INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids 2007; **54**:731–743
Published online 5 April 2007 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.1487

Semidiscrete formulations for transient transport at small time steps

Isaac Harari[1,*,†] and Guillermo Hauke[2]

[1]*Department of Solid Mechanics, Materials and Systems, Tel Aviv University, Ramat Aviv 69978, Israel*
[2]*Litec—Departamento de Mecánica de Fluidos, Centro Politécnico Superior, C/Maria de Luna 3, 50.018 Zaragoza, Spain*

SUMMARY

Solutions of direct time-integration schemes for transient advection–diffusion–reaction problems that converge in time to conventional semidiscrete formulations may be polluted at small time steps by spurious spatial oscillations. This degradation is not an artifact of the time-marching scheme, but rather a property of the solution of the semidiscrete Galerkin approximation itself. An analogy to steady advection–diffusion–reaction problems with a modified reaction coefficient by the Rothe method of discretizing in time prior to spatial discretization provides an upper bound on the time step for the onset of spatial instability. Spatial stabilization removes this pathology, leading to stabilized implicit time-integration schemes that are free of spurious oscillations at small time steps. Copyright © 2007 John Wiley & Sons, Ltd.

Received 22 December 2006; Revised 13 February 2007; Accepted 16 February 2007

KEY WORDS: semidiscrete advection–diffusion–reaction; small time step oscillation; Rothe method; spatial stabilization

1. INTRODUCTION

The common approach to transient analysis, called the method of lines, involves time integration of a semidiscrete formulation, obtained by spatial approximation. Thus, the approximation is carried out in two stages. First, spatial discretization, e.g. by standard finite element methods, leads to the semidiscrete formulation (a system of coupled ordinary differential equations in time). Then, temporal integration by time-marching schemes results in a system of algebraic equations at each time level. One of the most widely used family of direct time-integration schemes for unsteady transport phenomena governed by advection–diffusion–reaction equations is the generalized trapezoidal (or θ) methods. The unconditionally stable, second-order accurate, Crank–Nicolson scheme

*Correspondence to: Isaac Harari, Department of Solid Mechanics, Materials and Systems, Tel Aviv University, Ramat Aviv 69978, Israel.
†E-mail: harari@eng.tau.ac.il

(or trapezoidal rule) is, probably, the most commonly used implicit algorithm among the generalized trapezoidal family methods.

It is well known that higher modes of semidiscrete formulations are approximated poorly [1, Section 6.3]. As a result, algorithmic damping is often introduced in time-integration schemes in order to remove the participation of high-frequency modal components [2–4]. However, as the time step is reduced with a fixed mesh size, the deleterious effects of higher modes are inevitably admitted into the computation, even in the presence of algorithmic damping [5]. Thus, spurious spatial oscillations, along with attendant overshoot in time, may pollute the solution at small time steps of all algorithms that converge in time to standard consistent semidiscrete formulations [6, 7].

Conventional wisdom advocates that time step reduction be accompanied by corresponding refinement of the spatial mesh. In fact, procedures for time-step selection for explicit methods often advise against reducing time steps far below the critical values for temporal stability [8, p. 510]. Indeed, a recent analysis of the truncation error shows that in some cases accuracy degrades as the time step is reduced below a certain value [9]. Nevertheless, small time steps are often necessary in practice.

Many scientific applications involve the analysis of interaction problems which couple several physical phenomena, often with multiple time and length scales. For example, in typical reacting flows the time scales of the non-equilibrium chemical reactions are much smaller than those of the continuum transport [10, 11]. Extremely small time steps are required to resolve the chemistry, yet an implicit time-integration scheme is often preferred to deal with the stiff behaviour of such systems [12, Chapter IV]. Similar situations arise in fluid–solid interaction problems, where implicit time marching schemes are employed for long time integration, yet the motion may dictate very small time steps [13]. Several cases of spatial oscillations [14, 15] and instabilities [10, 11, 16, 17] at small time steps have been observed. These spurious phenomena are often viewed as a violation of basic qualitative characteristics, such as the maximum principle [18].

The present investigation is an extension of previous work on the pure parabolic problem of diffusion [7], to include the effects of convection and reaction. The key idea is to employ the Rothe method or the horizontal method of lines of first discretizing in time with a time-integration scheme, leading to a family of steady differential equations which are then approximated spatially on each discrete time level. This approach reveals that the time-discrete equation that is solved in each time level of implicit schemes is, in fact, a Galerkin approximation of a steady equation with a modified reaction coefficient, that can have destabilizing effects at small time steps. Standard analysis of the steady equation (with a modified coefficient) provides an upper bound on the time step for the onset of spatial instability. Any scheme that stabilizes the steady advection–diffusion–reaction equation, e.g. [19–22] removes this pathology. Similar ideas are explored in the context of enriched finite elements based on a multiscale approach [23].

Oscillations in transient computation were observed in [24], and essentially removed with a two-parameter Petrov–Galerkin method. The present analysis associates the oscillations with small time steps, provides explicit bounds on the time step for the onset of this pathology, and employs multiscale stabilization to eliminate the instabilities.

The remainder of this paper is organized as follows. In Section 2, we consider the generalized trapezoidal family of time-integration schemes for semidiscrete advection–diffusion–reaction. Stability analysis of the time-discrete analog of this problem obtained by the Rothe method in Section 3, characterizes the threshold of instability at small time steps, and introduces a stabilization procedure for implicit time-integration schemes. Section 4 reports on several computations

DOI: 10.1002/fld

that demonstrate the presence of spatial oscillations at small time steps and their absence from the spatially stabilized time integration. Conclusions are offered in Section 5.

2. ALGORITHMS FOR TRANSIENT ADVECTION–DIFFUSION–REACTION

Let $\Omega \subset \mathbb{R}^d$ be a d-dimensional, open, bounded spatial region with smooth boundary Γ. The open time interval of length $T>0$ is $(0, T)$.

2.1. Semidiscrete Galerkin formulation

Consider the (homogeneous Dirichlet) transient advection–diffusion–reaction problem of finding $u(\mathbf{x}, t)$, such that

$$u_{,t} - \nabla \cdot (\kappa \nabla u) + \mathbf{a} \cdot \nabla u - su = f \quad \text{in } \Omega \times (0, T) \tag{1}$$

$$u = 0 \quad \text{on } \Gamma \times (0, T) \tag{2}$$

$$(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega \tag{3}$$

Here, the known coefficients are the diffusivity $\kappa(\mathbf{x})>0$, the flow velocity $\mathbf{a}(\mathbf{x})$, and the source parameter $s(\mathbf{x})$, which is positive for production and negative for dissipation or absorption. In addition, $f(\mathbf{x}, t)$ is a prescribed load function, and u_0 is the specified initial value. Generalization of the results of the paper to problems with other types of boundary conditions is straightforward.

We partition Ω into non-overlapping regions (element domains, numbered with index e) in the usual way. The semidiscrete Galerkin approximation is stated in terms of the set of functions which *do not* depend on time $\mathscr{V}^h \subset H_0^1(\Omega)$. The standard finite element method is finding $u^h(\cdot, t) \in \mathscr{V}^h$ such that $\forall w^h \in \mathscr{V}^h$

$$(w^h, \dot{u}^h) + a(w^h, u^h) = (w^h, f) \tag{4}$$

$$(w^h, u^h(0)) = (w^h, u_0) \tag{5}$$

Here, $\mathbf{x}$ is suppressed as an argument of u, the superposed dot denotes time differentiation, and $(\cdot, \cdot)$ is the $L_2(\Omega)$ inner product. The form of the right-hand side assumes sufficiently smooth f. The bilinear operator is

$$a(w, u) = (\nabla w, \kappa \nabla u) + (w, \mathbf{a} \cdot \nabla u) - (w, su) \tag{6}$$

The matrix equations are obtained in the usual way (see, e.g. [8]). The functions w^h and u^h are expressed in terms of standard finite element shape functions which are not time dependent, whereas the unknown nodal values are time dependent.

The semidiscrete form of the initial/boundary-value problem for transient transport (1)–(3) is the initial-value problem of finding the vector of unknown nodal values, $\mathbf{d} = \mathbf{d}(t)$, satisfying the coupled system of ordinary differential equations

$$\mathbf{M}\dot{\mathbf{d}} + \mathbf{K}\mathbf{d} = \mathbf{F} \tag{7}$$

and initial conditions

$$\mathbf{d}(0) = \mathbf{d}_0 \tag{8}$$

DOI: 10.1002/fld

Here, $\mathbf{M}$ is the symmetric, positive-definite, mass matrix obtained from the first term on the left-hand side of (4), $\mathbf{K}$ is the matrix obtained from the remaining terms on the left-hand side of (4), $\mathbf{F}=\mathbf{F}(t)$ is the prescribed load vector obtained from the right-hand side of (4), and $\dot{\mathbf{d}}$ is the time derivative of $\mathbf{d}$. The initial conditions $\mathbf{d}_0$ are usually taken as nodal values of the given function $u_0(\mathbf{x})$.

Remark
The mass matrix that arises in the Galerkin semidiscrete approximation is the *consistent* mass representation. This is the representation that is considered subsequently, unless specified otherwise.

2.2. Time integration: the generalized trapezoidal method

The generalized trapezoidal method for integrating the semidiscrete equation (7) from t_n to $t_{n+1}=t_n+\Delta_t$ is expressed in terms of $\mathbf{d}_n$ and $\mathbf{v}_n$, the approximations to $\mathbf{d}(t_n)$ and $\dot{\mathbf{d}}(t_n)$, respectively, as follows:

$$\mathbf{M}\mathbf{v}_{n+1}+\mathbf{K}\mathbf{d}_{n+1}=\mathbf{F}(t_{n+1}) \tag{9}$$

$$\mathbf{d}_{n+1}=\widetilde{\mathbf{d}}_{n+1}+\gamma\Delta_t\mathbf{v}_{n+1} \tag{10}$$

Here the predictor is

$$\widetilde{\mathbf{d}}_{n+1}=\mathbf{d}_n+(1-\gamma)\Delta_t\mathbf{v}_n \tag{11}$$

The generalized trapezoidal algorithms are a one-step, one-parameter ($0\leqslant\gamma\leqslant1$) family of methods including: the first-order accurate, conditionally stable, explicit (assuming $\mathbf{M}$ is lumped) forward-Euler method ($\gamma=0$), the second-order accurate, unconditionally stable, implicit trapezoidal or midpoint rule, also known as the Crank–Nicolson scheme ($\gamma=1/2$), and the first-order accurate, unconditionally stable, implicit backward-Euler method ($\gamma=1$).

We consider an implementation of the method in the form

$$(\mathbf{M}+\gamma\Delta_t\mathbf{K})\mathbf{v}_{n+1}=\mathbf{F}(t_{n+1})-\mathbf{K}\widetilde{\mathbf{d}}_{n+1} \tag{12}$$

The initialization of the solution procedure is standard. At the beginning of each time step, the terms on the right-hand side of (12) are known. The equation is solved for $\mathbf{v}_{n+1}$, and $\mathbf{d}_{n+1}$ is then obtained from the update Equation (10).

3. STABILITY ANALYSIS: ROTHE FORMULATION

Standard implicit time-integration schemes of semidiscrete formulations for parabolic problems violate the maximum principle at small time steps [6, 7, 18]. These pathologies can be characterized, and later removed, by an alternative approach to the derivation of the discrete equations.

3.1. Steady model problem

The standard procedure of first discretizing in space to obtain the semidiscrete equation (7) and then discretizing in time is called the method of lines [25]. An alternative approach is the Rothe method [26] (or horizontal method of lines) of first discretizing in time and then in space on each discrete time level. By this procedure, we discretize the original differential equation (1)

DOI: 10.1002/fld

with the generalized trapezoidal method time-integration scheme in terms of $u_n(\mathbf{x})$ and $v_n(\mathbf{x})$, the approximations to $u(\mathbf{x}, t_n)$ and $u_{,t}(\mathbf{x}, t_n)$, respectively, as follows:

$$v_{n+1} - \nabla \cdot (\kappa \nabla u_{n+1}) + \mathbf{a} \cdot \nabla u_{n+1} - s u_{n+1} = f(\mathbf{x}, t_{n+1}) \tag{13}$$

$$u_{n+1} = \widetilde{u}_{n+1} + \Delta_t \gamma v_{n+1} \tag{14}$$

Here the predictor is

$$\widetilde{u}_{n+1} = u_n + (1 - \gamma)\Delta_t v_n \tag{15}$$

The Galerkin equation is expressed in terms of standard spatial finite element approximations

$$(w^h, v^h_{n+1}) + a(w^h, u^h_{n+1}) = (w^h, f(t_{n+1})) \tag{16}$$

Here, the bilinear operator is given by (6) and $\mathbf{x}$ is suppressed as an argument of f. Simple substitution of the update equation (14) yields

$$(w^h, v^h_{n+1}) + \gamma \Delta_t a(w^h, v^h_{n+1}) = (w^h, f(t_{n+1})) - a(w^h, \widetilde{u}^h_{n+1}) \tag{17}$$

The Rothe form reveals that the time-discrete equation that is solved in each time step of implicit schemes is, in fact, a Galerkin approximation of a *steady* advection–diffusion–reaction equation with a modified source parameter and load, cf. (12). Note that the term containing the predictor is integrated by parts in the standard discrete equation.

3.2. Spurious oscillations

Stability properties of Galerkin finite element approximation of the *steady* advection–diffusion–reaction equation are known [27]. The numerical solution is characterized by several dimensionless quantities: the element Péclet number $\alpha = |\mathbf{a}|h/(2\kappa)$ and the element Damköhler number $\sigma = sh/|\mathbf{a}|$, as well as the Courant–Friedrichs–Lewy number $\mathrm{CFL} = |\mathbf{a}|\Delta_t/h$, a non-dimensional measure of the time step. This additional quantity appears in the *modified* source parameter due to the implicit time stepping of the semidiscrete equation.

The standard analysis, with the source parameter suitably modified, indicates that spurious oscillations can occur in the solution when

$$\mathrm{CFL} < \mathrm{CFL}^{\mathrm{bound}} = \frac{1}{3\gamma}\left(\frac{1-\alpha}{\alpha} + \frac{\sigma}{3}\right)^{-1} \tag{18}$$

This is the upper bound on time steps for instability of the semidiscrete Galerkin equation of transient advection–diffusion–reaction with a linear finite element spatial discretization, integrated in time by the generalized trapezoidal method. Similar results may be obtained for other time-integration algorithms.

The case of transient advection–diffusion is of particular interest. The bound is obtained by simply eliminating the source parameter

$$\mathrm{CFL}^{\mathrm{bound}} = \frac{1}{3\gamma}\,\frac{\alpha}{1-\alpha} \tag{19}$$

Clearly, this result applies to the diffusion-dominated regime $\alpha < 1$ (Figure 1). For the advection-dominated regime $\alpha \geqslant 1$ there can be spurious oscillations at any time step, which is a classical result from the analysis of the steady equation.

DOI: 10.1002/fld

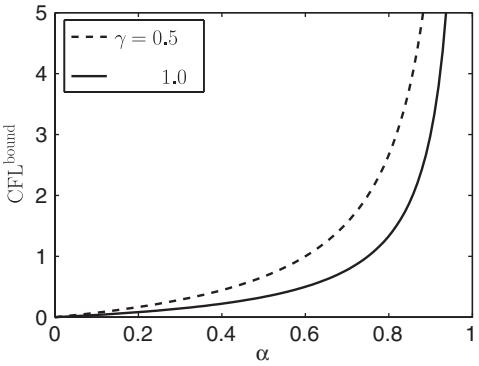

Figure 1. The CFL upper bound (19) for instability of the semidiscrete Galerkin equation of transient advection–diffusion with linear finite element spatial discretization, integrated in time by the generalized trapezoidal method.

Remark

It would appear that spurious oscillations can arise at any time step for the forward-Euler algorithm ($\gamma = 0$). However, this scheme is usually combined with mass lumping, a pointwise representation of the inertial term, in order to justify the use of this algorithm, which is conditionally stable in time. Mass lumping modifies the underlying semidiscrete formulation and precludes spurious oscillations in solutions obtained with linear elements [7, 28]. (See also recent work on selective lumping [29].) Unfortunately, this property is not shared by all higher-order elements. Furthermore, while the lumped representation is of the same order of spatial accuracy as the consistent representation on uniform meshes, the spatial accuracy of the lumped representation can degrade on non-uniform meshes, depending on the degree of variation in mesh size [30].

3.3. Stabilization

The Galerkin discretization (17) represents a steady advection–diffusion–reaction problem, which can be written as a function of a modified bilinear operator

$$\hat{a}(w^h, v^h_{n+1}) = (w^h, \hat{f}(t_{n+1})) \tag{20}$$

where

$$\hat{a}(w, u) = (\nabla w, \hat{\kappa}\nabla u) + (w, \hat{\mathbf{a}} \cdot \nabla u) - (w, \hat{s}u) \tag{21}$$

$$(w, \hat{f}(t_{n+1})) = (w, f(t_{n+1})) - a(w, \tilde{u}^h_{n+1}) \tag{22}$$

and

$$\tilde{\kappa} = \gamma \Delta_t \kappa \tag{23}$$

$$\tilde{\mathbf{a}} = \gamma \Delta_t \mathbf{a} \tag{24}$$

$$\tilde{s} = \gamma \Delta_t s - 1 \tag{25}$$

DOI: 10.1002/fld

Note that the right-hand side of the Galerkin method (20) $(w^h, \hat{f}(t_{n+1}))$ contains the load $f(t_{n+1})$ plus the effect of the predictor $\tilde{u}^h_{n+1}$ upon the velocity v_{n+1}, namely $a(w, \tilde{u}^h_{n+1})$. This term includes the viscous contribution of the predictor in integrated-by-parts form.

In order to stabilize the Galerkin discretization (20), the combined adjoint stabilization method [21] is implemented. This method adds two stabilization integrals to the Galerkin method (a least-squares plus a gradient least-squares term), and can be interpreted as an approximation to the exact variational multiscale method, where the cross moments of the element Green's function have been neglected. Each stabilization term possesses a parameter, adjusted for superconvergence of the two amplification factors present in advection–diffusion–reaction equations. Thus, the method results in nodally exact one-dimensional finite element solutions for problems considered here, for any range of dimensionless parameters and constant load vector.

The stabilized variational formulation reads

$$\hat{a}(w^h, v^h_{n+1}) - (\tau_0 \hat{\mathscr{L}}^* w^h, \hat{\mathscr{L}} v^h_{n+1} - \hat{f}(t_{n+1}))_{\tilde{\Omega}} - (\tau_1 \nabla \hat{\mathscr{L}}^* w^h, \nabla \hat{\mathscr{L}} v^h_{n+1} - \nabla \hat{f}(t_{n+1}))_{\tilde{\Omega}} = (w^h, \hat{f}(t_{n+1})) \tag{26}$$

where $\hat{\mathscr{L}}$ and $\hat{\mathscr{L}}^*$ denote, respectively, the standard differential operator and its adjoint, that is

$$\hat{\mathscr{L}} w = -\nabla \cdot (\hat{\kappa} \nabla w) + \hat{\mathbf{a}} \cdot \nabla w - \hat{s} \tag{27}$$

$$\hat{\mathscr{L}}^* w = -\nabla \cdot (\hat{\kappa} \nabla w) - \hat{\mathbf{a}} \cdot \nabla w - \hat{s} \tag{28}$$

The expression of the stabilization parameters τ_0, τ_1 can be found in [21].

Remark

Note that in (20), the Galerkin predictor diffusion contribution on the right-hand side emanates naturally in integrated-by-parts form. This has an important impact on accuracy and the same philosophy should be applied to the other predictor viscous terms on the stabilization integrals. This treatment was also implicit in [7] for the transient diffusion problem. For comparison, the method in [24] without this feature results in more dissipative numerical solutions.

In classical stabilization of semidiscrete transient equations, the time derivative is absent from the augmented stabilizing space (see [31, 32] and references therein), although it may be accounted for indirectly [33]. It is, however, recovered in the present method through the modified source term in the residual, the augmented stabilizing weighting space and the stabilizing parameter. This typically results in larger stabilization contributions.

4. NUMERICAL RESULTS

As examples of the preceding procedure, the following two transient advection–diffusion problems exhibit oscillatory solutions with conventional time-marching schemes at small time steps even in the diffusion-dominated regime. The proposed stabilization removes these pathologies.

4.1. Boundary layer

Consider the one-dimensional problem of a transient boundary layer in $x \in (0, L)$, with boundary conditions $u(0, t) = 0$ and $u(L, t) = 1$. The initial condition is the smooth function $u(x, 0) = u_0(x) = 1$.

DOI: 10.1002/fld

Under these conditions, the analytical solution is given by

$$u(x,t) = \frac{1-\exp\left(\dfrac{ax}{\kappa}\right)}{1-\exp\left(\dfrac{aL}{\kappa}\right)} + \exp\left(\frac{a}{2\kappa}x - \frac{a^2}{4\kappa}t\right)\sqrt{\frac{2}{L}}\sum_{i=1}^{\infty}\left\{\frac{4\sqrt{2L}\kappa^2 i\pi}{a^2L^2+4\kappa^2 i^2\pi^2}\exp\left(-\left(\frac{\pi i\sqrt{\kappa}}{L}\right)^2 t\right)\sin\left(\frac{\pi i}{L}x\right)\right\} \tag{29}$$

The following computations compare the Galerkin solution with the transient stabilized solution at $\alpha = 0.1$. For $\mathrm{CFL} = \mathrm{CFL}^{\mathrm{bound}}$, Figure 2 shows that, according to the theory, there are no oscillations for both, $\gamma = 1.0$ and 0.5. The $\mathrm{CFL}^{\mathrm{bound}}$ above is based on the Galerkin method.

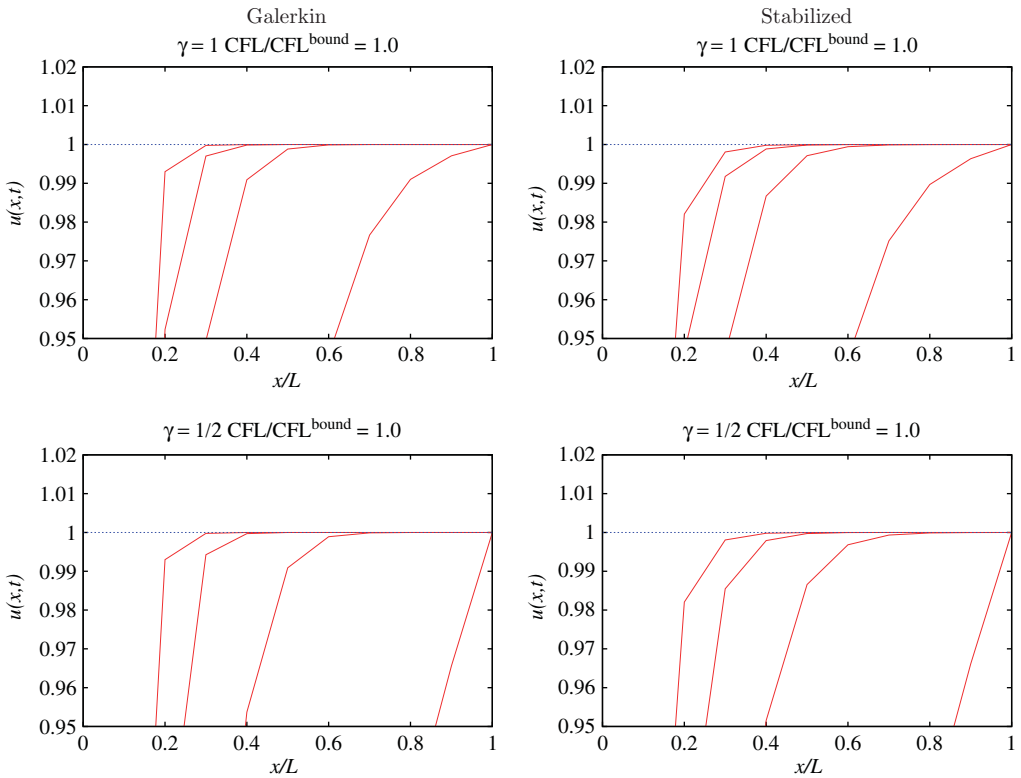

Figure 2. Boundary layer. Detail of the Galerkin (left) and transient stabilized (right) solutions during the first instances for $\gamma = 1$ and 0.5 at $\mathrm{CFL} = \mathrm{CFL}^{\mathrm{bound}}$.

DOI: 10.1002/fld

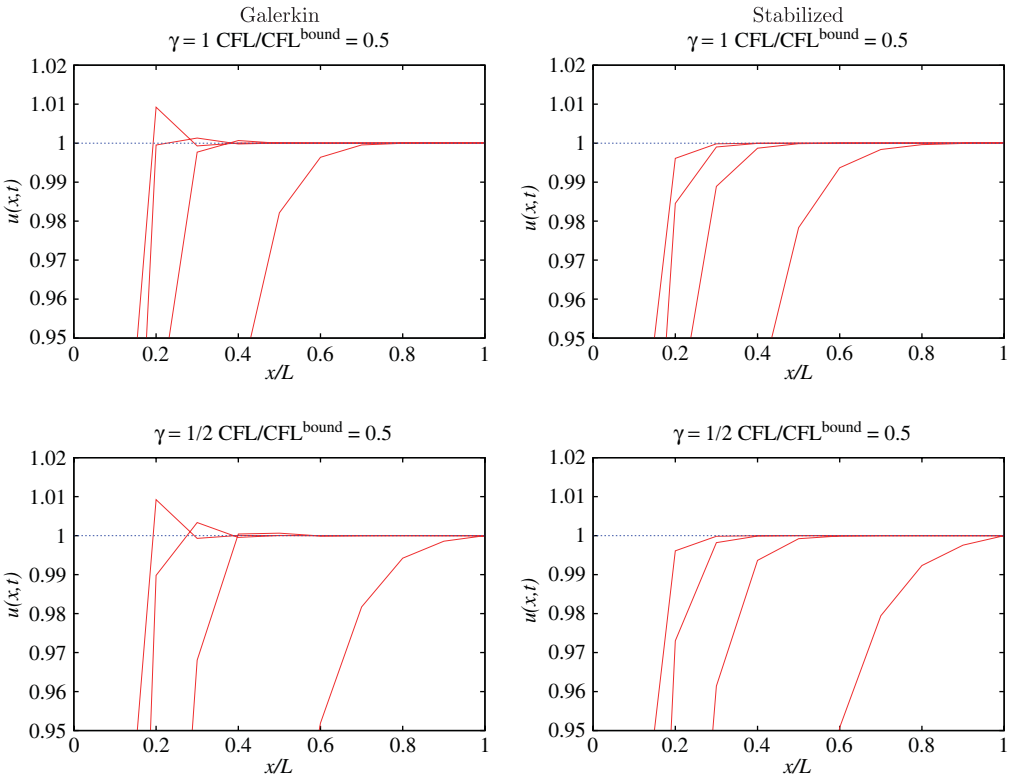

Figure 3. Boundary layer. Detail of the Galerkin (left) and transient stabilized (right) solutions during the first instances for $\gamma = 1$ and 0.5 at $\mathrm{CFL} = 0.5\mathrm{CFL}^{\mathrm{bound}}$.

When the time step is decreased, for instance to $\mathrm{CFL} = 0.5\mathrm{CFL}^{\mathrm{bound}}$, then the Galerkin solution shows the typical small time-step oscillations. These are eliminated by the transient stabilization introduced in this paper (see Figure 3).

4.2. *Transport of a diffused square wave*

Next, consider the transport by convection and diffusion of a one-dimensional square wave. The initial condition is depicted in Figure 4, a unit square pulse between $x_l = 0.2$ and $x_r = 0.7$. Lack of smoothness is apparent at the corners of the pulse.

The analytical solution for homogeneous Dirichlet boundary conditions, valid before the pulse reaches a boundary, can be approximated by

$$u(x,t) = 0.5(\mathrm{erf}((x - at - x_l)/\sqrt{4\kappa t}) - \mathrm{erf}((x - at - x_r)/\sqrt{4\kappa t})) \tag{30}$$

DOI: 10.1002/fld

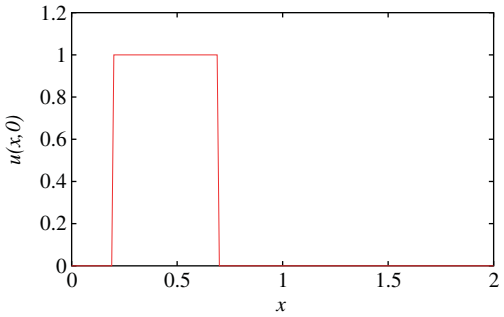

Figure 4. Square wave. Initial condition.

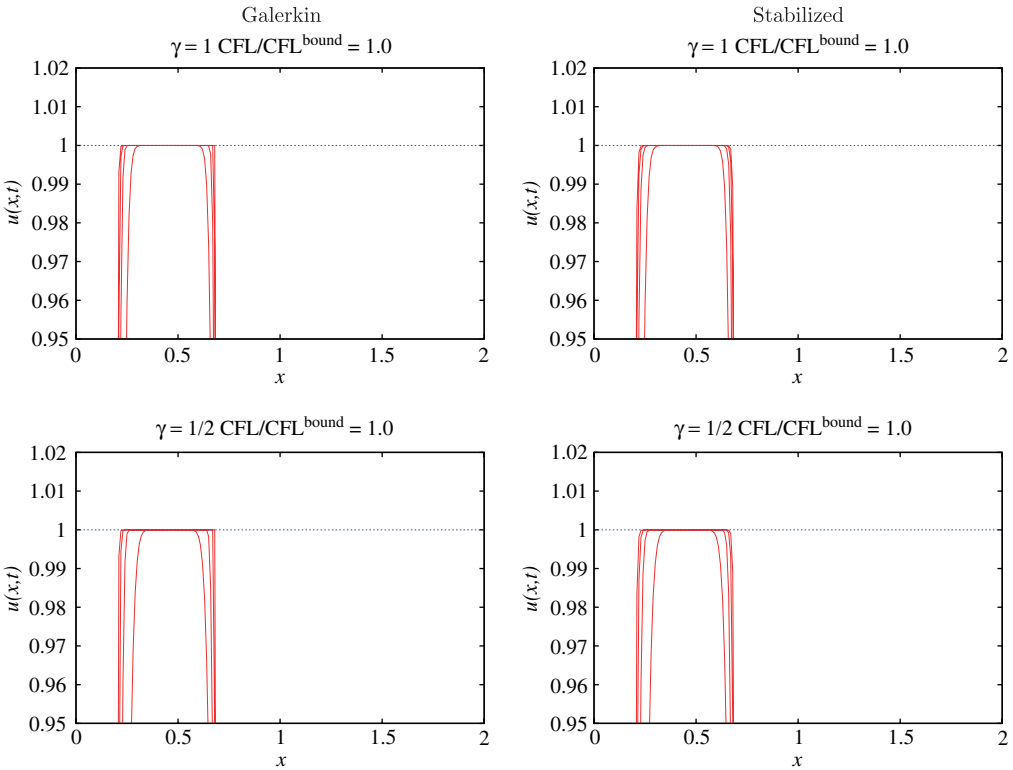

Figure 5. Square wave. Detail of the Galerkin (left) and transient stabilized (right) solutions during the first instances for $\gamma = 1$ and 0.5 at $\mathrm{CFL} = \mathrm{CFL}^{\mathrm{bound}}$.

As in the previous example, when $\mathrm{CFL} < \mathrm{CFL}^{\mathrm{bound}}$, small time step oscillations are induced in the Galerkin solution. Again, the transient stabilization applied to the Rothe discretization is able to get rid of them. This is demonstrated in Figures 5 and 6 for $\alpha = 0.1$.

DOI: 10.1002/fld

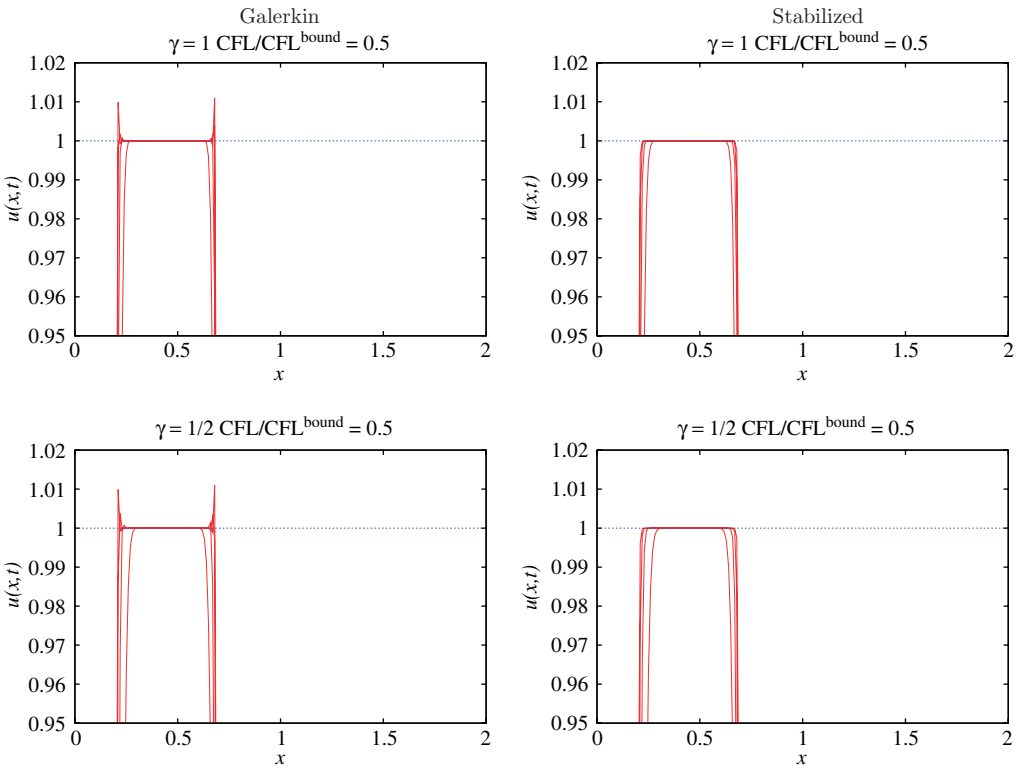

Figure 6. Square wave. Detail of the Galerkin (left) and transient stabilized (right) solutions during the first instances for $\gamma = 1$ and 0.5 at $\mathrm{CFL} = 0.5\mathrm{CFL}^{\mathrm{bound}}$.

5. CONCLUSIONS

The present investigation extends previous work on spatial stability of transient diffusion at small time steps to transient advection–diffusion–reaction problems. Solutions of the Galerkin semidiscrete formulation may exhibit spatial oscillations, due to poor approximation of higher modes. Consequently, all conventional direct time-integration schemes that are based on such semidiscrete formulations and are convergent in time will eventually admit these pathologies as the time step is reduced (with a fixed mesh size).

The Rothe method of first discretizing in time with a time-integration scheme, leads to a family of steady differential equations which are then approximated spatially on each discrete time level. This approach reveals that the time-discrete equation that is solved in each time level of implicit schemes is, in fact, a Galerkin approximation of a steady equation with a modified reaction coefficient, that can have destabilizing effects at small time steps. Standard analysis of the steady equation (with a modified coefficient) provides an upper bound on the time step for the onset of spatial instability. Any scheme that stabilizes the steady equation removes this pathology.

Future work will address the stabilization of advection- and reaction-dominated phenomena, as well as implementational issues such as the form of the time-marching schemes and initialization.

DOI: 10.1002/fld

ACKNOWLEDGEMENTS

The authors acknowledge conversations with Pavel Bochev, Victor Calo, Alvaro L. G. A. Coutinho, Thomas J. R. Hughes, and Arif Masud.

REFERENCES

1. Strang G, Fix GJ. *An Analysis of the Finite Element Method*. Prentice-Hall: Englewood Cliffs, NJ, 1973.
2. Chung J, Hulbert GM. A time integration algorithm for structural dynamics with improved numerical dissipation: the generalized-α method. *Journal of Applied Mechanics* (ASME) 1993; **60**(2):371–375.
3. Hilber HM, Hughes TJR, Taylor RL. Improved numerical dissipation for time integration algorithms in structural dynamics. *Earthquake Engineering Structural Dynamics* 1977; **5**(3):283–292.
4. Jansen KE, Whiting CH, Hulbert GM. A generalized-α method for integrating the filtered Navier–Stokes equations with a stabilized finite element method. *Computer Methods in Applied Mechanics and Engineering* 2000; **190** (3–4):305–319. *Fourth Japan—US Symposium on Finite Element Methods in Large-scale Computational Fluid Dynamics*, Tokyo, 1998.
5. Krenk S. State–space time integration with energy control and fourth-order accuracy for linear dynamic systems. *International Journal for Numerical Methods in Engineering* 2006; **65**(5):595–619.
6. Fujii H. Some remarks on finite element analysis of time-dependent field problems. In *Theory and Practice in Finite Element Structural Analysis*, Yamada Y, Gallagher RH (eds). University of Tokyo Press: Tokyo, 1973; 91–106.
7. Harari I. Stability of semidiscrete formulations for parabolic problems at small time steps. *Computer Methods in Applied Mechanics and Engineering* 2004; **193**(15–16):1491–1516.
8. Hughes TJR. *The Finite Element Method*. Dover: Mineola, NY, 2000 (Corrected reprint of the 1987 original).
9. Yang C, Gu Y. Minimum time-step criteria for the Galerkin finite element methods applied to one-dimensional parabolic partial differential equations. *Numerical Methods for Partial Differential Equations* 2006; **22**(2):259–273.
10. Bochev PB, Gunzburger MD, Shadid JN. On inf–sup stabilized finite element methods for transient problems. *Computer Methods in Applied Mechanics and Engineering* 2004; **193**(15–16):1471–1489.
11. Bochev PB, Shadid JN, Gunzburger MD. On stabilized finite element methods for transient problems with varying time scales. In *Proceedings of the Fifth World Congress* (*WCCM V*), Mang HA, Rammerstorfer FG, Eberhardsteiner J (eds). Vienna University of Technology: Austria, 2002.
12. Hairer E, Wanner G. *Solving Ordinary Differential Equations. II. Stiff and Differential-algebraic Problems*. Springer Series in Computational Mathematics, vol. 14. Springer: Berlin, 1991.
13. Masud A. Private communication. 2003.
14. Bradford SF, Katopodes ND. The anti-dissipative, non-monotone behavior of Petrov–Galerkin upwinding. *International Journal for Numerical Methods in Fluids* 2000; **33**(4):583–608.
15. Fabritz JE. A two-dimensional numerical model for simulating the movement and biodegradation of contaminants in a saturated aquifer. *Master's Thesis*, University of Washington, Seattle, Washington, 1995.
16. Behr M. Private communication. 2002.
17. Rannacher R. Finite element solution of diffusion problems with irregular data. *Numerische Mathematik* 1984; **43**(2):309–327.
18. Faragó I, Horváth R, Korotov S. Discrete maximum principle for linear parabolic problems solved on hybrid meshes. *Applied Numerical Mathematics* 2005; **53**(2–4):249–264.
19. Brezzi F, Hauke G, Marini LD, Sangalli G. Link-cutting bubbles for the stabilization of convection–diffusion–reaction problems. *Mathematical Models and Methods in Applied Sciences* 2003; **13**(3):445–461 (Dedicated to Jim Douglas, Jr. on the occasion of his 75th birthday).
20. El Alaoui L, Ern A. Nonconforming finite element methods with subgrid viscosity applied to advection–diffusion–reaction equations. *Numerical Methods for Partial Differential Equations* 2006; **22**(5):1106–1126.
21. Hauke G, Sangalli G, Doweidar ME. Combining adjoint stabilized methods for the advection–diffusion–reaction problem. *Mathematical Models and Methods in Applied Sciences* 2007; **17**(2):305–326.
22. Idelsohn S, Nigro N, Storti M, Buscaglia M. A Petrov–Galerkin formulation for advection–reaction–diffusion problems. *Computer Methods in Applied Mechanics and Engineering* 1996; **136**(1–2):27–46.
23. Franca LP, Ramalho JVA, Valentin F. Enriched finite element methods for unsteady reaction–diffusion problems. *Communications in Numerical Methods in Engineering* 2006; **22**(6):619–625.

DOI: 10.1002/fld

24. Idelsohn SR, Heinrich JC, Oñate E. Petrov–Galerkin methods for the transient advective–diffusive equation with sharp gradients. *International Journal for Numerical Methods in Engineering* 1996; **39**:1455–1473.
25. Berezin IS, Zhidkov NP. *Computing Methods*, vols. I and II. Pergamon: Oxford, 1965.
26. Rothe E. Zweidimensionale parabolische Randwertaufgaben als Grenzfall eindimensionaler Randwertaufgaben. *Mathematishe Annalen* 1930; **102**:650–670.
27. Harari I, Hughes TJR. Stabilized finite element methods for steady advection–diffusion with production. *Computer Methods in Applied Mechanics and Engineering* 1994; **115**(1–2):165–191.
28. Ikeda T. *Maximum Principle in Finite Element Models for Convection–Diffusion Phenomena*. Lecture Notes in Numerical and Applied Analysis, vol. 4. Kinokuniya Book Store Co Ltd.: Tokyo, 1983. North-Holland Mathematics Studies, 76.
29. Russell TF, Binning P. On no, not the wiggles again! A revisit of an old problem and a new approach. *Technical Report 205*, Center for Computational Mathematics, University of Colorado at Denver, Denver, Colorado, 2004.
30. Harari I, Turkel E. Accurate finite difference methods for time-harmonic wave propagation. *Journal of Computational Physics* 1995; **119**(2):252–270.
31. Hauke G, Doweidar MH. Fourier analysis of semi-discrete and space–time stabilized methods for the advective–diffusive–reactive equation: I. SUPG. *Computer Methods in Applied Mechanics and Engineering* 2005; **194**(1): 45–81.
32. Hauke G, Doweidar MH. Fourier analysis of semi-discrete and space-time stabilized methods for the advective–diffusive–reactive equation: II. SGS. *Computer Methods in Applied Mechanics and Engineering* 2005; **194**(6–8):691–725.
33. Tezduyar TE, Senga M. Stabilization and shock-capturing parameters in SUPG formulation of compressible flows. *Computer Methods in Applied Mechanics and Engineering* 2006; **195**(13–16):1621–1632.

DOI: 10.1002/fld