

# Cross-diffusion systems: RDS approximation and Numerical analysis \*

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## 1 Introduction

Cross-diffusion systems sometimes arise in population ecology. The well-known Lotka-Volterra competition diffusion system is one of the typical problem in population ecology. The system has been extensively investigated in order to understand spatial and temporal behaviours of interacting species. However, it covers only the case where the diffusive motions of different species are mutually non-interfering. The interactions between species are at each points. Apart from the point-interactions, Kerner [9] considered a motional type of interaction. He proposed a system in which diffusion of the first species depends not only on the density of the first species but also on the density of the second species, and vice versa. Such mixture of diffusion terms is called cross-diffusion, and such kind of systems are called cross-diffusion systems. Depending on the cross-diffusivities, in some cases the cross-diffusivities denote the movement of  $i^{\text{th}}$  species in the direction of lower concentration of  $j^{\text{th}}$  species, and in others the flux of  $i^{\text{th}}$  species is directed toward increasing population density of  $j^{\text{th}}$  species. Therefore, the cross-diffusion effects give rise to segregation or aggregation. During the past decades, several cross-diffusion systems have been proposed and analyzed, especially in the area of population ecology. The presences of cross-diffusion often complicate its analysis and numerical analysis. In this survey, we suggest an easy way to deal with cross-diffusion system.

This paper is concerned with the following type of nonlinear diffusion problems: Find  $\mathbf{z} = (z_1, \dots, z_M) : \bar{\Omega} \times [0, T] \rightarrow \mathbb{R}^M$  ( $M \in \mathbb{N}$ ) such that

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

Here,  $\Omega \subset \mathbb{R}^d$  ( $d \in \mathbb{N}$ ) is a bounded domain with smooth boundary  $\partial\Omega$ ,  $T$  is a positive constant,  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_M)$ ,  $\mathbf{f} = (f_1, \dots, f_M) : \mathbb{R}^M \rightarrow \mathbb{R}^M$  and  $\mathbf{z}^0 = (z_1^0, \dots, z_M^0) :$

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$\Omega \rightarrow \mathbb{R}^M$  are given functions,  $\nu$  is the unit outward normal vector to the boundary  $\partial\Omega$ . We note that the diffusivity  $\beta_i$  of the  $i^{\text{th}}$  component depends not only on the  $i^{\text{th}}$  variable but also on the  $j^{\text{th}}$  ( $j \neq i$ ) variables in general. Thus, the system (1) is a cross-diffusion system. This framework is so general as to include Shigesada-Kawasaki-Teramoto cross-diffusion system [14], a cooperative cross-diffusion system with fractional type of cross-diffusivities (e.g. [10]) and a cross-diffusion system with piecewise linear diffusivities [13]. The problem (1) also contains degenerate parabolic problems such as the Stefan problem and the porous medium equations. We can deal with such problems. But, in this paper, we do not describe the results for the degenerate problems. Each problem is interesting because of the cross-diffusivities. However, they are not easy to deal with because of the cross-diffusivities. It might be useful for analysis of the problems to remove the cross-diffusivities.

In an attempt to avoid the cross-diffusivities, we propose an approximation to (1) by a semilinear reaction-diffusion system. The solutions of the nonlinear cross-diffusion system (1) can be approximated by those of the semilinear reaction-diffusion system. This indicates that the mechanism of nonlinear diffusion might be captured by reaction-diffusion interaction. The reaction-diffusion system consists of simple reactions and linear diffusions. Resolving semilinear problems is typically easier than dealing with nonlinear problems. Since we can avoid the cross-diffusivities by means of a reaction-diffusion system approximation, we apply the theory to numerical analysis. Considering discretizations of the reaction-diffusion system, we provide a linear discrete-time scheme to approximate the cross-diffusion system (1). The scheme attains the optimal convergence rates. Furthermore, we employ finite volume technique to discretize the discrete-time scheme in space. The ensuing numerical scheme is unconditionally stable and very easy to implement.

Let us summarize our recent results ([10, 11, 12] $+\alpha$ ).

- A framework for analyzing uniqueness of the weak solution of (1) for  $L^2$  initial data is given.
- The regularities of the weak solution of (1) in the case where  $z^0 \in H^1(\Omega)^M$  are established.
- A semilinear reaction-diffusion system is provided as an approximation to (1), and rates of convergence of the semilinear approximation with respect to the approximation parameter are analyzed.
- A linear discrete-time scheme is proposed to approximate (1), and the optimal convergence rates are derived for the linear scheme.
- A fully discrete finite volume scheme to (1) is given and analyzed.

The rest of the paper is organized as follows. In the next section, we state assumptions and a weak formulation of (1). We give the reaction-diffusion system approximation in Section 3, discrete-time scheme in Section 4 and the finite volume scheme in Section 5.

## 2 Preliminaries

In this section we establish the assumptions on the data, state precisely the problems.

## 2.1 Assumptions

We deal with a general problem including both uniformly parabolic and weakly coupled cases. We treat the system (1) which possess block triangular diffusion matrices. The following notations are used:  $\mathbb{R}^M = \mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_l}$ ,

$$\begin{aligned} \mathbf{z} &= (z_1, \dots, z_M) = (z_{11}, \dots, z_{1m_1}, z_{21}, \dots, z_{2m_2}, \dots, z_{l1}, \dots, z_{lm_l}), \\ \boldsymbol{\beta} &= (\beta_1, \dots, \beta_M) = (\beta_{11}, \dots, \beta_{1m_1}, \beta_{21}, \dots, \beta_{2m_2}, \dots, \beta_{l1}, \dots, \beta_{lm_l}) \end{aligned}$$

and so on. We impose on  $\boldsymbol{\beta}$  and  $\mathbf{f}$  the following assumptions:

(H1)  $\boldsymbol{\beta}$  is a Lipschitz continuous function satisfying  $\boldsymbol{\beta}(\mathbf{0}) = \mathbf{0}$  and the following properties.

- For each  $i = 1, \dots, l-1$  and  $j = 1, \dots, m_i$ , the function  $\beta_{ij}$  is independent of the  $rs^{\text{th}}$  ( $r > i, s = 1, \dots, m_r$ ) variables.
- There exist positive constants  $a$  and  $K$  such that

$$\sum_{j=1}^{m_i} (\beta_{ij}(\boldsymbol{\xi}) - \beta_{ij}(\boldsymbol{\eta})) (\xi_{ij} - \eta_{ij}) \geq a \sum_{s=1}^{m_i} |\xi_{is} - \eta_{is}|^2 - K \sum_{r=1}^{i-1} \sum_{s=1}^{m_r} |\xi_{rs} - \eta_{rs}|^2$$

for all  $i = 1, \dots, l$  and almost all  $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^M$ .

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

A fixed parameter  $\mu$  appears in the approximations in this paper. We assume the following condition on the parameter:

(H3)  $\mu$  satisfies

$$0 < \mu < \frac{a}{2(a^2 + M^2 L_\phi^2)}.$$

Here  $L_\phi$  is a Lipschitz constant of  $\phi_i(\boldsymbol{\eta}) := \beta_i(\boldsymbol{\eta}) - a\eta_i$ .

## 2.2 Weak formulation

In this paper,  $\langle \cdot, \cdot \rangle$  denotes both the inner product in  $L^2(\Omega)$  and the duality pairing between  $H^1(\Omega)^*$  and  $H^1(\Omega)$ . The problem (1) will be understood in the sense of the following weak form:

**Definition 1** A function  $\mathbf{z} \in (L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^1(\Omega)^*))^M$  is said to be a weak solution of (1) if it fulfils

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

for all functions  $\varphi_i \in L^2(0, T; H^1(\Omega))$ ,  $i = 1, 2, \dots, M$ , and

$$\mathbf{z}(\cdot, 0) = \mathbf{z}^0 \quad \text{a.e. in } \Omega.$$

There exists a unique weak solution of (1) under the assumptions (H1) and (H2) [10, 11].

### 3 Reaction-diffusion system approximation

In order to avoid the nonlinearity of the diffusion, we proposed the following semilinear reaction-diffusion system as an approximation to (1) [10]:

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = \frac{1}{\mu} \Delta \mathbf{u} - \frac{1}{\varepsilon} (\mathbf{u} - \beta(\mu \mathbf{u} + \mathbf{v})) + \frac{1}{\mu} \mathbf{f}(\mu \mathbf{u} + \mathbf{v}) & \text{in } Q, \\ \frac{\partial \mathbf{v}}{\partial t} = \frac{\mu}{\varepsilon} (\mathbf{u} - \beta(\mu \mathbf{u} + \mathbf{v})) & \text{in } Q, \\ \frac{\partial \mathbf{u}}{\partial \nu} = \mathbf{0} & \text{on } \partial \Omega \times (0, T), \\ \mathbf{u}(\cdot, 0) = \mathbf{u}^{0,\varepsilon}, \quad \mathbf{v}(\cdot, 0) = \mathbf{v}^{0,\varepsilon} & \text{in } \Omega, \end{cases} \quad (2)$$

where  $\mu$  and  $\varepsilon$  are positive parameters, and  $\mathbf{u}^{0,\varepsilon}$  and  $\mathbf{v}^{0,\varepsilon}$  are approximations to  $\beta(\mathbf{z}^0)$  and  $\mathbf{z}^0 - \mu\beta(\mathbf{z}^0)$ , respectively. Let  $(\mathbf{u}^\varepsilon, \mathbf{v}^\varepsilon)$  be a weak solution of (2). The reaction-diffusion systems include only simple reactions and linear diffusions. Resolving semi-linear problems is typically easier than dealing with nonlinear problems. Therefore, our ideas are expected to reveal new and more effective approaches to the study of nonlinear problems.

We proved in [10] that  $\mu \mathbf{u}^\varepsilon + \mathbf{v}^\varepsilon$  converges to the weak solution  $\mathbf{z}$  of (1) as  $\varepsilon$  tends to zero in a certain sense. Quite recently, we obtain the following results about the rates of convergence with respect to  $\varepsilon$ :

**Theorem 1** *Assume that (H1)–(H3) hold. Let  $\mathbf{z}$  be the weak solution of (1) with an initial datum  $\mathbf{z}^0$  and  $\mathbf{z}^\varepsilon$  be the weak solution of (2) with initial data  $\mathbf{u}^{0,\varepsilon}$  and  $\mathbf{v}^{0,\varepsilon}$ , respectively. Set  $\mathbf{z}^\varepsilon = \mu \mathbf{u}^\varepsilon + \mathbf{v}^\varepsilon$  and  $\mathbf{z}^{0,\varepsilon} = \mu \mathbf{u}^{0,\varepsilon} + \mathbf{v}^{0,\varepsilon}$ . Then there exists a positive constant  $C$  depending only on  $M, T, a, K, L_\phi, |\Omega|, \mathbf{f}(\mathbf{0})$  and  $L_f$  such that*

$$\begin{aligned} E &:= \|\mathbf{z} - \mathbf{z}^\varepsilon\|_{L^2(Q)^M} + \left\| \int_0^t (\beta(\mathbf{z}) - \mathbf{u}^\varepsilon) \right\|_{L^\infty(0,T;H^1(\Omega))^M} \\ &\leq C \left( 1 + \|\mathbf{z}^{0,\varepsilon}\|_{L^2(\Omega)^M}^2 \right) (\varepsilon^{1/2} + \sigma(\varepsilon)). \end{aligned}$$

Here,  $\sigma(\varepsilon) = \|\mathbf{z}^0 - \mathbf{z}^{0,\varepsilon}\|_{L^2(\Omega)^M}$ . Moreover, if  $\mathbf{z}^0 \in H^1(\Omega)^M$ , then

$$E \leq C \left( 1 + \|\mathbf{z}^{0,\varepsilon}\|_{H^1(\Omega)^M}^2 \right) (\varepsilon + \sigma(\varepsilon)),$$

and

$$\|\beta(\mathbf{z}) - \mathbf{u}^\varepsilon\|_{L^2(0,T;H^1(\Omega))^M} \leq C \left( 1 + \|\mathbf{z}^{0,\varepsilon}\|_{H^1(\Omega)^M}^2 \right) (\varepsilon^{1/2} + \sigma(\varepsilon)/\varepsilon^{1/2}).$$

### 4 Linear scheme

We removed the nonlinearity of the diffusion by means of a reaction-diffusion system approximation. We apply the theory to numerical analysis to the nonlinear problem (1). To this end, in this section, we consider discrete-time schemes to approximate the solution of (1).



**Theorem 2** Assume that (H1)–(H3) hold. Let  $\mathbf{z}$  and  $\{\mathbf{U}^n, \mathbf{Z}^n\}$  be the weak solution of (1) and the solution of Problem DT, respectively. We denote by  $\mathbf{U}$  and  $\mathbf{Z}$  the piecewise constant interpolation in time of  $\{\mathbf{U}^n\}$  and  $\{\mathbf{Z}^n\}$ , respectively. Then there exists a positive constant  $C$  depending only on  $M, T, a, K, L_\phi, |\Omega|, \mathbf{f}(\mathbf{0}), L_f$  and  $\mu$  such that

$$\begin{aligned} E &:= \|\mathbf{z} - \mathbf{Z}\|_{L^2(Q)^M} + \left\| \int_0^t (\boldsymbol{\beta}(\mathbf{z}) - \mathbf{U}) \right\|_{L^\infty(0,T;H^1(\Omega))^M} \\ &\leq C \left( 1 + \|\mathbf{z}^{0,\tau}\|_{L^2(\Omega)^M} + \tau \|\nabla \mathbf{z}^{0,\tau}\|_{L^2(\Omega)^M} \right) (\tau^{1/2} + \sigma(\tau)). \end{aligned} \quad (5)$$

Here,  $\sigma(\tau) = \|\mathbf{z}^0 - \mathbf{z}^{0,\tau}\|_{L^2(\Omega)^M}$ . Moreover, if  $\mathbf{z}^0 \in H^1(\Omega)^M$ , then

$$E \leq C \left( 1 + \|\mathbf{z}^{0,\tau}\|_{H^1(\Omega)^M} \right) (\tau + \sigma(\tau)), \quad (6)$$

and

$$\|\boldsymbol{\beta}(\mathbf{z}) - \mathbf{U}\|_{L^2(0,T;H^1(\Omega))^M} \leq C \left( 1 + \|\mathbf{z}^{0,\tau}\|_{H^1(\Omega)^M} \right) (\tau^{1/2} + \sigma(\tau)/\tau^{1/2}). \quad (7)$$

These rates are sharp on account of the global regularity in time. Indeed, while the initial datum  $\mathbf{z}^0$  belongs to  $L^2(\Omega)^M$ , the following regularities are fulfilled:

$$\begin{aligned} \mathbf{z} &\in H^1(0, T; H^1(\Omega)^*)^M \cap L^2(0, T; H^1(\Omega))^M \subset H^{1/2}(0, T; L^2(\Omega))^M, \\ \int_0^t \boldsymbol{\beta}(\mathbf{z}) &\in H^1(0, T; H^1(\Omega))^M \subset C^{0,1/2}([0, T]; H^1(\Omega))^M. \end{aligned}$$

Thus, the order (5) is sharp. When  $\mathbf{z}^0 \in H^1(\Omega)^M$ , the following further regularity results hold:

$$\mathbf{z} \in H^1(0, T; L^2(\Omega))^M \text{ and } \boldsymbol{\beta}(\mathbf{z}) \in H^{1/2}(0, T; H^1(\Omega))^M.$$

Hence, (6) and (7) appear to be optimal.

The following type of nonlinear schemes have been studied by several authors (e.g. [1, 2, 5, 6, 8]):

$$\begin{cases} \frac{\mathbf{Z}^n - \mathbf{Z}^{n-1}}{\tau} = \Delta \boldsymbol{\beta}(\mathbf{Z}^n) + \mathbf{f}(\mathbf{Z}^n) & \text{in } \Omega, \\ \frac{\partial \boldsymbol{\beta}(\mathbf{Z}^n)}{\partial \nu} = \mathbf{0} & \text{on } \partial\Omega. \end{cases} \quad (8)$$

Fully implicit schemes show better stability and accuracy properties in practice. Therefore, the schemes (8) might be efficient. However, they are not easy to implement. For solving the corresponding nonlinear algebraic systems arising from fully implicit schemes, some iterative methods such as Newton method have to be used to linearize the schemes. The ensuing linear algebraic systems are large. For two or three dimensional problems and for three or four or more components systems, the implementation becomes complicated. Fully implicit schemes are unfriendly toward mathematicians and students who want to see numerical solutions but do not want to spend a lot of time and effort on programming. We analyzed the nonlinear scheme (8) and obtained the same rates of convergence as for the linear scheme (3) [11].

## 5 Finite volume scheme

In this section, we consider a fully discrete numerical scheme to (1).

Hereafter, we assume that  $\Omega \subset \mathbb{R}^d$ ,  $d = 2$  or  $d = 3$  is an open bounded polygonal or polyhedral connected domain. Following [7], we define a finite volume discretization of  $Q = \Omega \times (0, T)$ .

**Definition 2 (Admissible mesh)** *An admissible mesh  $\mathcal{M}$  of  $\Omega$  is given by a set of open, bounded subsets of  $\Omega$  (control volumes) and a family of points (one per control volume), satisfying the following properties*

1. *The closure of the union of all the control volumes is  $\overline{\Omega}$ . We denote by  $m_K$  the measure of each volume element  $K$ .*
2.  *$K \cap L = \emptyset$  for any  $(K, L) \in \mathcal{M}^2$ , such that  $K \neq L$ . If  $\overline{K} \cap \overline{L} \neq \emptyset$ , then it is a subset of a hyperplane in  $\mathbb{R}^d$ . Let us denote by  $\mathcal{E} \subset \mathcal{M}^2$  the set of pairs  $(K, L)$ , such that  $K \neq L$  and the  $d - 1$  Lebesgue measure of  $\overline{K} \cap \overline{L}$  is strictly positive. For  $(K, L) \in \mathcal{E}$  we write  $K|L$  for the set  $\overline{K} \cap \overline{L}$  and  $m_{K|L}$  for the  $d - 1$  Lebesgue measure of  $K|L$ .*
3. *For any  $K \in \mathcal{M}$  we also define  $\mathcal{N}_K = \{L \in \mathcal{M}, (K, L) \in \mathcal{E}\}$  and assume that  $\partial K = \overline{K} \setminus K = (\overline{K} \cap \partial\Omega) \cup \left(\bigcup_{L \in \mathcal{N}_K} K|L\right)$ .*
4. *There exists a family of points  $(x_K)_{K \in \mathcal{M}}$ , such that if  $L \in \mathcal{N}_K$  then the straight line  $(x_K, x_L)$  is orthogonal to  $K|L$ . We set*

$$d_{K|L} = d(x_K, x_L) \quad \text{and} \quad T_{K|L} = \frac{m_{K|L}}{d_{K|L}},$$

where the last quantity is sometimes called the transmissibility across the edge  $K|L$ .

We then define a discretization of the whole domain  $Q$  in the following way.

**Definition 3 (Discretization of  $Q$ )** *Let  $\tau = T/N_T$  ( $N_T \in \mathbb{N}$ ) be a time step size and set  $t^n = n\tau$ . Then, a finite volume discretization  $\mathcal{D}$  of  $Q$  is defined as*

$$\mathcal{D} = (\mathcal{M}, \mathcal{E}, \{x_K\}_{K \in \mathcal{M}}, \{t^n\}_{n \in \{0, \dots, N_T\}}),$$

where  $\mathcal{M}$ ,  $\mathcal{E}$  and  $\{x_K\}_{K \in \mathcal{M}}$  are given in Definition 2. The mesh size is defined by

$$\text{size}(\mathcal{D}) = \max \left\{ \max_{K \in \mathcal{M}} m_K, \tau \right\}.$$

We present below the finite volume scheme which we use and define approximate solutions. We assume that (H1)–(H3) are satisfied and suppose that  $\mathcal{D}$  is an admissible discretization of  $Q$  in the sense of Definition 3. We prescribe the approximate initial condition

$$z_{iK}^0 = \frac{1}{m_K} \int_K z_i^{0,\tau}(x) dx. \quad (9)$$

For  $n \in \{1, \dots, N_T\}$  and  $K \in \mathcal{M}$ , find  $\mathbf{u}_K^n = (u_{1K}^n, \dots, u_{MK}^n)$  such that

$$m_K (u_{iK}^n - \beta_i(z_K^{n-1})) - \frac{\tau}{\mu} \sum_{L \in \mathcal{N}_K} T_{K|L} (u_{iL}^n - u_{iK}^n) = \frac{\tau}{\mu} m_K f_i(z_K^{n-1}), \quad (10)$$

and then calculate  $\mathbf{z}_K^n = (z_{1K}^n, \dots, z_{MK}^n)$  by

$$z_{iK}^n = z_{iK}^{n-1} + \mu (u_{iK}^n - \beta_i(\mathbf{z}_K^{n-1})). \quad (11)$$

For  $x \in \Omega$  and  $t \in (0, T]$ , let  $K \in \mathcal{M}$  be such that  $x \in K$  and  $n \in \{1, \dots, N_T\}$  be such that  $t \in (t^{n-1}, t^n]$ . We then define the approximate solutions to  $\mathbf{z}$  and  $\beta(\mathbf{z})$  by

$$\mathbf{z}_{\mathcal{D}}(x, t) = \mathbf{z}_K^n \quad \text{and} \quad \mathbf{u}_{\mathcal{D}}(x, t) = \mathbf{u}_K^n. \quad (12)$$

The unique existence of the approximate solutions is well known because (10) is the finite volume discretization of the linear elliptic equation.

The matrix corresponding to the ensuing algebraic problem is symmetric, positive definite and independent of  $n$  and  $i$ . Therefore, the full power of numerical linear algebra can be used to solve efficiently the resulting algebraic systems. Our algorithm ensures the mass conservation while  $\mathbf{f} \equiv \mathbf{0}$ .

We have the following convergence result [12]:

**Theorem 3** *For  $k \in \mathbb{N}$ , let  $\mathcal{D}_k$  be an admissible mesh in the sense of Definitions 2 and 3. Assume that  $\text{size}(\mathcal{D}_k) \rightarrow 0$  as  $k \rightarrow \infty$  and that (H1)–(H3) are satisfied. Let  $\mathbf{z}$  be the weak solution of (1), and  $\mathbf{z}_{\mathcal{D}_k}$  and  $\mathbf{u}_{\mathcal{D}_k}$  be given by (9)–(12) with  $\mathcal{D} = \mathcal{D}_k$ . Then, there exist a subsequence of the admissible meshes, still denoted by  $\mathcal{D}_k$ , such that*

$$\begin{aligned} \mathbf{z}_{\mathcal{D}_k} &\rightarrow \mathbf{z}, \\ \mathbf{u}_{\mathcal{D}_k} &\rightarrow \beta(\mathbf{z}) \end{aligned} \quad \text{strongly in } L^2(Q)^M \text{ and a.e. in } Q$$

as  $k$  tends to infinity.

We also proved that the finite volume scheme is unconditionally stable. Implementation is almost same as that for the implicit method for the linear heat equation. The computational cost is less than  $M$  times that for the linear heat equation because the ensuing linear algebraic system involves the same matrix for all time steps and for all  $i \in \{1, \dots, M\}$ . The scheme is versatile. When you want to consider other nonlinearity, all you have to do is to rewrite the function  $\beta$ . Thus, the scheme (9)–(11) is a versatile, very easy to implement, unconditionally stable, conservative, convergent numerical scheme.

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