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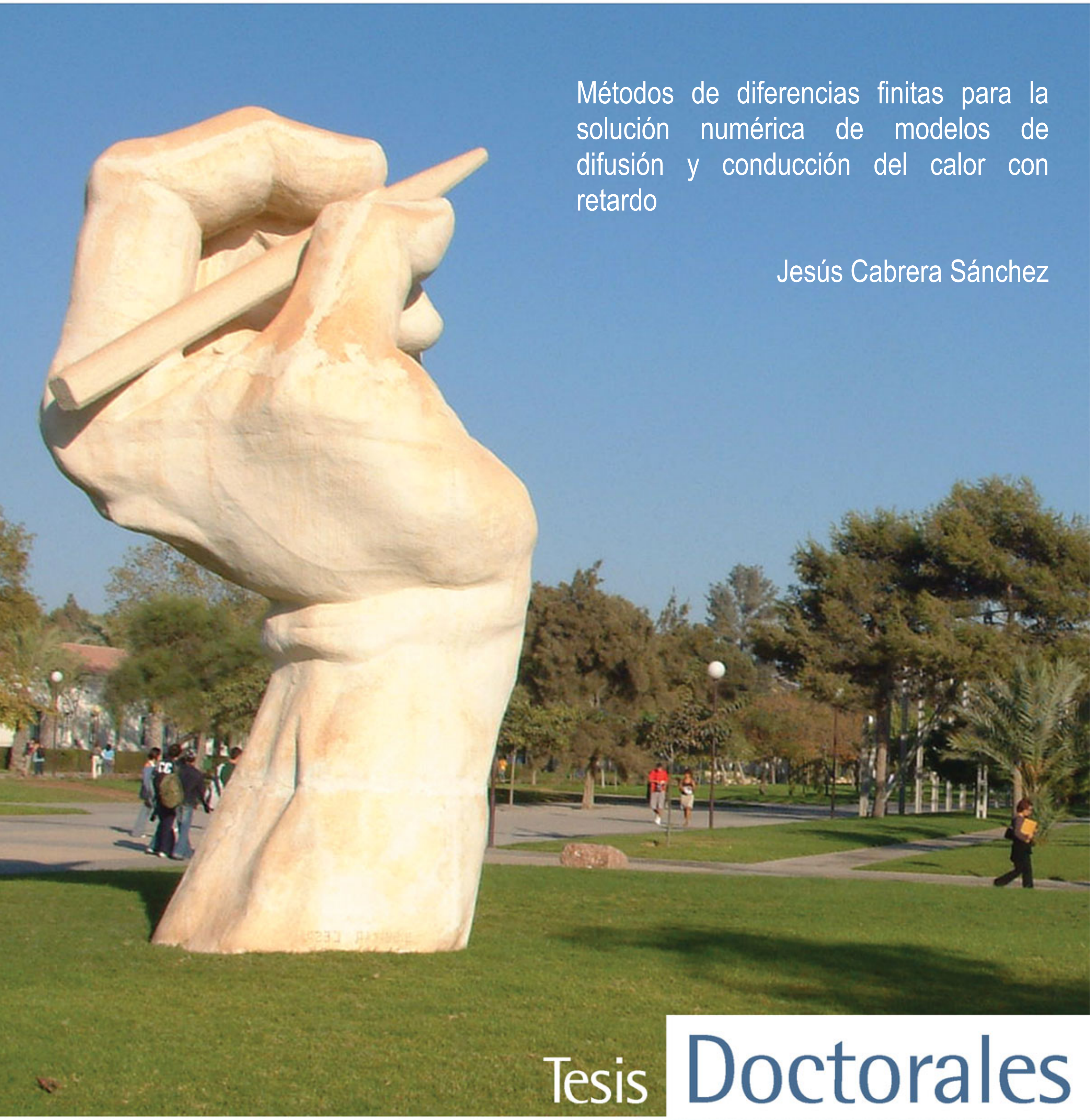
Métodos de diferencias finitas para la solución numérica de modelos de difusión y conducción del calor con retardo

Jesús Cabrera Sánchez



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Métodos de diferencias finitas para la solución numérica de modelos de difusión y conducción del calor con retardo

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A Mª Ángeles y Fernando

Agradecimientos

Parte del trabajo desarrollado en esta tesis se ha llevado a cabo en el marco del proyecto *"Obtención de soluciones exactas y construcción de aproximaciones numéricas mediante esquemas en diferencias para ecuaciones de difusión que incorporan fenómenos de retardo"* (GRE12-08), financiado por la Universidad de Alicante.

El grupo de investigación de *"Ecuaciones diferenciales con retardo"*, en cuyo seno se ha realizado el trabajo, ha recibido financiación de la Universidad de Alicante a través de las sucesivas convocatorias anuales de ayudas a grupos de investigación (VIGROB-038).

Índice general

Parte I

Síntesis

Capítulo 1

Objetivos, estructura y resumen de la tesis

Esta tesis se presenta en la modalidad de *tesis por compendio de publicaciones*. La normativa vigente en la Universidad de Alicante sobre presentación de tesis según esta modalidad, que es de obligado cumplimiento para las tesis presentadas dentro de los nuevos programas de doctorado dependientes de la Escuela de Doctorado de la Universidad de Alicante, define de forma detallada, y en ciertos aspectos de forma bastante rígida, tanto la estructuración de los contenidos de la memoria como diversas especificaciones concretas sobre cuestiones de formato. Por ello, la estructura general de esta memoria de tesis viene determinada por dicha normativa, tal como se indica a continuación.

La memoria debe incluir una sección inicial de síntesis, en la que se presenten, en una de las dos lenguas oficiales de la Comunidad Autónoma, los objetivos e hipótesis, los trabajos presentados y se justifique la unidad temática, debiendo incorporar un resumen global de los resultados obtenidos, de la discusión de estos resultados y de las conclusiones finales, proporcionando una idea precisa del contenido de la tesis.

La segunda sección debe contener los artículos o capítulos de libro publicados, bajo el título de *Trabajos publicados*. Cada uno de los trabajos publicados debe aparecer como un capítulo diferenciado, incluyendo la referencia bibliográfica completa, y puede consistir en una versión maquetada para la tesis del trabajo publicado, debiendo incluirse en este caso una reproducción de la primera página de la publicación. La última sección de la tesis debe estar formada por las conclusiones de la misma.

De acuerdo con esta normativa, en este primer capítulo se presenta el conjunto de aspectos que corresponden a la sección de *Síntesis*. En particular, en este capítulo se incluye un resumen de todos los contenidos de las publicaciones incorporadas en los siguientes capítulos de la memoria. Puesto que en los artículos incluidos en la sección de *Trabajos publicados* ya se ha llevado a cabo una importante labor de síntesis de los resultados obtenidos, el cumplimiento de la normativa en este aspecto hace inevitable una repetición de parte de los contenidos presentes en las publicaciones, aunque estos aparecen en este capítulo de forma conjunta y en una de las lenguas oficiales de la Comunidad Valenciana.

1.1. Antecedentes, objetivos y desarrollo del trabajo de investigación

Es bien conocido que los modelos basados en ecuaciones diferenciales, ordinarias o parciales, constituyen una de las herramientas básicas de la modelización matemática. Sin embargo, en una gran variedad de problemas reales de la ciencia y la técnica es preciso tener en cuenta que el comportamiento de un sistema puede depender o estar afectado por momentos anteriores o por el conjunto de la historia previa del mismo. En estos casos, resulta preciso utilizar ecuaciones diferenciales funcionales, con el fin de poder elaborar modelos adecuados para estos procesos. En particular, las ecuaciones diferenciales con retardo (EDR) y las ecuaciones en derivadas parciales con retardo (EDPR) permiten de forma relativamente simple incorporar en los modelos que las utilizan las características fundamentales de los procesos en los que existen efectos hereditarios o retardados.

Ejemplos de aplicaciones de modelos basados en EDR y EDPR en problemas y campos muy variados, incluyendo, entre otros, problemas de dinámica de poblaciones, transmisión de calor, control de procesos y propiedades de materiales viscoelásticos pueden encontrarse en los manuales sobre EDR y EDPR (véase, p. ej., [1–7] y las referencias allí incluidas).

Los problemas básicos que se consideran en esta memoria son problemas de difusión o conducción del calor en los que aparecen fenómenos de retardo. El modelo clásico para describir procesos de difusión, transmisión del calor o fenómenos de transporte o dispersión es la ecuación de difusión, o de conducción del calor,

$$u_t(t,x) = a^2 u_{xx}(t,x). \tag{1.1}$$

La incorporación de efectos de retardo en estos procesos da lugar a la ecuación generalizada de difusión con retardo

$$u_t(t,x) = a^2 u_{xx}(t,x) + b^2 u_{xx}(t-\tau,x), \tag{1.2}$$

donde $\tau > 0$ es el valor del retardo. Esta ecuación se reduce al modelo clásico para $b = 0$ o, de forma equivalente, cuando $\tau = 0$, de modo que no existe retardo.

En dos tesis anteriores [8, 9], desarrolladas dentro del grupo de *Ecuaciones diferenciales con retardo* de la Universidad de Alicante, se abordó la construcción de soluciones exactas y numéricas de problemas mixtos para la ecuación generalizada de difusión con retardo del tipo

$$u_t(t,x) = a^2 u_{xx}(t,x) + b^2 u_{xx}(t-\tau,x),\ t > \tau,\ 0 \leq x \leq l, \tag{1.3}$$

con condición inicial

$$u(t,x) = \varphi(t,x), \qquad 0 \leq t \leq \tau, \quad 0 \leq x \leq l, \tag{1.4}$$

y condiciones de contorno de tipo Dirichlet

$$u(t,0) = u(t,l) = 0, \qquad t \geq 0. \tag{1.5}$$

En el caso de la conducción del calor, es preciso tener en cuenta fenómenos de retardo cuando se analizan procesos de conducción del calor a nivel de microescala, tanto desde el punto de vista temporal o espacial. En estas situaciones se ponen de manifiesto propiedades que no se corresponden con la ley de Fourier clásica [10] y, como se explica más adelante, algunos de los modelos más usuales para incorporar estos comportamientos se traducen en modelos de EDPR o en modelos basados en aproximaciones de distinto orden.

Uno de los métodos clásicos para obtener soluciones numéricas de las ecuaciones en derivadas parciales es la utilización de esquemas en diferencias. Esta estrategía clásica también está siendo utilizada con éxito para la resolución numérica de ecuaciones en derivadas parciales con retardo [11, 12].

El objetivo general planteado en el proyecto de investigación de esta tesis es la obtención de métodos en diferencias finitas para la obtención de soluciones numéricas de modelos de difusión y de conducción del calor con retardo.

Dado el enorme interés registrado en los últimos años por los modelos no clásicos de conducción del calor, debido a la necesidad de considerar fenómenos de conducción del calor a nivel de microescala en diversas aplicaciones técnicas recientes (láseres ultrarrápidos, nanofluidos, etc...) entre los objetivos de esta investigación está la obtención de esquemas en diferencias para algunos de los modelos de conducción del calor con retardo, propuestos en la literatura, obtenidos mediante aproximaciones de mayor orden de los modelos con retardo de fase dual (dual-phase-lagging), en adelante modelos DPL, basados en la ley no-Fourier de la conductividad térmica.

Asimismo, estamos interesados en proporcionar esquemas en diferencias para un modelo de difusión con retardo con coeficientes variables dependientes del tiempo, generalización del modelo (1.3), extendiendo así los resultados obtenidos en [9], permitiendo con ello ampliar el rango de problemas y aplicaciones en los que podrían ser de utilidad resultados similares a los obtenidos en aquella tesis.

En todos los casos, se estudia la convergencia de los esquemas propuestos, determinando así la idoneidad de las soluciones proporcionadas por los mismos.

De forma algo más detallada, los objetivos de este trabajo de tesis se concretan en los siguientes puntos:

1. Desarrollo de esquemas en diferencias para la obtención de soluciones aproximadas de modelos DPL de segundo orden de aproximación.

   Se considera un modelo general que engloba a los modelos DPL obtenidos mediante aproximaciones de segundo orden en el flujo de calor y de primer o segundo orden en el gradiente de la temperatura.

   Utilizando aproximaciones en diferencias finitas de las derivadas implicadas en el modelo, inspiradas en las que dan lugar al esquema de Crank-Nicolson para la ecuación de difusión clásica, se deduce un esquema en diferencias para este modelo general.

   Considerando aproximaciones compactas de cuarto orden de las derivadas, se deduce un esquema en diferencias finitas compacto con mayor orden de precisión que el esquema anterior.

   Se demuestra la convergencia de los esquemas propuestos, expresándolos para ello como esquemas de dos niveles y estudiando su estabilidad y su consistencia.

   En todos los casos, los algoritmos desarrollados se implementan mediante sistemas de cálculo numérico.

2. Obtención de un esquema en diferencias para la obtención de soluciones aproximadas de un modelo de difusión con retardo con

coeficientes variables dependientes del tiempo.

Se adapta un esquema en diferencias propuesto en [9] para la ecuación de difusión con retardo con coeficientes constantes a la ecuación con coeficientes variables dependientes del tiempo.

Se demuestra la convergencia del esquema propuesto, expresándolo para ello como esquema de dos niveles y estudiando la estabilidad y la consistencia.

A lo largo del desarrollo del trabajo de tesis los resultados parciales obtenidos se han ido presentando en diversos congresos y recogido en diferentes publicaciones, tal como se enumera a continuación. Las publicaciones más relevantes son las incluidas en la siguiente sección de la memoria, *Trabajos publicados*, según se indica en el siguiente listado.

Comunicaciones a congresos

1. Cabrera, J.; Castro, M.A.; Rodríguez, F. y Martín, J.A.
   Difference schemes for numerical solutions of lagging models of heat conduction.
   Mathematical Modelling in Engineering & Human Behaviour 2011, Valencia, 2011.

2. Castro, M.A.; Rodríguez, F.; Cabrera, J. y Martín, J.A.
   Difference schemes for time dependent heat conduction models with delay.
   Mathematical Modelling in Engineering & Human Behaviour 2012, Valencia, 2012.

3. Castro, M.A.; Rodríguez, F.; Cabrera, J. y Martín, J.A.
   A compact difference scheme for numerical solutions of second order dual-phase-lagging models of microscale heat transfer.
   Mathematical Modelling in Engineering & Human Behaviour 2014, Valencia, 2014.

Publicaciones

1. Cabrera, J.; Castro, M.A.; Rodríguez, F. y Martín, J.A.
   Difference schemes for numerical solutions of lagging models of heat conduction.
   En: L. Jódar; L. Acedo; J. C. Cortés (eds.), Modelling for Engineering and Human Behaviour 2011, pp. 189–193. Instituto de Matemática Multidisciplinar, Valencia, 2012. ISBN: 978-84-695-2143-4

2. Cabrera, J.; Castro, M.A.; Rodríguez, F. y Martín, J.A.
   Difference schemes for numerical solutions of lagging models of heat conduction.
   Mathematical and Computer Modelling 57, 2013, pp. 1625-1632.
   Publicación incluida como Capítulo 2 de la memoria.

3. Castro, M.A.; Rodríguez, F.; Cabrera, J. y Martín, J.A.
   A compact difference scheme for numerical solutions of second order dual-phase-lagging models of microscale heat transfer.
   Journal of Computational and Applied Mathematics, 291, 2016, pp. 432-440.
   Publicación incluida como Capítulo 3 de la memoria.

4. Castro, M.A.; Rodríguez, F.; Cabrera, J. y Martín, J.A.

An explicit difference scheme for time dependent heat conduction models with delay.
En: L. Jódar; L. Acedo; J. C. Cortés; F. Pedroche (eds.), Modelling for Engineering and Human Behaviour 2012, pp. 132–136. Instituto de Matemática Multidisciplinar, Valencia, 2013. ISBN: 978-84-695-6701-2

5. Castro, M.A.; Rodríguez, F.; Cabrera, J. y Martín, J.A.
Difference schemes for time dependent heat conduction models with delay.
International Journal of Computer Mathematics 91(1), 2014, pp. 53-61.
Publicación incluida como Capítulo 4 de la memoria.

A continuación se presenta un resumen de los principales resultados correspondientes a las publicaciones incluidas en los siguientes capítulos de la memoria. Previamente se exponen, de forma muy resumida, los principales conceptos sobre esquemas en diferencias para problemas de valores iniciales.

1.2. Esquemas en diferencias

Se resume a continuación la teoría básica acerca de la aproximación de la solución de un problema de valores iniciales lineales mediante esquemas en diferencias lineales de dos o más niveles [13, Capítulos 3 y 7].

En problemas de valores iniciales

$$\frac{d}{dt}v\left(t\right)=Av\left(t\right),\ 0\leq t\leq T, \tag{1.6}$$

$$v(0) = v_0, \tag{1.7}$$

donde A es un operador lineal y v_0 es un elemento de un espacio de Banach $\mathcal{B}$, la solución $v(t)$ en cada instante de tiempo t es un elemento de $\mathcal{B}$ que verifica la ecuación y las condiciones impuestas en el problema (1.6)-(1.7).

Los esquemas en diferencias aproximan la solución por una secuencia de puntos de $\mathcal{B}$, U_0, $U_1, \ldots,$ tal que U_n se supone una aproximación de $v(nk)$, donde k es un incremento pequeño. Las ecuaciones en diferencias del esquema son

$$U_{n+1} = C(k)\, U_n, \;\; n \geq 0 \tag{1.8}$$

o de forma más general

$$U_{n+1} = C_{q-1}(k)\, U_n + C_{q-2}(k)\, U_{n-1} + \cdots + C_0(k)\, U_{n-q+1}, \;\; n \geq q-1 \tag{1.9}$$

donde $C_i(k)$, $i = 0, 1, \ldots, q$, son operadores en diferencias lineales acotados que pueden depender de los incrementos de la variable temporal y los incrementos de las variables espaciales, así como de las variables espaciales, y q es un natural fijo. Su solución está determinada de forma única por q puntos iniciales $U_0, U_1, \ldots, U_{q-1}$. La ecuación (1.9) recibe el nombre de esquema multinivel de $q+1$ niveles, siendo por tanto (1.8) un esquema de dos niveles.

La teoría general de la aproximación de problemas de valores iniciales por ecuaciones en diferencias aportada por Peter Lax, estudia la idoneidad de la solución de los esquemas en diferencias para aproximar la solución de un problema de valores iniciales. Dicha teoría se construye sobre la base de que el problema (1.6)-(1.7) es un problema "*properly posed*" en el siguiente sentido:

Sea $\mathcal{D}$ el conjunto de elementos v_0 de $\mathcal{B}$ para los que existe una única solución $v\,(t)$ de (1.6) tal que $v\,(0) = v_0$.

Se dice que el problema de valores iniciales (1.6)-(1.7) determinado por el operador lineal A es "*properly posed*" si se verifica que el conjunto $\mathcal{D}$ es denso en $\mathcal{B}$ y existe una constante K tal que para cualquier v_0 de $\mathcal{D}$, la solución $v\,(t)$ para $v\,(0) = v_0$ verifica $\|v\,(t)\| \leq K\,\|v_0\|\,,\ 0 \leq t \leq T$.

La propiedad fundamental que un esquema en diferencias debe tener para ser útil es la de ser un *esquema convergente*. Operando sobre v_0 n veces con $C\,(k)$ da $U_n = C\,(k)^n\,v_0$, que es esperable que aproxime a $v\,(nk)$. Se dice que el esquema (1.8) proporciona una aproximación convergente para el problema de valores iniciales (1.6)-(1.7) si se verifica que para cualquier secuencia $k_1, k_2, \ldots$ de incrementos de tiempo que tiende a cero, si t es fijo, $0 \leq t \leq T$, y n_j, para cada $j = 1, 2, \ldots$, es un entero tal que $n_j k_j \to t$ cuando $j \to +\infty$, se verifica que

$$\|C\,(k_j)^{n_j}\,v_0 - v\,(t)\| \to 0, \text{ cuando } j \to +\infty$$

para cada $u_0 \in \mathcal{B}$.

El estudio de la convergencia de un esquema en diferencias se realiza a través del estudio de la consistencia y la estabilidad del esquema (Teorema de equivalencia de Lax).

La familia de operadores $C\,(k)$ que define el esquema (1.8) proporciona una aproximación *consistente* para el problema de valores iniciales (1.6)-(1.7) si, para cada $v\,(t)$ en una clase $\mathcal{U}$ de soluciones cuyos elementos iniciales u_0 son densos en $\mathcal{B}$ se verifica

$$\left\| \frac{v\left(t+k\right)-C\left(k\right)v\left(t\right)}{k} \right\| \to 0, \text{ cuando } k\to 0,\ 0\leq t\leq T.$$

Se llama *error de truncación* en un instante t, $0 \leq t \leq T$, a la cantidad

$$\frac{v\left(t+k\right)-C\left(k\right)v\left(t\right)}{k}.$$

La aproximación dada por (1.8) se dice que es *estable*, si para algún $k_0 > 0$, la familia infinita de operadores

$$C\left(k\right)^n, \begin{array}{l} 0<k<k_0, \\ 0\leq nk\leq T, \end{array}$$

está uniformemente acotada.

El Teorema de equivalecia de Lax establece que para un problema de valores iniciales *properly posed* y una aproximación en diferencias para éste que satisface la condición de consistencia, la estabilidad es una condición necesaria y suficiente para la convergencia.

En esquemas multinivel, dado que la condición inicial del problema de valores iniciales está dada en $t = 0$, se toma $U_0 = v_0$ y el resto de los valores de arranque para la ecuación en diferencias (1.9), esto es las aproximaciones $U_1, U_2, \ldots, U_{q-1}$, en $t = k$, $t = 2k$, $\ldots$, $t = (q-1)\,k$, se obtienen de la condición inicial del problema de valores iniciales mediante alguna aproximación, para conseguir iniciar los cálculos en (1.9). Se supone $U_j \to v_0$ cuando $k \to 0$, para $j = 1, 2, \ldots, q-1$.

Un vector columna cuyas $q-$componentes son elementos de $\mathcal{B}$ puede ser considerado como un elemento de un espacio de Banach auxiliar $\mathcal{B}^*$.

Así si definimos U_n^* como el vector

$$U_n^* = \begin{bmatrix} U_n \\ U_{n-1} \\ \vdots \\ U_{n-q+2} \\ U_{n-q+1} \end{bmatrix},$$

y $C^*(k)$ como la siguiente matriz de operadores

$$C^*(k) = \begin{bmatrix} C_{q-1}(k) & C_{q-2}(k) & \cdots & C_1(k) & C_0(k) \\ I & 0 & \cdots & 0 & 0 \\ 0 & I & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & I & 0 \end{bmatrix},$$

donde I es el operador identidad, entonces la ecuación (1.9) se transforma en el esquema de dos niveles

$$U_{n+1}^* = C^*(k)\, U_n^*, \tag{1.10}$$

siendo las definiciones de convergencia, consistencia y estabilidad para el esquema (1.10) las conocidas para un esquema de dos niveles. De esta manera el esquema (1.9) es convergente, consistente y estable si lo es el esquema equivalente de dos niveles (1.10), siendo equivalente la convergencia del esquema a su estabilidad, siempre que el problema de valores iniciales sea *properly posed* y el esquema consistente (Teorema de Lax).

1.3. Esquemas en diferencias para modelos DPL

Los modelos DPL [10, 14, 15] constituyen una familia de modelos no-Fourier de conducción del calor.

Los avances técnicos en nanomateriales y en las aplicaciones de láseres ultrarápidos han llevado en las dos últimas décadas a incrementar el interés en los modelos no-Fourier de condicción del calor [16–20]. Cuando se estudia la transferencia de calor a nivel microscópico, esto es, en intervalos de tiempo muy cortos o en dimensiones espaciales muy pequeñas, puede ser necesario considerar la presencia de retardos de tiempo en el flujo de calor y el gradiente de la temperatura para tener en cuenta fenómenos tales como la velocidad finita de propagación, los comportamientos ondulatorios y las respuestas retardadas a perturbaciones térmicas [10, 21], que no están presentes en el modelo de difusión clásico. De esta forma, estos modelos han encontrado aplicación en los últimos años en un amplio rango de problemas de transferencia del calor de ingeniería y en problemas de transferencia de calor biomédicos, como en el tratamiento con láser ultrarápido de estructuras ultrafinas [16, 22], la transferencia de calor en nanofluidos [17, 18], o la transferencia de calor en tejidos biológicos durante terapias térmicas o en tejidos sometidos a irradiación láser [19, 20, 23]. En consecuencia, se han propuesto soluciones analíticas y métodos para la computación numérica de aproximaciones para algunos modelos no-Fourier particulares en diferentes escenarios.

Los modelos con retardo de conducción de calor, como los modelos DPL, que incorporan retardos de tiempo en el flujo de calor y en el gradiente de la temperatura, y algunos de sus casos particulares y aproximaciones, dan lugar a ecuaciones de conducción de calor en forma de ecuaciones en derivadas parciales hiperbólicas o retardadas.

En el modelo DPL, la ley clásica de Fourier,

$$\mathbf{q}(\mathbf{r}, t) = -k\nabla T(\mathbf{r}, t), \tag{1.11}$$

que relaciona el vector de flujo de calor $\mathbf{q}(\mathbf{r}, t)$ y el gradiente de la temperatura $\nabla T(\mathbf{r}, t)$, en un tiempo t para un punto $\mathbf{r}$ en el dominio espacial, se reemplaza por

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k\nabla T(\mathbf{r}, t + \tau_T), \tag{1.12}$$

donde τ_q y τ_T son los correspondientes retardos de fase. El modelo con retardo de fase simple (single-phase-lag model, en adelante SPL) [24] es el caso particular con $\tau_T = 0$.

En orden a determinar $\mathbf{q}$ y T, la ecuación (1.11) se combina con la ecuación de la energía establecida en un tiempo general t durante el proceso transitorio

$$\nabla \bullet \mathbf{q}(\mathbf{r}, t) + Q(\mathbf{r}, t) = C_p \frac{\partial T}{\partial t}(\mathbf{r}, t) \tag{1.13}$$

siendo C_p la capacidad calorífica y Q la fuente de calor. Combinando la ley de Fourier y el principio de conservación de la energía, se obtiene la ecuación clásica de difusión, que en ausencia de fuente de calor está dada por

$$\frac{\partial T}{\partial t}(\mathbf{r}, t) = \alpha \nabla^2 T(\mathbf{r}, t), \tag{1.14}$$

donde $\alpha = \dfrac{k}{C_p}$ es la difusividad térmica.

De forma similar, usando (1.12) en lugar de la ley de Fourier, se obtiene una ecuación en derivadas parciales con retardo [25, 26]. Si suponemos también ausencia de fuente de calor, esta ecuación viene dada por

$$\frac{\partial T}{\partial t}(\mathbf{r}, t + \tau_q) = \alpha \nabla^2 T(\mathbf{r}, t + \tau_T). \tag{1.15}$$

Sin embargo, es frecuente usar aproximaciones de primer orden en (1.12),

$$\mathbf{q}(\mathbf{r}, t) + \tau_q \frac{\partial \mathbf{q}}{\partial t}(\mathbf{r}, t) \cong -k \left(\nabla T(\mathbf{r}, t) + \tau_T \frac{\partial}{\partial t} \nabla T(\mathbf{r}, t) \right), \tag{1.16}$$

llamándose usualmente modelo DPL a la ecuación derivada [14],

$$\frac{\partial}{\partial t} T(\mathbf{r}, t) + \tau_q \frac{\partial^2}{\partial t^2} T(\mathbf{r}, t) = \alpha \left(\Delta T(\mathbf{r}, t) + \tau_T \Delta \frac{\partial}{\partial t} T(\mathbf{r}, t) \right). \tag{1.17}$$

El clásico modelo de Cattaneo-Vernotte [27–29] es el caso particular de (1.17) con $\tau_T = 0$.

También se puede considerar aproximaciones de mayor orden en (1.12) [30, 31]. En este trabajo, denotaremos al modelo (1.17) por DPL(1,1), mientras que los modelos que resultan correspondientes a aproximaciones de segundo orden en τ_q y aproximaciones de primer o segundo orden en τ_T se denotarán, respectivamente, por DPL(2,1),

$$\frac{\partial}{\partial t} T(\mathbf{r}, t) + \tau_q \frac{\partial^2}{\partial t^2} T(\mathbf{r}, t) + \frac{\tau_q^2}{2} \frac{\partial^3}{\partial t^3} T(\mathbf{r}, t) = \alpha \left(\Delta T(\mathbf{r}, t) + \tau_T \Delta \frac{\partial}{\partial t} T(\mathbf{r}, t) \right),$$

y DPL(2,2),

$$\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)+\frac{\tau_q^2}{2}\frac{\partial^3}{\partial t^3}T(\mathbf{r},t)=\alpha\left(\Delta T(\mathbf{r},t)+\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t)\right.$$
$$\left.+\frac{\tau_T^2}{2}\Delta\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)\right).$$

En particular, consideramos una barra finita con extremos aislados en $x=0$ y $x=l$, de modo que

$$T(0,t)=T(l,t)=0, \quad t\geq 0, \tag{1.18}$$

y distribución de temperatura inicial

$$\begin{aligned} &T(x,0)=\phi(x),\\ &\frac{\partial}{\partial t}T(x,0)=\varphi(x), \quad x\in[0,l],\\ &\frac{\partial^2}{\partial t^2}T(x,0)=\psi(x), \end{aligned} \tag{1.19}$$

con conducción de calor, para $t>0$ y $x\in[0,l]$, dado por el modelo DPL(2,2)

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{1}{\alpha}T(x,t)+\frac{\tau_q}{\alpha}\frac{\partial}{\partial t}T(x,t)+\frac{\tau_q^2}{2\alpha}\frac{\partial^2}{\partial t^2}T(x,t)\right)=\frac{\partial^2}{\partial x^2}\Big(T(x,t)\\ +\tau_T\frac{\partial}{\partial t}T(x,t)+\frac{1}{2}\tau_T^2\frac{\partial^2}{\partial t^2}T(x,t)\Big). \end{aligned} \tag{1.20}$$

En realidad, consideraremos una ecuación más general,

$$\begin{aligned}\frac{\partial}{\partial t}\left(AT\left(x,t\right)+B\frac{\partial}{\partial t}T\left(x,t\right)+C\frac{\partial^2}{\partial t^2}T\left(x,t\right)\right)=\frac{\partial^2}{\partial x^2}\Big(T\left(x,t\right)\\ +D\frac{\partial}{\partial t}T\left(x,t\right)+E\frac{\partial^2}{\partial t^2}T\left(x,t\right)\Big),\end{aligned} \tag{1.21}$$

donde el modelo DPL(2,2) se obtiene con

$$A=\frac{1}{\alpha},\quad B=\frac{\tau_q}{\alpha},\quad C=\frac{\tau_q^2}{2\alpha},\quad D=\tau_T,\quad E=\frac{\tau_T^2}{2},$$

mientras el modelo DPL(2,1) es el caso particular con $E=0$.

La construcción de soluciones numéricas para el modelo DPL(1,1) y variaciones en distintos escenarios se ha abordado en trabajos previos (por ejemplo, [32–39]). En este trabajo, se desarrollan dos esquemas numéricos para el modelo (1.21), y en particular para los modelos DPL(2,1) y DPL(2,2) en una dimensión para la variable espacial, con condiciones inicial y de contorno descritas anteriormente, caracterizando sus propiedades de convergencia y estabilidad. El primero es un esquema tipo Crank-Nicholson en cuanto que está basado en aproximaciones en diferencias finitas de las derivadas implicadas en el modelo inspiradas en las que dan lugar al esquema de Crank-Nicolson para la ecuación de difusión clásica. En el segundo se consideran aproximaciones compactas de cuarto orden de las derivadas, lo que da lugar a un esquema compacto con mayor orden de precisión que el esquema anterior.

Se considera la malla uniforme $\{(x_j,t_n), j=0\dots P, n=0\dots N\}$, del dominio acotado $[0,l]\times[0,T_M]$, para algún $T_M>0$ fijo, definida por los incrementos $h=\Delta x$ y $k=\Delta t$, tales que $l=Ph$ y $T_M=Nk$.

Denotaremos el valor de una función cualquiera w en un punto (x_j, t_n) de la malla por w_j^n.

1.3.1. Esquema tipo Crank-Nicolson

En el Capítulo 2 se propone un esquema en diferencias tipo Crank-Nicolson para el modelo (1.21). Después de introducir nuevas variables para escribir (1.21) como un sistema de primer orden en t, se desarrolla el esquema en diferencias, se analiza la convergencia, demostrando primero la estabilidad del método, expresado como esquema de dos niveles, y probando después su consistencia, dando cotas de los errores de truncación. Finalmente, se presentan ejemplos numéricos.

Para escribir (1.21) como un sistema de primer orden en t se introducen dos nuevas variables. Estas variables son

$$v\left(x,t\right) = BT\left(x,t\right) + C\frac{\partial}{\partial t}T\left(x,t\right) \tag{1.22}$$

y

$$u\left(x,t\right) = AT\left(x,t\right) + \frac{\partial}{\partial t}v\left(x,t\right). \tag{1.23}$$

Así, la Eq. 1.21 se puede escribir

$$\frac{\partial}{\partial t}u\left(x,t\right) = \frac{\partial^2}{\partial x^2}\left(aT\left(x,t\right) + bv\left(x,t\right) + cu\left(x,t\right)\right), \tag{1.24}$$

donde

$$a = (C^2 + EB^2 - BDC - ACE)/C^2, \quad b = (DC - BE)/C^2, \quad c = E/C.$$

Por lo tanto, de (1.22) y (1.23) se obtiene

$$\frac{\partial}{\partial t}T\left(x,t\right)=\frac{1}{C}\left(v\left(x,t\right)-BT\left(x,t\right)\right) \tag{1.25}$$

y

$$\frac{\partial}{\partial t}v\left(x,t\right)=u\left(x,t\right)-AT\left(x,t\right). \tag{1.26}$$

El problema mixto dado por Eq. 1.21 con condiciones de contorno (1.18) y condiciones iniciales (1.19) es equivalente a el sistema formado por las ecuaciones (1.24)-(1.26), con condiciones de contorno

$$\begin{aligned} &u(0,t)=u(l,t)=0, \\ &T(0,t)=T(l,t)=0, \quad t\geq 0, \\ &v(0,t)=v(l,t)=0, \end{aligned} \tag{1.27}$$

y condiciones iniciales

$$\left.\begin{aligned} &u\left(x,0\right)=A\phi\left(x\right)+B\varphi\left(x\right)+C\psi\left(x\right), \\ &T\left(x,0\right)=\phi\left(x\right), \\ &v\left(x,0\right)=B\phi\left(x\right)+C\varphi\left(x\right), \end{aligned}\right. \qquad x\in\left[0,l\right]. \tag{1.28}$$

El esquema en diferencias finitas propuesto para el modelo DPL(2,2) se derivará de las siguientes aproximaciones por diferencias finitas en las ecuaciones (1.24)-(1.26),

$$\begin{aligned}
\frac{u_j^{n+1}-u_j^n}{k} &= \frac{1}{2}\delta_x^2\left(aT_j^n+bv_j^n+cu_j^n\right), &(1.29)\\
&+ \frac{1}{2}\delta_x^2\left(aT_j^{n+1}+bv_j^{n+1}+cu_j^{n+1}\right)\\
\frac{T_j^{n+1}-T_j^n}{k} &= -\frac{B}{C}\left(\frac{T_j^{n+1}+T_j^n}{2}\right)+\frac{1}{C}\left(\frac{v_j^{n+1}+v_j^n}{2}\right), &(1.30)\\
\frac{v_j^{n+1}-v_j^n}{k} &= \frac{1}{2}\left(u_j^{n+1}+u_j^n\right)-\frac{A}{2}\left(T_j^{n+1}+T_j^n\right), &(1.31)
\end{aligned}$$

donde

$$\delta_x^2 w_j^n = \frac{w_{j-1}^n-2w_j^n+w_{j+1}^n}{h^2}.$$

La discretizaciones de las condiciones de contorno e iniciales, correspondientes a (1.27) y (1.28), están dadas por

$$u_0^n=u_P^n,\quad T_0^n=T_P^n=0,\quad v_0^n=v_P^n=0,\quad n=0\ldots N, \tag{1.32}$$

y

$$\begin{aligned}
u_j^0 &= A\phi(jh)+B\varphi(jh)+C\psi(jh),\\
T_j^0 &= \phi(jh), \qquad\qquad j=0,\ldots,P. &(1.33)\\
v_j^0 &= B\phi(jh)+C\varphi(jh),
\end{aligned}$$

Introduciendo, para $n=0,\ldots,N$, los vectores U^n, T^n, y V^n, donde U^n apila los $P-1$ valores $u_j^n, j=1,\ldots,P-1$, y de forma similar para T^n y V^n, y denotando por M a la matriz tridiagonal $(P-1)\times(P-1)$

$M = tridiag\,(1, -2, 1)$ y por $r = h/k^2$,

$$\begin{aligned} x_k &= 4C + 2Bk + Ak^2, \\ y_k &= 4C - 2Bk - Ak^2, \\ z_k &= 4C + 2Bk - Ak^2, \end{aligned}$$

$$\begin{aligned} \alpha_k &= \frac{r}{2}\left(c + \frac{x_k + z_k}{x_k}\frac{bk}{4} + \frac{ak^2}{x_k}\right), \\ \beta_k &= \frac{r}{2}\left(a + \frac{ay_k}{x_k} - \frac{x_k + y_k}{x_k}\frac{bAk}{2}\right), \\ \gamma_k &= \frac{r}{2}\left(b + \frac{4ak}{x_k} + \frac{bz_k}{x_k}\right), \end{aligned}$$

las ecuaciones del esquema se pueden dar en forma matricial como sigue,

$$(I - \alpha_k M)\,U^{n+1} = (I + \alpha_k M)\,U^n + \beta_k M T^n + \gamma_k M V^n, \tag{1.34}$$

$$T^{n+1} = \frac{k^2}{x_k}U^n + \frac{y_k}{x_k}T^n + \frac{4k}{x_k}V^n + \frac{k^2}{x_k}U^{n+1}, \tag{1.35}$$

y

$$V^{n+1} = \frac{x_k + z_k}{4x_k}kU^n - \frac{x_k + y_k}{2x_k}AkT^n + \frac{z_k}{x_k}V^n + \frac{x_k + z_k}{4x_k}kU^{n+1}, \tag{1.36}$$

donde I denota la matriz identidad de orden $(P-1)\times(P-1)$.

De aquí, partiendo de los valores iniciales dados por (1.33), y teniendo en cuenta las condiciones de contorno (1.32), el método puede avanzar del paso n al paso $n+1$, calculando U^{n+1} de (1.34), lo cual se puede hacer de forma eficiente, ya que los coeficientes de U^{n+1} forman también una matriz tirdiagonal, y substituyendo en las ecuaciones (1.35) y (1.36), obtener T^{n+1} y V^{n+1}.

Para probar la convergencia del esquema, se demuestra que el método es incondicionalmente estable, para cualquier valor finito de $r = h/k^2$, y que es consistente con la ecuación en derivadas parciales original. Así, del teorema de equivalencia de Lax [13], se deduce la convergencia.

En primer lugar, el método se escribe como esquema de dos niveles. Resolviendo para U^{n+1} en (1.34), y escribiendo

$$X_k = (I - \alpha_k M), \quad Y_k = (I + \alpha_k M),$$

se obtiene

$$U^{n+1} = X_k^{-1} Y_k U^n + \beta_k X_k^{-1} M T^n + \gamma_k X_k^{-1} M V^n, \tag{1.37}$$

y, substituyendo en (1.35) y (1.36),

$$\begin{aligned} T^{n+1} &= \frac{k^2}{x_k} \left(I + X_k^{-1} Y_k\right) U^n + \left(\frac{y_k}{x_k} I + \frac{k^2}{x_k} \beta_k X_k^{-1} M\right) T^n, & (1.38)\\ &+ \left(\frac{4k}{x_k} I + \frac{k^2}{x_k} \gamma_k X_k^{-1} M\right) V^n \\ V^{n+1} &= \frac{x_k + z_k}{4x_k} k \left(I + X_k^{-1} Y_k\right) U^n + \left(-\frac{x_k + y_k}{2x_k} A k\right. & (1.39)\\ &+ \left.\frac{x_k + z_k}{4x_k} k \beta_k X_k^{-1} M\right) T^n + \left(\frac{z_k}{x_k} I + \frac{x_k + z_k}{4x_k} k \gamma_k X_k^{-1} M\right) V^n. \end{aligned}$$

Considerando el vector apilado $[U^n, T^n, V^n]^T$, donde el superíndice T denota la transpuesta, el método se puede escribir como esquema de dos niveles

$$\left[U^{n+1}, T^{n+1}, V^{n+1}\right]^T = Q_k \left[U^n, T^n, V^n\right]^T, \tag{1.40}$$

donde la matriz del esquema, Q_k, es la matriz por bloques, 3×3, determinada por los coeficientes de U^n, T^n y V^n en (1.37)–(1.39) y cuya expresión está dada en la página 72.

Se prueba la estabilidad del método. Para ello se introduce la matriz límite

$$Q = \lim_{k \to 0} Q_k = \begin{bmatrix} X^{-1}Y & raX^{-1}M & rbX^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix},$$

con

$$X^{-1} = \left(I - \frac{1}{2}rcM\right)^{-1}, \quad Y = \left(I + \frac{1}{2}rcM\right),$$

y se calculan explícitamente las potencias de Q,

$$Q^n = \begin{bmatrix} \left(X^{-1}Y\right)^n & -\frac{a}{c}\left(I - \left(X^{-1}Y\right)^n\right) & -\frac{b}{c}\left(I - \left(X^{-1}Y\right)^n\right) \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}, \tag{1.41}$$

deduciéndose su acotación uniforme de la de la matriz del esquema de Crank-Nicolson para el ecuación clásica de difusión, $X^{-1}Y$. Usando la forma del lema de Gronwall que se da en [40, pp. 186], se obtiene una acotación uniforme de $\|Q_k^n - Q^n\|$ y de aquí que el esquema es estable, incondicionalmente, en el sentido de Lax [13].

Para el estudio de la consistencia se considera la solución exacta del problema dado por (1.24)-(1.26), definida en $[0, l] \times [0, T_M]$ y denotada por $w = \left(\widetilde{u}, \widetilde{T}, \widetilde{v}\right)$. Para un $t = nk$ dado fijo, los puntos de la malla

$$(ih, nk), \ i = 0, 1, \ldots, P,$$

tienen asociados el vector

$$W_h^k(nk) = \left[\widetilde{U}^n, \widetilde{T}^n, \widetilde{V}^n\right]^T \in \mathbb{R}^{3(P-1)}, \tag{1.42}$$

donde

$$\begin{aligned}
\widetilde{U}^n &= \left[\widetilde{u}(h,nk), \widetilde{u}(2h,nk), \ldots, \widetilde{u}((P-1)h,nk)\right]^T, \\
\widetilde{T}^n &= \left[\widetilde{T}(h,nk), \widetilde{T}(2h,nk), \ldots, \widetilde{T}((P-1)h,nk)\right]^T, \\
\widetilde{V}^n &= \left[\widetilde{v}(h,nk), \widetilde{v}(2h,nk), \ldots, \widetilde{v}((P-1)h,nk)\right]^T.
\end{aligned}$$

El error de truncación del esquema de dos niveles (1.40), en $t = nk$, es el vector de $\mathbb{R}^{3(P-1)}$

$$\mathfrak{T}_h^k(nk) = \frac{1}{k}\left(W_h^k((n+1)k) - Q_k W_h^k(nk)\right). \tag{1.43}$$

El esquema en diferencias (1.40) verifica la condición de consistencia si la solución w del problema (1.24)-(1.26) satisface

$$\lim_{k\to 0} \frac{1}{k}\left\|W_h^k((n+1)k) - Q_k W_h^k(nk)\right\|_\infty = 0, \text{ for } 0 \leq nk \leq T_M, \tag{1.44}$$

para cada conjunto de funciones iniciales que garanticen suficientes condiciones de regularidad de w.

El error de truncación local en el punto de la malla (jh, nk), [13, p. 20], está dado por

$$\left(\mathcal{T}_{1,j}^n, \mathcal{T}_{2,j}^n, \mathcal{T}_{3,j}^n\right) = \mathcal{L}w_j^n,$$

donde $\mathcal{L} = (\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3)$ es el operador en diferencias asociado al esquema [41, p. 42].

Se puede comprobar que

$$\mathfrak{T}_h^k(nk) = E_k\left[\mathcal{T}_1^n, \mathcal{T}_2^n, \mathcal{T}_3^n\right]^T, \tag{1.45}$$

donde $\mathcal{T}_i^n = \left[\mathcal{T}_{i,1}^n, \mathcal{T}_{i,2}^n, \ldots, \mathcal{T}_{i,P-1}^n\right]^T$, $i = 1, 2, 3$, y E_k es la matriz 3×3 cuyos elementos están definidos en la página 75, y

$$E = \lim_{k\to 0} E_k = \begin{bmatrix} X^{-1} & \frac{ra}{2}X^{-1}M & \frac{br}{2}X^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}. \tag{1.46}$$

Utilizando desarrollos de Taylor de segundo y tercer orden en puntos apropiados para una función genérica g, se obtiene

$$\frac{g_j^{n+1} - g_j^n}{k} = \frac{\partial g}{\partial t}\left(jh, \left(n + \frac{1}{2}\right)k\right) + O\left(k^2\right), \tag{1.47}$$

$$\frac{g_j^n + g_j^{n+1}}{2} = g\left(jh, \left(n + \frac{1}{2}\right)k\right) + O\left(k^2\right). \tag{1.48}$$

$$\frac{1}{2}\left[\delta_x^2 g_j^m + \delta_x^2 g_j^{m+1}\right] = \frac{\partial^2 g}{\partial x^2}\left(jh, \left(m + \frac{1}{2}\right)k\right) + O\left(k^2\right) + O\left(h^2\right). \tag{1.49}$$

De las estimaciones proporcionadas por (1.47), (1.48) y (1.49), aplicadas a las componentes del error de truncación local, se sigue que

$$\begin{aligned} \mathcal{T}_{1,j}^n &= O\left(k^2\right) + O\left(h^2\right), \\ \mathcal{T}_{2,j}^n &= O\left(k^2\right), \\ \mathcal{T}_{3,j}^n &= O\left(k^2\right). \end{aligned}$$

Así, ya que de (1.46) se sigue que E_k tiene norma acotada, se puede deducir que el esquema es consistente con la ecuación en derivadas parciales, y también que el error de truncación satisface

$$\left\|\mathfrak{T}_h^k\,(nk)\right\|_\infty = O\left(k^2\right) + O\left(h^2\right),$$

de donde se deduce la consistencia del esquema y, por tanto, su convergencia.

1.3.2. Esquema compacto

En la publicación incluida en el Capítulo 3, se considera de nuevo el modelo (1.21) y se propone y estudia un esquema en diferencias compacto para este modelo.

Primero se introducen dos nuevas variables , $v(x,t)$ y $u(x,t)$, en orden a expresar (1.21) como un sistema de primer orden en t,

$$v\,(x,t) = BT\,(x,t) + C\frac{\partial}{\partial t}T\,(x,t)\,, \tag{1.50}$$

y

$$u\,(x,t) = AT\,(x,t) + \frac{\partial}{\partial t}v\,(x,t)\,. \tag{1.51}$$

Así, usando (1.50) y (1.51), se puede probar que la Eq. 1.21 se puede escribir como

$$\frac{\partial}{\partial t}u\,(x,t) = a\frac{\partial^2}{\partial x^2}T\,(x,t) + b\frac{\partial^2}{\partial x^2}v\,(x,t) + c\frac{\partial^2}{\partial x^2}u\,(x,t)\,, \tag{1.52}$$

donde

$$a = (C^2 + EB^2 - BDC - ACE)/C^2,\ b = (DC - BE)/C^2,\ c = E/C.$$

En consecuencia, escribiendo (1.50) y (1.51) de la forma

$$\frac{\partial}{\partial t} T\left(x,t\right) = \frac{1}{C}\left(v\left(x,t\right) - BT\left(x,t\right)\right) \tag{1.53}$$

y

$$\frac{\partial}{\partial t} v\left(x,t\right) = u\left(x,t\right) - AT\left(x,t\right), \tag{1.54}$$

las ecuaciones (1.52)-(1.54), con condiciones de contorno

$$\begin{aligned} &u(0,t) = u(l,t) = 0, \\ &T(0,t) = T(l,t) = 0, \qquad t \geq 0, \\ &v(0,t) = v(l,t) = 0, \end{aligned} \tag{1.55}$$

y condiciones iniciales

$$\begin{aligned} &u\left(x,0\right) = A\phi\left(x\right) + B\varphi\left(x\right) + C\psi\left(x\right), \\ &T\left(x,0\right) = \phi\left(x\right), \qquad\qquad x \in [0,l] \\ &v\left(x,0\right) = B\phi\left(x\right) + C\varphi\left(x\right), \end{aligned} \tag{1.56}$$

dan un problema equivalente al que consiste de la ecuación (1.21), con condiciones de contorno (1.18), y condiciones iniciales (1.19).

Para derivar el nuevo esquema numérico para el modelo DPL(2,2) se usarán las siguientes aproximaciones en diferencias finitas en las ecuaciones (1.53) y (1.54),

$$\frac{1}{k}\left(T_j^{n+1}-T_j^n\right) = -\frac{B}{2C}\left(T_j^{n+1}+T_j^n\right)+\frac{1}{2C}\left(v_j^{n+1}+v_j^n\right), \quad (1.57)$$

$$\frac{1}{k}\left(v_j^{n+1}-v_j^n\right) = \frac{1}{2}\left(u_j^{n+1}+u_j^n\right)-\frac{A}{2}\left(T_j^{n+1}+T_j^n\right). \quad (1.58)$$

Para la ecuacón (1.52), se puede seguir dos planteamientos distintos. Escribiendo

$$f(x,t)=\frac{\partial^2}{\partial x^2}T(x,t), \quad g(x,t)=\frac{\partial^2}{\partial x^2}v(x,t), \quad s(x,t)=\frac{\partial^2}{\partial x^2}u(x,t),$$

usando en (1.52) las aproximaciones finitas

$$\frac{1}{k}\left(u_j^{n+1}-u_j^n\right)=\frac{a}{2}\left(f_j^{n+1}+f_j^n\right)+\frac{b}{2}\left(g_j^{n+1}+g_j^n\right)+\frac{c}{2}\left(s_j^{n+1}+s_j^n\right),$$

y considerando para las funciones f, g, y s la aproximación en diferencias finitas de cuarto orden compacta [42],

$$\frac{1}{10}f_{j-1}^n+f_j^n+\frac{1}{10}f_{j+1}^n=\frac{6}{5}\delta_x^2T_j^n,$$

donde

$$\delta_x^2 w_j^n=\frac{1}{h^2}\left(w_{j-1}^n-2w_j^n+w_{j+1}^n\right),$$

con aproximaciones análogas para g y s, tras algunas manipulaciones algebraicas se obtiene la expresión

$$\begin{aligned}&u_{j-1}^{n+1}+10u_j^{n+1}+u_{j+1}^{n+1}-\left(u_{j-1}^n+10u_j^n+u_{j+1}^n\right)=\\&6ak\delta_x^2\left(T_j^{n+1}+T_j^n\right)+6bk\delta_x^2\left(v_j^{n+1}+v_j^n\right)+6ck\delta_x^2\left(u_j^{n+1}+u_j^n\right)\end{aligned} \quad (1.59)$$

Este planteamiento, análogo al usado en [35] para el correspondiente modelo DPL(1,1), enfatiza la obtención del esquema a partir de la clase de aproximaciones finitas compactas presentadas en [42], y sugiere la forma de generalizar usando otras aproximaciones en diferencias finitas compactas de alto orden de [42].

Sin embargo, se puede obtener una derivación mucho más directa de (1.59) usando en la ecuación (1.52) las siguientes aproximaciones en diferencias,

$$\begin{aligned}&\frac{1}{12k}\left(u_{j+1}^{n+1}-u_{j+1}^{n}\right)+\frac{5}{6k}\left(u_{j}^{n+1}-u_{j}^{n}\right)+\frac{1}{12k}\left(u_{j-1}^{n+1}-u_{j-1}^{n}\right)=\\&\frac{a}{2}\delta_x^2\left(T_j^{n+1}+T_j^{n}\right)+\frac{b}{2}\delta_x^2\left(v_j^{n+1}+v_j^{n}\right)+\frac{c}{2}\delta_x^2\left(u_j^{n+1}+u_j^{n}\right),\end{aligned}$$

que son análogas a las que dan lugar a un método clásico para la ecuación de difusión [13, p. 191], y lleva de forma inmediata a la Eq. (1.59) Además de una derivación más simple, la ventaja de este planteamiento es que relaciona el nuevo esquema con un método en diferencias para la ecuación clásica del calor que se sabe que es incondicionalmente estable, proporcionando la base para un análisis directo de la estabilidad del nuevo método.

Así, el nuevo esquema está definido por las ecuaciones (1.57), (1.58), y (1.59), junto a las condiciones de contorno e iniciales discretizadas correspondientes a (1.55) y (1.56),

$$u_0^n=u_P^n,\ T_0^n=T_P^n=0,\ v_0^n=v_P^n=0,\ n=0\ldots N, \tag{1.60}$$

y

$$\begin{aligned} u_j^0 &= A\phi(jh) + B\varphi(jh) + C\psi(jh), \\ T_j^0 &= \phi(jh), \qquad\qquad\qquad\qquad j = 0, \ldots, P. \\ v_j^0 &= B\phi(jh) + C\varphi(jh), \end{aligned} \tag{1.61}$$

A continuación, el esquema se expresará en forma matricial. Considerando, para $n = 0, \ldots, N$, los vectores U^n, T^n, y V^n, donde U^n, respectivamente T^n y V^n, apilan los $P-1$ valores u_j^n, respectivamente T_j^n y v_j^n, para $j = 1, \ldots, P-1$. Escribiendo $r = h/k^2$, e introduciendo las dos matrices tridiagonales $(P-1) \times (P-1)$, $M = tridiag\,(1, -2, 1)$ y $S = tridiag\,(1, 10, 1)$, esto es, matrices con unos en las diagonales inferior y superior y con -2, para M, o con 10, para S, en la diagonal principal, la expresión del esquema como un sistema de ecuaciones matricial está dado por

$$\begin{aligned} S\left(U^{n+1} - U^n\right) =& 6r\left(aM\left(T^{n+1} + T^n\right) + bM\left(V^{n+1} + V^n\right)\right. \\ & \left. + cM\left(U^{n+1} + U^n\right)\right), \end{aligned} \tag{1.62}$$

$$\frac{1}{k}\left(T^{n+1} - T^n\right) = -\frac{B}{2C}\left(T^{n+1} + T^n\right) + \frac{1}{2C}\left(V^{n+1} + V^n\right), \tag{1.63}$$

y

$$\frac{1}{k}\left(V^{n+1} - V^n\right) = \frac{1}{2}\left(U^{n+1} + U^n\right) - \frac{A}{2}\left(T^{n+1} + T^n\right). \tag{1.64}$$

Se pueden obtener expresiones más prácticas despejando T^{n+1} y V^{n+1} de (1.63) y (1.64), y sustituyendo en (1.62). Tras simplificar y escribiendo

$$x_k = 4C + 2Bk + Ak^2,\; y_k = 4C - 2Bk - Ak^2,\; z_k = 4C + 2Bk - Ak^2,$$

y

$$
\begin{aligned}
\alpha_k &= r\left(c+\frac{x_k+z_k}{x_k}\frac{bk}{4}+\frac{ak^2}{x_k}\right),\\
\beta_k &= r\left(a+\frac{ay_k}{x_k}-\frac{x_k+y_k}{x_k}\frac{bAk}{2}\right),\\
\gamma_k &= r\left(b+\frac{4ak}{x_k}+\frac{bz_k}{x_k}\right),
\end{aligned}
$$

se obtienen las siguientes expresiones,

$$(S-6\alpha_k M)\,U^{n+1}=(S+6\alpha_k M)\,U^n+6\beta_k MT^n+6\gamma_k MV^n, \qquad (1.65)$$

$$T^{n+1}=\frac{y_k}{x_k}T^n+\frac{4k}{x_k}V^n+\frac{k^2}{x_k}U^n+\frac{k^2}{x_k}U^{n+1}, \qquad (1.66)$$

$$V^{n+1}=-\frac{4kAC}{x_k}T^n+\frac{z_k}{x_k}V^n+\frac{2C+Bk}{x_k}kU^n+\frac{2C+Bk}{x_k}kU^{n+1}, \qquad (1.67)$$

que muestran que, usando los valores iniciales dados por (1.61) y las condiciones de contorno (1.60), la aplicación del método para obtener la aproximación numérica que corresponde al paso siguiente $n+1$ consiste en resolver (1.65) para obtener U^{n+1} y sustitir en las ecuaciones (1.66) y (1.67) para calcular T^{n+1} y V^{n+1}. Nótese que el coeficiente de U^{n+1} en (1.65) es una matriz tridiagonal, lo que permite un cálculo muy eficiente de U^{n+1}.

Para analizar la estabilidad del método, primero lo escribimos como un esquema de dos niveles. Después, usando un argumento límite y una forma del lema de Gronwall, se probará que las potencias de la matriz del esquema están uniformemente acotadas y de aquí se deducirá la estabilidad incondicional del método.

Escribiendo

$$X_k = I - 6\alpha_k S^{-1}M, \quad Y_k = I + 6\alpha_k S^{-1}M),$$

donde I denota la matriz identidad $(P-1)\times(P-1)$, de (1.65) se obtiene,

$$U^{n+1} = X_k^{-1}Y_k U^n + 6\beta_k X_k^{-1}S^{-1}MT^n + 6\gamma_k X_k^{-1}S^{-1}MV^n, \tag{1.68}$$

y, de (1.66) y (1.67),

$$\begin{aligned} T^{n+1} &= \frac{2k^2}{x_k}X_k^{-1}U^n \\ &+\frac{y_k}{x_k}X_k^{-1}\left(I - 6\left(\alpha_k - \beta_k\frac{k^2}{y_k}\right)S^{-1}M\right)T^n \\ &+\frac{4k}{x_k}X_k^{-1}\left(I - 6\left(\alpha_k - \frac{1}{4}\gamma_k k\right)S^{-1}M\right)V^n, \end{aligned} \tag{1.69}$$

y

$$\begin{aligned} V^{n+1} &= \frac{2\,(2C+Bk)\,k}{x_k}X_k^{-1}U^n \\ &-\frac{4kAC}{x_k}X_k^{-1}\left(I - 6\left(\alpha_k + \beta_k\frac{(2C+Bk)}{4AC}\right)S^{-1}M\right)T^n \\ &+\frac{z_k}{x_k}X_k^{-1}\left(I - 6\left(\alpha_k - \gamma_k\frac{(2C+Bk)\,k}{z_k}\right)S^{-1}M\right)V^n. \end{aligned} \tag{1.70}$$

Así, introduciendo el vector apilado $[U^n, T^n, V^n]^T$, donde el superíndice T denota la transpuesta, el método se puede escribir como el esquema de dos niveles

$$\left[U^{n+1}, T^{n+1}, V^{n+1}\right]^T = Q_k\left[U^n, T^n, V^n\right]^T, \tag{1.71}$$

donde la matriz del esquema, Q_k, es la matriz por bloques, 3×3, determinada por los coeficientes de U^n, T^n y V^n en (1.68)–(1.70) dada en la página 99.

Escribiendo

$$X^{-1} = \left(I - 6rcS^{-1}M\right)^{-1}, \quad Y = I + 6rcS^{-1}M,$$

se puede probar que la matriz $Q = \lim_{k \to 0} Q_k$ está dada por

$$Q = \begin{bmatrix} X^{-1}Y & 12raX^{-1}S^{-1}M & 12rbX^{-1}S^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.$$

Entonces, como las matrices M, S, X, y Y conmutan, se puede obtener la siguiente expresión de las potencias de la matriz límite Q,

$$Q^n = \begin{bmatrix} \left(X^{-1}Y\right)^n & -\frac{a}{c}\left(I - \left(X^{-1}Y\right)^n\right) & -\frac{b}{c}\left(I - \left(X^{-1}Y\right)^n\right) \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.$$

Aquí, la matriz $X^{-1}Y$ es similar a la matriz de un esquema incondicionalmente estable y convergente para la ecuación clásica de difusión [13, p. 191, esquema 12], y por tanto sus potencias están uniformemente acotadas, es decir, existen constantes $k_0 > 0$ y $C > 0$ tales que, para $0 < k < k_0$ y $0 \leq nk \leq T_M$, se tiene que

$$\|Q^n\| \leq C.$$

Se puede comprobar directamente que $\|Q_k - Q\| = O(k)$, por tanto existe una constante $\alpha > 0$ tal que, para $0 < k < k_0$,

$$\|Q_k - Q\| \leq \alpha k.$$

Entonces, escribiendo

$$Q_k^n - Q^n = \sum_{j=0}^{n-1} \left(Q_k^{n-1-j} - Q^{n-1-j}\right)(Q_k - Q)\, Q^j + \sum_{j=0}^{n-1} Q^{n-1-j}(Q_k - Q)\, Q^j,$$

se obtiene que

$$\|Q_k^n - Q^n\| \leq C\alpha k \sum_{j=0}^{n-1} \left\|Q_k^j - Q^j\right\| + C^2 \alpha T_M.$$

De la desigualdad anterior, usando la forma del lema de Gronwall que dada en [40, pp. 186], se puede obtener la siguiente acotación uniforme de $\|Q_k^n - Q^n\|$

$$\|Q_k^n - Q^n\| \leq C^2 \alpha T_M e^{T_M C \alpha},$$

para todo $n \geq 0$. Así, para $0 < k < k_0$ y $0 \leq nk \leq T_M$, se tiene que las matrices Q_k^n están uniformemente acotadas,

$$\|Q_k^n\| = \|Q_k^n - Q^n + Q^n\| \leq C^2 \alpha T_M e^{T_M C \alpha} + C,$$

y de aquí que el esquema es estable, incondicionalmente, en el sentido de Lax [13].

Seguidamente, se obtienen cotas de los errores de truncación del esquema, y así, asumiendo que la solución sea suficientemente suave, se deduce la consistencia del método, la cual, junto con la estabilidad incondicional del método garantiza su convergencia. En lo que sigue, se denotará por $w = \left(\widetilde{u}, \widetilde{T}, \widetilde{v}\right)$ a la solución exacta del problema (1.52)-(1.54).

Sea $\mathcal{L} = (\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3)$ el operador en diferencias asociado al esquema [41, p. 42], donde

$$\begin{aligned}
\mathcal{L}_1 w_j^n &= \frac{1}{10k}\left(\widetilde{u}_{j-1}^{n+1} - \widetilde{u}_{j-1}^{n} + 10\left(\widetilde{u}_{j}^{n+1} - \widetilde{u}_{j}^{n}\right) + \widetilde{u}_{j+1}^{n+1} - \widetilde{u}_{j+1}^{n}\right) \\
&\quad -\frac{3}{5}\left(a\delta_x^2\left(\widetilde{T}_j^{n+1} + \widetilde{T}_j^{n}\right) + b\delta_x^2\left(\widetilde{v}_j^{n+1} + \widetilde{v}_j^{n}\right) + c\delta_x^2\left(\widetilde{u}_j^{n+1} + \widetilde{u}_j^{n}\right)\right), \\
\mathcal{L}_2 w_j^n &= \frac{1}{k}\left(\widetilde{T}_j^{n+1} - \widetilde{T}_j^{n}\right) + \frac{B}{2C}\left(\widetilde{T}_j^{n+1} + \widetilde{T}_j^{n}\right) - \frac{1}{2C}\left(\widetilde{v}_j^{n+1} + \widetilde{v}_j^{n}\right), \\
\mathcal{L}_3 w_j^n &= \frac{1}{k}\left(\widetilde{v}_j^{n+1} - \widetilde{v}_j^{n}\right) - \frac{1}{2}\left(\widetilde{u}_j^{n+1} + \widetilde{u}_j^{n}\right) + \frac{A}{2}\left(\widetilde{T}_j^{n+1} + \widetilde{T}_j^{n}\right),
\end{aligned}$$

de modo que el error de truncación local en el punto (jh, nk), [13, p. 20], está dado por $\left(\mathcal{T}_{1,j}^n, \mathcal{T}_{2,j}^n, \mathcal{T}_{3,j}^n\right) = \mathcal{L}w_j^n$.

Usando desarrollos en serie de Taylor apropiados, se consiguen las siguientes acotaciones,

$$\mathcal{T}_{1,j}^n = O\left(k^2\right) + O\left(h^4\right), \ \mathcal{T}_{2,j}^n = O\left(k^2\right), \ \mathcal{T}_{3,j}^n = O\left(k^2\right). \tag{1.72}$$

Considerando los vectores de las soluciones exactas en los puntos de la malla,

$$\begin{aligned}
\widetilde{U}^n &= \left[\widetilde{u}_1^n, \widetilde{u}_2^n, \ldots, \widetilde{u}_{P-1}^n\right]^T, \\
\widetilde{T}^n &= \left[\widetilde{T}_1^n, \widetilde{T}_2^n, \ldots, \widetilde{T}_{P-1}^n\right]^T, \\
\widetilde{V}^n &= \left[\widetilde{v}_1^n, \widetilde{v}_2^n, \ldots, \widetilde{v}_{P-1}^n\right]^T,
\end{aligned}$$

y el vector apilado $W^n = \left[\widetilde{U}^n, \widetilde{T}^n, \widetilde{V}^n\right]^T \in \mathbb{R}^{3(P-1)}$, el error de truncación del esquema de dos niveles (1.71), en $t = nk$, es el vector

$$\mathfrak{T}^n = \frac{1}{k}\left(W^{n+1} - Q_k W^n\right), \tag{1.73}$$

y se puede comprobar que

$$\mathfrak{T}^n = E_k \left[\mathcal{T}_1^n, \mathcal{T}_2^n, \mathcal{T}_3^n\right]^T, \tag{1.74}$$

donde $\mathcal{T}_i^n = \left[\mathcal{T}_{i,1}^n, \mathcal{T}_{i,2}^n, \ldots, \mathcal{T}_{i,P-1}^n\right]^T$, $i = 1, 2, 3$, y E_k es la matriz 3×3 cuyos elementos están definidos en la página 105.

No es difícil comprobar que la matriz $E = \lim_{k\to 0} E_k$ está dada por

$$E = \begin{bmatrix} 10X^{-1}S^{-1} & 6raX^{-1}S^{-1}M & 6rbX^{-1}S^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}, \tag{1.75}$$

y de aquí se deduce que E_k tiene norma acotada. Por tanto, de (1.72) y (1.74), se tiene que, para $0 \leq nk \leq T_M$,

$$\lim_{k\to 0} \frac{1}{k} \left\| W_h^k\left((n+1)k\right) - Q_k W_h^k(nk) \right\|_\infty = 0, \tag{1.76}$$

de modo que el esquema es consistente con la ecuación en derivadas parciales. También se deduce que el error de truncación verifica

$$\left\|\mathfrak{T}^n\right\|_\infty = O\left(k^2\right) + O\left(h^4\right). \tag{1.77}$$

Como consecuencia, dado que el método es incondicionalmente estable, para cualquier valor finito de $r = h/k^2$, y es consistente con la ecuación en derivadas parciales original, a partir del Teorema de equivalencia de Lax [13] se concluye que el método es también incondicionalmente convergente de orden $O(k^2) + O(h^4)$.

1.4. Esquema en diferencias para el modelo de difusión con retardo y coeficientes variables

Cuando el modelo con retardo de fase dual (1.12) se combina con el principio de conservación de la energía (1.13), se obtiene una ecuación de conducción del calor, que se reduce a la ecuación clásica de difusión cuando $\tau_q = \tau_T = 0$. En otro caso, da lugar a una ecuación en derivadas parciales con retardo, un modelo retardado cuando $\tau_T = 0$, i.e., en el modelo SPL [24], y también si $\tau = \tau_q - \tau_T > 0$, o en una ecuación avanzada si $\tau_q - \tau_T < 0$ [25, 26]. Si utilizamos aproximaciones de diversos órdenes con respecto a los retardos en (1.12), se obtienen los ya mencionados modelos DPL [30, 31], que incluyen, cuando se consideran aproximaciones de primer orden y $\tau_T = 0$, el modelo de Cattaneo-Vernotte [27, 29].

Algunos de estos modelos no-Fourier pueden presentar problemas de estabilidad [30, 43] y/o violar principios físicos [44]. Además, los efectos no clásicos son evidentes sólo en comportamientos transitorios, cuando el tiempo de respuesta es del mismo orden de magnitud que el tiempo de relajación [10, 26], estando disponible el modelo de difusión clásico para proporcionar descripciones exactas para tiempos mucho más largos. De ahí, podría ser razonable considerar un modelo de conducción de calor que combine tanto términos clásicos como retardados, con el tiempo variando el peso, de modo que el término con retardo finalmente se haga insignificante, y el modelo se acerque a la difusión clásica a largo plazo, garantizando también su estabilidad.

En la publicación recogida en el Capítulo 4, se ha considerado el siguiente modelo de conducción de calor en una varilla finita con extremos aislados, la ecuación en derivadas parciales con término de retardo y no retardo, y con coeficientes dependientes del tiempo,

$$\frac{\partial T}{\partial t}(x,t) = a(t)\frac{\partial^2 T}{\partial x^2}(x,t) + b(t)\frac{\partial^2 T}{\partial x^2}(x,t-\tau), \qquad \begin{array}{l} 0 \leq x \leq l, \\ t > \tau, \end{array} \tag{1.78}$$

con condición inicial

$$T(x,t) = \phi(x,t), \ \ 0 \leq x \leq l, \ 0 \leq t \leq \tau, \tag{1.79}$$

y condición de contorno de Dirichlet

$$T(0,t) = T(l,t) = 0, \ t \geq 0, \tag{1.80}$$

donde $\tau > 0$, y $a(t)$, $b(t)$ son funciones reales positivas.

En la literatura científica podemos encontrar trabajos en los que se proponen esquemas numéricos para obtener soluciones aproximadas de diferentes tipos de modelos no-Fourier de conducción de calor con coeficientes constantes, por ejemplo [32, 33, 37–39] o los trabajos recogidos en los Capítulos 2 y 3. También se han propuesto esquemas en diferencias para problemas parabólicos con retardo, por ejemplo [45–48], incluyendo el problema (1.78) en el caso de coeficientes constantes [11, 12].

En el trabajo incluido en el Capítulo 4 se construye un esquema en diferencias explícito para el problema dependiente del tiempo (1.78)–(1.80), caracterizando sus propiedades de convergencia. El esquema se expresa forma matricial y como esquema de dos niveles para facilitar el estudio de la convergencia, que dependerá de la geometría de la malla considerada lo que se ilustra con ejemplos numéricos.

Se considera un dominio acotado $[0, l] \times [0, M\tau]$, para algún entero fijo $M > 1$, y la malla uniforme $\{(x_p, t_n), p = 0 \dots P, n = 0 \dots MN\}$, definida por los incrementos $h = \Delta x$ y $k = \Delta t$, tales que $l = Ph$ y $\tau = Nk$. Los valores de una función w en los puntos de la malla, $w(x_p, t_n)$, se denotan $w_{p,n}$. El esquema se puede aplicar en cualquier dominio acotado $[0, l] \times [0, T_{\mathsf{max}}]$, considerando M tal que $T_{\mathsf{max}} \leq M\tau$.

Se denota por $u(x, t)$ la aproximación numérica de $T(x, t)$ que se obtendrá con el esquema. Se usan aproximaciones en diferencias finitas de las derivadas parciales en (1.78), como en el esquema explícito clásico para la ecuación de la difusión [41, pp. 6-8], o en el esquema explícito para el caso de coeficientes constantes [11],

$$\frac{\partial u}{\partial t}(x_p, t_n) \approx \frac{1}{k}\delta_t u_{p,n} = \frac{1}{k}\left(u_{p,n+1} - u_{p,n}\right),$$

$$\frac{\partial^2 u}{\partial x^2}(x_p, t_n) \approx \frac{1}{h^2}\delta_x^2 u_{p,n} = \frac{1}{h^2}\left(u_{p-1,n} - 2u_{p,n} + u_{p+1,n}\right),$$

Escribiendo $\alpha = k/h^2$, $a_n = a\,(nk)$, y $b_n = b\,(nk)$, de (1.78)–(1.80) se obtiene el sistema de ecuaciones en diferencias

$$\begin{aligned} & u_{p,n+1} = u_{p,n} + \alpha a_n \delta_x^2 u_{p,n} + \alpha b_n \delta_x^2 u_{p,n-N}, \\ & p = 1, 2, \ldots, P-1, \quad n = N, N+1, \ldots, MN-1, \end{aligned} \tag{1.81}$$

con condiciones iniciales

$$u_{p,n} = \phi\,(ph, kn,)\,,\ p = 0, 1, \ldots, P,\ n = 0, 1, \ldots, N, \tag{1.82}$$

y condiciones de contorno

$$u_{0,n} = u_{P,n} = 0,\ n = 0, 1, \ldots, MN. \tag{1.83}$$

Usando (1.81)–(1.83), se pueden calcular los valores de $u_{p,n}$ para todos los puntos de la malla recursivamente, y después extenderlos por continuidad para obtener aproximaciones numéricas $u(x,t)$ para $(x,t) \in [0,l] \times [0, M\tau]$.

Introduciendo los vectores $\boldsymbol{u}_n = [u_{1,n}, u_{2,n}, \cdots, u_{P-1,n}]^T$, para $n = 0, 1, \ldots, MN$, donde el superíndice T denota la transpuesta, y la matriz $(P-1) \times (P-1)$ tridiagonal

$$\mathbf{M} = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & -2 \end{bmatrix},$$

y escribiendo la matriz identidad $(P-1) \times (P-1)$ como $\mathbf{I}$, las ecuaciones del esquema se pueden dar de forma matricial como

$$\boldsymbol{u}_{n+1} = (\mathbf{I} + \alpha a_n \mathbf{M})\, \boldsymbol{u}_n + \alpha b_n \mathbf{M} \boldsymbol{u}_{n-N},\ n = N, N+1, \ldots, MN-1, \quad (1.84)$$

con condición inicial

$$\boldsymbol{u}_n = \boldsymbol{\phi}_n,\ n = 0, 1, \ldots, N, \quad (1.85)$$

donde $\boldsymbol{\phi}_n = [\phi(h, nk), \phi(2h, nk), \ldots, \phi((P-1)h, nk)]^T$, para $n = 0, 1, \ldots, N$.

El esquema se expresa como un esquema de dos niveles, en orden a facilitar el análisis de sus propiedades. Introduciendo los vectores apilados

$$\boldsymbol{u}_n^* = [\boldsymbol{u}_n, \boldsymbol{u}_{n-1}, \cdots, \boldsymbol{u}_{n-N}]^T,\ n = N, N+1, \ldots, MN,$$

y

$$\boldsymbol{\phi}^* = [\boldsymbol{\phi}_N, \boldsymbol{\phi}_{N-1}, \ldots, \boldsymbol{\phi}_0]^T,$$

y las matrices por bloques

$$\mathbf{C}_n^* = \begin{bmatrix} \mathbf{I} + \alpha a_n \mathbf{M} & 0 & \cdots & 0 & \alpha b_n \mathbf{M} \\ \mathbf{I} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & \mathbf{I} & 0 \end{bmatrix},\ n = N, N+1, \ldots, MN, \quad (1.86)$$

las ecuaciones (1.84) y (1.85) se pueden escribir de la forma

$$\boldsymbol{u}_{n+1}^* = \mathbf{C}_n^* \boldsymbol{u}_n^*,\ n = N, N+1, \ldots, MN-1, \quad (1.87)$$

$$\boldsymbol{u}_N^* = \boldsymbol{\phi}^*. \tag{1.88}$$

Se establecen condiciones que garantizan la convergencia del esquema en diferencias propuesto. Primero, se proporciona una expresión del error de truncación del esquema, de donde se establece su consistencia. Después, dando condiciones para la estabilidad de una transformación del esquema original, se prueba directamente la convergencia del método. En lo que sigue, v denotará la solución exacta del problema (1.78)–(1.80).

Sea L el operador en diferencias asociado con el esquema [41, p. 42],

$$Lu_{p,n} = \frac{1}{k}\left(u_{p,n+1} - u_{p,n} - \alpha a_n \delta_x^2 u_{p,n} - \alpha b_n \delta_x^2 u_{p,n-N}\right), \tag{1.89}$$

de forma que el error de truncación local [49, p. 165], [13, p. 20], en el punto (ph, nk) está dado por $\mathcal{T}_{p,n} = Lv_{p,n}$. Se demuestra que si existen $\dfrac{\partial^2}{\partial t^2} v\left(x,t\right)$ y $\dfrac{\partial^4}{\partial x^4} v\left(x,t\right)$ y son continuas, el error de truncación local del esquema explíto definido en (1.84) está dado por

$$\begin{aligned}\mathcal{T}_{p,n} =& \frac{k}{2}\frac{\partial^2 v}{\partial t^2}\left(ph, \left(n+\theta_1\right)k\right) - \frac{h^2}{12}\Bigg(a_n \frac{\partial^4 v}{\partial x^4}\left(\left(p-1+2\theta_2\right)h, nk\right) \\ &+ b_n \frac{\partial^4 v}{\partial x^4}\left(\left(p-1+2\theta_3\right)h, \left(n-N\right)k\right)\Bigg),\end{aligned} \tag{1.90}$$

donde $\theta_1, \theta_2, \theta_3 \in (0,1)$.

Este resultado se puede obtener fácilmente usando desarrollos en serie de Taylor apropiados. Las condiciones sobre la regularidad de la solución exacta v están garantizadas si la función inicial y los coeficientes son suficientemente regulares, por ejemplo, si $\phi\left(x,\cdot\right)$, $a(\cdot)$ y $b(\cdot)$ son continuamente diferenciables dos veces, $\phi\left(\cdot,t\right)$ es continuamente diferenciable cuatro veces, y la función inicial ϕ satisface algunas condiciones.

Introduciendo los vectores, $\mathfrak{T}_n = \left[\mathcal{T}_{1,n}, \mathcal{T}_{2,n}, \ldots, \mathcal{T}_{P-1,n}\right]^T$, y los vectores apilados,

$$\mathfrak{T}_n^* = \left[\mathfrak{T}_n, 0, \ldots, 0\right]^T,$$

de los errores de truncación, y, de forma similar, los correspondientes vectores para la solución exacta en los puntos de la malla,

$$\boldsymbol{v}_n = \left[v_{1,n}, v_{2,n}, \cdots, v_{P-1,n}\right]^T$$

y

$$\boldsymbol{v}_n^* = \left[\boldsymbol{v}_n, \boldsymbol{v}_{n-1}, \cdots, \boldsymbol{v}_{n-N}\right]^T,$$

se comprueba que

$$\mathfrak{T}_n^* = \frac{1}{k}\left(\boldsymbol{v}_{n+1}^* - \mathbf{C}_n^* \boldsymbol{v}_n^*\right), \tag{1.91}$$

el cual es el error de truncación local del esquema, expresado en forma de esquema de dos niveles, como se definió en (1.87).

De forma inmediata se deduce que si $\dfrac{\partial^2}{\partial t^2} v(x,t)$ y $\dfrac{\partial^4}{\partial x^4} v(x,t)$ existen y son continuas en $[0,l] \times [\tau, M\tau]$, el esquema explícito definido en (1.84), o equivalentemente en (1.87), es consistente con la ecuación en derivadas parciales (1.78), y el error de truncación local verifica

$$\left\|\mathfrak{T}_n^*\right\|_\infty = O(k) + O\left(h^2\right).$$

A continuación, se usa la forma diagonal de la matriz $\mathbf{M}$ para transformar (1.87) en un esquema de dos niveles con matriz diagonal por bloques, el cual se prueba que es estable y facilita una demostarción directa de la convergencia del método.

Los valores propios de la matriz $\mathbf{M}$ son, [41, p. 52],

$$\lambda_p = -4\sin^2\frac{\pi p}{2P},\ p = 1,\ldots,P-1, \tag{1.92}$$

que forman una sucesión estrictamente decreciente, verificándose las acotaciones $-4 < \lambda_p < 0$, para $p = 1,\ldots,P-1$. La matriz $\mathbf{M}$ se puede expresar en forma diagonal como $\mathbf{M} = \mathbf{A}\mathbf{D}\mathbf{A}^{-1}$, donde $\mathbf{A}$ es la matriz correspondiente a la base de vectores propios

$$\mathcal{X}_p = \left[\sin\frac{\pi p}{P}, \sin\frac{2\pi p}{P}, \ldots, \sin\frac{(P-1)\,\pi p}{P}\right]^T,\ p = 1,\ldots,P-1, \tag{1.93}$$

y $\mathbf{D} = \operatorname{diag}\left[\lambda_1,\ldots,\lambda_{P-1}\right]$. De aquí, introduciendo la matriz $(N+1)\times(N+1)$ diagonal por bloques $\mathbf{A}^* = \operatorname{diag}\left[\mathbf{A},\mathbf{A},\ldots,\mathbf{A}\right]$, y la matriz por bloques

$$\mathbf{D}_n^* = \begin{bmatrix} \mathbf{I}+\alpha a_n\mathbf{D} & 0 & \cdots & 0 & \alpha b_n\mathbf{D} \\ \mathbf{I} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & \mathbf{I} & 0 \end{bmatrix}, \tag{1.94}$$

se obtiene

$$\mathbf{C}_n^* = \mathbf{A}^*\mathbf{D}_n^*\left(\mathbf{A}^*\right)^{-1}. \tag{1.95}$$

Sea $\boldsymbol{\varphi}_n = \left[\varphi_{1,n},\varphi_{2,n},\ldots,\varphi_{P-1,n}\right]^T$ el vector $\boldsymbol{\varphi}_n = \mathbf{A}^{-1}\boldsymbol{u}_n$. El vector apilado $\boldsymbol{\varphi}_n^* = \left[\boldsymbol{\varphi}_n,\boldsymbol{\varphi}_{n-1},\cdots,\boldsymbol{\varphi}_{n-N}\right]^T$ verifica que $\boldsymbol{\varphi}_n^* = \left(\mathbf{A}^*\right)^{-1}U_n^*$, y de aquí, de (1.87), se obtiene

$$\boldsymbol{\varphi}_{n+1}^* = \mathbf{D}_n^*\boldsymbol{\varphi}_n^*. \tag{1.96}$$

Las componentes en esta última ecuación se pueden reordenar para obtener la expresión equivalente

$$\boldsymbol{\psi}^*_{n+1} = \mathbf{G}^*_n \boldsymbol{\psi}^*_n, \tag{1.97}$$

donde $\boldsymbol{\psi}^*_n = [\boldsymbol{\psi}_{1,n}, \boldsymbol{\psi}_{2,n}, \cdots, \boldsymbol{\psi}_{P-1,n}]^T$, con $\boldsymbol{\psi}_{p,n} = [\varphi_{p,n}, \varphi_{p,n-1}, \cdots, \varphi_{p,n-N}]^T$, y $\mathbf{G}^*_n$ es la matriz diagonal por bloques $\mathbf{G}^*_n = \mathrm{diag}\left[\mathbf{G}_{1,n}, \mathbf{G}_{2,n}, \ldots, \mathbf{G}_{P-1,n}\right]$, con

$$\mathbf{G}_{p,n} = \begin{bmatrix} 1+\alpha a_n \lambda_p & 0 & \ldots & 0 & \alpha b_n \lambda_p \\ 1 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \end{bmatrix}. \tag{1.98}$$

El esquema en diferencias (1.96) es estable, [49, p. 159], si existe $k_0 > 0$ tal que para todo $0 < k < k_0$ la familia de matrices

$$\left\{ \prod_{i=1}^{n-N} \mathbf{D}^*_{n-i},\ n = N+1, N+2, \ldots, MN \right\} \tag{1.99}$$

está uniformemente acotada, independientemente de k.

Si $\mathbf{P}$ es la matriz de permutación de filas tal que $\boldsymbol{\psi}^*_{n+1} = \mathbf{P}\boldsymbol{\varphi}^*_{n+1}$, se sigue, de (1.96) y (1.97), que $\mathbf{G}^*_n = \mathbf{P}\mathbf{D}^*_n\mathbf{P}^{-1}$. Dado que $\|\mathbf{P}\|_\infty = \|\mathbf{P}^{-1}\|_\infty = 1$, se verifica que

$$\left\| \prod_{i=1}^{n-N} \mathbf{G}^*_{n-i} \right\|_\infty = \left\| \prod_{i=1}^{n-N} \mathbf{D}^*_{n-i} \right\|_\infty,$$

de modo que la estabilidad de los esquemas (1.96) y (1.97) son equivalentes.

Se prueba que si

$$b\,(t) < a\,(t) \;\text{ y } \alpha \leq \frac{1}{2\,(a(t)+b(t))},\; \text{para } \tau < t \leq M\tau, \tag{1.100}$$

entonces

$$\left\| \prod_{i=1}^{n-N} \mathbf{G}^*_{n-i} \right\|_\infty \leq 1,\; n = N+1, N+2, \ldots, MN, \tag{1.101}$$

y de aquí el esquema definido por (1.96) es estable.

En lo que sigue, se asumirá que se verifican las condiciones (1.100). No es difícil probar, como se hizo en [11, Teorema 5] para el caso de coeficientes constantes, que bajo estas condiciones el esquema definido en (1.84) es asintóticamente estable.

Se prueba que bajo las condiciones dadas para la consistencia del esquema (1.84) y la estabilidad del esquema (1.96) se verifica que existe $K = K\,(\phi, M\tau, \alpha)$ tal que

$$\left\| \prod_{i=1}^{n-N} \mathbf{C}^*_{n-i} \boldsymbol{\phi}^* - \boldsymbol{v}^*_n \right\|_\infty \leq Kh, \quad \tau < nk \leq M\tau.$$

y por tanto el esquema propuesto es convergente.

Nótese que el esquema se aplica con un α fijo, de modo que la constante K depende de la geometría de la malla, ya que depende de α, pero es independiente de sus tamaños. Este resultado, sin embargo, no garantiza el orden correcto de convergencia, que debe ser $O(h^2)$ como se prueba en el error de truncación local, pero parece difícil conseguir una demostración alternativa de la convergencia que proporcione una estimación de la precisión de segundo orden para h.

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Parte II

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Capítulo 2

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Difference schemes for numerical solutions of lagging models of heat conduction

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ABSTRACT

Non-Fourier models of heat conduction are increasingly being considered in the modeling of microscale heat transfer in engineering and biomedical heat transfer problems. The dual-phase-lagging model, incorporating time lags in the heat flux and the temperature gradient, and some of its particular cases and approximations, result in heat conduction modeling equations in the form of delayed or hyperbolic partial differential equations.

In this work, the application of difference schemes for the numerical solution of lagging models of heat conduction is considered. Numerical schemes for some DPL approximations are developed, characterizing their properties of convergence and stability. Examples of numerical computations are included.

1. Introduction

Different non-Fourier models of heat conduction have been developed that, unlike the classical diffusion equation, imply finite speeds of propagation and may account for phenomena that appear in transient responses at the microscale level, such as thermal "inertia", heat waves and delayed responses to thermal disturbances (see [1,2]). They are increasingly being considered in the modeling of microscale heat transfer in engineering and biomedical heat transfer problems, as in ultrafast laser processing of thin-film engineering structures [3,4], heat transfer in nanofluids [5,6], or bio-heat transfer during thermal therapy or laser irradiation of biological tissues [7–9].

Lagging models of heat conduction, as the dual-phase-lag (DPL) model [2,10,11], which incorporates time lags in the heat flux and the temperature gradient, and some of its particular cases and approximations, result in heat conduction equations in the form of delayed or hyperbolic partial differential equations.

In the DPL model, classical Fourier law relating the heat flux vector $\mathbf{q}(\mathbf{r}, t)$ and the temperature gradient $\nabla T(\mathbf{r}, t)$, at time t for a point $\mathbf{r}$ in the space domain, is replaced by

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k\nabla T(\mathbf{r}, t + \tau_T), \tag{1}$$

where τ_q and τ_T are the corresponding phase lags. The single-phase-lag model [12] is the particular case with $\tau_T = 0$.

Combining Fourier law and the conservation of energy principle, the classical diffusion equation is obtained. In a similar way, using (1) instead of the Fourier law, a delayed partial differential equation is obtained [13,14]. However, it is common to use first-order approximations in (1),

$$\mathbf{q}(\mathbf{r}, t) + \tau_q \frac{\partial \mathbf{q}}{\partial t}(\mathbf{r}, t) \cong -k\left(\nabla T(\mathbf{r}, t) + \tau_T \frac{\partial}{\partial t}\nabla T(\mathbf{r}, t)\right), \tag{2}$$

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2.1. Introduction

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In the DPL model, classical Fourier law relating the heat flux vector $\mathbf{q}(\mathbf{r}, t)$ and the temperature gradient $\nabla T(\mathbf{r}, t)$, at time t for a point $\mathbf{r}$ in the space domain, is replaced by

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k\nabla T(\mathbf{r}, t + \tau_T), \tag{2.1}$$

where τ_q and τ_T are the corresponding phase lags. The single-phase-lag model [12] is the particular case with $\tau_T = 0$.

Combining Fourier law and the conservation of energy principle, the classical diffusion equation is obtained. In a similar way, using (2.1) instead of the Fourier law, a delayed partial differential equation is obtained [13, 14]. However, it is common to use first-order approximations in (2.1),

$$\mathbf{q}(\mathbf{r},t)+\tau_q\frac{\partial \mathbf{q}}{\partial t}(\mathbf{r},t)\cong -k\left(\nabla T(\mathbf{r},t)+\tau_T\frac{\partial}{\partial t}\nabla T(\mathbf{r},t)\right), \qquad (2.2)$$

referring to the derived equation as the DPL model [10],

$$\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)=\alpha\left(\Delta T(\mathbf{r},t)+\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t)\right). \qquad (2.3)$$

The well-known Cattaneo-Vernotte model [15–17] is the particular case of (2.3) with $\tau_T=0$.

Higher order approximations in (2.1) can also be considered [18, 19]. In this work, model (2.3) will be denoted DPL(1,1), while corresponding models resulting from second order approximation in τ_q and first or second order approximations in τ_T will be denoted, respectively, as DPL(2,1),

$$\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)+\frac{\tau_q^2}{2}\frac{\partial^3}{\partial t^3}T(\mathbf{r},t)=\alpha\left(\Delta T(\mathbf{r},t)+\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t)\right),$$

and DPL(2,2),

$$\begin{aligned}\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)+\frac{\tau_q^2}{2}\frac{\partial^3}{\partial t^3}T(\mathbf{r},t)=&\alpha\left(\Delta T(\mathbf{r},t)+\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t)\right.\\&\left.+\frac{\tau_T^2}{2}\Delta\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)\right).\end{aligned}$$

Finite differences schemes to obtain numerical approximations for DPL(1,1) models and variations, in different spatial domains, have been proposed in [20–27]. In this work, numerical schemes for DPL(2,2) models in one spatial dimension, with appropriate initial and boundary conditions, as well as particular cases, are developed, characterizing their properties of convergence and stability.

In particular, consider a finite rod with insulated ends at $x = 0$ and $x = l$, so that

$$T(0,t) = T(l,t) = 0, \quad t \geq 0, \tag{2.4}$$

and initial temperature distribution

$$T(x,0) = \phi(x), \quad \frac{\partial}{\partial t}T(x,0) = \varphi(x), \quad \frac{\partial^2}{\partial t^2}T(x,0) = \psi(x), \quad x \in [0,l], \tag{2.5}$$

with heat conduction, for $t > 0$ and $x \in [0,l]$, given by DPL(2,2) model

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{1}{\alpha}T(x,t) + \frac{\tau_q}{\alpha}\frac{\partial}{\partial t}T(x,t) + \frac{\tau_q^2}{2\alpha}\frac{\partial^2}{\partial t^2}T(x,t)\right) &= \frac{\partial^2}{\partial x^2}\big(T(x,t) \\ &+\tau_T\frac{\partial}{\partial t}T(x,t) + \frac{1}{2}\tau_T^2\frac{\partial^2}{\partial t^2}T(x,t)\big). \end{aligned}$$

In fact, a more general equation,

$$\begin{aligned} \frac{\partial}{\partial t}\left(AT(x,t) + B\frac{\partial}{\partial t}T(x,t) + C\frac{\partial^2}{\partial t^2}T(x,t)\right) &= \frac{\partial^2}{\partial x^2}\big(T(x,t) \\ &+D\frac{\partial}{\partial t}T(x,t) + E\frac{\partial^2}{\partial t^2}T(x,t)\big), \end{aligned} \tag{2.6}$$

will be considered, where DPL(2,2) is obtained with

$$A = \frac{1}{\alpha}, \quad B = \frac{\tau_q}{\alpha}, \quad C = \frac{\tau_q^2}{2\alpha}, \quad D = \tau_T, \quad E = \frac{\tau_T^2}{2},$$

while DPL(2,1) is the particular case with $E = 0$.

In the next section, after introducing new variables to write (2.6) as a first order system in t, a Crank-Nicholson type difference scheme is developed. In Section 3, convergence is analyzed, first showing the stability of the method, written as a two-level scheme, and then proving its consistency, giving bounds on the truncation errors. Finally, in Section 4, some numerical examples are presented.

2.2. Finite difference scheme

Introducing the two new variables

$$v(x,t) = BT(x,t) + C\frac{\partial}{\partial t}T(x,t) \tag{2.7}$$

and

$$u(x,t) = AT(x,t) + \frac{\partial}{\partial t}v(x,t), \tag{2.8}$$

Eq. 2.6 can be written as

$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}\left(T(x,t) + D\frac{\partial}{\partial t}T(x,t) + E\frac{\partial^2}{\partial t^2}T(x,t)\right),$$

or, since from (2.7) and (2.8)

$$\frac{\partial}{\partial t}T(x,t) = \frac{1}{C}\left(v(x,t) - BT(x,t)\right),$$

$$\frac{\partial^2}{\partial t^2}T(x,t) = \frac{1}{C}\left(u(x,t) - AT(x,t) - B\frac{\partial}{\partial t}T(x,t)\right),$$

and

$$\frac{\partial^2}{\partial t^2}T\left(x,t\right)=\frac{1}{C}\left(u\left(x,t\right)-AT\left(x,t\right)-\frac{B}{C}v\left(x,t\right)+\frac{B^2}{C}T\left(x,t\right)\right),$$

Eq. 2.6 can be expressed as

$$\frac{\partial}{\partial t}u\left(x,t\right)=\frac{\partial^2}{\partial x^2}\left(aT\left(x,t\right)+bv\left(x,t\right)+cu\left(x,t\right)\right), \tag{2.9}$$

where

$$a=(C^2+EB^2-BDC-ACE)/C^2, \quad b=(DC-BE)/C^2, \quad c=E/C.$$

Hence, since from (2.7) and (2.8) one gets

$$\frac{\partial}{\partial t}T\left(x,t\right)=\frac{1}{C}\left(v\left(x,t\right)-BT\left(x,t\right)\right) \tag{2.10}$$

and

$$\frac{\partial}{\partial t}v\left(x,t\right)=u\left(x,t\right)-AT\left(x,t\right), \tag{2.11}$$

the mixed problem given by Eq. 2.6 with boundary conditions (2.4) and initial conditions (2.5) is equivalent to the system consisting of equations (2.9)-(2.11), with boundary conditions

$$\begin{aligned} u(0,t)&=u(l,t)=0,\\ T(0,t)&=T(l,t)=0, \quad t\geq 0,\\ v(0,t)&=v(l,t)=0, \end{aligned} \tag{2.12}$$

and initial conditions

$$\begin{aligned} u\left(x,0\right) &= A\phi\left(x\right)+B\varphi\left(x\right)+C\psi\left(x\right), \\ T\left(x,0\right) &= \phi\left(x\right), \qquad\qquad\qquad\qquad x\in\left[0,l\right]. \\ v\left(x,0\right) &= B\phi\left(x\right)+C\varphi\left(x\right), \end{aligned} \tag{2.13}$$

In what follows, a bounded domain $[0,l]\times[0,T_M]$, for some fixed $T_M>0$, will be considered, together with the uniform mesh $\{(x_j,t_n), j=0\dots P, n=0\dots N\}$, defined by the increments $h=\Delta x$ and $k=\Delta t$, such that $l=Ph$ and $T_M=Nk$. The value of any function w at a point (x_j,t_n) in the mesh will be denoted w_j^n.

The proposed finite difference scheme for DPL(2,2) model will be derived from the following finite difference approximations in equations (2.9)-(2.11),

$$\begin{aligned} \frac{u_j^{n+1}-u_j^n}{k} &= \frac{1}{2}\delta_x^2\left(aT_j^n+bv_j^n+cu_j^n\right) \\ &+ \frac{1}{2}\delta_x^2\left(aT_j^{n+1}+bv_j^{n+1}+cu_j^{n+1}\right), \end{aligned} \tag{2.14}$$

$$\frac{T_j^{n+1}-T_j^n}{k} = -\frac{B}{C}\left(\frac{T_j^{n+1}+T_j^n}{2}\right)+\frac{1}{C}\left(\frac{v_j^{n+1}+v_j^n}{2}\right), \tag{2.15}$$

$$\frac{v_j^{n+1}-v_j^n}{k} = \frac{1}{2}\left(u_j^{n+1}+u_j^n\right)-\frac{A}{2}\left(T_j^{n+1}+T_j^n\right), \tag{2.16}$$

where

$$\delta_x^2 w_j^n = \frac{w_{j-1}^n-2w_j^n+w_{j+1}^n}{h^2}.$$

Discretized boundary and initial conditions, corresponding to (2.12) and

(2.13), are given by

$$u_0^n = u_P^n, \quad T_0^n = T_P^n = 0, \quad v_0^n = v_P^n = 0, \quad n = 0 \dots N, \tag{2.17}$$

and

$$\begin{aligned} u_j^0 &= A\phi(jh) + B\varphi(jh) + C\psi(jh), \\ T_j^0 &= \phi(jh), \\ v_j^0 &= B\phi(jh) + C\varphi(jh), \end{aligned} \qquad j = 0, \dots, P. \tag{2.18}$$

Solving for T_j^{n+1} and v_j^{n+1} in (2.15) and (2.16), substituting into (2.14), and writing $r = h/k^2$,

$$\begin{aligned} x_k &= 4C + 2Bk + Ak^2, \\ y_k &= 4C - 2Bk - Ak^2, \\ z_k &= 4C + 2Bk - Ak^2, \\ \alpha_k &= \frac{r}{2}\left(c + \frac{x_k + z_k}{x_k}\frac{bk}{4} + \frac{ak^2}{x_k}\right), \\ \beta_k &= \frac{r}{2}\left(a + \frac{ay_k}{x_k} - \frac{x_k + y_k}{x_k}\frac{bAk}{2}\right), \\ \gamma_k &= \frac{r}{2}\left(b + \frac{4ak}{x_k} + \frac{bz_k}{x_k}\right), \end{aligned}$$

the following expressions for the scheme can be obtained,

$$T_j^{n+1} = \frac{k^2}{x_k}u_j^n + \frac{y_k}{x_k}T_j^n + \frac{4k}{x_k}v_j^n + \frac{k^2}{x_k}u_j^{n+1}, \tag{2.19}$$

$$v_j^{n+1} = \frac{x_k + z_k}{4x_k} k u_j^n - \frac{x_k + y_k}{2x_k} A k T_j^n + \frac{z_k}{x_k} v_j^n + \frac{x_k + z_k}{4x_k} k u_j^{n+1}, \quad (2.20)$$

and

$$u_j^{n+1} - \alpha_k \left(u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}\right) = u_j^n + \alpha_k \left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \beta_k \left(T_{j-1}^n - 2T_j^n + T_{j+1}^n\right) + \gamma_k \left(v_{j-1}^n - 2v_j^n + v_{j+1}^n\right). \quad (2.21)$$

Introducing, for $n = 0 \ldots N$, the vectors U^n, T^n, and V^n, where U^n stacks up the $P-1$ values $u_j^n, j = 1, \ldots, P-1$, and similarly for T^n and V^n, and writing M for the tridiagonal $(P-1) \times (P-1)$ matrix $M = tridiag\,(1, -2, 1)$, the equations of the scheme can be given in matrix form as follows,

$$(I - \alpha_k M)\, U^{n+1} = (I + \alpha_k M)\, U^n + \beta_k M T^n + \gamma_k M V^n, \quad (2.22)$$

$$T^{n+1} = \frac{k^2}{x_k} U^n + \frac{y_k}{x_k} T^n + \frac{4k}{x_k} V^n + \frac{k^2}{x_k} U^{n+1}, \quad (2.23)$$

and

$$V^{n+1} = \frac{x_k + z_k}{4x_k} k U^n - \frac{x_k + y_k}{2x_k} A k T^n + \frac{z_k}{x_k} V^n + \frac{x_k + z_k}{4x_k} k U^{n+1}, \quad (2.24)$$

where I denotes the $(P-1) \times (P-1)$ identity matrix.

Hence, starting from the initial values given by (2.18), and taking into account the boundary conditions (2.17), the method can progress from step n to step $n+1$, solving for U^{n+1} in (2.22), which can be done very efficiently, since the coefficient of U^{n+1} is also a tridiagonal matrix, and substituting into equations (2.23) and (2.24), to obtain T^{n+1} and V^{n+1}.

2.3. Convergence, stability and consistency

To prove the convergence of the scheme introduced above, it will be shown in this section that the method is unconditionally stable, for any finite value of $r = h/k^2$, and that it is consistent with the original partial differential equation. Thus, from Lax equivalence theorem [28], convergence will follow.

First, the method will be written as a two-level scheme. Solving for U^{n+1} in (2.22), and writing

$$X_k = (I - \alpha_k M), \quad Y_k = (I + \alpha_k M),$$

one gets

$$U^{n+1} = X_k^{-1} Y_k U^n + \beta_k X_k^{-1} M T^n + \gamma_k X_k^{-1} M V^n,$$

and, substituting into (2.23) and (2.24),

$$\begin{aligned}
T^{n+1} &= \frac{k^2}{x_k}\left(I + X_k^{-1}Y_k\right)U^n + \left(\frac{y_k}{x_k}I + \frac{k^2}{x_k}\beta_k X_k^{-1}M\right)T^n \\
&+ \left(\frac{4k}{x_k}I + \frac{k^2}{x_k}\gamma_k X_k^{-1}M\right)V^n \\
V^{n+1} &= \frac{x_k + z_k}{4x_k}k\left(I + X_k^{-1}Y_k\right)U^n \\
&+ \left(-\frac{x_k + y_k}{2x_k}Ak + \frac{x_k + z_k}{4x_k}k\beta_k X_k^{-1}M\right)T^n \\
&\quad + \left(\frac{z_k}{x_k}I + \frac{x_k + z_k}{4x_k}k\gamma_k X_k^{-1}M\right)V^n
\end{aligned}$$

Considering the stack vector $[U^n, T^n, V^n]^T$, where the superindex T denotes the transpose, the method can be written as the two-level scheme

$$\left[U^{n+1}, T^{n+1}, V^{n+1}\right]^T = Q_k \left[U^n, T^n, V^n\right]^T, \tag{2.25}$$

where the matrix of the scheme, Q_k, is given by

$$Q_k = \begin{bmatrix} Q_k^{1,1} & Q_k^{1,2} & Q_k^{1,3} \\ Q_k^{2,1} & Q_k^{2,2} & Q_k^{2,3} \\ Q_k^{3,1} & Q_k^{3,2} & Q_k^{3,3} \end{bmatrix}, \tag{2.26}$$

where

$$\begin{aligned}
Q_k^{1,1} &= X_k^{-1} Y_k, \\
Q_k^{1,2} &= \beta_k X_k^{-1} M, \\
Q_k^{1,3} &= \gamma_k X_k^{-1} M, \\
Q_k^{2,1} &= \frac{k^2}{x_k}\left(I + X_k^{-1} Y_k\right), \\
Q_k^{2,2} &= \frac{8C - x_k}{x_k} I + \frac{k^2}{x_k} \beta_k X_k^{-1} M, \\
Q_k^{2,3} &= \frac{4k}{x_k} I + \frac{k^2}{x_k} \gamma_k X_k^{-1} M, \\
Q_k^{3,1} &= \frac{2C + Bk}{x_k} k \left(I + X_k^{-1} Y_k\right), \\
Q_k^{3,2} &= -\frac{4CAk}{x_k} I + \frac{2C + Bk}{x_k} k \beta_k X_k^{-1} M, \\
Q_k^{3,3} &= \frac{z_k}{x_k} I + \frac{2C + Bk}{x_k} k \gamma_k X_k^{-1} M.
\end{aligned}$$

It can be shown that, writing

$$X^{-1} = \left(I - \frac{1}{2}rcM\right)^{-1}, \quad Y = \left(I + \frac{1}{2}rcM\right),$$

$$Q = \mathop{\mathrm{lím}}_{k\to 0} Q_k = \begin{bmatrix} X^{-1}Y & raX^{-1}M & rbX^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.$$

Also, taking into account that matrices M, X, and Y commute, one gets

$$Q^n = \begin{bmatrix} (X^{-1}Y)^n & -\frac{a}{c}\left(I - (X^{-1}Y)^n\right) & -\frac{b}{c}\left(I - (X^{-1}Y)^n\right) \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.$$

The matrix $X^{-1}Y$ is similar to the matrix of the Crank-Nicolson scheme for the classical diffusion equation, and so its powers are uniformly bounded [28–30]. Thus, matrices Q^n are also uniformly bounded, and from here it can be derived that the scheme is stable in the sense of Lax [28].

2.3.1. Consistency

Consider the exact solution of the problem given by (2.9)-(2.11), defined in $[0, l] \times [0, T_M]$, which will be denoted $w = \left(\widetilde{u}, \widetilde{T}, \widetilde{v}\right)$ in this section. For a given $t = nk$ fixed, the mesh points

$$(ih, nk)\,, \ i = 0, 1, \ldots, P,$$

have the associated vector

$$W_h^k(nk) = \left[\widetilde{U}^n, \widetilde{T}^n, \widetilde{V}^n\right]^T \in \mathbb{R}^{3(P-1)}, \tag{2.27}$$

where

$$\begin{aligned} \widetilde{U}^n &= \left[\widetilde{u}(h,nk), \widetilde{u}(2h,nk), \ldots, \widetilde{u}((P-1)h,nk)\right]^T, \\ \widetilde{T}^n &= \left[\widetilde{T}(h,nk), \widetilde{T}(2h,nk), \ldots, \widetilde{T}((P-1)h,nk)\right]^T, \\ \widetilde{V}^n &= \left[\widetilde{v}(h,nk), \widetilde{v}(2h,nk), \ldots, \widetilde{v}((P-1)h,nk)\right]^T. \end{aligned}$$

The truncation error of the two-level scheme (2.25), at $t = nk$, is the vector in $\mathbb{R}^{3(P-1)}$

$$\mathfrak{T}_h^k(nk) = \frac{1}{k}\left(W_h^k((n+1)k) - Q_k W_h^k(nk)\right). \tag{2.28}$$

The difference scheme (2.25) verifies the consistency condition if the solution w of the problem (2.9)-(2.11) satisfies

$$\lim_{k\to 0} \frac{1}{k}\left\|W_h^k((n+1)k) - Q_k W_h^k(nk)\right\|_\infty = 0, \text{ for } 0 \le nk \le T_M, \tag{2.29}$$

for every set of initial functions guaranteeing sufficient conditions of regularity of w.

The local truncation error at the point in the mesh (jh, nk), [28, p. 20], is given by

$$\left(\mathcal{T}_{1,j}^n, \mathcal{T}_{2,j}^n, \mathcal{T}_{3,j}^n\right) = \mathcal{L} w_j^n,$$

where $\mathcal{L} = (\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3)$ is the difference operator associated with the scheme [31, p. 42], that is

$$
\begin{aligned}
\mathcal{L}_1 w_j^n &= \frac{\widetilde{u}_j^{n+1} - \widetilde{u}_j^n}{k} - \frac{1}{2}\delta_x^2\left(a\widetilde{T}_j^n + b\widetilde{v}_j^n + c\widetilde{u}_j^n\right) \\
&- \frac{1}{2}\delta_x^2\left(a\widetilde{T}_j^{n+1} + b\widetilde{v}_j^{n+1} + c\widetilde{u}_j^{n+1}\right), \\
\mathcal{L}_2 w_j^n &= \frac{\widetilde{T}_j^{n+1} - \widetilde{T}_j^n}{k} + \frac{B}{2C}\left(\widetilde{T}_j^{n+1} + \widetilde{T}_j^n\right) - \frac{1}{2C}\left(\widetilde{v}_j^{n+1} + \widetilde{v}_j^n\right), \\
\mathcal{L}_3 w_j^n &= \frac{\widetilde{v}_j^{n+1} - \widetilde{v}_j^n}{k} - \frac{\widetilde{u}_j^{n+1} + \widetilde{u}_j^n}{2} + \frac{A}{2}\left(\widetilde{T}_j^{n+1} + \widetilde{T}_j^n\right),
\end{aligned}
$$

where $\left(\widetilde{u}_j^n, \widetilde{T}_j^n, \widetilde{v}_j^n\right)$ are the values of the exact solution at the points in the mesh.

One can verify that

$$
\mathfrak{T}_h^k(nk) = E_k\left[\mathcal{T}_1^n, \mathcal{T}_2^n, \mathcal{T}_3^n\right]^T, \tag{2.30}
$$

where $\mathcal{T}_i^n = \left[\mathcal{T}_{i,1}^n, \mathcal{T}_{i,2}^n, \ldots, \mathcal{T}_{i,P-1}^n\right]^T$, $i = 1, 2, 3$, and

$$
E_k = \begin{bmatrix} E_k^{1,1} & E_k^{1,2} & E_k^{1,3} \\ E_k^{2,1} & E_k^{2,2} & E_k^{2,3} \\ E_k^{3,1} & E_k^{3,2} & E_k^{3,3} \end{bmatrix},
$$

where

$$
\begin{aligned}
E_k^{1,1} &= X_k^{-1}, \\
E_k^{1,2} &= \frac{rC\left(2a - kAb\right)}{x_k} X_k^{-1} M, \\
E_k^{1,3} &= \frac{r\left(ka + b\left(2C + Bk\right)\right)}{x_k} X_k^{-1} M,
\end{aligned}
$$

$$
\begin{aligned}
E_k^{2,1} &= \frac{k^2}{x_k} X_k^{-1}, \\
E_k^{2,2} &= \frac{4C}{x_k} I + \frac{rCk^2 \left(2a - kAb\right)}{x_k^2} X_k^{-1} M, \\
E_k^{2,3} &= \frac{2k}{x_k} I + \frac{rk^3 \left(a + b\left(2C + Bk\right)\right)}{x_k^2} X_k^{-1} M, \\
E_k^{3,1} &= \frac{2C + Bk}{x_k} k X_k^{-1}, \\
E_k^{3,2} &= -\frac{2C}{x_k} k \left(AI - \frac{r\left(2C + Bk\right)\left(2a - kAb\right)}{2x_k} X_k^{-1} M \right), \\
E_k^{3,3} &= \frac{2\left(2C + Bk\right)}{x_k} \left(I + \frac{r\left(ka + b\left(2C + Bk\right)\right)}{2x_k} k X_k^{-1} M \right),
\end{aligned}
$$

with

$$
E = \lim_{k \to 0} E_k = \begin{bmatrix} X^{-1} & \frac{ra}{2} X^{-1} M & \frac{br}{2} X^{-1} M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}. \tag{2.31}
$$

For a generic function g, to estimate the values g_j^n and g_j^{n+1}, the Taylor expansion

$$
\begin{aligned}
g\left(x, t\right) \quad = \quad & g\left(x_0, t_0\right) + \left[\frac{\partial g}{\partial t}\left(x_0, t_0\right) \cdot \left(t - t_0\right) + \frac{\partial g}{\partial x}\left(x_0, t_0\right) \cdot \left(x - x_0\right) \right] + \\
& + \frac{1}{2} \left[\frac{\partial^2 g}{\partial t^2}\left(x_0, t_0\right) \cdot \left(t - t_0\right)^2 \right. \\
& + 2 \frac{\partial^2 g}{\partial t \partial x}\left(x_0, t_0\right) \cdot \left(t - t_0\right)\left(x - x_0\right) \\
& \quad \left. + \frac{\partial^2 g}{\partial x^2}\left(x_0, t_0\right) \cdot \left(x - x_0\right)^2 \right] + R_2\left(x, t\right),
\end{aligned}
$$

with remainder

$$R_2(x,t) = \frac{1}{6}\left[\sum_{i=0}^{3} \frac{3!}{(3-i)!i!} \frac{\partial^3 g}{\partial t^{3-i}\partial x^i}(\xi,\tau)\cdot(t-t_0)^{3-i}(x-x_0)^i\right].$$

can be applied to $g(x,t)$ in the points $(x_0,t_0) = \left(jh,\left(n+\frac{1}{2}\right)k\right)$ and $(x_0,t_0) = (jh,(n+1)k)$, obtaining

$$\frac{g_j^{n+1}-g_j^n}{k} = \frac{\partial g}{\partial t}\left(jh,\left(n+\frac{1}{2}\right)k\right) + O\left(k^2\right), \tag{2.32}$$

$$\frac{g_j^n+g_j^{n+1}}{2} = g\left(jh,\left(n+\frac{1}{2}\right)k\right) + O\left(k^2\right). \tag{2.33}$$

Finding expressions for g_{j+1}^{m+1}, g_j^{m+1}, and g_{j-1}^{m+1} using a third order Taylor's expansion for $g(x,t)$ in the point $\left(jh,\left(m+\frac{1}{2}\right)k\right)$, one gets

$$\frac{1}{2}\left[\delta_x^2 g_j^m + \delta_x^2 g_j^{m+1}\right] = \frac{\partial^2 g}{\partial x^2}\left(jh,\left(m+\frac{1}{2}\right)k\right) + O\left(k^2\right) + O\left(h^2\right). \tag{2.34}$$

From the estimations provided by (2.32), (2.33) and (2.34), applied to the components of the local truncation error, it follows that

$$\begin{aligned}
\mathcal{T}_{1,j}^n &= O\left(k^2\right) + O\left(h^2\right),\\
\mathcal{T}_{2,j}^n &= O\left(k^2\right),\\
\mathcal{T}_{3,j}^n &= O\left(k^2\right).
\end{aligned}$$

Thus, since from (2.31) it follows that E_k has bounded norm, it can be deduced that the scheme is consistent with the partial differential equation, and also that the truncation error satisfies

$$\left\|\mathfrak{T}_h^k\left(nk\right)\right\|_\infty = O\left(k^2\right) + O\left(h^2\right).$$

2.4. Numerical examples

In this section examples of DPL(2,2) and DPL(2,1) models, with simple initial functions so that the exact solutions can be computed, are presented, comparing the exact values with the numerical approximations provided by the difference scheme.

Consider the mixed problem given by Eq. 2.6, with $l = 1$, parameters $\alpha = \alpha_{Cu} = 1{,}1283 \cdot 10^{-4}$ m^2/s, $\tau_q = \tau_{Cu} = 0{,}4648$ ps, and $\tau_T = \tau_{Cu} = 70{,}833$ ps, corresponding to those experimentally found in Copper [2, p. 123], and with boundary conditions (2.4) and initial conditions

$$\left.\begin{aligned} T(x,0) &= \sin(\pi x), \\ \frac{\partial}{\partial t}T(x,0) &= -\alpha_{Cu}\pi^2\sin(\pi x), \\ \frac{\partial^2}{\partial t^2}T(x,0) &= 0, \end{aligned}\right. \qquad x \in [0,l]\,.$$

In Figure 1, the exact solution for this problem (left), and the differences with DPL(2,1) model (right) is presented. In Fig. 2, maximum errors of the approximate solutions, in terms of time, are presented for DPL(2,2) model (top) and DPL(2,1) model (down), showing the expected order of approximation in relation with the size of the mesh (right).

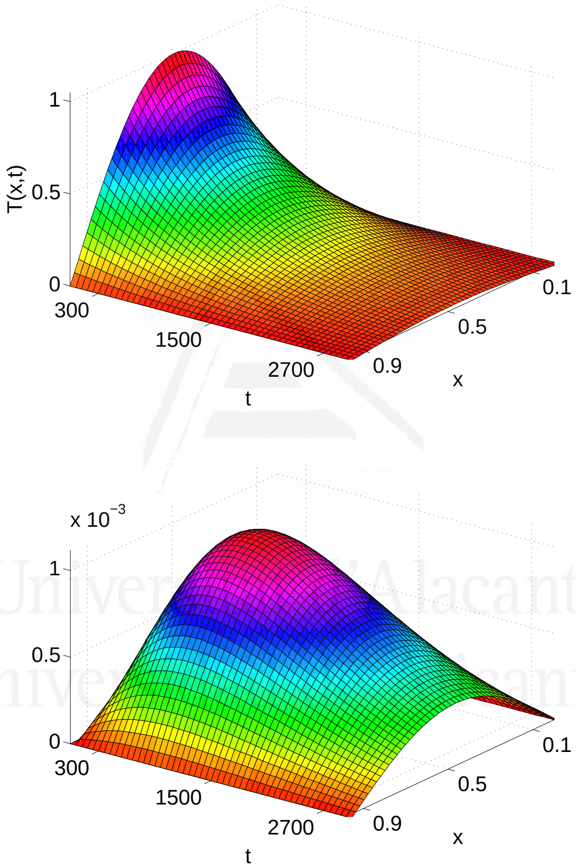

Figura 2.1: Temperature evolution for DPL(2,2) model (up), and absolute differences with DPL(2,1) model (down).

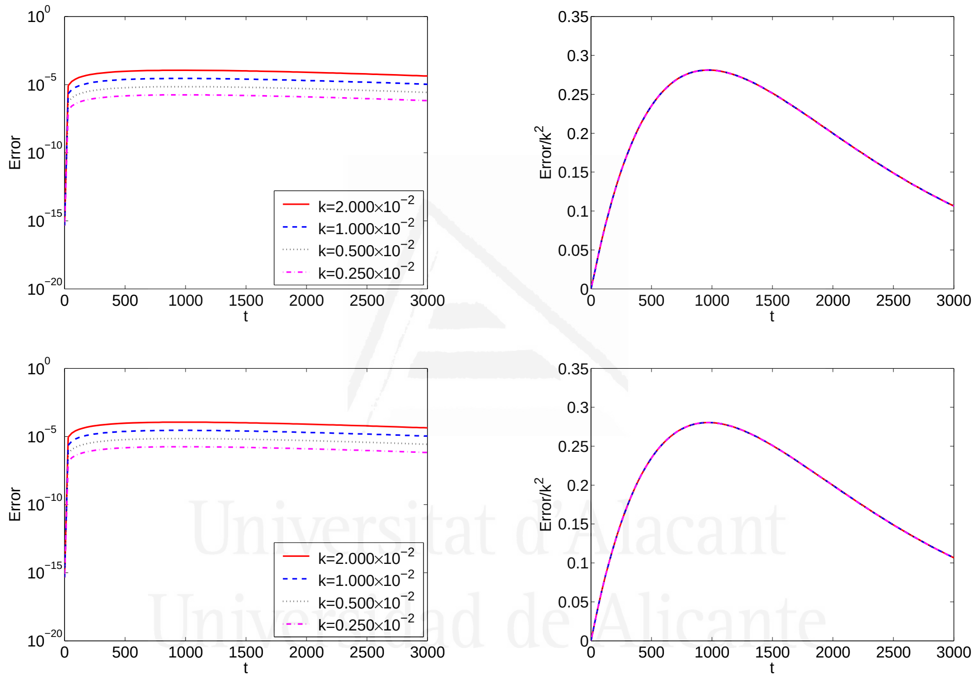

Figura 2.2: Maximum errors of the approximate solutions, in terms of time, for DPL(2,2) model (top, left) and DPL(2,1) model (down, left), and relation with the size of the mesh (right).

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Capítulo 3

A compact difference scheme for numerical solutions of second order dual-phase-lagging models of microscale heat transfer

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A compact difference scheme for numerical solutions of second order dual-phase-lagging models of microscale heat transfer

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ABSTRACT

Dual-phase-lagging (DPL) models constitute a family of non-Fourier models of heat conduction that allow for the presence of time lags in the heat flux and the temperature gradient. These lags may need to be considered when modeling microscale heat transfer, and thus DPL models have found application in the last years in a wide range of theoretical and technical heat transfer problems. Consequently, analytical solutions and methods for computing numerical approximations have been proposed for particular DPL models in different settings.

In this work, a compact difference scheme for second order DPL models is developed, providing higher order precision than a previously proposed method. The scheme is shown to be unconditionally stable and convergent, and its accuracy is illustrated with numerical examples.

1. Introduction

Technical advances in nanomaterials and in the applications of ultrafast lasers have lead in last two decades to an increasing interest in non-Fourier models of heat conduction [1–5]. These models try to account for phenomena, such as finite speeds of propagation and wave behaviors, that appear when studying heat transfer at the microscale level, i.e., in very short time intervals or at very small space dimensions [6,7].

The basis for the dual-phase-lagging (DPL) family of models is the introduction of two time lags into the Fourier law [7–9],

$$\mathbf{q}(\mathbf{r}, t+\tau_q) = -k\nabla T(\mathbf{r}, t+\tau_T), \tag{1}$$

where τ_q and τ_T are, respectively, the phase lags in the heat flux vector, $\mathbf{q}$, and the temperature gradient, ∇T, t and $\mathbf{r}$ are the time and spatial coordinates, and k is the conductivity.

When both lags are zero, so that the classical Fourier law is recovered, the combination of (1) with the conservation of energy principle leads to the diffusion or classical heat conduction equation. Otherwise, a partial differential equation with delay is obtained [10,11].

Most commonly, though, first or higher order approximations in the time lags in (1) are used [8,12,13]. In this work, the heat equation resulting from first order approximations,

$$\frac{\partial}{\partial t}T(\mathbf{r}, t) + \tau_q \frac{\partial^2}{\partial t^2}T(\mathbf{r}, t) = \alpha\left(\Delta T(\mathbf{r}, t) + \tau_T \Delta \frac{\partial}{\partial t}T(\mathbf{r}, t)\right), \tag{2}$$

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When both lags are zero, so that the classical Fourier law is recovered, the combination of (3.1) with the conservation of energy principle leads to the diffusion or classical heat conduction equation. Otherwise, a partial differential equation with delay is obtained [10, 11].

Most commonly, though, first or higher order approximations in the time lags in (3.1) are used [8, 12, 13]. In this work, the heat equation resulting from first order approximations,

$$\frac{\partial}{\partial t}T(\mathbf{r}, t) + \tau_q \frac{\partial^2}{\partial t^2}T(\mathbf{r}, t) = \alpha \left(\Delta T(\mathbf{r}, t) + \tau_T \Delta \frac{\partial}{\partial t} T(\mathbf{r}, t) \right), \tag{3.2}$$

usually referred to as the DPL model [8], will be denoted DPL(1,1), and the equations derived from second order approximation in τ_q and up to second order approximation in τ_T will be denoted DPL(2,1),

$$\begin{aligned}\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)+\frac{\tau_q^2}{2}\frac{\partial^3}{\partial t^3}T(\mathbf{r},t)&=\alpha\Delta T(\mathbf{r},t)\\&+\alpha\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t),\end{aligned}\tag{3.3}$$

and DPL(2,2),

$$\begin{aligned}\frac{\partial}{\partial t}T(\mathbf{r},t)+\tau_q\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)+\frac{\tau_q^2}{2}\frac{\partial^3}{\partial t^3}T(\mathbf{r},t)&=\alpha\Delta T(\mathbf{r},t)\\&+\alpha\tau_T\Delta\frac{\partial}{\partial t}T(\mathbf{r},t)+\alpha\frac{\tau_T^2}{2}\Delta\frac{\partial^2}{\partial t^2}T(\mathbf{r},t)).\end{aligned}\tag{3.4}$$

The construction of numerical solutions for DPL(1,1) model and variations in different settings has been addressed in previous works (e.g., [14–19]). For DPL(2,2) models, a Crank-Nicholson type difference scheme was presented in [20]. The objective of this work is to develop a higher order, compact difference scheme for the same problem considered in [20], in an similar way as was done in [17] for DPL(1,1) models but employing a more direct approach to construct the scheme and prove its stability and convergence.

As in [20], a general equation for heat conduction in one dimension will be considered,

$$\begin{aligned}\frac{\partial}{\partial t}\left(AT\left(x,t\right)+B\frac{\partial}{\partial t}T\left(x,t\right)+C\frac{\partial^2}{\partial t^2}T\left(x,t\right)\right)&=\frac{\partial^2}{\partial x^2}\big(T\left(x,t\right)\\&+D\frac{\partial}{\partial t}T\left(x,t\right)+E\frac{\partial^2}{\partial t^2}T\left(x,t\right)\big),\end{aligned}\tag{3.5}$$

which includes DPL(2,2), as given by (3.4), by taking

$$A = \frac{1}{\alpha}, \quad B = \frac{\tau_q}{\alpha}, \quad C = \frac{\tau_q^2}{2\alpha}, \quad D = \tau_T, \quad E = \frac{\tau_T^2}{2}, \tag{3.6}$$

and reduces to DPL(2,1) when $E = 0$. The problem is stated for a finite domain $x \in [0, l]$, with Dirichlet boundary conditions,

$$T(0,t) = T(l,t) = 0, \ t \geq 0, \tag{3.7}$$

and initial conditions

$$T(x,0) = \phi(x), \ \frac{\partial}{\partial t}T(x,0) = \varphi(x), \ \frac{\partial^2}{\partial t^2}T(x,0) = \psi(x), \ x \in [0,l]\,. \tag{3.8}$$

The rest of the paper is organized as follows. In the next section, the new compact difference scheme for DPL(2,2) model is constructed. In Section 3, after expressing the method as a two-level scheme, the unconditional stability of the method is proved. Next, in Section 4, assuming sufficient regularity of the solution, the consistency of the method is shown, and bounds on the truncation errors are obtained. In the last section, numerical examples are presented, illustrating the higher accuracy of the new method in comparison with the scheme previously proposed in [20].

3.2. Construction of the compact finite difference scheme

First, two new variables, $v(x,t)$ and $u(x,t)$, are introduced in order to express (3.5) as a first order system in t,

$$v\left(x,t\right) = BT\left(x,t\right) + C\frac{\partial}{\partial t}T\left(x,t\right), \tag{3.9}$$

and

$$u\left(x,t\right) = AT\left(x,t\right) + \frac{\partial}{\partial t}v\left(x,t\right). \tag{3.10}$$

Thus, using (3.9) and (3.10), it can be shown that Eq. 3.5 can be written as

$$\frac{\partial}{\partial t}u\left(x,t\right) = a\frac{\partial^2}{\partial x^2}T\left(x,t\right) + b\frac{\partial^2}{\partial x^2}v\left(x,t\right) + c\frac{\partial^2}{\partial x^2}u\left(x,t\right), \tag{3.11}$$

where

$$\begin{aligned} a &= (C^2 + EB^2 - BDC - ACE)/C^2, \\ b &= (DC - BE)/C^2, \\ c &= E/C. \end{aligned} \tag{3.12}$$

Consequently, writing (3.9) and (3.10) in the form

$$\frac{\partial}{\partial t}T\left(x,t\right) = \frac{1}{C}\left(v\left(x,t\right) - BT\left(x,t\right)\right) \tag{3.13}$$

and

$$\frac{\partial}{\partial t}v\left(x,t\right) = u\left(x,t\right) - AT\left(x,t\right), \tag{3.14}$$

an equivalent problem to that consisting of equation (3.5), boundary conditions (3.7), and initial conditions (3.8) is given by the system of equations (3.11)-(3.14), with boundary conditions

$$\begin{aligned} u(0,t) &= u(l,t) = 0, \\ T(0,t) &= T(l,t) = 0, \quad t \geq 0, \\ v(0,t) &= v(l,t) = 0, \end{aligned} \tag{3.15}$$

and initial conditions

$$\begin{aligned} u\left(x,0\right) &= A\phi\left(x\right) + B\varphi\left(x\right) + C\psi\left(x\right), \\ T\left(x,0\right) &= \phi\left(x\right), & x \in \left[0,l\right]. \\ v\left(x,0\right) &= B\phi\left(x\right) + C\varphi\left(x\right), \end{aligned} \tag{3.16}$$

Numerical solutions will be computed inside a bounded domain $[0,l] \times [0,T_M]$, for some fixed $T_M > 0$, at the points of the mesh $\{(x_j,t_n), j = 0 \ldots P, n = 0 \ldots N\}$, where $l = Ph$ and $T_M = Nk$ for spatial increment $h = \Delta x$ and temporal increment $k = \Delta t$. In what follows, for any function w, w_j^n will denote its value at the point (x_j,t_n).

To derive the new numerical scheme for DPL(2,2) model, the following finite difference approximations will be used in equations (3.13) and (3.14),

$$\frac{1}{k}\left(T_j^{n+1} - T_j^n\right) = -\frac{B}{2C}\left(T_j^{n+1} + T_j^n\right) + \frac{1}{2C}\left(v_j^{n+1} + v_j^n\right), \tag{3.17}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = \frac{1}{2}\left(u_j^{n+1} + u_j^n\right) - \frac{A}{2}\left(T_j^{n+1} + T_j^n\right). \tag{3.18}$$

For Eq. 3.11, two different approaches may be followed. Writing

$$f(x,t) = \frac{\partial^2}{\partial x^2} T(x,t), \quad g(x,t) = \frac{\partial^2}{\partial x^2} v(x,t), \quad s(x,t) = \frac{\partial^2}{\partial x^2} u(x,t),$$

using in (3.11) the finite approximations

$$\frac{1}{k}\left(u_j^{n+1} - u_j^n\right) = \frac{a}{2}\left(f_j^{n+1} + f_j^n\right) + \frac{b}{2}\left(g_j^{n+1} + g_j^n\right) + \frac{c}{2}\left(s_j^{n+1} + s_j^n\right),$$

and considering for the functions f, g, and s the compact fourth order finite difference approximation [21],

$$\frac{1}{10} f_{j-1}^n + f_j^n + \frac{1}{10} f_{j+1}^n = \frac{6}{5}\delta_x^2 T_j^n,$$

where

$$\delta_x^2 w_j^n = \frac{1}{h^2}\left(w_{j-1}^n - 2w_j^n + w_{j+1}^n\right),$$

with analogous approximations for g and s, after some algebraic manipulations one can get to the expression

$$\begin{aligned} & u_{j-1}^{n+1} + 10u_j^{n+1} + u_{j+1}^{n+1} - \left(u_{j-1}^n + 10u_j^n + u_{j+1}^n\right) = 6ak\delta_x^2\left(T_j^{n+1} + T_j^n\right) \\ & + 6bk\delta_x^2\left(v_j^{n+1} + v_j^n\right) + 6ck\delta_x^2\left(u_j^{n+1} + u_j^n\right). \end{aligned} \tag{3.19}$$

This approach, analogous to that used in [17] for the corresponding DPL(1,1) model, emphasizes the obtention of the scheme from the class of compact finite approximations presented in [21], suggesting the way for generalizations by using other higher-order compact finite difference from [21].

However, a much more direct derivation of (3.19) can be obtained by using for Eq. 3.11 the following finite difference approximations,

$$\frac{1}{12k}\left(u_{j+1}^{n+1}-u_{j+1}^{n}\right)+\frac{5}{6k}\left(u_{j}^{n+1}-u_{j}^{n}\right)+\frac{1}{12k}\left(u_{j-1}^{n+1}-u_{j-1}^{n}\right)=$$
$$\frac{a}{2}\delta_x^2\left(T_j^{n+1}+T_j^n\right)+\frac{b}{2}\delta_x^2\left(v_j^{n+1}+v_j^n\right)+\frac{c}{2}\delta_x^2\left(u_j^{n+1}+u_j^n\right),$$

which are analogous to those leading to a classical method for the diffusion equation [22, p. 191], and let immediately to equation (3.19). Besides its simpler derivation, the advantage of this approach is that it relates the new scheme to a difference method for classical heat conduction that is known to be unconditionally stable, providing the basis for a direct analysis of the stability of the new method in the next section.

Thus, the new scheme is defined by equations (3.17), (3.18), and (3.19), together with the discretized boundary and initial conditions, corresponding to (3.15) and (3.16),

$$u_0^n=u_P^n,\ T_0^n=T_P^n=0,\ v_0^n=v_P^n=0,\ n=0\ldots N, \tag{3.20}$$

and

$$\begin{aligned}
u_j^0 &= A\phi(jh)+B\varphi(jh)+C\psi(jh), \\
T_j^0 &= \phi(jh), \qquad\qquad j=0,\ldots,P. \\
v_j^0 &= B\phi(jh)+C\varphi(jh),
\end{aligned} \tag{3.21}$$

Next, the scheme will be expressed in matrix form. Consider, for $n=0\ldots N$, the vectors U^n, T^n, and V^n, where U^n, respectively T^n and V^n, stacks up the $P-1$ values u_j^n, respectively T_j^n and v_j^n, for $j=1,\ldots,P-1$. Writing $r=h/k^2$, and introducing the two tridiagonal $(P-1)\times(P-1)$ matrices $M=tridiag\,(1,-2,1)$ and $S=tridiag\,(1,10,1)$, i.e., tridiagonal matrices with ones in the upper and lower diagonals and with -2, for M, or with 10, for S, in the main diagonal, the expression of the scheme as a system of matrix equations is given by

$$\begin{aligned} S\left(U^{n+1}-U^{n}\right) =&6r\left(aM\left(T^{n+1}+T^{n}\right)+bM\left(V^{n+1}+V^{n}\right)\right. \\ &\left.+\,cM\left(U^{n+1}+U^{n}\right)\right), \end{aligned} \tag{3.22}$$

$$\frac{1}{k}\left(T^{n+1}-T^{n}\right)=-\frac{B}{2C}\left(T^{n+1}+T^{n}\right)+\frac{1}{2C}\left(V^{n+1}+V^{n}\right), \tag{3.23}$$

and

$$\frac{1}{k}\left(V^{n+1}-V^{n}\right)=\frac{1}{2}\left(U^{n+1}+U^{n}\right)-\frac{A}{2}\left(T^{n+1}+T^{n}\right). \tag{3.24}$$

More practical expressions can be obtained by solving for T^{n+1} and V^{n+1} in (3.23) and (3.24), and substituting into (3.22). After some rearrangements, and writing

$$x_k=4C+2Bk+Ak^2,\ y_k=4C-2Bk-Ak^2,\ z_k=4C+2Bk-Ak^2, \tag{3.25}$$

and

$$\begin{aligned} \alpha_k &= r\left(c+\frac{x_k+z_k}{x_k}\frac{bk}{4}+\frac{ak^2}{x_k}\right), \\ \beta_k &= r\left(a+\frac{ay_k}{x_k}-\frac{x_k+y_k}{x_k}\frac{bAk}{2}\right), \\ \gamma_k &= r\left(b+\frac{4ak}{x_k}+\frac{bz_k}{x_k}\right), \end{aligned} \tag{3.26}$$

the following expressions can be obtained,

$$\left(S-6\alpha_k M\right)U^{n+1}=\left(S+6\alpha_k M\right)U^{n}+6\beta_k MT^{n}+6\gamma_k MV^{n}, \tag{3.27}$$

$$T^{n+1} = \frac{y_k}{x_k}T^n + \frac{4k}{x_k}V^n + \frac{k^2}{x_k}U^n + \frac{k^2}{x_k}U^{n+1}, \tag{3.28}$$

$$V^{n+1} = -\frac{4kAC}{x_k}T^n + \frac{z_k}{x_k}V^n + \frac{2C+Bk}{x_k}kU^n + \frac{2C+Bk}{x_k}kU^{n+1}, \tag{3.29}$$

which show that, using the initial values given by (3.21) and the boundary conditions (3.20), the application of the method to obtain the numerical approximations corresponding to the next step time $n+1$ consists of solving for U^{n+1} in (3.27) and substituting into equations (3.28) and (3.29) to compute T^{n+1} and V^{n+1}. Note that the coefficient of U^{n+1} in (3.27) is a tridiagonal matrix, which allows for a very efficient computation of U^{n+1}.

Pseudocode of the algorithm used to implement the new scheme is presented in Table 3.1.

3.3. Unconditional stability of the method

To analyze the stability of the method, first it will be written as a two-level scheme. Then, using a limit argument and a form of Gronwall lemma, it will be shown that the powers of the matrix of the scheme are uniformly bounded, and hence the unconditional stability of the method will follow.

Writing

$$X_k = I - 6\alpha_k S^{-1}M, \quad Y_k = I + 6\alpha_k S^{-1}M,$$

where I denotes the $(P-1)\times(P-1)$ identity matrix, from (3.27) one

Table 3.1: Pseudocode of the algorithm for the new difference scheme

Input data

input DPL problem parameters, α, τ_T, τ_q, l, and functions giving the initial conditions, ϕ, φ, and ψ

set $A = 1/\alpha$, $B = \tau_q/\alpha$, $C = \tau_q^2/2\alpha$, $D = \tau_T$, $E = \tau_T^2/2$

input domain and mesh parameters, T_M, h, and k

set $P = l/h$, $N = T_M/k$, $r = k/h^2$

Compute auxiliary coefficients and matrices

compute a, b, and c (Eq. 3.12), and x_k, y_k, and z_k (Eq. 3.25)

compute α_k, β_k, and γ_k (Eq. 3.26)

compute tridiagonal matrices $M = tridiag\,(1, -2, 1)$ and $S = tridiag\,(1, 10, 1)$

Initial values (Eq. 3.21)

for $j = 1$ to $P - 1$ do $T_j^0 = \phi(jh)$; $V_j^0 = BT_j^0 + C\varphi(jh)$; $U_j^0 = AT_j^0 + B\varphi(jh) + C\psi(jh)$; end for

Advance computation to next time step until done (saving partial computations and reusing memory)

for $n = 1$ to N do

Compute vector U^1 by solving the tridiagonal system given by Eq. 3.27

$(S - 6\alpha_k M)\, U^1 = (S + 6\alpha_k M)\, U^0 + 6\beta_k M T^0 + 6\gamma_k M V^0$

Compute vectors V^1 and T^1 (Eqs. 3.28 and 3.29)

$T^1 = \frac{y_k}{x_k} T^0 + \frac{4k}{x_k} V^0 + \frac{k^2}{x_k} U^0 + \frac{k^2}{x_k} U^1$

$V^1 = -\frac{4kAC}{x_k} T^0 + \frac{z_k}{x_k} V^0 + \frac{2C+Bk}{x_k} k U^0 + \frac{2C+Bk}{x_k} k U^1$

Save n-step numerical approximation, T^1

Reuse memory, $T^0 = T^1$, $V^0 = V^1$, $U^0 = U^1$

end for

gets,

$$U^{n+1} = X_k^{-1} Y_k U^n + 6\beta_k X_k^{-1} S^{-1} M T^n + 6\gamma_k X_k^{-1} S^{-1} M V^n,$$

and, from (3.28) and (3.29),

$$\begin{aligned} T^{n+1} &= \frac{2k^2}{x_k} X_k^{-1} U^n + \frac{y_k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \beta_k \frac{k^2}{y_k} \right) S^{-1} M \right) T^n \\ &\quad + \frac{4k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \frac{1}{4} \gamma_k k \right) S^{-1} M \right) V^n, \end{aligned}$$

and

$$\begin{aligned} V^{n+1} &= \frac{2\left(2C + Bk\right) k}{x_k} X_k^{-1} U^n \\ &\quad - \frac{4kAC}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k + \beta_k \frac{\left(2C + Bk\right)}{4AC} \right) S^{-1} M \right) T^n \\ &\quad + \frac{z_k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \gamma_k \frac{\left(2C + Bk\right) k}{z_k} \right) S^{-1} M \right) V^n. \end{aligned}$$

Thus, introducing the stack vector $[U^n, T^n, V^n]^T$, with superindex T denoting the transpose, the method can be written as the two-level scheme

$$\left[U^{n+1}, T^{n+1}, V^{n+1}\right]^T = Q_k \left[U^n, T^n, V^n\right]^T, \tag{3.30}$$

where the matrix of the scheme, Q_k, is given by

$$Q_k = \begin{bmatrix} Q_k^{1,1} & Q_k^{1,2} & Q_k^{1,3} \\ Q_k^{2,1} & Q_k^{2,2} & Q_k^{2,3} \\ Q_k^{3,1} & Q_k^{3,2} & Q_k^{3,3} \end{bmatrix}, \tag{3.31}$$

with

$$
\begin{aligned}
Q_k^{1,1} &= X_k^{-1} Y_k, \\
Q_k^{1,2} &= 6\beta_k X_k^{-1} S^{-1} M, \\
Q_k^{1,3} &= 6\gamma_k X_k^{-1} S^{-1} M, \\
Q_k^{2,1} &= \frac{2k^2}{x_k} X_k^{-1}, \\
Q_k^{2,2} &= \frac{y_k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \beta_k \frac{k^2}{y_k} \right) S^{-1} M \right), \\
Q_k^{2,3} &= \frac{4k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \frac{1}{4} \gamma_k k \right) S^{-1} M \right), \\
Q_k^{3,1} &= \frac{2\,(2C + Bk)\,k}{x_k} X_k^{-1}, \\
Q_k^{3,2} &= -\frac{4kAC}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k + \beta_k \frac{(2C + Bk)}{4AC} \right) S^{-1} M \right), \\
Q_k^{3,3} &= \frac{z_k}{x_k} X_k^{-1} \left(I - 6 \left(\alpha_k - \gamma_k \frac{(2C + Bk)\,k}{z_k} \right) S^{-1} M \right).
\end{aligned}
$$

Writing

$$
X^{-1} = \left(I - 6rcS^{-1}M \right)^{-1}, \quad Y = I + 6rcS^{-1}M,
$$

it can be shown that the matrix $Q = \text{lím}_{k\to 0} Q_k$ is given by

$$
Q = \begin{bmatrix} X^{-1}Y & 12raX^{-1}S^{-1}M & 12rbX^{-1}S^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.
$$

Then, since the matrices M, S, X, and Y commute, one gets the following expression for the powers of the limit matrix Q,

$$Q^n = \begin{bmatrix} (X^{-1}Y)^n & -\frac{a}{c}\left(I-(X^{-1}Y)^n\right) & -\frac{b}{c}\left(I-(X^{-1}Y)^n\right) \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}.$$

Here, the matrix $X^{-1}Y$ is similar to the matrix of an unconditionally stable and convergent scheme for the classical diffusion equation [22, p. 191, scheme 12], and so its powers are uniformly bounded, i.e., there are constants $k_0 > 0$ and $C > 0$ such that, for $0 < k < k_0$ and $0 \leq nk \leq T_M$, it holds that $\|Q^n\| \leq C$.

It can be checked, by direct computation, that $\|Q_k - Q\| = O\left(k\right)$, so that there is a constant $\alpha > 0$ such that, for $0 < k < k_0$,

$$\|Q_k - Q\| \leq \alpha k.$$

Then, writing

$$\begin{aligned} Q_k^n - Q^n &= \sum_{j=0}^{n-1} Q_k^{n-1-j}\left(Q_k - Q\right)Q^j \\ &= \sum_{j=0}^{n-1}\left(Q_k^{n-1-j} - Q^{n-1-j} + Q^{n-1-j}\right)\left(Q_k - Q\right)Q^j \\ &= \sum_{j=0}^{n-1}\left(Q_k^{n-1-j} - Q^{n-1-j}\right)\left(Q_k - Q\right)Q^j \\ &\quad + \sum_{j=0}^{n-1} Q^{n-1-j}\left(Q_k - Q\right)Q^j, \end{aligned}$$

it follows that

$$\begin{aligned}\|Q_k^n - Q^n\| &\leq \sum_{j=0}^{n-1} \left\|Q_k^{n-1-j} - Q^{n-1-j}\right\| \|Q_k - Q\| \left\|Q^j\right\| \\ &\quad + \sum_{j=0}^{n-1} \left\|Q^{n-1-j}\right\| \|Q_k - Q\| \left\|Q^j\right\| \\ &\leq C\alpha k \sum_{j=0}^{n-1} \left\|Q_k^{n-1-j} - Q^{n-1-j}\right\| + nC^2\alpha k \\ &\leq C\alpha k \sum_{j=0}^{n-1} \left\|Q_k^j - Q^j\right\| + C^2\alpha T_M.\end{aligned}$$

From the last inequality, a uniform bound for $\|Q_k^n - Q^n\|$ can be obtained, by using the form of Gronwall lemma stated next [23, pp. 186].

Lemma 1 (Gronwall inequality)**.** *Let $u(n)$, $f(n)$, p, and q be nonnegative such that*

$$u(n) \leq p + q \sum_{j=a}^{n-1} f(j)\, u(j), \quad n \geq a,$$

then

$$u(n) \leq p \prod_{j=a}^{n-1} (1 + qf(j)), \quad n \geq a.$$

Thus, taking

$$u(n) = \|Q_k^n - Q^n\|, \; p = C^2\alpha T_M, \; q = C\alpha k, \; a = 0, \; f(j) = 1,$$

one gets, for all $n \geq 0$,

$$\|Q_k^n - Q^n\| \leq C^2\alpha T_M (1 + C\alpha k)^n.$$

Taking into account that $(1 + C\alpha k)^n \leq (1 + C\alpha k)^{T_M/k}$, and that $(1 + C\alpha k)^{T_M/k}$ increases with k decreasing, with

$$\lim_{k\to 0} (1 + C\alpha k)^{T_M/k} = e^{T_M C\alpha},$$

it follows that,

$$\|Q_k^n - Q^n\| \leq C^2 \alpha T_M e^{T_M C\alpha},$$

for all $n \geq 0$. Thus, for $0 < k < k_0$ and $0 \leq nk \leq T_M$, it holds that the matrices Q_k^n are uniformly bounded,

$$\|Q_k^n\| = \|Q_k^n - Q^n + Q^n\| \leq C^2 \alpha T_M e^{T_M C\alpha} + C,$$

and hence the scheme is stable, unconditionally, in the sense of Lax [22].

3.4. Truncation errors, consistency, and convergence

Next, bounds on the truncations errors of the scheme will be obtained, and thus, assuming sufficient smoothness of the solution, the consistency of the method will follow, which, together with the results of the last section, will assure its convergence. In what follows, the exact solution of the problem (3.11)-(3.14) will be denoted $w = \left(\widetilde{u}, \widetilde{T}, \widetilde{v}\right)$.

Let $\mathcal{L} = (\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3)$ be the difference operator associated with the scheme [24, p. 42], where

$$\begin{aligned}
\mathcal{L}_1 w_j^n &= \frac{1}{10k}\left(\widetilde{u}_{j-1}^{n+1}-\widetilde{u}_{j-1}^{n}+10\left(\widetilde{u}_{j}^{n+1}-\widetilde{u}_{j}^{n}\right)+\widetilde{u}_{j+1}^{n+1}-\widetilde{u}_{j+1}^{n}\right)\\
&\quad -\frac{3}{5}\left(a\delta_x^2\left(\widetilde{T}_j^{n+1}+\widetilde{T}_j^{n}\right)+b\delta_x^2\left(\widetilde{v}_j^{n+1}+\widetilde{v}_j^{n}\right)+c\delta_x^2\left(\widetilde{u}_j^{n+1}+\widetilde{u}_j^{n}\right)\right)\\
\mathcal{L}_2 w_j^n &= \frac{1}{k}\left(\widetilde{T}_j^{n+1}-\widetilde{T}_j^{n}\right)+\frac{B}{2C}\left(\widetilde{T}_j^{n+1}+\widetilde{T}_j^{n}\right)-\frac{1}{2C}\left(\widetilde{v}_j^{n+1}+\widetilde{v}_j^{n}\right)\\
\mathcal{L}_3 w_j^n &= \frac{1}{k}\left(\widetilde{v}_j^{n+1}-\widetilde{v}_j^{n}\right)-\frac{1}{2}\left(\widetilde{u}_j^{n+1}+\widetilde{u}_j^{n}\right)+\frac{A}{2}\left(\widetilde{T}_j^{n+1}+\widetilde{T}_j^{n}\right),
\end{aligned}$$

so that the local truncation error at the point (jh, nk), [22, p. 20], is given by $\left(\mathcal{T}_{1,j}^n, \mathcal{T}_{2,j}^n, \mathcal{T}_{3,j}^n\right) = \mathcal{L} w_j^n$.

Using appropriate Taylor series expansions, it is not difficult to show that the following bounds hold,

$$\mathcal{T}_{1,j}^n = O\left(k^2\right) + O\left(h^4\right),\ \mathcal{T}_{2,j}^n = O\left(k^2\right),\ \mathcal{T}_{3,j}^n = O\left(k^2\right). \tag{3.32}$$

Considering the vectors of exact solutions at the points in the mesh,

$$\begin{aligned}
\widetilde{U}^n &= \left[\widetilde{u}_1^n, \widetilde{u}_2^n, \ldots, \widetilde{u}_{P-1}^n\right]^T,\\
\widetilde{T}^n &= \left[\widetilde{T}_1^n, \widetilde{T}_2^n, \ldots, \widetilde{T}_{P-1}^n\right]^T,\\
\widetilde{V}^n &= \left[\widetilde{v}_1^n, \widetilde{v}_2^n, \ldots, \widetilde{v}_{P-1}^n\right]^T.
\end{aligned}$$

and the stack vector $W^n = \left[\widetilde{U}^n, \widetilde{T}^n, \widetilde{V}^n\right]^T \in \mathbb{R}^{3(P-1)}$, the truncation error of the two-level scheme (3.30), at $t = nk$, is the vector

$$\mathfrak{T}^n = \frac{1}{k}\left(W^{n+1} - Q_k W^n\right), \tag{3.33}$$

and one can verify that

$$\mathfrak{T}^n = E_k \left[\mathcal{T}_1^n, \mathcal{T}_2^n, \mathcal{T}_3^n\right]^T, \tag{3.34}$$

where $\mathcal{T}_i^n = \left[\mathcal{T}_{i,1}^n, \mathcal{T}_{i,2}^n, \dots, \mathcal{T}_{i,P-1}^n\right]^T$, $i = 1, 2, 3$, and

$$E_k = \begin{bmatrix} E_k^{1,1} & E_k^{1,2} & E_k^{1,3} \\ E_k^{2,1} & E_k^{2,2} & E_k^{2,3} \\ E_k^{3,1} & E_k^{3,2} & E_k^{3,3} \end{bmatrix},$$

with

$$\begin{aligned}
E_k^{1,1} &= 10 X_k^{-1} S^{-1}, \\
E_k^{1,2} &= \frac{12rC}{x_k} \left(2a - bAk\right) X_k^{-1} S^{-1} M, \\
E_k^{1,3} &= \frac{12r}{x_k} \left(2bC + \left(Bb + a\right) k\right) X_k^{-1} S^{-1} M, \\
E_k^{2,1} &= 10 \frac{k^2}{x_k} X_k^{-1} S^{-1}, \\
E_k^{2,2} &= \frac{4C}{x_k} X_k^{-1} \left(I - 6\left(\alpha_k - \frac{k^2 r}{2x_k}\left(2a - bAk\right)\right) S^{-1} M\right), \\
E_k^{2,3} &= \frac{2k}{x_k} X_k^{-1} \left(I - 6\left(\alpha_k - \frac{kr}{x_k}\left(2bC + \left(Bb + a\right) k\right)\right) S^{-1} M\right), \\
E_k^{3,1} &= 10 \frac{\left(2C + Bk\right) k}{x_k} X_k^{-1} S^{-1}, \\
E_k^{3,2} &= -\frac{2ACk}{x_k} X_k^{-1} \left(I - 6\left(\alpha_k + r\frac{2C + Bk}{Ax_k}\left(2a - bAk\right)\right) S^{-1} M\right), \\
E_k^{3,3} &= \frac{2\left(2C + Bk\right)}{x_k} X_k^{-1} \left(I - 6\left(\alpha_k - \frac{kr}{x_k}\left(2bC + \left(Bb + a\right) k\right)\right) S^{-1} M\right).
\end{aligned}$$

It is not difficult to verify that the matrix $E = \text{lím}_{k\to 0} E_k$ is given by

$$E = \begin{bmatrix} 10X^{-1}S^{-1} & 6raX^{-1}S^{-1}M & 6rbX^{-1}S^{-1}M \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix}, \tag{3.35}$$

and hence it follows that E_k has bounded norm. Therefore, from (3.32) and (3.34), it holds that, for $0 \leq nk \leq T_M$,

$$\text{lím}_{k\to 0} \frac{1}{k} \left\| W_h^k \left((n+1)\, k \right) - Q_k W_h^k \left(nk \right) \right\|_\infty = 0, \tag{3.36}$$

so that the scheme is consistent with the partial differential equation. Also, it can be deduced that the truncation error satisfies

$$\left\| \mathfrak{T}^n \right\|_\infty = O\left(k^2\right) + O\left(h^4\right). \tag{3.37}$$

As a result, since the method is unconditionally stable, for any finite value of $r = h/k^2$, and it is consistent with the original partial differential equation, from Lax equivalence theorem [22] it follows that the method is also unconditionally convergent of order $O\left(k^2\right) + O\left(h^4\right)$.

3.5. Numerical examples

In this section, two examples of application of the new scheme to DPL(2,2) models are presented, comparing its accuracy with that of the previous method in [20]. The selected problems include simple initial functions, allowing for the computation of exact solutions, so that the errors of the numerical approximations provided by the scheme, with respect to the exact values, can be illustrated.

Consider the problem (3.5)-(3.7), with initial conditions

$$T(x,0)=\sin(\pi x),\ \frac{\partial}{\partial t}T(x,0)=-\alpha_{Cu}\pi^2\sin(\pi x),\ \frac{\partial^2}{\partial t^2}T(x,0)=0,\ x\in[0,l]\,,$$

and with parameters $l = 1$, and α, τ_q, and τ_T corresponding to those experimentally found in copper [7, p. 123], $\alpha = 1{,}1283\cdot 10^{-4}$ m^2/s, $\tau_q = 0{,}4648$ ps, and $\tau_T = 70{,}833$ ps.

In Figure 1, the absolute differences between the exact solution and the numerical approximations,

$$\left|\widetilde{T}\,(x,t)-T\,(x,t)\right|,$$

obtained either with the new scheme, left subfigures, or with the previous method in [20], right subfigures, are presented, using two different mesh sizes in the same domain.

A more detailed illustration of the error properties of the new scheme, and its better accuracy as compared with the method in [20], is presented in Figures 2 and 3, for a similar DPL(2,2) model but with initial conditions

$$\left.\begin{aligned}T(x,0)&=\sin(\pi x),\\ \frac{\partial}{\partial t}T(x,0)&=-\pi^2\sin(\pi x),\\ \frac{\partial^2}{\partial t^2}T(x,0)&=\pi^4\sin(\pi x),\end{aligned}\right.\quad x\in[0,l]\,,$$

and with parameters $l=1$, $\alpha=1$, $\tau_q=\frac{1}{16}$, and $\tau_T=\frac{2}{\pi^2}-\frac{1}{16}$.

In Fig. 2, left, the maximum absolute errors of the approximate solu-

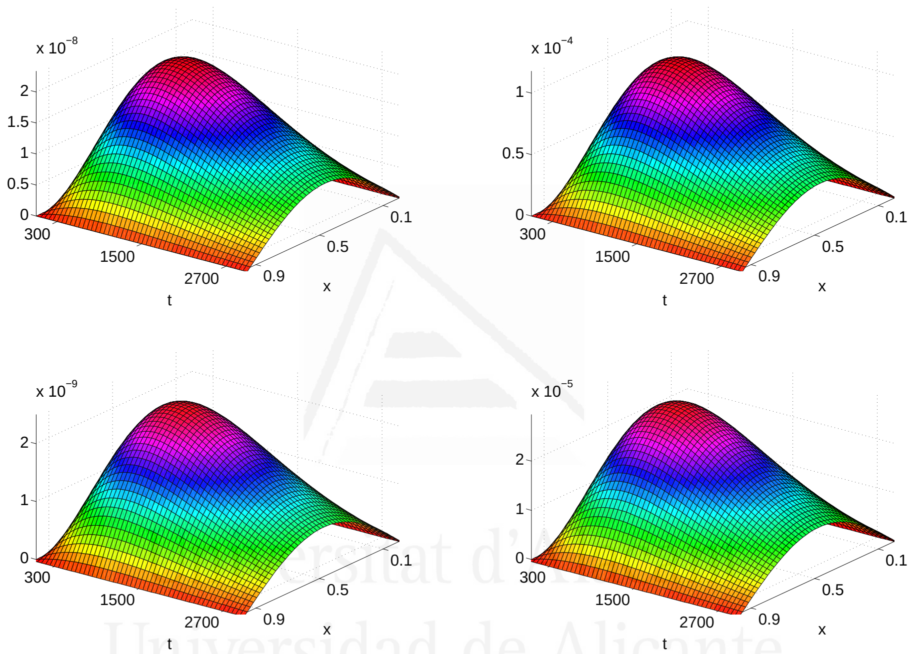

Figura 3.1: Absolute errors, $\left|\widetilde{T}\,(x,t) - T\,(x,t)\right|$, with respect to the exact values $\widetilde{T}(x,t)$, for the numerical approximations of DPL(2,2) model, $T(x,t)$, obtained with the scheme of this work (left), and with the method in [20] (right), for two different mesh sizes (top: $\Delta x = \Delta t = 0{,}02$; bottom: $\Delta x = \Delta t = 0{,}01$).

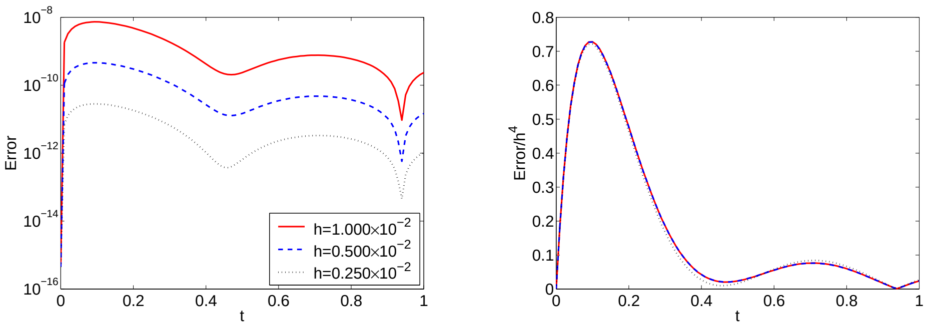

Figura 3.2: Maximum errors of the approximate solutions, in terms of time, for three different mesh sizes (left), and relation with the size of the mesh (right).

tion obtained with the new method as a function of time is presented, for three different mesh sizes. The right subfigure shows the relative errors in relation with the mesh size, in agreement with the order of the method.

In Fig. 3, the absolute errors in Fig. 2 (left) are compared with the corresponding errors of the previous method in [20], showing the higher accuracy of the new scheme.

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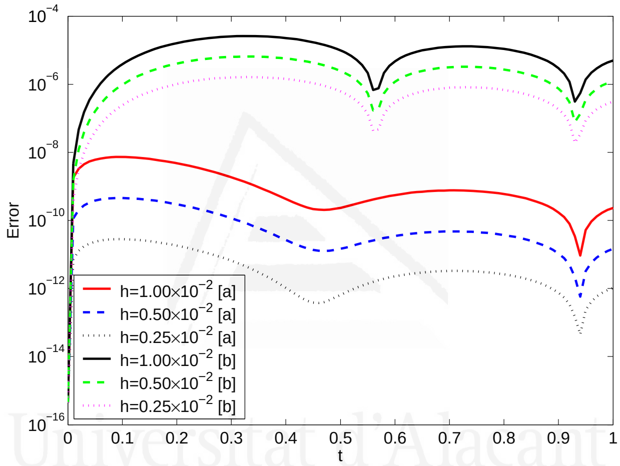

Figura 3.3: Comparison of the absolute errors for the new scheme developed in this work and the previous method in [20], for three different mesh sizes. New scheme: lower three lines, [a] (as in Fig. 2 left). Previous method: upper three lines, [b].

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Capítulo 4

Difference schemes for time–dependent heat conduction models with delay

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Difference schemes for time-dependent heat conduction models with delay

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Different non-Fourier models of heat conduction, that incorporate time lags in the heat flux and/or the temperature gradient, have been increasingly considered in the last years to model microscale heat transfer problems in engineering. Numerical schemes to obtain approximate solutions of constant coefficients lagging models of heat conduction have already been proposed. In this work, an explicit finite difference scheme for a model with coefficients variable in time is developed, and their properties of convergence and stability are studied. Numerical computations showing examples of applications of the scheme are presented.

Keywords: non-Fourier heat conduction; finite differences; convergence and stability

2010 AMS Subject Classifications: 65M06; 65M12; 65Q20; 35R10; 80M20

1. Introduction

Different non-Fourier models of heat conduction have been considered to model microscale heat transfer in engineering problems to properly account for non-classical effects such as heat waves, delayed responses, and finite speed of propagation (see [12,23] and references therein). These models are being increasingly used in a variety of technical applications, as in ultrafast laser processing of thin-film structures, heat transfer in nanofluids, or in laser irradiation of biological tissues (see, e.g. [14,15,24,26,30,33,34]).

In the dual-phase-lag model [22,23], time lags are incorporated into Fourier law that relates heat flux $\mathbf{q}(\mathbf{r}, t)$ and temperature gradient $\nabla T(\mathbf{r}, t)$ for a point $\mathbf{r}$ at time t

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k\nabla T(\mathbf{r}, t + \tau_T), \tag{1}$$

where τ_q and τ_T are the corresponding phase lags. Combining Equation (1) with the principle of energy conservation, an equation for heat conduction is obtained, which reduces to the classical diffusion equation when $\tau_q = \tau_T = 0$. Otherwise, it results into a partial differential equation with delay, a delayed model when $\tau_T = 0$, that is, in the single-phase-lag model [20], and also if $\tau = \tau_q - \tau_T > 0$, or an equation of advanced type if $\tau_q - \tau_T < 0$ [13,29]. It is also common to use first-order approximations with respect to the lags in Equation (1), referring to the resulting heat conduction equation as the DPL model [22], which includes as a particular case, when

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4.1. Introduction

Different non-Fourier models of heat conduction have been considered to model microscale heat transfer in engineering problems, to properly account for non-classical effects such as heat waves, delayed responses, and finite speed of propagation [see 12, 23, and references therein]. These models are being increasingly used in a variety of technical applications, as in ultrafast laser processing of thin-film structures, heat transfer in nanofluids, or in laser irradiation of biological tissues [see, e.g., 15, 16, 24, 28, 30, 33, 34].

In the dual-phase-lag model [22, 23], time lags are incorporated into Fourier law, that relates heat flux $\mathbf{q}(\mathbf{r}, t)$ and temperature gradient $\nabla T(\mathbf{r}, t)$, for a point $\mathbf{r}$ at time t,

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k\nabla T(\mathbf{r}, t + \tau_T), \tag{4.1}$$

where τ_q and τ_T are the corresponding phase lags. Combining (4.1) with the principle of energy conservation, an equation for heat conduction is obtained, which reduces to the classical diffusion equation when $\tau_q = \tau_T = 0$. Otherwise, it results into a partial differential equation with delay, a delayed model when $\tau_T = 0$, i.e., in the single-phase-lag model [20], and also if $\tau = \tau_q - \tau_T > 0$, or an equation of advanced type if $\tau_q - \tau_T < 0$ [13, 29]. It is also common to use first order approximations with respect to the lags in (4.1), referring to the resulting heat conduction equation as the DPL model [22], which includes as a particular case, when $\tau_T = 0$, the Cattaneo-Vernotte model [4, 25], but higher order approximations have also been considered [14, 21].

Some of these non-Fourier models may present stability problems [11, 14] and/or violate physical principles [5]. Also, non-classical effects are only apparent in transient behaviours, when the response time of interest is of the same order of magnitude as the relaxation time [23, 29], the classical diffusion model being able to provide accurate descriptions for much longer times. Hence, it could be reasonable to consider a model of heat conduction combining both classical and delayed terms, with time varying strength, so that the term with delay eventually becomes negligible, and the model approaches classical diffusion in the long term, also guaranteeing its stability.

In this work, the following model for heat conduction in a finite rod with insulated ends will be considered, the partial differential equation with delay and non-delay terms, and with time dependent coefficients,

$$\frac{\partial T}{\partial t}(x,t) = a(t)\frac{\partial^2 T}{\partial x^2}(x,t) + b(t)\frac{\partial^2 T}{\partial x^2}(x,t-\tau), \; 0 \le x \le l, \; t > \tau, \quad (4.2)$$

with initial condition

$$T(x,t) = \phi(x,t), \; 0 \le x \le l, \; 0 \le t \le \tau, \quad (4.3)$$

and Dirichlet boundary condition

$$T(0,t) = T(l,t) = 0, \; t \ge 0, \quad (4.4)$$

where $\tau > 0$, and $a(t)$, $b(t)$ are positive real functions.

Numerical schemes to obtain approximate solutions of different types of constant coefficients non-Fourier models of heat conduction have already been developed [see, e.g., 3, 6, 7, 26, 27, 31]. Difference schemes for parabolic problems with delay have also been proposed [see, e.g., 1, 2, 18, 32], including problem (4.2) in the constant coefficients case [8, 9]. The aim of this work is the construction of an explicit difference scheme for the time dependent problem (4.2)–(4.4), characterising its convergence properties. In the next section, the proposed difference scheme is formulated, expressed in matrix form and as a two-level scheme. In Section 3, conditional convergence of the method is proved, which is illustrated in Section 4 with numerical examples. Finally, conclusions are presented and future work is suggested.

4.2. Construction of the difference scheme

Consider a bounded domain $[0,l]\times[0,M\tau]$, for some fixed integer $M>1$, and the uniform mesh $\{(x_p,t_n), p=0\ldots P, n=0\ldots MN\}$, defined by the increments $h=\Delta x$ and $k=\Delta t$, such that $l=Ph$ and $\tau=Nk$. In what follows, the values of a function w at the points of the mesh, $w(x_p,t_n)$, will be denoted $w_{p,n}$. Note that the scheme can be applied in any bounded domain $[0,l]\times[0,T_{\mathsf{max}}]$, by considering M such that $T_{\mathsf{max}}\le M\tau$.

Let $u(x,t)$ denote the numerical approximation to $T(x,t)$ to be obtained with the scheme. Using finite differences approximations to partial derivatives in (4.2), as in the classical explicit scheme for the diffusion equation [19, pp. 6-8], or in the explicit scheme for the constant coefficients case [8],

$$\frac{\partial u}{\partial t}(x_p,t_n)\approx\frac{1}{k}\delta_t u_{p,n}=\frac{1}{k}\left(u_{p,n+1}-u_{p,n}\right),$$

$$\frac{\partial^2 u}{\partial x^2}(x_p, t_n) \approx \frac{1}{h^2}\delta_x^2 u_{p,n} = \frac{1}{h^2}\left(u_{p-1,n} - 2u_{p,n} + u_{p+1,n}\right),$$

and writing $\alpha = k/h^2$, $a_n = a(nk)$, and $b_n = b(nk)$, from (4.2)–(4.4) one gets the system of difference equations

$$\begin{aligned} u_{p,n+1} = u_{p,n} + \alpha a_n \delta_x^2 u_{p,n} + \alpha b_n \delta_x^2 u_{p,n-N}, \\ p = 1, 2, \ldots, P-1, \quad n = N, N+1, \ldots, MN-1, \end{aligned} \tag{4.5}$$

with initial conditions

$$u_{p,n} = \phi(ph, kn,), \; p = 0, 1, \ldots, P, \; n = 0, 1, \ldots, N, \tag{4.6}$$

and boundary conditions

$$u_{0,n} = u_{P,n} = 0, \; n = 0, 1, \ldots, MN. \tag{4.7}$$

Hence, using (4.5)–(4.7), the values of $u_{p,n}$ for all the points in the mesh can be recursively computed, and then extended by continuity to obtain the numerical approximation $u(x,t)$ for $(x,t) \in [0,l] \times [0, M\tau]$.

Introducing the vectors $\boldsymbol{u}_n = [u_{1,n}, u_{2,n}, \cdots, u_{P-1,n}]^T$, for $n = 0, 1, \ldots, MN$, where the superindex T denotes the transpose, and the $(P-1)\times(P-1)$ tridiagonal matrix

$$\mathbf{M}=\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & -2 \end{bmatrix},$$

and writing $\mathbf{I}$ for the $(P-1)\times(P-1)$ identity matrix, the equations of the scheme can be given in matrix form as

$$\boldsymbol{u}_{n+1}=\left(\mathbf{I}+\alpha a_n\mathbf{M}\right)\boldsymbol{u}_n+\alpha b_n\mathbf{M}\boldsymbol{u}_{n-N},\ n=N,N+1,\ldots,MN-1, \quad (4.8)$$

with initial condition

$$\boldsymbol{u}_n=\boldsymbol{\phi}_n,\ n=0,1,\ldots,N, \quad (4.9)$$

where $\boldsymbol{\phi}_n = \left[\phi\left(h,nk\right),\phi\left(2h,nk\right),\ldots,\phi\left((P-1)h,nk\right)\right]^T$, for $n=0,1,\ldots,N$.

Next, the scheme will be expressed as a two-level scheme, in order to facilitate the analysis of its properties. Introducing the stack vectors

$$\boldsymbol{u}_n^*=\left[\boldsymbol{u}_n,\boldsymbol{u}_{n-1},\cdots,\boldsymbol{u}_{n-N}\right]^T,\ n=N,N+1,\ldots,MN,$$

and

$$\boldsymbol{\phi}^*=\left[\boldsymbol{\phi}_N,\boldsymbol{\phi}_{N-1},\ldots,\boldsymbol{\phi}_0\right]^T,$$

and the block matrices

$$\mathbf{C}_n^* = \begin{bmatrix} \mathbf{I} + \alpha a_n \mathbf{M} & 0 & \cdots & 0 & \alpha b_n \mathbf{M} \\ \mathbf{I} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & \mathbf{I} & 0 \end{bmatrix}, \; n = N, N+1, \ldots, MN, \tag{4.10}$$

equations (4.8) and (4.9) can be written in the form

$$\boldsymbol{u}_{n+1}^* = \mathbf{C}_n^* \boldsymbol{u}_n^*, \; n = N, N+1, \ldots, MN-1, \tag{4.11}$$

$$\boldsymbol{u}_N^* = \boldsymbol{\phi}^*. \tag{4.12}$$

4.3. Convergence of the method

In this section, conditions that guarantee the convergence of the proposed difference scheme will be established. First, an expression for the truncation error of the scheme will be provided, and hence its consistency will be established. Then, by giving conditions for the stability of a transformation of the original scheme, the convergence of the method will be directly proved. In what follows, v will denote the exact solution of the problem (4.2)–(4.4).

Let L be the difference operator associated with the scheme [19, p. 42],

$$Lu_{p,n} = \frac{1}{k}\left(u_{p,n+1} - u_{p,n} - \alpha a_n \delta_x^2 u_{p,n} - \alpha b_n \delta_x^2 u_{p,n-N}\right), \tag{4.13}$$

so that the local truncation error [10, p. 165],[17, p. 20], at the point

(ph, nk) is given by $\mathcal{T}_{p,n} = Lv_{p,n}$. An expression for this error is given in the next proposition.

Proposition 1. *If* $\frac{\partial^2}{\partial t^2} v(x,t)$ *and* $\frac{\partial^4}{\partial x^4} v(x,t)$ *exist and are continuous, the local truncation error of the explicit scheme defined in (4.8) is given by*

$$\begin{aligned}\mathcal{T}_{p,n} =& \frac{k}{2}\frac{\partial^2 v}{\partial t^2}\left(ph, (n+\theta_1)k\right) - \frac{h^2}{12}\left(a_n \frac{\partial^4 v}{\partial x^4}\left((p-1+2\theta_2)h, nk\right)\right. \\ &\left. + b_n \frac{\partial^4 v}{\partial x^4}\left((p-1+2\theta_3)h, (n-N)k\right)\right),\end{aligned} \tag{4.14}$$

where $\theta_1, \theta_2, \theta_3 \in (0,1)$.

This result can be easily obtained using appropriate Taylor series expansions. It is to be noted that the conditions in this proposition about the regularity of the exact solution v are guaranteed if the initial function and the coefficients are sufficiently regular, e.g., if $\phi(x,\cdot)$, $a(\cdot)$ and $b(\cdot)$ are twice continuously differentiable, $\phi(\cdot,t)$ is four times continuously differentiable, and the initial function ϕ satisfies some matching conditions.

Introducing the vectors, $\mathfrak{T}_n = \left[\mathcal{T}_{1,n}, \mathcal{T}_{2,n}, \ldots, \mathcal{T}_{P-1,n}\right]^T$, and stack vectors,

$$\mathfrak{T}_n^* = \left[\mathfrak{T}_n, 0, \ldots, 0\right]^T,$$

of local truncation errors, and, similarly, the corresponding vectors for the exact solutions at the points in the mesh, $\boldsymbol{v}_n = \left[v_{1,n}, v_{2,n}, \cdots, v_{P-1,n}\right]^T$ and

$$\boldsymbol{v}_n^* = \left[\boldsymbol{v}_n, \boldsymbol{v}_{n-1}, \cdots, \boldsymbol{v}_{n-N}\right]^T,$$

it can be verified that

$$\mathfrak{T}_n^* = \frac{1}{k}\left(\boldsymbol{v}_{n+1}^* - \mathbf{C}_n^* \boldsymbol{v}_n^*\right), \tag{4.15}$$

which is the local truncation error for the scheme, expressed in the form of a two-level scheme, as defined in (4.11).

The next result follows immediately from (4.15) and Proposition 1.

Proposition 2. *If* $\frac{\partial^2}{\partial t^2} v(x,t)$ *and* $\frac{\partial^4}{\partial x^4} v(x,t)$ *exist and are continuous in* $[0,l] \times [\tau, M\tau]$*, the explicit scheme defined in (4.8), or equivalently in (4.11), is consistent with the partial functional differential equation (4.2), and the local truncation error verifies*

$$\|\mathfrak{T}_n^*\|_\infty = O(k) + O\left(h^2\right).$$

Next, the diagonal form of the matrix $\mathbf{M}$ will be used to transform (4.11) into a two-level scheme with block-diagonal matrix, which will be shown to be stable and will lead to a direct proof of the convergence of the method.

The eigenvalues of the matrix $\mathbf{M}$ are, [19, p. 52],

$$\lambda_p = -4\sin^2 \frac{\pi p}{2P},\ p = 1, \ldots, P-1, \tag{4.16}$$

which form a strictly decreasing sequence, verifying the bounds $-4 < \lambda_p < 0$, for $p = 1, \ldots, P-1$. The matrix $\mathbf{M}$ can be expressed in diagonal form as $\mathbf{M} = \mathbf{A}\mathbf{D}\mathbf{A}^{-1}$, where $\mathbf{A}$ is the matrix corresponding to the base of eigenvectors

$$\mathcal{X}_p = \left[\sin\frac{\pi p}{P}, \sin\frac{2\pi p}{P}, \ldots, \sin\frac{(P-1)\,\pi p}{P}\right]^T, \; p = 1, \ldots, P-1, \tag{4.17}$$

and $\mathbf{D} = \operatorname{diag}[\lambda_1, \ldots, \lambda_{P-1}]$. Hence, introducing the $(N+1) \times (N+1)$ block diagonal matrix $\mathbf{A}^* = \operatorname{diag}[\mathbf{A}, \mathbf{A}, \ldots, \mathbf{A}]$, and the block matrix

$$\mathbf{D}_n^* = \begin{bmatrix} \mathbf{I} + \alpha a_n \mathbf{D} & 0 & \cdots & 0 & \alpha b_n \mathbf{D} \\ \mathbf{I} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & \mathbf{I} & 0 \end{bmatrix}, \tag{4.18}$$

one gets

$$\mathbf{C}_n^* = \mathbf{A}^* \mathbf{D}_n^* \left(\mathbf{A}^*\right)^{-1}. \tag{4.19}$$

Let $\boldsymbol{\varphi}_n = [\varphi_{1,n}, \varphi_{2,n}, \ldots, \varphi_{P-1,n}]^T$ be the vector $\boldsymbol{\varphi}_n = \mathbf{A}^{-1}\boldsymbol{u}_n$. The stack vector $\boldsymbol{\varphi}_n^* = [\boldsymbol{\varphi}_n, \boldsymbol{\varphi}_{n-1}, \cdots, \boldsymbol{\varphi}_{n-N}]^T$ verifies that $\boldsymbol{\varphi}_n^* = (\mathbf{A}^*)^{-1} U_n^*$, and hence, from (4.11), one gets

$$\boldsymbol{\varphi}_{n+1}^* = \mathbf{D}_n^* \boldsymbol{\varphi}_n^*. \tag{4.20}$$

The components in this last equation can be reordered to obtain the equivalent expression

$$\boldsymbol{\psi}_{n+1}^* = \mathbf{G}_n^* \boldsymbol{\psi}_n^*, \tag{4.21}$$

where $\boldsymbol{\psi}_n^* = [\boldsymbol{\psi}_{1,n}, \boldsymbol{\psi}_{2,n}, \cdots, \boldsymbol{\psi}_{P-1,n}]^T$, with $\boldsymbol{\psi}_{p,n} = [\varphi_{p,n}, \varphi_{p,n-1}, \cdots, \varphi_{p,n-N}]^T$, and $\mathbf{G}_n^*$ is the block-diagonal matrix $\mathbf{G}_n^* = \operatorname{diag}[\mathbf{G}_{1,n}, \mathbf{G}_{2,n}, \ldots, \mathbf{G}_{P-1,n}]$, with

$$\mathbf{G}_{p,n} = \begin{bmatrix} 1+\alpha a_n\lambda_p & 0 & \dots & 0 & \alpha b_n \lambda_p \\ 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix}. \tag{4.22}$$

The difference scheme (4.20) is stable, [10, p. 159], if there is $k_0 > 0$ such that for all $0 < k < k_0$ the family of matrices

$$\left\{ \prod_{i=1}^{n-N} \mathbf{D}^*_{n-i},\ n = N+1, N+2, \dots, MN \right\} \tag{4.23}$$

is uniformly bounded, independently of k.

If $\mathbf{P}$ is the row permutation matrix such that $\boldsymbol{\psi}^*_{n+1} = \mathbf{P}\boldsymbol{\varphi}^*_{n+1}$, it follows, from (4.20) and (4.21), that $\mathbf{G}^*_n = \mathbf{P}\mathbf{D}^*_n\mathbf{P}^{-1}$. Since $\|\mathbf{P}\|_\infty = \|\mathbf{P}^{-1}\|_\infty = 1$, it holds that

$$\left\| \prod_{i=1}^{n-N} \mathbf{G}^*_{n-i} \right\|_\infty = \left\| \prod_{i=1}^{n-N} \mathbf{D}^*_{n-i} \right\|_\infty,$$

so that the stability of the schemes (4.20) and (4.21) are equivalent.

The next proposition gives conditions for the scheme defined in (4.20) to be stable.

Proposition 3. *If $b(t) < a(t)$, and $\alpha \le \dfrac{1}{2(a(t)+b(t))}$, for $\tau < t \le M\tau$, then*

$$\left\| \prod_{i=1}^{n-N} \mathbf{G}^*_{n-i} \right\|_\infty \le 1,\ n = N+1, N+2, \dots, MN, \tag{4.24}$$

and hence the scheme defined by (4.20) is stable.

Proof

It is immediate that

$$\left\|\mathbf{G}^*_{n-i}\right\|_\infty = \text{máx}\left\{\|\mathbf{G}_{p,n-i}\|_\infty, p = 1, 2, \ldots, P-1\right\},$$

and that

$$\|\mathbf{G}_{p,n-i}\|_\infty = \text{máx}\left\{1, |1+\alpha a_{n-i}\lambda_p| - \alpha b_{n-i}\lambda_p\right\},\ p = 1, 2, \ldots, P-1.$$

If $-\alpha a_{n-i}\lambda_p \leq 1$, then

$$|1+\alpha a_{n-i}\lambda_p| - \alpha b_{n-i}\lambda_p = 1 + \alpha\lambda_p\left(a_{n-i} - b_{n-i}\right) < 1,$$

since $a_{n-i} - b_{n-i} > 0$ and $\lambda_p < 0$. Otherwise, if $1 < -\alpha a_{n-i}\lambda_p$, then

$$|1+\alpha a_{n-i}\lambda_p| - \alpha b_{n-i}\lambda_p = -1 - \alpha\lambda_p\left(a_{n-i} + b_{n-i}\right) < 1,$$

since $\alpha \leq \dfrac{1}{2\left(a_{n-i} + b_{n-i}\right)}$ and $-\lambda_p < 4$. Therefore, the result is established.

In what follows, the conditions of Proposition 3 will be assumed to hold. It is not difficult to prove, as was done in [8, Theorem 5] for the constant coefficients case, that under these conditions the scheme defined in (4.8) is asymptotically stable.

Next, the convergence of the method will be established. From (4.19), Proposition 3, and the bounds

$$\|\mathbf{A}^*\|_\infty \leq \frac{2l}{\pi h}, \qquad \left\|(\mathbf{A}^*)^{-1}\right\|_\infty \leq \frac{4}{\pi},$$

it holds that

$$\left\|\prod_{i=1}^{n-N}\mathbf{C}_{n-i}^{*}\right\|_{\infty}\leq\frac{8l}{\pi^{2}h},\; n=N+1,N+2,\ldots,MN. \tag{4.25}$$

Eq. 4.15 can be written as a recurrence relation,

$$\boldsymbol{v}_{n+1}^{*}=\mathbf{C}_{n}^{*}\boldsymbol{v}_{n}^{*}+k\mathfrak{T}_{n}^{*},$$

and, since $\boldsymbol{v}_{N}^{*}=\boldsymbol{\phi}^{*}$, one gets, for $n=N+1,N+2,\ldots,MN$,

$$\boldsymbol{v}_{n}^{*}=\prod_{i=1}^{n-N}\mathbf{C}_{n-i}^{*}\boldsymbol{\phi}^{*}+k\sum_{m=0}^{n-N-1}\prod_{i=1}^{n-N-m-1}\mathbf{C}_{n-i}^{*}\mathfrak{T}_{N+m}^{*}. \tag{4.26}$$

From (4.25) and (4.26) it follows that

$$\left\|\prod_{i=1}^{n-N}\mathbf{C}_{n-i}^{*}\boldsymbol{\phi}^{*}-\boldsymbol{v}_{n}^{*}\right\|_{\infty}\leq\frac{8lk}{\pi^{2}h}\sum_{m=0}^{n-N-1}\left\|\mathfrak{T}_{N+m}^{*}\right\|_{\infty},$$

and, from Proposition 2, since $k=\alpha h^{2}$, there is $K_{0}>0$ such that

$$\left\|\mathfrak{T}_{N+m}^{*}\right\|_{\infty}\leq K_{0}k,$$

so that

$$\left\|\prod_{i=1}^{n-N}\mathbf{C}_{n-i}^{*}\boldsymbol{\phi}^{*}-\boldsymbol{v}_{n}^{*}\right\|_{\infty}\leq\frac{8l}{\pi^{2}}\alpha K_{0}\left(kn-\tau\right)h.$$

Therefore, the convergence of the method has been proved, as stated in the next theorem.

Theorem 1. *Under the conditions of Proposition 3, and for any initial* *function ϕ guaranteeing the conditions of Proposition 2, there is $K = K(\phi, M\tau, \alpha)$ such that*

$$\left\| \prod_{i=1}^{n-N} \mathbf{C}^*_{n-i} \boldsymbol{\phi}^* - \boldsymbol{v}^*_n \right\|_\infty \leq Kh, \quad \tau < nk \leq M\tau.$$

Note that the scheme is applied with a fixed α, so that the constant K depends on the geometry of the mesh, as given by α, but is independent of its size. This theorem, however, does not guarantee the right order of convergence, which should be $O(h^2)$ as shown in the local truncation error, but an alternative proof of the convergence of the method providing an estimate for accuracy of second order of h seems to be elusive.

4.4. Numerical examples

In this section, the numerical solution for a particular problem will be computed using the explicit difference scheme defined in Section 2, with two different mesh sizes to show the sharpness of the condition on α required in Theorem 1 for the convergence of the method.

Consider problem (4.2)–(4.4), with parameters $l = 1$ and $\tau = 1$, initial condition

$$\phi(x,t) = te^{-t} \sin(\pi x), \; 0 \leq x \leq 1, \; 0 \leq t \leq 1,$$

and coefficients $a(t) = 1 + e^{-t^2}$ and $b(t) = 1 - (1+t^2)^{-1}$.

Let $\alpha_L(t)$ be the function defined by

$$\alpha_L(t) = \frac{1}{2\left(a(t) + b(t)\right)}.$$

It is not difficult to see that, in this case, the greatest of the lower bounds of $\alpha_L(t)$ is 0.25, and thus, from Theorem 1, for any value $\alpha = k/h^2$ not greater than 0.25 the difference scheme is convergent.

In Fig. 4.1 and Fig. 4.2, the numerical solution $u(x,t)$ for the above problem is computed using a mesh with $h = 0{,}01$ and two different time increments, $k = 0{,}25 \times 10^{-4}$ and $k = 0{,}26 \times 10^{-4}$, that correspond with values of $\alpha = 0{,}25$ and $\alpha = 0{,}26$, respectively, the first one verifying the condition established in Theorem 1 and the second one being slightly greater than the limit of convergence. Numerical solutions seem to be similar for not too large times (Fig. 4.1), but, on the contrary, for large times the solution of the problem takes very small values and the method behaves well for $\alpha = 0{,}25$ (Fig. 4.2, left), but not for $\alpha = 0{,}26$ (Fig. 4.2, right).

4.5. Conclusions

In this work, a model of heat conduction combining time dependent classical and delayed terms has been considered. To allow the computation of numerical solutions for this model, an explicit difference scheme has been constructed, expressed in matrix form and also as a two-level scheme. Bounds on the local truncation error of the scheme have been provided, its properties of consistency and stability have been analysed, and conditions for the convergence of the method have been established and illustrated

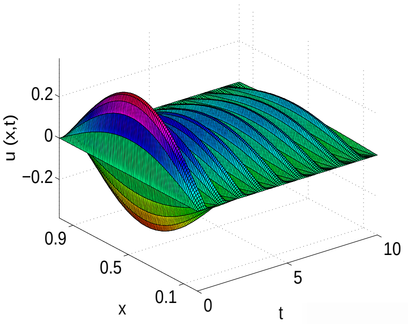

Figura 4.1: Numerical solution u of the problem in Section 4, using a mesh with $h = 0{,}01$ and time increments $k = 0{,}25 \times 10^{-4}$, corresponding to $\alpha = 0{,}25$ (up), and $k = 0{,}26 \times 10^{-4}$, corresponding to $\alpha = 0{,}26$ (down), for $t \in [0, 10]$.

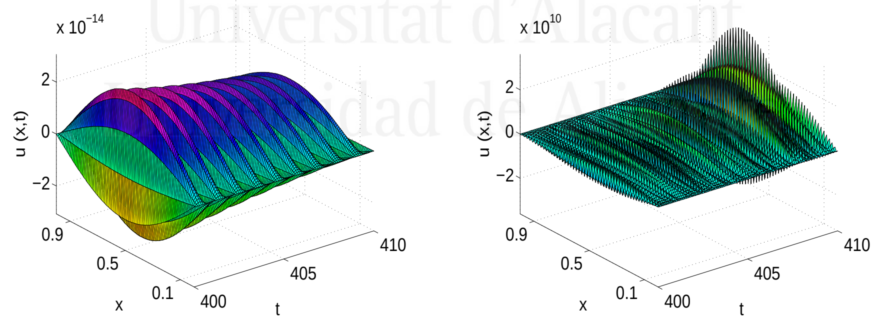

Figura 4.2: Numerical solution u of the problem in Section 4, using a mesh with $h = 0{,}01$ and time increments $k = 0{,}25 \times 10^{-4}$, corresponding to $\alpha = 0{,}25$ (up), and $k = 0{,}26 \times 10^{-4}$, corresponding to $\alpha = 0{,}26$ (down), for $t \in [400, 410]$.

with numerical examples. Open problems for future work would include to formally derive the mixed delayed model from physical foundations, as was done in [29] for the pure delayed model, and the development of higher order implicit schemes, in a similar way to those proposed in [9] for the constant coefficients case.

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Parte III

Conclusiones

Conclusiones generales

El esquema propuesto en el artículo recogido en el Capítulo 2, dado por las ecuaciones (2.22)–(2.24), proporciona soluciones aproximadas del modelo (2.6) con condiciones de contorno (2.4) y condiciones iniciales (2.5) y en particular de las aproximaciones de segundo orden del modelo con doble retardo de fase, esto es, de los modelos de conducción del calor DPL(2,1) y DPL(2,2). La solución aproximada por el esquema converge a la solución exacta cuando los incrementos espacial $h = \Delta x$ y temporal $k = \Delta t$, que determinan la geometría de la malla, se aproximan a cero, manteniendo fija la relación $r = \frac{k}{h^2}$, siendo el error del orden de $O\left(k^2\right) + O\left(h^2\right)$, como se ilustra en los experimentos numéricos mostrados en la Figura 2.2.

La utilización de aproximaciones compactas de mayor orden de las derivadas permite la construcción de esquemas más eficientes. Así, en el trabajo incluido en el Capítulo 3 se ha propuesto un esquema compacto, dado por (3.27)–(3.29), para la obtención de soluciones numéricas del modelo (3.5) con condiciones de contorno (3.7) y condiciones iniciales (3.8), que convergen a la solución exacta con error $O\left(k^2\right) + O\left(h^4\right)$. De este modo, si la malla se construye de forma que $k = O\left(h^2\right)$ entonces, con el primer esquema se obtienen aproximaciones con error del orden de $O(h^2)$ mientras que con el segundo esquema el error es del orden de $O(h^4)$, como se ilustra en los experimentos numéricos mostrados en las Figuras 3.1–3.3.

En la publicación recogida en el Capítulo 4, se ha considerado un modelo de conducción de calor que combina los términos clásico y retardado dependientes del tiempo dado por (4.2)–(4.4). Se ha construido el esquema en diferencias explícito (4.5)–(4.7) que permite el cálculo de soluciones numéricas de este modelo. Su expresión en forma matricial (4.8)–(4.9) y como esquema de dos niveles (4.11)–(4.12) facilitan el estudio de la convergencia del esquema.

En la Proposición 1, pág. 125, se da una expresión del error de truncación local del esquema y en la Proposición 2, pág. 126, se proporcionan cotas del error de truncación del esquema estableciéndose la consistencia del mismo.

En la Proposición 3, pág. 128, se da una condición sobre el parámetro $\alpha = \frac{k}{h^2}$, que determina la geometría de la malla, para que el esquema (4.20) sea estable. Este esquema es la transformación por la Transformada Discreta Seno del esquema propuesto. Bajo esta condición y las condiciones sobre la función inicial que garantizan la consistencia del esquema, se establece en el Teorema 1, página 130, la convergencia del esquema propuesto. Estas condiciones para la convergencia del método se han ilustrado con ejemplos numéricos, Figuras 4.1 y 4.2.