Time-accurate solution of stabilized convection-diffusion-reaction equations: I. Time and space discretization

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SUMMARY

The paper addresses the development of time accurate methods for solving transient convection-diffusion-reaction problems using finite elements. Multi-stage time stepping schemes of high accuracy are used. They are first combined with a Galerkin formulation to briefly recall the time space discretization. Then spatial stabilization techniques are combined with high-order time stepping schemes. Moreover, a least-squares formulation is also developed for these high-order time schemes combined with C^0 finite elements (in spite of the diffusion operator and without reducing the strong form into a system of first-order differential equations). The weak forms induced by the SUPG, GLS, SGS and least-squares formulations are presented and compared. In a companion paper (Part II of this work), the phase and damping properties of the developed schemes are analyzed and numerical examples are included to confirm the effectiveness of the proposed methodology for solving time dependent convection-diffusion-reaction problems.

KEY WORDS: convection-diffusion-reaction, time stepping schemes, stabilization, least-squares, finite element method

1. INTRODUCTION

A great deal of effort has been devoted in recent years to the development of finite element methods for the numerical approximation of transport problems involving convective, diffusive and reactive processes. It is well-known that the standard Galerkin finite element method is not ideally suited to deal with the spatial discretization of convection dominated transport problems [16, 9]. Thus spatial stabilization techniques are necessary to introduce a suitable amount of numerical dissipation in the presence of internal or boundary layers.

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In truly transient problems, which are of interest in the present paper, the basic issue is not merely a question of adding artificial diffusion. Another equally important aspect being to ensure an adequate coupling between the spatial approximation provided by the finite element method and the time discretization. As noted in [8], it has been shown that the combination of a standard Galerkin spatial discretization with classical, second order accurate, time stepping schemes, such as the Lax-Wendroff, leap-frog, and Crank-Nicolson methods, fails to produce satisfactory numerical results when convection dominates the transport process. Actually, the above second order time integration methods properly combine with linear finite elements in convection problems only for small values of the time step, thus severely undermining the utility of such time integration schemes in practical applications. Moreover, multi-step explicit schemes [14, 15], which can go beyond second order, suffer from severe restrictions on the allowable time step in both convection and diffusion dominated areas [7].

With these two issues in mind it seems reasonable to go beyond second order schemes stabilized with techniques originally designed for steady problems, see [13, 20, 4], and high-order time stepping schemes designed exclusively for pure convection problems [10, 5, 1, 6],and mixed least-squares finite element formulations [18, 2].

Moreover, another important issue motivates the use of high-order integration schemes. The computational cost of transient problems is directly related to the size of the time step. Thus, increasing the order of the time stepping algorithm allows to use larger time steps maintaining the overall accuracy (which, obviously, must be comparable to the spatial accuracy). For instance, moving from a second to a fourth order time integration scheme implies an increase of the time step size by a factor of $1/\sqrt{\triangle t}$ (where $\triangle t$ is the time step employed in the second order method). This can only be done if the properties of the higher order algorithm (for instance, stability) are not degraded and the cost is not dramatically increased. Note that such a factor means that, from an accuracy point of view, a second order scheme with a dimensionless time step of $\triangle t = 0.01$ is approximately equivalent to a fourth order scheme with $\triangle t = 0.1$ (ten times larger!).

Here, high-order implicit time stepping schemes combined with classical stabilization techniques are proposed which adequately combine with C^0 finite elements in convection-diffusion-reaction problems because of their simultaneous A-stability and high-order accuracy. The issue of coupling stabilized C^0 continuous spatial finite elements with highly accurate time stepping algorithms is not trivial. On one hand, the time stepping scheme can only involve first time derivatives (u_t is coupled with second order spatial derivatives by the differential equation). And at the same time, the stabilization technique must induce weak forms with approximating functions belonging to $\mathcal{H}^1$. This is standard in stabilization schemes such as *streamline-upwind Petrov-Galerkin* (SUPG), *Galerkin least-squares* (GLS), and *sub-grid scale* (SGS) methods. Note however, that the usual formulations of such methods do not go beyond second-order time schemes. Here this limitation is precluded. A standard *least-squares* (LS) formulation of the convection-diffusion equation would require functions belonging to $\mathcal{H}^2$ or the use of mixed approximations, *i.e.* increasing the number of nodal unknowns, see [18, 2]. This is also avoided in the present formulation.

Note that the proposed methods follow the classical structure: finite differences in time — finite elements in space. Other alternatives are possible, namely space-time finite elements, see for instance [17, 20], but they are not addressed here.

2. PROBLEM STATEMENT

We are concerned with a time accurate finite element solution of the following convection-diffusion-reaction initial boundary value problem:
Given the velocity field $\boldsymbol{a}(\boldsymbol{x},t)$, the diffusion coefficient $\nu(\boldsymbol{x},t)$, the reaction $\sigma(\boldsymbol{x},t)$, the source term $s(\boldsymbol{x},t)$, and the necessary initial and boundary conditions, find $u(\boldsymbol{x},t)$ such that

$$u_t + \boldsymbol{a}\cdot\nabla u - \nu\nabla^2 u + \sigma u = s \qquad\qquad \text{in } \Omega\times(0,T), \qquad (1\text{a})$$

$$u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) \qquad\qquad \text{on } \Omega, \qquad (1\text{b})$$

$$u = u_D \qquad\qquad \text{on } \partial\Omega\backslash\Gamma, \qquad (1\text{c})$$

$$\nu\,\boldsymbol{n}\cdot\nabla u = \varrho(\boldsymbol{n}\cdot\boldsymbol{a})(u - u_e) + \eta \qquad\qquad \text{on } \Gamma, \qquad (1\text{d})$$

where the first boundary condition, (1c), is Dirichlet (u_D is given), and the second one, (1d), is either Neumann o Robin depending on the parameters ϱ and η (u_e is also given).

The exact conditions for existence and unicity of the solution can be found in [19, Chap. 12] or [16, Thm 2.5.1], among others. In convection dominated problems, it is sufficient for existence and unicity to impose that $\nu \geq \nu_0 > 0$ and $0 < \mu_0 \leq \sigma - \frac{1}{2}\nabla\cdot\boldsymbol{a} \leq \mu_1$ in Ω. With these conditions, the bilinear form associated with the spatial operator (in a Galerkin formulation) is continuous and coercive, with a coercivity constant $\alpha = \min\{\nu_0, (\nu_0 + C_\Omega\mu_0)/(1 + C_\Omega)\}$, where C_Ω is the Poincaré inequality constant ($\int_\Omega v^2 d\Omega \leq C_\Omega \int_\Omega |\nabla v|^2 d\Omega$). That is, the Lax-Milgram Lemma can be applied.

Symbolically the partial differential equation (1a) may be rewritten as:

$$u_t + \mathcal{L}(u) = s, \qquad (2)$$

where the spatial differential operator is defined as

$$\mathcal{L} := \boldsymbol{a}\cdot\nabla - \nu\nabla^2 + \sigma \qquad (3)$$

The numerical solution of such a convection-diffusion-reaction problem clearly involves a double discretization process, that is, time discretization and space discretization.

3. TIME DISCRETIZATION

A key point in this paper is that time discretization precedes the spatial discretization. Which discretization is performed first is not an issue for linear spatial operators $\mathcal{L}$, see Eq. (3), with constant coefficients and a Galerkin formulation. Here, however, the objective is to stabilize the equations and, consequently, time discretization must be performed first.

For illustration purposes, only implicit multi-stage methods are presented. A more complete (and unified presentation as Padé approximations) can be found in [7, 8].

These schemes can be written in incremental form as

$$\frac{\triangle\boldsymbol{u}}{\triangle t} - \mathbf{W}\triangle\boldsymbol{u}_t = \mathbf{w}\,u_t^n, \qquad (4)$$

where the unknown $\triangle\boldsymbol{u} \in \mathbb{R}^{\mathbf{n}_{\text{stages}}}$ is a vector whose dimension varies with the number of stages, $\mathbf{n}_{\text{stages}}$. The vector $\triangle\boldsymbol{u}_t$ is the partial derivative of $\triangle\boldsymbol{u}$ with respect to time. The time derivatives in (4) are replaced by spatial derivatives using the original differential equation.

For instance, in the case of a linear operator $\mathcal{L}$ with constant coefficients, see (3), equation (4) becomes

$$\frac{\triangle \boldsymbol{u}}{\triangle t} + \mathbf{W}\mathcal{L}(\triangle \boldsymbol{u}) = \mathbf{w}\big[s^n - \mathcal{L}(u^n)\big] + \mathbf{W}\triangle \boldsymbol{s}. \tag{5}$$

The precise definition of $\triangle \boldsymbol{u}$ (recall that $\triangle \boldsymbol{u}_t$ is simply $\partial \triangle \boldsymbol{u}/\partial t$), $\triangle \boldsymbol{s}$, $\mathbf{w}$, and $\mathbf{W}$ depends on each particular method. In the present paper, reference will be made to the classical second-order and a fourth-order method, namely:

Second order Padé approximation: R_{11} **(Crank-Nicolson)**

$$\triangle \boldsymbol{u} = u^{n+1} - u^n, \qquad \triangle \boldsymbol{s} = s^{n+1} - s^n,$$
$$\mathbf{W} = \frac{1}{2}, \qquad\qquad \mathbf{w} = 1. \tag{6}$$

Note that in this case $\mathbf{n_{stages}} = 1$ and, consequently, the vectors and matrix in (4) become scalars.

Fourth order Padé approximation: R_{22}

$$\triangle \boldsymbol{u} = \left\{ \begin{array}{c} u^{n+1/2} - u^n \\ u^{n+1} - u^{n+1/2} \end{array} \right\}, \qquad \triangle \boldsymbol{s} = \left\{ \begin{array}{c} s^{n+1/2} - s^n \\ s^{n+1} - s^{n+1/2} \end{array} \right\},$$
$$\mathbf{W} = \frac{1}{24}\left[\begin{array}{cc} 7 & -1 \\ 13 & 5 \end{array} \right], \qquad\qquad \mathbf{w} = \frac{1}{2}\left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\}. \tag{7}$$

Note that a three-stage sixth order method can be developed along the same lines from Padé approximation R_{33} [8].

Both equations (4) and (5) with the corresponding initial and boundary conditions, Eqs. (1b) (1c) and (1d), define a problem in *strong form*, which must be solved at each time step. For simplicity, the truncation errors are not explicitly shown in (4), and (5). Note, however, that if these truncation errors are accounted for, equations (1a) and (4) are equivalent, and the exact solution verifies the new strong form. The spatially continuous differential equations, (4) or (5), are the basis for the finite element discretization.

4. STANDARD GALERKIN APPROXIMATION

Application of the Galerkin formulation to the time stepping schemes defined by (4) results in the following weak form

$$\big(\boldsymbol{v}, \frac{\triangle \boldsymbol{u}}{\triangle t}\big)_\Omega - \big(\boldsymbol{v}, \mathbf{W}\triangle \boldsymbol{u}_t\big)_\Omega = \big(\boldsymbol{v}, \mathbf{w}\, u_t^n\big)_\Omega \tag{8}$$

for all $\boldsymbol{v} \in [\mathcal{V}_0^h]^{\mathbf{n_{stages}}}$. With $\mathcal{V}_0^h$ subset of the usual functional space $\mathcal{H}_0^1 = \{v \mid v \in \mathcal{H}^1, v = 0 \text{ on } \partial\Omega\backslash\Gamma\}$, and with the standard definition of the vector scalar product $\big(\boldsymbol{v}, \boldsymbol{u}\big)_\Omega = \int_\Omega \boldsymbol{u}\cdot\boldsymbol{v}\, d\Omega$.

Note that the right-hand side of (8) is known, and that the second term of the left-hand side (*i.e.* $\triangle \boldsymbol{u}_t$) includes the Laplace operator, which is integrated by parts. Reference [8] provides a complete derivation, analysis and illustration of these time schemes with the Galerkin formulation; the proposed extension to stabilized formulations is presented next.

5. EXTENSION TO STABILIZED METHODS

In order to stabilize the convective term in a consistent manner, *i.e.* ensuring that the solution of the differential equation is also a solution of the weak form, Hughes and co-workers have proposed several techniques. They follow the rationale: an extra term weighted over the element interiors is added to the Galerkin weak form. This added term is a function of the residual of the differential equation to ensure consistency. These methods are originally designed for the steady convection-diffusion equation and subsequently extended to transient problems with second order time schemes and to space-time formulations. In this literature, the spatial discretization precedes the time discretization and consequently, the residual employed in the stabilization term includes time derivatives. The implementation of multi-stage time stepping schemes is, in such a case, not trivial.

Here, standard stabilization techniques are implemented with high-order time stepping schemes such as (4). The standard stabilization techniques used in the present context are the *streamline-upwind Petrov-Galerkin* (SUPG), *Galerkin least-squares* (GLS), and *sub-grid scale* (SGS) methods. Moreover, a *least-squares* (LS) stabilization procedure is also proposed.

In order to have a consistent stabilization a residual must be defined. The residual, in this case, is chosen after time discretization. Thus, from (4) one gets

$$\mathcal{R}(\triangle \boldsymbol{u}) := \triangle \boldsymbol{u}/\triangle t - \mathbf{W} \triangle \boldsymbol{u}_t - \mathbf{w}\, u_t^n, \tag{9}$$

and the consistently stabilized weak form is

$$\left(\boldsymbol{v}, \frac{\triangle \boldsymbol{u}}{\triangle t}\right)_{\Omega} - \left(\boldsymbol{v}, \mathbf{W} \triangle \boldsymbol{u}_t\right)_{\Omega} + \underbrace{\sum_{e} \left(\tau \mathcal{P}(\boldsymbol{v}), \mathcal{R}(\triangle \boldsymbol{u})\right)_{\Omega^e}}_{\text{Stabilization term}} = \left(\boldsymbol{v}, \mathbf{w}\, u_t^n\right)_{\Omega} \tag{10}$$

with $\boldsymbol{v} \in [\mathcal{H}_0^1]^{\mathrm{n_{stages}}}$. Note that the stabilization term is added to the Galerkin weak form, see (8). In the stabilization term a free parameter appears τ (the intrinsic time scale), see [21, 4], and the operator $\mathcal{P}$ characterizes the stabilization technique (*i.e.* SUPG, GLS, SGS, or LS).

Again, the truncation errors are not explicitly indicated. But as noted earlier the truncation error, *i.e.* a term $\mathcal{O}(\triangle t^m)$, can be added to (9) and (10). This would ensure that the solution of (1) is also the unique solution of (9) (and the unique solution of (10) because the added term is a function of the residual). If the truncation error is neglected, the precision in time is characterized by the order of this error, $m = 2$ or 4, depending on the particular scheme chosen, respectively (6) or (7).

In order to better visualize the spatial differential structure of (9), this equation is rewritten for the particular case of linear $\mathcal{L}$ with constant coefficients, *i.e.* from (5),

$$\mathcal{R}(\triangle \boldsymbol{u}) = \frac{\triangle \boldsymbol{u}}{\triangle t} + \mathbf{W}\mathcal{L}(\triangle \boldsymbol{u}) - \mathbf{w}\big[s^n - \mathcal{L}(u^n)\big] - \mathbf{W}\triangle \boldsymbol{s}, \tag{11}$$

where, from the second term on the right-hand side, one can observe that the operator $\mathcal{L} = \boldsymbol{a} \cdot \nabla - \nu \nabla^2 + \sigma$ acts on each component of $\triangle \boldsymbol{u}$.

In order to completely define the stabilized method, (10), the perturbation operator, $\mathcal{P}$, must be defined, see for instance [3] for a general presentation in a framework of single-step time integration methods, *i.e.* at most second order in time, or a space-time approach.

5.1. Streamline-upwind Petrov-Galerkin stabilization

This stabilization technique is defined by taking,

$$\mathcal{P}(\boldsymbol{v}) := \mathbf{W}(\boldsymbol{a} \cdot \nabla)\boldsymbol{v}. \tag{12}$$

Note that the matrix $\mathbf{W}$, which affects the convection term in (11), induces a *non scalar* stabilization (each equation of the multi-stage time algorithm is affected by different coefficients). The weak form for the SUPG method is obtained after substitution of the perturbation, *i.e.* (12), in equation (8). The non symmetric structure of the stabilization term induces some technical difficulties in the stability analysis of the SUPG method. This is avoided in the Galerkin least-squares stabilization technique because it introduces a symmetric stabilization term in a consistent manner.

5.2. Galerkin least-squares stabilization

The need for a previous time discretization is clear in this method. The GLS stabilization uses as perturbation operator $\mathcal{P}$ the spatial differential operator of the strong form, which in this case is affected by the time discretization. Note that the present approach differs from the standard space-time GLS formulation (no time derivatives appear in $\mathcal{P}$ and thus there is no need for multi-corrector algorithms), see [3, 20]. In the case of a linear convection-diffusion-reaction equation with constant coefficients, from (11) one deduces the operator $\mathcal{P}$, namely

$$\mathcal{P}(\boldsymbol{v}) := \frac{\boldsymbol{v}}{\triangle t} + \mathbf{W}\,\mathcal{L}(\boldsymbol{v}). \tag{13}$$

From a practical point of view there is no major difference between SUPG and GLS methods. Note that both methods are not identical, as in steady problems, for convection-diffusion (no reaction) and with linear elements (the second order derivatives are zero in the element interiors). Moreover, the qualitative influence of each term in the definition of $\mathcal{P}$, Eq. (13), may be interpreted as follows,

$$\mathcal{P}(\boldsymbol{v}) = \frac{\boldsymbol{v}}{\triangle t} + \mathbf{W}\,\mathcal{L}(\boldsymbol{v}) = \underbrace{\frac{\boldsymbol{v}}{\triangle t}}_{\text{Galerkin}} + \mathbf{W}\Big[\underbrace{(\boldsymbol{a}\cdot\nabla)\boldsymbol{v}}_{\text{SUPG}} - \underbrace{\nabla\cdot(\nu\nabla\boldsymbol{v})}_{0} + \underbrace{\sigma\boldsymbol{v}}_{\text{Galerkin}}\Big].$$

The first term is a Galerkin weighting, the second term corresponds to the SUPG stabilization, the third term is zero for linear elements, and the fourth term is also a Galerkin weighting. Thus, for linear elements and a constant positive reaction, GLS is SUPG with the Galerkin term weighted $1 + \tau(C\sigma + 1/\triangle t)$ times more (with C a constant related to $\mathbf{W}$). This implies, that the instabilities introduced by Galerkin are a little bit more amplified in GLS compared with SUPG. This minor problem of the GLS stabilization technique is overcome in the simplest version of the sub-grid scale (SGS) method, see next section.

In the case of the nonlinear convection-diffusion-reaction equation it is helpful to define the quasi-linear operator related to (3), see for instance the discussion in [11]. This quasi-linear operator is then used in (13). Note finally, that the stabilization term is symmetric but the complete weak form, *i.e.* (10) with (13), is in general non-symmetric.

5.3. Sub-grid scale stabilization

The simplest version of SGS assumes that $\mathcal{P}$ is minus the adjoint operator used in GLS, *i.e.*

$$\mathcal{P}(\boldsymbol{v}) := -\frac{\boldsymbol{v}}{\triangle t} - \mathbf{W}\,\mathcal{L}^*(\boldsymbol{v}) = -\frac{\boldsymbol{v}}{\triangle t} + \mathbf{W}\big[(\boldsymbol{a}\cdot\nabla)\boldsymbol{v} + \nabla\cdot(\nu\nabla\boldsymbol{v}) - \sigma\boldsymbol{v}\big], \qquad (14)$$

where $\mathcal{L}^*$ is the adjoint operator of $\mathcal{L}$. Following the same rationale as in the previous section to qualitatively determine the influence of the Galerkin term in SGS compared with SUPG, one gets that in SGS the Galerkin term is weighted $1 - \tau(C\sigma + 1/\triangle t)$ times more than in SUPG. Thus it has less influence than in SUPG and GLS.

5.4. Least-squares stabilization

The correct implementation of a standard least-squares formulation for (1) requires to work in $\mathcal{H}^2$ unless a mixed least-squares formulation is used, see [18, 2]. Here an alternative procedure is proposed which allows to use standard $\mathcal{C}^0$ finite element interpolation and test functions and does not increase the number of nodal unknowns. Standard least-squares use directly the spatial strong form to construct the integral equation. Here, since time discretization is already performed, equation (4) or (5) is used. Consequently, one gets: find $\triangle\boldsymbol{u} \in [\mathcal{H}^2]^{\mathrm{n_{stages}}}$ such that

$$\big(\frac{\boldsymbol{v}}{\triangle t} + \mathbf{W}\,\mathcal{L}(\boldsymbol{v}), \mathcal{R}(\triangle\boldsymbol{u})\big)_\Omega = 0 \qquad \forall\boldsymbol{v} \in [\mathcal{H}^2]^{\mathrm{n_{stages}}}. \qquad (15)$$

However, an "equivalent" form following the same rationale as for standard stabilized methods, see Eq. (10), can be devised. It is equivalent in the sense that its unique solution is also the unique solution of (1) and also solution of (15). The first argument in (15) is split by linearity and the term containing $\mathcal{L}(\boldsymbol{v})$ is only evaluated on the element interiors, namely

$$\big(\boldsymbol{v}, \mathcal{R}(\triangle\boldsymbol{u})\big)_\Omega + \sum_e \big(\triangle t\,\mathbf{W}\,\mathcal{L}(\boldsymbol{v}), \mathcal{R}(\triangle\boldsymbol{u})\big)_{\Omega_e} = 0. \qquad (16)$$

Now the interpolation and tests functions can be taken in a subspace of $[\mathcal{H}^{1+}]^{\mathrm{n_{stages}}}$, where $\mathcal{H}^1 \subsetneq \mathcal{H}^{1+} := \{w \in \mathcal{H}^1(\Omega) \;/\; w|_{\Omega_e} \in \mathcal{H}^2(\Omega_e) \text{ for all element } \Omega_e\} \subsetneq \mathcal{H}^2$. The formulation is symmetric (this is not the case for the other stabilization techniques because $\mathbf{W}$ is, in general, not symmetric), and $\mathcal{C}^0$ finite elements can be used. This approach can also be viewed as a stabilization technique: the first term accounts for the Galerkin part of the weak form, and the second term introduces the desired stabililization with the following definition of τ and $\mathcal{P}$

$$\tau := \triangle t, \text{ and } \mathcal{P}(\boldsymbol{v}) := \mathbf{W}\,\mathcal{L}(\boldsymbol{v}). \qquad (17)$$

In fact, the GLS formulation neglecting the "inertia term" is used in common practice [22]. It corresponds to the same perturbation operator and uses the standard τ instead of $\triangle t$.

6. SUMMARY AND CONCLUSIONS

This paper proposes a methodology for the finite element computation of truly transient transport-reaction problems that is both time accurate and spatially stable. By performing the time discretization before the spatial one, standard stabilization techniques can be adapted to implicit multi-stage time stepping algorithms of high accuracy. The proposed approach uses

time stepping schemes, such as implicit multi-stage methods, which only involve up to second order spatial derivatives. Then, viewing the time-discretized equation as a spatial problem, which must be solved at each time step, consistent (residual based) stabilization techniques can be applied. Moreover, a least-squares formulation is also proposed. It can be used with C^0 finite elements and it is not restricted to systems of first-order differential equations. The accuracy analysis of these methods and some examples are presented in a companion paper [12].

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