

A geometric singular perturbation analysis of regularised reaction-nonlinear diffusion models including shocks

Bronwyn Bradshaw-Hajek¹, Ian Lizarraga², Robert Marangell², and Martin Wechselberger^{*2}

¹UniSA STEM, University of South Australia, Mawson Lakes, South Australia, Australia

²School of Mathematics and Statistics, University of Sydney, NSW, Australia

1 Motivation

Wave fronts are ubiquitous in nature. In the context of population dynamics, such waves may be viewed as representing patterns or structure in migrating populations. Reaction-diffusion equations, such as the extensively studied Fisher equation [5], are used to model population growth dynamics combined with a simple Fickian diffusion process, and are typically capable of exhibiting travelling wave solutions.

In cell migration, advection (or transport) is another important model mechanism. It may represent, e.g., tactically-driven movement, where cells migrate in a directed manner in response to a concentration gradient. Such a concentration gradient develops, for example, in a soluble fluid (chemotaxis) or as a gradient of cellular adhesion sites or of substrate-bound chemoattractants (haptotaxis). Well studied examples of individual cells exhibiting directed motion in response to a chemical gradient include bacteria chemotactically migrating towards a food source. Wound healing, angiogenesis or malignant tumor invasion are just a few examples of chemotactic and/or haptotactic cell movement where the migrating cells form part of a dense population of cells as may be found in tissues. Such migrating cell populations not only form travelling waves but may also develop sharp interfaces in the wave form.

From a classical PDE point of view, these advection-reaction models may represent hyperbolic balance laws (hyperbolic conservation laws with source terms), and the formation of shock fronts is well known. In general, shocks are problematic because as the wave front steepens (and a shock forms) the solution becomes multivalued and physically nonsensical. The model breaks down and it becomes impossible to compute the temporal evolution of the solution [9].

To account for shocks, modellers have employed the technique of *regularisation* – adding small higher order terms to these models to smooth out the shocks. In the context of hyperbolic conservation/balance laws, these are usually small viscous (diffusive) regularisations, e.g., the viscous Burgers equation. Due to dissipative mechanisms, these physical shocks are observed as narrow transition regions with steep gradients of field variables. Mathematically, questions of existence

*corresponding author & presenter (martin.wechselberger@sydney.edu.au)

and uniqueness of such viscous shock profiles are fundamental.¹

Another source for the formation of sharp interfaces can be found in density-dependent nonlinear diffusion processes. Through sensing the local cell density, cells make informed decisions, i.e., they perform a ‘biased walk’. This could lead to, e.g., the tendency to cluster or aggregate with other nearby cells; think of flocking or swarming which might be perceived as an advantageous situation for the cell population. Such aggregation mechanism can be achieved through, e.g., negative (or backward) diffusion. Such reaction-nonlinear diffusion (RND) models may form shocks. Again, modellers have employed the technique of *regularisation* – adding small higher order terms to these models to ‘smooth’ the shocks, but these are not so well-known, at least in the bioscientific community. Possible shock formation in such regularised RND models is the main focus of this presentation, and we will use the tools from geometric singular perturbation theory and dynamical systems theory to tackle this problem.

2 The setup for RND Models

We start by considering a dimensionless reaction–nonlinear diffusion model of the form

$$u_t = (D(u)u_x)_x + f(u) = \Phi(u)_{xx} + f(u) \quad (1)$$

where $x \in \mathbb{R}$ denotes the spatial domain, $t \in \mathbb{R}_+$ denotes the time domain, $u \in \mathbb{R}_+$ denotes a (population/agent) density, $D(u)$ models a (population/agent) density dependent diffusivity. $\Phi(u)$ is an anti-derivative of $D(u)$, i.e. $\Phi'(u) = D(u)$, referred to as the *potential*. The (dimensionless) population/agent density u is scaled such that $u \in [0, 1]$ forms the domain of interest where $u = 1$ is the carrying capacity of the population/agent density. This domain of interest is also reflected in the reaction term $f(u)$ which is modelled either as *logistic growth*, $f(u) = f_l(u) = u(1 - u)$, or as *bistable growth*, $f(u) = f_b(u) = u(u - \alpha)(1 - u)$, $0 < \alpha < 1$.

We focus on RND models where not only diffusion is present but also *aggregation* (or *backward diffusion*) [2, 6, 4, 10, 11]. The heuristic motivation for this modelling assumption is based on the observation that population tend to cluster for, e.g., safety (to avoid easy predation). By imposing different motility rates for agents that are isolated, compared to other agents, one obtains density dependent nonlinear diffusion [7]. Aggregation will manifest itself in these models in sign changes of the density dependent diffusion coefficient $D(u)$. The simplest density-dependent nonlinear diffusion coefficient model that we consider is of the polynomial form

$$D(u) = \beta(u - \gamma_1)(u - \gamma_2) \quad (2)$$

with $0 < \gamma_1 < \gamma_2 < 1$, i.e., diffusion-aggregation-diffusion (DAD) in the domain of interest. For sparse population density diffusive behaviour is assumed, while for intermediate population density aggregation will happen which again turns into diffusive behaviour for large population densities (close to carrying capacity).

¹Another option is dispersive regularisation, e.g., the KdV equation. Note that both regularisations (viscous and dispersive) deal with the same equation (inviscid Burgers) and create very different outcomes.

2.1 Shock fronts in the RND model (1)

It is well-known that in the case of a nonlinear advection-reaction model which defines a hyperbolic balance law (under certain assumptions) shock formation is a well-known phenomenon. Similarly, negative diffusivity $D(u)$ can also cause shock formation in an RND model [4, 12, 13].

Let us look for one of the simplest coherent structures in such RND models (1), travelling waves with wave speed $c \in \mathbb{R}$ that connect the asymptotic end states $u_- = 1 \rightarrow u_+ = 0$, i.e., population/agents invade the unoccupied domain with constant speed. A travelling wave analysis introduces a co-moving frame $z = x - ct$ in (1), $c \in \mathbb{R}$. Stationary solutions, i.e., $u_t = 0$, in this co-moving frame include travelling waves/fronts, and they are found as special (heteroclinic) solutions of the corresponding ODE problem $-cu_z - (D(u)u_z)_z = f(u)$. Define $v := -cu - D(u)u_z$ to obtain the corresponding 2D dynamical system

$$\begin{aligned} u_z &= -\frac{(v + cu)}{D(u)} \\ v_z &= f(u). \end{aligned}$$

We are interested in a travelling front/wave in this system corresponding to a heteroclinic connection from one steady state ($u = 1$) to the other ($u = 0$) or vice versa. In our setup of the RND model, such a solution (if it exists) cannot be smooth, because the zeros of the diffusion coefficient $D(u)$ which exist in the relevant domain of interest $u \in [0, 1]$ define singularities in this problem. To avoid these singularities, discontinuous jumps (shocks) would be necessary to define ‘weak’ solutions of the original PDE problem (1).

2.2 Regularisations of RND models

To account for these shocks, we employ the technique of regularisation to this RND problem. Regularisation of RND models is typically considered in one of two ways [11, 12]. The first method of regularisation accounts for *viscous relaxation* by adding a small temporal change in the diffusivity:

$$u_t = (\Phi(u) + \varepsilon u_t)_{xx} + f(u), \quad 0 \leq \varepsilon \ll 1. \quad (3)$$

The second of these involves adding a small change in the potential to account for *nonlocal effects*, leading to:

$$u_t = (\Phi(u) - \varepsilon^2 u_{xx})_{xx} + f(u), \quad 0 \leq \varepsilon \ll 1. \quad (4)$$

These regularisation techniques have been widely employed in models of chemical phase-separation, though they have gone relatively unnoticed in biological models until very recently.

In this presentation, we study the possible effects of *both* regularisations in a single RND model, i.e.,

$$u_t = (\Phi(u) + \varepsilon a u_t - \varepsilon^2 u_{xx})_{xx} + f(u), \quad 0 \leq \varepsilon \ll 1, a \geq 0. \quad (5)$$

Since we only consider small perturbative regularisations $0 < \varepsilon \ll 1$, these models are so-called *singularly perturbed systems* and, as a consequence, the powerful machinery of geometric singular perturbation theory (GSPT) is applicable [3, 8, 16], as we shall explain in this presentation.

Remark 2.1 *This regularised RND model (5) can be derived from the history dependent energy functional*

$$E(u) = \int_{\Omega} \left(F(u) + \varepsilon a \int_0^t u_s^2 ds + \frac{\varepsilon^2}{2} |u_x|^2 \right) dx,$$

where $F(u) = \int \Phi(u)du$ is the free energy density function of the homogeneous state. The interfacial energy, $\frac{\varepsilon^2}{2}|u_x|^2$, introduces smoothing effects in regions with large gradients, and so does the memory term, $\varepsilon a \int_0^t u_s^2 ds$, which can be interpreted as visco-elastic potential energy; see, e.g., [18].

Remark 2.2 Continuum macroscale models can also be derived from lattice-based microscale models; see [7] for leading order RND models and [1] for regularised RND models (albeit more complicated).

3 Travelling wave analysis of the regularised RND model (5)

We derive conditions based on the specific functions $D(u)$ and $f(u)$ that lead to travelling waves with sharp interfaces (shocks) in one spatial dimension. We introduce a travelling wave coordinate $z = x - ct$ for waves with speed $c \in \mathbb{R}$. This transforms the regularised RND model (5) into a fourth order ordinary differential equation

$$-cu_z = \Phi(u)_{zz} - \varepsilon a c u_{zzz} - \varepsilon^2 u_{zzzz} + f(u), \quad (6)$$

which we can recast as a *singularly perturbed dynamical system* in standard form

$$\begin{aligned} \varepsilon u_z &= \hat{u} \\ \varepsilon \hat{u}_z &= w + \Phi(u) - \delta \hat{u} \\ v_z &= f(u) \\ w_z &= v + cu. \end{aligned} \quad (7)$$

where $(u, \hat{u}) \in \mathbb{R}^2$ are ‘fast’ variables, $(v, w) \in \mathbb{R}^2$ are ‘slow’ variables, and $\varepsilon \ll 1$ is the singular perturbation parameter.

Rescaling the ‘slow’ independent travelling wave variable $dz = \varepsilon dy$ in (7) gives the equivalent fast system

$$\begin{aligned} u_y &= \hat{u} \\ \hat{u}_y &= w + \Phi(u) - \delta \hat{u} \\ v_y &= \varepsilon f(u) \\ w_y &= \varepsilon(v + cu). \end{aligned} \quad (8)$$

with the ‘fast’ independent travelling wave variable y . These equivalent dynamical systems (7) respectively (8) have a symmetry

$$(\hat{u}, v, c, y) \leftrightarrow (-\hat{u}, -v, -c, -y), \quad \text{resp.} \quad (\hat{u}, v, c, z) \leftrightarrow (-\hat{u}, -v, -c, -z).$$

The aim is to use methods from GSPT to analyse the travelling wave problem in its ‘slow’ and ‘fast’ singular limit, and to obtain results on the existence (and stability) of travelling waves in the full regularised RND problem.

3.1 The limit on the ‘fast’ scale - the layer problem

We begin with the ‘fast’ system (8). Here the limit $\varepsilon \rightarrow 0$ gives the *layer problem*

$$\begin{aligned}
u_y &= \hat{u} \\
\hat{u}_y &= w + \Phi(u) - \delta \hat{u} \\
v_y &= w_y = 0,
\end{aligned} \tag{9}$$

i.e., (v, w) are considered parameters. Hence, the flow is along two-dimensional fast fibers $\mathcal{L} := \{(u, \hat{u}, v, w) \in \mathbb{R}^4 : (v, w) = \text{const}\}$. The set of equilibria of the layer problem,

$$S := \{(u, \hat{u}, v, w) \in \mathbb{R}^4 : \hat{u} = \hat{u}(u, v) = 0, w = w(u, v) = -\Phi(u)\}, \tag{10}$$

forms the two-dimensional *critical manifold* of the problem which is a graph over (u, v) -space. The stability property of this set of equilibria S is determined by the two non-trivial eigenvalues of the layer problem, i.e., the eigenvalues of the Jacobian evaluated along S ,

$$J = \begin{pmatrix} 0 & 1 \\ D(u) & -\delta \end{pmatrix}. \tag{11}$$

This matrix has $\text{tr}J = -\delta$ and $\det J = -D(u)$. Hence, for $D(u) > 0$ equilibria are of saddle-type while for $D(u) < 0$ equilibria are of focus/node/centre-type. Loss of normal hyperbolicity happens along the one-dimensional set(s)

$$F := \{(u, \hat{u}, v, w) \in S : D(u) = 0\}. \tag{12}$$

In the assumed diffusion-aggregation-diffusion (DAD) setup of (2), we have $F = F_l \cup F_r = \{(u, \hat{u}, v, w) \in S : u = \gamma_1\} \cup \{(u, \hat{u}, v, w) \in S : u = \gamma_2\}$, i.e., we have a splitting of the critical manifold $S = S_s^l \cup F_l \cup S_m \cup F_r \cup S_s^r$ where

$$S_s^l := \{(u, \hat{u}, v, w) \in \mathbb{R}^4 : \hat{u} = \hat{u}(u, v) = 0, w = w(u, v) = -\Phi(u), u < \gamma_1\}$$

$$S_s^r := \{(u, \hat{u}, v, w) \in \mathbb{R}^4 : \hat{u} = \hat{u}(u, v) = 0, w = w(u, v) = -\Phi(u), u > \gamma_2\}$$

denote saddle-type outer branches and, for $\delta \neq 0$,

$$S_m := \{(u, \hat{u}, v, w) \in \mathbb{R}^4 : \hat{u} = \hat{u}(u, v) = 0, w = w(u, v) = -\Phi(u), \gamma_1 < u < \gamma_2\}$$

denotes the (node/focus-type) middle branch. For $\delta = 0$ this middle branch S_m is of centre-type (where normal hyperbolicity is lost as well).

3.1.1 The $\delta = 0$ case

In this case, the layer problem (9),

$$\begin{aligned}
u_y &= \hat{u} \\
\hat{u}_y &= w + \Phi(u)
\end{aligned} \tag{13}$$

is Hamiltonian with

$$H(u, \hat{u}) = \frac{\hat{u}^2}{2} - \int (w + \Phi(u)) du. \tag{14}$$

Trajectories of this layer problem are confined to level sets of the Hamiltonian (14), i.e., $H(u, \hat{u}) = k$. Possible trajectories that are able to connect equilibrium points on different branches of the critical manifold S are confined to the saddle branches $S_s^{l/r}$ including the boundaries $F_{l/r}$. The corresponding equilibrium points $p_{l/r} = (u_{l/r}, 0, v_{l/r}, -\Phi(u_{l/r})) \in S_s^{l/r} \cup F_{l/r}$ of such connections must fulfill $v_l = v_r$ and $\Phi(u_l) = \Phi(u_r)$ since v and w are constant.

Remark 3.1 This creates a bound on possible w -values, $w \in [-\Phi(u_{f-}), -\Phi(u_{f+})]$ where $D(u_{f\mp}) = 0$, i.e., confined to region between the local extrema of Φ .

Without loss of generality, set $H(u_l, \hat{u} = 0) = 0$, i.e., $H(u, \hat{u}) = \frac{\hat{u}^2}{2} - \int_{u_l}^u (w + \Phi(u)) du$. Then $H(u_r, \hat{u} = 0)$ must be equal zero as well for the existence of a layer connection between these two points. This constraint leads to the well-known ‘equal area rule’ (see, e.g. [12]),

$$\int_{u_l}^{u_r} (w_h + \Phi(u)) du = 0. \quad (15)$$

This rule allows for $S_s^{l/r}$ to $S_s^{r/l}$ connections, but not to the boundaries $F_{l/r}$ or the centre-type middle branch S_m . Due to the symmetry ($\hat{u} \leftrightarrow -\hat{u}$), there exists automatically a pair of such heteroclinic connections for fixed $w = w_h$, i.e., $\Gamma_+(w_h, 0) : p_l \rightarrow p_r$ and $\Gamma_-(w_h, 0) : p_r \rightarrow p_l$.

Remark 3.2 The equal area rule (15) determines the value $w = w_h$ for which this integral vanishes. For $a = 0$, it is independent of the possible wave speed $c \in \mathbb{R}$.

3.1.2 The small $|\delta|$ case

For sufficiently small $|\delta| > 0$, we show that nearby heteroclinic connections to the same asymptotic end states still exist. This is done via a *Melnikov-type* argument; see, e.g., [15, 17]:

Define $x = (u, \hat{u})^\top$ and $f(x; w, \delta) = (\hat{u}, w + \Phi(u) - \delta \hat{u})^\top$ such that the layer problem is given in vector form by $x' = f(x; w, \delta)$, $x \in \mathbb{R}^2$. This system possesses heteroclinic orbits $\Gamma_\pm(y)$ for $w = w_h$ and $\delta = 0$, i.e., $\Gamma' = f(\Gamma_\pm; w_h, 0)$. Let $x = \Gamma_\pm + X$, $X \in \mathbb{R}^2$ which transforms the layer problem to the non-autonomous problem $X' = A(y)X + g(X, y; w, \delta)$ with the non-autonomous matrix $A(y) := D_x f(\Gamma_\pm; w_h, 0)$ and the nonlinear remainder $g(X, y; w, \delta) = f(\Gamma_\pm + X; w, \delta) - f(\Gamma_\pm; w_h, 0) - A(y)X$. The linear equation $X' = A(y)X$ is the *variational equation* along Γ_\pm . The corresponding *adjoint equation* is given by $\Psi' + A^\top(y)\Psi = 0$. Solutions of the variational and its adjoint equation preserve a constant angle along Γ_\pm , i.e., $D_y(\Psi^\top(y)X(y)) = 0, \forall y \in \mathbb{R}$. We can use this fact to define a splitting of the vector space \mathbb{R}^2 along Γ_\pm . Without loss of generality, we define it at $y = 0$ in the following way: $\mathbb{R}^2 = \text{span}\{f(\Gamma_\pm(0); w_h, 0)\} \oplus W$ where W is spanned by the solutions of the adjoint equation that decay exponentially for $y \rightarrow \pm\infty$; here, this space is one-dimensional and we denote the corresponding solution by $\psi(y) = (\psi_1(y), \psi_2(y))^\top$.

We measure the distance $\Delta \in \mathbb{R}$ between the one-dimensional stable and unstable manifolds emanating from the saddle-equilibria in a suitable cross section Σ . We denote these manifold segments by X_\pm . Based on our setup, we choose $\Sigma = W$. This distance function depends on the system parameters, i.e., $\Delta = \Delta(w, \delta)$. In the previous section, we established $\Delta(w_h, 0) = 0$. In general, one cannot solve $\Delta(w, \delta) = 0$ explicitly. Thus one aims to solve $\Delta(w, \delta) = 0$ near $(w, \delta) = (w_h, 0)$ approximately by means of the implicit function theorem: e.g., if $D_w \Delta(w_h, 0) \neq 0$ then $w = w_h(\delta) = w_h + b\delta + O(\delta^2)$ solves $\Delta(w_h(\delta), \delta) = 0$ for $\delta \in (-\delta_0, +\delta_0)$. The leading order expansion parameter b is then given by

$$b = -\frac{D_\delta \Delta(w_h, 0)}{D_w \Delta(w_h, 0)}.$$

These first-order expansion terms of the distance function Δ are known as first-order *Melnikov integrals*. They can be calculated as follows:

$$(D_w\Delta(w_h, 0), D_\delta\Delta(w_h, 0)) = \left(\int_{-\infty}^{\infty} (\psi(s)^\top D_w f(\Gamma_\pm(0); w_h, 0)) ds, \int_{-\infty}^{\infty} (\psi(s)^\top D_\delta f(\Gamma_\pm(0); w_h, 0)) ds \right)$$

We have $D_w f(\Gamma_\pm(0); w_h, 0) = (0, 1)^\top$ and, hence,

$$D_w\Delta(w_h, 0) = \int_{-\infty}^{\infty} (\psi(s)^\top D_w f(\Gamma_\pm(0); w_h, 0)) ds = \int_{-\infty}^{\infty} \psi_2(s) ds \neq 0,$$

based on the geometric observation that the ψ_2 -component does not change sign along Γ_\pm . The measure is well-defined since $\psi_2(y)$ is decaying exponentially for $y \rightarrow \pm\infty$. Hence, $w = w_h(\delta) = w_h + b\delta + O(\delta^2)$ solves $\Delta(w(\delta), \delta) = 0$ for $\delta \in (-\delta_0, +\delta_0)$. We also have $D_\delta f(\Gamma_\pm(0); w_h, 0) = (0, -\hat{u}(y))^\top$ and, hence,

$$D_\delta\Delta(w_h, 0) = \int_{-\infty}^{\infty} (\psi(s)^\top D_\delta f(\Gamma_\pm(0); w_h, 0)) ds = - \int_{-\infty}^{\infty} \hat{u}(s)\psi_2(s) ds \neq 0,$$

based on a similar geometric observation as above, i.e., both terms do not change sign under the variation along Γ_\pm . Hence,

$$b = \frac{D_\delta\Delta(w_h, 0)}{D_w\Delta(w_h, 0)} = - \frac{\int_{-\infty}^{\infty} \hat{u}(s)\psi_2(s) ds}{\int_{-\infty}^{\infty} \psi_2(s) ds} \neq 0$$

and we have a leading order affine solution $w(\delta)$ to $\Delta(w, \delta) = 0$ near $(w_h, 0)$.

Remark 3.3 *Only for $(w, \delta) = (w_h, 0)$ there exist two heteroclinics Γ_\pm simultaneously. For fixed small $\delta \neq 0$, the two heteroclinics exist for distinct w -values. There is also the symmetry $\delta \leftrightarrow -\delta$. Thus one only needs to continue one heteroclinic in (w, δ) -space. The other is given through the symmetry.*

Remark 3.4 *The leading order linear growth found in the Melnikov analysis cannot continue indefinitely since the saddle equilibria $p_{l/r}$ are confined to w -values between the local extrema of Φ ; see Remark 3.1. These extrema indicate saddle-node bifurcations of equilibria.*

3.1.3 The $\delta = O(1)$ case

What is the fate of the heteroclinic branches established in the previous section? Do they exist for large $|\delta|$ as well? Note, the heteroclinic orbits are confined to the upper (Γ_+) or lower (Γ_-) half-plane in (u, \hat{u}) -space. In these half-planes, the u -motion is monotone. Hence, all heteroclinics Γ_\pm are graphs over the u -coordinate chart in (u, \hat{u}) -space, i.e., $\Gamma_\pm : \hat{u}(u) : u \in (u_l, u_r)$. We consider Γ_+ . Such a heteroclinic orbit $\hat{u}(u)$ must fulfill

$$\begin{aligned} \frac{d\hat{u}}{du} &= \frac{w + \Phi(u) - \delta\hat{u}}{\hat{u}}, \quad \forall u \in (u_l, u_r) \\ \implies \frac{d}{du} \left(\frac{\hat{u}^2}{2} \right) &= \frac{d}{du} \int (w + \Phi(u) - \delta\hat{u}) du, \quad \forall u \in (u_l, u_r) \\ \implies \frac{\hat{u}^2}{2} &= \int_{u_l}^u (w + \Phi(u) - \delta\hat{u}) du, \quad \forall u \in (u_l, u_r). \end{aligned}$$

For $u \rightarrow u_l$, the last line is fulfilled since $\hat{u}(u_l) = 0$. For $u \rightarrow u_r$, where $\hat{u}(u_r) = 0$, we obtain a condition for the existence of a heteroclinic orbit,

$$\boxed{\int_{u_l}^{u_r} (w + \Phi(u)) du = \delta \int_{u_l}^{u_r} \hat{u}(u) du,} \quad (16)$$

which, for $\delta = 0$, gives the equal area rule as established previously. For $\delta \neq 0$ this formula provides a generalised ‘equal area rule’, i.e., the left hand side must move away from its ‘equal area’ position given for $w = w_h(0)$ to counteract the right hand side contribution. This gives $w = w_h(\delta)$.

For sufficiently large $|\delta| = \delta_m$, w will reach its limit w_{sn} where one of the saddle equilibria $p_{l/r}$ goes through a saddle-node bifurcation. Until then, the heteroclinic connection is along the hyperbolic direction, but afterwards it will be along the centre direction which is non-unique and, hence, replaces the codimension-one role of the w variation. Hence, for fixed $w = w_{sn}$ and for sufficiently large $|\delta| > \delta_m$, there exists always a heteroclinic orbit.

Remark 3.5 For $w = w_{sn}$, the rhs of (16) is fixed. One concludes that for sufficiently large $|\delta| > \delta_m$, there is a $\hat{u}(u)$ that fulfills the generalised equal area rule, i.e., that fixes the right hand side $\delta \int \hat{u} du$ to the correct value.

Figure 1 summarizes our results on the existence of shocks in the regularised RND model, i.e., the solution branches of $\Delta(w, \delta) = 0$. The important insight here is that viscous relaxation regularisation is dominant for $|\delta| > |\delta_m|$

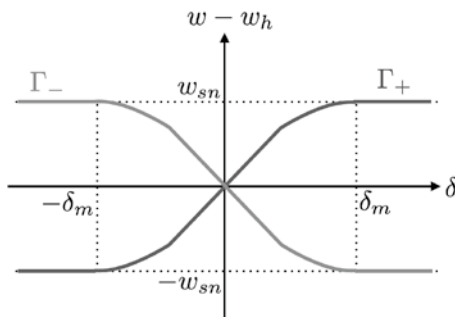


Figure 1: sketch of complete bifurcation diagram for heteroclinic connections Γ_{\pm} in (δ, w) -space centered at $(w_h, 0)$.

3.2 The limit on the slow scale - the reduced problem

For the slow system (7), the limit $\varepsilon \rightarrow 0$ gives the *reduced problem*

$$\begin{aligned} 0 &= \hat{u} \\ 0 &= w + \Phi(u) - \delta \hat{u} \\ v_z &= f(u) \\ w_z &= v + cu. \end{aligned} \quad (17)$$

It describes the ‘evolution’ of the slow variables (v, w) constrained to the 2D critical manifold S (10). Here, the critical manifold S is given as a graph over the (u, v) -space, i.e., $S : \psi(u, v) \in \mathbb{R}^4$.

Therefore, we aim to study the corresponding reduced flow on S in this (u, v) -coordinate chart. By definition, the main requirement on the reduced vector field $R(u, v) \in \mathbb{R}^2$ is that, when mapped onto S via $D\psi$ it has to correspond to the (leading order) slow component of the full four-dimensional vector field constraint to S , i.e.,

$$D\psi(u, v)R(u, v) = \Pi^S G(\psi(u, v)) = \left(\frac{v + cu}{-D(u)}, 0, f(u), v + cu \right)^\top$$

where $\Pi^S G(\psi(u, v))$ is the (oblique) projection of the vector field $G = (0, 0, f(u), v + cu)^\top$ onto the tangent bundle TS of the critical manifold S along fast fibres spanned by $\{(1, 0, 0, 0)^\top, (0, 1, 0, 0)^\top\}$. Thus the reduced vector field $R(u, v)$ in the (u, v) -coordinate chart is given by

$$\begin{aligned} -D(u)u_z &= v + cu \\ v_z &= f(u). \end{aligned} \tag{18}$$

Note that this dynamical system is singular along the folds F^\pm where $D(u) = 0$. To be able to study the reduced problem (18) in a neighbourhood of F^\pm , we make an auxiliary state-dependent time transformation $dz = D(u)d\zeta$ which gives the so-called *desingularised problem*

$$\begin{aligned} u_\zeta &= -(v + cu) \\ v_\zeta &= D(u)f(u). \end{aligned} \tag{19}$$

This problem is topologically equivalent to (18) on the saddle-type outer branches of S while one has to reverse the orientation on the middle node-focus-centre-type branch of S to obtain the equivalent flow. We classify all singularities of the reduced problem (18) by analysing the auxiliary system, the desingularised problem (19).

Remark 3.6 *We emphasize that the desingularised system is only a proxy system to study the problem near the folds. To completely understand the original flow near the folds, one has to use additional techniques such as the blow-up method [14].*

The asymptotic end states of the travelling waves form equilibrium states of the desingularised (and the reduced) problem defined by $f(u_\pm) = 0$, and $v_\pm = -cu_\pm$. Our focus is on asymptotic end states given by the equilibria $(u_\mp, v_\mp) = (1, -c)$ and $(u_\pm, v_\pm) = (0, 0)$. In the case of the bistable reaction term, there exists an additional equilibrium in the domain of interest defined by $f(u_b = \alpha) = 0$ which gives $(u_b, v_b) = (\alpha, -c\alpha)$. We assume $\gamma_1 < \alpha < \gamma_2$, i.e. this additional equilibrium is located on the middle branch S_m . The Jacobian evaluated at any of these equilibria $(u_{\pm,b}, v_{\pm,b})$ is given by

$$J = \begin{pmatrix} -c & -1 \\ D(u_{\pm,b})f'(u_{\pm,b}) & 0 \end{pmatrix}$$

which has $\text{tr } J = -c$ and $\det J = D(u_{\pm,b})f'(u_{\pm,b})$. The types of equilibria of the reduced problem are summarized in the following table.

Remark 3.7 *The auxiliary system (19) defines another type of singularities for the reduced problem through $D(u) = 0$ which exist on the folds $F_{l/r}$ and are known as folded singularities; see, e.g., [16]. If time permits, I will briefly discuss this in my presentation.*

$D(u)$	$f(u)$	(u_-, v_-)	(u_+, v_+)	$(u_b, v_b), \gamma_1 < \alpha < \gamma_2$
DAD	logistic	Saddle	stable NF	-
DAD	bistable	Saddle	Saddle	Saddle

Table 1: Type of equilibria on critical manifold S

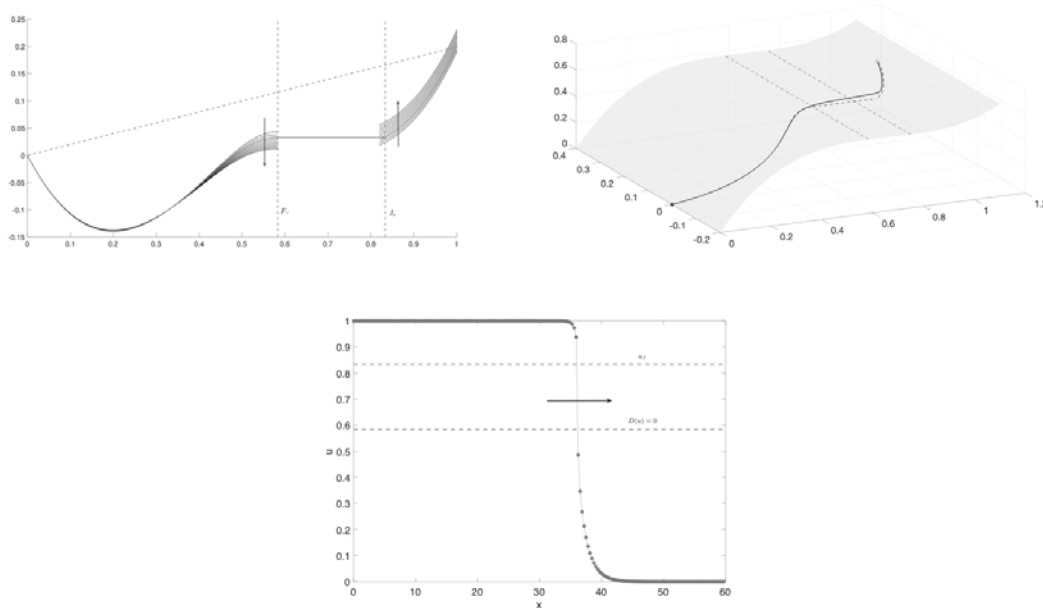


Figure 2: (Top Left) construction of singular heteroclinic orbit in (u, v) sub-space for $\delta > \delta_m$. The shock connects from $J_a \in S_s^r$ to F^- with asymptotic end states $u_- = 1$ and $u_+ = 0$. (Top Right) shows the singular heteroclinic orbit (dashed red, $\varepsilon = 0$) as well as the perturbed shock-fronted travelling wave (black solid, $0 < \varepsilon \ll 1$) in (u, v, w) -space. (Bottom) The corresponding travelling wave profile with sharp interface for $0 < \varepsilon \ll 1$

3.3 Construction of heteroclinic orbits that give shock waves

The final task is to concatenate solutions from the two limiting problems to construct singular heteroclinic orbits. Figure 2 shows an example for $|\delta| > |\delta_m|$; see Figure 1. In this case, the shock location is at (one of) the folds of the critical manifold. From a regularisation point-of-view, this indicates that viscous relaxation (u_{xxt} -term) dominates the nonlocal effects (u_{xxxx} -term).

The power of geometric singular perturbation theory is to show the persistence of travelling waves with smooth and sharp interfaces (shocks) constructed above under sufficiently small perturbations $0 < \varepsilon \ll 1$ by means of geometric properties of invariant manifolds. Figure 2 (Bottom) indicates that this is indeed the case.

Remark 3.8 *If time permits, I will also discuss some of the intricacies of numerical schemes to resolve the predicted analytical shock location. Similarly, if time permits, I briefly discuss (spectral) stability properties of these solutions.*

Acknowledgement

This work has been funded by the Australian Research Council DP200102130 grant.

References

- [1] K. Anguige and C. Schmeiser. A one-dimensional model of cell diffusion and aggregation, incorporating volume filling and cell-to-cell adhesion. *Journal of Mathematical Biology*, 58(3):395–427, jun 2008.
- [2] J. W. Cahn. On spinoidal decomposition. *Acta. Metall.*, 9(795-801), 1961.
- [3] N. Fenichel. Geometric singular perturbation theory. *J Differential Equations*, 31:53–98, 1979.
- [4] A. E. Fernando, K. A. Landman, and M. J. Simpson. Nonlinear diffusion and exclusion processes with contact interactions. *Physical Review E*, 81, January 2010.
- [5] R. A. Fisher. The wave of advance of advantageous genes. *Annals of Eugenics*, 7:355–369, 1937.
- [6] J. Hilliard. Spinodal decomposition. in phase transformations. *Am. Soc. Metals*, pages 497–560, 1970.
- [7] S. T. Johnston, R. E. Baker, D. L. S. McElwain, and M. J. Simpson. Co-operation, competition and crowding: a discrete framework linking allee kinetics, nonlinear diffusion, shocks and sharp-fronted travelling waves. *Scientific Reports*, 7(42134), 2017.
- [8] C. K. R. T. Jones. Geometric singular perturbation theory. in *Dynamical Systems, Springer Lecture Notes Math.*, 1609:44–120, 1995.
- [9] P. K. Maini, L. Malaguti, C. Marcelli, and S. Matucci. Aggregative movement and front propagation for bi-stable population models. *Mathematical Models and Methods in Applied Sciences*, 17(9):1351–1368, 2007.
- [10] J.D. Murray. *Mathematical Biology I: An introduction*, volume 1 of *Interdisciplinary Applied Mathematics*. Springer, Hong Kong, 3rd edition, 2002.
- [11] V. Padron. Effect of aggregation on population recovery modelled by a forward-backward pseudoparabolic equation. *Transactions of the American Mathematical Society*, 356(7):2739–2756, 2003.
- [12] R. L. Pego. Front migration in the nonlinear Cahn–Hilliard equation. *Proc. R. Soc. Lond. A*, 422:261–278, 1989.
- [13] C. J. Penington, B. D. Hughes, and K. A. Landman. Building macroscale models from microscale probabilistic models: A general probabilistic approach for nonlinear diffusion and multispecies phenomena. *Physical Review E*, 84, October 2011.
- [14] P. Szmolyan and M. Wechselberger. Canards in \mathbb{R}^3 . *J Differential Equations*, 177:419–453, 2001.

- [15] André Vanderbauwhede. Bifurcation of degenerate homoclinics. *Results in Mathematics*, 21(1-2):211–223, mar 1992.
- [16] M. Wechselberger and G. J. Pettet. Folds, canards and shocks in advection-reaction-diffusion models. *Nonlinearity*, 23:1949–1969, 2010.
- [17] Martin Wechselberger. Extending Melnikov theory to invariant manifolds on non-compact domains. *Dynamical Systems*, 17(3):215–233, aug 2002.
- [18] T.P. Witelski. The structure of internal layers for unstable nonlinear diffusion equations. *Studies in Applied Mathematics*, 96:277–300, 1996.