Monotonicity condition for the θ-scheme for diffusion equations

J. Frederic Bonnans, Xiaolu Tan

To cite this version:

J. Frederic Bonnans, Xiaolu Tan. Monotonicity condition for the θ-scheme for diffusion equations. [Research Report] RR-7778, INRIA. 2011, pp.6. inria-00634417

HAL Id: inria-00634417
https://hal.inria.fr/inria-00634417

Submitted on 21 Oct 2011

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Monotonicity condition for the θ-scheme for diffusion equations

J. Frédéric BONNANS — Xiaolu TAN

N° 7778

Octobre 2011

Thème NUM

Rapport de recherche

ISSN 0249-6399 ISRN INRIA/RR--7778--FR+ENG

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

INRIA

centre de recherche SACLAY – ÎLE-DE-FRANCE

Monotonicity condition for the θ-scheme for diffusion equations*

J. Frédéric BONNANS† , Xiaolu TAN‡

Thème NUM — Systèmes numériques
Équipes-Projets Commands

Rapport de recherche n° 7778 — Octobre 2011 — 6 pages

Abstract: We derive the necessary and sufficient condition for the $L^\infty-$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.

* We thank Nizar Touzi (CMAP) for fruitful discussions.

† INRIA-Saclay and CMAP, École Polytechnique, 91128 Palaiseau, and Laboratoire de Finance des Marchés d'Énergie, France (Frederic.Bonnans@inria.fr).

‡ CMAP, École Polytechnique, 91128 Palaiseau, France (xiaolu.tan@polytechnique.edu), research supported by the Chair *Financial Risks* of the *Risk Foundation* sponsored by Société Générale, the Chair *Derivatives of the Future* sponsored by the Fédération Bancaire Française, and the Chair *Finance and Sustainable Development* sponsored by EDF and CA-CIB.

Centre de recherche INRIA Saclay – Île-de-France
Parc Orsay Université
4, rue Jacques Monod, 91893 ORSAY Cedex
Téléphone : +33 1 72 92 59 00

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

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

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*

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

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*

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

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 :

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

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*

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

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

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

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:

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

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* $\alpha = \frac{\sigma_0^2 \Delta t}{\Delta x^2} \leq \frac{3}{2}$.

References

[1] G. Allaire, *Numerical analysis and optimization*, Oxford University Press, Oxford, 2007. An introduction to mathematical modelling and numerical simulation, Translated from the French by Alan Craig.

[2] G. Barles and P.E. Souganidis, *Convergence of approximation schemes for fully nonlinear second order equations*, Asymptotic Anal., 4(3):271-283, 1991.

Centre de recherche INRIA Saclay – Île-de-France
Parc Orsay Université - ZAC des Vignes
4, rue Jacques Monod - 91893 Orsay Cedex (France)

Centre de recherche INRIA Bordeaux – Sud Ouest : Domaine Universitaire - 351, cours de la Libération - 33405 Talence Cedex
Centre de recherche INRIA Grenoble – Rhône-Alpes : 655, avenue de l'Europe - 38334 Montbonnot Saint-Ismier
Centre de recherche INRIA Lille – Nord Europe : Parc Scientifique de la Haute Borne - 40, avenue Halley - 59650 Villeneuve d'Ascq
Centre de recherche INRIA Nancy – Grand Est : LORIA, Technopôle de Nancy-Brabois - Campus scientifique
615, rue du Jardin Botanique - BP 101 - 54602 Villers-lès-Nancy Cedex
Centre de recherche INRIA Paris – Rocquencourt : Domaine de Voluceau - Rocquencourt - BP 105 - 78153 Le Chesnay Cedex
Centre de recherche INRIA Rennes – Bretagne Atlantique : IRISA, Campus universitaire de Beaulieu - 35042 Rennes Cedex
Centre de recherche INRIA Sophia Antipolis – Méditerranée : 2004, route des Lucioles - BP 93 - 06902 Sophia Antipolis Cedex

Éditeur
INRIA - Domaine de Voluceau - Rocquencourt, BP 105 - 78153 Le Chesnay Cedex (France)
http://www.inria.fr
ISSN 0249-6399