MATRIX-EQUATION-BASED STRATEGIES FOR CONVECTION-DIFFUSION EQUATIONS

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Abstract. We are interested in the numerical solution of nonsymmetric linear systems arising from the discretization of convection-diffusion partial differential equations with separable coefficients and dominant convection. Preconditioners based on the matrix equation formulation of the problem are proposed, which naturally approximate the original discretized problem. For certain types of convection coefficients, we show that the explicit solution of the matrix equation can effectively replace the linear system solution. Numerical experiments with data stemming from two and three dimensional problems are reported, illustrating the potential of the proposed methodology.

Key words. Convection-diffusion equations, iterative solvers, preconditioning, matrix equations.

AMS subject classifications. 65F10, 65F30

1. Introduction. We are interested in the numerical solution of the convection-diffusion partial differential equation

\[-\varepsilon \Delta u + \mathbf{w} \cdot \nabla u = f, \quad \text{in } \Omega \subset \mathbb{R}^d,\]  

with \(d = 2, 3\), where \(\mathbf{w}\) is the convection vector, while \(\varepsilon\) is the viscosity parameter. In particular, we consider the dominant convection case, that is \(|\mathbf{w}| \gg \varepsilon\), and we assume that \(\mathbf{w}\) is incompressible, that is \(\text{div}(\mathbf{w}) = 0\). Moreover, we assume that the components of \(\mathbf{w}\) are separable functions in the space variables. For simplicity the equation is equipped with Dirichlet boundary conditions; the analyzed procedures could be used with Neumann boundary conditions as well.

Standard finite difference or finite element discretizations yield the algebraic large nonsymmetric linear system

\[Au = f, \quad \text{with } A \in \mathbb{R}^{N \times N}.\]  

The discretization phase is crucial to obtain a reliable numerical solution to (1.1), as spurious oscillations may occur in the approximate solution in the dominant convection regime; see, e.g., [10]. A variety of strategies is available, which either take a fine enough discretization, or appropriately modify the differential operator so as to limit the convection side-effects [14]; see [30] for a recent essay on the subject. In our numerical experiments we used the former approach, though the proposed methodology could also be adapted to handle, e.g., SUPG techniques [23].

We are interested in exploring preconditioning strategies for solving (1.2), that stem from knowledge of the differential operator and its discretization. In particular, a computationally cheap approximation to the original differential operator will be employed, that exploits the original matrix equation structure of the problem. The idea of using a simplified operator as a preconditioner is well known in the convection-diffusion equation literature. More precisely, classical strategies use the symmetric
part of the operator – see, e.g., [13],[1], and in particular the discussion in [19] – due to the fact that a symmetric problem is usually cheaper to solve than the original nonsymmetric system if fast solvers such as fast Fourier transform, cyclic reduction or multigrid can be employed. In the case of nonsymmetric preconditioners, attempts have focussed on simplifying the operator so as to still use fast solvers, and this is achieved, e.g., by imposing constant coefficients or by dropping some of the first order terms; see, e.g., [2],[7],[9],[13]. However, their effectiveness and computational cost of their application have not been clearly assessed. Finally, most publications aim at analyzing the two-dimensional (2D) problem, whereas the three-dimensional (3D) problem represents a challenging task, especially from a computational point of view.

We exploit the matrix structure of the discretized problem to construct a cost-effective nonsymmetric approximation: the application of the new preconditioner amounts to solving a Sylvester matrix equation, whose coefficient matrices are tightly related to the original discretized problem. Other authors have used matrix equations either as a solver or as a preconditioner for the system stemming from (1.1); see, e.g., [32], [33], [29], [26]. However, on the one hand, only very simplified models have been considered, on the other hand, to the best of our knowledge no performance evaluation has ever been performed with respect to more common multilevel techniques. We derive a new preconditioning operator by first writing down the full multiterm matrix equation corresponding to finite difference discretization of the two or three-dimensional problem and then by appropriately simplifying the operator; then we iteratively solve the associated Sylvester equation so as to achieve good performance of the overall preconditioning phase. The choice of the Sylvester equation solver is crucial for assessing the preconditioning costs. In the literature, ADI and cheap solvers for the Kronecker formulation were suggested for various (e.g. symmetric) variants of the problem [7],[15],[33]; here we exploit a recently developed efficient iterative solver for the Sylvester equation, whose cost per inner iteration for a 2D problem may be as low as \(O(n)\), where \(n\) is the one-dimensional problem size; this solver allows us to preserve the leading coefficients of the two first order derivatives without losing efficiency.

Our preliminary numerical results are promising and clearly illustrate the potential of this approach: the overall solution compares rather well with state-of-the-art and finely tuned algebraic multigrid preconditioners. When used as a solver, in both 2D and 3D problems, its performance is superior to other available approaches. Finally, our numerical experiments confirm theoretical results in the literature on the robustness of the approach with respect to the mesh parameter, namely the number of iterations of the system solver is essentially independent of the problem size.

Our aim is to derive a proof-of-concept preconditioning procedure for the finite difference discretization of the problem on rectangular and parallelepipidal domains, as a first step towards its higher level development for the finite element discretization on more general domains.

Here is a synopsis of the paper. In section 2 we derive the matrix formulation of the two-dimensional discretized problem, from which the standard form (1.2) is derived by means of Kronecker product expansion. Section 3 describes how the boundary conditions can be embedded in the matrix formulation. Section 4 uses the previously derived form to define the preconditioning operator and its associated Sylvester matrix equation, while implementation details are given in section 4.1. The procedure is then generalized to three dimensional problems in section 5, while numerical experiments with systems stemming from both two and three dimensional data are reported in
section 6. Finally, our conclusions are given in section 7.

2. A matrix oriented formulation. In this section we reformulate the algebraic problem (1.1) in terms of a multiterm linear matrix equation. This derivation will be used to introduce our preconditioner, to be applied to a Krylov subspace method as an acceleration strategy for solving (1.2). For the ease of presentation, we shall first concentrate on the two-dimensional problem, and then extend our derivation to the three-dimensional case in section 5.

We start by recalling the matrix equation associated with the discretization by five-point stencil finite differences of the Poisson equation $-\Delta u = f$ on a rectangular domain $\Omega \subset \mathbb{R}^2$. For the sake of simplicity, we shall assume that $\Omega = (0, 1)^2$. Let $\Omega_h$ be a uniform discretization of $\Omega$, with nodes $(x_i, y_j)$, $i, j = 1, \ldots, n$. Then assuming homogeneous Dirichlet boundary conditions are used, centered finite difference discretization leads to the linear system (1.2) with

$$A = T_{n-1} \otimes I_{n-1} + I_{n-1} \otimes T_{n-1},$$

and $T_{n-1} = \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{(n-1) \times (n-1)}$ is the symmetric tridiagonal matrix approximating the second-order derivative in one-dimension, while the entries of $u$ contain an approximation to $u$ at the nodes, having used a lexicographic order of the entries.

We thus take a step back, and describe in details the process leading to the Kronecker formulation, with the aim of deriving its matrix counterpart. This description will allow us to also include the boundary conditions in a systematic manner.

Let $\bar{\Omega}_h$ be a uniform discretization of the closed domain $\bar{\Omega}$, with equidistant points in each direction, $(x_i, y_j)$, $i, j = 0, \ldots, n$. Analogously, $U_{i,j} = U(x_i, y_j)$ is the value of the approximation $U$ to $u$ at the nodes. For each $i, j = 1, \ldots, n - 1$ we have the usual approximations

$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} = \frac{1}{h^2} [1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix},$$

and analogously for the $y$ direction, but from the right,

$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = \frac{1}{h^2} [U_{i,j-1}^T, U_{i,j}^T, U_{i,j+1}^T]^{-1} [-2, 1].$$

Let

$$T = -\frac{1}{h^2} \begin{pmatrix} * & * & & & & & \\
\star & -2 & 1 & & & & \\
& 1 & \ddots & \ddots & & & \\
& & \ddots & 1 & \ddots & & \\
& & & \ddots & \ddots & \ddots & \\
& & & & 1 & -2 & * \\
& & & & \star & * & \star \end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}; \quad (2.1)$$

the unspecified values $\ast$ are associated with boundary values of $U$ and will be discussed in section 3. Collecting these relations for all rows $i$'s and for all columns $j$'s, for the whole domain we obtain

$$-u_{xx} \approx TU, \quad -u_{yy} \approx UT.$$
With these approximations we can write the following classical matrix form of the finite difference discretization of the Poisson equation on a square domain (see, e.g., [31])

$$TU + UT = F,$$

where $F_{i,j} = f(x_i, y_j) + b.c.$ (2.2)

Except for the boundary conditions, the Kronecker formulation of (2.2) gives the same form as (1.2).

For the convection-diffusion equation with separable coefficients a similar derivation provides a multiterm linear matrix equation. We state the result in the following proposition, where separable convection coefficients are assumed. To this end, we define the matrix

$$B = \frac{1}{2h} \begin{bmatrix}
* & * \\
* & 0 & 1 \\
& -1 & \ddots & \ddots \\
& \ddots & \ddots & 1 \\
& -1 & 0 & * \\
* & * \\
\end{bmatrix} \in \mathbb{R}^{(n+1) \times (n+1)},$$

(2.3)

which represents the centered finite difference approximation of the first order one dimensional (1D) derivative on a uniformly discretized interval.

**Proposition 2.1.** Assume that the convection vector $w = (w_1, w_2)$ satisfies $w_1 = \phi_1(x)\psi_1(y)$ and $w_2 = \phi_2(x)\psi_2(y)$. Let $(x_i, y_j) \in \bar{\Omega}_h$, $i, j = 0, \ldots, n$ and set $\Phi_k = \text{diag}(\phi_k(x_0), \ldots, \phi_k(x_n))$ and $\Psi_k = \text{diag}(\psi_k(y_0), \ldots, \psi_k(y_n))$, $k = 1, 2$. Then with the previous notation, the centered finite-difference discretization of the differential operator in (1.1) leads to the following operator:

$$\mathcal{L}_h : U \rightarrow \epsilon TU + \epsilon UT + (\Phi_1 B)U\Psi_1 + \Phi_2 U(B^T\Psi_2).$$

(2.4)

**Proof.** The first two terms of $\mathcal{L}_h(U)$ were derived for (2.2). We are left with showing that the first order term can be expressed in terms of the 1D discretization matrix $B$ in (2.3). We have

$$\phi_1(x_i)\psi_1(y_j)u_x(x_i, y_j) \approx \phi_1(x_i)\frac{u(x_{i+1}, y_j) - u(x_{i-1}, y_j)}{2h} \psi_1(y_j)$$

$$= \frac{1}{2h} \phi_1(x_i)[-1, 0, 1] \begin{bmatrix}
U_{i-1,j} \\
U_{i,j} \\
U_{i+1,j} \\
\end{bmatrix} \psi_1(y_j),$$

and analogously,

$$\phi_2(x_i)\psi_2(y_j)u_y(x_i, y_j) \approx \frac{1}{2h} \phi_2(x_i)[U_{i,j-1}, U_{i,j}, U_{i,j+1}] \begin{bmatrix}
-1 \\
0 \\
1 \\
\end{bmatrix} \psi_2(y_j).$$

Collecting these results for all grid nodes and recalling that $U_{i,j} = U(x_i, y_j)$, we obtain

$$(\phi_1(x_i)\psi_1(y_j)u_x(x_i, y_j))_{i,j=0,\ldots,n} \approx \Phi_1 BU\Psi_1,$$

$$(\phi_2(x_i)\psi_2(y_j)u_y(x_i, y_j))_{i,j=0,\ldots,n} \approx \Phi_2 U(B^T\Psi_2),$$
and the result follows.

The operator in (2.4) is a linear multiterm matrix function, and it is a general variant of the matrix equations already present in the early literature on difference methods [4]. This type of equations now often arises in the discretization of partial differential equations with stochastic terms; see [28] for a description of this and other contexts where these operators arise. In the deterministic setting, however, the difficulty of explicitly dealing with all terms have led the scientific community to abandon this form, in favor of the Kronecker formulation.

3. Imposing the boundary conditions. The algebraic problem needs to be completed by imposing the boundary values. These will fill up the undefined entries in the coefficient matrices, and in the right-hand side matrix. To this end, we recall that with the given ordering of the elements in $U$, the first and last columns, $Ue_1$ and $Ue_{n+1}$ resp., correspond to the boundary sides $y = 0$ and $y = 1$, whereas the first and last rows take up the values at the boundary sides $x = 0$ and $x = 1$. With this notation, we wish to complete the corners of the matrices $T$ and $B$, giving rise to the matrices $T_1, T_2$ and $B_1, B_2$, respectively, so that the following matrix equation is well defined for $(x, y) \in \bar{\Omega}_h$:

$$
\varepsilon T_1 U + \varepsilon UT_2 + \Phi_1 B_1 U \Psi_1 + \Phi_2 U B_2 \Psi_2 = F.
$$

(3.1)

With the same notation as for $U$, the entries of $F$ corresponding to $i, j \in \{0, n\}$ will contain contributions from the boundary values of $U$, which are determined next.

For the boundary conditions to be satisfied, the operator $L_h(U) = \varepsilon T_1 U + \varepsilon UT_2 + \Phi_1 B_1 U \Psi_1 + \Phi_2 U B_2 \Psi_2$ should act as the (scaled) identity operator for points at the boundary. To this end, from the generic matrix $T$ we define the matrix $T_1$ as follows:

$$
T_1 = -\frac{1}{h^2} \begin{pmatrix}
-1 & 0 & 1 & -2 & 1 & & \\
1 & -2 & 1 & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
0 & -1 & & & & & \\
\end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)},
$$

while the matrix corresponding to the first order operator ($B$ in the generic case) can be written as

$$
B_1 = \frac{1}{2h} \begin{pmatrix}
0 & 0 & 1 & & & & \\
-1 & 0 & 1 & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
-1 & 0 & 1 & & & & \\
0 & 0 & & & & & \\
\end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}.
$$

For the derivative in the $y$ direction, right multiplication should also act like the identity, therefore we can define $T_2 = T_1^T$ and correspondingly, $B_2 = B_1^T$. We are thus ready to define the missing entries in $F$ so that (3.1) holds. For the first column, that is for the side $y = 0$, we write

$$
F e_1 = (\varepsilon T_1 U + \varepsilon UT_2 + \Phi_1 B_1 U \Psi_1 + \Phi_2 U B_2 \Psi_2) e_1 \\
= \varepsilon T_1 U e_1 + \varepsilon UT_2 e_1 + \Phi_1 B_1 U \Psi_1 e_1 + \Phi_2 U B_2 \Psi_2 e_1 \\
= \varepsilon T_1 U e_1 + \frac{\varepsilon}{h^2} U e_1 + \Psi_1(y_0) \Phi_1 B_1 U e_1,
$$
where we used the fact that $B_2 \Psi_2 e_1 = 0$. Similar reasonings ensure that the boundary values at $y = 1$ are imposed, thus defining $F e_{n+1}$. For the side $x = 0$ we have

$$c_1^T F = e_1^T (c T_1 U + c U T_2 + \Phi_1 B_1 U \Psi_1 + \Phi_2 U B_2 \Psi_2) = e_1^T F$$

$$= e_1^T c T_1 U + e_1^T c U T_2 + e_1^T \Phi_1 B_1 U \Psi_1 + e_1^T \Phi_2 U B_2 \Psi_2$$

$$= \frac{e}{h^2} e_1^T U + e \epsilon^T U T_2 + \phi_2(x_0) e_1^T U B_2 \Psi_2,$$

where the fact that $e_1^T \Phi_1 B_1 = 0$ was used. The definition of $e_{n+1}^T F$ follows analogously.

We stress that maintaining the same boundary conditions in the designed preconditioner has other benefits, in addition to accurately reproducing the original operator. Indeed, it was shown in [20] that if the preconditioner is itself a matrix arising from the discretization of an elliptic operator, then under certain regularity assumptions the $L_2$-norm of the preconditioned matrix $AP^{-1}$ is uniformly bounded with respect to the discretization parameter.

4. The new preconditioner. The main obstacle in directly solving equation (2.4) is given by its many general terms. Indeed, had the equation terms with coefficient matrices on either side of the unknown matrix, the problem would be readily recognized as a matrix Sylvester equation. This scenario does occur whenever some of the convection terms have a simplified structure, so that those terms only depend on some of the variables. This is the case, for instance, with the operator $L(u) = -\Delta u + \phi_1(x) u_x$, which gives rise to $L_h(U) = T_1 U + UT_2 + \Phi_1 B_1 U = (T_1 + \Phi_1 B_1) U + UT_2$. In this case, computational strategies based on the matrix equation can be employed; see, e.g., [32],[29], and [8] and its references for some early methods; see also section 6 for some examples with state-of-the-art approaches. In the general multiterm case, a simplified version of the left-hand side in (2.4) can be used as an acceleration operator, in the form of a matrix equation solver; a similar strategy was adopted in [7], with encouraging numerical results with early solution methods. Let

$$L_h : Y \mapsto c T_1 Y + c Y T_2 + (\Phi_1 B_1) Y \Psi_1 + \Phi_2 Y (B_2 \Psi_2)$$

be the operator associated with (3.1). Then $L_h$ can be approximated by replacing two of the diagonal coefficient matrices, namely

$$\Psi_1 \approx \bar{\psi}_1 I, \quad \Phi_2 \approx \bar{\phi}_2 I,$$

where the scalars $\bar{\psi}_1$ and $\bar{\phi}_2$ represent some average of the functions $\psi_1$ and $\phi_2$ on the given domain. In our experiments we used

$$\bar{\psi}_1 := \frac{1}{n + 1} \sum_i \psi_1(x_i), \quad \bar{\phi}_2 := \frac{1}{n + 1} \sum_i \phi_2(y_i),$$

but other strategies may be considered. Substituting the approximations (4.1) in $L_h$, the matrix $Y$ can be collected, yielding the following approximation to $L_h$:

$$P : Y \mapsto (c T + \bar{\psi}_1 \Phi_1 B) Y + Y (c T + \bar{\phi}_2 B^T \Psi_2).$$

The use of $P$ in an acceleration context consists of applying $P^{-1}$ to a given matrix $G$. This corresponds to solving the following Sylvester equation

$$P(Y) = G \quad \Leftrightarrow \quad (c T_1 + \bar{\psi}_1 \Phi_1 B_1) Y + Y (c T_2 + B_2 \Psi_2 \bar{\phi}_2) = G.$$
This matrix equation has a unique solution for any $G \neq 0$ if and only if the spectra of $\epsilon T_1 + \bar{\psi}_1 \Phi B_1$ and $-(\epsilon T_2 + B_2 \bar{\phi}_2)$ have no common eigenvalues. This is ensured for instance if both coefficient matrices in (4.3) have eigenvalues in $\mathbb{C}^+$. The numerical solution of (4.3) will be discussed in section 4.1.

We would like to point out that the approximation in (4.1) corresponds to introducing the following modified convection vector

$$\bar{w} := (\bar{\psi}_1 \phi_1(x), \bar{\phi}_2 \psi_2(y)) \approx w.$$  \hfill (4.4)

so that the continuous operator $L(u) = -\epsilon \Delta u + w \cdot \nabla u$ is approximated by $\bar{L}(u) = -\epsilon \Delta u + \bar{w} \cdot \nabla u$. Similar preconditioning strategies relying on simplified (non-self-adjoint) versions of the operator $L$ have been developed in the past, see, e.g., [2], [7], [9], [13]; some of them use a matrix equation oriented formulation, which allows one to significantly lower the computational cost, compared with the Kronecker form, while keeping non-constant coefficients. In all these cases, however, no performance assessment has been clearly analyzed, and in fact, the overall cost heavily depends on the complexity of the method used to apply the preconditioner. By employing a matrix equation formulation, the computational cost is in general significantly lower than if one were to solve at each iteration a nonsymmetric linear system that is very close to the original one (unless special strategies can be designed for the latter), see, e.g., the discussion in [2, page 1514]. We refer to [23] for experimental comparisons with inner-outer procedures that explore incomplete LU preconditioners.

In the continuous case, our strategy determines a preconditioner that is \(^1\) “compact – equivalent” to the original operator $L$ [2, Proposition 3.5]. In particular, this property implies that if one were to use the conjugate gradient method to the normal equation associated with our preconditioned problem, its convergence rate would be bounded by a quantity that is independent of the mesh parameter [2, Theorem 4.7]. In our numerical experiments we did not employ the normal equation, but we can still empirically infer that mesh independence is maintained. Finally, we should mention that this property does not necessarily imply that the preconditioner is good, that is that a low number of iterations is obtained.

4.1. Implementation details. Since $A$ in (1.2) is nonsymmetric, the Krylov subspace solver GMRES ([25]) for nonsymmetric problems can be used, and the operator preconditioner $P^{-1}$ is applied from the right. In a standard implementation, at each iteration $k$ of GMRES the preconditioner is applied to a vector as $y_k = P^{-1}g_k$, where $g_k$ is a vector with $N = (n + 1)^2$ components. In our matrix strategy, we first transform the vector $g_k$ into the matrix $G_k$ such that $g_k = \text{vec}(G_k)$, and then obtain $y_k = \text{vec}(Y_k)$ as the solution to the Sylvester equation

$$\begin{bmatrix} \epsilon T_1 + \bar{\psi}_1 \Phi B_1 & Y \\ Y & \epsilon T_2 + B_2 \bar{\phi}_2 \Psi_2 \end{bmatrix} \begin{bmatrix} Y \end{bmatrix} = G_k,$$  \hfill (4.5)

where the coefficient matrices have both dimensions $n + 1$. For $n$ up to a few hundreds, this equation may be efficiently solved by means of the Bartels-Stewart method [3], whose computational cost is $O((n + 1)^3)$. This cost should be compared with the cost of solving an inner system of size $(n + 1)^2 \times (n + 1)^2$ by either a sparse direct solver, or by a fast solver if applicable. If a different number of nodes is used in each direction, or a three-dimensional problem is solved, then the two coefficient matrices will have

\(^3\)Roughly speaking, two elliptic operators are compact – equivalent if their principal parts coincide up to a constant factor, and they have homogeneous Dirichlet conditions on the same part of the boundary.
different size, without any significant impact on the solution process, though the cost will change accordingly.

For larger \( n \), the application of the Bartels-Stewart method may become too expensive to be competitive, therefore an iterative method should be employed. In this case, the Sylvester equation is solved up to a certain tolerance, so that only an approximation to \( Y \) is obtained. To make the strategy cost and memory effective when using state-of-the-art iterative methods, the right-hand side should be low rank. Therefore, \( G_k \) is also approximated by a low-rank matrix by means of a truncated singular value decomposition. The overall effectiveness of the acceleration process thus depends on how much information the truncation retains, and how accurate the iterative solution will be. These require the tuning of three parameters (the truncation and stopping tolerances, and the maximum rank allowed for \( G_k \)) that we set a-priori in all our numerical experiments: \( \text{tol}_{\text{truncation}}=10^{-2}, \text{tol}_{\text{inner}}=10^{-4}, r_{\text{max}}=10 \). The performance did not seem to be influenced by small variations of the values of these parameters.

Finally, we mention that if an iterative solver is used for (4.3), then the preconditioning step makes the overall process a nonlinear operation, as the inexact operator \( \mathcal{P}^{-1} \) “changes” at each system solver iteration. As a consequence, the flexible version of GMRES, named FGMRES in the following [24], is used, giving rise to an inner-outer iteration.

The iterative solution of the Sylvester equation is performed by means of the Extended Krylov subspace method (KPIK), originally proposed in [27] for the Lyapunov equation, and then adapted to solving the Sylvester equation in [6]. The relative residual norm is used as stopping criterion, and the residual is checked at every other iteration, as suggested in [27]. Other efficient Sylvester equation solvers could be used, see the recent survey [28]. However, in a preconditioning framework, the fact that the coefficient matrices can be factorized once for all makes KPIK very appealing in terms of computational costs; see [27] for further details.

5. The three-dimensional case. The 3D convection-diffusion equation can be stated as in (1.1), for \( \Omega \subset \mathbb{R}^3 \). To convey our idea, we again first focus on the Poisson equation, and then generalize the matrix formulation to the finite difference discretization of the non-self-adjoint problem (1.1). For the sake of simplicity, we shall assume that \( \Omega = (0,1)^3 \), though more general parallelepipedal domains could also be considered. We discretize \( \Omega \) with equidistant nodes in each direction, \((x_i, y_j, z_k)\), for \( i,j,k = 0, \ldots, n \). To fix the ideas, let \( U^{(k)}_{i,j} = U(x_i, y_j, z_k) \) denote the value of the approximation \( U \) to \( u \) at the node \((x_i, y_j, z_k)\) (other orderings may be more convenient depending on the equation properties). We also define the tall matrix

\[
\mathbf{U} = \begin{bmatrix} U^{(0)} & \vdots & U^{(n)} \end{bmatrix} = \sum_{k=0}^{n} (e_{k+1} \otimes U^{(k)}) \in \mathbb{R}^{(n+1)^2 \times (n+1)},
\]

where \( e_j \) is the \( j \)th canonical vector of \( \mathbb{R}^{n+1} \).
Let $T$ be as defined in (2.1). Then, for $I \in \mathbb{R}^{(n+1) \times (n+1)}$ the identity matrix,

$$
-u_{xx} \approx \sum_{k=0}^{n} (e_{k+1} \otimes TU^{(k)}) = (I \otimes T) \sum_{k=0}^{n} (e_{k+1} \otimes U^{(k)}) = (I \otimes T) \mathcal{U},
$$

$$
-u_{yy} \approx \sum_{k=0}^{n} (e_{k+1} \otimes U^{(k)}T) = \sum_{k=0}^{n} (e_{k+1} \otimes U^{(k)})T = UT,
$$

$$
-u_{zz} \approx (T \otimes I) \mathcal{U}.
$$

With these approximations we can thus obtain the following matrix form of the finite difference discretization of the Poisson equation:

$$
(I \otimes T) \mathcal{U} + UT + (T \otimes I) \mathcal{U} = F,
$$

(5.1)

where $F = \sum_{k=0}^{n} (e_{k+1} \otimes F^{(k)}) \in \mathbb{R}^{(n+1)^2 \times (n+1)}$ and $(F^{(k)})_{i,j} = f(x_i, y_j, z_k)$. The Kronecker formulation of the matrix equation (5.1) determines the usual approximation of the Laplacian operator by seven-point stencil finite differences,

$$
\Delta \approx I \otimes I \otimes T + I \otimes T \otimes I + T \otimes I \otimes I \in \mathbb{R}^{(n+1)^3 \times (n+1)^3}.
$$

For the convection-diffusion equation with separable coefficients a similar derivation provides a multiterm linear matrix equation. We state the result in the following proposition.

**Proposition 5.1.** Assume that the convection vector $\mathbf{w} = (w_1, w_2, w_3)$ satisfies $w_1 = \phi_1(x) \psi_1(y) v_1(z)$, $w_2 = \phi_2(x) \psi_2(y) v_2(z)$, and $w_3 = \phi_3(x) \psi_3(y) v_3(z)$. Let $(x_i, y_j, z_k)$, $i, j, k = 0, \ldots, n$ be the grid nodes discretizing $\bar{\Omega}$ with mesh size $h$, and set $\Phi_i = \text{diag}(\phi_i(x_0), \ldots, \phi_i(x_n))$, $\Psi_j = \text{diag}(\psi_j(y_0), \ldots, \psi_j(y_n))$, and $\Upsilon_\ell = \text{diag}(\psi_\ell(z_0), \ldots, \psi_\ell(z_n))$, $\ell = 1, 2, 3$.

Then, with $B$ as defined in (2.3), the centered finite-difference discretization of the differential operator in (1.1) leads to the following operator:

$$
\mathcal{L}_h : U \rightarrow (I \otimes T) \mathcal{U} + UT + (T \otimes I) \mathcal{U} + (T_1 \otimes \Phi_1 B) \mathcal{U} \Psi_1 + (T_2 \otimes \Phi_2 B T^T) \Psi_2 + ([\Upsilon_3 B] \otimes \Phi_3 ) \mathcal{U} \Psi_3.
$$

(5.2)

**Proof.** The second order terms of $\mathcal{L}_h(U)$ correspond to a multiple of (5.1). We are thus left with showing that the first order term can be expressed by means of the 1D discretization matrix $B$. We first fix $k = \bar{k}$ and we have

$$
\phi_1(x_i) \psi_1(y_j) v_1(z_k) u_{x}(x_i, y_j, z_k) \approx v_1(z_k) \phi_1(x_i) \frac{u(x_{i+1}, y_j, z_k) - u(x_{i-1}, y_j, z_k)}{2h} \psi_1(y_j).
$$

$$
= \frac{1}{2h} v_1(z_k) \phi_1(x_i) \begin{bmatrix} U^{(k)}_i & U^{(k)}_{i-1, j} \\ U^{(k)}_{i+1, j} & U^{(k)}_j \end{bmatrix} \begin{bmatrix} -1 \\ 0 \end{bmatrix} \psi_1(y_j).
$$

Analogously,

$$
\phi_2(x_i) \psi_2(y_j) v_2(z_k) u_{y}(x_i, y_j, z_k) \approx \frac{1}{2h} v_2(z_k) \phi_2(x_i) \begin{bmatrix} U^{(k)}_{i, j-1} & U^{(k)}_{i, j} \\ U^{(k)}_{i, j+1} & U^{(k)}_{i+1, j} \end{bmatrix} \begin{bmatrix} -1 \\ 0 \end{bmatrix} \psi_2(y_j).
$$

Collecting these results for all grid nodes $(x_i, y_j, z_k)$, $i, j = 0, \ldots, n$ and recalling that $U^{(k)}_{i, j} = U(x_i, y_j, z_k)$, we obtain

$$
(\phi_1(x_i) \psi_1(y_j) v_1(z_k) u_{x}(x_i, y_j, z_k))_{i, j = 0, \ldots, n} \approx v_1(z_k) \Phi_1 B U^{(k)} \Psi_1,
$$

and similarly for the other terms.
and
\[
(\phi_2(x_i)\psi_2(y_j)v_2(z_k)u_y(x_i, y_j, z_k))_{i,j=0,...,n} \approx v_2(z_k)\Phi_2U^{(k)}B^T\Psi_2.
\]

Therefore, for all \( z \) nodes,
\[
(\phi_1(x_i)\psi_1(y_j)v_1(z_k)u_x(x_i, y_j, z_k))_{i,j,k=0,...,n}
\approx [\Upsilon_1 \otimes I] \sum_{k=0}^n (e_{k+1} \otimes \Phi_1 B^T)^{(k)} \Psi_1 = [\Upsilon_1 \otimes I](I \otimes \Phi_1 B)[\sum_{k=0}^n (e_{k+1} \otimes U^{(k)})] \Psi_1
\]
\[
= [\Upsilon_1 \otimes I](I \otimes \Phi_1 B)\mathcal{U}\Psi_1 = (\Upsilon_1 \otimes \Phi_1 B)\mathcal{U}\Psi_1,
\]
and
\[
(\phi_2(x_i)\psi_2(y_j)v_2(z_k)u_y(x_i, y_j, z_k))_{i,j,k=0,...,n}
\approx [\Upsilon_2 \otimes I] \sum_{k=0}^n (e_{k+1} \otimes \Phi_2 U^{(k)}) B^T \Psi_2 = [\Upsilon_2 \otimes I](I \otimes \Phi_2)[\sum_{k=0}^n (e_{k+1} \otimes U^{(k)})] B^T \Psi_2
\]
\[
= [\Upsilon_2 \otimes I](I \otimes \Phi_2)\mathcal{U}B^T\Psi_2 = (\Upsilon_2 \otimes \Phi_2)\mathcal{U}B^T\Psi_2.
\]

On the other hand, for the \( z \) direction it holds
\[
\phi_3(x_i)\psi_3(y_j)v_3(z_k)u_z(x_i, y_j, z_k) \approx v_3(z_k)\phi_3(x_i) \frac{u(x_i, y_j, z_k+1) - u(x_i, y_j, z_k-1)}{2h}
\]
\[
\approx \frac{1}{2h} v_3(z_k)\phi_3(x_i) \begin{bmatrix} U_{i,j}^{(k-1)} \\ U_{i,j}^{(k)} \\ U_{i,j}^{(k+1)} \end{bmatrix} \psi_3(y_j).
\]

Collecting this relation for all blocks,
\[
(\phi_3(x_i)\psi_3(y_j)v_3(z_k)u_z(x_i, y_j, z_k))_{i,j,k=0,...,n}
\approx (\Upsilon_3 B \otimes I) \sum_{k=0}^n (e_{k+1} \otimes (\Phi_3 U^{(k)})) \Psi_3 = (\Upsilon_3 B \otimes I)(I \otimes \Phi_3)[\sum_{k=0}^n (e_{k+1} \otimes U^{(k)})] \Psi_3
\]
\[
= (\Upsilon_3 B \otimes I)(I \otimes \Phi_3)\mathcal{U}\Psi_3 = [(\Upsilon_3 B) \otimes \Phi_3] \mathcal{U}\Psi_3.
\]

and the result follows. \( \Box \)

Imposing the boundary conditions completely determines the entries of \( T \) in all three instances, as well as the missing entries in \( B \). Following the same steps as for the 2D case, the matrix equation (5.2) can be written as
\[
((I \otimes T_1) + (T_2^T \otimes I)) U + U T_3 + (\Upsilon_1 \otimes \Phi_1 B_1) \mathcal{U} \Psi_1 + (\Upsilon_2 \otimes \Phi_2) \mathcal{U} B_3 \Psi_2 + [(\Upsilon_3 B_3^T) \otimes \Phi_3] \mathcal{U} \Psi_3 = F,
\]
highlighting the presence of five distinct terms in the matrix equation. With this ordering of the variables, it holds that \( B_3 = B_2 \) and \( T_3 = T_2 \). Note that a tensorial formulation could also be obtained by further “unrolling” the Kronecker products in some of the terms. All three directions of the tensor would have dimension \( n + 1 \), thus being the natural generalization of the 2D problem. In future research we will explore the possibility of explicitly solving the fully tensorized equation (with three terms), possibly using recently developed strategies [16],[18].

The matrix equation above may take the form of a standard Sylvester equation depending on whether some of the coefficients \( \phi_\ell, \psi_\ell \) and \( \psi_\ell, \ell = 1, 2, 3 \) vanish; see
Example 6.5. In the generic case, a preconditioning operator can still be derived, e.g., by averaging the values of some of the coefficients, the way it was done in the 2D case. The new preconditioner then consists of an approximation of the equation (5.2). For instance, by approximating $\Psi_1, \Psi_3$ as
$$
\Psi_1 \approx \tilde{\psi}_1 I, \quad \Psi_3 \approx \tilde{\psi}_3 I,
$$
and also using $\Phi_2 \otimes \Upsilon_2 \approx \chi I$, the following operator is obtained,
$$
P : V \rightarrow \left( (I \otimes T_1) + (T_2^2 \otimes I) + \tilde{\psi}_1 (T_1 \otimes \Phi_1 B_1) + \tilde{\psi}_3 [(T_3 B_2^2) \otimes \Phi_3] \right) V + V (T_3 + \tilde{\chi} B_3 \Psi_2)
$$
whose application entails the solution of a Sylvester equation with coefficient matrices of size $(n + 1)^2 \times (n + 1)^2$ and $(n + 1) \times (n + 1)$, respectively.

6. Numerical experiments. In this section several numerical experiments are presented using both two and three dimensional problems. Performance with respect to the problem parameter – the viscosity – and the discretization parameter – the meshsize – are considered.

In both dimensional settings we first consider the case when the matrix equation framework can be used as a solver for the original equation: this corresponds to problems where the first order term coefficients only depend on the same variable as the corresponding derivative. Comparisons with either sparse direct solvers or with iterative solvers are shown. Then we report on our experience when using the matrix equation strategy as a preconditioner for more general convection-diffusion problems with separable coefficients. We compare the performance of the new approach with that of state-of-the-art algebraic multigrid preconditioners; experimental comparisons with (less performing) ILU-type preconditioners can be found in [23]. More precisely, we shall consider both the algebraic multigrid preconditioner MI20 [5] with GMRES as a solver, and AGMG [21] with flexible GMRES as a solver (in AGMG all default parameters were used, while in MI20, control.one_pass_coarsen was set to 1). Both strategies have been shown to be applicable to convection-diffusion equations, and in particular, for AGMG it was shown in [22] that this variable preconditioning strategy is well suited for both 2D and 3D problems.

We stress that our experimental comparisons somewhat penalize our approach, as the other preconditioners are in fact fortran90 fully compiled codes, for which a mex file was made available. Their performance is thus expected to be superior to interpreted Matlab functions, on which our preconditioner is based. Nonetheless, the reported results show that the new strategy is still competitive.

Except for Example 6.3, all problem data were obtained by centered finite difference discretization on the given domain; for all experiments the grid fineness was chosen so as to avoid spurious oscillations in the numerical solution for the coarsest grid used.

All experiments were performed with Matlab Version 7.13.0.564 (R2011b) on a Dell Latitude laptop running ubuntu 14.04 with 4 CPUs at 2.10GHz.

6.1. Two-dimensional problems. Whenever the convection vector has the simplified form $w = (w_1, w_2) = (\phi_1(x), \psi_2(y))$, that is $\psi_1$ and $\phi_2$ are constant functions, the matrix formulation (2.4) reduces to
$$
\epsilon T_1 U + \epsilon UT_2 + (\Phi_1 B_1) U + U (B_2 \Psi_2) = F,
$$
which is a Sylvester matrix equation, and can thus be solved directly, with no further approximation. In the first two examples, we thus consider equations leading to this
simplified form, and we compare the performance of either two direct solvers – in the
matrix and vector equation regimes respectively, or of two iterative solvers.

Example 6.1. We consider the convection-diffusion (1.1) with $\Omega = (0,1)^2$, $f = 0$, $w = (1 + (x+1)^2/4, 0)$, and the following Dirichlet boundary conditions:

\[
\begin{align*}
\{ & u(x, 0) = 1 \quad x \in [0,1], \\
& u(x, 1) = 0 \quad x \in [0,1].
\end{align*}
\]

With these data, equation (2.4) reduces to $\epsilon T_1 U + \epsilon U T_2 + (\Phi_1 B_1) U = F$, that is to the following Sylvester equation,

\[(\epsilon T_1 + \Phi_1 B_1) U + \epsilon U T_2 = F;\]  

(6.1)

where the right-hand side $F$ contains the Dirichlet boundary conditions (see section 3). We solve this matrix equation using the \texttt{lyap} function in Matlab, from the Control Toolbox, and its “vectorized” version (i.e. its Kronecker formulation) by means of a sparse direct solver (Matlab backslash operation). The results are reported in Table 6.1 (left), for a variety of mesh dimensions and viscosity values; the same number of grid nodes, $n_x$ and $n_y$, was used in the $x$ and $y$ directions, respectively. The numbers show the superiority of the use of the (dense) Sylvester solver, compared with that of a general-purpose sparse direct solver.

The right portion of Table 6.1 reports the same type of experiments for the rectangular domain $\Omega = (0,1) \times (0,2)$. A grid consisting of small squares was still used, so that a different number of nodes in the two directions was imposed. Both methods are sensitive to the unbalanced dimension growth in the two directions, although the matrix oriented approach is still faster. Note that for the largest grid, the performance of the dense solver \texttt{lyap} deteriorates more significantly. For such large problems, an iterative solver should be preferred.

| $\epsilon$ | $n_x$ | $n_y$ | Vect. CPU time | Matrix CPU time | $\epsilon$ | $n_x$ | $n_y$ | Vect. CPU time | Matrix CPU time |
|-------|-------|-------|---------------|----------------|-------|-------|-------|---------------|----------------|
| 0.0333 | 65    |       | 0.02          | 0.008          | 0.0333 | 65    | 130   | 0.04          | 0.025          |
| 0.0333 | 129   |       | 0.07          | 0.030          | 0.0333 | 129   | 258   | 0.15          | 0.081          |
| 0.0333 | 257   |       | 0.37          | 0.159          | 0.0333 | 257   | 514   | 0.76          | 0.415          |
| 0.0333 | 513   |       | 2.01          | 0.898          | 0.0333 | 513   | 1026  | 4.28          | 2.410          |
| 0.0333 | 1025  | 10.95 | 6.389         |                |        |       |       |               |                |
| 0.0167 | 65    |       | 0.02          | 0.005          | 0.0167 | 65    | 130   | 0.03          | 0.016          |
| 0.0167 | 129   |       | 0.08          | 0.029          | 0.0167 | 129   | 258   | 0.15          | 0.093          |
| 0.0167 | 257   |       | 0.39          | 0.155          | 0.0167 | 257   | 514   | 0.70          | 0.435          |
| 0.0167 | 513   | 1.91  | 0.899         |                | 0.0167 | 513   | 1026  | 5.18          | 2.376          |
| 0.0167 | 1025  | 10.95 | 6.354         |                | 0.0167 | 1025  | 2050  | 35.31         | 28.691         |
| 0.0083 | 65    |       | 0.01          | 0.006          | 0.0083 | 65    | 130   | 0.03          | 0.018          |
| 0.0083 | 129   |       | 0.08          | 0.032          | 0.0083 | 129   | 258   | 0.16          | 0.087          |
| 0.0083 | 257   | 0.38  | 0.154         |                | 0.0083 | 257   | 514   | 0.88          | 0.631          |
| 0.0083 | 513   | 1.92  | 0.891         |                | 0.0083 | 513   | 1026  | 5.15          | 3.245          |
| 0.0083 | 1025  | 11.03 | 6.443         |                | 0.0083 | 1025  | 2050  | 29.99         | 24.735         |

Table 6.1

Example 6.1. Total CPU time for a sparse direct solver and the function \texttt{lyap}, as the viscosity and the problem dimension change. Left: square domain. Right: rectangular domain with same mesh size and different number of nodes in $x$ and $y$ directions.

Example 6.2. We consider solving the algebraic problem stemming from the equation of Example 6.1 (in $\Omega = (0,1)^2$) by means of an iterative solver. In the case of the linear system (the Kronecker version of (6.1)), both MI20 and AGMG were
considered as preconditioners. As discussed in section 4.1, the iterative solver for the Sylvester equation \((6.1)\) was the extended Krylov subspace method [27] (KPIK in the following). In both solvers, the stopping criterion was based on the relative residual 2-norm, with stopping tolerance equal to \(10^{-8}\). Numerical results are reported in Table 6.2 as the viscosity and number of grid nodes in each direction change. We observe that the number of iterations varies for all methods as the mesh is refined, and in a more significant manner for KPIK. However, we recall from section 4.1 that memory requirements in this case are not an issue, as the extended Krylov subspace actually generated is a subset of \(\mathbb{R}^{nx}\). For the two algebraic multigrid preconditioners, a mildly varying number of iterations with respect to \(nx\) has been largely observed in the literature, at least experimentally. All methods are not very sensitive to changes in viscosity. In terms of CPU times, the method based on the matrix equation shows the best performance, especially as the problem size increases. In summary, iteratively solving the problem by resorting to its matrix equation formulation pays off in this case. A comparison with the timings of Table 6.1 is also of interest. Note that for the largest size, the iterative solvers should be preferred, whereas for most other sizes, especially in the linear system formulation, the direct solver is superior. This fact is typical of two-dimensional problems, for which sparse direct solvers remain attractive over iterative ones, also for very fine discretizations when the Kronecker formulation is used.

In the next two examples we consider problems where the convection coefficients both depend on both variables, although in a separable manner. The matrix-equation-based strategy is then used as a preconditioner, in which the original operator is approximated via a Sylvester operator.

**Example 6.3.** We consider the convection-diffusion equation in \(\Omega = (0,1)^2\) with
\[
\mathbf{w} = (2y(1-x^2), -2x(1-y^2)),
\]
and the Dirichlet boundary conditions \(u(0,y) = 0, u(1,y) = 0, u(x,0) = 0\) and \(u(x,1) = 1\). This is a simple model for the temperature distribution in a cavity with a ‘hot’ external wall \((\{1\} \times [0,1])\) and the wind characterized by \(\mathbf{w}\) determines a recirculating flow; this model was used as a test example in [14]. Data were generated with the IFISS package [12], which uses a uniform finite element discretization on
a rectangular grid. The coefficient matrices of the Sylvester operator preconditioner were generated by finite differences and the corresponding equation solved with KPIK. Thanks to the chosen uniform discretization in IFISS, the obtained preconditioning operator was still effective, in spite of the different discretization technique. Numerical results are reported in Table 6.3, where a stopping tolerance of $10^{-6}$ was used. The preconditioner MI20 broke down several times on this example, therefore its results were not included. Instead, the last column shows timings for the Matlab default sparse solver (backslash operator).

The numbers in the table show a very good performance of the new approach with respect to the number of iterations, but timings are in general higher than with AGMG preconditioning; better performance of FGMRES+KPIK may be obtained with a compiled code. Note that both iterative solvers are largely superior to the sparse direct method.

| $\epsilon$ | $n_x$ | FGMRES+AGMG | FGMRES+KPIK | DIRECT |
| --- | --- | --- | --- | --- |
| 0.005 | 129 | 0.0377 (6) | 0.1301 (10) | 0.0786 |
| 0.005 | 257 | 0.1216 (6) | 0.2509 (9) | 0.4338 |
| 0.005 | 513 | 0.5970 (6) | 0.7709 (8) | 3.3971 |
| 0.005 | 1025 | 3.1946 (7) | 6.0621 (8) | 19.0872 |
| 0.0025 | 129 | 0.0634 (7) | 0.1306 (10) | 0.0824 |
| 0.0025 | 257 | 0.1073 (5) | 0.2173 (9) | 0.4223 |
| 0.0025 | 513 | 0.5029 (5) | 0.7151 (8) | 2.4794 |
| 0.0025 | 1025 | 2.5261 (6) | 5.3601 (7) | 16.1251 |
| 0.0013 | 129 | 0.1882 (10) | 0.1686 (10) | 0.1117 |
| 0.0013 | 257 | 0.2531 (7) | 0.2283 (9) | 0.4317 |
| 0.0013 | 513 | 0.5075 (5) | 0.7088 (8) | 3.2329 |
| 0.0013 | 1025 | 2.1558 (5) | 3.9864 (6) | 24.6895 |

Table 6.3. CPU time and number of iterations for different preconditioners and a sparse direct solver, as the viscosity and mesh parameter vary.

Example 6.4. We consider a variant of Example V in [11] in $\Omega = (0, 1)^2$, where the convection vector was modified so as to obtain a divergence free convection term, and so as not to have zero mean, namely

$$w = \left(y(1 - (2x + 1)^2), -2(2x + 1)(1 - y^2)\right),$$

together with zero Dirichlet boundary conditions except for the side $y = 0$ where

$$\begin{cases}
  u(x, 0) = 1 + \tanh[10 + 20(2x - 1)], & 0 \leq x \leq 0.5, \\
  u(x, 0) = 2, & 0.5 < x \leq 1.
\end{cases}$$

The problem was discretized using centered finite differences, and the grid was selected fine enough so as not to have spurious oscillations. As in the previous example, we compare the performance of various preconditioners, as the viscosity and the mesh parameter change. Results are reported in Table 6.4, where the stopping tolerance $10^{-6}$ was used.

This is a recognized hard problem due to the strong layer appearing near the boundary $y = 0$. This appears to be the only problem where FGMRES+AGMG gives much worse results than the other methods, both in terms of variability on the number of iterations, and in terms of CPU time. On the other hand, MI20 and KPIK worked very well as preconditioners, with an either constant or even decreasing number of iterations, and lower CPU times, with somewhat lower values for the matrix-equation-based approach.
Example 6.4. CPU time and number of iterations for different preconditioners, as the viscosity and mesh parameter vary.

6.2. Three-dimensional problems. Like in the previous section, we first report on the case where the discretized problem can be directly solved as a Sylvester equation, and then on the case when the Sylvester equation serves as preconditioner for the more involved problem.

Example 6.5. We consider the 3D problem $-\epsilon \Delta u + w \cdot \nabla u = 1$, in $\Omega = (0,1)^3$, with convection term

$$w = (x \sin x, y \cos y, e^{xz} - 1),$$

and zero Dirichlet boundary conditions. After a centered finite difference discretization with $n_x = n_y = n_z$ nodes in each direction, the equation (5.2) takes the form

$$(I \otimes T_1) U + U T_3 + (T_2^T \otimes I) U + (I \otimes \Phi_1 B_1) U + U B_3 Y_3 + [(\Psi_2 B_2)^T \otimes I] U = 11^T,$$

where $1$ is the vector of all ones, and this corresponds to the following Sylvester equation in $U$,

$$[I \otimes (T_1 + \Phi_1 B_1) + (T_2 + \Psi_2 B_2)^T \otimes I] U + U (T_3 + B_3 Y_3) = 11^T. \tag{6.2}$$

Note that the fact that the forcing term in the original equation yields a low rank right-hand side in the matrix equation is crucial for the solution process.

We solved this matrix equation by means of KPIK, and compared its performance with the solution of the corresponding linear system (via its Kronecker formulation) with GMRES preconditioned by MI20, and with flexible GMRES preconditioned by AGMG. Results are reported in Table 6.5, with stopping tolerance equal to $10^{-9}$.

As in the corresponding 2D problem (Table 6.2), the number of iterations is quite stable for both algebraic multigrid preconditioners, whereas it varies, though very mildly, when KPIK is used. On the other hand, CPU time is very much in favor of the matrix equation solver, whose computation exploited the lower order complexity of the problem. One order of magnitude lower timings can be observed in some instances. All strategies seem not to be sensitive to the choice of viscosity in the considered range.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
$\epsilon$ & $n_x$ & FGMRES+AGMG & GMRES+MI20 & FGMRES+KPIK \\
& & CPU time (# its) & CPU time (# its) & CPU time (# its) \\
\hline
0.1000 & 128 & 0.1081 (11) & 0.1000 & 0.5743 (11) \\
0.1000 & 256 & 0.3812 (4) & 0.1000 & 0.5351 (7) \\
0.1000 & 512 & 1.7394 (1) & 0.1000 & 1.0543 (7) \\
0.1000 & 1024 & 4.3287 (4) & 0.1000 & 2.6372 (6) \\
0.1000 & 2048 & 16.7394 (5) & 0.1000 & 2.6372 (6) \\
\hline
0.0500 & 128 & 0.2269 (4) & 0.0500 & 0.5168 (10) \\
0.0500 & 256 & 0.3812 (4) & 0.0500 & 0.6455 (9) \\
0.0500 & 512 & 1.2380 (4) & 0.0500 & 1.1769 (8) \\
0.0500 & 1024 & 4.3345 (4) & 0.0500 & 3.0812 (7) \\
0.0500 & 2048 & 14.9237 (10) & 0.0500 & 3.0812 (7) \\
\hline
0.0333 & 128 & 0.2368 (4) & 0.0333 & 0.6428 (11) \\
0.0333 & 256 & 0.4218 (4) & 0.0333 & 0.8149 (11) \\
0.0333 & 512 & 1.1977 (4) & 0.0333 & 1.3786 (9) \\
0.0333 & 1024 & 4.4130 (4) & 0.0333 & 3.7214 (9) \\
0.0333 & 2048 & 20.1120 (4) & 0.0333 & 17.9188 (7) \\
\hline
\end{tabular}
\caption{Example 6.4. CPU time and number of iterations for different preconditioners, as the viscosity and mesh parameter vary.}
\end{table}
Table 6.5

| $\epsilon$ | $n_x$ | FGMRES+AGMG | GMRES+MI20 | KPIK |
|------------|-------|-------------|------------|------|
|            |       | CPU time (# its) | CPU time (# its) | CPU time (# its) |
| 0.0050     | 50    | 0.6044 (13)   | 1.0591 (6)   | 0.1353 (18)   |
| 0.0050     | 60    | 1.1250 (14)   | 1.6022 (7)   | 0.1734 (18)   |
| 0.0050     | 70    | 2.0385 (14)   | 3.4253 (7)   | 0.2326 (20)   |
| 0.0050     | 80    | 3.4903 (14)   | 4.4297 (7)   | 0.3583 (20)   |
| 0.0050     | 90    | 5.7324 (15)   | 6.8705 (7)   | 0.4999 (22)   |
| 0.0050     | 100   | 8.0207 (15)   | 9.7207 (7)   | 0.5677 (22)   |
| 0.0010     | 50    | 0.6556 (13)   | 1.1306 (6)   | 0.1811 (18)   |
| 0.0010     | 60    | 1.3011 (14)   | 1.7854 (7)   | 0.2386 (18)   |
| 0.0010     | 70    | 1.9509 (14)   | 2.7829 (7)   | 0.2346 (20)   |
| 0.0010     | 80    | 3.5291 (14)   | 4.6576 (7)   | 0.4096 (20)   |
| 0.0010     | 90    | 5.1344 (14)   | 6.8176 (7)   | 0.4253 (22)   |
| 0.0010     | 100   | 7.6815 (14)   | 9.4935 (7)   | 0.5446 (22)   |
| 0.0005     | 50    | 0.7039 (14)   | 1.0530 (6)   | 0.1751 (16)   |
| 0.0005     | 60    | 1.2560 (14)   | 1.7341 (6)   | 0.2314 (18)   |
| 0.0005     | 70    | 2.2242 (14)   | 2.9667 (7)   | 0.2301 (20)   |
| 0.0005     | 80    | 3.4558 (14)   | 4.5964 (7)   | 0.3472 (22)   |
| 0.0005     | 90    | 4.8076 (14)   | 6.4841 (7)   | 0.4257 (22)   |
| 0.0005     | 100   | 7.3914 (14)   | 9.6274 (7)   | 0.5927 (24)   |

Example 6.5. CPU time and number of iterations for different preconditioners, as the viscosity and mesh parameter vary.

Example 6.6. Finally, we consider the 3D convection-diffusion equation in $\Omega = (0,1)^3$, with $f = 1$ and convection vector $w = (yz(1-x^2),0,e^z)$, and zero Dirichlet boundary conditions. Due to the structure of $w$, we can treat separately the $(z)$ variable and the $(x,y)$ variables. With this variable ordering in mind, we can define $U$ of size $n_z \times (n_x n_y)$, and the following corresponding matrix equation

$$T_3 U + \mathcal{U}(I \otimes T_2 + T_2^T \otimes I) + \Upsilon_3 B_3 U + \Upsilon_1 \mathcal{U}(I \otimes \Phi_1 B_1) = 11^T.$$  

With the approximation $\Upsilon_1 \approx \bar{\upsilon}_1 I$, the matrix-equation-based preconditioner is given by

$$P : V \rightarrow (T_3 + \Upsilon_3 B_3) V + \mathcal{V}(I \otimes T_2 + T_2^T \otimes I + I \otimes \bar{\upsilon}_1 \Phi_1 B_1),$$

with coefficient matrices of dimension $n_z \times n_z$ and $n_x n_y \times n_x n_y$. We compare the performance of flexible GMRES with this preconditioner (the Sylvester equation is iteratively solved as described in section 4.1), with that of flexible GMRES preconditioned by AGMG, and of GMRES with MI20, both applied to the corresponding linear system. The stopping tolerance was set to $10^{-9}$. The results of our numerical experiments are shown in Table 6.6. We readily notice that GMRES+MI20 did not perform well, and we had to stop the solution process for the two smaller values of the viscosity, due to the excessive CPU time necessary for building the preconditioner. The other preconditioning strategies perform comparably all the way up to $10^6$ unknowns, with a steadily lower number of iterations for the matrix-equation-based preconditioner, which in turns implies lower memory requirements of flexible GMRES.

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\(^2\)Other variable aggregations are possible. The one we chose allowed us to explicitly treat the first derivative in the $z$ direction in the preconditioner.
In terms of CPU time performance is comparable, although the new strategy usually requires lower time; we expect that the use of a compiled implementation of this new strategy will make this difference more remarkable.

| $\epsilon$ | $n_x$ | FGMRES+AGMG | GMRES+MI20 | FGMRES+KPIK |
|------------|-------|-------------|------------|-------------|
| 0.5000     | 50    | 0.6239 (15) | 0.9182 (6) | 0.9291 (6)  |
| 0.5000     | 60    | 1.2095 (15) | 1.8236 (7) | 1.2027 (6)  |
| 0.5000     | 70    | 2.1041 (15) | 3.1649 (7) | 1.6585 (6)  |
| 0.5000     | 80    | 3.7370 (16) | 4.9765 (7) | 2.4943 (6)  |
| 0.5000     | 90    | 7.5874 (16) | 9.2040 (8) | 3.2513 (6)  |
| 0.5000     | 100   | 7.7626 (16) | 11.9912 (8)| 4.7548 (6)  |
| 0.1000     | 50    | 0.8041 (17) | 75.8874 (6)| 1.4610 (8)  |
| 0.1000     | 60    | 2.1310 (18) | - ( -)    | 1.5299 (8)  |
| 0.1000     | 70    | 2.8043 (18) | - ( -)    | 1.8926 (8)  |
| 0.1000     | 80    | 5.1219 (19) | - ( -)    | 3.2928 (9)  |
| 0.1000     | 90    | 7.3179 (19) | - ( -)    | 4.6429 (9)  |
| 0.1000     | 100   | 9.5759 (19) | - ( -)    | 6.5590 (9)  |
| 0.0500     | 50    | 0.6780 (17) | 168.5447 (6)| 1.1999 (10)|
| 0.0500     | 60    | 1.4318 (18) | - ( -)    | 1.7296 (10)|
| 0.0500     | 70    | 2.8427 (19) | - ( -)    | 2.5215 (10)|
| 0.0500     | 80    | 4.9616 (20) | - ( -)    | 3.6615 (10)|
| 0.0500     | 90    | 7.1038 (20) | - ( -)    | 5.0098 (10)|
| 0.0500     | 100   | 10.7181 (21)| - ( -)    | 6.8661 (10)|

Table 6.6: CPU time and number of iterations for different preconditioners, as the viscosity and mesh parameter vary. “-” stands for excessive CPU time in building the preconditioner.

7. Conclusions and outlook. We have implemented a new matrix-equation-based strategy for solving or preconditioning a variety of two and three-dimensional convection-diffusion problems. Our preliminary numerical experiments show that the new approach performs comparably well with respect to state-of-the-art algebraic multigrid preconditioners. As opposed to earlier attempts with this type of approaches, we have shown that recently developed Sylvester equation solvers can make the matrix equation strategy very appealing whenever the original partial differential equation has separable coefficients.

Our current implementation is limited to the use of uniform meshes for rectangular or parallelepipedal domains. We plan to generalize the approach to more general settings in the future. The restriction to separable convection terms can be relaxed by appropriately approximating the operator at the preconditioning level, by designing special corresponding separable approximations. These possibilities will also be explored.

Our description could be generalized to tensor structures with more than three dimensions, as they occur in many emerging applications [16],[17],[18]. We will explore the possibility of extending our algorithmic methodology to this setting, taking into account the role of the convection terms in this more advanced framework.

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