Explicit time integration scheme with large time steps for first order transient problems using finite increment calculus

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Abstract

We present an explicit integration scheme for solving the transient heat conduction equation that allows larger time steps than the standard forward Euler scheme. The derivation starts from a higher order form of the governing differential equations of the problem obtained using a Finite Increment Calculus (FIC) procedure. The efficiency of the new explicit integration scheme in terms of substantial gains in the time step size versus the forward Euler scheme is verified in an example of application. The method is readily extendible to other problems in mechanics governed by the first order transient differential equation.

1 INTRODUCTION

Many transient problems in engineering and applied sciences are modeled by first and second order partial differential equations. Examples of first order transient problems involving a single scalar variable are found in heat conduction, seepage in porous media, gas diffusion, magnetostatics and Reynolds film lubrication, among others. Relevant first order problems involving more than one variable are creep of solids, Stokes flows and compressible gas flows, just to cite a few.

Second order transient problems, on the other hand, are typical in structural dynamics and wave propagation problems [3, 5, 17, 48]. The transient solution of first and second order transient problems can be found using implicit and explicit time integration schemes, or a combination of both [2, 9, 14, 15, 16, 17, 18, 41].

Explicit integration schemes are much simpler than implicit ones, as they do not requiere the inversion of a matrix, and for many problems are the only feasible alternative. Evidences of this are found in the analysis with the finite element method (FEM) of structural dynamics problems involving complex frictional contact conditions [3, 17, 48], and in the solution of problems in particle mechanics using the discrete element method (DEM) [8, 36], for instance.

Explicit time integration schemes for the first and second order transient equations have also been popular in the context of the so-called dynamic relaxation methods. These procedures aim to obtain the quasi-static response of a complex mechanical system in a simpler manner by solving an auxiliary first order transient problem [18, 47], or an auxiliary second order problem with an adequate selection of the mass and damping parameters [46].

The explicit time integration of first and second order transient problems is restricted by the size of the time step, which governs the stability of the numerical solution. The critical time step ensuring a stable solution for both types of transient problems depends on the inverse of the maximum eigenvalue of the system. This invariably leads to the need of very small time steps when very fine meshes are used, with the corresponding burden in the computational cost of the transient solution. Paradoxically, as it is typical in the explicit integration of the transient equations in mechanics, the physical solution of the problem is governed by the low frequency modes of the dynamic system, while the highest eigenvalue, depending on the level of mesh refinement, rules the computational efficiency of the explicit integration scheme.

Overcoming the curse of the critical time step size for explicit time integration schemes is still one of the big challenges in computational mechanics.

No information has been reported, to the authors knowledge, on explicit time integration schemes for solving the first order transient equations using time steps larger than those governed by the standard stability rule mentioned above.

On the other hand, several efforts to reduce the dependency of the time step size of explicit integration schemes with the largest eigenvalue of the system have been reported for the second order partial differential equation with applications to elasto-dynamics and structural dynamics problems. The general aim is to alleviate the step size limitation imposed by the higher frequencies (i.e. the mesh frequencies) whose response components contribute very little to the overall response of the dynamic system, which is typically dominated by the lower modes, as above mentioned. The most popular strategies to achieve this goal follow the so-called elemental and global mass scaling procedures [1, 6, 19, 21, 22, 44, 45, 46]. A different approach reported by Gonzalez and Park [12] uses a mass-tailoring technique for filtering out the high-frequency response components. Many mass scaling approaches have been used for deriving efficient explicit time relaxation methods [4, 13, 23, 39, 40, 43, 44, 46].

The aim of this work is to derive an explicit integration scheme for the first order transient equation that allows larger time steps than standard explicit schemes. The strategy to achieve this challenging objective is to solve a set of modified transient differential equations derived via the Finite Increment Calculus (FIC) procedure [25, 30]. The characteristic time parameters of the FIC equations allow us to derive a new explicit integration scheme with larger time steps than the critical value for the original differential equations, while retaining the accuracy of the transient solution sought.

The content of the paper is organized as follows. In the next section we formulate the FIC form of the first order transient equation. For the sake of clarity, and without loss of generality, we will focus here in the solution of the transient heat conduction problem. The derivation of an explicit integration scheme for the FIC form of the transient heat conduction equation is detailed. The stability conditions leading to the expression of the limit time step size are derived. The gain versus the standard explicit time integration scheme is shown. Again, for the sake of clarity the comparisons in this work will be referred to the forward Euler explicit scheme applied to the standard transient heat conduction equation. The advantages in efficiency, in terms of gains in the time step size, and accuracy of the new explicit time integration scheme are confirmed in an example of application.

2 FINITE INCREMENT CALCULUS FORM OF THE TRANSIENT HEAT CONDUCTION EQUATION

2.1 The standard transient heat conduction equation

The discretized form of the transient heat conduction equation using the FEM has the following standard form [17, 49]

$$\mathbf{C}\dot{\mathbf{a}} + \mathbf{K}\mathbf{a} - \mathbf{f} = \mathbf{0} \qquad \text{in } [\Omega, t] \tag{1}$$

In Eq.(1) t and Ω are respectively the time and the space domain where Eq.(1) holds, $\mathbf{a}$ is the vector of the nodal temperatures, $\dot{(\cdot)}$ denotes the time derivative, $\mathbf{C}$ is the heat capacity matrix, $\mathbf{K}$ is the conductivity matrix and $\mathbf{f}$ is the flux vector containing contributions from the internal and external heat sources. Eq.(1) is completed with the appropriate boundary conditions specifying the prescribed values of the temperature and the normal heat flux at the boundary, and with the initial temperature field on Ω.

The expressions of the matrices and vectors of Eq.(1) and the boundary conditions can be found in many text books [17, 49]. The derivation of Eq.(1) is briefly described in Appendix A.

In this work we will assume a diagonal form of matrix $\mathbf{C}$.

The explicit solution of Eq.(1) can be written, using the forward Euler scheme [2, 17, 49], as

$$\frac{1}{\Delta t}\mathbf{C}(\mathbf{a}^{n+1} - \mathbf{a}^n) + \mathbf{K}\mathbf{a}^n - \mathbf{f}^n = 0 \tag{2}$$

where $(\cdot)^n$ denotes values at time $t = t_n$.

From Eq.(2) we can find

$$\mathbf{a}^{n+1} = \mathbf{C}^{-1}\left[(\mathbf{I} - \Delta t\mathbf{K})\mathbf{a}^n + \Delta t\mathbf{f}^n\right] \tag{3}$$

where $\mathbf{I}$ is the identify matrix.

Eq.(3) shows that for a diagonal form of $\mathbf{C}$, the time evolution of the nodal temperatures can be found without solving a system of equations.

The stability of the forward Euler scheme is found using standard procedures [2, 17, 49]. A summary is given next.

The solution of the transient problem will be assumed of the form

$$\mathbf{a}(\mathbf{x}, t) = \sum_{i=1}^{N} \boldsymbol{\phi}_i(\mathbf{x}) a_i(t) \tag{4}$$

where N is the number of nodal temperatures in the discretized system and $a_i(t)$ and $\boldsymbol{\phi}$ are, respectively the i-th modal amplitude and the i-th modal vector of the eigenvalue system

$$|\mathbf{K} - \lambda_i \mathbf{M}|\boldsymbol{\phi}_i = 0 \tag{5}$$

and $\lambda_1, \cdots, \lambda_N$ are the eigenvalues of the system ordered from the smallest one, λ_1, to the largest one, λ_N.

Substituting Eq.(4) into (3) for $\mathbf{f}^n = 0$, and using the orthogonality properties of the modal vectors $\boldsymbol{\phi}_i$ versus the matrices $\mathbf{C}$ and $\mathbf{K}$, we can obtain after little algebra

$$a_i^{n+1} = (1 - p_i) a_i^n \tag{6}$$

with

$$p_i = \frac{k_i}{c_i}\Delta t = \lambda_i \Delta t \tag{7}$$

where $\lambda_i = \frac{k_i}{c_i}$, and

$$k_i = \boldsymbol{\phi}_i^T \mathbf{K} \boldsymbol{\phi}_i \quad , \quad c_i = \boldsymbol{\phi}_i^T \mathbf{C} \boldsymbol{\phi}_i \tag{8}$$

Assuming a stable solution of the type $a_i^{n+1} = \gamma_i a_i^n$, with γ_i being the amplification factor, we can rewrite Eq.(6) as

$$\gamma_i = (1 - p_i) \tag{9}$$

The stability condition, ensuring that $|\gamma_i| < 1$ is

$$-1 < (1 - p_i) < 1 \qquad \text{for } i = 1, N \tag{10}$$

From Eq.(10) we deduce the stability and the time step limits for $i = N$, as

$$p_N < 2 \qquad \text{and} \qquad \Delta t \leq \Delta t_l = \frac{2}{\lambda_N} \tag{11}$$

where Δt_l is the limit time step that guarantees the stability of the explicit solution.

In order to avoid non-physical oscillatory solutions, the following additional condition must be satisfied

$$0 < \gamma_i < 1 \qquad , \quad \text{for } i = 1, m \tag{12}$$

where m is the number of low order modes that govern the solution of the transient problem. In practice it suffices that $0 < \gamma_1 < 1$.

2.2 FIC form of the transient heat conduction equation

The differential equation for the transient heat conduction problem is typically found by establishing the balance of heat fluxes in an infinitesimal space-time domain belonging to $[\Omega, t]$ (Appendix A). From the original governing differential equation and the adequate boundary conditions, the discretized form of Eq.(1) can be found using the FEM, for instance [17, 49].

In this work the solution of the transient problem governed by Eq.(1) will be found by solving a modified higher order form of Eq.(1), written as

$$\mathbf{r} - \tau_1 \dot{\mathbf{r}} + \tau_2^2 \ddot{\mathbf{r}} = 0 \tag{13}$$

where

$$\mathbf{r} := \mathbf{C}\dot{\mathbf{a}} + \mathbf{K}\mathbf{a} - \mathbf{f} \tag{14}$$

is a residual vector of nodal heat fluxes that vanishes for the exact solution, and τ_1 and τ_2 are characteristic time parameters.

The modified governing equations leading to Eq.(13) can be found from physical arguments using a Finite Increment Calculus (FIC) procedure based in establishing the balance of heat fluxes in a space-time domain of dimensions $[d\Omega, \tau]$ where $d\Omega = dxdy$, in two dimensions (2D), and τ is *finite time interval* defined as a proportion of the time step parameter Δt of the time integration scheme ([24, 25, 26] and Appendix A). In this work, we will take

$$\tau_1 = \delta_1 \Delta t \qquad \text{and} \qquad \tau_2 = \sqrt{\delta_2}\Delta t \tag{15}$$

where δ_1 and δ_2 are arbitrary parameters that govern the stability of the time integration scheme. The selection of δ_1 and δ_2 is detailed in Section 4.

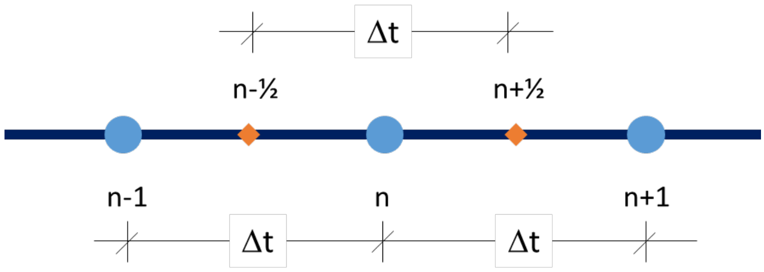

Figure 1: Stencil of three time instants at t^{n-1}, t^n and t^{n+1} with $t^{n+1} = t^n + \Delta t$.

Clearly for values of $\tau_1 = \tau_2 = 0$ the standard "infinitesimal" form of the discretized heat conduction equation (Eq.(1)) is recovered.

The derivation of Eq.(13) using the mechanical arguments mentioned in the above paragraph is presented in the Appendix A. Further details are given in [25, 26]. Eq.(13) can also be interpreted from a mathematical view point, as the second-order Taylor expansion in time of all the terms in Eq.(1).

The solution of the FIC form of the transient heat conduction equation (Eq.(13)) can now be attempted using any time discretization procedure. It is interesting that, similarly as for the 1D quasi-static advection-diffusion problem [25], the exact analytical solution of the original differential equations can be found by choosing adequately the characteristic time parameters of the FIC equations. This is, however, not possible for most practical problems and, hence, the transient solution of Eq.(13) will typically be an approximation of the numerical solution obtained for the infinitesimal form (Eq.(1)).

The FIC approach for formulating higher order forms of the differential equation in mechanics has been successfully used, in conjunction with standard numerical methods, such as the FEM and meshless procedures, for finding accurate and stable solutions for steady state and transient problems, such as convection-diffusion-radiation, fluid dynamics and quasi-incompressible solids, among others [7, 10, 11, 20, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 37, 38, 42].

In this work Eq.(13) will be the starting point for deriving a new explicit integration scheme for the transient heat conduction equation, allowing larger time steps than the standard forward Euler scheme for the original equation (Eq.(1)), while retaining a high accuracy in the transient numerical solution.

3 EXPLICIT TIME INTEGRATION OF THE FIC FORM OF THE TRANSIENT HEAT CONDUCTION EQUATION

The FIC form of the transient heat conduction equation at time $t = t_n$ is written using Eqs.(13) and (15) as

$$\mathbf{r}^n - \delta_1 \Delta t \dot{\mathbf{r}}^n + \delta_2 \Delta t^2 \ddot{\mathbf{r}}^n = 0 \tag{16}$$

where $\mathbf{r}^n = \mathbf{r}(\Omega, t_n)$.

The explicit computation of vectors $\dot{\mathbf{r}}^n$ and $\ddot{\mathbf{r}}^n$ is detailed next.

3.1 Explicit computation of $\dot{\mathbf{r}}^n$

From Figure 1 we can write

$$\dot{\mathbf{r}}^n = \mathbf{C}\dot{\mathbf{a}}^n + \mathbf{K}\dot{\mathbf{a}}^n - \dot{\mathbf{f}}^n = \frac{1}{\Delta t}\mathbf{C}(\dot{\mathbf{a}}^{n+1/2} - \dot{\mathbf{a}}^{n-1/2}) + \frac{1}{\Delta t}\mathbf{K}(\mathbf{a}^n - \mathbf{a}^{n-1}) - \frac{1}{\Delta t}(\mathbf{f}^n - \mathbf{f}^{n-1}) \quad (17)$$

From the original differential equation (Eq.(1)) and the definition of $\mathbf{r}$ of Eq.(14), we will assume that $\mathbf{r}^{n-1/2} = 0$ for the exact solution. Under this assumption we can deduce, after particularizing Eq.(1) for $t = t_{n-1/2}$,

$$\mathbf{C}\dot{\mathbf{a}}^{n-1/2} = -(\mathbf{K}\mathbf{a}^{n-1/2} - \mathbf{f}^{n-1/2}) = -\frac{1}{2}\mathbf{K}\left(\mathbf{a}^n + \mathbf{a}^{n-1}\right) + \frac{1}{2}(\mathbf{f}^n + \mathbf{f}^{n-1}) \quad (18)$$

On the other hand, we can write

$$\dot{\mathbf{a}}^{n+1/2} = \frac{1}{\Delta t}(\mathbf{a}^{n+1} - \mathbf{a}^n) \quad (19)$$

Substituting Eqs.(18) and (19) into (17) and grouping terms yields the sought expression,

$$\dot{\mathbf{r}}^n = \frac{1}{\Delta t^2}(\mathbf{a}^{n+1} - \mathbf{a}^n) + \frac{1}{2}\mathbf{K}(3\mathbf{a}^n - \mathbf{a}^{n-1}) - \frac{1}{2}(3\mathbf{f}^n - \mathbf{f}^{n-1}) \quad (20)$$

3.2 Explicit computation of $\ddot{\mathbf{r}}^n$

From Figure 1 we can write

$$\ddot{\mathbf{r}}^n = \mathbf{C}\ddot{\mathbf{a}}^n + \mathbf{K}\ddot{\mathbf{a}}^n - \ddot{\mathbf{f}}^n = \frac{1}{\Delta t}\mathbf{C}(\ddot{\mathbf{a}}^{n+1/2} - \ddot{\mathbf{a}}^{n-1/2}) + \frac{2}{\Delta t}\mathbf{K}(\dot{\mathbf{a}}^n - \dot{\mathbf{a}}^{n-1/2}) - \frac{2}{\Delta t}(\dot{\mathbf{f}}^n - \dot{\mathbf{f}}^{n-1/2}) \quad (21)$$

We will also assume that the following expressions hold

$$\frac{1}{\Delta t}\mathbf{C}\ddot{\mathbf{a}}^{n+1/2} = \frac{1}{\Delta t^3}\mathbf{C}(\mathbf{a}^{n+1} - 2\mathbf{a}^n + \mathbf{a}^{n-1}) \quad (22a)$$

$$\mathbf{C}\dot{\mathbf{a}}^{n-1} = -\mathbf{K}\mathbf{a}^{n-1} + \mathbf{f}^{n-1} \quad (22b)$$

The derivation of Eq.(22b) follows from assuming that Eq.(1) holds for $t = t_{n-1}$. Using Eq.(22b) we can obtain,

$$\frac{1}{\Delta t}\mathbf{C}\ddot{\mathbf{a}}^{n-1/2} = \frac{1}{\Delta t^2}\mathbf{C}(\dot{\mathbf{a}}^n - \dot{\mathbf{a}}^{n-1}) = \frac{1}{\Delta t^3}\mathbf{C}(\mathbf{a}^n - \mathbf{a}^{n-1}) + \frac{1}{\Delta t^2}\mathbf{K}\mathbf{a}^{n-1} - \frac{1}{\Delta t^2}\mathbf{f}^{n-1} \quad (23)$$

Also,

$$\begin{aligned}\frac{2}{\Delta t}\mathbf{K}(\dot{\mathbf{a}}^n - \dot{\mathbf{a}}^{n-1/2}) &= \frac{2}{\Delta t^2}\mathbf{K}(\mathbf{a}^n - \mathbf{a}^{n-1}) + \frac{2}{\Delta t}(\mathbf{C}\ddot{\mathbf{a}}^{n-1/2} - \dot{\mathbf{f}}^{n-1/2}) = \frac{2}{\Delta t^2}\mathbf{K}(\mathbf{a}^n - \mathbf{a}^{n-1}) \\ &+ \frac{2}{\Delta t^3}\mathbf{C}(\mathbf{a}^{n+1} - 2\mathbf{a}^n + \mathbf{a}^{n-1}) - \frac{2}{\Delta t}\dot{\mathbf{f}}^{n-1/2} \quad (24)\end{aligned}$$

For the computation of $\ddot{\mathbf{a}}^{n-1/2}$in Eq.(24) we have used the same expression as in Eq.(22a). Also, in the derivation of Eq.(24) we have assumed that Eq.(1) holds for $t = n - \frac{1}{2}$.

Substituting Eqs.(22a), (23) and (24) into (21) gives

$$\ddot{\mathbf{r}}^n = \frac{1}{\Delta t^3}\mathbf{C}(3\mathbf{a}^{n+1} - 7\mathbf{a}^n + 4\mathbf{a}^{n-1}) + \frac{1}{\Delta t^2}\mathbf{K}(2\mathbf{a}^n - 3\mathbf{a}^{n-1}) - \frac{1}{\Delta t^2}(2\mathbf{f}^n - 3\mathbf{f}^{n-1}) \tag{25}$$

In the derivation of Eq.(25) we have computed $\dot{\mathbf{f}}^n$ in Eq.(21), as $\dot{\mathbf{f}}^n = \frac{1}{\Delta t}(\mathbf{f}^n - \mathbf{f}^{n-1})$.

Substituting the expressions of $\dot{\mathbf{r}}^n$ and $\ddot{\mathbf{r}}^n$ of Eqs.(20) and (25) into Eq.(16) and using Eqs.(14) and (2), gives finally, after grouping terms

$$\boxed{\begin{aligned}(1-\delta_1+3\delta_2)\mathbf{C}\mathbf{a}^{n+1} + \left[-(1-\delta_1+7\delta_2)\mathbf{C} + \Delta t\left(1-\frac{3}{2}\delta_1+2\delta_2\right)\mathbf{K}\right]\mathbf{a}^n + \\ + \left[4\delta_2\mathbf{C} + \Delta t\left(\frac{\delta_1}{2}-3\delta_2\right)\mathbf{K}\right]\mathbf{a}^{n-1} - \Delta t\left[\left(1-\frac{3}{2}\delta_1+2\delta_2\right)\mathbf{f}^n + \left(\frac{\delta_1}{2}-3\delta_2\right)\mathbf{f}^{n-1}\right] = \mathbf{0}\end{aligned}} \tag{26}$$

Eq.(26) provides an explicit scheme for computing $\mathbf{a}^{n+1}$ in terms of $\mathbf{a}^n$, $\mathbf{a}^{n-1}$, $\mathbf{f}^n$ and $\mathbf{f}^{n-1}$.

Remark 1. The explicit scheme of Eq.(26) is a consequence of the strategy for computing the terms in $\dot{\mathbf{r}}^n$ and $\ddot{\mathbf{r}}^n$, as explained in Sections 3.1 and 3.2. Indeed, other explicit schemes, with possibly better performance, can be found using other alternatives for evaluating these terms.

4 STABILITY OF THE EXPLICIT SCHEME FOR THE FIC FORM OF THE TRANSIENT HEAT CONDUCTION EQUATION

4.1 Computation of the critical time step

The stability of the explicit scheme of Eq.(26) can be studied by the same procedure explained in Section 2.1.

Substituting Eq.(4) into (26) and using the orthogonality properties of the eigenvectors $\boldsymbol{\phi}_i$ versus the matrices $\mathbf{C}$ and $\mathbf{K}$ we obtain after little algebra

$$\begin{aligned}(1-\delta_1+3\delta_2)a_i^{n+1} + \left[-(1-\delta_1+7\delta_2) + \left(1-\frac{3}{2}\delta_1+2\delta_2\right)p_i\right]a_i^n + \\ + \left[4\delta_2 + \left(\frac{\delta_1}{2}-3\delta_2\right)p_i\right]a_i^{n-1} = 0\end{aligned} \tag{27}$$

where p_i is given by Eq.(7).

Assuming again a solution of the type $a_i^{n+1} = \gamma_i a_i^n$ with $|\gamma_i| < 1$ we can obtain the characteristic equation for the amplification factor of each mode, γ_i, as

$$A\gamma_i^2 + B\gamma_i + C = 0 \tag{28}$$

where

$$\begin{aligned}A &= 1-\delta_1+3\delta_2 \\ B &= -(1-\delta_1+7\delta_2) + \left(1-\frac{3}{2}\delta_1+2\delta_2\right)p_i \\ C &= 4\delta_2 + \left(\tfrac{\delta_1}{2}-3\delta_2\right)p_i\end{aligned} \tag{29}$$

The coefficients of Eq.(29) ensuring $-1 < \gamma_i < 1$ can be found by direct analysis of the roots of Eq.(28), or via the Routh-Hurwitz criterion. A good explanation of the later approach is given in Belytschko et al. ([3], pp. 338–339).

The three stability conditions are the following:

1. $A + B + C > 0$

$$(1 - \delta_1 - \delta_2)p_i \geq 0 \tag{30}$$

This gives

$$1 - \delta_1 - \delta_2 \geq 0 \tag{31}$$

2. $A - C \geq 0$

$$(1 - \delta_1 - \delta_2) + \left(3\delta_1 - \frac{\delta_2}{2}\right) p_i \geq 0 \tag{32}$$

Taking into account Eq.(31), Eq.(32) is satisfied if

$$\delta_2 \leq \frac{1}{6}\delta_1 \tag{33}$$

Condition (31) becomes (using $\delta_2 = \frac{\delta}{6}$)

$$1 - \frac{7}{6}\delta_1 \geq 0\,, \quad \text{or} \quad \delta_1 \leq \frac{6}{7} \tag{34}$$

3. $A - B + C \geq 0$

$$2(1 - \delta_1 + 7\delta_2) + (-1 + 2\delta_1 - 5\delta_2)p_i \geq 0 \tag{35}$$

Eq.(34) gives the limiting value for p_i as

$$p_i \leq \frac{2(1 - \delta_1 + 7\delta_2)}{1 - 2\delta_1 + 5\delta_2} \qquad i = 1, N \tag{36}$$

Substituting the condition for δ_2 of Eq.(33) (for the identity case) into (36) gives

$$p_i \leq 2\left[1 + \frac{8\delta_1}{6 - 7\delta_1}\right] \qquad i = 1, N \tag{37}$$

Condition (37) must be satisfied for all the modes. Particularizing condition (37) for the largest mode ($i = N$) leads to the expression of the allowable time increment, Δt, as

$$\boxed{\Delta t \leq \Delta t_l = \frac{2}{\lambda_N}\left(1 + \frac{8\delta_1}{6 - 7\delta_1}\right)} \tag{38}$$

Note that for $\delta_1 = 0$ we recover the expression $\Delta t_l = \frac{2}{\lambda_N}$ of the forward Euler scheme for the standard transient heat conduction equation (Eq.(11)).

It is easy to verify that expression (38) yields larger critical time steps than those allowed for the forward Euler scheme.

Remark 2. From the general explicit scheme of Eq.(26) we can obtain a particular simpler form by choosing $\delta_2 = \frac{1}{6}\delta_1$, as

$$\boxed{\begin{aligned}\left(1-\frac{\delta_1}{2}\right)\mathbf{C}\mathbf{a}^{n+1}+\left[-\left(1+\frac{\delta_1}{6}\right)+\Delta t\left(1-\frac{7}{6}\delta_1\right)\mathbf{K}\right]\mathbf{a}^n+\\ +\frac{2}{3}\delta_1\mathbf{C}\mathbf{a}^{n-2}-\Delta t\left(1-\frac{7}{6}\delta_1\right)\mathbf{f}^n=0\end{aligned}} \tag{39}$$

Eq.(39) is the expression recommended for the practical application of the new explicit scheme and, as such, it will be used for solving the demonstrative example presented in Section 5.

Remark 3. The new explicit time integration scheme is termed ETF11. The letters ETF emanate from the initials of **E**xplicit **T**ime integration, **F**IC procedure. The first digit 1 refers to the first order transient equation, while the second digit 1 denotes that the scheme is the outcome of the option chosen in this work for the computation of the terms $\dot{\mathbf{r}}^n$ and $\ddot{\mathbf{r}}^n$ in Section 3 and for choosing $\delta_2 = \frac{1}{6}\delta_1$ (Eq.(34)). Other ways of computing these terms and the value of δ_2 will lead to other ETF1 schemes, as mentioned in Remark 1.

The speed-up (SUP) of the new ETF11 integration scheme is defined as

$$SUP = \frac{\Delta t_l^{ETF11}}{\Delta t_l^{FE}} = \left(1+\frac{8\delta_1}{6-7\delta_1}\right) \tag{40}$$

where Δt_l^{ETF11} and Δt_l^{FE} denote the limit time steps of the ETF11 and the forward Euler (FE) schemes given by Eqs.(11) and (38), respectively.

Note that in Eq.(40) δ_1 should not exceed $\frac{6}{7}$, as specified by Eq.(34).

Table 1 gives the SUP values in terms of the time integration parameter δ_1. It can be seen that values of SUP > 1 (meaning gains in the time step size versus the forward Euler scheme) are obtained for $\delta_1 > 0$. In particular, large SUP values are obtained for values of δ_1 exceeding 0.7. Clearly, the limit value of $\delta_1 \simeq \frac{6}{7}$ will yield an (unrealistic) infinite value of the SUP value.

δ_1	SUP
0	1
0.5	2.6
0.7	3.66
0.73	7.292
0.75	9.00
0.8	17.0
0.825	30.33
0.85	136

Table 1: Speed-up (SUP) values of the new explicit ETF11 scheme versus the forward Euler scheme in terms of the time integration parameter δ_1

4.2 Critical value of the δ_1 parameter

Following the explanation given in Section 3 (Eq.(12)), the SUP gains of the ETF11 scheme are limited in practice by the condition

$$0 < \gamma_1 < 1 \tag{41}$$

so that no spurious oscillations are found in the transient solution. The value of γ_1 can be obtained by solving the characteristic equation (28) for the lowest eigenvalue of the system, for every particular problem.

Particularizing the characteristic equation (28) for γ_1 using $\delta_2 = \frac{\delta_1}{6}$ we obtain the following quadratic equation

$$\left(1 - \frac{\delta_1}{2}\right)\gamma_1^2 + (2r_1 - 1)\left(1 + \frac{\delta_1}{6}\right)\gamma_1 + \frac{2\delta_1}{3} = 0 \tag{42}$$

where

$$r_1 = \frac{\lambda_1}{\lambda_N} \tag{43}$$

is the ratio between the lowest and larger eigenvalues of the system.

In the derivation of Eq.(42) we have used the expression $p_1 = \Delta t \lambda_1 = \frac{\lambda_1}{\lambda_n} p_n = r_1 p_n$ with p_n given by Eq.(37), as

$$p_n = 2\left[1 + \frac{8\delta_1}{6 - 7\delta_1}\right] \tag{44}$$

The absence of oscillatory solutions can be guaranteed by a non-negative expression of the discriminant of Eq.(42), i.e.

$$(2r_1 - 1)^2\left(1 + \frac{\delta_1}{6}\right)^2 - \frac{8}{3}\delta_1\left(1 - \frac{\delta_1}{2}\right) \geq 0 \tag{45}$$

After grouping terms we find

$$\left(4 + \frac{C_1}{12}\right)\delta_1^2 + [C_1 - 8]\delta_1 + 3C_1 \geq 0 \tag{46}$$

with $C_1 = (2r_1 - 1)^2$.

The minor solution of Eq.(46) (for the equality case) gives the critical value of the δ_1 parameter (termed δ_1^{crit}) ensuring no oscillatory solutions. It is straight-forward to find

$$\delta_1^{crit} = \frac{1}{(8 + \frac{1}{6}C_1)}\left[(8 - C_1) - 8(1 - C_1)^{1/2}\right] \tag{47}$$

It can be verified that $\delta_1^{crit} < \delta_1^{lim} = \frac{6}{7}$.

It is interested that the value of δ_1^{crit} approaches δ_1^{lim} as $C_1 \to 1$. This is the case for very fine meshes for which $r_1 \to 0$ and $C_1 \to 1$.

The efficiency of the ETF11 scheme versus the forward Euler scheme is demonstrated in the example presented in the next section.

5 EXAMPLES

The example chosen to show the efficiency of the new ETF11 scheme for the transient heat conduction equation is the time evolution of the temperature in a square prismatic domain of unit thickness with an internal circle (Figure 2).

The material properties of the heat conduction problem are the following,

$$\rho = 2698,4\, Kg/m^3, \quad k = 237\, J/^{\circ}Cms, \quad c = 900 J/^{\circ}CKg$$

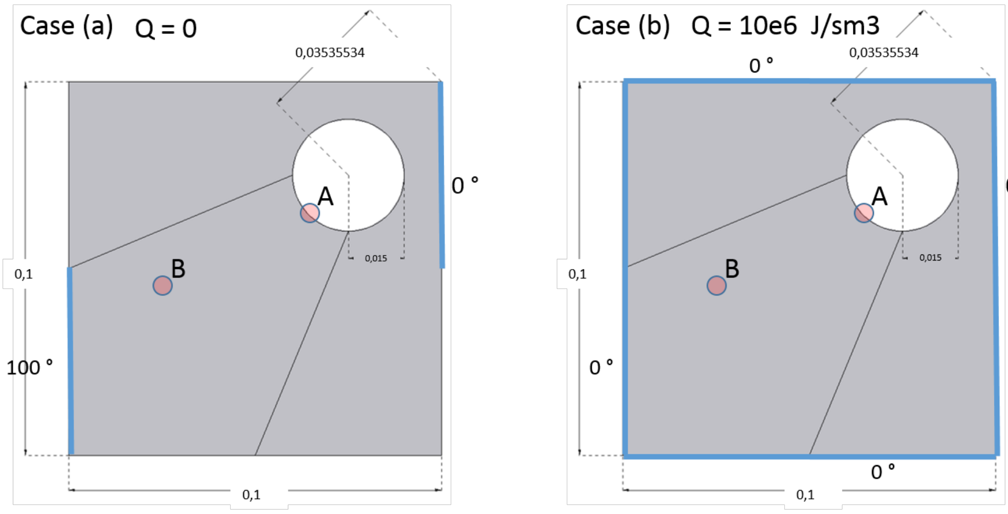

Figure 2: Square domain of unit thickness with internal hole. Zero initial temperature at all the internal points. Case (a): $Q = 0$. Temperature prescribed to 100°C and 0°C along half the lateral sides as shown. Zero normal flux prescribed at all the other boundaries. Case (b): $Q = 10^6$. Temperature prescribed to 0°C at the square sides. Zero normal flux prescribed at the boundary of the internal circle. Sampling points $A(0.064, 0.064)$ and $B(0.021, 0.044)$. Dimensions in meters.

Case (a). $Q = 0$

The first case considered assumes that the distributed heat source Q is zero (Appendix A.1). The initial temperature at all the internal points of the domain is prescribed to zero, with exception of the values at the mid-length of the lateral sides where the initial temperature is prescribed (and kept fixed) at 100°C and 0°C, as shown in Figure 2. A zero flux condition is specified at all the other boundaries.

The problem has been analyzed with the four unstructured meshes of 151, 6.146, 12.630 and 58.076 3-noded linear triangles shown in Figure 3.

We have used the forward Euler (FE) scheme with a value of $\Delta t^{FE} = 0.99 \times \Delta t_l$ (with $\Delta t_l = \frac{2}{\lambda_N}$), and the new ETF11 scheme Δt^{ETF11} given by Eq.(38).

Table 2 shows the minimum and maximum eigenvalues for the three meshes used, as well as the limit value of $\delta_1^{lim}(= 6/7)$, the critical value δ_1^{crit} (Eq.(47)) and the actual value of δ_1 used in the computations. We have verified that the values of δ_1 satisfy Eq.(41) and yield accurate transient solutions at all points in the domain. The time steps used for each analysis are shown in Figure 3.

The SUP gains in time step size of the ETF11 scheme versus the forward Euler scheme are shown in the last column of Table 2. The advantage of the new explicit time integration scheme is clearly evidenced.

Figure 4 shows the steady state distribution of the temperature over the analysis domain obtained with the ETF11 scheme. The ETF11 results are indistinguishable from those obtained with the forward Euler scheme.

The curves of Figure 5 show the temperature evolution at a point A over the boundary of the internal circle with coordinates $(0.064, 0.064)$ and at an internal point B located at $(0.021, 0.044)$ computed with the forward Euler and the ETF11 schemes for the four meshes considered. Excellent agreement between both solutions is found at both points, as well as in the rest of the points of the analysis domain with a distinct advantage in terms of SUP in the computations using the new explicit scheme.

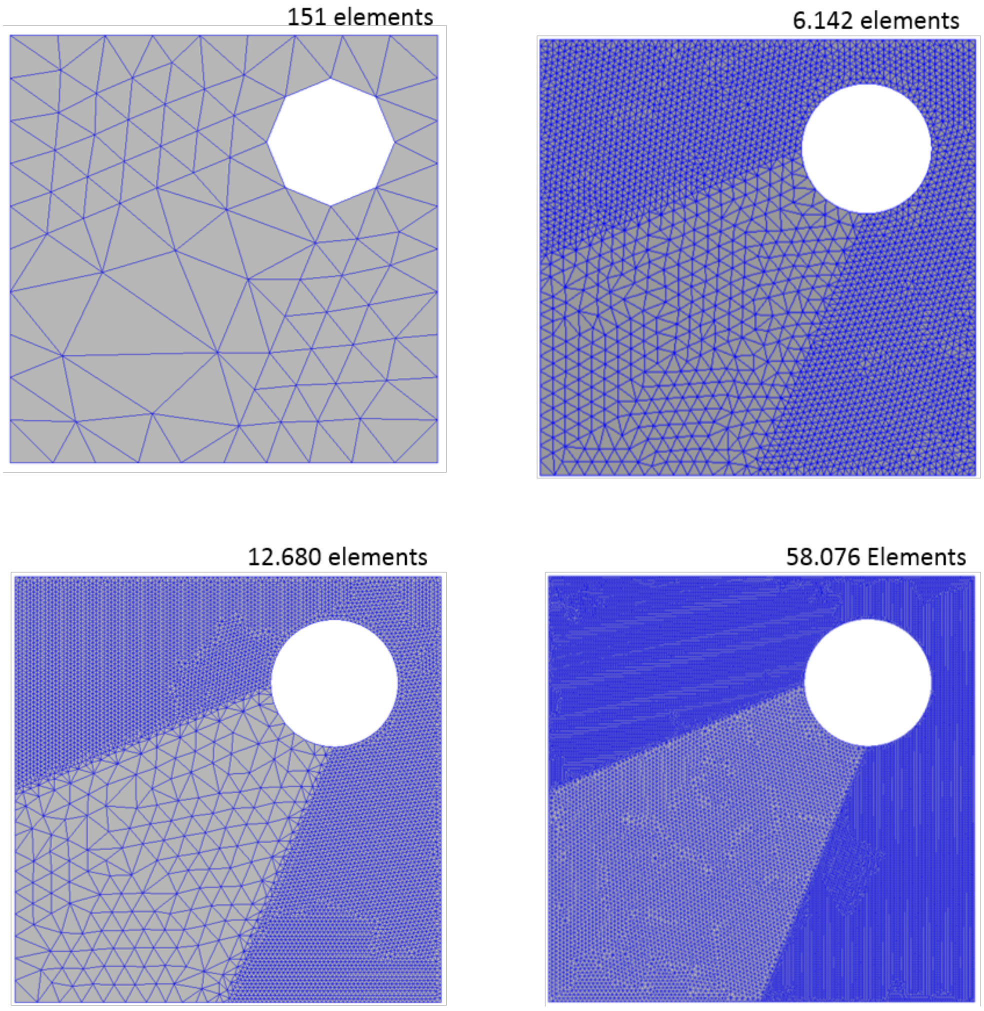

Figure 3: Finite element meshes of 3-noded triangles used for the transient analysis.

Case (b). $Q = 10^6$

The conditions of the problem of Case (a) have been changed as follows:

- The temperature at the edges of the square domain has been prescribed to 0°C.
- A constant heat source of $Q = 10^6 \ \frac{J}{sm^2}$ has been applied over the whole domain.

The rest of the conditions and the material properties are the same as for Case (a).

The values of λ_1, λ_N, δ_1^{crit}, δ_1 and SUP for this problem are shown in Table 3. Numerical results obtained using the FE and the ETF11 schemes are again coincident, with considerable gains is speed-up using the new explicit scheme.

Figure 6 shows the temperature contours at steady stated obtained with both schemes. Figure 7 shows the evolution of the temperature at points A and B using the FE and ETF11 schemes. The coincidence of the results is clearly visible.

We note, finally, that, as expected, both the forward Euler and the ETF11 solutions for Cases (a) and (b) coincide with the more costly implicit solution using the time step of the ETF11 scheme.

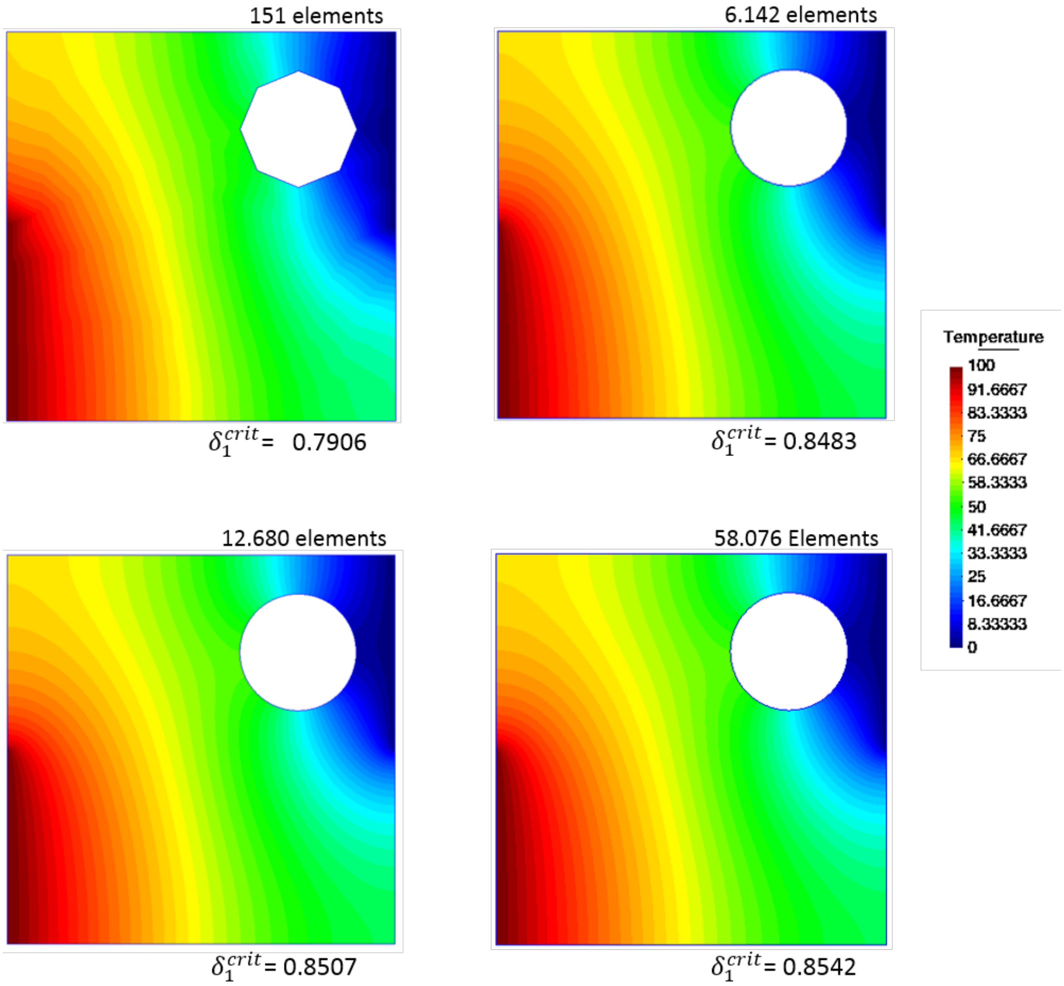

Figure 4: Temperature contours at steady state obtained with the forward Euler scheme and the new ETF11 scheme. The results are practically identical for both schemes.

6 CONCLUSIONS

The FIC form of the first order transient heat conduction equation provides a pathway for deriving a new explicitly time integration scheme allowing considerable larger time steps than the standard forward Euler scheme. The procedure is readily applicable to other problems governed by the first order parabolic differential equation. The approach can be also extended for enhancing the time step limit of other standard explicit schemes for solving these type of equations. The simple demonstrative examples presented have shown that accurate solutions can be obtained using time increments much larger that for the forward Euler scheme.

The ETF11 integration scheme will have many advantages in the fast transient solution of practical problems governed by the first order parabolic equation using any of the well known space discretization procedures. Typical examples are heat conduction, Stokes flows, compressible gas flows and creep of solids, among others. Another interesting application would be the Lagrangian transport of substances accounting for conductive heat effects.

A promising utilization of the new ETF11 scheme is the fast explicit computation

	λ_1	λ_N	δ_1^{lim}	δ_1^{crit}	δ_1	SUP
Mesh 1 $N_{el} = 151$	4.571×10^{-2}	8.4	0.857	0.796	3.99	3.99
Mesh 2 $N_{el} = 6.142$	4.169×10^{-2}	476.56	0.857	0.848	0.823	28.55
Mesh 3 $N_{el} = 12.680$	4.157×10^{-2}	903.42	0.850	0.847	0.825	30.33
Mesh 4 $N_{el} = 58.076$	4.129×10^{-2}	4144.11	0.857	0.8542	0.840	57.00

Table 2: Case (a), $Q = 0$ (Figure 2a). Minimum and maximum eigenvalues for the four meshes used. δ_1^{lim}, δ_1^{crit} and δ_1 denote respectively, the limit and critical values of δ_1 and the value of δ_1 used in the ETF11 computations. SUP is the speed up versus the forward Euler scheme

	λ_1	λ_N	δ_1^{lim}	δ_1^{crit}	δ_1	SUP
Mesh 1 $N_{el} = 151$	0.1825	0.685	0.857	0.718	0.620	2.60
Mesh 2 $N_{el} = 6.142$	0.1839	377.77	0.857	0.836	0.780	12.50
Mesh 3 $N_{el} = 12.680$	0.1838	717.74	0.857	0.842	0.800	17.0
Mesh 4 $N_{el} = 58.076$	0.1839	4144.11	0.857	0.851	0.8325	39.60

Table 3: Case (b), $Q = 10^6$ (Figure 2b). Minimum and maximum eigenvalues for the four meshes used. δ_1^{lim}, δ_1^{crit} and δ_1 denote respectively, the limit and critical values of δ_1 and the value of δ_1 used in the ETF11 computations. SUP is the speed up versus the forward Euler scheme

of steady-state solutions via time relaxation. This topic has been the objective of much research in the previous decades [2, 3, 17]. Indeed, the combination of the ETF11 scheme with adequate diagonal forms of matrix **C** will pave the way for deriving new families of enhanced time relaxation procedures.

The possible competitive advantage of the new ETF11 scheme with large time steps versus the implicit scheme will also be a topic of future research.

We note, finally, that the ETF11 is a particular member of the family of new explicit time integration schemes for the first order transient equation derived via the FIC approach, as started in Remarks 1, 2 and 3.

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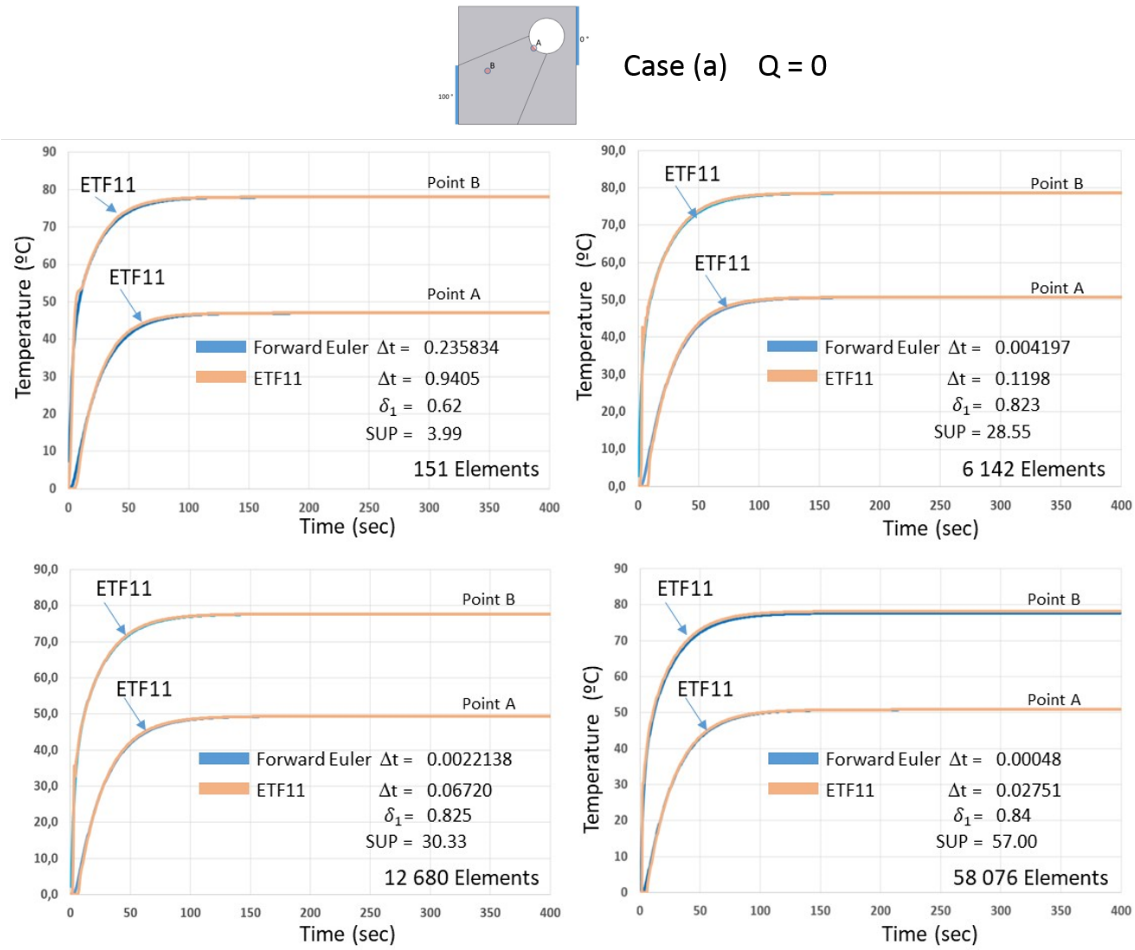

Figure 5: Case (a). Time evolution of the temperature at points A and B. The graphs show results obtained with forward Euler scheme and the ETF11 scheme for the values of δ_1 given in Table 2. The time steps used and the speed-up (SUP) versus the forward Euler scheme is shown for each mesh.

A APPENDIX A. FIC FORM OF THE TRANSIENT HEAT CONDUCTION EQUATION

A.1 Infinitesimal form of the transient heat conduction equation

Consider a one-dimensional (1D) heat conduction problem in a bar of lenght L. Figure A.1 shows the space-time domain where balance of heat fluxes is enforced. The balance equation can be written as

$$\underbrace{q_A dt + S dx dt}_{\text{flux in}} - \underbrace{q_B dt}_{\text{flux out}} = 0 \tag{A.1}$$

where

$$S = Q - \rho c \frac{\partial \phi}{\partial t} \tag{A.2}$$

In Eqs.(A.2) ϕ is the temperature, q is the heat flux, Q is a distributed heat source and ρ and c are the density and the specific heat capacity, respectively.

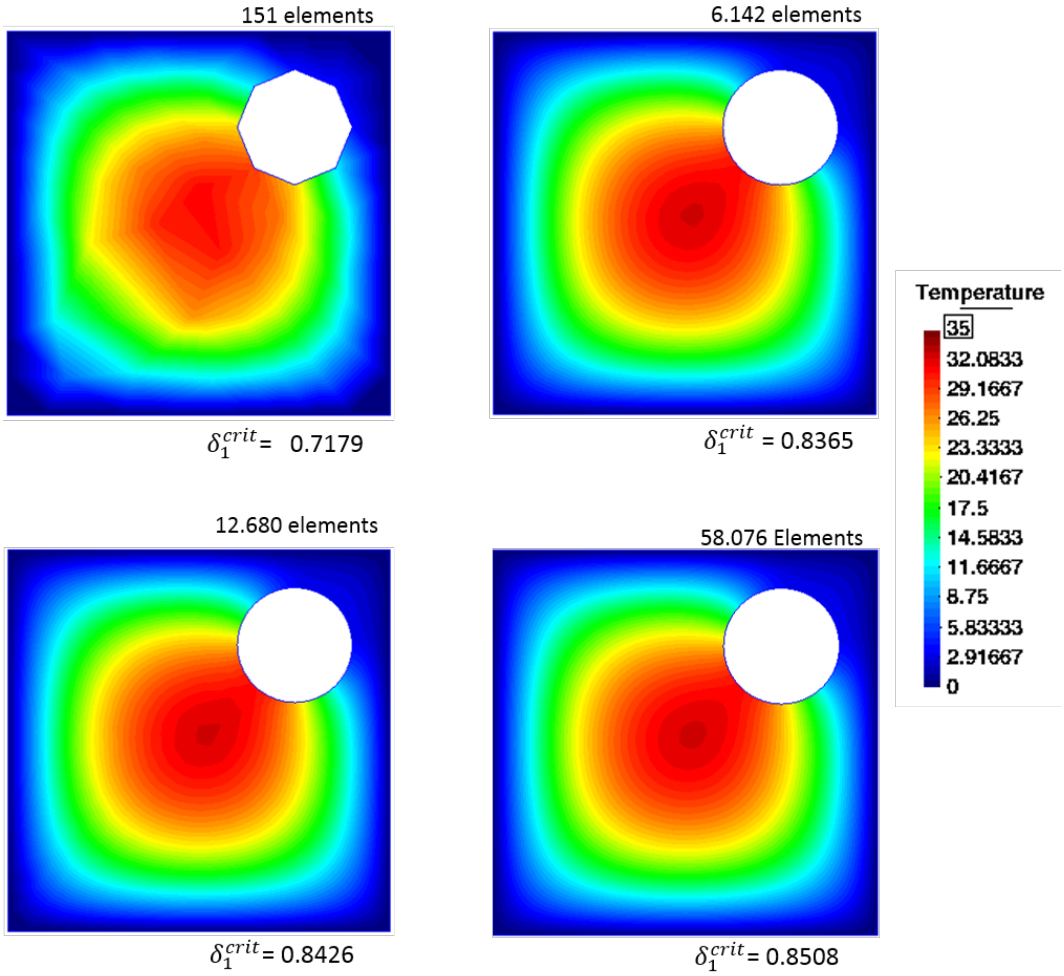

Figure 6: Temperature contours at steady state obtained with the forward Euler scheme an the new ETF11 scheme. The results are practically identical for both schemes.

The flux q_B can be expressed in terms of q_A using a Taylor expansion as

$$q_B = q_A + dx \left.\frac{dq}{dx}\right|_A + HOT(dx)^2 \tag{A.3}$$

where HOT denotes the higher order terms.

Substituting Eq.(A.2) into (A.1) and assuming that the space and time domains are infinitesimal, yields

$$\rho c \frac{\partial \phi}{\partial t} + \frac{\partial q}{\partial x} - Q = 0 \qquad \text{in } [L, t] \tag{A.4}$$

The heat flux is related to the temperature by the Fourier expression,

$$q = -k \frac{\partial \phi}{\partial x} \tag{A.5}$$

where k is the thermal conductivity.

Substituting Eq.(A.5) into (A.4) yields the standard form of the 1D heat condition equation as

$$\rho c \frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x}\left(k \frac{\partial \phi}{\partial x}\right) - Q = 0 \qquad \text{in } [L, t] \tag{A.6}$$

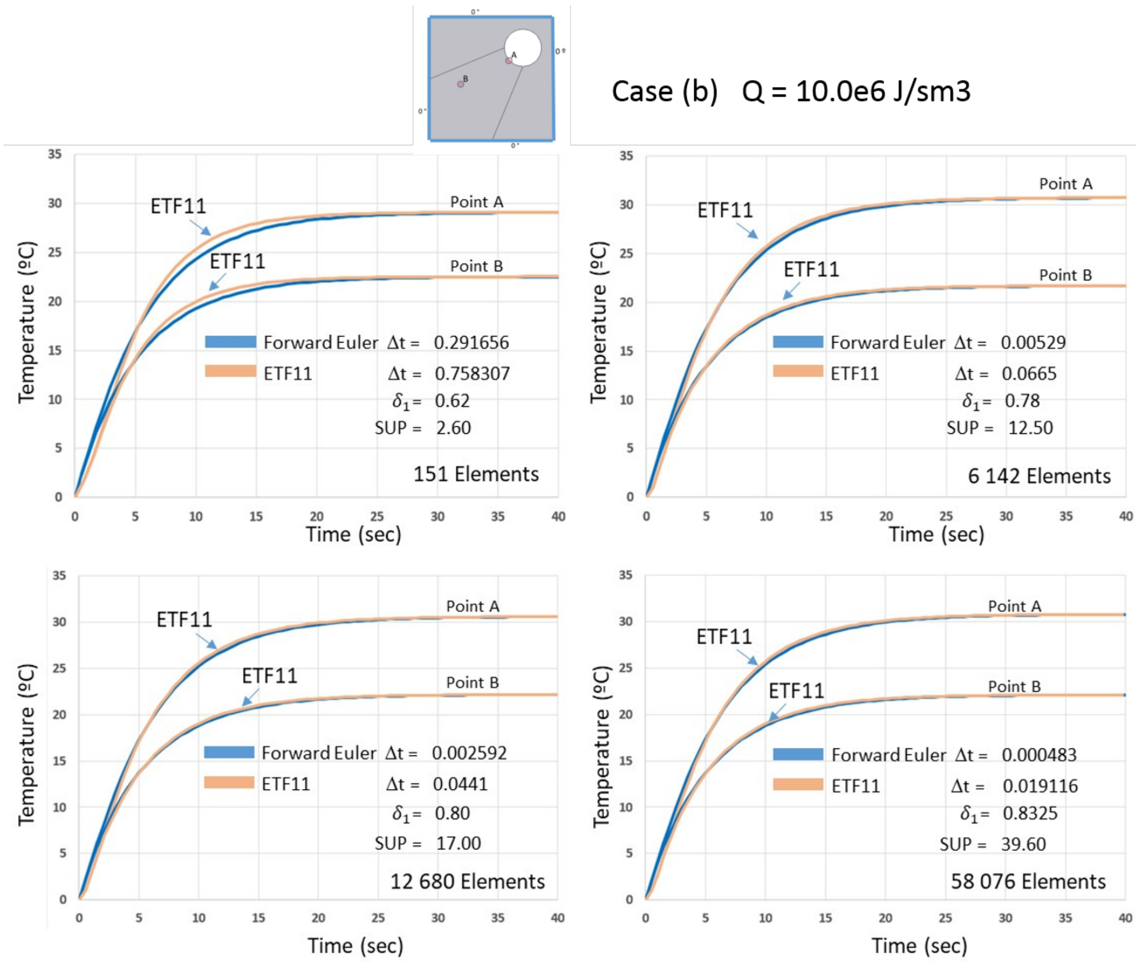

Figure 7: Case (b). Time evolution of the temperature at points A and B. The graphs show results obtained with forward Euler scheme and the ETF11 scheme for the values of δ_1 given in Table 2. The time steps used and the speed-up (SUP) versus the forward Euler scheme is shown for each mesh.

Eq.(A.5) is completed with the standard boundary condition on the temperature and the normal heat flux at the Dirichlet and Neumann boundaries, as well as with the initial temperature field at $t = t_0$.

Application of the standard Galerkin FEM [17, 49] to the solution of Eq.(A.6), leads to the matrix form

$$\mathbf{C}\dot{\mathbf{a}} + \mathbf{K}\mathbf{a} - \mathbf{f} = \mathbf{0} \tag{A.7}$$

where $\mathbf{a}$ is the vector of nodal temperatures, $\mathbf{a} = [\phi_1, \phi_2, \cdots \phi_N]^T$ and N is the number of nodes in the finite element mesh discretizing the analysis domain.

The details of the matrices and vectors in Eq.(A.7) can be found in many text books [17, 49].

A.2 FIC form of the transient heat conduction equation

The new heat balance domain $[dx, \tau]$ is shown in Figure A.2, where τ is a finite time increment.

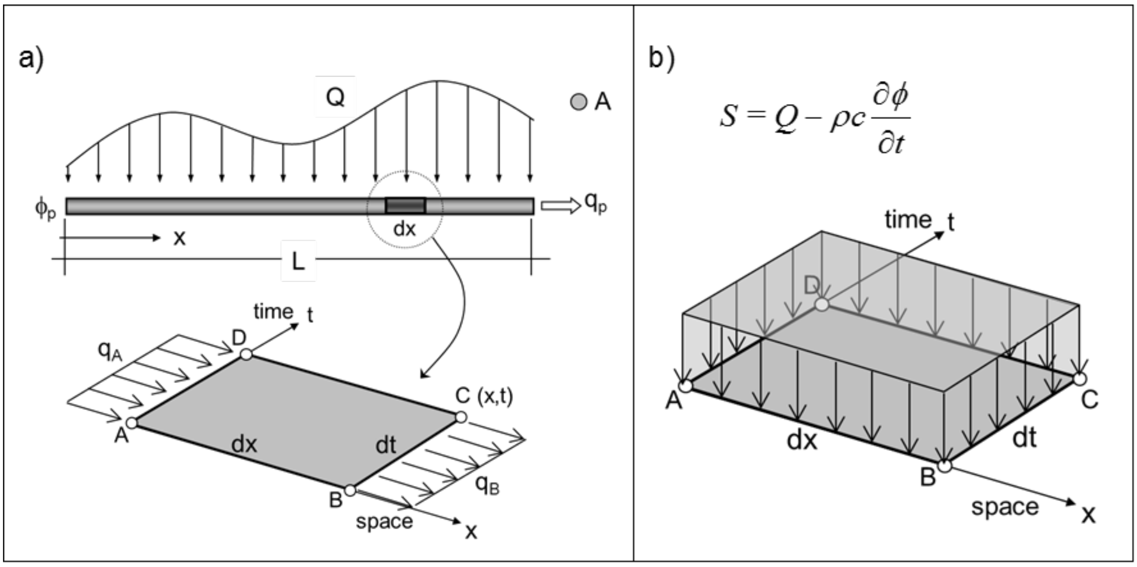

Figure A.1: (a) Space-time domain of dimensions (dx, dt) for the balance of heat fluxes in the transient 1D heat conduction problem. (b) Space-time domain for computing the contribution of the distributed heat source S

The equation expressing the balance of fluxes in the domain is written as

$$\iint_{AD} q d\Omega - \iint_{ABCD} S dx dt - \int_{BC} q dt = 0 \tag{A.8}$$

where S is given in Eq.(A.2).

The heat fluxes q and S at points A, B and D are expressed in terms of the fluxes at point C. For example,

$$\begin{aligned} q_A = \; & q_C - \left(dx \frac{\partial q}{\partial x} + \tau \frac{\partial q}{\partial t} \right)_C + \left(\frac{(dx)^2}{2} \frac{\partial^2 q}{\partial x^2} + \frac{\tau dx}{4} \frac{\partial^2 q}{\partial x \partial t} + \frac{\tau^2}{2} \frac{\partial^2 q}{\partial t^2} \right)_C - \\ & - \left(\frac{(dx)^3}{24} \frac{\partial^3 q}{\partial x^3} + \frac{\tau (dx)^2}{12} \frac{\partial^3 q}{\partial x^2 \partial t} + \frac{\tau^2 dx}{12} \frac{\partial^3 q}{\partial x \partial t^2} + \frac{\tau^3}{24} \frac{\partial^3 q}{\partial t^3} \right)_C + \\ & + HOT(dx^4, \tau^4) \end{aligned} \tag{A.9}$$

Similar expressions can be found for q_B, q_D and S_A, S_B and S_C.

Substituting these expressions into Eq.(A.8), and taking into account Eq.(A.5) leads to the following higher order differential equation

$$r - \tau_1 \frac{\partial r}{\partial t} + \tau_2^2 \frac{\partial^2 r}{\partial t^2} = 0 \tag{A.10}$$

where

$$r := \rho c \frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) - Q \tag{A.11}$$

In Eq.(A.10) τ_1 and τ_2 are time increments such that $\tau_1 = \frac{\tau}{2}$ and τ_2 accounts for the higher order terms disregarded in the truncated form of Eq.(A.9).

In the derivation of Eq.(A.10) we have neglected the terms involving products by $(dx)^2$, τ^2, τdx and higher order expressions of dx and τ [24, 25].

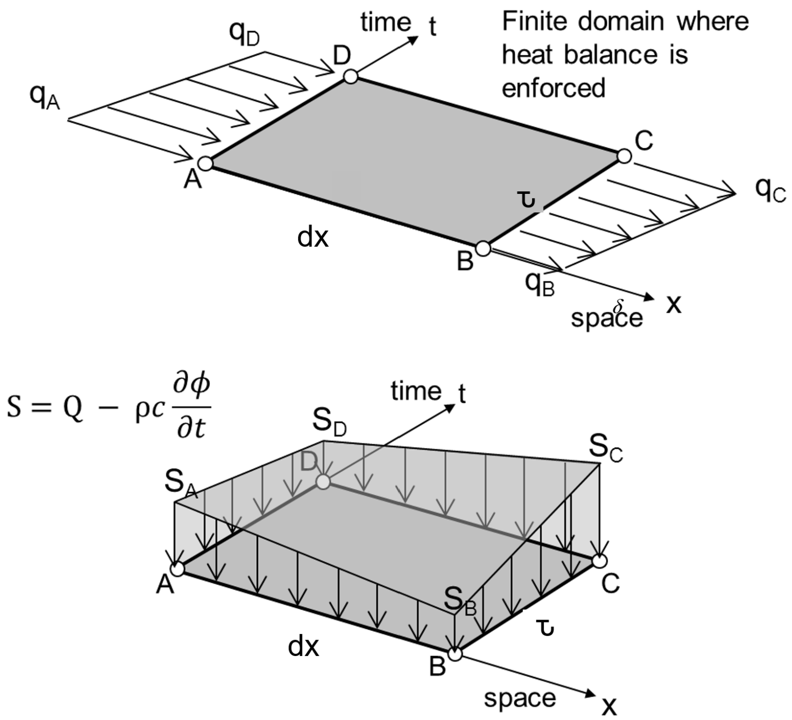

Figure A.2: Space-time domain of dimensions (dx, τ) for the balance of heat in the transient 1D heat conduction problem (upper figure). Lower figure: Space-time domain for computing the contribution of the distributed heat source S

The Galerkin FEM form of Eq.(A.10) can be readily found as

$$\mathbf{r} - \tau_1 \dot{\mathbf{r}} + \tau_2^2 \ddot{\mathbf{r}} = 0 \tag{A.12}$$

which is the sought FIC expression, coincident with Eq.(13).

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