Numerical methods for time dependent partial differential equations

1 Introduction

There are many phenomena of interest in biological and life sciences that are modelled by time dependent partial differential equations of the form

$$\frac{\partial c}{\partial t} + \mathbf{u}(x,t)\cdot\nabla c = A\Delta c + f(t,c) \text{ in } D\times(0,T], \tag{1.1}$$

in $D\times(0,T]$, where $D\subset\mathbf{R}^d(d=1,2$ ó $3)$ denotes the spatial domain where the phenomena take place, $(0,T)$ is a time interval and $c(x,t)$ denotes the dependent variable representing the magnitude that is modelled. Equation (1.1) is the mathematical expression of a conservation law satisfied for $c(x,t)$. To explain the meaning of terms of (1.1) we assume that $d=2$. $A\Delta c \equiv A(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2})$, Δ being the Laplace operator, is the **diffusion term**; $\mathbf{u}(x,t) = (u_1(x,t),u_2(x,t))$ is a velocity field such that the term $\frac{\partial c}{\partial t}+\mathbf{u}(x,t)\cdot\nabla c = \frac{\partial c}{\partial t}+u_1(x,t)\frac{\partial c}{\partial x_1}+u_2(x,t)\frac{\partial c}{\partial x_2}$ represents the variation of $c(x,t)$ following the trajectories described by $\mathbf{u}(x,t)$. This variation is also known as the material derivative of $c(x,t)$ and is denoted by $\frac{Dc}{Dt}$. Many phenomena take place in a medium where there is no velocity field, so that $\mathbf{u}=\mathbf{0}$ and $\frac{Dc}{Dt}\equiv\frac{\partial c}{\partial t}$. Finally, the term $f(t,c)$ is a function of c representing internal interactions among the different components of the system, such term is known as the **reaction term**.

We shall learn how to calculate an approximate solution of (1.1) by the method of finite differences both in space and time in an step by step procedure. First, we consider that $\mathbf{u}=\mathbf{0}$ and the function f does not have any dependence on c. These simplifying assumptions reduce (1.1) to a lineal diffusion equation, which is the prototype equation for what the mathematicians call linear parabolic problems. Then, we will assume $\mathbf{u} \neq \mathbf{0}$, but still keeping f as independent of c. Finally, we shall end up assuming that $f = f(c)$.

2 Numerical methods for linear parabolic problems

We consider the model problem

$$\begin{cases} \dfrac{\partial c}{\partial t} = A\Delta c + f(\mathbf{x}, t) \text{ in } D \times (0, T], \\ \quad c(\mathbf{x}, 0) = c_0(\mathbf{x}),\ \mathbf{x} \in D, \\ \quad c\mid_{\partial D} = g(\mathbf{x},t) \text{ for all } t > 0, \end{cases} \tag{2.1}$$

where $f(\mathbf{x}, t)$ is the forcing function, $g(\mathbf{x}, t)$ is the value of c on the boundary ∂D and $c_0(\mathbf{x})$ is the initial value. To avoid unnecessary complications in the presentation of the numerical schemes, we shall assume in the sequel, unless otherwise stated, that *i)* $f(\mathbf{x}, t)$ and $g(\mathbf{x},t)$ are sufficiently smooth. *ii)* $\overline{D} \equiv D \cup \partial D \equiv [a, b] \times [c, d]$, a, b, c, d are real, this means that $\overline{D}$ is a rectangular region in the plane. *iii)* $\overline{D}$ is covered by a uniform rectangular grid of grid spacing $\Delta x = \Delta y$. *iv)* A constant time step Δt. *v)* Given positive integers I, J and N, such that $(I - 1) \times \Delta x =\mid b - a \mid$, $(J - 1) \times \Delta y =\mid d - c \mid$ and $N \times \Delta t = T$, the region $\overline{D}$ is approximated by the computational domain $\overline{D}_h = \{(x_i, y_j) \in \overline{D} : 1 \leq i \leq I, \text{ and } 1 \leq j \leq J\}$. Next, we introduce some notation. If $u(x, y, t)$ is a function defined on $\overline{D} \times [0, T]$, we set $u^n_{ij} \equiv u(x_i, y_j, t_n)$.The derivatives are approximated by finite difference operators. Let z denote either x or y, we have

forward difference operators Δ^+_z, Δ^+_t and *backward difference operators* Δ^-_z, Δ^-_t

$$\Delta^+_z u^n_i := u^n_{i+1} - u^n_i,\ \Delta^-_z u^n_i := u^n_i - u^n_{i-1},$$
$$\Delta^+_t u^n_i := u^{n+1}_i - u^n_i,\ \Delta^-_1 u^n_i := u^n_i - u^{n-1}_i;$$

central difference operators δ_z, δ_t

$$\delta_z u^n_i := u^n_{i+\frac{1}{2}} - u^n_{i-\frac{1}{2}},$$
$$\delta_t u^n_i := u^{n+\frac{1}{2}}_i - u^{n-\frac{1}{2}}_i;$$

Some times, instead of the central difference operator $\delta_{(\cdot)}$, it is used the double interval central difference operator $\Delta_{0(\cdot)}$

$$\Delta_{0z}u_i^n := u_{i+1}^n - u_{i-1}^n,$$
$$\Delta_{0t}u_i^n := u_i^{n+1} - u_i^{n-1};$$

second order central difference $\delta_z^2,\ \delta_t^2$

$$\delta_z^2 u_i^n := u_{i+1}^n - 2u_i^n + u_{i-1}^n,$$
$$\delta_t^2 u_i^n ;= u_i^{n+1} - 2u_i^n + u_i^{n-1}.$$

By using Taylor series expansion and assuming u is sufficiently smooth we can obtain the following approximations

$$\Delta_z^+ u_i^n \text{ and } \Delta_z^- u_i^n = (\frac{\partial u}{\partial z})_{z=ih} + O(h),$$
$$\delta_z u_i^n \text{ and } \Delta_{0z}u_i^n = (\frac{\partial u}{\partial z})_{z=ih} + O(h^2),$$
$$\delta_z^2 u_i^n = (\frac{\partial^2 u}{\partial z^2})_{z=ih} + O(h^2),$$

Analogous approximations hold for $\Delta_t^+ u_i^n,\ \Delta_t^- u_i^n,\ \delta_t u_i^n,\ \Delta_{0t}u_i^n$ and $\delta_t^2 u_i^n$, respectively.

The approximate solution of (2.1) at (x_i, y_j, t_n) is denoted by C_{ij}^n. Sometimes, if there is no confusion, we shall write C^n instead of C_{ij}^n.

2.1 Euler explicit scheme (EBTCS)

The simplest numerical scheme we can use to compute the numerical solution of (2.1) is the Euler explicit scheme, also known as **b**ackwards in **t**ime **c**entral in **s**pace (BTCS), which is expressed by

$$C_{ij}^{n+1} = C_{ij}^n + (r_x\delta_x^2 + r_y\delta_y^2)C_{ij}^n + \Delta t f_{ij}^n,\ 1 < i < I,\ 1 < j < J \text{ and } n > 0, \tag{2.2a}$$

with the boundary conditions:

a) on the left and right walls

$$\text{for } 1 \le j \le J \textit{ and } n > 0,\ C_{1j}^n = g(a, j\Delta y, t_n) \textit{ and } C_{Ij}^n = g(b, j\Delta y, t_n), \tag{2.2b}$$

b) on the lower un upper walls

$$\text{for } 1 \le i \le I \textit{ and } n > 0,\ C_{i1}^n = g(i\Delta x, c, t_n) \textit{ and } C_{iJ}^n = g(i\Delta x, d, t_n), \tag{2.2c}$$

and the initial condition

$$\text{for } all\ i\ and\ j,\ C_{ij}^0 = c_0(x_i, y_j) \tag{2.2d}$$

The parameters r_x and r_y are given by

$$r_x = \frac{A\Delta t}{\Delta x^2}, r_y = \frac{A\Delta t}{\Delta y^2}. \tag{2.3}$$

The scheme is explicit because there is only one unknown value C^{n+1} at the new time level.

2.1.1 Analysis of Euler explicit scheme

Our next concern is to study **consistency, stability** and **convergence** of this scheme

Truncation error. Consistency

Let $T(x, y, t)$ denote the pointwise truncation error at $(x, y, t) \in \overline{D}_h \times [0, T]$. For the scheme EBTCS, $T(x, y, t)$ is calculated by substituting the solution of $c(x, t)$ in (2.2a). The result is

$$T_{ij}^n = \frac{c_{ij}^{n+1} - c_{ij}^n}{\Delta t} - A(\frac{\delta_x^2}{\Delta x^2} - \frac{\delta_y^2}{\Delta y^2})c_{ij}^n - F_{ij}^n. \tag{2.4}$$

Assuming that c is sufficiently smooth, we expand in a Taylor series around (x_i, y_j, t_n) the terms of this expression and get

$$\begin{cases} T_{ij}^n = (\frac{\partial c}{\partial t} - A\Delta c - F) \mid_{(x_i, y_j t_n)} + \\ \{\frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} \mid_{(x_i, y_j, \eta)} - \frac{A}{12}\Delta x^2(\frac{\partial^4 c}{\partial x^4} + \frac{\partial^4 c}{\partial y^4})\} \mid_{(\varepsilon, \zeta, t_n)}, \end{cases}$$

where $t_n < \eta < t_{n+1}$ and $(x_i - \Delta x, y_j - \Delta y) < (\varepsilon, \zeta) < (x_i + \Delta x, y_j + \Delta y)$. Let $\| \cdot \|_\infty$ denotes the maximum norm, and K_1, K_2 and K_3 be bounds in such a norm for $\frac{\partial^2 c}{\partial t^2}$, $\frac{\partial^4 c}{\partial x^4}$ and $\frac{\partial^4 c}{\partial y^4}$ for all t, then we have that

$$\| T_{ij}^n \|_\infty \leq \frac{\Delta t}{2}K_1 + \frac{A}{12}(\Delta x^2 K_2 + \Delta y^2 K_3) \tag{2.5}$$

We recall the definition of **consistency** of a numerical method given in the lectures of IVP.

Definition1 *A method is consistent in the* $\| \cdot \|$ *−norm if*

$$\lim \| T^n \| = 0 \text{ as } \Delta t \to 0 \text{ and } (\Delta x, \Delta y) \to 0.$$

Moreover, the method is consistent of order (p,q) if

$$\| T^n \| = O(\Delta t^p + \Delta x^q + \Delta y^q)$$

Then, by virtue of (2.5) we say that the scheme EBTCS is **consistent** in the maximum norm with order $(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$.

Stability.

Definition 2 *A numerical method is said to be stable in the* $\| \cdot \|$ *−norm, if there exist positive constants* Δt_0, h_0 *and* K_T *such that for all* $n \geq 0$

$$\| C^n \| \leq K_T,$$

for $0 < \Delta t \leq \Delta t_0$ *and* $0 < \Delta x, \Delta y \leq h_0$. *The constant* K_T *may depends on* t*, but is independent of* n. Therefore, this definition says that the stability is an intrinsic property of the method to keep the solution not growing without bound. A simple but very practical method to study the stability of the scheme (2.2a) makes use of the discrete Fourier transform assuming the domain is infinite and that there are no forcing terms and boundary conditions. This approach will give a necessary condition for stability of the scheme applied to solve the initial boundary value problem (2.1). For details see Thomas (1994). From a practitioner point of view, the way to apply the method is as follows. Take one discrete Fourier mode and set

$$C_{pq}^n \sim \lambda^n e^{i(k_x p \Delta x + k_y q \Delta y)}, \tag{2.6}$$

where $\mathbf{k} = (k_x, k_y)$ is a wave number. Substituting this expression into (2.2a) and using Euler formula ($e^{ia} = \cos a + i \sin a$) we obtain the amplification factor

$$\lambda(\mathbf{k}) = 1 - 4(r_x \sin^2 \frac{k_x}{2} \Delta x + r_y \sin^2 \frac{k_y}{2} \Delta y) \tag{2.7}$$

The method is stable -the solution will remain bounded- if

$$| \lambda | \leq 1. \tag{2.8}$$

Then, from (2.7) it follows that (2.8) is satisfied if

$$r_x + r_y \leq \frac{1}{2}. \tag{2.10}$$

(2.8) is known as the discrete von Neuman stability condition Note that this condition is not sufficient because we have forgotten the boundary effects. However, if the region D were infinite or periodic, then the above condition would also be sufficient. Moreover, it is worth noticing that if the initial boundary value problem is solvable by a finite Fourier series then (2.10) is also a necessary and sufficient condition for stability of the EBTCS scheme when is applied to solve (1.2).

Convergence

Definition 3 *We recall that a numerical scheme approximating a continuous initial boundary value problem is a convergent scheme at any* $t \in [0, T]$ *in a given* $\| \cdot \|$ *−norm, if for any sequence of partitions* $\{\Delta x, \Delta y\}_l$

$$\| C^{n+1} - c^{n+1} \|_l \to 0$$

as $(n+1)\Delta t \to t$*,* $l \to \infty$ *and* $\Delta t \to 0$*.*

To study the convergence of the scheme (2.2) we set

$$e_{ij}^n = c_{ij}^n - C_{ij}^n \tag{2.11}$$

So that, substracting (2.2a) from (2.4) gives

$$e_{ij}^{n+1} = (1 - 2r_x - 2r_y)e_{ij}^n + r_x(e_{i+1j}^n + e_{i-1j}^n) + r_y(e_{ij+1}^n + e_{ij-1}^n) * \Delta t T_{ij}^n. \tag{2.12}$$

Let $E^n = \| e_{ij}^n \|_\infty$. If $(1 - 2r_x - 2r_y)$ is positive, the coefficients on the right hand side are all positive, so that

$$E^{n+1} \leq E^n + \Delta t \| T^n \|_\infty$$

or equivalently

$$E^{n+1} \leq E^0 + n\Delta t \| T^n \|_\infty . \tag{2.13}$$

If $E^0 \to 0$ as Δt and $(\Delta x, \Delta y) \to 0$, then by virtue of (2.5) it follows from (2.13) that $E^{n+1} \to 0$ as Δt and $(\Delta x, \Delta y) \to 0$ and hence EBTCS is convergent.

Note that the important points of the proof are: *a)* $(1 - 2r_x - 2r_y) \geq 0$, which is the stability condition, and b) consistency. EBTCS scheme has the good property of being easy to implement in all types of computer architectures, however if Δx is small and the coefficient A takes moderate values, the stability condition requires a very small value for Δt, so that one has to take an enormous number of time steps to complete the calculations. This sometimes makes the scheme inefficient. In such cases one may prefer implicit schemes, which are unconditionally stable and do not have to satisfy stability constraints that put conditions on the size of Δx and Δt. Accuracy is the only reason to determine the size of Δt and Δx. The most common implicit schemes used to compute the approximate solution of (2.1) are Euler implicit, also known as IBTCS (**i**mplicit **b**ackward in **t**ime **c**entral in **s**pace) and Crank-Nicolson (CN).

2.2 Euler implicit scheme (IBTCS)

For $1 < i < I, 1 < j < J$ and $n > 0$, the expression of this scheme is

$$C_{ij}^{n+1} - (r_x\delta_x^2 + r_y\delta_y^2)C_{ij}^{n+1} = C_{ij}^n + \Delta t F_{ij}^{n+1} \tag{2.14}$$

and (2.2b)-(2.2d) for the boundary and initial conditions.

Following the method used for the analysis of the scheme EBTCS we can prove very easily that for the scheme IBTCS

$$\| T^n \|_\infty = O(\Delta t) + O(\Delta x^2) + O(\Delta y^2) \ for\ all\ n > 0.$$

Furthermore, it is *unconditionally stable* and *convergent*. However, there is another approach, known as the operator or matrix approach, to analyze difference schemes, which is very convenient for the analysis of difference schemes for initial boundary value problems. Assembling (2.14) in matrix-vector form yields

$$Q_1 C^{n+1} = C^n + \Delta t(F^{n+1} + B^{n+1}), \tag{2.15a}$$

where $C^{n+1} = [C_1^{n+1}, ..., C_K^{n+1}]^T, K = (I-2)\times(J-2),\ Q_1$ is a $K \times K$ matrix of the form

$$Q_1 = \begin{bmatrix} B & -r_yI & \Theta & - \\ -r_yI & B & -r_yI & \\ - & - & - & -r_yI \\ - & \Theta & -r_yI & B \end{bmatrix},$$

where I is the $(I-2)\times(I-2)$ unitary matrix, Θ is the null matrix and B is an $(I-2)\times(I-2)$ tridiagonal matrix of the form

$$B = \begin{bmatrix} 1+2r_x+2r_y & -r_x & 0 & - \\ -r_x & 1+2r_x+2r_y & -r_x & - \\ - & - & - & -r_x \\ - & 0 & -r_x & 1+2r_x+2r_y \end{bmatrix},$$

B^n is the column vector which contains boundary condition values. Q_1 is a symmetric positive definite matrix, so that (2.15a) can be written as

$$C^{n+1} = QC^n + \Delta t G^{n+1}, \tag{2.15b}$$

where $G^{n+1} = Q(F^{n+1} + B^{n+1})$ and $Q = Q_1^{-1}$.

2.2.1 Analysis of Euler implicit scheme

We analyze the scheme IBTCS written in operator form (2.15). Of course, we proceed by studying **consistency, stability** and **convergence**; however, now it is convenient to do so in terms of a general norm $\|\cdot\|$, rather than the pointwise approach used above.

Truncation error. Consistency.

Let c^n be the vector $[c_1^n, ..., c_K^n]^T$, where c_i^n denotes the value of the exact solution at (x_i, t_n). Using(2.15b) we express the truncation error as

$$\Delta t T^n = c^{n+1} - Qc^n - \Delta t G^n. \tag{2.16}$$

To calculate $\| T^n \|$ one has to calculate each component T_i^n in a manner similar to the computation of the pointwise truncation error, and then apply the definition of the norm. By so doing, it is easy to see that

scheme (2.15b) is of order $(1,2)$ **in the norms** $\|\cdot\|_2, \|\cdot\|_1$**and .**$\|\cdot\|_\infty$

Stability.

Another way (equivalent to Definition 2) to define stability of a numerical method written in operator form is the following

Definition 4 *A numerical scheme of the form*

$$C^{n+1} = QC^n,\ n \geq 0$$

is stable with respect to a norm $\|\cdot\|$, *if there exist* $\Delta t_0,\ h_0$ *and a positive constant* β *such that*

$$\| C^{n+1} \| \leq (1+\beta\Delta t) \| C^n \|$$

for all $(n+1)\Delta t = t,\ 0 < \Delta t < \Delta t_0,\ 0 < \Delta x, \Delta y < h_0$.

Then, by virtue of (2.15b), with $G^n \equiv 0$, and the definition of the operator norm $\| Q \|$, i.e., $\| Q \| = \sup \frac{\|Qa\|}{\|a\|}$ for all $a \neq 0$, the scheme IBTCS is stable if and only if

$$\| Q \| \leq (1+\beta\Delta t) \tag{2.17}$$

The point here is how to obtain a useful estimate for $\| Q \|$ in terms of properties of the matrix Q which are easy to calculate. From a first course on numerical analysis, we know that for any matrix Q, $\| Q \|_2 \geq \sigma(Q)$, where $\sigma(Q) = \max\{| \lambda_i |: \lambda_i$ are eigenvalues of $Q\}$ is known as spectral radius of Q, and $\| Q \|_2$ is the l_h^2. But, if Q is a Hermitian matrix, then $\| Q \|_2 = \sigma(Q)$. Hence, the stability of a symmetric scheme such as (2.15b) is intimately linked to the spectrum of the matrix of the scheme. It is difficult to obtain the eigenvalues of a matrix; however, we can bound them by virtue of Gerschgoring circle theorem, which is stated next without proof.

Gerschgoring Circle Theorem. *Let* $A = (a_{ij})_{K\times K}$ *a* $K \times K$ *matrix and for all* $i = 1, .., K$, $\rho_i = \sum_{j=}^{K} | a_{ij} |$, *with* $i \neq j$. *For each eigenvalue* λ *of* Q *there exists an* i *such that*

$$| \lambda - a_{ii} | \leq \rho_i.$$

By virtue of this theorem, the eigenvalue λ_i *of* Q_1 *satisfy*

$$1 \leq \lambda_i \leq 1 + 4(r_x + r_y),$$

for all $i = 1, 2, ..., K$. *Hence, the eigenvalue* μ_i *of* $Q = Q_1^{-1}$ *satisfy for all* i.

$$\frac{1}{1+4(r_x+r_y)} \leq \mu_i \leq 1.$$

These inequalities guaranty that the scheme IBTCS is unconditionally stable in the l_h^2-norm according to (2.17).

Moreover, since Q_1 is a symmetric positive definite diagonalizable matrix, it can be shown by application of Gerschgoring circle theorem that the scheme is also unconditionally stable in the maximum and l_h^1 norms.

Convergence.

We study the convergence of the IBTCS scheme in the norm $\| \cdot \|$, which stands for the $l_h^2,\ l_h^1$ or the maximum norm. Recalling that $e^n := c^n - C^n$, then by virtue of (2.15b) and (2.16) we obtain that

$$\| e^{n+1} \| \leq \| Q \| \| e^n \| + \Delta t \| T^n \| \leq \| e^n \| + \Delta t \| T^n \|,$$

and by stability

$$\| e^{n+1} \| \leq \| e^0 \| + t_n \| T^n \| .$$

Since the scheme is consistent of order $(1, 2)$, then it follows that as $\Delta t \to 0$ and $(\Delta x, \Delta y) \to 0$, $\| e^{n+1} \| \to 0$ for all n. So that, the scheme is convergent in the norm $\| \cdot \|$.

2.3 Crank-Nicolson scheme (CN)

For $1 < i < I, 1 < j < J$ and $n > 0$, the expression of this scheme is

$$C_{ij}^{n+1} - \frac{1}{2}(r_x\delta_x^2 + r_y\delta_y^2)C_{ij}^{n+1} = C_{ij}^n + \frac{1}{2}(r_x\delta_x^2 + r_y\delta_y^2)C_{ij}^n + \frac{\Delta t}{2}(F_{ij}^{n+1} + F_{ij}^n), \quad (2.17)$$

plus the boundary and initial terms (2.2b)-(2.2d)

In matrix form this scheme reads as

$$Q_1 C^{n+1} = PC^n + \Delta t(\overline{F}^n + \overline{B}^n), \quad (2.18)$$

where $\overline{F}^n = \frac{1}{2}(F_{ij}^{n+1} + F_{ij}^n)$, $\overline{B}^n = \frac{1}{2}(B_{ij}^{n+1} + B_{ij}^n)$, and Q_1 and P are $K \times K$ matrices. Some properties of them are:

i) $Q_1 = I + B,\ P = I - B$, where I is the $K \times K$ identity matrix and B is a $K \times K$ symmetric positive definite matrix.

ii) The eigenvalues λ_i of B satisfy for all $i = 1, 2, .., K$,

$$0 \leq \lambda_i \leq r_x + r_y.$$

iii) Let μ_i be an eigenvalue of $Q_1^{-1}P$. The for all i,

$$\mu_i = \frac{1 - \lambda_i}{1 + \lambda_i}. \quad (2.19)$$

2.3.1 Analysis of Crank-Nicolson scheme

Our analysis of CN scheme is restricted, as in the previous schemes, to calculate the truncation error and to study the stability and convergence.

Truncation error. Consistency.
From (2.19) it follows that

$$\Delta t T^n = Q_1 c^{n+1} - P c^n - \Delta t(\overline{F}^n + \overline{B}^n). \tag{2.20}$$

To estimate each component T_i^n we essentially follow the method used in the scheme IBTCS. We have that the truncation error of the Crank-Nicolson scheme in the $\| \cdot \| -$ norm is $O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2)$. So that, CN is, for almost the same computational work, more accurate than the scheme IBTCS.

Stability.
To study the stability of CN in the $\| \cdot \|$-norm, we consider the scheme being applied to a homogeneous problem. Then (2.18) becomes

$$C^{n+1} = Q_1^{-1} P C^n.$$

By virtue of (2.19) it follows that

$$\| Q_1^{-1} P \| \leq 1, \; hence \; \| C^{n+1} \| \leq \| C^n \| \tag{2.21}$$

so that the CN scheme is unconditionally stable in the $\| \cdot \|$-norm.

Convergence.
We study the convergence of CN in the $\| \cdot \|$ $-$norm. Let $e^n = c^n - C^n$, then by virtue of (2.18) and (2.10) we have that

$$Q_1 e^{n+1} - P e^n = \Delta t T^n$$

Hence by using (2.21) we obtain that

$$\| e^{n+1} \| \leq \| e^n \| + \Delta t \| T^n \| .$$

Thus,

$$\| e^{n+1} \| \leq \| e^0 \| + t_n \| T^n \| .$$

Since the scheme is consistent of order $(2, 2)$, then as $\Delta t \to 0$ and $(\Delta x, \Delta y) \to 0$, $\| e^{n+1} \| \to 0$ for all n.

2.4 Neuman boundary conditions

So far, we have studied the numerical schemes with Dirichlet boundary conditions (prescribed data of the solution on the boundary); however, there are many problems in which the normal derivative of the solution is the prescribed datum on the boundary. Specifically,

$$\frac{\partial c}{\partial n} |_{\partial D} = g \quad \text{for all } t.$$

There are various methods to impose this condition in a numerical difference scheme. We explain two of them, which are used very often, considering a one dimensional problem. To this end, let $x_1 \equiv a$ and $x_I \equiv b$ be the end points of the interval on which Neuman boundary condition are prescribed

$$-\frac{\partial c}{\partial x} |_{x=x_1} = g(a, t_n) \text{ and } \frac{\partial c}{\partial x} |_{x=x_I} = g(b, t_n) \quad \text{for all } t_n.$$

Method 1 (First order method) In this method we discretize the first order derivative of c as

$$\begin{cases} -\dfrac{\partial c^n}{\partial x} |_{x=x_1} \simeq -\dfrac{C_2^n - C_1^n}{\Delta x} = g_1^n, \\ \dfrac{\partial c^n}{\partial x} |_{x=x_I} \simeq \dfrac{C_I^n - C_{I-1}^n}{\Delta x} = g_I^n. \end{cases}$$

Method 2 (Second order method) In this method we add artificial points to the domain such that we can discretize by central differences the first order derivative. Thus, adding the points $x_0 = a - \Delta x$ and $x_{I+1} = b + \Delta x$, we approximate the Neuman boundary condition as

$$\begin{cases} -\dfrac{\partial c^n}{\partial x} |_{x=x_1} \simeq -\dfrac{C_2^n - C_0^n}{2\Delta x} = g_1^n, \\ \dfrac{\partial c^n}{\partial x} |_{x=x_I} \simeq \dfrac{C_{I+1}^n - C_{I-1}^n}{2\Delta x} = g_I^n. \end{cases}$$

2.5 Explicit versus Implicit schemes

We have studied standard explicit and implicit schemes to solve linear parabolic problems. We next summarize some of the relevant properties of such schemes.

Explicit schemes

- They have to satisfy a stability condition that in many multidimensional problems may be very restrictive. So that, Δt may be very small and consequently a large number of time steps have to be taken to carry out a large scale experiment.

- They are easy to implement and good for parallel computers.

Implicit schemes

- The discretization parameters are chosen by accuracy reasons rather than by stability constraints.

- The parameter Δt can be much larger than in explicit schemes regardless the size of Δx.

- To find the numerical solution of implicit schemes one has to invert a matrix. In one dimensional problems this may not cause any trouble, but in multidimensional problems things can be more difficult. However, for symmetric matrices, there are efficient iterative methods, such as the **Conjugate Gradient Method** with preconditioning and **Multigrid Methods** that can significantly alleviate this task.

It is difficult to state categorically which kind of schemes is better. That depends upon the problem to be solved, the computer used in the calculations, the programming abilities, the accuracy with which one wants to calculate etc. Although, things are not clearly defined, one recommendation is that for strongly stiff problems problems one must prefer implicit schemes with time step control.

2.6 ADI schemes

These scheme were invented long time ago (in the mid fifties) when the computers were slow and had a limited amount of memory, so that solving multidimensional problems with implicit schemes, such as CN, was a difficult task. The purpose of ADI (Alternative Direction Implicit) schemes was to speed up the computations of implicit schemes without using too much memory. To achieve this goal, *the idea is to break the multidimensional difference scheme, such as (2.1), into a sequence of one dimensional schemes which can be solved relatively fast (and using a small amount of memory) by inverting a tridiagonal matrix.* In order to apply this idea in an optimal way, the geometry of the domain D should be simple, for instance, a rectangle or square in two dimensional problems or a hexaedra in three dimensions. Among the various ADI schemes proposed by several authors, we shall consider the **Peaceman- Rachford scheme** that can be formulated as follows.

For $1 < i < I, 1 < j < J$ and $n > 0$, let

$$\begin{cases} i) \quad \dfrac{C_{ij}^{n+1/2} - C_{ij}^{n}}{\Delta t/2} = \frac{A}{\Delta x^2}\delta_x^2 C_{ij}^{n+1/2} + \frac{A}{\Delta y^2}\delta_y^2 C_{ij}^{n} + F_{ij}^{n}, \\ ii) \quad \dfrac{C_{ij}^{n+1} - C_{ij}^{n+1/2}}{\Delta t/2} = \frac{A}{\Delta x^2}\delta_x^2 C_{ij}^{n+1/2} + \frac{A}{\Delta y^2}\delta_y^2 C_{ij}^{n+1} + F_{ij}^{n+1}. \end{cases} \tag{2.22}$$

plus the boundary and initial conditions.

2.6.1 Analysis of ADI schemes

Truncation error. Consistency.

To study the truncation error of ADI schemes we combine $i)$ and $ii)$ in such way that (2.22) can be written as

$$(1 - \frac{r_x}{2}\delta_x^2)(1 - \frac{r_y}{2}\delta_y^2)C_{ij}^{n+1} = (1 + \frac{r_x}{2}\delta_x^2)(1 + \frac{r_y}{2}\delta_y^2)C_{ij}^{n} + \Delta t\overline{F}^n \tag{2.23}$$

Hence

$$\begin{aligned} \Delta t T_{ij}^n = & (1 - \tfrac{r_x}{2}\delta_x^2 - \tfrac{r_y}{2}\delta_y^2)c_{ij}^{n+1} - (1 + \tfrac{r_x}{2}\delta_x^2 + \tfrac{r_y}{2}\delta_y^2)c_{ij}^{n} \\ & -\Delta t\overline{F}^n + \frac{\Delta t}{4}\frac{\delta_x^2}{\Delta x^2}\frac{\delta_y^2}{\Delta y^2}(c_{ij}^{n+1} - c_{ij}^{n}). \end{aligned} \tag{2.24a}$$

By a Taylor expansion around $(x_i, y_j, t_n + \frac{\Delta t}{2})$ it follows that for all n

$$\| T^n \| = O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2) + O(\Delta t \Delta x^2) + O(\Delta y \Delta y^2). \tag{2.24b}$$

Stability

We prove that the Peaceman-Rachford scheme is unconditionally stable by using the discrete Fourier method Thus, we let

$$C_{lm}^n = \lambda^n \exp i(lp\pi\Delta x + mq\pi\Delta y)$$

in (2.23). The result that follows is

$$\lambda = \frac{(1 - 2r_x \sin^2(\frac{p\pi\Delta x}{2}))(1 - 2r_y \sin^2(\frac{q\pi\Delta y}{2}))}{(1 + 2r_x \sin^2(\frac{p\pi\Delta x}{2}))(1 + 2r_y \sin^2(\frac{q\pi\Delta y}{2}))}$$

Hence. $| \lambda | \leq 1$ for any (p, q). So that the scheme is unconditionally stable.

Convergence

We leave as an exercise the discussion of the convergence of the Peaceman-Rachford scheme using the same approach as in the Crank Nicolson scheme.

To calculate the solution C^{n+1} of (2.22) we have to solve first $(J-2)$ tridiagonal systems to obtain $C^{n+1/2}$ according to i), and then $(I-2)$ tridiagonal systems according to ii). Since the tridiagonal matrices of the systems are diagonal dominant, then Gaussian elimination (**Thomas algorithm)** can be implemented very efficiently.

3 Transport-diffusion problems

We can make more general the model problem (1.1) by adding transport terms, which show up when the diffusion mechanism takes place in an environment in which there is a flow field This type of problems appear quite often in biological and environmental modelling. Our model problem is now

$$\begin{cases} \dfrac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = A\Delta c + f(\mathbf{x}, t) \text{ in } D \times (0, T], \\ c(x, 0) = c_0(x),\, x \in D, \\ c\,|_{\partial D} = g(x,t) \text{ for all } t\ > 0, \end{cases} \tag{3.1}$$

where $\mathbf{u}(x,t)$ is a velocity vector. A first approach to find the numerical solution of (3.1) may consist of using some of the schemes we have explained for pure diffusion problems. This is a valid strategy whenever $\mathbf{u}\cdot\nabla c$ is not the dominant term in the equation, but if the term $\mathbf{u} \cdot \nabla c$ is much larger than. $A\Delta c$, then the schemes studied for parabolic problems can have troubles, because the mathematical properties of the solution are quite different, since the character of the solution of (3.1) is mostly determined by $\dfrac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c$. This bring us to discuss some basic ideas on linear hyperbolic problems.

3.1 Linear hyperbolic problems

Let us consider the 1-dimensional partial differential equation

$$\begin{array}{c} \dfrac{\partial c}{\partial t} + u(x, t)\dfrac{\partial c}{\partial x} = 0,\ x \in \mathbf{R},\ t \in (0, T] \\ c(x, 0) = c_0(x).\ \textit{prescribed} \end{array} \tag{3.2a}$$

This is one of the simplest partial differential equations, although to approximate it numerically is not a trivial task at all. The analytical solution of (3.2a) is easily obtained by observing that c is constant along curves, called the **characteristics,** which are solution of the IVP

$$\begin{gathered}\frac{dx}{dt} = u(x,t) \\ x(0)\ prescribed,\end{gathered} \tag{3.2b}$$

since the time derivative of $c(x,t)$ along such curves

$$\frac{dc(x,t)}{dt} = \frac{\partial c}{\partial t} + \frac{dx}{dt}\frac{\partial c}{\partial x} = 0, \tag{3.2c}$$

implies that $c(c,t) = cons\tan t$. If $u(x,t)$ is constant, then the solution of (3.2b) is the family of parallel straight lines $x - ut = cons\tan t$, so that $c(x,t) = c_0(x - ut)$. On the contrary, if $u(x,t)$ depends on x and t, the solution of (3.2b) is the family of lines

$$x - \int_0^t u(x(\tau),\tau)d\tau = cons\tan t,$$

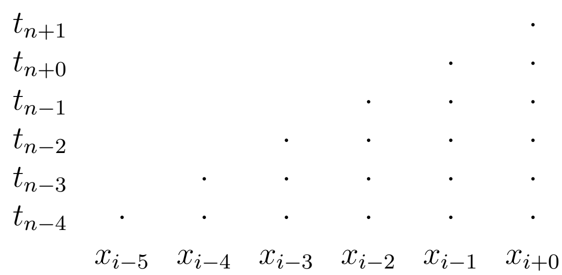
and $c(x,t) = c_0(x - \int_0^t u(x(\tau),\tau)d\tau)$. Furthermore, in the nonlinear problem in which u is a function of c, i.e.,$u = u(c)$, the characteristics are straight lines because c is constant along each, although they are not parallel. In this case too, $c(x,t) = c_0(x - u(c)t)$ until the characteristics break down, that is, they cross each other. The important role played by the characteristics in the analytical solution of (3.2a) must be reproduced by the numerical methods designed to approximate the solution, otherwise the method will not converge. In this spirit, a necessary condition that a numerical method must satisfy for convergence is the so called CFL condition, after the names of the important mathematicians Courant Friedrichs and Lewy (1928), who formulated such a condition in term of the concept of *domain of dependence.* To understand this concept we consider the model problem (3.2a) with $u > 0$ constant. The **domain of dependence** of the point (x,t) is defined as the set of all points in the plain (x,t) that the solution of (3.2a) is dependent upon. Since at (x_i,t_n) the solution is obtained by drawing through this point the characteristic $x - ut = cons\tan t$ back to where it meets the line $t = 0$; then the domain of influence of (x_i,t_n) is the segment of $x - ut = cons\tan t$ that joins the points $(x(0),0)$ with (x_i,t_n).Analogously, we can define the domain of dependence for the numerical solution. To this end, we compute the numerical solution of (3.2a) by the finite difference explicit upwind scheme

$$C_i^{n+1} = C_i^n - \upsilon(C_i^n - C_{i-1}^n) \tag{3.3a}$$

where

$$\upsilon = \frac{u\Delta t}{\Delta x} \tag{3.3b}$$

The value of C_i^{n+1} depends on the values of C_i^n and C_{i-1}^n, that is, the value at the point (x_i, t_{n+1}) depends on the values at the points (x_{i-1}, t_n) and (x_i, t_n) and so on. As illustrated in the figure below, the value of C_i^{n+1} depends on data give in a **triangle with vertex** (x_{i+0}, t_{n+1}) for time levels $n+1$ up to $n-4$, and ultimately, on data on data at the points on the initial line $(t = 0)$ $x_{i-n-1}, x_{i-n-2}, ..., x_i$. This triangle is the **numerical domain of dependence** of C_i^{n+1}.



The CFL condition states that for a convergent finite difference scheme the domain of dependence of the partial differential equation must lie within the domain of dependence of the numerical solution. And this condition is satisfied if $\upsilon \leq 1$. Note that if $\upsilon > 1$, the domain of dependence of the partial differential equation is not contained in the domain of dependence of the numerical solution and, therefore, the numerical solution will not converge to the true solution. What we have just obtained is a necessary stability condition for an explicit numerical scheme which is used to calculate the solution of (3.2a). We must emphasize that CFL condition is not a sufficient condition for the stability of a scheme.

Based on the properties of the characteristics, we present next a method which can be used to calculate the numerical solution of (3.1) when the transport terms are dominant.

3.2 Modified method of characteristics (MMC)

We assume that the velocity $\mathbf{u}$ is not constant and denote by $X(x, s; t)$ the characteristics of the total derivative operator

$$\frac{Dc}{Dt} := \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c$$

$X(x, s; t)$ are the solution curves of

$$\begin{cases} \frac{dX}{dt} = \mathbf{u}(X(x, s; t) \\ X(x, s; s) = x. \end{cases}$$

The MMC associates to each spatial grid point $\mathbf{x}_k = (x_i, y_j)$ at time level t_{n+1} a particle and ask by the position occupied by such a particle at time level t_n. Suppose we know such a position, then we approximate the total derivative of c_{ij} at time t_{n+1} as

$$\frac{Dc_{ij}}{Dt} \mid_{t=t_{n+1}} \simeq \frac{c_{ij}^{n+1} - c^n(X(x_i, y_j, t_{n+1}; t_n))}{\Delta t}.$$

The problem that appears in this approach is how to determine $c^n(X(x_i, y_j, t_{n+1}; t_n))$ since $X(x_i, y_j, t_{n+1}; t_n)$ is in general not a grid point. The discretization of $\frac{Dc}{Dt}$ suggests the following scheme to approximate the solution of (3.1).

For $1 < i < I, 1 < j < J$ and $n > 0$ do:

*Step*1 Calculate $\mathbf{X}(x_i, y_j, t_{n+1}; t_n)$ by solving

$$\begin{cases} \frac{dX}{dt} = \mathbf{u}(X(x_i, y_j, t_{n+1}; t), \quad t_n < t \leq t_{n+1}, \\ X(x_i, y_j, t_{n+1}; t_{n+1}) = (x_i, y_j). \end{cases} \tag{3.4a}$$

*Step*2 Compute $C^n(X(x_i, y_j, t_{n+1}; t_n))$ by quadratic or higher degree Lagrange interpolation of C^n at the points $X(x_i, y_j, t_{n+1}; t_n)$.

*Step*3 Let

$$C_{ij}^{n+1} - (r_x\delta_x^2 + r_y\delta_y^2)C_{ij}^{n+1} = C^n(X(x_i, y_j, t_{n+1}; t_n)) + \Delta t F_{ij}^{n+1} \tag{3.4b}$$

Note that (3.4b) looks like the IBTCS scheme with initial condition $C^n(\mathbf{X}(x_i, y_j, t_{n+1;}t_n)$ instead of C^n. A crucial point for the performance of the MMC scheme is the solution of (3.4a). There are many methods that can be applied, but for accuracy of second order in time, what is sufficient with (1.29), any second order Runge-Kutta method is valid.

Few remarks are now in order.

1) It can be proven that scheme (3.4a)-(3.4b) is unconditionally stable with truncation error $O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$. The analysis that gives such results is more difficult than the analysis of conventional schemes studied before, and is beyond the scope of these lectures.

2) Although the asymptotic error of the schemes based on the MMC may be of the same order as the error of conventional schemes, however the actual error is smaller. We illustrate this assertion through several tough example that we will show in class.

3.3 Crank-Nicolson scheme

This scheme will work well in transport-diffusion problems whenever the **convective term is moderate**. If such a term takes large values, or is the dominant term in the equation, CN schemes can still be used but the grid must be refined.

For $1 < i < I, 1 < j < J$ and $n > 0$, the expression of the scheme is

$$\left\{ \begin{array}{c} (1 + \frac{1}{2}\alpha_{ij}^{n+1/2}\delta_{0x} + \frac{1}{2}\beta_{ij}^{n+1/2}\delta_{0y} - \frac{1}{2}r_x\delta_x^2 - \frac{1}{2}r_y\delta_y^2)C_{ij}^{n+1} = \\ (1 - \frac{1}{2}\alpha_{ij}^{n+1/2}\delta_{0x} - \frac{1}{2}\beta_{ij}^{n+1/2}\delta_{0y} + \frac{1}{2}r_x\delta_x^2 + \frac{1}{2}r_y\delta_y^2)C_{ij}^{n} + \frac{\Delta t}{2}(F_{ij}^{n+1} + F_{ij}^{n}), \end{array} \right. \tag{3.5}$$

where $(\alpha_{ij}^{n+1/2}, \beta_{ij}^{n+1/2}) = (v_{1ij}^{n+1/2}\frac{\Delta t}{2\Delta x}, v_{2ij}^{n+1/2}\frac{\Delta t}{2\Delta y})$

3.3.1 Analysis of Crank-Nicolson

We can apply the same methodology as in the previous section to calculate the truncation error and study the stability of the scheme (3.5).

Truncation error. Consistency

The truncation error at (x_i, y_j, t_n) is given by

$$\begin{array}{l} \Delta t T_{ij}^n = (1 + \frac{1}{2}\alpha_{ij}^{n+1/2}\delta_{0x} + \frac{1}{2}\beta_{ij}^{n+1/2}\delta_{0y} - \frac{1}{2}r_x\delta_x^2 - \frac{1}{2}r_y\delta_y^2)c_{ij}^{n+1} \\ -(1 - \frac{1}{2}\alpha_{ij}^{n+1/2}\delta_{0x} - \frac{1}{2}\beta_{ij}^{n+1/2}\delta_{0y} + \frac{1}{2}r_x\delta_x^2 + \frac{1}{2}r_y\delta_y^2)c_{ij}^{n} - \Delta t\overline{F}_{ij}^{n}. \end{array} \tag{3.6a}$$

Performing a Taylor expansion around the point $(x_i, y_j, t_n + \frac{\Delta t}{2})$. and after a series of simple but tedious operations, we can obtain that if $\mathbf{u}(x,t)$ is sufficiently smooth then

$$\| T^n \| = O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2). \tag{3.6b}$$

Stability.

It can be proved by means of the operator (matrix) approach or the L^2-norm technique that the scheme (3.5) is in general **unconditionally stable**.

Note that by assembling (3.5) we get the expression

$$Q_1 C^{n+1} = PC^n + \Delta t(\overline{F}^n + \overline{B}^n), \tag{1}$$

where $Q_1 = I + B$ and $P = I - B$. Here, I is the $K \times K$ identity matrix and B is now a $K \times K$ non symmetric matrix. It can be shown that there exists Q_1^{-1}, so that (3.5) has a unique solution.

The solution of (3.5) can be obtained by iterative methods suitable for non symmetric systems. A good choice for is the **BiCGSTAB** method with diagonal preconditioning. However, we must say that solving non symmetric systems is always more expensive than solving symmetric ones, in particular, when the convective terms are large. A good scheme to deal with such a case is the modified method of characteristics

4 Numerical Methods for Reaction-Diffusion Models

We consider a further generalization of the diffusive model, which consists of adding a non linear term of the form $f(c)$ representing non linear interactions rates. The model equation is then termed reaction-diffusion equation. Rather than on a single reaction-diffusion equation, the practical interest lies on reaction-diffusion systems of equations; however, in order to make clear our point, we shall concentrate on numerical methods to solve reaction-diffusion models that consist of a single equation. To extend such methods to systems is not difficult. Our model problem is now

$$\left\{ \begin{array}{c} \dfrac{\partial c}{\partial t} = A\Delta c + f(c) \text{ in } D \times (0,T], \\ c(\mathbf{x},0) = c_0(\mathbf{x}),\ \mathbf{x} \in D, \\ \frac{\partial c}{\partial n} \mid_{\partial D} = 0. \end{array} \right. \tag{4.1}$$

We assume the following:

$H1$) There exists a region $S = (a,b) \subset \mathbf{R}$ where the non linear function $f(c)$ satisfies

$H2$) $f \in C^2(S, \mathbf{R})$, $f(0) = 0$.

$H3$) $f(c)n_s \leq 0$,

where n_s is the outward normal to S. Then, it is known that S is an invariant region for $c(\mathbf{x},t)$.

$H4$) There exist a positive constant K such that $\left|\dfrac{\partial f}{\partial c}\right| \leq K$.

$H5$) As $T \to \infty$ the solution c approaches an equilibrium solution $\overline{c}(\mathbf{x})$ which satisfies

$$\left\{ \begin{array}{c} A\Delta\overline{c} + f(\overline{c}) = 0 \text{ in } D, \\ \dfrac{\partial \overline{c}}{\partial n} \mid_{\partial D} = 0. \end{array} \right.$$

$H6$) $\overline{c}$ is asymptotically stable.

The non linear term $f(c)$ introduces further difficulties in the procedure to find the numerical solution of (31)- If $\left|\dfrac{\partial f}{\partial c}\right|$ is large, then fully implicit methods are recommended; however, if $\left|\dfrac{\partial f}{\partial c}\right|$ takes low or moderate values, as is the case in many biological and ecological problems, then explicit or semi-implicit schemes may be a good choice. As a first approach to the numerical solution of (4.1), we shall consider explicit schemes only. There are many explicit scheme which can be used to integrate (4.1); however, the simplest one is the scheme EBTCS. This scheme has the trouble with the fulfillment of a severe stability criterium, but, on the other hand , it has a good asymptotic behavior. There are many people who use it in their research.

4.1 EBTCS for Reaction-Diffusion Equations

The formulation of the scheme is

$$C_{ij}^{n+1} = C_{ij}^{n}+(r_x\delta_x^2+r_y\delta_y^2)C_{ij}^{n}+\Delta t f_{ij}^{n},\ 1 < i < I,\ 1 < j < J \text{ and } n > 0, \tag{4.2}$$

where $f_{ij}^n \equiv f(C_{ij}^n)$. (33) has to be modified at the boundary nodes according to the method chosen to impose Neuman boundary conditions.

4.1.1 Analysis

Truncation error: Consistency.

The expression for the truncation error is

$$T_{ij}^{n} = \frac{c_{ij}^{n+1} - c_{ij}^{n}}{\Delta t} - A(\frac{\delta_x^2}{\Delta x^2} - \frac{\delta_y^2}{\Delta y^2})c_{ij}^{n} - f_{ij}^{n} \tag{4.3a}$$

Performing Taylor series expansion and assuming that c_{tt} and c_{xxxx} and c_{yyyy} are bounded , we can see

$$\parallel T^n \parallel = O(\Delta t) + O(\Delta x^2) + O(\Delta y^2). \tag{4.3b}$$

Note that, the presence of the non linear term $f(c)$ does not introduce any difference as for the truncation error is concerned. The study of the stability is more delicate.

Stability.

First we note that by virtue of $H2$

$$f(C_{ij}^n) = \frac{\partial f}{\partial C}(\widetilde{c}_{ij}^n)C_{ij}^n.$$

The, by writing (32) in matrix form yields

$$C^{n+1} = \overline{Q}C^n,$$

where $\overline{Q} = Q + diag\dfrac{\partial f}{\partial C}$, with $Q = I + B$, B being the matrix generated by assembling $r_x\delta_x^2 + r_y\delta_y^2$. Since $\overline{Q}$ is symmetric, then the scheme is stable if and only if $\| \overline{Q} \| \leq 1$. Let us consider, for instance, the max norm. Thus, we have that

$$\| Q \|_\infty \leq | \, 1 + 4\Delta t A(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}) + K),$$

where K is the constant of $H4$. Hence, if

$$\Delta t \leq \frac{2}{4A(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}) + K} \tag{3.6}$$

the scheme is stable.

Convergence.

To study the convergence it is convenient to define for each $r > 0$ the ball

$$B_r = \{C \in \mathbf{R}^M : \| C - \overline{c} \|_\infty \leq r\}.$$

Next, let $e_{ij}^n = c_{ij}^n - C_{ij}^n$. Then

$$e_{ij}^{n+1} = e_{ij}^n + (r_x\delta_x^2 + r_y\delta_y^2)e_{ij}^n + \Delta t \left(f(c_{ij}^n) - f(C_{ij}^n) \right) + \Delta t T_{ij}^n.$$

Applying a Taylor expansion to the term $f(c_{ij}^n) - f(C_{ij}^n)$ it follows that

$$\begin{cases} e_{ij}^{n+1} = e_{ij}^n + (r_x\delta_x^2 + r_y\delta_y^2)e_{ij}^n + \Delta t f'(\overline{c}_{ij})e_{ij}^n + \\ \qquad \Delta t f''(\eta_{ij}^n)[(c_{ij}^n - \overline{c}_{ij}) + \gamma_{ij}^n e_{ij}^n] + \Delta t T_{ij}^n, \end{cases}$$

where $0 < \gamma < 1$ and η_{ij}^n is an intermediate point of $(c_{ij}^n, \overline{c}_{ij}, C_{ij}^n)$.
Hence,

$$\| e^{n+1} \| \leq \| I + \Delta t B^* \| \| e^n \| + \Delta t R K_1 \| e^n \| + \Delta t \| T^n \|, \tag{3.7}$$

where $\| \cdot \|$ is now the l_h^2-norm, K_1 is a bound for f'' and $I + \Delta t B^* \equiv Q + diag(\dfrac{\partial f}{\partial c}(\overline{c}_{ij}))$. Taking into account that $I + \Delta t B^*$ is a symmetric matrix , so that $\| I + \Delta t B^* \| = \rho(I + \Delta t B^*)$, and applying Gershgoring lemma we have the bound

$$\| I + \Delta t B^* \| \leq 1 - \alpha \Delta t,$$

where $\alpha > 0$. Taking R sufficiently small (independent of the grid spacing) it follows that

$$\| e^{n+1} \| \leq (1 - \Delta t \beta) \| e^n \| + \Delta t \| T^n \|$$

By applying Gronwall inequality yields that there is a positive bounded constant K_2 such that for all n

$$\| e^{n+1} \| \leq K_2(\Delta t + \Delta x^2 + \Delta y^2). \tag{3.8}$$

5 Basic bibliography

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