TAYLOR-GALERKIN-BASED SPECTRAL ELEMENT METHODS FOR CONVECTION-DIFFUSION PROBLEMS

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SUMMARY

Several explicit Taylor-Galerkin-based time integration schemes are proposed for the solution of both linear and non-linear convection problems with divergence-free velocity. These schemes are based on second-order Taylor series of the time derivative. The spatial discretization is performed by a high-order Galerkin spectral element method. For convection-diffusion problems an operator-splitting technique is given that decouples the treatment of the convective and diffusive terms. Both problems are then solved using a suitable time scheme. The Taylor-Galerkin methods and the operator-splitting scheme are tested numerically for both convection and convection-diffusion problems.

KEY WORDS Convection-diffusion problems Operator-splitting Taylor-Galerkin time integration Spectral element method

1. INTRODUCTION

The point of departure in this paper is the unsteady convection-diffusion equation for divergencefree velocity fields **u**,

$$\frac{\partial \mathbf{c}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{c} - (\nabla \cdot \eta \nabla)\mathbf{c} = \mathbf{f} \quad \text{in } \Omega,$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega.$$
(1)

with $\Omega \subset \mathbb{R}^d$ an open and bounded region with boundary Γ (*d* is the dimension of space). The velocity field $\mathbf{u}(\mathbf{x}, t)$ in $\overline{\Omega} = \Omega \cup \Gamma$ is given for $t \in [0, T]$. Note that the case $\mathbf{c} = \mathbf{u}$ yields a non-linear Burgers equation. For convenience, homogeneous Dirichlet boundary conditions are assumed, given by

$$\mathbf{c}(\mathbf{x}, t) = \mathbf{0}, \quad \mathbf{x} \text{ on } \Gamma, \quad t \ge 0.$$
(2)

The initial conditions are given by

$$\mathbf{c}(\mathbf{x},0) = \mathbf{c}_0, \quad \mathbf{x} \text{ in } \mathbf{\bar{\Omega}}. \tag{3}$$

Equation (1) is important for several classes of problems.

- 1. General convection-diffusion problems (energy equation, constitutive equations in viscoelastic flow). In this case the viscosity η is positive but it can be a function of c.
- 2. Pure convection problems (particle tracking or free boundary problems). In the case $\eta = 0$ equation (1) results in a convection (or transport) problem and describes the convection of

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the quantity c. A convection problem also arises if an operator-splitting method is applied to (1). This case is discussed in the subsequent sections.

3. Splitting methods and pressure correction (projection) methods for the incompressible Navier-Stokes equations. In this case the equations are non-linear ($\mathbf{c} = \mathbf{u}$).

Standard Galerkin approximations of convection-diffusion problems are often unstable and show spurious oscillations or 'wiggles' related to the fact that the resulting system matrix is no longer diagonally dominant. Especially if the convection part dominates the problem, these oscillations can only be suppressed by severe mesh and time step refinement, which is often not practical.

An overview of recently developed methods that stabilize the numerical approximation of convection-dominated problems is given by Donea.¹ For steady problems a common approach is the use of some kind of upwinding. Among these techniques are streamline upwind (SU) methods,² streamline upwind/Petrov–Galerkin (SUPG) methods^{3,4} and Galerkin least squares (GLS) methods.⁵

For unsteady problems various generalized Galerkin methods have been developed in the last decade. An important class of these methods is formed by the Taylor–Galerkin methods. These methods, introduced for finite elements by Donea,⁶ add in a natural way a stabilizing diffusion term to the numerical scheme, using Taylor series expansions in time including second- and third-order terms. In the finite difference context similar techniques are provided by Lax–Wendroff schemes.⁷ In contrast with the general procedure, Taylor–Galerkin methods usually consider the time integration before the spatial discretization. A recent analysis of Taylor–Galerkin schemes is given by Donea and Quartapelle.⁸

In this study a Galerkin high-order spectral element method is chosen for the spatial discretization. Spectral element methods are domain decomposition methods using high-order p-type weighted residual approximation for the solution of partial differential equations. The key feature of p-type methods is that they achieve convergence by increasing the degree of the approximation. Spectral element methods were first presented by Patera;⁹ a recent overview is given by Maday and Patera.¹⁰ Spectral element methods have the geometric flexibility of all other domain decomposition methods such as the well-known h-type finite element method.^{11,12}

The spectral element technique belongs to the large class of spectral methods.^{13,14} Spectral methods are characterized by the property that for problems with a solution that is sufficiently smooth, exponential accuracy is obtained by expanding the solution in a series of special expansion functions. These expansion functions are solutions of singular Sturm-Liouville problems. Owing to their high-order character, spectral element methods are appropriate for problems in which high-order regularity is guaranteed or (in any case) not the exception, such as is the case for incompressible flow problems. If the regularity of the solution is low or if the required accuracy is not very high, spectral element methods are domain decomposition techniques, complex geometries (even singularities) and physically originated difficulties such as boundary layers can be treated by local mesh refinement.

In this paper Taylor–Galerkin tine integration is combined with a spectral element spatial discretization for the approximation of convection–diffusion problems. In Section 2 an operator-splitting approach is described which decouples a convection–diffusion problem into a pure convection problem and a pure diffusion problem. The splitting method is based on the classical splitting methods,^{15,16} but also follows an approach proposed by Maday *et al.*¹⁷ In Section 3 several Taylor–Galerkin schemes are deduced that are specifically suited for (non-linear)

convection problems with time-dependence and divergence-free velocity. The schemes are applied to several convection problems, both linear and non-linear. In Section 4 the full operator-splitting scheme is given for convection-diffusion problems. Numerical results are given also for this scheme. Finally, in Section 5 conclusions are drawn.

2. OPERATOR-SPLITTING APPROACH

With respect to the choice of time integration it is preferable to decouple the treatment of convection and diffusion. For spectral-type methods the eigenvalues of the diffusion system are real and strictly negative and grow like $\mathcal{O}(N^4)$ as $N \to \infty$.¹⁴ Here N is the maximum of the number of degrees of freedom in each spatial direction. As a consequence the diffusion (or stiff) part requires a time integration with a stability area that includes the negative real axis ($A(\alpha)$ -stable time integration¹⁸). As is well known, some type of (semi-)implicit time integration is then in order. For the diffusive part the system matrix does not depend on time and suitable iterative solvers such as finite element preconditioning^{19,20} can be applied in each time step. On the other hand, especially in the case where the problem is non-linear or in the case where the velocity u is time-dependent, an implicit time integration of the convective terms requires an evaluation of the convective matrix in each time step. Therefore, explicit time integration is virtually necessary to ensure efficiency of the numerical scheme; in this case the solution of the system only involves matrix-vector products which can be evaluated using an element-by-element procedure. Moreover, for the convective part the eigenvalues are complex and grow 'only' like $\mathcal{O}(N^2)$ as $N \to \infty$. The restriction on the time step is therefore not too severe if explicit time integration is applied to the convective part.

In view of this it appears appropriate to treat unsteady convection-diffusion problems by an operator-splitting technique in which the problem is decomposed into a pure convection problem and a pure diffusion problem. Both problems are then solved by suitable time integrations, with different time steps if necessary.

Hereto the convection-diffusion problem (1) is rewritten as

$$\partial \mathbf{c}/\partial t = \mathcal{D}(\mathbf{c}) + \mathscr{C}(\mathbf{c}) + \mathbf{f},$$
(4)

where $\mathscr{D}(\mathbf{c}) = (\nabla \cdot \eta \nabla)\mathbf{c}$ is the diffusion operator and $\mathscr{C}(\mathbf{c}) = -(\mathbf{u} \cdot \nabla)\mathbf{c}$ is the convection operator. Following the idea of Maday *et al.*,¹⁷ equation (4) is written in terms of an integration factor in \mathscr{C} as

$$\frac{\partial}{\partial t} \left(\mathscr{Q}_{c}^{(t^{*},t)} \mathbf{c}(t) \right) = \mathscr{Q}_{c}^{(t^{*},t)} (\mathscr{D}(\mathbf{c}) + \mathbf{f}), \tag{5}$$

with t^{*} an arbitrary fixed time. The integrating factor $\mathcal{Q}_{c}^{(t^*,t)}$ is defined by

$$\frac{\partial}{\partial t} \mathcal{Q}_{c}^{(t^{*},t)} = -\mathcal{Q}_{c}^{(t^{*},t)} \mathscr{C}(\mathbf{c}), \qquad \mathcal{Q}_{c}^{(t^{*},t^{*})} = \mathscr{I}, \qquad (6)$$

where \mathscr{I} is the identity operator. Equation (5) is integrated by a suitable time integration for the diffusion operator $\mathscr{D}(\mathbf{c})$. A useful class of $A(\alpha)$ -stable time integration methods is given by the so-called 'backward difference formulae',¹⁸ These schemes are accurate for all components around the origin in the stability diagram and absolutely stable away from the origin in the left imaginary plane. Thus it is possible to use high-order backward difference schemes without the severe constraints on the time step that are needed for general high-order multistep schemes such as the Adams-Moulton methods, which are not $A(\alpha)$ -stable for any order higher than two.²¹ Application of a backward difference scheme to equation (5) gives the semidiscrete system

$$\frac{\gamma_0 \mathbf{c}^{n+1} - \sum_{i=1}^k \beta_i \mathcal{Q}_c^{(t^{n+1}, t^{n+1-i})} \mathbf{c}^{n+1-i}}{\Delta t} = \mathscr{D}(\mathbf{c}^{n+1}) + \mathbf{f}^{n+1}, \tag{7}$$

where e.g. the superscript n+1 denotes the approximation at time $t^{n+1} = (n+1)\Delta t$, with Δt the time step. For consistency it is required that

$$\gamma_0 = \sum_{i=1}^k \beta_i. \tag{8}$$

The coefficients of the first-order scheme (k = 1), which is in fact a backward Euler scheme, are $\gamma_0 = 1$ and $\beta_1 = 1$. For the second-order scheme (k = 2) they read $\gamma_0 = \frac{3}{2}$, $\beta_1 = 2$ and $\beta_2 = -\frac{1}{2}$. To evaluate the terms $\mathcal{Q}_c^{(i^{n+1},i^{n+1-i})} \mathbf{c}^{n+1-i}$ (i = 1, 2, ...,), the following associated initial value

problem is solved:

$$\partial \tilde{\mathbf{c}}(s) / \partial s = \mathscr{C}(\tilde{\mathbf{c}})(s), \quad 0 < s < i\Delta t,$$

$$\tilde{\mathbf{c}}(0) = \mathbf{c}^{n+1-i},$$
(9)

from which it then follows that

$$\mathscr{Q}_{c}^{(t^{n+1},t^{n+1-i})}\mathbf{c}^{n+1-i} = \tilde{\mathbf{c}}(i\Delta t).$$
⁽¹⁰⁾

Problem (9), accounting fro the convection part, can be solved using a suitable (and preferably explicit) scheme with a time step Δs which can be taken different from Δt . In the next section several Taylor-Galerkin time integration methods appropriate for both linear and non-linear convection problems are proposed and discussed. Note that the integrating factor $\mathcal{Q}_{c}^{(t^{n+1},t^{n+1-i})}$ is in fact never constructed explicitly; rather, the 'action' of the integrating factor is evaluated through solution of the associated convection problem (9).

Remark. An alternative approach for the diffusion is to use the θ -method or the trapezoidal method. The semidiscrete equation for the diffusion operator then becomes

$$\frac{\mathbf{c}^{n+1} - \mathcal{Q}_{c}^{(t^{n+1},t^{n})}\mathbf{c}^{n}}{\Delta t} = \theta(\mathscr{D}(\mathbf{c}^{n+1}) + \mathbf{f}^{n+1}) + (1-\theta)\mathcal{Q}_{c}^{(t^{n+1},t^{n})}(\mathscr{D}(\mathbf{c}^{n}) + \mathbf{f}^{n}).$$
(11)

The terms $\mathcal{D}_{c}^{(t^{n+1},t^{n})}\mathbf{c}^{n}$ and $\mathcal{D}_{c}^{(t^{n+1},t^{n})}(\mathcal{D}(\mathbf{c}^{n}) + \mathbf{f}^{n})$ are calculated according to a convection problem similar to (9).

For $\theta = \frac{1}{2}$ this scheme results in a second-order-accurate Crank-Nicolson method. This scheme is commonly used for diffusion problems. In Navier-Stokes calculations it is frequently applied to the viscous and pressure terms. Although the Crank-Nicolson scheme is $A(\alpha)$ -stable for such terms, it has the disadvantage that it damps high-frequency components very weakly, whereas these components in reality decay very rapidly. In cases where this is undesirable, a possible strategy is to use $\theta = \frac{1}{2} + \delta \Delta t$, where δ is a small positive constant. This method damps all components of the solution and is formally second-order in time.

3. TAYLOR-GALERKIN TIME INTEGRATION

3.1. Schemes for linear convection

Taylor-Galerkin time integration methods are an extension of some typical time-stepping methods on the basis of Taylor series expansions including up to third-order terms. They are appropriate for pure convection problems, both linear and non-linear, since a stabilizing diffusion term is added to the numerical scheme in a natural way as part of the time integration.

Taylor-Galerkin methods were first proposed by Donea⁶ for linear convection equations with both constant and variable, but not time-dependent, velocity.

In this section several Taylor-Galerkin schemes for linear convection problems are discussed (the Galerkin discretization is in fact given in Section 3.3). For reasons mentioned in the previous section, explicit schemes are preferable. An overview is given of second-order methods that lead to explicit schemes, with special emphasis on convection problems with a time-dependent and divergence-free velocity field. For velocity fields that are not divergence-free, some of the schemes are not applicable. Keeping in mind possible applications, e.g. the incompressible Navier-Stokes equations, this seems to be a valid assumption. In Reference 6 third-order methods are given; however, these result in semi-implicit schemes.

Consider the linear convection equation

$$\frac{\partial \mathbf{c}}{\partial s} = -(\mathbf{u} \cdot \nabla) \mathbf{c} \quad \text{in } \mathbf{\Omega},$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \mathbf{\Omega},$$
(12)

with initial and boundary conditions. Following the notation of the previous section, the variable s is used for the time in a convection problem. The velocity field u(x, s) can depend both on space and on time.

Explicit Euler Taylor-Galerkin (EETG). The schemes for linear convection are Euler schemes, i.e. the Taylor series of the time derivative is based on forward differences. The approximation of **c** at $s = m\Delta s$ is denoted by **c**^m. The discretization in time is derived from the explicit Taylor series

$$\mathbf{c}^{m+1} = \mathbf{c}^m + \Delta s \left. \frac{\partial \mathbf{c}}{\partial s} \right|^m + \frac{\Delta s^2}{2} \left. \frac{\partial^2 \mathbf{c}}{\partial s^2} \right|^m + \mathcal{O}(\Delta s^3).$$
(13)

Using the original differential equation (12), the second derivative can be expressed as

$$\frac{\partial^2 \mathbf{c}}{\partial s^2} = -\frac{\partial \mathbf{u}}{\partial s} \cdot \Delta \mathbf{c} + \mathbf{u} \cdot \nabla (\mathbf{u} \cdot \nabla \mathbf{c}). \tag{14}$$

Substitution of (14) and the original equation into (13) yields a second-order EETG method

$$\mathbf{c}^{m+1} = \mathbf{c}^m - \Delta s \left[\left(\mathbf{u}^m + \frac{\Delta s}{2} \frac{\partial \mathbf{u}}{\partial s} \middle|^m \right) \cdot \nabla \right] \mathbf{c}^m + \frac{\Delta s^2}{2} \left(\mathbf{u}^m \cdot \nabla \right) (\mathbf{u}^m \cdot \nabla) \mathbf{c}^m + \mathcal{O}(\Delta s^3).$$
(15)

The third term on the right-hand side is not to be thought of as an artificial diffusion term but rather as part of the time integration. It possesses the tensorial structure similar to the streamline upwind/Petrov-Galerkin formulation proposed by Brooks and Hughes.³

In fact, the derivation of this scheme is similar to that of the schemes proposed by Donea *et al.*²² for convection-diffusion problems. However, if there is a diffusion term, the method becomes a semi-implicit one. The coefficient of the convective term in (15), containing the time derivative of the velocity, can be approximated either implicitly as

$$\mathbf{u}^{m} + \frac{\Delta s}{2} \frac{\partial \mathbf{u}}{\partial s} \Big|^{m} = \mathbf{u}^{m} + \frac{\Delta s}{2} \left(\frac{\mathbf{u}^{m+1} - \mathbf{u}^{m}}{\Delta s} + \mathcal{O}(\Delta s) \right)$$
$$= \frac{\mathbf{u}^{m} + \mathbf{u}^{m+1}}{2} + \mathcal{O}(\Delta s^{2})$$
$$= \mathbf{u}^{m+1/2} + \mathcal{O}(\Delta s^{2})$$
(16)

or explicitly as

$$\mathbf{u}^{m} + \frac{\Delta s}{2} \frac{\partial \mathbf{u}}{\partial s} \Big|^{m} = \mathbf{u}^{m} + \frac{\Delta s}{2} \left(\frac{\mathbf{u}^{m} - \mathbf{u}^{m-1}}{\Delta s} + \mathcal{O}(\Delta s) \right)$$
$$= \frac{3\mathbf{u}^{m} - \mathbf{u}^{m-1}}{2} + \mathcal{O}(\Delta s^{2})$$
$$= \mathbf{u}^{m-1/2} + \mathcal{O}(\Delta s^{2})$$
(17)

In equation (17) the notation $\mathbf{u}^{m-1/2}$ is introduced for simplicity. If the implicit approximation (16) is applied, only one old velocity \mathbf{u}^m has to be stored; in the explicit case (17) two old velocities \mathbf{u}^m and \mathbf{u}^{m-1} must be stored. However, it is not always possible to have the velocity at the time level m+1 available, e.g. in non-linear or coupled problems. In this case the explicit approximation has to be applied.

The two-step EETG scheme. Equation (13) can be rewritten as

$$\mathbf{c}^{m+1} + \mathbf{c}^m + \Delta s \left. \frac{\partial \mathbf{c}}{\partial s} \right|^{m+1/2} + \mathcal{O}(\Delta s^3), \tag{18}$$

where

$$\frac{\partial \mathbf{c}}{\partial s} \bigg|^{m+1/2} = \frac{\partial \mathbf{c}}{\partial s} \bigg|^m + \frac{\Delta s}{2} \frac{\partial^2 \mathbf{c}}{\partial s^2} \bigg|^m. \tag{19}$$

Substituting the original equation (12) at the time level $m + \frac{1}{2}$ into equation (18) yields

$$\mathbf{c}^{m+1} = \mathbf{c}^m - \Delta s(\mathbf{u}^{m+1/2} \cdot \nabla) \mathbf{c}^{m+1/2} + \mathcal{O}(\Delta s^3).$$
⁽²⁰⁾

The explicit Taylor series for $c^{m+1/2}$ reads

$$\mathbf{c}^{m+1/2} = \mathbf{c}^m + \frac{\Delta s}{2} \frac{\partial \mathbf{c}}{\partial s} \bigg|^m + \mathcal{O}(\Delta s^2).$$
(21)

Again substituting the original equation, now at time level *m*, gives

$$\mathbf{c}^{m+1/2} = \mathbf{c}^m - \frac{\Delta s}{2} \left(\mathbf{u}^m \cdot \nabla \right) \mathbf{c}^m.$$
(22)

Equations (20) and (22) give a second-order-accurate two-step explicit scheme. Morgan *et al.*²³ propose this scheme for general linear conservation problems. The same scheme is classified in Reference 24 as a second-order Runge-Kutta predictor-corrector method. For convection problems the two-step scheme is not asymptotically stable. However, it is quite useful for integration over a fixed time interval. Since the growth rate of the numerical solution is proportional to Δs^3 , one need merely to choose the time step sufficiently small so that the numerical growth of the solution is insignificant. This property is often referred to as weak instability.¹⁴

The two-step scheme possesses the same accuracy as the EETG method. However, there is no need to evaluate the 'expensive' second-order term. Moreover, application of a Galerkin spatial discretization (spectral elements) to this scheme is simpler than is the case for the EETG scheme. This aspect will be discussed in Section 3.3.

3.2. Schemes for non-linear convection

In this subsection Taylor-Galerkin schemes for non-linear convection problems are discussed. Although most schemes are practically the same as the schemes for linear convection, several aspects must be addressed separately. Consider the non-linear convection equation (Burgers equation with zero diffusivity)

$$\partial \mathbf{u}/\partial s = -(\mathbf{u} \cdot \nabla)\mathbf{u} \quad \text{in } \mathbf{\Omega},$$

 $\nabla \cdot \mathbf{u} = 0 \quad \text{in } \mathbf{\Omega},$
(23)

with initial and boundary conditions.

Explicit Euler Taylor-Galerkin (EETG). The derivation of a second-order-accurate explicit Euler Taylor-Galerkin scheme for the non-linear Burgers equation for divergence-free velocity is completely analogous to the linear case. The scheme reads

$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s \left[\left(\mathbf{u}^m + \frac{\Delta s}{2} \frac{\partial \mathbf{u}}{\partial s} \middle|^m \right) \cdot \nabla \right] \mathbf{u}^m + \frac{\Delta s^2}{2} \left(\mathbf{u}^m \cdot \nabla \right) \left(\mathbf{u}^m \cdot \nabla \right) \mathbf{u}^m + \mathcal{O}(\Delta s^3).$$
(24)

In order to keep the scheme explicit, the coefficient of the convective term must now be approximated according to (17).

A different Taylor-Galerkin scheme for non-linear convection equations is proposed by Laval and Quartapelle.²⁵ Their scheme is more general in the sense that the velocity is not required to be divergence-free. Moreover, the treatment of the time derivative of the velocity differs from the one proposed in equation (17). Since the equations are non-linear, in their scheme the original equation (23) is substituted for the time derivative of the velocity; this leads to a rather complicated scheme, especially if a Galerkin spatial discretization is applied. The treatment of the time derivative of the velocity proposed here is quite simple and does not lower the second-order accuracy of the original scheme.

The two-step EETG scheme. Again analogously to the linear case, the two-step Euler Taylor-Galerkin scheme can be written as

$$\mathbf{u}^{m+1/2} = \mathbf{u}^m - \frac{\Delta s}{2} (\mathbf{u}^m \cdot \nabla) \mathbf{u}^m,$$

$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s (\mathbf{u}^{m+1/2} \cdot \nabla) \mathbf{u}^{m+1/2}.$$
(25)

Analogously to the linear case, this method can easily be extended to a three-step method. For non-linear problems another way to construct a two- step EETG scheme is to substitute in the second equation of (25) the following Taylor series for $\mathbf{u}^{m+1/2}$:

$$\mathbf{u}^{m+1/2} = \mathbf{u}^m + \frac{\Delta s}{2} \frac{\partial \mathbf{u}}{\partial s} \bigg|^m + \mathcal{O}(\Delta s^2)$$
$$= \mathbf{u}^m - \frac{\Delta s}{2} (\mathbf{u}^m \cdot \nabla) \mathbf{u}^m + \mathcal{O}(\Delta s^2).$$
(26)

Then for divergence-free velocity fields the following scheme is obtained:

$$\mathbf{u}^{m+1/2} = \mathbf{u}^m - \frac{\Delta s}{2} (\mathbf{u}^m \cdot \nabla) \mathbf{u}^m$$
$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s (\mathbf{u}^{m+1/2} \cdot \nabla) \mathbf{u}^m + \frac{\Delta s^2}{2} (\mathbf{u}^m \cdot \nabla) (\mathbf{u}^m \cdot \nabla) \mathbf{u}^m.$$
(27)

This scheme can be viewed as a stabilized version of the original two-step scheme (25). The second equation of (27) is similar to the one-step EETG scheme (24). The difference is that since the problem is non-linear, it is possible to derive the coefficient for the convective term using the original equation. The most efficient and easiest-to-implement scheme is, also for non-linear convection problems, the two-step scheme (25), especially in an operator-splitting procedure.

3.3. Galerkin spectral element discretization

Application of the spectral element discretization to the semidiscrete systems of the previous subsections is done in the standard Galerkin way. In the spectral element approximation the domain is divided into non-overlapping, conforming elements. The discretization process is based on a variational or weak formulation of the partial differential equation. The main effect of the variational approach is that the continuity requirements at element boundaries are lowered. The integral equations appearing in the variational formulation are integrated by high-order Legendre Gauss-Lobatto quadrature. The variables in each element are expanded in a series of high-order polynomial basis functions. For reasons of efficiency, in more dimensions a tensorial basis is used. The discrete matrix-vector system is generated in the standard Galerkin way, leading to a block-banded system.

Since the schemes for linear convection can be derived from those for non-linear convection, only the latter schemes are considered. As already stated in Section 1, only homogeneous boundary conditions are considered for simplicity. The Galerkin weighted residual formulation of the EETG method (24) is given by

$$(\mathbf{u}^{m+1},\mathbf{v}) = (\mathbf{u}^m,\mathbf{v}) - \Delta s((\mathbf{u}^{m-1/2}\cdot\nabla)\mathbf{u}^m,\mathbf{v}) + \frac{\Delta s^2}{2}((\mathbf{u}^m\cdot\nabla)(\mathbf{u}^m\cdot\nabla)\mathbf{u}^m,\mathbf{v}),$$
(28)

with v the standard Galerkin test function. Application of Green's formula to the second-order term and substituting $\nabla \cdot \mathbf{u}^m = 0$ gives the variational or weak formulation

$$(\mathbf{u}^{m+1},\mathbf{v}) = (\mathbf{u}^m,\mathbf{v}) - \Delta s((\mathbf{u}^{m-1/2}\cdot\nabla)\mathbf{u}^m,\mathbf{v}) + \frac{\Delta s^2}{2}((\mathbf{u}^m\cdot\nabla)\mathbf{u}^m,(\mathbf{u}^m\cdot\nabla)\mathbf{v}).$$
(29)

For non-homogeneous boundary conditions also a non-trivial boundary integral must be taken into account. Applying the spectral element discretization then leads to

$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s \mathbf{M}^{-1} \mathbf{C}^{m-1/2} \mathbf{u}^m - \frac{\Delta s^2}{2} \mathbf{M}^{-1} \mathbf{D}^m \mathbf{u}^m.$$
(30)

The matrix $\mathbb{C}^{m-1/2}$ is the convective matrix with velocity $\mathbf{u}^{m-1/2}$ (see equation (17)); the matrix \mathbb{D}^m is a symmetric diffusion matrix arising in a natural way as part of the time integration. The matrix \mathbf{M} is the mass matrix, which is diagonal owing to the Legendre Gauss-Lobatto quadrature. Consequently, the solution of equation (3) (and of every other subsequent system)

does not involve the inversion of a matrix but only matrix-vector products which are evaluated using an element-by-element procedure. In general, for low-order methods the consistent mass matrix approach has advantages as regards the accuracy of the numerical scheme (see e.g. Reference 26). For high-order methods it is shown numerically by Timmermans and Van de Vosse²⁷ that the use of a diagonal mass matrix approach is valid, with relatively little loss of accuracy compared with low-order methods.

In an analogous way the spectral element discretization of the two-step EETG scheme (25) reads

$$\mathbf{u}^{m+1/2} = \mathbf{u}^m - \frac{\Delta s}{2} \mathbf{M}^{-1} \mathbf{C}^m \mathbf{u}^m,$$

$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s \mathbf{M}^{-1} \mathbf{C}^{m+1/2} \mathbf{u}^{m+1/2}.$$
(31)

Likewise for the extended stabilized two-step scheme (27)

$$\mathbf{u}^{m+1/2} = \mathbf{u}^m - \frac{\Delta s}{2} \mathbf{M}^{-1} \mathbf{C}^m \mathbf{u}^m,$$

$$\mathbf{u}^{m+1} = \mathbf{u}^m - \Delta s \mathbf{M}^{-1} \mathbf{C}^{m+1/2} \mathbf{u}^m - \frac{\Delta s^2}{2} \mathbf{M}^{-1} \mathbf{D}^m \mathbf{u}^m.$$
 (32)

For the two-step scheme (31) no boundary integral arises in the case of non-homogeneous boundary conditions owing to the absence of the second-order term. This scheme is therefore not only the most efficient but also the easiest to implement.

3.4. Numerical results

In this subsection the performance of the explicit Taylor-Galerkin methods and the spectral element approximation is tested by applying the numerical schemes to several convection problems of varying difficulty. First the proposed schemes are compared by means of a one-dimensional linear test case, the convection of a Gaussian hill. As an example of one-dimensional non-linear convection a non-linear Burgers problem is approximated. In more dimensions the efficiency of the scheme becomes rather important. The fast two-step EETG scheme is applied to several two- dimensional linear problems, both smooth and non-smooth.

One-dimensional linear convection. Consider as a test case for the Taylor-Galerkin schemes for linear convection problems in one dimension the convection of a Gaussian hill described by

$$c(x, t) = \exp\left(-\frac{(x - x_0 - ut)^2}{2\sigma^2}\right).$$
 (33)

The initial hill (t = 0) is centred around $x_0 = 0.15$ and has a standard deviation $\sigma = 0.04$. The hill is convected with constant velocity u = 1 and $t \in [0, 0.6]$.

For this problem the Taylor-Galerkin schemes for linear convection are compared with a Crank-Nicolson time integration. The spatial discretization is a spectral element one using $n_e = 16$ elements of degrees of approximation n = 2, 4 and 8. The discrete maximum error $\varepsilon = ||c - c_h||_{\infty,gl}$ for these cases is given in Table I. Here c_h denotes the approximate solution and the subscript ∞ ,gl means that the maximum error is evaluated in the Gauss-Lobatto points of the spectral element approximation. The exact solution and the approximation for $n_e = 16$, n = 4 using 256 time steps are shown in Figure 1.

Method		Number of time steps			
	n	128	256	512	1024
Two-step EETG	2 4 8	0.20×10^{0} 0.44×10^{-1} Unstable	0.21×10^{0} 0.10×10^{-1} Unstable	$\begin{array}{c} 0.21 \times 10^{0} \\ 0.90 \times 10^{-2} \\ 0.30 \times 10^{-2} \end{array}$	$ \begin{array}{r} 0.21 \times 10^{0} \\ 0.91 \times 10^{-2} \\ 0.74 \times 10^{-3} \end{array} $
One-step EETG	2 4 8	0.16×10^{0} 0.47×10^{-1} Unstable	0.19×10^{0} 0.10×10^{-1} 0.12×10^{-1}	$\begin{array}{c} 0.20 \times 10^{0} \\ 0.77 \times 10^{-2} \\ 0.30 \times 10^{-2} \end{array}$	$\begin{array}{c} 0.21 \times 10^{0} \\ 0.84 \times 10^{-2} \\ 0.74 \times 10^{-3} \end{array}$
Crank-Nicolson	2 4 8	$\begin{array}{c} 0.22 \times 10^{0} \\ 0.30 \times 10^{-1} \\ 0.24 \times 10^{-1} \end{array}$	0.22×10^{0} 0.13×10^{-1} 0.59×10^{-2}	0.21×10^{0} 0.93×10^{-2} 0.15×10^{-2}	$\begin{array}{c} 0.21 \times 10^{0} \\ 0.92 \times 10^{-2} \\ 0.37 \times 10^{-3} \end{array}$

Table I. Discrete maximum error $||c - c_h||_{\infty, gl}$ for the convection of a Gaussian hill; $n_e = 16$ elements with varying degree of approximation n

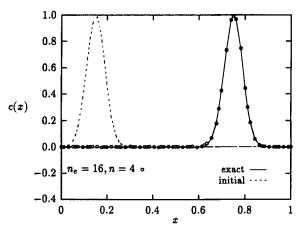


Figure 1. Convection of a Gaussian hill; exact solution and two-step EETG approximation for $n_e = 16$, n = 4 using 256 time steps

The results show that the one-step and two-step EETC methods are comparable with respect to accuracy. Both schemes need more time steps to become stable as the degree of approximation of the spatial discretization increases, the one-step scheme being a little more stable. Note also that the solution becomes much more accurate as the degree of approximation increases. the Crank–Nicolson scheme is only slightly more accurate. All schemes show second-order accuracy if the degree of approximation is large enough. Taking into account that the explicit Taylor– Galerkin schemes require far less processing time, it is obvious that they are in fact preferable for this problem.

One-dimensional non-linear convection. Consider the one-dimensional non-linear Burgers equation (23) with domain $\Omega = (0, 4)$ and $t \in [0, 2]$. The initial condition is given by

$$u(x, 0) = g(x) = \begin{cases} a - b \cos(2\pi x), & 0 \le x \le 1, \\ a - b, & \text{elsewhere,} \end{cases}$$
(34)

with a = 1 and b = 0.01. The boundary conditions are given by

$$u(0, t) = u(4, t) = a - b.$$
(35)

The exact solution to this problem is given by²⁸

$$u(x, t) = g(y), \qquad x = y + u(g(y))t.$$
 (36)

For this initial solution no shock arises in the given time segment.

This non-linear problem is solved with the explicit two-step EETG scheme and compared with a time-linearized Crank-Nicolson scheme. The latter scheme was in fact used to solve this problem in Reference 27. Since the boundary conditions are non-homogeneous, for this case the two-step scheme is easier to implement than the one-step EETG scheme (30) and the extended two-step scheme (32), both of which involve the evaluation of a boundary integral. The spectral element method uses the same number of elements and degrees of approximation as in the linear case. Since the solution only varies over an interval of 0.02, the numerical solution is verified with respect to the relative error

$$\varepsilon = \frac{\|\boldsymbol{u} - \boldsymbol{u}_{\mathbf{h}}\|_{\infty, \mathbf{gl}}}{0.02}.$$
(37)

The results for the relative error of the three different spectral element discretizations are given in Table II.

For non-linear convection the results are much the same as for the linear convection problem, although no second-order accuracy is achieved owing to the non-linearity. The two-step EETG scheme is quite comparable in accuracy with the Crank-Nicolson scheme. Again, for an increasing degree of approximation the solution becomes much more accurate, but then also more time steps are needed to obtain a stable numerical scheme. However, as already stated in the linear convection case, owing to the efficiency of the two-step scheme, it is more suited for this problem than the Crank-Nicolson method.

Two-dimensional linear convection. In more dimensions the choice of the time integration becomes more and more important with respect to efficiency. From the previous subsections it appears that the two-step EETG scheme (31) is the most suitable for large more-dimensional problems. In order to check the performance of the two-step scheme, consider the unsteady

· <u>······</u> ·····		Number of time steps			
Method	n	128	256	512	1024
Two-step EETG	2 4 8	0.92×10^{-1} 0.21×10^{-1} Unstable	0.99×10^{-1} 0.14×10^{-1} Unstable	$ \begin{array}{c} 0.10 \times 10^{0} \\ 0.11 \times 10^{-1} \\ 0.33 \times 10^{-2} \end{array} $	$\begin{array}{c} 0.10 \times 10^{0} \\ 0.11 \times 10^{-1} \\ 0.16 \times 10^{-2} \end{array}$
Crank-Nicolson	2 4 8	$\begin{array}{c} 0.11 \times 10^{0} \\ 0.22 \times 10^{-1} \\ 0.15 \times 10^{-1} \end{array}$	0.10×10^{0} 0.15×10^{-1} 0.57×10^{-2}	$\begin{array}{c} 0.10 \times 10^{0} \\ 0.12 \times 10^{-1} \\ 0.29 \times 10^{-2} \end{array}$	0.10×10^{0} 0.12×10^{-1} 0.18×10^{-2}

Table II. Relative discrete maximum error $||u - u_h||_{\infty,gl}/0.02$ for the Burgers proglem; $n_e = 16$ elements with varying degree of approximation n

rotation of a Gaussian hill described by the convection equation in two dimensions with domain $\Omega = (-1, 1) \times (-1, 1)$ and $t \in [0, 0.5]$. The time-dependent velocity is given by

$$\mathbf{u}(\mathbf{x}, t) = [-\pi^2 \sin((2\pi t)x_2), \pi^2 \sin((2\pi t)x_1)]^{\mathrm{T}}.$$
(38)

The initial solution is given by

$$c(\mathbf{x}, t) = 0.01^{4[(x_1 + 1/2)^2 + x_2^2]}.$$
(39)

It represents a smooth Gaussian hill with height equal to 1 and radius equal to $\frac{1}{4}$ centred at $(-\frac{1}{2}, 0)$. At t = 0.5 the hill is rotated halfway without diffusion and therefore without loss of shape.

The problem is solved using the two-step EETG scheme. Two types of convergence are examined. To check the *p*-convergence, the number of elements is kept fixed at $n_e = 4$ and the degree of approximation is varied (n = 4, 8, 12, 16). To check the *h*-convergence, the degree of approximation is kept fixed at n = 2 and the number of elements varied ($n_e = 16$, 64, 144, 256). The total number of degrees of freedom in the corresponding discretizations is the same. The results for the discrete maximum error $\varepsilon = ||c - c_h||_{\infty, gl}$ for the first discretization are given in Table III and for the second discretization in Table IV.

It is evident that the two-step scheme performs very well for this problem. The results of Table III show that the Gaussian hill is convected very accurately as the degree of approximation increases (*p*-convergence). These results are in good agreement with those for the steady rotation of a Gaussian hill presented by Timmermans and Van de Vosse.²⁷ From Table IV it can be deduced that *h*-convergence is also obtained; the solutions obtained upon increasing the degree of approximation, however, are much more accurate. In Figure 2 (left) the solution for n = 8 is shown. There are still some 'wiggles' visible in this solution. Figure 2 (right) shows the solution for n = 16, which is convected in an extremely accurate way.

It is also interesting to observe how the two-step and the spectral element discretization perform if the solution is no longer smooth. Consider again a linear convection problem in two

Time steps	<i>n</i> = 4	n = 8	n = 12	<i>n</i> = 16
256	$0.33 \times 10^{\circ}$	0.67×10^{-1}	0.17×10^{-1}	Unstable
512 1024	$0.33 \times 10^{\circ}$ $0.33 \times 10^{\circ}$	0.67×10^{-1} 0.67×10^{-1}	0.29×10^{-2} 0.29×10^{-2}	0.29×10^{-2} 0.33×10^{-3}

Table III Discrete maximum error $||c - c_h||_{\infty, gl}$ for the rotation of a Gaussian hill; number of elements $n_e = 4$ fixed, with varying degree of approximation n

Table IV Discrete maximum error $||c - c_h||_{\infty, gl}$ for the rotation of a Gaussian hill; degree of approximation n = 2 fixed, with varying degree of elements n_e

Time steps	$n_{e} = 16$	$n_e = 64$	$n_{\rm e} = 144$	$n_{\rm e} = 256$
256	$0.53 \times 10^{\circ}$	0.18×10^{0}	0.77×10^{-1}	0.34×10^{-1}
512	$0.53 \times 10^{\circ}$	0.19×10^{0}	0.82×10^{-1}	0.37×10^{-1}
1024	$0.53 \times 10^{\circ}$	$0.19 \times 10^{\circ}$	0.82×10^{-1}	0.38×10^{-1}

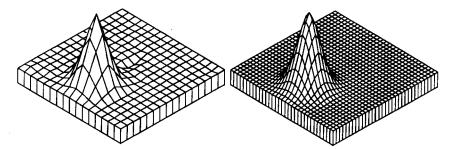


Figure 2. Unsteady rotation of a Gaussian hill; two-step EETG approximation using 1024 time steps for $n_e = 4$, n = 8 (left) and for $n_e = 4$, n = 16 (right)

dimensions with domain $\Omega = (-1, 1) \times (-1, 1)$ and $t \in [0, 1]$. The initial solution is given by

$$c(\mathbf{x},0) = \begin{cases} 1 - 4\sqrt{\left[(x_1 - \frac{1}{2})^2 + x_2^2\right]}, & (x_1 - \frac{1}{2})^2 + x_2^2 \le \frac{1}{16}, \\ 0, & (x_1 - \frac{1}{2})^2 + x_2^2 > \frac{1}{16}. \end{cases}$$
(40)

It represents a non-smooth cone with height equal to 1 and radius equal to $\frac{1}{4}$ centred at $(\frac{1}{2}, 0)$. The velocity is now given by

$$\mathbf{u}(\mathbf{x}, t) = \begin{bmatrix} -2\pi x_2, 2\pi x_1 \end{bmatrix}^{\mathrm{T}},\tag{41}$$

resulting in a steady rotation of the initial cone. Since there is no diffusion present, the end solution at t = 1 is exactly the same as the initial solution.

Again both p- and h-convergence are examined. The discretizations are the same as in the approximation of the Gaussian hill. The results for the first discretization are given in Table V and for the second discretization in Table VI.

Table V. Discrete maximum error $||c - c_h||_{\infty,gl}$ for the rotation of a cone; number of elements $n_e = 4$ fixed, with varying degree of approximation n

Time steps	<i>n</i> = 4	n = 8	n = 12	n = 16
256	$0.58 \times 10^{\circ}$	$0.30 \times 10^{\circ}$	Unstable	Unstable
512	0.58×10^{0}	$0.23 \times 10^{\circ}$	0.32×10^{1}	Unstable
1024	0.58×10^{0}	$0.21 \times 10^{\circ}$	0.17×10^{0}	0.38×10^{1}
2⇐↓¶		$0.21 \times 10^{\circ}$	0.17×10^{0}	0.97×10^{-1}

Table VI. Discrete maximum error $||c - c_h||_{\infty,g1}$ for the rotation of a cone; degree of approximation n = 2 fixed, with varying degree of elements n_e

Time steps	$n_{\rm e} = 16$	$n_{\rm e} = 64$	$n_{\rm e} = 144$	$n_{\rm e} = 256$
256	0.11×10^{1}	$0.54 \times 10^{\circ}$	$0.26 \times 10^{\circ}$	Unstable
512	0.11×10^{1}	$0.54 \times 10^{\circ}$	$0.29 \times 10^{\circ}$	$0.14 \times 10^{\circ}$
1024	0.11×10^{1}	$0.54 \times 10^{\circ}$	$0.29 \times 10^{\circ}$	$0.15 \times 10^{\circ}$
2048	0.11×10^{1}	$0.54 \times 10^{\circ}$	$0.29 \times 10^{\circ}$	0.15×10^{0}

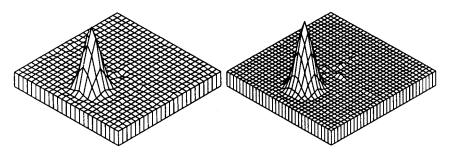


Figure 3. Steady rotation of a cone; two-step EETG approximation using 1024 time steps for $n_e = 4$, n = 12 (left) and using 2048 time steps for $n_e = 4$, n = 16 (right)

The results of Table V show that for this problem no clear *p*-convergence is obtained. This is of course due to the fact that the solution is non-smooth. However, good results are still obtained if the degree of approximation and the number of time steps are large enough, as can be seen in Figure 3, where the solutions are shown for $n_e = 4$, n = 12 using 1024 time steps (left) and for $n_e = 4$, n = 16 using 2048 time steps (right). As regards the results of Table VI, it is seen that no clear *h*-convergence is obtained either. The solution improves slightly as the number of elements is increased. With respect to accuracy and efficiency one may conclude that the high-order elements are preferable up to degree n = 8. For a higher degree of approximation the solution is indeed more accurate but also more expensive than the solutions obtained with elements of degree n = 2. Concluding, it can be said that one has to look for an optimal combination of *p*- and *h*-convergence when approximating non-smooth problems. The spectral element method can then be a very useful tool.

4. OPERATOR-SPLITTING FOR CONVECTION-DIFFUSION

4.1. The time integration scheme

Combining the semi-implicit backward difference schemes for the diffusion operator with the explicit Taylor-Galerkin time integration of the previous section, a full operator-splitting scheme for convection-diffusion problems can be derived, based on the theory of Section 2. As an example the two-step Taylor-Galerkin method is chosen for the associated convection problem (9).

According to equation (7), the diffusion step reads (again only the non-linear case is considered)

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \sum_{i=1}^{k_1} \beta_i \mathcal{Q}_c^{(t^{n+1}, t^{n+1-i})} \mathbf{u}^{n+1-i}}{\Delta t} = \mathcal{D}(\mathbf{u}^{n+1}) + \mathbf{f}^{n+1}.$$
(42)

The terms $\mathcal{Q}^{(t^{n+1-i},t^n)}\mathbf{u}^n$ (i = 1, 2, ...) are calculated according to the two-step explicit EETG scheme with initial condition $\tilde{\mathbf{u}}^0 = \mathbf{u}^{u+1-i}$ using a time step Δs such that $\Delta t = j\Delta s$ with j an integer. The semidiscrete convection step then reads

$$\tilde{\mathbf{u}}^{m+1/2} = \tilde{\mathbf{u}}^m - \frac{\Delta s}{2} (\tilde{\mathbf{u}}^m \cdot \nabla) \tilde{\mathbf{u}}^m,$$

$$\tilde{\mathbf{u}}^{m+1} = \tilde{\mathbf{u}}^m - \Delta s (\tilde{\mathbf{u}}^{m+1/2} \cdot \nabla) \tilde{\mathbf{u}}^{m+1/2}.$$
(43)

Analogously to equation (10), it then follows that

$$\tilde{\mathbf{u}}^{n+1-i} = \tilde{\mathbf{u}}^{i(j+1)},\tag{44}$$

where the simpler notation $\tilde{\mathbf{u}}^{n+1-i} = \mathcal{Q}^{(t^{n+1-i},t^n)}\mathbf{u}^n$ is introduced.

4.2. Galerkin spectral element discretization

The application of Galerkin spectral element discretization to the splitting scheme of the previous subsection is straightforward. The weighted residual formulation of the diffusion step is given by (again homogeneous boundary conditions are assumed)

$$\left(\gamma_0 \mathbf{u}^{n+1} - \sum_{i=1}^{k_1} \beta_i \tilde{\mathbf{u}}^{n+1-i}, \mathbf{y}\right) = \Delta t(\mathscr{D}(\mathbf{u}^{n+1}) + \mathbf{f}^{n+1}, \mathbf{v}),$$
(45)

leading to

$$\mathbf{M}\left(\gamma_0 \mathbf{u}^{n+1} - \sum_{i=1}^{k_1} \beta_i \tilde{\mathbf{u}}^{n+1-i}\right) = \Delta t (-\mathbf{D} \mathbf{u}^{n+1} + \mathbf{M} \mathbf{f}^{n+1}).$$
(46)

The terms $\tilde{\mathbf{u}}^{n+1-i}$ are evaluated through

$$\tilde{\mathbf{u}}^{m+1/2} = \tilde{\mathbf{u}}^m - \frac{\Delta s}{2} \mathbf{M}^{-1} \mathbf{C}^m \tilde{\mathbf{u}}^m,$$

$$\tilde{\mathbf{u}}^{m+1} = \tilde{\mathbf{u}}^m - \Delta s \mathbf{M}^{-1} \mathbf{C}^{m+1/2} \tilde{\mathbf{u}}^{m+1/2},$$
(47)

with initial condition $\tilde{\mathbf{u}}^0 = \mathbf{u}^{n+1-i}$.

Remark. If a Crank-Nicolson scheme (see equation (11)) is used to treat the diffusion step, the discrete Galerkin system for the diffusion step becomes

$$\mathbf{M}(\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^n) = \frac{1}{2}\Delta t(-\mathbf{D}\mathbf{u}^{n+1} + \mathbf{M}\mathbf{f}^{n+1}) + \frac{1}{2}\Delta t \tilde{\mathbf{d}}^n,$$
(48)

where

$$\tilde{\mathbf{u}}^{n} = \mathscr{Q}_{c}^{(t^{n+1},t^{n})}\mathbf{u}^{n},$$

$$\tilde{\mathbf{d}}^{n} = \mathscr{Q}_{c}^{(t^{n+1},t^{n})}(-\mathbf{D}\mathbf{u}^{n} + \mathbf{M}\mathbf{f}^{n}).$$
(49)

The term $\tilde{\mathbf{u}}^n$ is evaluated through the solution of the two-step scheme (47) with initial condition $\tilde{\mathbf{u}}^0 = \mathbf{u}^n$. The term $\tilde{\mathbf{d}}^n$ is evaluated according to the two-step scheme

$$\tilde{\mathbf{d}}^{m+1/2} = \tilde{\mathbf{d}}^m - \frac{\Delta s}{2} \mathbf{M}^{-1} \mathbf{C}^m \tilde{\mathbf{d}}^m,$$

$$\tilde{\mathbf{d}}^{m+1} = \tilde{\mathbf{d}}^m - \Delta s \mathbf{M}^{-1} \mathbf{C}^{m+1/2} \tilde{\mathbf{d}}^{m+1/2}.$$
(50)

The initial condition to equation (50) reads

$$\tilde{\mathbf{d}}^0 = \mathbf{d}^n = -\mathbf{M}^{-1}\mathbf{D}\mathbf{u}^n + \mathbf{f}^n.$$
⁽⁵¹⁾

If the term $\tilde{\mathbf{d}}^n$ in equation (48) is replaced by \mathbf{d}^n , such as is the case in splitting methods based on the classical splitting approach,¹ the second-order accuracy of the diffusion step is lost. This will be shown numerically in the next subsection. Note that in the case of a backward difference scheme there is no need to convect the diffusion operator itself, thus prohibiting 'expensive' evaluations like (51).

4.3. Numerical results

In order to test the performance of the operator-splitting approach, in this section a one-dimensional convection-diffusion problem is solved using an implicit time integration for the diffusion step and the explicit two-step EETG scheme (31) for the convection step.

Consider as a test case for the operator-splitting scheme the problem of a Gaussian hill in one dimension travelling with a constant velocity u = 1 and spreading isotropically with a viscosity $\eta = 0.05$. This problem is adapted from a test case in Reference 22. The exact solution has the form

$$c(x,t) = \frac{\sigma(0)}{\sigma(t)} \exp\left(-\frac{(x-x_0-ut)^2}{2\sigma(t)^2}\right),$$
(52)

where $\sigma(t) = \sqrt{(\sigma(0) + 2\eta t)}$. The initial hill (t = 0) is centred around $x_0 = 0.15$ and has a standard deviation $\sigma(0) = 0.04$. The hill is convected with constant velocity u = 1 and $t \in [0, 0.3]$.

This problem is solved using the splitting scheme described above for both a first- and a second-order backward difference (BDF) scheme and for a Crank-Nicolson scheme (CN-new). Moreover, it is checked whether the second-order accuracy of the Crank-Nicolson splitting scheme is lost if the term $\tilde{\mathbf{d}}^n$ in equation (48) is replaced by \mathbf{d}^n (CN-classical). The number of time steps for the convection step is equal to 64. The spectral element discretization uses $n_e = 16$ elements with degree of approximation n = 4. The discrete maximum error $\varepsilon = ||c - c_h||_{\infty, gl}$ is given in Table VII. Figure 4 shows the exact solution and the approximation for $n_e = 16$, n = 4 using a second-order backward difference scheme with four diffusion time steps.

The performance of the operator-splitting scheme is quite good. Only very few expensive diffusion steps are needed to obtain accurate solutions. It can also be seen that the backward difference schemes and the Crank-Nicolson scheme achieve the theoretical order of accuracy for sufficient diffusion steps. The performance of the 'classical' Crank-Nicolson approach is very poor compared with the other results. For the small number of diffusion steps that are needed to obtain accuracy for the other schemes, the solution is not very accurate. The large number of convection steps in each diffusion cycle does not require much extra processing time, since each convection step is solved explicitly.

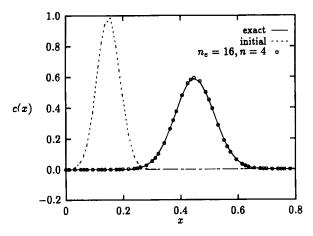


Figure 4. Convection and diffusion of a Gaussian hill; exact solution and two-step EETG/second-order backward difference approximation for $n_e = 16$, n = 4 using four diffusion steps containing 64 convection steps each

Diffusion steps	BDF 1st-order	BDF 2nd-order	CN-new	CN-classical
2	0.42×10^{-1}	0.24×10^{-1}	0.58×10^{-2}	$0.23 \times 10^{\circ}$
4	0.22×10^{-1}	0.39×10^{-2}	0.16×10^{-2}	$0.26 \times 10^{\circ}$
8	0.11×10^{-1}	0.87×10^{-3}	0.42×10^{-3}	0.11×10^{0}
16	0.58×10^{-2}	0.31×10^{-3}	0.24×10^{-3}	0.43×10^{-1}
32	0.30×10^{-2}	0.17×10^{-3}	0.17×10^{-3}	0.20×10^{-1}

Table VII. Discrete maximum error $||c - c_h||_{\infty, gl}$ for the convection and diffusion of a Gaussian hill; $n_e = 16$ elements of degree n = 4; 64 two-step EETG convection steps per diffusion step

5. CONCLUSIONS

In this paper a closer look has been taken at the application of a Galerkin high-order spectral element method to convection-diffusion problems with a time-dependent and divergence-free velocity field. In order to decouple the treatment of the convection operator and the stiff diffusion operator, an operator-splitting integrating factor approach has been presented. The decoupled problems are then solved with suitable time integrations, if necessary using different time steps.

For pure convection problems explicit time integration is virtually necessary to obtain an efficient numerical scheme, especially in the case where the problem is non-linear. A possible strategy to stabilize the numerical oscillations that often occur in the solution of convection-dominated problems is to make use of so-called Taylor–Galerkin methods. Several explicit second-order schemes have been proposed and analysed for both linear and non-linear convection problems with time-dependent and divergence-free velocity. The schemes have been tested by means of several model test cases. With respect to accuracy the Taylor–Galerkin schemes are quite comparable with an implicit Crank–Nicolson scheme; as regards efficiency, the explicit schemes are much faster than the implicit time integration. Also, for non-linear and for more-dimensional problems the Taylor–Galerkin schemes appear to be very well suited.

For convection-diffusion problems the operator-splitting technique gives good results. The splitting scheme has been applied to a one-dimensional test case. The convection part is treated with a suitable Taylor-Galerkin scheme. The diffusion or stiff part of the equation can be solved with a second-order (semi-)implicit backward difference scheme or with a trapezoidal method (e.g. Crank-Nicolson), the former being the more efficient. Only very few diffusion steps are needed to obtain a second-order-accurate splitting scheme. The number of convection steps can be taken relatively large, since the Taylor-Galerkin schemes are explicit.

Finally, with respect to the spectral element spatial discretization it can be concluded that if the number of time steps is large enough, a clear p-convergence for smooth problems to the exact solution is seen. In the operator-splitting technique proposed here the larger number of time steps required for a higher-order spectral element approximation is not a problem with respect to efficiency. The number of 'expensive' diffusion steps is very low compared with the number of 'cheap' convection steps. Moreover, since the application of a high-order method validates the use of a diagonal mass matrix (much more so than in the case of a low-order method), the explicit convection steps only involve matrix-vector products and not the inversion of a matrix to solve the system. When the problem is no longer smooth, an optimum has to be found between p- and h-convergence. In this case the spectral element method is a very useful tool, since both types of convergence can be realized by it.

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