison of $\|\varepsilon^0_T\|_{**}$ for test 4, different boundary conditions.

	Dirichlet for y		Neumann for y	
h	$\|T^0_{ex}\|_{**}$	$\|\varepsilon^0_T\|_{**}$	$\|T^0_{ex}\|_{**}$	$\|\varepsilon^0_T\|_{**}$
2^{-5}	1.6e+5	6.8e+4	9.2e+5	7.5e+3
2^{-6}	9.0e+5	3.8e+5	5.2e+5	2.1e+4
2^{-7}	5.1e+6	2.2e+6	2.9e+6	6.1e+4
	$h^{-5/2}$	$h^{-5/2}$	$h^{-5/2}$	$h^{\mathbf{-3/2}}$

One can conclude from table 5 that behavior of $\|\varepsilon^0_T\|_{**}$ is slightly better for Neumann than for Dirichlet boundary conditions. However, even for Neumann boundary conditions the norm $\|\cdot\|_{**}$ of the initial heat flux error can behave as $h^{-3/2}$, which for $\tau \sim h$ implies very weak convergence with order $h^{1/2}$ in L_2-norm.

4.1.2. *Nonuniform mesh.* Consider the following nonuniform mesh in $[0, 1]^2$ is given:

$$h = \begin{cases} h_1, & y \le 1/2, \\ h_2, & y > 1/2. \end{cases}$$

In tables 6 and 7 we study heat flux error and behavior $\|\varepsilon^0_T\|_{**}$ for test 1 and test 2 on the nonuniform mesh.

Table 6. Heat flux error for nonuniform mesh, $\frac{\tau}{h} = 3.2$, tests $1-2$.

h		test 1		test 2	
h_1	h_2	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$
1/30	1/36	1.8e+2	3.4e+1	3.9e+2	7.2e+1
1/60	1/72	1.8e+2	2.4e+1	3.9e+2	5.1e+1
1/120	1/144	1.8e+2	1.7e+1	5.14e+2	4.8e+1
		h^0	$h^{1/2}$	h^{0-}	$h^{1/2}$

Table 7. Behavior of $\|\varepsilon_T^0\|_{**}$ for nonuniform mesh, test $1-2$.

h		test 1		test 2	
h_1	h_2	$\|T_{ex}^0\|_{**}$	$\|\varepsilon_T^0\|_{**}$	$\|T_{ex}^0\|_{**}$	$\|\varepsilon_T^0\|_{**}$
1/30	1/36	1.4e+4	2.3e+5	1.1e+6	4.9e+5
1/60	1/72	1.4e+4	1.3e+6	6.4e+6	2.8e+6
1/120	1/144	1.4e+4	7.4e+6	3.6e+7	1.6e+7
		h^0	$h^{-5/2}$	$h^{-5/2}$	$h^{-5/2}$

Apparently, if the mesh is nonuniform the behavior of the norm $\|\varepsilon_T^0\|_{**}$ and convergence cannot get better than for uniform case. The main remark here is that it actually does not make the situation worse (at least, when the mesh step changes in a finite h-independent number of points) despite the fact that approximation of high-order derivatives in $\|\varepsilon_T^0\|_{**}$ gets worse around the places where the mesh step changes.

Remark. (variable heat conductivity)

If the heat conductivity is no longer constant the same convergence issues happen as considered above.

4.2. **Flux splitting scheme based on predictor-corrector scheme.** According to results of section 3 flux splitting scheme (11) does not suffer from conditional convergence issues as scheme (5)-(6) , since scheme (11) belongs to the predictor-corrector type of scheme with stable predictor. In tables 8 and 9 heat flux error is presented for test $1-3$ on uniform and nonuniform meshes respectively, cf. with tables 1 and 5.

Table 8. Heat flux error for tests $1-3$, $\frac{\tau}{h} = 3.2$, uniform mesh.

	test 1		test 2		test 3	
h	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$
2^{-5}	2.6e-1	1.8e-1	3.2e-1	1.2e-1	1.1e-2	6.2e-3
2^{-6}	7.3e-2	5.2e-2	9.0e-2	3.4e-2	2.7e-3	1.5e-3
2^{-7}	1.8e-2	1.3e-2	2.3e-2	8.3e-3	6.7e-4	3.8e-4
	h^2	h^2	h^2	h^2	h^2	h^2

Table 9. Heat flux error for tests $1-2$, $\frac{\tau}{h} = 3.2$, nonuniform mesh.

h		test 1		test 2	
h_1	h_2	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$	$\parallel \varepsilon_w \parallel_C$	$\parallel \varepsilon_w \parallel_{L_2}$
1/30	1/36	2.6e-1	1.8e-1	3.1e-1	1.2e-1
1/60	1/72	7.4e-2	5.2e-2	8.9e-2	3.5e-2
1/120	1/144	1.8e-2	1.3e-2	2.3e-2	8.5e-3
		h^2	h^2	h^2	h^2

As expected, for all test solutions one has convergence with second order. Non-uniformity of mesh does not spoil convergence order as well as overall accuracy.

5. Conclusion

In this work we study previously observed convergence issues for the flux splitting scheme based on alternating direction scheme for flux divergence. It is shown that conditional convergence for some tests is in full agreement with a priori estimates proved before. The obtained results show that for convergence of flux splitting scheme based on alternating direction scheme for flux divergence it is required to have exact values of the initial heat flux as initial data.

The main drawback of the scheme is that its heat flux has nonzero component in the kernel of discrete divergence operator which is in turn very sensitive to the small approximation errors in the orthogonal complement. Theoretical analysis of a priori estimates behavior was carried out using results from [11] where an explicit form of the eigensystem was obtained in one-dimensional case. On the basis of eigenvectors decomposition we derive sufficient conditions on discrete Fourirer coefficients to guarantee convergence of the flux splitting scheme based on alternating direction scheme for certain test solutions.

Based on the provided analysis and results of numerical experiments we consider the idea that if one takes scalar splitting scheme of predictor-corrector type, then constructs within the proposed general approach the corresponding vector splitting scheme for the heat flux then the resulting scheme for the flux will enjoy simple stability estimates and will not suffer from any convergence issues. Numerical results confirm this theoretical suggestion. Therefore, we conclude that predictor-corrector type of schemes are much more preferable than others due to the presence of simple stability estimates and efficiency from the viewpoint of implementation.

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