1.4 Symmetrization in Cross-diffusions

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Introduction

The term *diffusion* stems from the Latin word *diffundere*, which means *to spread*.

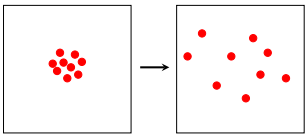


Fig. 1: *Diffusing particles*

Diffusion is an irreversible process governing the movement of particles from regions of higher to regions of lower concentration. The phenomenon of diffusion is ubiquitous in nature and can be observed in gas, liquids, and even in solids. Everyday examples include the spread of perfume, smoke, and other airborne particles through the surrounding air, and the dispersion of a droplet of ink in a glass of water until the solution becomes uniformly colored. The continuum approach, which treats diffusion as a continuous process rather than focusing on individual particles, traces back to Fick's laws in the 19th century. This approach, which we adopt in this article, is well-suited for studying physical systems from a macroscopic viewpoint.

In systems with multiple components, diffusive processes can become intricate, and the flux of a species S_1 may be influenced by the density gradient of a second species S_2. This is when cross-diffusion occurs. Physical systems that can exhibit cross-diffusive behavior comprise electrolytes, temperature-responsive materials, and thermoelectric materials where a temperature gradient may induce an electric current.

The mathematical concept of cross-diffusion also encompasses certain biological processes, including chemotaxis and cross-effects arising in predator-prey systems. Cross-diffusion may induce intriguing patterns in reaction–diffusion systems. It may lead to the surprising phenomenon of uphill diffusion, which in contrast to the classical Fickian diffusion downhill, i.e., in the direction of the negative density gradient, describes a movement uphill, towards higher density. For an illustration in one space dimension we refer to Figure 2, where, loosely speaking, in the region $x \approx 0.5$ the red species gets pushed away uphill by the blue species. (Detailed descriptions of the numerical experiments will be omitted in this short highlight article.)

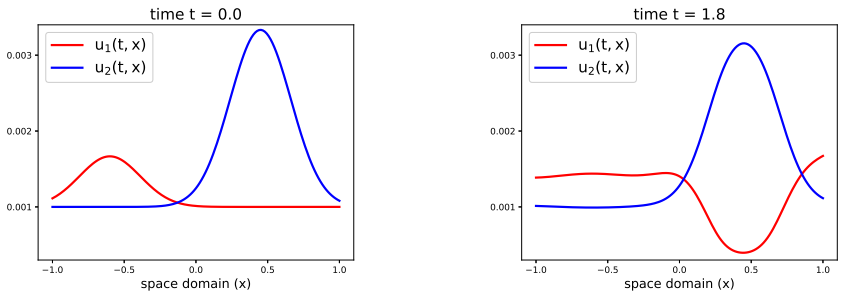


Fig. 2: *Uphill diffusion in the segregation cross-diffusion system (6) (n=2, k_1=17, k_2=1 & no-flux boundary c)*

(a) Density profiles at initial time

(b) Effect of uphill diffusion in u_1

Cross-diffusion systems are challenging to analyze mathematically, and explicit solution formulas are rarely available. Effective methods for their analysis often rely on specific structural conditions. In this article, we outline our recent results on the analysis of cross-diffusion systems enjoying a structure motivated by thermodynamics: the systems considered are driven by an entropy, and

dissipative effects are induced by a symmetric and positive semidefinite tensor acting on the driving forces. The symmetry of the dissipation tensor is linked to the famous *reciprocal relations*, also called *Onsager symmetry*—a concept attributed to the Nobel Prize laureate Lars Onsager that expresses a symmetry property of the transport coefficients in nonequilibrium systems modeling an irreversible thermodynamic process.

In the next section, we introduce key notions with a focus on parabolic cross-diffusion and briefly discuss the example in [2, 3]. Subsequently, we focus on a cross-diffusion system of hyperbolic–parabolic type, which arises in mathematical biology, and describe our approach in [1] towards its analysis. Certain types of symmetry properties turn out to be useful if not indispensable when it comes to deriving *a priori* estimates.

Entropy structure and Onsager symmetry

Consider a quasilinear second-order system of partial differential equations (PDEs) of the form

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathbb{A}(u)\nabla u), \quad \text{where } u = (u_1, \dots, u_n)^T,\ \mathbb{A}(u) \in \mathbb{R}^{n\times n}. \tag{1}$$

Formally, cross-diffusion is characterized by the presence of a non-vanishing off-diagonal term in the so-called *diffusion matrix* $\mathbb{A}(u)$. A fundamental question in the mathematical analysis of PDEs such as (1) concerns their well-posedness, which comprises three properties: the existence of a solution, its uniqueness, and the continuous dependence of the solution on the data. In order for system (1) to be well posed for suitable initial and boundary conditions, it is necessary to impose a structural condition on the matrix $\mathbb{A}$. Sufficient for the well-posedness on a short time interval is the spectral condition $\sigma(\mathbb{A}(u)) \subset \{z \in \mathbb{C} : \Re(z) > 0\}$, in which case the system is *parabolic* (in the sense of Petrovskii). For understanding the global well-posedness, spectral properties alone are insufficient.

Diffusive systems arising in thermodynamics often exhibit a formal gradient-flow structure, expressed as (cf. [6])

$$\dot{u} = -\mathcal{K}(u)D\mathcal{H}(u), \tag{2}$$

where $\dot{u} = \frac{\mathrm{d}}{\mathrm{d}t}u$, $\mathcal{H}$ denotes a (differentiable) driving functional and $\mathcal{K}$ the Onsager operator, a symmetric and positive semidefinite linear operator, whose symmetry property reflects the Onsager principle. In this article, we focus on systems (2) with $u = u(t,x) \in [0,\infty)^n, t > 0, x \in \mathbb{T}^d, n, d \in \mathbb{N}$, where $\mathcal{H}$ is given by an integral functional $\mathcal{H}(u) = \int_{\mathbb{T}^d} h(u)$ with $h \in C^2$ strictly convex and where the Onsager operator takes the form $\mathcal{K}(u)\xi = -\nabla \cdot (\mathbb{M}(u)\nabla\xi)$ with $\mathbb{M}(u) \in \mathbb{R}^{n\times n}$ symmetric and positive semidefinite. Inserting these choices into (2) yields (1) with

$$\mathbb{A}(u) = \mathbb{M}(u)D^2h(u). \tag{3}$$

Observe that the matrix $\mathbb{A}(u)$ need not be symmetric. But identity (3) implies that $\mathbb{A}(u)$ is diagonalizable over $\mathbb{R}$ and all its eigenvalues are nonnegative. Thus, if in addition $\operatorname{rank}\mathbb{A}(u) = n$, the PDE system (1) is parabolic. For parabolic cross-diffusion systems, the structure (3) is very useful in the construction of global-in-time weak solutions.

Entropy variables and symmetrization

Given an entropy function h on a convex domain $\widehat{\mathcal{D}} \subseteq (0,\infty)^n$, the so-called *entropy variable* $v := Dh(u)$ plays an important role in the construction of global (weak) solutions and the design of suitable approximation schemes. Notice that for h strongly convex and smooth, the differential Dh is a diffeomorphism onto its image. Recovering u from v via $u = (Dh)^{-1}(v) = Dh^*(v)$, where h^* is the Legendre transform of h, we deduce $u \in \widehat{\mathcal{D}}$ and thus $u_i \geq 0$ for all $i = 1,\dots,n$—a conclusion that can be seen as a substitute for a weak form of the maximum principle. Importantly, the change to entropy variables brings the PDE system (1), (3) in a symmetric form

$$D^2h^*(v)\partial_t v = \nabla\cdot(\mathbb{M}(u)\nabla v), \tag{4}$$

in which the entropy estimate is derived by taking as a test function the unknown v itself.

Example: Soret and Dufour effect

The Soret effect, also called *thermodiffusion*, refers to the occurrence of a diffusion flux caused by a thermal gradient. Its counterpart, according to Onsager symmetry, is the Dufour effect—a heat flux induced by a density gradient. In the joint paper [2], we established a global existence result for nonisothermal reaction–diffusion systems accounting for cross-effects of Soret and Dufour type. The approximation scheme in [2] is based on a variant of (4) including a higher-order elliptic regularization term. The usefulness of the thermodynamic structure for establishing weak–strong uniqueness of nonisothermal reaction–diffusion systems has been observed in [3] (see also [4]).

Cross-diffusion with incomplete diffusion

The condition $\operatorname{rank}\mathbb{A}(u) = n$ is not satisfied in all applications. For instance, biological tissue tends to separate into distinct regions, a behavior known as segregation, which is incompatible with complete diffusive mixing. In this context, we considered in [1, 5] the following cross-diffusion system

$$\partial_t u_i = \nabla\cdot(u_i\nabla(\mathbb{B}u)_i), \qquad i = 1,\dots,n, \tag{5}$$

where $\mathbb{B} \in \mathbb{R}^{n\times n}$ is such that $\mathbb{B}\mathbb{D}(\lambda) \in \mathbb{R}^{n\times n}$ is symmetric and positive semidefinite for some $\lambda \in (0,\infty)^n$, where $\mathbb{D}(\lambda) := \operatorname{diag}(\lambda_1,\dots,\lambda_n)$. This system generalizes the equations

$$\partial_t u_i = \nabla\cdot(k_i u_i \nabla p), \quad i = 1,\dots,n, \qquad \text{where } p = \sum_{i=1}^n u_i,\ k_i > 0, \tag{6}$$

obtained by the choice $\mathbb{B} = \mathbf{k}\otimes\mathbf{1}$, $\mathbf{1} := (1,\dots,1)^T$, $\mathbf{k} := (k_1,\dots,k_n)^T$, which is admissible with $\lambda = \mathbf{k}$. Equations (6) have been proposed in the mathematical biology literature and describe the mass-preserving transport of a system of n species with densities u_i, $i = 1,\dots,n$, along the velocity fields $-k_i\nabla p$, each of which points in the direction of fastest spatial decay of the total density p. Thus, the equations model species undergoing a directed motion in order to avoid spatial crowding.

System (5) has a gradient-flow structure of the form (3). Indeed, letting

$$h(u) = \sum_{i=1}^{n} \frac{1}{\lambda_i}(u_i \log u_i - u_i) \quad \text{and} \quad \mathbb{M}(u) = \mathbb{D}(u)\mathbb{B}\mathbb{D}(\lambda)\mathbb{D}(u),$$

we recognize in the product $\mathbb{M}(u)D^2h(u)$ the diffusion matrix $\mathbb{A}(u) = \mathbb{D}(u)\mathbb{B}$. Notice that $\operatorname{rank}\mathbb{A}(u) = \operatorname{rank}\mathbb{B}$ for all $u \in (0,\infty)^n$. Hence, if $r := \operatorname{rank}\mathbb{B} < n$, the PDE system is not parabolic, and we are faced with a borderline case, where local well-posedness cannot directly be inferred from classical literature, but may still be expected given the nonnegativity of all eigenvalues of $\mathbb{A}(u)$.

Normal form

To analyze the local well-posedness of (5), we introduced in [1] a change of variables that brings the system in a more canonical form, a so-called *normal form*.

Change of variables. Let $\Phi : (0,\infty)^n \to \mathcal{D} \subseteq \mathbb{R}^n$ be a diffeomorphism with inverse Ψ, and define $w := \Phi(u)$. Then, the equation for w takes the form

$$\partial_t w = \nabla \cdot (\hat{\mathbb{A}}(w)\nabla w) - (\nabla D\Psi(w)^{-1}) \cdot \mathbb{A}(\Psi(w))D\Psi(w)\nabla w, \tag{7}$$

where the diffusion matrix $\hat{\mathbb{A}}(w) := D\Psi(w)^{-1}\mathbb{A}(\Psi(w))D\Psi(w)$ is conjugate to $\mathbb{A}(\Psi(w))$. In particular, the two matrices share their spectrum and rank, which implies that $\operatorname{rank}\hat{\mathbb{A}}(\Phi(u)) = \operatorname{rank}\mathbb{A}(u) = r$ for $u \in (0,\infty)^n$.

A key point of the normal form is to choose Φ in such a way that $\hat{\mathbb{A}}(w)$ has a block structure

$$\hat{\mathbb{A}}(w) = \begin{pmatrix} \mathbf{0}_{(n-r)\times(n-r)} & \mathbf{0}_{(n-r)\times r} \\ \mathbf{0}_{r\times(n-r)} & \mathbb{A}_*^{\mathrm{II}}(w) \end{pmatrix}, \text{ where } \mathbb{A}_*^{\mathrm{II}}(w) \in \mathbb{R}^{r\times r} \text{ has full rank.} \tag{8}$$

In this case, the last r components $w_{\mathrm{II}} := (w_{n-r+1},\dots,w_n)$ satisfy a parabolic subsystem, and it remains to understand the structure of the $(n-r)\times(n-r)$ first-order subsystem that governs the evolution of $w_{\mathrm{I}} := (w_1,\dots,w_{n-r})$.

Symmetrization of first-order subsystem. If $r < n-1$, the quasilinear first-order subsystem of (7) satisfied by w_{I} is nonscalar, in which case its local well-posedness, for w_{II} fixed, becomes nontrivial. Crucial for the derivation of *a priori* bounds from energy estimates is *symmetrizability* (in a sense different from the Onsager principle). A first-order PDE system of the form

$$\mathbb{A}_0\partial_t v + \sum_{j=1}^{d} \mathbb{A}_j\partial_{x_j} v + F = 0, \tag{9}$$

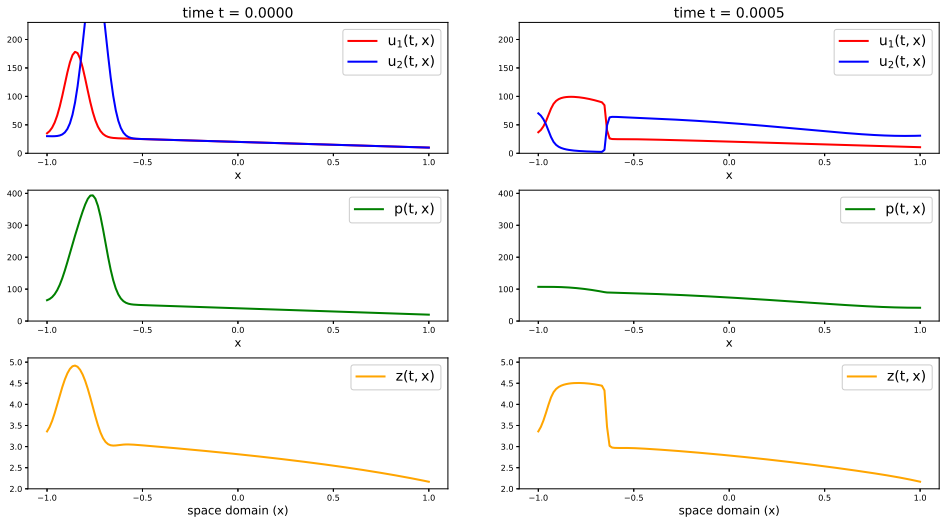
where $v = (v_1,\dots,v_m)$, $\mathbb{A}_j = \mathbb{A}_j(t,x) \in \mathbb{R}^{m\times m}$, $F = F(t,x) \in \mathbb{R}^m$, is called *symmetric hyperbolic* if the matrices $\mathbb{A}_j$, $j = 0,\dots,m$, are symmetric and if $\mathbb{A}_0$ is positive definite. System (9) is called *symmetrizable* if it can be cast in a symmetric hyperbolic form upon left-multiplication by a nonsingular matrix $\widetilde{\mathbb{A}}_0(t,x)$. Symmetrizability is classical for hyperbolic systems of conservation

laws with an entropy structure. However, the symmetrizability of the first-order subsystem in (7) (assuming (8)) is not immediate. In [1], we have established it by an explicit calculation for a (nonlinear) change of variables Φ based on an eigenbasis of the symmetric matrix $\mathbb{BD}(\lambda)$. As a matter of fact, in the new variables $w = \Phi(u)$ we obtained in [1] a system in normal form of symmetric hyperbolic–parabolic type, which reads as

$$\mathbb{A}_0^{\mathrm{I}}(w)\partial_t w_{\mathrm{I}} + \sum_{j=1}^{d} \mathbb{A}_1^{\mathrm{I}}(w, \partial_{x_j} w_{\mathrm{II}})\partial_{x_j} w_{\mathrm{I}} = f_{\mathrm{I}}(w, \nabla w_{\mathrm{II}}),$$
$$\mathbb{A}_0^{\mathrm{II}}\,\partial_t w_{\mathrm{II}} - \nabla \cdot \left(\mathbb{A}_*^{\mathrm{II}}(w)\nabla w_{\mathrm{II}}\right) = 0,$$

where $\mathbb{A}_0^{\mathrm{I}} : \mathcal{D} \longrightarrow \mathbb{R}^{(n-r)\times(n-r)}_{\mathrm{spd}}$, where $\mathbb{A}_1^{\mathrm{I}} : \mathcal{D} \times \mathbb{R}^r \longrightarrow \mathbb{R}^{(n-r)\times(n-r)}_{\mathrm{sym}}$ is linear in its second argument, and where $f_{\mathrm{I}} : \mathcal{D} \times \mathbb{R}^{dr} \longrightarrow \mathbb{R}^{n-r}$ is quadratic in its second argument. Furthermore, $\mathbb{A}_0^{\mathrm{II}} \in \mathbb{R}^{r\times r}_{\mathrm{spd}}$ is constant, and $\mathbb{A}_*^{\mathrm{II}} : \mathcal{D} \longrightarrow \mathbb{R}^{r\times r}_{\mathrm{spd}}$. By $\mathbb{R}^{m\times m}_{\mathrm{spd}}$, we denote the cone of symmetric positive definite real $m\times m$ matrices.

This normal form allowed us to apply existing methods for symmetric hyperbolic systems and (symmetric) parabolic systems separately to the respective subsystem. A short-time classical solution to the coupled hyperbolic–parabolic system, and thus also to (5), was then obtained by a contraction mapping argument.



(a) Profiles at initial time

(b) Shock in z at a later time

Fig. 3: *Parabolic (middle) & hyperbolic (bottom) part of normal form (11), and densities u_1, u_2 (top) (k_1=1, k_2=17)*

Example

For system (6) with $n = 2$, the change of variables introduced in [1] takes the form

$$w = (z, p) := (\Phi_{\mathrm{I}}(u), \Phi_{\mathrm{II}}(u)) = \left(\log(u_1^{1/k_1}/u_2^{1/k_2}), u_1+u_2\right), \tag{10}$$

and the PDE system in the new variables becomes an inhomogeneous quasilinear transport equation coupled to a quasilinear parabolic equation:

$$\begin{aligned} \partial_t z - c(w)\nabla p \cdot \nabla z &= f(w, \nabla p), \\ \partial_t p &= \nabla \cdot (a(w)\nabla p), \end{aligned} \tag{11}$$

where (with $u = \Phi^{-1}(w)$)

$$c(w) = k_1 + (k_2 - k_1)\frac{k_1 u_1}{a(w)} > 0, \quad f(w, \nabla p) = -\frac{(k_2 - k_1)}{a(w)}|\nabla p|^2, \quad a(w) = \sum_{i=1}^{2} k_i u_i.$$

Figure 3 illustrates the change of variables (10) leading to the normal form. The hyperbolic character of the z-evolution becomes apparent through the shock-type singularity that emerges when passing from Figure 3 (a) to (b).

Conclusion and outlook

Thermodynamic structures give rise to effective methods to analyze cross-diffusion, including change to entropy variables and symmetrization. For cross-diffusion with incomplete diffusion, local-in-time well-posedness in spaces of smooth functions relies on a change of variables that brings the underlying PDE system in a normal form. In this context, it would be interesting to identify, in more generality, the relevant structural properties that ensure symmetrizability of the resulting first-order subsystem. Another challenging question concerns the possibility of a finite-time breakdown of the local classical solution to (6), which we have only captured numerically so far (cf. Figure 3). Concerning the important questions of a global-in-time analysis of (5) for large data based on generalized solution concepts as well as numerical approximations preserving the thermodynamic structure, we refer to our recent preprint [5].

References

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