# ON THE SOLUTION OF THE TIME-DEPENDENT CONVECTION-DIFFUSION EQUATION BY THE FINITE ELEMENT METHOD

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## RESUMEN

Presentamos un método de elementos finitos basado en una formulación de Petrov-Galerkin para la ecuación de convección y difusión con dependencia de tiempo. El esquema se basa en funciones de base bilineales en espacio y tiempo y en funciones de peso no-conformes cuadráticas en tiempo y lineales en el espacio. Obtenemos esquemas de segundo orden en el tiempo y tercer orden de exactitud en el espacio, libres de efectos de difusión y dispersión numérica. Presentamos resultados numéricos que demuestran que el esquema posee exelentes propiedades de aproximación.

## ABSTRACT

A Petrov-Galerkin finite element method is presented for the time-dependent convection-diffusion equation. The scheme is based on bilinear time-space trial and quadratic in time-linear in space test functions, the latter being non-conforming. Second order in time and third order in space accuracy is obtained, and the schemes are free of numerical diffusion and dispersion effects. Numerical results are presented which show excellent approximation properties.

## INTRODUCTION

The use of the finite element method via Petrov-Galerkin formulations of various forms has been extremely effective in the numerical solution of convection-dominated problems. Initially, the methods were developed for steady-state equations with no time dependence [1, 2]. Later, by means of rather ad-hoc extensions, they were applied to time-dependent equations [3, 4]; however, these extensions were mostly justified by means of numerical experimentation, and a formal analysis is lacking. Moreover, a local analysis technique used in [5] showed that the direct extension of the Petrov-Galerkin method to time-dependent convection-dominated problems can generate algorithms that introduce excessive numerical damping and are incapable of describing the time evolution of the solution with adequate accuracy.

In this work, we present a possible extension of the Petrov-Galerkin method for steady-state equations introduced in [6, 7] to time-dependent problems. This is done by means of time-space elements, so the algorithms are by necessity implicit. We only consider one-step algorithms, i.e., we assume the solution is known at time $t = t_n$ and we calculate an approximation for time $t_{n+1} = t_n + \Delta t$. A local analysis, such as the one used in [5], allows us to determine two parameters introduced in the algorithm in an element-by-element fashion so as to optimize the approximation properties.

For the case of a constant coefficient equation on a uniform mesh, we can construct algorithms that are second-order accurate in time and third-order accurate in space. We can also identify, in certain cases, values of the parameters for which superconvergence occurs. The analysis shows that to obtain optimal convergence rates in this class of algorithms, we must compromise the stability and we can only find optimal schemes that are conditionally stable.

The numerical examples show that the algorithm is extremely accurate, and the simplicity of its formulation makes it attractive to use in more complex engineering problems.

## SPACE-TIME PETROV-GALERKIN METHOD

Let us consider the time-dependent convection-diffusion equation in the interval $a \leq x \leq b$

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = K\frac{\partial^2 \phi}{\partial x^2} + Q \tag{1}$$

$$\phi(x, 0) = \phi_0(x) \tag{2}$$

$$\phi(a, t) = \phi_a \tag{3a}$$

$$A\phi(b, t) + B\frac{\partial \phi}{\partial x}(b, t) = C \tag{3b}$$

where $\phi$ is the transported quantity. For simplicity, we assume that the convective velocity u and the diffusion coefficient K are positive constants, Q represents sources and sinks, and, initially, $Q = 0$.

We consider bilinear space-time trial functions (Figure 1) given in isoparametric coordinates $-1 \leq \xi \leq 1$, $-1 \leq \eta \leq 1$ by

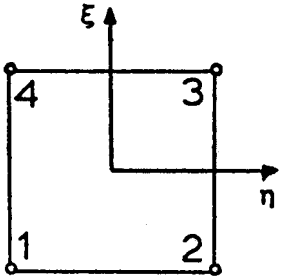


Figure 1. Nodal numbering for four-noded space-time elements in isoparametric coordinates.

$$N^1(\xi, \eta) = \frac{1}{4}(1 - \xi)(1 - \eta) \tag{4a}$$

$$N^2(\xi, \eta) = \frac{1}{4}(1 + \xi)(1 - \eta) \tag{4b}$$

$$N^3(\xi, \eta) = \frac{1}{4}(1 + \xi)(1 + \eta) \tag{4c}$$

$$N^4(\xi, \eta) = \frac{1}{4}(1 - \xi)(1 + \eta) \tag{4d}$$

Only two test functions are needed to define the algorithm on each element; these will be of the form

$$W^i(\xi, \eta) = M^i(\xi, \eta) + \alpha \frac{\partial M^i}{\partial \xi} + \beta \frac{\partial^2 M^i}{\partial \xi \partial \eta} \tag{5}$$

where i = 3, 4 and

$$M^3(\xi, \eta) = \frac{1}{2}(1 + \xi)(1 - \eta^2) \tag{6a}$$

$$M^4(\xi, \eta) = \frac{1}{2}(1 - \xi)(1 - \eta^2) \tag{6b}$$

The parameters $\alpha$ and $\beta$ will be determined later.

Note that the weighting functions are of the form

$$w = v + p \tag{7}$$

where v is a function quadratic in time and p is a perturbation function discontinuous at the nodal points.

To formulate the variational problem, first define the 'jump' operator

$$[\phi]_x \equiv \phi^+(x) - \phi^-(x) \tag{8}$$

where $\phi^+$ and $\phi^-$ denote the limits approaching from the right and left, respectively.

We can now write the following residual equation

$$\int_t^{t+\Delta t}\left\{\int_a^b\left[v\left(\frac{\partial\phi}{\partial t}+u\frac{\partial\phi}{\partial x}\right)+K\frac{\partial v}{\partial x}\frac{\partial\phi}{\partial x}-vQ\right]dx+vg\Big|_{x=b}\right.$$
$$\left.+\sum_{e_i}\int_{e_i}p\left(\frac{\partial\phi}{\partial t}+u\frac{\partial\phi}{\partial x}-K\frac{\partial^2\phi}{\partial x^2}-Q\right)dx\right\}dt=0 \tag{9}$$

where

$$g=\begin{cases}0 & \text{if } \beta=0\\ \frac{K}{\beta}[C-A\phi(b,t)] & \text{if } \beta\neq 0\end{cases} \tag{10}$$

and the summation is over all element interiors $e_i$. Equation (9) is equivalent to

$$\int_t^{t+\Delta t}\left\{\sum_{e_i}\int_{e_i}w\left(\frac{\partial\phi}{\partial t}+u\frac{\partial\phi}{\partial x}-K\frac{\partial^2\phi}{\partial x^2}-Q\right)dx+\sum_i v\left[K\frac{\partial\phi}{\partial x}\right]_{x_i}\right.$$
$$\left.+v\left(K\frac{\partial\phi}{\partial x}+g\right)_{x=b}\right\}dt=0 \tag{11}$$

From here we find that the Euler-Lagrange equations are equation (1) restricted to the element interiors, equation (3b) if $\beta\neq 0$, and the continuity conditions

$$\left[K\frac{\partial\phi}{\partial x}\right]_{x_i}=0 \tag{12}$$

at all nodes.

To determine the parameters $\alpha$ and $\beta$, we perform a local analysis on the difference equations generated by this algorithm; the latter is, for a typical node i

$$\frac{1}{9\Delta t}[(\phi_{i-1}^{n+1}-\phi_{i-1}^{n})+4(\phi_i^{n+1}-\phi_i^{n})+(\phi_{i+1}^{n+1}-\phi_{i+1}^{n})]-\frac{\alpha}{6\Delta t}[(\phi_{i+1}^{n+1}-\phi_{i+1}^{n})-(\phi_{i-1}^{n+1}-\phi_{i-1}^{n})]$$
$$+\frac{u}{6h}(\phi_{i+1}^{n+1}-\phi_{i-1}^{n+1})-\frac{\alpha u}{6h}(\phi_{i+1}^{n+1}-2\phi_i^{n+1}+\phi_{i-1}^{n+1})+\frac{\beta u}{6h}(\phi_{i+1}^{n+1}-2\phi_i^{n+1}+\phi_{i-1}^{n+1})$$
$$+\frac{u}{6h}(\phi_{i+1}^{n}-\phi_{i-1}^{n})-\frac{\alpha u}{6h}(\phi_{i+1}^{n}-2\phi_i^{n}+\phi_{i-1}^{n})-\frac{\beta u}{6h}(\phi_{i+1}^{n}-2\phi_i^{n}+\phi_{i-1}^{n}) \tag{13}$$
$$-\frac{K}{3h^2}(\phi_{i+1}^{n+1}-2\phi_i^{n+1}+\phi_{i-1}^{n+1})-\frac{K}{3h^2}(\phi_{i+1}^{n}-2\phi_i^{n}+\phi_{i-1}^{n})=0$$

where h is the uniform mesh size. Expanding in Taylor series and using the original differential equation to rewrite the higher order derivatives in the expansion, we can write the total truncation error $\tau$ in the form

$$\tau = \left\{1 - \left[\alpha + \frac{2}{\gamma}\right]\tanh\frac{\gamma}{2}\right\}\sinh\gamma\left[\left[\left(\frac{2K}{3\gamma}\right)(\phi_i^{n+1})_{xx} + \left(\frac{2h}{3\gamma^2}\right)(\phi_i^{n+1})_{tx}\right]\right.$$

$$+\left(\frac{h^2}{3}\right)\left\{\frac{\alpha}{\gamma} + \frac{\beta C}{2} - \frac{C^2}{6} + \frac{2}{\gamma^3}\sinh\gamma\left[1 - \tanh\frac{\gamma}{2}\right] - \frac{4}{\gamma^4}(\cosh\gamma - 1)\right\}(\phi_i^{n+1})_{txx} \tag{14}$$

$$+\left(\frac{h^3}{3}\right)\left\{\frac{C^2}{3}\left[\frac{1}{\gamma} - \frac{C-\alpha}{4}\right] - \frac{\alpha}{2}\left[\frac{1}{6} - \frac{C}{\gamma} - \frac{2}{\gamma^2}\right] - \frac{1}{6\gamma} + \frac{\beta C^2}{4} + \frac{2}{\gamma^2}\sinh\gamma\left[1 - \tanh\frac{\gamma}{2}\right]\right.$$

$$\left.\left. - \frac{4}{\gamma^5}(\cosh\gamma - 1)\right\}(\phi_i^{n+1})_{txxx} + \text{HOT}\right.$$

where the cell Peclet number $\gamma$ and the Courant number $C$ are given by

$$\gamma = \frac{uh}{K} \tag{15}$$

$$C = \frac{u\Delta t}{h} \tag{16}$$

The subindices t and x denote partial differentiation with respect to time and space, and HOT stands for higher order terms.

We can now choose $\alpha$ so as to make the first term in (14) vanish. This gives

$$\alpha = \coth\frac{\gamma}{2} - \frac{2}{\gamma} \tag{17}$$

Notice that this is the same value obtained previously for the steady-state case [1, 2]. The parameter $\beta$ can then be found as a function of $\alpha$ so as to make the second term in (14) vanish. This gives

$$\beta = \frac{C}{3} - \frac{2\alpha}{\gamma C} \tag{18}$$

and, in general, leads to a scheme that is of the order of $h^3$.

The stability of the present Petrov-Galerkin scheme can be studied using standard methods and shows that the scheme is unconditionally stable if $\beta = 0$ for any value of $\alpha$. If $\beta \neq 0$, however, the scheme is only conditionally stable with a stability limit given by $C \leq 1$. It appears that it is not possible to improve on this condition within the framework of the present algorithm's architecture; however, numerical experimentation with $\beta = 0$ when the algorithm is unconditionally stable indicates that the condition $C \leq 1$ is necessary for accurate tracking of the time evolution of solution.

## COMMENTS

1. The present algorithm is only one of several that have been studied in detail. It is also the most accurate one. Other possible algorithms and their analyses will be reported in future publications.

2. The weighting functions defined in (5) and (6) are not unique. There are many ways to construct weighting functions that lead to equivalent algorithms. In our opinion, this representation is the easiest to use.

3. If $\alpha$ and $\beta$ are calculated according to (17) and (18) and we choose C to be a real root of

$$\frac{\alpha}{12}C^3 + \frac{1}{3\gamma}C^2 = \frac{1}{6\gamma} + \frac{\alpha}{12} - \frac{\alpha}{\gamma^2} \tag{19}$$

then the third term in the expression for the truncation error (14) vanishes and a fourth-order scheme is obtained. It can be easily shown that (19) always has a root such that $0 < C < 1$ and such that $C \to 0$ as $\gamma \to 0$ and $C \to 1$ as $\gamma \to \infty$.

4. If $\alpha = \beta = 0$, the scheme reduces to a Crank-Nicolson Galerkin method using linear space elements. Also, when $\gamma \to 0$, the pure diffusion case, expression (17) gives $\alpha = 0$ and equation (13) is independent of $\beta$ so that the scheme automatically reduces to the Crank-Nicolson Galerkin form for the pure diffusion equation, as expected.

5. In the limit where $\gamma \to \infty$, we get $\alpha \to 1$ and $\beta \to C/3$. This algorithm retains the third-order accuracy and is fourth-order accurate when $C = 1$.

6. The scheme exhibits no numerical damping when $C = 1$. For $C < 1$, very little damping is introduced, stemming mainly from the inability of the mesh to capture the peaks.

7. The algorithm can be immediately extended to variable coefficients, $Q \neq 0$, and non-uniform meshes by local evaluation of the parameters in an element-wise fashion.

## EXAMPLES

The performance of the proposed algorithm is illustrated by means of two numerical examples. The first example involves the transport and diffusion of a Gaussian wave form of unit initial amplitude centered at $x = 0.25$. The exact solution is given by

$$\phi(x, t) = \frac{1}{\sqrt{1 + t}}\, e^{-\frac{(x-u(t+1))^2}{4K(t+1)}} \tag{20}$$

and we set the function equal to zero when $|\phi| < 10^{-10}$. Equation (1) is solved in the interval $[0, 2]$, and the solution is followed over two full wavelengths. In Figure 2, we show the solution obtained numerically for $C = 0.9$ and $\gamma = 20$. The left peak is the initial condition, the middle one is the solution after $t = 2.07$ seconds, and the third after $t = 4.05$ seconds. The exact and numerical solutions have been superimposed on Figure 2 and practically no difference can be observed. The same problem was solved for five different meshes, keeping the Courant number constant at $C = 0.9$. The maximum relative errors, at time $t = 2.07$ seconds, referred to the maximum magnitude of the exact solution are shown in Table 1.

In Figure 3, we have plotted the maximum relative error against the mesh size in a log-log curve. It shows the expected linear relation with slope 2.7. This is the actual convergence rate and is in excellent agreement with the theoretical value of 3.

The second example involves variable coefficients and a variable source term. Equation (1) now takes the form

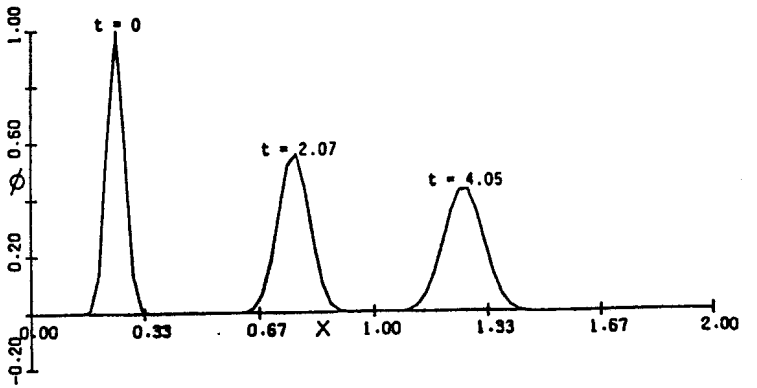


Figure 2. Numerical and analytical solution to the first example at times t = 0, 2.07, and 4.05 seconds.

Table 1. Maximum errors for the first example for different mesh sizes.

| Mesh Size | Maximum Absolute Error | Maximum Relative Error (%) |
|---|---|---|
| 0.06250 | 0.149 | 26.2 |
| 0.05000 | 0.077 | 14.0 |
| 0.04167 | 0.046 | 8.7 |
| 0.02500 | 0.012 | 2.2 |
| 0.01250 | 0.002 | 0.3 |

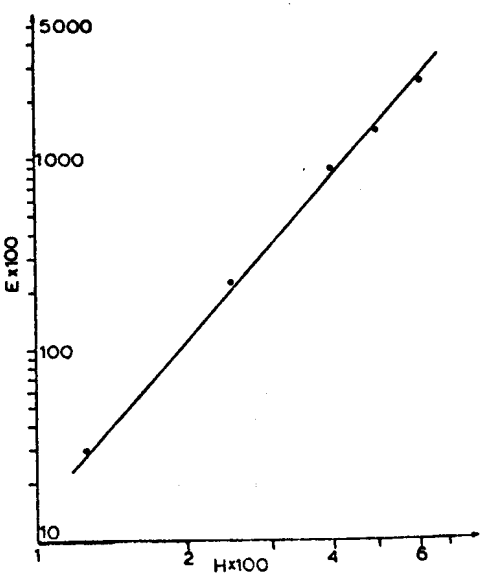


Figure 3. Maximum relative errors versus mesh size for the first example.

$$\frac{\partial \phi}{\partial t} = u\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial x}\left[a^2 e^{x^2}\frac{\partial \phi}{\partial x}\right]$$

$$+ 2a\left[1 + 2x(x - u(t+1)) - \frac{2}{a}(x - u(t+1))^2\right]e^{x^2} e^{-\frac{(x-u(t+1))^2}{a}} \tag{21}$$

and the analytical solution is

$$\phi(x, t) = e^{-\frac{(x-u(t+1))^2}{a}} \tag{22}$$

Expression (22) represents a wave that translates without changing its shape or amplitude. In Figure 4, we show numerical solutions at times $t = 0$, $t = 2.0$, and $t = 4.0$ seconds obtained using (a) $\alpha = \beta = 0$, (b) $\alpha \neq 0$ and $\beta = 0$, and (c) $\alpha \neq 0$ and $\beta \neq 0$. The parameters used in this calculation are

$$a = 0.00359$$
$$u = 0.3$$
$$c = 0.9$$

The parameter $\gamma$ varies between $10 < \gamma < 580$. The first two cases represent algorithms that are unconditionally stable; however, they show significant numerical dispersion, especially case (a) which is the Crank-Nicolson Galerkin algorithm. Both of these solutions also show a significant phase lag. Case (b) is equivalent to a direct extension to the time-dependent case of the Petrov-Galerkin methods developed in [1, 2] for steady-state equations by combining the weighted residuals formulation in space with a Crank-Nicolson scheme in time. It shows less numerical dispersion than (a), but it suffers from stronger damping and is out of phase.

The results of our proposed algorithm, shown in (c), show no dispersion or phase errors. A small amount of numerical damping is, however, evident. This is unavoidable when the mesh does not always agree with the location of the maximum and minimum peaks. We should point out that if $C = 1$ is used, the exact solution is obtained to two significant digits.

## CONCLUSIONS

We have presented a new Petrov-Galerkin finite element method for the time-dependent convection-diffusion equation. The method has been fully analyzed locally, although not so in the energy norms, and shows second order in time and third order in space convergence rates. The numerical examples show excellent approximation properties. The scheme shows virtually no phase error and very little numerical damping when tracking the time evolution of the solutions.

Extensions to this work are being pursued for both multidimensional and nonlinear situations and will be reported in the near future.

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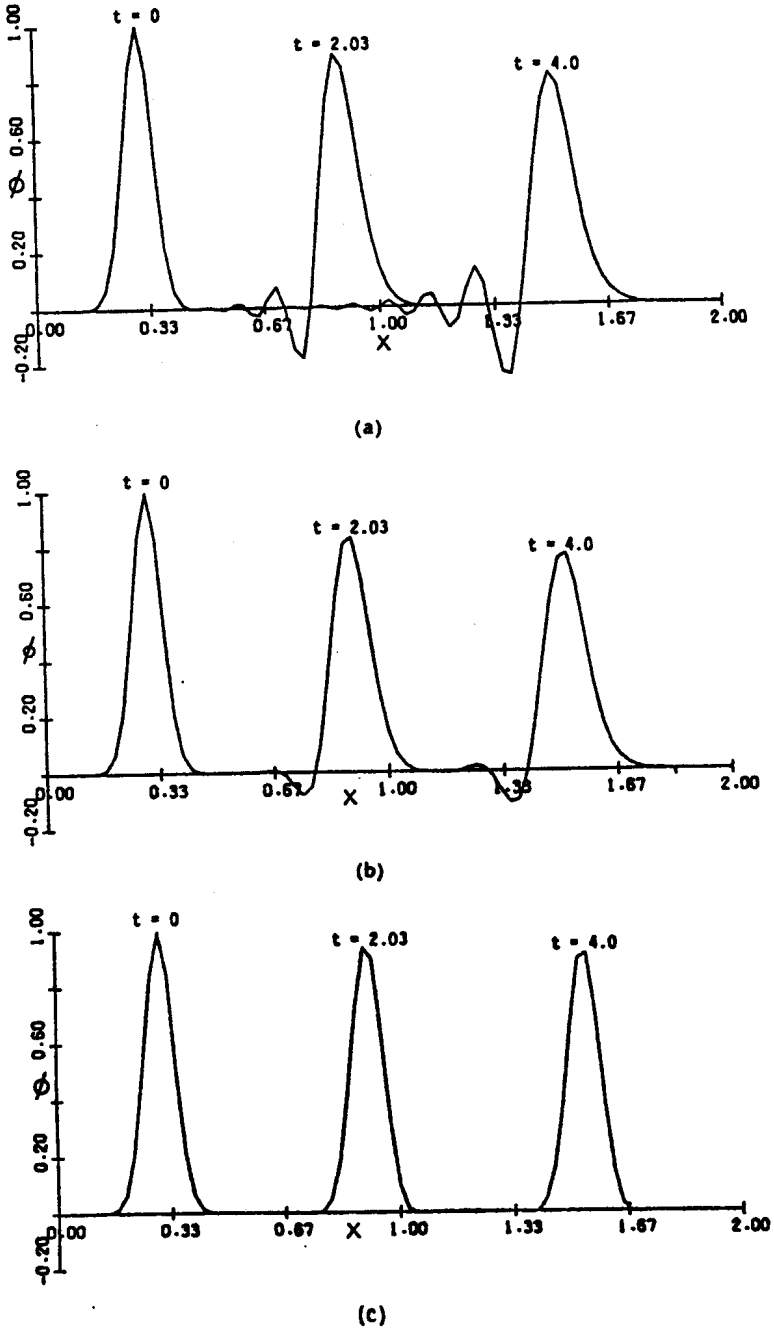


Figure 4. Numerical solutions to the second example at times t = 0, 2.03, and 4.0 seconds:

(a) $\alpha = \beta = 0$
(b) $\alpha \neq 0, \beta = 0$
(c) $\alpha \neq 0, \beta \neq 0$

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