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Numerical solution of nonlinear cross-diffusion systems by a linear scheme

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Abstract.

This paper introduces a linear scheme to approximate the solutions of the general nonlinear cross-diffusion system. After discretizing the scheme in space, we obtain a versatile, easy to implement and stable numerical scheme for the cross-diffusion system. Numerical experiments are carried out to examine rates of convergence with respect to the time step and the spatial mesh sizes.

§1. Introduction

This paper deals with numerical schemes to approximate the following nonlinear problem: Find $\boldsymbol{z} = (z_1, \ldots, z_M) : \overline{\Omega} \times [0, T) \to \mathbb{R}^M$ $(M \in \mathbb{N})$ such that

$$
(1) \qquad \begin{cases} \dfrac{\partial \boldsymbol{z}}{\partial t} = \Delta \boldsymbol{\beta}(\boldsymbol{z}) + \boldsymbol{f}(\boldsymbol{z}) & \text{in} \quad Q := \Omega \times (0, T), \\ \dfrac{\partial \boldsymbol{\beta}(\boldsymbol{z})}{\partial \nu} = \boldsymbol{0} & \text{on} \quad \partial\Omega \times (0, T), \\ \boldsymbol{z}(\cdot, 0) = \boldsymbol{z}_0 & \text{in} \quad \Omega. \end{cases}
$$

Here, $\Omega \subset \mathbb{R}^d$ $(d \in \mathbb{N})$ is a bounded domain with smooth boundary $\partial\Omega$, T is a positive constant, $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_M)$, $\boldsymbol{f} = (f_1, \ldots, f_M)$: $\mathbb{R}^M \to \mathbb{R}^M$ and $\boldsymbol{z}_0 = (z_{01}, \ldots, z_{0M})$: $\Omega \to \mathbb{R}^M$ are given functions, ν is the unit outward normal vector to the boundary $\partial\Omega$. We note that the diffusivity β_i of the ith component depends not only on the ith variable but also on the jth $(j \neq i)$ variables in general. This mixture of diffusion terms

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is called cross-diffusion. Numerous problems of this type have been proposed in the literature, especially in the area of population ecology.

One of the typical examples of nonlinear cross-diffusion systems is the following model which was proposed by Shigesada, Kawasaki and Teramoto [14] to understand spatial and temporal behaviours of two animal species under the influence of the population pressure due to intra- and interspecific interferences:

$$(2) \qquad \begin{cases} \dfrac{\partial z_1}{\partial t} = \Delta\left[(a_{10} + a_{11}z_1 + a_{12}z_2)z_1\right] + (c_{10} - c_{11}z_1 - c_{12}z_2)z_1, \\ \dfrac{\partial z_2}{\partial t} = \Delta\left[(a_{20} + a_{21}z_1 + a_{22}z_2)z_2\right] + (c_{20} - c_{21}z_1 - c_{22}z_2)z_2, \end{cases}$$

where a_{ij}, c_{ij} $(i = 1, 2,\ j = 0, 1, 2)$ are non-negative constants. Here, z_i represents the population density of ith species. The virtual diffusivity of the ith species $a_{i0} + a_{i1}z_1 + a_{i2}z_2$ is dependent on intra- and interspecific population pressure. The cross-diffusion terms describe tendencies such that the ith species keeps away from high-density areas of the jth species. The spatially segregating coexistence of two competing species occurs by the cross-diffusion effect.

There are a number of other exciting cross-diffusion systems. For instance, Kadota and Kuto [9] investigated a prey-predator cross-diffusion system. In the system, the diffusivity of the prey is the same type of (2), but that of the predator is a fractional type which implies the population pressure of the predator weakens in high-density areas of the prey, i.e., the predator migrates towards areas of high concentration of the prey. Murakawa and Ninomiya [13] considered a three-component reaction-diffusion system with a reaction rate parameter, and investigate its singular limit as the reaction rate tends to infinity. The limit problem is described by a nonlinear cross-diffusion system which possesses piecewise linear nonlinear diffusions. Moreover, they proved that the cross-diffusion system is a weak form of a free boundary problem with triple junctions.

Thus, there are a lot of interesting and important cross-diffusion systems. We would like to carry out numerical experiments for various type of nonlinearities. However, there are few results on numerical analysis for the cross-diffusion systems. There are theoretical results on numerical methods for the Shigesada–Kawasaki–Teramoto model (2). Galiano, Garzón and Jüngel [6] considered a fully implicit discrete-time scheme. They proved that convergence in one space dimension. Barrett and Blowey [2] considered a fully discrete finite element approximation with a regularization technique. Their method is also fully implicit. They showed that convergence in space dimensions $d \leq 3$, and presented numerical experiments in one space dimension. Chen and Jüngel employed a finite difference technique [4] and a Euler–Galerkin method [5] to discretize in space. They took advantage of the fully discrete schemes to prove the existence of a weak solution of the system (2). Andreianov, Bendahmane and Ruiz-Baier [1] proved convergence of a positivity-preserving finite volume scheme. Their scheme is applicable to slightly general problem. However, it can not be applied to, for example, the linear cross-diffusion system [7] and the cross-diffusion system appeared in [13] in which the solutions can be positive or negative. All of them treated nonlinear implicit schemes to the system (2). Implicit schemes show better stability and accuracy properties in general. Therefore, their schemes might be efficient. However, for three or four or more components systems and for high dimensional simulations, the implementation becomes complicated. Moreover, their analysis can not apply to other cross-diffusion systems. There may be cases where we want to see numerical solutions easily and where many numerical simulations are carried out by changing not only the coefficients but also the nonlinearity itself. These schemes are not suitable in such cases.

In response to this, the author proposed a linear discrete-time scheme to approximate general nonlinear cross-diffusion system [12]. After discretizing the scheme in space, versatile, easy to implement and stable numerical schemes are obtained. In this paper, we introduce the linear scheme and carry out numerical simulations in order to investigate the efficiency of the scheme.

§2. A linear scheme and results

In this section we present a linear scheme to approximate the solutions of the general cross-diffusion system (1) and state our theoretical results.

2.1. A linear scheme

We denote by $\tau = T/N_T$ ($N_T \in \mathbb{N}$) the time step size. The following linear scheme was proposed by the author [12]: Put

$$\boldsymbol{Z}^0 = \boldsymbol{z}_0^\tau.$$

Here, $\boldsymbol{z}_0^\tau \in H^1(\Omega)^M$ is an approximation to $\boldsymbol{z}_0 \in L^2(\Omega)^M$. For $n = 1, 2, \ldots, N_T$, find $\boldsymbol{Z}^n$ and $\boldsymbol{U}^n$ such that

$$
(3) \qquad \begin{cases} \boldsymbol{U}^n - \dfrac{\tau}{\mu}\Delta \boldsymbol{U}^n = \boldsymbol{\beta}(\boldsymbol{Z}^{n-1}) + \dfrac{\tau}{\mu}\boldsymbol{f}(\boldsymbol{Z}^{n-1}) & \text{in} \quad \Omega, \\ \dfrac{\partial \boldsymbol{U}^n}{\partial \nu} = \boldsymbol{0} & \text{on} \quad \partial\Omega, \\ \boldsymbol{Z}^n = \boldsymbol{Z}^{n-1} + \mu(\boldsymbol{U}^n - \boldsymbol{\beta}(\boldsymbol{Z}^{n-1})) & \text{in} \quad \Omega, \end{cases}
$$

where μ is a fixed positive constant. We assert that $\boldsymbol{Z}^n$ approximates $\boldsymbol{z}(\cdot, \tau n)$. This scheme is quite simple. The scheme amounts to solving M linear elliptic equations, followed by explicit algebraic corrections at each time step. After discretizing the scheme in space, we obtain a versatile, easy to implement and efficient numerical scheme for the cross-diffusion system.

The scheme (3) can be regarded as an extension of a linear scheme based on the nonlinear Chernoff formula for the degenerate parabolic equations, i.e. $M = 1$, which was proposed by Berger, Brezis and Rogers [3]. The extension of the scheme to the system is very easy and natural. However, the theory can not be applied to the system. We proved the stability and the convergence of the linear scheme by means of the theory of reaction-diffusion system approximation [11, 12].

2.2. Assumptions

The general cross-diffusion system is quite difficult to deal with. Even for the problem (2), only partial results are available on the existence of solutions (see [4], [5] and references therein). We impose the following assumptions:

(H1) $\boldsymbol{\beta}$ is a Lipschitz continuous function satisfying $\boldsymbol{\beta}(\boldsymbol{0}) = \boldsymbol{0}$. Moreover, there exists a positive constant a such that

$$
\sum_{i=1}^{M}\sum_{j=1}^{M}(\beta_i)_j(\boldsymbol{\eta})\xi_i\xi_j \geq a|\boldsymbol{\xi}|^2
$$

for almost all $\boldsymbol{\eta}, \boldsymbol{\xi} \in \mathbb{R}^M$.

Here, $(\beta_i)_j$ denotes the derivative of the ith component of $\boldsymbol{\beta}$ with respect to the jth variable.

(H2) $\boldsymbol{f}$ is a Lipschitz continuous function.

Let L be a positive constant satisfying

$$
|(\beta_i)_j(\boldsymbol{\eta}) - a\delta_{ij}| \leq L
$$

for almost all $\boldsymbol{\eta} \in \mathbb{R}^M$ and all $i, j \in \{1, 2, \ldots, M\}$, where δ_{ij} is the Kronecker delta.

(H3) μ satisfies

$$0 < \mu < \frac{a}{a^2 + M^2 L^2}.$$

(H4) $\boldsymbol{z}_0 \in L^2(\Omega)^M$. $\boldsymbol{z}_0^\tau \in H^1(\Omega)^M$ satisfy

$$\|\boldsymbol{z}_0^\tau\|_{L^2(\Omega)^M} + \sqrt{\tau}\, \|\boldsymbol{z}_0^\tau\|_{H^1(\Omega)^M} \le C$$

for some positive constant C independent of τ. Moreover,

$$\boldsymbol{z}_0^\tau \rightharpoonup \boldsymbol{z}_0 \quad \text{weakly in } L^2(\Omega)^M \text{ as } \tau \to 0.$$

The assumption (H1) implies the system is uniformly parabolic. We also proved convergence for non-uniformly parabolic cross-diffusion systems. But they are weakly coupled. They have triangular diffusion matrices. See [12] for the details.

2.3. Weak formulation

The problem (1) will be understood in the sense of the following weak form:

Definition 2.1. *A function $\boldsymbol{z}$ is said to be a weak solution of* (1) *if it fulfils $\boldsymbol{z} \in (L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^1(\Omega)^*))^M$, $\boldsymbol{z}(\cdot,0) = \boldsymbol{z}_0$ a.e. in Ω and*

$$\int_0^T \left\langle \frac{\partial z_i}{\partial t}, \varphi_i \right\rangle + \int_0^T \langle \nabla \beta_i(\boldsymbol{z}), \nabla \varphi_i \rangle = \int_0^T \langle f_i(\boldsymbol{z}), \varphi_i \rangle$$

for all functions $\varphi_i \in L^2(0,T;H^1(\Omega))$, $i = 1,2,\dots,M$. Here, $\langle \cdot, \cdot \rangle$ denotes both the inner product in $L^2(\Omega)$ and the duality pairing between $H^1(\Omega)^*$ and $H^1(\Omega)$.

2.4. Main results

We now state our main results.

Theorem 1. *Assume that* (H1)–(H4) *are satisfied. Let $\{\boldsymbol{Z}^n, \boldsymbol{U}^n\}_{n=0}^{N_T}$ be the solution of* (3). *We denote by $\boldsymbol{Z}^{(\tau)}$ and $\boldsymbol{U}^{(\tau)}$ the functions obtained by piecewise constant interpolation in time of $\{\boldsymbol{Z}^n\}$ and $\{\boldsymbol{U}^n\}$, respectively. Then, there exist subsequences $\{\boldsymbol{Z}^{(\tau_k)}\}$, $\{\boldsymbol{U}^{(\tau_k)}\}$ of $\{\boldsymbol{Z}^{(\tau)}\}$, $\{\boldsymbol{U}^{(\tau)}\}$ and a weak solution $\boldsymbol{z}$ of* (1) *such that*

$$\boldsymbol{Z}^{(\tau_k)} \to \boldsymbol{z}, \quad \boldsymbol{U}^{(\tau_k)} \to \boldsymbol{\beta}(\boldsymbol{z})$$

strongly in $L^2(Q)^M$, a.e. in Q and weakly in $L^2(0,T;H^1(\Omega))^M$ as τ_k tends to zero.

Remark. The strong convergence of $\boldsymbol{U}^{(\tau_k)}$ was not obtained in [12] because slightly general scheme has been treated in [12]. However, the following estimate holds for the scheme (3):

$$\tau \sum_{n=1}^{N_T} \|\boldsymbol{U}^n - \boldsymbol{\beta}(\boldsymbol{Z}^n)\|^2_{L^2(\Omega)^M} \le C\tau.$$

Here, C is a positive constant independent of τ. This estimate and the strong convergence property of $\boldsymbol{Z}^{(\tau_k)}$ lead the assertion.

§3. Numerical experiments

In this section, one-dimensional numerical experiments are carried out to examine rates of convergence. We deal with the system (2) in a finite domain $\Omega = (0, L) = (0, 2)$. The following coefficients and initial functions are adopted: $a_{10} = 0.01, a_{11} = 0, a_{12} = 0.1, a_{20} = 0.01, a_{21} = 2, a_{22} = 0,\ c_{10} = 2.8, c_{11} = 1.1, c_{12} = 1, c_{20} = 3, c_{21} = 1, c_{22} = 1.1,$

$$z_{01}(x) = 8/21 \times (1 + 0.01\cos(\pi x)), \quad z_{02}(x) = 50/21 \times (1 - 0.01\sin(\pi x)).$$

We employ the finite-difference method to discretize (3) in space. The spatial mesh size is denoted by $h = L/N_X$, where $N_X + 1$ is the number of mesh points. Let $Z_i^{j,n}$ be the numerical approximation of $z_i(jh, n\tau)$. The fully discrete numerical scheme is as follows. For given $\{Z_i^{j,n-1}\}_{i=1,\dots,M,\ j=0,\dots,N_X}$ $(n = 1, \dots, N_T)$, solve the following linear system to find $\{U_i^{j,n}\}_{i=1,\dots,M,\ j=0,\dots,N_X}$:

$$\begin{aligned}
&U_i^{j,n} - \frac{\tau}{\mu h^2}(U_i^{j+1,n} - 2U_i^{j,n} + U_i^{j-1,n}) = \beta_i(\boldsymbol{Z}^{j,n-1}) + \frac{\tau}{\mu} f_i(\boldsymbol{Z}^{j,n-1}),\\
&U_i^{-1,n} = U_i^{1,n}, \quad U_i^{N_X+1,n} = U_i^{N_X-1,n}.
\end{aligned}$$

Thereafter, compute $\{Z_i^{j,n}\}_{i=1,\dots,M,\ j=0,\dots,N_X}$ by

$$Z_i^{j,n} = Z_i^{j,n-1} + \mu(U_i^{j,n} - \beta_i(\boldsymbol{Z}^{j,n-1})).$$

Because of the lack of exact solution, we regard a fine grid numerical solution with $N_X = 2^{11}$, $\tau = 2^{-20}$ and $\mu = 0.25$ as a 'solution'. The 'solution' is shown in Fig. 1.

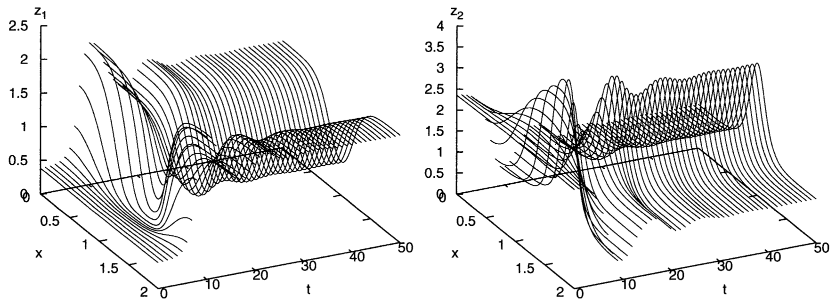

Fig. 1. The 'solution' until $t = 50$

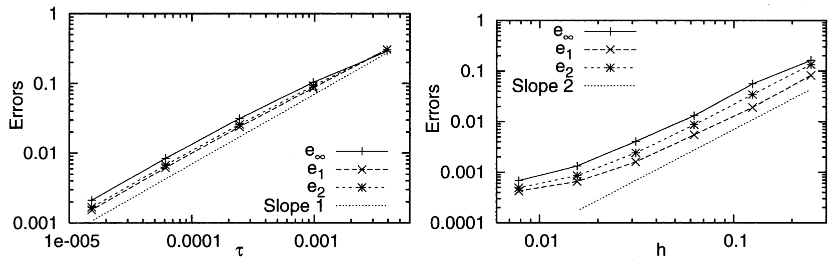

Fig. 2. Numerical results at $t = 10$

We denote by e_p^n $(p = 1, 2, \infty)$ the discrete relative $L^p(\Omega)$-norm of errors at time $t = n\tau$, namely,

$$e_p^n = \left(\sum_{\substack{i=1,2 \\ 0 \le j \le N_X}} \left| Z_i^{j,n} - z_i(jh, n\tau) \right|^p \Big/ \sum_{\substack{i=1,2 \\ 0 \le j \le N_X}} |z_i(jh, n\tau)|^p \right)^{1/p}, \quad p = 1, 2,$$

$$e_\infty^n = \max_{\substack{i=1,2 \\ 0 \le j \le N_X}} \left| Z_i^{j,n} - z_i(jh, n\tau) \right| \Big/ \max_{\substack{i=1,2 \\ 0 \le j \le N_X}} |z_i(jh, n\tau)| .$$

We inquire into rates of convergence with respect to the time step size τ. To this end, numerical simulations are done with $\mu = 0.25$ and $N_X = 2^{10}$ fixed. The left figure of Fig. 2 shows the numerical results at time $t = 10$ with $\tau = 2^{-8}, 2^{-10}, 2^{-12}, 2^{-14}, 2^{-16}$. The errors are along a straight line having slope 1, which implies numerical rates of convergence with respect to τ are of order τ for different norms. Numerical rates of convergence with respect to the spatial mesh size h at $t = 10$ are observed

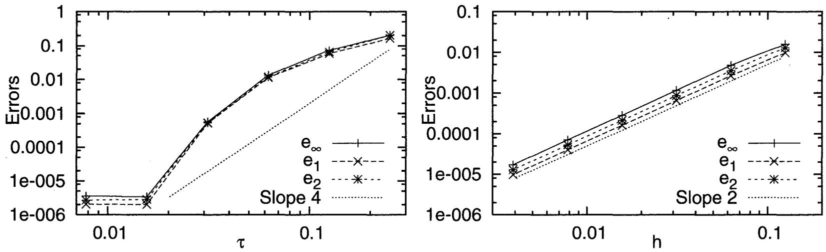

Fig. 3. Numerical results at $t = 100$

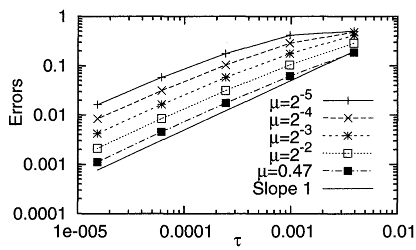

Fig. 4. Results for various choices of the parameter μ

in the right figure. In this simulation, we used $\mu = 0.25$, $\tau = 2^{-18}$ and $N_X = 2^3, 2^4, \ldots, 2^8$. The numerical results represent that the rates are almost of order h^2. This order is similar to that of the fully implicit scheme examined by Andreianov et al. [1]. Fig. 3 shows numerical results at $t = 100$. At this time, the 'solution' is almost close to a steady state. We used $\mu = 0.25$ and $N_X = 2^{10}$ fixed in the left figure and $\tau = 2^{-10}$ fixed in the right. Numerical convergence rates with respect to h are observed to be of order h^2 and numerical solutions seem to converge very rapidly with respect to τ.

We investigate a relationship between the parameter μ and errors. Fig. 4 sums up the numerical errors e_∞ for $N_X = 2^{10}$ fixed and various choices of τ and μ. The convergence rate is of order τ for every choice of μ. However, the errors are dependent on μ. We can observe that the larger μ, the smaller the errors become. On the other hand, the numerical solutions are unstable when we take $\mu \geq 0.48$. Therefore, we would like to estimate the optimal upper bound of the parameter μ. Jäger and Kačur [8] have studied the linear scheme (3) for the nonlinear diffusion equation (1), i.e., $M = 1$. They improved the scheme by replacing the constant parameter μ with a function. Thereby, we expect that we can construct a highly accurate numerical method by changing the constant μ into a suitable function. This will be a subject of a forthcoming paper.

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