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Abstract: We derive the necessary and sufficient condition for the L^∞−monotonicity of finite difference θ-scheme for a diffusion equation. We confirm that the discretization ratio $\Delta t = O(\Delta x^2)$ is necessary for the monotonicity except for the implicit scheme. In case of the heat equation, we get an explicit formula, which is weaker than the classical CFL condition.

Key-words: Theta-scheme, monotonicity.

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La condition de la monotonie du $\theta-$schéma pour les équations de diffusion

Résumé : Nous nous intéressons à la condition nécessaire et suffissante de la monotonie du $\theta-$schéma pour l'équation de diffusion en dimension un. Notre résultat confirme que le ratio de discrétisation $\Delta t = O(\Delta x^2)$ est nécéssaire pour la monotonice sauf le schéma implicite. Dans le cas de l'équation de la chaleur, nous obtenons la formule explicite, qui est plus faible que la condition CFL.

Mots-clés : Theta-schéma, monotonie.

1 Introduction

The monotonicity of a numerical scheme is an important issue in numerical analysis. For example, in the convergence analysis in Chapiter 2 of Allaire [1], the author uses the $L^\infty-$monotonicity to derive the stability of the scheme, which gives a proof of convergence. In the viscosity solution convergence context of Barles and Souganidis [2], the $L^\infty-$monotonicity is a key criterion to guarantee the convergence of the numerical scheme.

We are here interested in the finite difference $\theta-$scheme for the diffusion equation:

$$\partial_t v \ - \ \sigma^2(x)\ D^2_{xx} v \ \ = \ \ 0, \qquad (t,x) \in \mathbb{R}^+ \times \mathbb{R}. \tag{1.1}$$

with initial condition $v(0,x) = g(x)$.

2 The $\theta-$scheme and CFL condition

Let $h = (\Delta t, \Delta x) \in (\mathbb{R}^+)^2$ be the discretization in time and space, denote $t_n := n\Delta t$, $x_i := i\Delta x$, $\sigma_i := \sigma(x_i)$ and by u^n_i the numerical solution of v at point (t_n, x_i), let $\mathcal{N} := \{x_i : i \in \mathbb{N}\}$ be a discrete grid on $\mathbb{R}$. The finite difference $\theta-$scheme $(0 \le \theta \le 1)$ for diffusion equation (1.1) is a countable infinite dimensional linear system on $\mathcal{N}$:

$$\frac{u^{n+1}_i - u^n_i}{\Delta t} \ - \ \sigma^2_i \Big(\theta \frac{u^{n+1}_{i+1} - 2u^{n+1}_i + u^{n+1}_{i-1}}{\Delta x^2} + (1-\theta) \frac{u^n_{i+1} - 2u^n_i + u^n_{i-1}}{\Delta x^2} \Big) \ = \ 0, \tag{2.1}$$

with initial condition $u^0_i = g(x_i)$.

Let $(u^n) := (u^n_i)_{i \in \mathbb{Z}}$ be a $\mathbb{Z}-$dimentional vector, denote $\alpha_i := \frac{\sigma_i^2 \Delta t}{\Delta x^2}$ and $\beta_i := \frac{\theta \alpha_i}{1+2\theta\alpha_i}$, we define $\mathbb{Z} \times \mathbb{Z}$ diensional matrices I, D, T and E as follows: I is the identity matrix, D is a diagonal matrix with $D_{i,i} = \alpha_i$, T is a tridiagonal matrix with $T_{i,i-1} = T_{i,i+1} = \alpha_i$ and $T_{i,i} = 0$, and $E := \theta[I + 2\theta D]^{-1}T$ which is a tridiagonal matrix with $E_{i,i-1} = E_{i,i+1} = \beta_i$ and $E_{i,i} = 0$. Then the system (2.1) can be written as

$$\big[I + 2\theta D - \theta T\big]\ (u^{n+1}) \ \ = \ \ \big[I - 2(1-\theta)D + (1-\theta)T\big]\ (u^n),$$

or equivalently

$$\big[I + 2\theta D\big]\ \big[I - E\big]\ (u^{n+1}) \ \ = \ \ \big[I - 2(1-\theta)D + (1-\theta)T\big]\ (u^n). \tag{2.2}$$

Proposition 2.1. *Suppose that the function g is bounded on $\mathcal{N}$ and there is constant $\bar\sigma > 0$ such that $|\sigma_i| \le \bar\sigma$ for every $i \in \mathbb{Z}$, then the $\mathbb{Z} \times \mathbb{Z}$ matrix $I - E$ is invertible and its inversion B is given by*

$$B \ \ := \ \ I \ + \ \sum_{n=1}^{\infty} E^n. \tag{2.3}$$

And therefore, there is a unique solution for system (2.1) *(or* (2.2)*) given by*

$$(u^{n+1}) \ \ = \ \ B\ \big[I + 2\theta D\big]^{-1}\ \big[I - 2(1-\theta)D + (1-\theta)T\big]\ (u^n). \tag{2.4}$$

Proof. First, $(\alpha_i)_{i\in\mathbb{N}}$ defined by $\alpha_i = \frac{\sigma_i^2 \Delta t}{\Delta x^2}$ are uniformly bounded by $\bar\alpha := \frac{\bar\sigma^2 \Delta t}{\Delta x^2}$ since $(\sigma_i)_{i\in\mathbb{Z}}$ are uniformly bounded by $\bar\sigma$. It follows that $\beta_i = \frac{\theta\alpha_i}{1+2\theta\alpha_i} \le \rho := \frac{\theta\bar\alpha}{1+2\theta\bar\alpha} < \frac{1}{2}$.

Denote by $B(\mathcal{N})$ the space of all bounded functions defined on $\mathcal{N}$, then E can be viewed as an operator on $B(\mathcal{N})$ and its $L^\infty-$norm is defined by

$$\|E\|_\infty \;:=\; \sup_{u\in B(\mathcal{N}),u\neq 0} \frac{|Eu|_\infty}{|u|_\infty}.$$

Clearly, $\|E\|_\infty \leq 2\rho < 1$, and therefore, B in (2.3) is well defined and one can easily verify that B is the inverse of $\big[I-E\big]$. □

Definition 2.2. *A numerical scheme for equation* (1.1) *given by* $u_i^{n+1} = \mathbf{T}_h[u^n]_i$ *is said to be* $L^\infty-$*monotone if*

$$u_i^{1,n} \;\leq\; u_i^{2,n}, \;\; \forall i\in\mathbb{Z} \quad\Rightarrow\quad \mathbf{T}_h[u^{1,n}]_i \;\leq\; \mathbf{T}_h[u^{2,n}]_i, \;\; \forall i\in\mathbb{Z}.$$

Remark 2.3. *It is well-known that in the case* $\theta = 1$*, system* (2.2) *is an implicit scheme, and it is automatically* $L^\infty-$*monotone for every discretization* $(\Delta t, \Delta x)$*. When* $\theta < 1$*, a sufficient condition to gurantee the* $L^\infty-$*monotonicity of system* (2.2) *is the CFL(Courant-Friedrichs-Lewy) condition*

$$\bar{\alpha} \;:=\; \frac{\bar{\sigma}^2\Delta t}{\Delta x^2} \;\leq\; \frac{1}{2(1-\theta)}, \qquad \textit{for}\;\; \bar{\sigma} := \sup_{i\in\mathbb{Z}} \sigma_i. \tag{2.5}$$

The CFL condition is a sufficient condition for the monotonicity of $\theta-$scheme, and it implies a discretization ratio $\Delta t = O(\Delta x^2)$. We shall confirm that this ratio is necessary to guarantee the monotonicity in the following.

3 The necessary and sufficient condition

Let $\gamma_i := \frac{(1-\theta)\alpha_i}{1+2\theta\alpha_i} = \frac{(1-\theta)}{\theta}\beta_i$ and $b_{i,j}$ be elements of the matrix B, i.e. $B = (b_{i,j})_{(i,j)\in\mathbb{Z}^2}$. It is clear that $b_{i,j} \geq 0$ for every $(i,j)\in\mathbb{Z}^2$ by the definition of B in (2.3). Therefore, it follows from (2.4) that the necessary and sufficient condition for monotonicity of system (2.1) can be written as :

$$b_{i,j-1}\gamma_{j-1} \;+\; b_{i,j}\Big(\frac{1}{1+2\theta\alpha_j} - 2\gamma_j\Big) \;+\; b_{i,j+1}\gamma_{j+1} \;\;\geq\;\; 0, \qquad \forall (i,j)\in\mathbb{Z}^2. \tag{3.1}$$

Theorem 3.1. *Suppose that* $|\sigma_i| \leq \bar{\sigma} < \infty$ *for every* $i\in\mathbb{Z}$*, and let* $\theta\in(0,1)$*. Then the necessary and sufficient condition of monotonicity for the* $\theta-$*scheme in* (2.1) *is*

$$\alpha_i \;=\; \frac{{\sigma_i}^2\Delta t}{\Delta x^2} \;\leq\; \frac{1}{2(1-\theta)} \;+\; \frac{b_{i,i}-1}{2\theta(1-\theta)}, \qquad \forall i\in\mathbb{Z}. \tag{3.2}$$

Proof. First, since B is the inversion of $I-E$, we have $B\,\big[I-E\big] = I$, and it follows that

$$b_{i,j-1}\beta_{j-1} \;+\; b_{i,j+1}\beta_{j+1} \;\;=\;\; \begin{cases} b_{ij}-1, & \text{for } i=j,\\ b_{ij}, & \text{for } i\neq j.\end{cases}$$

Therefore, in case that $i\neq j$, (3.1) is equivalent to:

$$b_{i,j}\,\Big(\frac{1-\theta}{\theta} + \frac{1}{1+2\theta\alpha_j} - 2\gamma_j\Big) \;\geq\; 0. \tag{3.3}$$

Since $b_{i,j} \geq 0$, the inequality (3.3) holds as soon as

$$(1-\theta)(1+2\theta\alpha_j) \ + \ \theta \ - \ 2\theta(1-\theta)\alpha_j \quad \geq \quad 0,$$

which is always true.

In case that $i = j$, (3.1) is equivalent to:

$$b_{i,i}\left(\frac{1-\theta}{\theta} + \frac{1}{1+2\theta\alpha_i} - 2\gamma_i\right) \ - \ \frac{1-\theta}{\theta} \quad \geq \quad 0,$$

i.e.

$$\alpha_i \quad \leq \quad \frac{1}{2(1-\theta)} \ + \ \frac{b_{i,i}-1}{2\theta(1-\theta)}.$$

which is the required inequality (3.2). □

Remark 3.2. *Since $b_{i,i} < \infty$ for every $i \in \mathbb{Z}$, it follows from Theorem 3.1 that the ratio $\Delta t = O(\Delta x^2)$ is necessary for the monotonicity of $\theta-$scheme ($0 < \theta < 1$) as soon as $\sigma_i \neq 0$ for some $i \in \mathbb{Z}$.*

4 The heat equation

In this section, les us suppose that $\sigma(x) \equiv \sigma_0$ with a positive constant σ_0, then the diffusion equation turns to be the heat equation:

$$\partial_t v \ - \ \sigma_0^2 \ D_{xx}^2 v \quad = \quad 0, \qquad (t,x) \in \mathbb{R}^+ \times \mathbb{R}. \tag{4.1}$$

In this case, we can compute $b_{i,i}$ and then get an explicit formula for the monotonicity condition (3.2). Let

$$A \text{ be a } \mathbb{Z}\times\mathbb{Z} \text{ tridiagonal matrix such that } A_{i,i-1} = A_{i,i+1} = 1 \text{ and } A_{i,i} = 0, \tag{4.2}$$

then clearly, $E = \beta A$ with $\beta = \frac{\theta\alpha}{1+2\theta\alpha} < \frac{1}{2}$, $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2}$ and

$$B \quad = \quad \Big[I - \beta A\Big]^{-1} \quad := \quad \sum_{n=0}^{\infty} \beta^n A^n. \tag{4.3}$$

Lemma 4.1. *Denote by A^n the $n-$th exponentiation of matrix A in (4.2) for $n \in \mathbb{N}$, we rewritten $A^n = (a_{i,j}^{(n)})_{(i,j)\in\mathbb{Z}\times\mathbb{Z}}$. Then,*

$$a_{i,j}^{(n)} \quad = \quad \begin{cases} C_n^{(n+i-j)/2}, & \text{if } \frac{n+i-j}{2} \in \mathbb{Z} \cap [0,n], \\ 0, & \text{otherwise.} \end{cases} \tag{4.4}$$

Proof. We proceed by induction. First, it is clearly that (4.4) holds true for $n = 1$. Suppose that the (4.4) is true in case that $n = m$. Since $A^{m+1} = A^m \ A$, we then have $a_{i,j}^{m+1} = a_{i,j-1}^m + a_{i,j+1}^m$. It follows from $C_n^k = C_{n-1}^k + C_{n-1}^{k-1}$ that (4.4) holds still true for the case $n = m+1$. We then conclude the proof. □

By Lemma 4.1 and equality (4.3), we get $b_{i,i} = \sum_{k=0}^{\infty} C_{2k}^k \beta^{2k}$ with the convention that $C_0^0 := 1$. As a result, the monotonicity condition (3.2) of $\theta-$scheme reduces to

$$\alpha \quad \leq \quad \frac{1}{2(1-\theta)} \ + \ \frac{f(\beta)}{2\theta(1-\theta)}, \tag{4.5}$$

where

$$f(x) \ := \ \sum_{k=1}^{\infty} C_{2k}^k \ x^{2k} \qquad \text{for} \ \ -\frac{1}{2} < x < \frac{1}{2}.$$

Remark 4.2. *We can verify that* $C_{2k}^k \approx \frac{1}{\sqrt{\pi k}} 4^k$ *as* $k \to \infty$ *by Stirling's formula, thus the radius of convergence of* $f(x)$ *is* $\frac{1}{2}$.

Let us now compute the function $f(x)$. Since $C_{2k}^k = 2 \ \frac{2k-1}{k} \ C_{2(k-1)}^{k-1}$, it follows that for $|x| < \frac{1}{2}$,

$$\begin{aligned} f'(x) &= \sum_{k=1}^{\infty} 2k \ C_{2k}^k \ x^{2k-1} \ = \ \sum_{k=1}^{\infty} 4 \ (2k-1) \ C_{2(k-1)}^{k-1} \ x^{2k-1} \\ &= 4x \ + \sum_{k=1}^{\infty} (8k+4) \ C_{2k}^k \ x^{2k+1} \ = \ 4x \ + \ 4x^2 f'(x) \ + \ 4x f(x). \end{aligned}$$

We are then reduced to the ordinary differential equation

$$f'(x) \ = \ \frac{4x}{1-4x^2} \ (f(x)+1), \qquad \text{with} \ \ f(0) \ = \ 0,$$

whose solution is $f(x) = \frac{1}{\sqrt{1-4x^2}} - 1$. Inserting this solution into (4.5), and by a direct manipulation, it follows that (4.5) is equivalent to

$$\alpha \ \leq \ \frac{1}{2(1-\theta)} \ + \ \frac{\theta}{4(1-\theta)^2}. \tag{4.6}$$

We get the following theorem:

Theorem 4.3. *The necessary and sufficient condition for the* $L^\infty-$*monotonicity of* $\theta-$*scheme* $(0 < \theta < 1)$ *of the heat equation* (4.1) *is*

$$\alpha \ = \ \frac{\sigma_0^2 \Delta t}{\Delta x^2} \ \leq \ \frac{1}{2(1-\theta)} \ + \ \frac{\theta}{4(1-\theta)^2}. \tag{4.7}$$

Remark 4.4. *In particular, when* $\theta = \frac{1}{2}$, *the CFL condition is* $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq 1$, *and the necessary and sufficient condition of the monotonicity is* $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq \frac{3}{2}$.

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