

COMPUTATION OF BIFURCATED BRANCHES IN A FREE BOUNDARY PROBLEM ARISING IN COMBUSTION THEORY*

OLIVIER BACONNEAU¹, CLAUDE-MICHEL BRAUNER¹ AND ALESSANDRA LUNARDI²

Abstract. We consider a parabolic 2D Free Boundary Problem, with jump conditions at the interface. Its planar travelling-wave solutions are orbitally stable provided the bifurcation parameter u_* does not exceed a critical value u_*^c . The latter is the limit of a decreasing sequence (u_*^k) of bifurcation points. The paper deals with the study of the 2D bifurcated branches from the planar branch, for small k . Our technique is based on the elimination of the unknown front, turning the problem into a *fully nonlinear* one, to which we can apply the Crandall-Rabinowitz bifurcation theorem for a local study. We point out that the *fully nonlinear* reformulation of the FBP can also serve to develop efficient numerical schemes in view of global information, such as techniques based on arc length continuation.

Résumé. On s'intéresse à un problème à frontière libre bidimensionnel, avec conditions de saut à l'interface. Le problème parabolique admet comme solutions des ondes progressives planes, qui sont orbitalement stables si le paramètre u_* ne dépasse pas la valeur u_*^c . Ce point critique est la limite d'une suite décroissante de points de bifurcation (u_*^k) . Dans cet article, on étudie la structure des branches bifurquées 2D à partir de la branche triviale formée des ondes planes, pour k petit. Notre technique consiste à éliminer le front inconnu, pour se ramener à un problème *totalelement non linéaire* équivalent, auquel on applique le théorème de bifurcation de Crandall-Rabinowitz pour une étude locale. La reformulation *totalelement non linéaire* du problème s'avère également bien adaptée à la mise en œuvre de méthodes numériques pour le suivi global des branches bifurquées, en particulier par continuation.

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¹ Mathématiques Appliquées de Bordeaux, Université Bordeaux I, 33405 Talence Cedex, France.
e-mail: Olivier.Baconneau@math.u-bordeaux.fr; Claude-Michel.Brauner@math.u-bordeaux.fr

² Dipartimento di Matematica, Università di Parma Via D'Azeglio 85/A, 43100 Parma, Italy.
e-mail: lunardi@prmat.math.unipr.it

1. INTRODUCTION

In this paper we study the bifurcated branches of travelling-wave solutions to the parabolic two-dimensional Free Boundary Problem,

$$\left\{ \begin{array}{l} u_t(t, z, y) = \Delta u(t, z, y) + u(t, z, y)u_z(t, z, y), \quad t \geq 0, \quad z \neq \xi(t, y), \quad y \in [-1, 1], \\ u(t, \xi(t, y), y) = u_* > 0, \quad [\partial u / \partial \nu](t, \xi(t, y), y) = -1, \quad t \geq 0, \quad y \in [-1, 1], \\ \partial \xi / \partial \nu(t, y) = 0, \quad t \geq 0, \quad y = \pm 1, \\ \partial u / \partial \nu(t, z, y) = 0, \quad t \geq 0, \quad z \neq \xi(t, y), \quad y = \pm 1, \\ u(t, -\infty, y) = 0, \quad u(t, +\infty, y) = u_\infty > 0, \quad t \geq 0, \quad y \in [-1, 1], \end{array} \right. \tag{1.1}$$

where the unknowns are the interface $\xi = \xi(t, y)$ and the (normalized) temperature $u = u(t, z, y)$. By $[f](\zeta)$ we mean $f(\zeta^+) - f(\zeta^-)$ at a point of possible discontinuity ζ .

Problem (1.1) arises as a multidimensional version of a system introduced by Stewart and Ludford [10] as a tentative model to describe the transition from a low speed combustion wave (deflagration) to a high speed combustion wave (detonation). Although this model has been ruled out as an accurate model of the physical situation, since then it has received constant attention because of its very unusual features as a Free Boundary Problem (see the survey [11]).

By travelling-wave solutions of (1.1) we mean solutions such that $\xi(t, y) = -ct + s(y)$, $u(t, z, y) = U(z + ct, y)$ for some $c \in \mathbb{R}$ and $U : \mathbb{R} \times [-1, 1] \rightarrow \mathbb{R}$. Replacing z by $z + ct$, the triplet (c, s, U) must satisfy

$$\left\{ \begin{array}{l} cU_z(z, y) = \Delta U(z, y) + U(z, y)U_z(z, y), \quad z \neq s(y), \quad y \in [-1, 1], \\ U(s(y), y) = u_*, \quad [\partial U / \partial \nu](s(y), y) = -1, \quad y \in [-1, 1], \\ \partial U / \partial y(x, \pm 1) = 0, \quad x \neq s(y), \\ \partial s / \partial y = 0, \quad y = \pm 1, \\ U(-\infty, y) = 0, \quad U(+\infty, y) = u_\infty, \quad y \in [-1, 1]. \end{array} \right. \tag{1.2}$$

It is easy to see that for certain values of the parameters [10] (precisely, for $u_\infty > \sqrt{2}$, $2/u_\infty < u_* < 2/u_\infty + u_\infty$) problem (1.2) has a one-dimensional or “planar” travelling-wave solution, unique up to translations, with $c = c_0 = u_\infty/2 + 1/u_\infty$ independent of u_* , $s \equiv 0$, and where $U(z, y) \equiv U_0(z)$ verifies:

$$\left\{ \begin{array}{l} c_0 U_0'(z) = U_0''(z) + U_0(z)U_0'(z), \quad z \neq 0, \\ U_0(0) = u_*, \quad [U_0'](0) = -1, \\ U_0(-\infty) = 0, \quad U_0(+\infty) = u_\infty, \end{array} \right. \tag{1.3}$$

whose solution is explicit. We denote this one-dimensional solution by the triplet $(c_0, 0, U_0)$. Numerically, we take hereafter $u_\infty = 2$, hence $c_0 = 3/2$.

The stability of such planar travelling-wave has been studied in [6]: it is orbitally stable iff the *bifurcation parameter* u_* does not exceed a critical value u_*^c . In [3], u_*^c has been shown to be the limit of a decreasing

sequence $(u_*^k)_{k \in \mathbb{N}^*}$ such that, for k large enough, u_*^k is a bifurcation point of a branch of nonplanar (*i.e.*, genuinely two-dimensional) travelling-wave solutions to (1.1), see Figure 1.

The proof in [3] is based on the elimination of the front s by an appropriate splitting of U , namely $U = U_0 + sU_0' + w$. The problem for w turns out to be *fully nonlinear* (see Sect. 2). The points u_*^k are characterized as those values of u_* at which the kernel of the linearized operator L acting on w is two-dimensional.

In contrast to [3], the paper deals with the two-dimensional bifurcated branches from the planar branch $(c_0, 0, U_0)$ for the small values of k . Our proofs rely on numerics. First, we prove that u_*^k is a bifurcation point by checking numerically the transversality condition. Then we study the shape of the bifurcated branches near u_*^k and show that they occur for u_* in a right neighborhood of u_*^k , for k small. Each two-dimensional branch (c, s, U) is parametrized by

$$u_* = u_*^k + \mu(\sigma), \quad c = c(\sigma), \quad s = s(\sigma), \quad U = U(\sigma), \quad -\delta_k < \sigma < \delta_k,$$

$(-\delta_k, \delta_k)$ being a small neighborhood of 0, and $\mu(0) = 0, c(0) = c_0, s(0) = 0, U(0) = U_0$. While it is not hard to see that $\dot{\mu}(0) = d\mu/d\sigma(0) = 0$, the computation of $\ddot{\mu}(0)$ is more difficult, and needs numerical treatment.

As usual, the information provided by the classical Crandall-Rabinowitz bifurcation theorem are only local. Global informations about the behaviour of bifurcated branches can be obtained by numerical methods, such as techniques based on arc length continuation [8].

Our aim is to point out that the idea of a *fully nonlinear* reformulation used in the theoretical proofs, *via* the elimination of the front s , can also serve to develop new numerical schemes for Free Boundary Problems. The price to pay (as in the continuous problem) is that the discretized system contains approximations of second order derivatives. In Section 4 we show how to handle the method practically, especially the question of the linear algebra. The method has appeared to be quite efficient in the computation of the first two-dimensional bifurcated branches.

2. EXISTENCE OF THE BIFURCATED BRANCHES

Problem (1.2) is studied fixing the free boundary by the change of coordinate

$$x = z - s(y)$$

and eliminating the unknown s by the splitting

$$U(x, y) = U_0(x) + s(y)U_0'(x) + w(x, y), \tag{2.1}$$

i.e. introducing the new unknown w . The boundary conditions give then

$$s(y) = [w(0, y)],$$

where by $[f(0, y)] = f(0^+, y) - f(0^-, y)$ we indicate from now on the jump at $x = 0$. Substituting into (1.2), one gets the *fully nonlinear problem* for (c, w) ,

$$\left\{ \begin{array}{l} (c - c_0)(U_0' + [w(0, y)]U_0'' + w_x) = \mathcal{L}w(x, y) + \mathcal{F}(w)(y), \quad x \neq 0, \quad y \in [-1, 1], \\ \mathcal{B}w = 0, \quad \mathcal{C}w = \mathcal{G}(w), \quad y \in [-1, 1], \\ \frac{\partial w}{\partial y} = 0, \quad x \neq 0, \quad y = \pm 1, \\ w(-\infty, y) = w(+\infty, y) = 0, \quad y \in [-1, 1], \end{array} \right. \tag{2.2}$$

with

$$\mathcal{L}v(x, y) = \Delta v(x, y) - c_0 v_x(x, y) + \frac{\partial}{\partial x} (U_0(x)v(x, y)), \quad x \neq 0, \quad y \in [-1, 1], \tag{2.3}$$

$$\mathcal{B}v(y) = v(0^-, y)U_0'(0^+) - v(0^+, y)U_0'(0^-), \quad y \in [-1, 1], \tag{2.4}$$

$$\mathcal{C}v(y) = [v_x(0, y)] + (u_* - c_0)[v(0, y)], \quad y \in [-1, 1], \tag{2.5}$$

and

$$\begin{aligned} \mathcal{F}(v)(x, y) &= (\partial_y[v(0, y)])^2(-U_0''(x) + [v(0, y)]U_0'''(x) + v_{xx}) + \frac{1}{2} \frac{\partial}{\partial x}(v + [v]U_0'(x))^2 \\ &- 2v_{xy}(x, y)\partial_y[v(0, y)] - \partial_{yy}[v(0, y)]([v(0, y)]U_0''(x) + v_x(x, y)), \end{aligned} \tag{2.6}$$

$$\mathcal{G}(v)(y) = 1 - (1 + (\partial_y[v(0, y)])^2)^{-1/2}. \tag{2.7}$$

The trivial branch of problem (1.2), that is $(c = c_0, s(y) = 0, U(z, y) = U_0(z))$, is transformed into the trivial branch for (2.2)

$$(c = c_0, w \equiv 0).$$

To state the bifurcation theorem, we need some preliminaries about the spectrum of the realization of \mathcal{L} in suitable functional spaces. The functional spaces where the problem is set are, as usual, weighted Hölder spaces [9]; if $0 < \alpha < 1$, then

$$\begin{aligned} X^\alpha &= \{w \in L^\infty(\mathbb{R} \times [-1, 1]) : (x, y) \mapsto q_-(x)w(x, y) \in C^\alpha(\mathbb{R}_- \times [-1, 1]), \\ &(x, y) \mapsto q_+(x)w(x, y) \in C^\alpha(\mathbb{R}_+ \times [-1, 1])\}, \\ \|w\|_{X^\alpha} &= \|q_-(x)w(x, y)\|_{C^\alpha(\mathbb{R}_+ \times [-1, 1])} + \|q_+(x)w(x, y)\|_{C^\alpha(\mathbb{R}_+ \times [-1, 1])}, \end{aligned}$$

with $q_-(x) = e^{-c_0x/2}$, $q_+(x) = e^{(u_\infty/2 - 1/u_\infty)x/2}$, in which the realization of the operator \mathcal{L} , with homogeneous boundary conditions, has good spectral properties. Together with the space X^α we shall use also the spaces $X^{k+\alpha}$, with $k \in \mathbb{N}$, defined similarly, as is C^α replaced by $C^{k+\alpha}$.

The realization of \mathcal{L} in X^α is the operator L defined by

$$\begin{aligned} D(L) &= \{w \in X^{2+\alpha}, \mathcal{B}w = \mathcal{C}w = 0 \text{ at } x = 0, \partial w / \partial y = 0 \text{ at } \mathbb{R} \times \{-1, 1\}\}, \\ L : D(L) &\mapsto X^\alpha, \quad Lw = \mathcal{L}w. \end{aligned}$$

Its spectrum is given by [6]

$$\sigma(L) = \{\lambda = \lambda_1 + \lambda_2 : \lambda_1 \in \sigma_1, \lambda_2 \in \sigma_2\},$$

where

$$\sigma_1 = \{-k^2\pi^2/4 : k \in \mathbb{N}\}$$

is the spectrum of the second-order derivative (acting on the variable y) with Neumann boundary condition at $y = \pm 1$, and

$$\sigma_2 = (-\infty, -c_0^2/4 + 1/2] \cup \{0\} \cup \{\tilde{\lambda}\}$$

is the spectrum of the operator (acting on the variable x) $v \mapsto v_{xx} - c_0v_x + \partial/\partial x(U_0v)$ in X^α , with boundary conditions $\mathcal{B}v(0, y) = \mathcal{C}v(0, y) = 0$. Note that $-c_0^2/4 + 1/2 < 0$. When it exists, $\tilde{\lambda}$ is a real eigenvalue depending

on u_* . The following properties hold:

- (a) if $2/u_\infty < u_* \leq u_0$, $\tilde{\lambda} < 0$;
- (b) if $u_0 < u_* \leq u_*^c$, $\tilde{\lambda}$ does not exist;
- (c) if $u_*^c < u_* < u_\infty + 2/u_\infty = 2c_0$, $\tilde{\lambda} > 0$,

where $u_0 = c_0 - \sqrt{c_0^2 - 1} - \sqrt{2c_0^2 - 3}$ and $u_*^c = c_0 + \sqrt{c_0^2 - 1}$. Moreover, $\lim_{u_* \downarrow u_*^c} \tilde{\lambda} = +\infty$, $\lim_{u_* \uparrow u_\infty + 2/u_\infty} \tilde{\lambda} = 0$, and the function $u_* \mapsto \tilde{\lambda}(u_*)$ is decreasing on the interval $(u_*^c, u_\infty + 2/u_\infty)$.

For each $k \in \mathbb{N}^*$, define u_*^k as the (unique) value of u_* such that (see Fig. 1)

$$\tilde{\lambda}(u_*) = \frac{k^2 \pi^2}{4}. \tag{2.8}$$

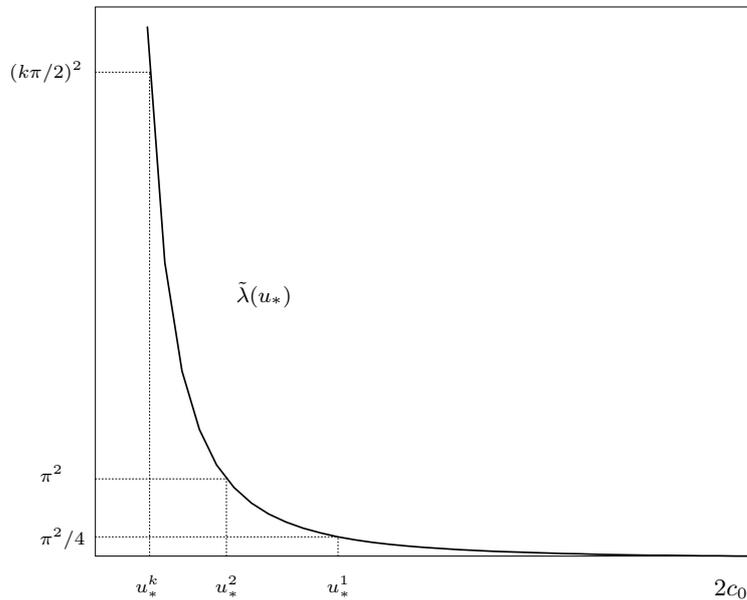


FIGURE 1. The figure shows the decreasing curve of the eigenvalue $\tilde{\lambda}$ versus the bifurcation parameter u_* . On the vertical axis, we put the $(k\pi)^2/4$ which define, by intersection with the decreasing curve, the values of the sequence of bifurcation points u_*^k , accumulating at u_*^c . Numerically, with $u_\infty = 2$, $c_0 = 3/2$, we find $u_*^1 \simeq 2.758 > u_*^2 \simeq 2.6936 > u_*^3 \simeq 2.6694 > u_*^4 \simeq 2.6569 > \dots > u_*^c \simeq 2.6182$.

Then [3], at $u_* = u_*^k$, 0 is a semisimple eigenvalue of L , and the kernel of L is two-dimensional. The values $u_* = u_*^k$ are the natural candidates to be bifurcation points of branches of nonplanar solutions to (1.2).

Theorem 2.1. Fix $\alpha \in (0, 1)$. For each small $k \in \mathbb{N}^*$, there exist $\delta_k > 0$ and three regular functions,

$$\mu_k : (-\delta_k, \delta_k) \mapsto \mathbb{R}, \quad c_k : (-\delta_k, \delta_k) \mapsto \mathbb{R}, \quad w_k : (-\delta_k, \delta_k) \mapsto X^{2+\alpha},$$

such that $\mu_k(0) = 0$, $c_k(0) = c_0$, $w_k(0) = 0$, and for each $\sigma \in (-\delta_k, \delta_k)$, the couple $(c_k(\sigma), w_k(\sigma))$ is a solution of (2.2) for $u_* = u_*^k + \mu_k(\sigma)$. Moreover $w_k(\sigma) \neq 0$ and $c_k(\sigma) > c_0$ for $\sigma \neq 0$.

The couple $(c_k(\sigma), w_k(\sigma))$ is the unique nontrivial solution of (2.2) for $u_* = u_*^k + \mu_k(\sigma)$ near the planar trivial branch $(c = c_0, w = 0)$.

Proof. We recall here the parts of the proof of [3, theorem 2.7] which will be used in the sequel.

We introduce the following notation: if Y is any Banach space of functions defined in $[-1, 1]$ or in $\mathbb{R} \times [-1, 1]$, we define $Y_{\partial y}$ to be the subset of Y consisting of those functions whose derivative w.r.t. y at ± 1 vanishes.

Proposition 2.2. *Let us consider the linear operator*

$$X_{\partial y}^{2+\alpha} \mapsto X^\alpha \times C_{\partial y}^{2+\alpha}([-1, 1]) \times C_{\partial y}^{1+\alpha}([-1, 1]),$$

$$u \mapsto Au = (\mathcal{L}u, \mathcal{B}u, \mathcal{C}u).$$

At $u_* = u_*^k$, 0 is a semisimple eigenvalue of A , and the kernel of A is spanned by the functions $\Phi_1(x, y) = U'_0(x)$, $\Phi_2(x, y) = \varphi(x)\eta_k(y)$ where

$$\eta_k(y) \begin{cases} = \sin(k\pi y/2), & \text{if } k \text{ is odd,} \\ = \cos(k\pi y/2), & \text{if } k \text{ is even,} \end{cases} \tag{2.9}$$

$$\varphi(x) = \frac{d}{dx} \frac{e^{p_1(k^2\pi^2/4)x}}{\tilde{\varphi}(x)}, \quad x < 0, \quad \varphi(x) = \frac{d}{dx} \frac{e^{-(p_2(k^2\pi^2/4)-c_0)x}}{\tilde{\varphi}(x)}, \quad x > 0, \tag{2.10}$$

$$p_1(\lambda) = (c_0 + \sqrt{c_0^2 + 4\lambda})/2, \quad p_2(\lambda) = (c_0 + \sqrt{c_0^2 + 4\lambda - 2})/2,$$

$$\tilde{\varphi}(x) = \exp\left(\frac{1}{2} \int_0^x U_0(s) ds\right) = \begin{cases} \frac{u_*}{2c_0} e^{c_0x} + 1 - \frac{u_*}{2c_0}, & x < 0, \\ \frac{u_\infty(u_\infty - u_*)}{u_\infty^2 - 2} e^{x/u_\infty} + \frac{u_\infty u_* - 2}{u_\infty^2 - 2} e^{u_\infty x/2}, & x > 0. \end{cases}$$

The spectral projection on the kernel is given by

$$\begin{aligned} Pv(x, y) &= \frac{1}{2u_\infty} \int_{-1}^1 \int_{\mathbb{R}} v(s, r) ds dr U'_0(x) + \int_{-1}^1 \int_{\mathbb{R}} v(s, r) \varphi^*(s) \eta_k(r) ds dr \varphi(x) \eta_k(y) \\ &= P_1v(x, y) + P_2v(x, y). \end{aligned}$$

where

$$\varphi^*(x) = \frac{\varphi(x)}{U'_0(x)}. \tag{2.11}$$

The range of A consists of the triplets (f, g_0, g_1) such that

$$\begin{aligned} \mathcal{Q}_1(f, g_0, g_1) &= \frac{1}{2u_\infty} \int_{-1}^1 \int_{\mathbb{R}} f(x, y) dx dy + \frac{1}{2u_\infty} \int_{-1}^1 g_1(y) dy = 0, \\ \mathcal{Q}_2(f, g_0, g_1) &= \int_{-1}^1 \int_{\mathbb{R}} f(x, y) \varphi^*(x) \eta_k(y) dx dy \\ &+ \frac{\varphi^*(0^+)}{U'_0(0^-)} \int_{-1}^1 \eta_k(y) g_0(y) dy + \varphi^*(0) \int_{-1}^1 \eta_k(y) g_1(y) dy = 0. \end{aligned} \tag{2.12}$$

Theorem 2.1 is proved by a Lyapunov–Schmidt procedure, reducing first the dimension of the kernel and the codimension of the range to 1; this is done by expressing c in terms of w ,

$$c = c_0 + \frac{1}{2u_\infty} \left(\int_{-1}^1 \left\{ |\partial_y[w(0, y)]|^2 (1 - Cw) \right\} dy - \int_{-1}^1 \mathcal{G}(w) dy \right) \tag{2.13}$$

and using the translation invariance of the problem to look for a solution w belonging to $(I - P_1)(X_{\partial y}^\alpha)$. The final equation is

$$\tilde{F}(w, \mu) = (0, 0, 0) \tag{2.14}$$

where $\mu = u_* - u_*^k$, and

$$\tilde{F} : (I - P_1)(X_{\partial y}^{2+\alpha}) \times \mathbb{R} \rightarrow \{(f, g_0, g_1) \in X_{\partial y}^\alpha \times C^{2+\alpha} \times C^{1+\alpha} : \mathcal{Q}_1(f, g_0, g_1) = 0\}$$

$$\tilde{F}(w, \mu) = (\mathcal{L}w + \mathcal{F}(w) + \mathcal{H}(w), Bw, Cw - \mathcal{G}(w)),$$

\mathcal{H} being defined by

$$\mathcal{H}(w) = -\frac{1}{2u_\infty} (U_0' + [w(0, y)]U_0'' + w_x) \int_{-1}^1 \{ \partial_y[w(0, y)]^2 (1 - Cw) - \mathcal{G}(w) \} dy.$$

Here the trivial branch is $w = 0$. The linear part $\tilde{L} = \tilde{F}_w(0, 0) = (\mathcal{L}, \mathcal{B}, \mathcal{C})$ has the following properties:

- 0 is a simple eigenvalue of \tilde{L} ,
- $\text{Ker } \tilde{L}$ is spanned by $\Phi_2(x, y) = \varphi(x)\eta_k(y)$,
- the range of \tilde{L} has codimension 1,
- $\tilde{F}_{\mu w}(0, 0) \cdot \Phi_2 \notin \text{Im } \tilde{L}$ iff $T_k \neq 0$ (*transversality condition*),

where

$$T_k = \int_{\mathbb{R}} \frac{\partial}{\partial x} \left(\frac{\partial U_0}{\partial u_*} \varphi \right) \varphi^* dx + [\varphi] \left(\varphi^*(0) - (c_0 - u_*^k) \varphi^{*'}(0^+) \frac{1}{U_0'(0^-)} \right). \tag{2.15}$$

For the small values of k , it is easy to compute a very accurate value of T_k by solving numerically (2.15), see Figure 2. We find that T_k is positive for k small, more precisely $T_k > 39$. Since the transversality condition is verified, it is possible to apply the Crandall–Rabinowitz Theorem [7] to obtain the statement. \square

3. STUDY OF CONCAVITY

To describe the bifurcated branches near the bifurcation points, we use the expansions given by the Crandall–Rabinowitz Theorem:

$$w_k(\sigma) = w_k(0) + \sigma \dot{w}_k(0) + \frac{\sigma^2}{2} \ddot{w}_k(0) + \text{H.O.T.}, \tag{3.1}$$

$$\mu_k(\sigma) = \mu_k(0) + \sigma \dot{\mu}_k(0) + \frac{\sigma^2}{2} \ddot{\mu}_k(0) + \text{H.O.T.}, \tag{3.2}$$

where $\sigma \in (-\delta_k, \delta_k)$. The dot “.” indicates the derivative with respect to σ . To simplify notation we do not mention explicitly the dependence of w on x and y .

The concavity of each branch depends on the first nonvanishing term in the expansion of μ_k .

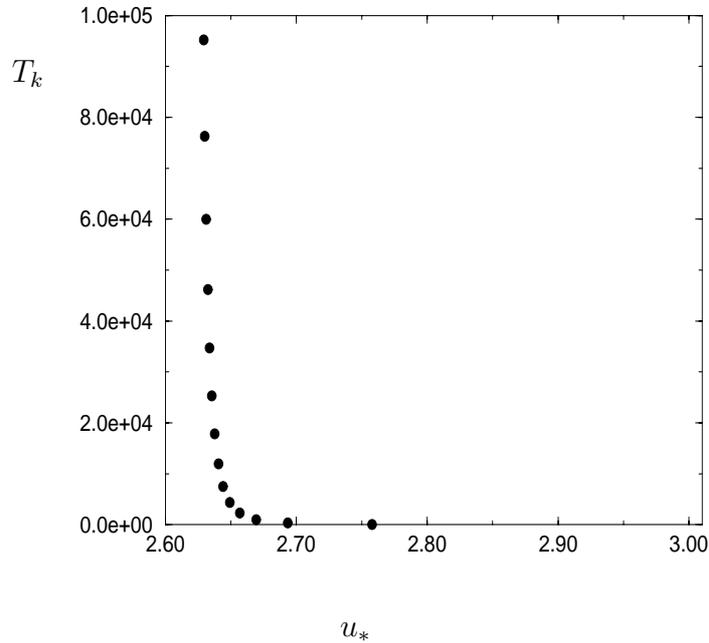


FIGURE 2. Transversality condition: T_k vs. u_*^k , $k = 1, 2, \dots$

Theorem 3.1. For every $k \in \mathbb{N}^*$ we have $\dot{\mu}_k(0) = 0$. For small k , we have

$$\ddot{\mu}_k(0) > 0. \tag{3.3}$$

Remark 3.2. It follows immediately that the bifurcated branches are “parabolic” near u_*^k , and the concavity of the first ones is towards the right hand side, so that they occur for $u_* > u_*^k$.

Proof. Of course to prove Theorem 3.1, we have to differentiate several times with respect to σ the identity (2.14), namely

$$\tilde{F}(w_k(\sigma), \mu_k(\sigma)) = 0, \quad \sigma \in (-\delta_k, \delta_k). \tag{3.4}$$

We warn the reader that several expressions below are triplets: the first component is defined on the domain $\mathbb{R}^* \times [-1, 1]$, the two others are defined on the interface $\{0\} \times [-1, 1]$. This is very natural in view of the structure of the problem involving the operator \mathcal{L} and the boundary operators \mathcal{B} and \mathcal{C} . For simplicity, the index k will be skipped.

Differentiating (3.4) once at $\sigma = 0$ does not provide any further information, since we already know that $w(0) = 0$, $\dot{w}(0) = \Phi_2$, $\mu(0) = 0$. Differentiating it twice, we get at $\sigma = 0$

$$2\tilde{F}_{\mu w}(\mu(0), w(0))\dot{w}(0)\dot{\mu}(0) + \tilde{F}_{ww}(\mu(0), w(0))(\dot{w}(0), \dot{w}(0)) = -\tilde{F}_w(\mu(0), w(0))\ddot{w}(0), \tag{3.5}$$

so the left-hand side of (3.5) is in the range of $\tilde{F}_w(\mu(0), w(0))$. Using its characterization in terms of \mathcal{Q}_2 we get

$$\dot{\mu}(0) = -\frac{\mathcal{Q}_2\left(\tilde{F}_{ww}(0,0) \cdot (\Phi_2, \Phi_2)\right)}{2\mathcal{Q}_2\left(\tilde{F}_{\mu w}(0,0) \cdot \Phi_2\right)}. \tag{3.6}$$

The denominator of the fraction is nothing but $2T_k$ (see (2.15)), and it does not vanish. Moreover,

$$\tilde{F}_{ww}(0,0)(\Phi_2, \Phi_2) = \begin{cases} 2\left(\Phi_2 + [\Phi_2(0,y)]U_0'(x, u_*^k)\right)\left(\partial_x \Phi_2 + [\Phi_2(0,y)]U_0''(x, u_*^k)\right) \\ -2\partial_y[\Phi_2(0,y)]^2(U_0''(x, u_*^k)) - 4\partial_{xy}\Phi_2 \partial_y[\Phi_2(0,y)] \\ -2\Delta[\Phi_2(0,y)]\left([\Phi_2(0,y)]U_0''(x, u_*^k) + \partial_x \phi_2\right) \\ -\frac{U_0'(x, u_*^k)}{2u_\infty} \int_{-1}^1 \partial_y[\Phi_2(0,y)]^2 dy, \quad x \neq 0, y \in [-1, 1], \\ 0, \quad y \in [-1, 1], \\ -\partial_y[\Phi_2(0,y)]^2, \quad y \in [-1, 1]. \end{cases} \tag{3.7}$$

Substituting into (3.6) and computing the integrals in the definition of \mathcal{Q}_2 , we get

$$\dot{\mu}(0) = 0.$$

Differentiating once again (3.4) at $\sigma = 0$ yields

$$\begin{aligned} 3\tilde{F}_{\mu w}(0,0) \cdot \Phi_2 \ddot{\mu}(0) + \tilde{F}_{www}(0,0) \cdot (\Phi_2, \Phi_2, \Phi_2) + 3\tilde{F}_{ww}(0,0) \cdot (\Phi_2, \ddot{w}(0)) \\ = -\tilde{F}_w(0,0) \cdot (\Phi_2, \partial_{\sigma\sigma\sigma} w(0)). \end{aligned} \tag{3.8}$$

Since the left-hand side of (3.8) is in the range of $\tilde{F}_w(0,0)$ we obtain a final formula for $\ddot{\mu}(0)$:

$$\ddot{\mu}(0) = -\frac{\mathcal{Q}_2\left(\tilde{F}_{www}(0,0) \cdot (\Phi_2, \Phi_2, \Phi_2)\right)}{3\mathcal{Q}_2\left(\tilde{F}_{\mu w}(0,0) \cdot \Phi_2\right)} - \frac{\mathcal{Q}_2\left(\tilde{F}_{ww}(0,0) \cdot (\Phi_2, \ddot{w}(0))\right)}{\mathcal{Q}_2\left(\tilde{F}_{\mu w}(0,0) \cdot \Phi_2\right)}. \tag{3.9}$$

The two addenda in the expression for $\ddot{\mu}(0)$ give different difficulties. We will compute the summands numerically which obviously restricts our proof to the small values of k .

(i) As far as the first one is concerned, $\mathcal{Q}_2\left(\tilde{F}_{www}(0,0) \cdot (\Phi_2, \Phi_2, \Phi_2)\right)$ may be expressed as an integral of a known function over \mathbb{R} . After tedious computations,

$$\tilde{F}_{www}(0,0) \cdot (\Phi_2, \Phi_2, \Phi_2) = \begin{cases} 6\partial_y[\Phi_2(0,y)]^2\left([\Phi_2(0,y)]U_0^{(3)} + \partial_{xx}\phi_2\right) \\ -\frac{3}{2u_\infty}([\Phi_2(0,y)]U_0'' + \partial_x \Phi_2) \int_{-1}^1 \partial_y[\Phi_2(0,y)]^2 dy, \\ x \neq 0, y \in [-1, 1], \\ 0, \quad y \in [-1, 1], \\ 0, \quad y \in [-1, 1]. \end{cases} \tag{3.10}$$

Applying \mathcal{Q}_2 to (3.10), we find explicitly that

$$\begin{aligned} \mathcal{Q}_2\left(\tilde{F}_{www}(0,0) \cdot (\Phi_2, \Phi_2, \Phi_2)\right) &= -\frac{3k^2\pi^2}{8u_\infty}(c_0 - p_1 - p_2)^2 \int_{\mathbb{R}} \left(U_0''(c_0 - p_1 - p_2) + \varphi'\right) \varphi^* dx \\ &\quad + \frac{3k^2\pi^2}{8}(c_0 - p_1 - p_2)^2 \int_{\mathbb{R}} \left(U_0^{(3)}(c_0 - p_1 - p_2) + \varphi''\right) \varphi^* dx, \end{aligned} \quad (3.11)$$

which can be computed numerically with high accuracy.

(ii) The second summand is more complicated because $\ddot{w}(0)$ is not explicitly known, and one has to compute it by a suitable numerical method. We first return to formula (3.5) to obtain a system for $\ddot{w}(0)$, namely

$$\tilde{F}_w(\mu(0), w(0))\ddot{w}(0) = -\tilde{F}_{ww}(\mu(0), w(0))(\dot{w}(0), \dot{w}(0)). \quad (3.12)$$

The operator $\tilde{F}_w(\mu(0), w(0))$ is nothing but the triplet $(\mathcal{L}, \mathcal{B}, \mathcal{C})$, therefore (3.12) can be easily solved by a finite-difference scheme. Next, one computes numerically the 3 components of $\tilde{F}_{ww}(0,0)(\Phi_2, \ddot{w}(0))$, by (writing r for $\ddot{w}(0)$):

$$\tilde{F}_{ww}(0,0)(\Phi_2, r) = \begin{cases} 2\partial_y[\Phi_2(0, y)] \partial_y[r(0, y)] (-U_o''(x, u_*^k)) - 2\partial_{xy}\Phi_2 \partial_y[r(0, y)] \\ -2\partial_{xy}r \partial_y[\Phi_2(0, y)] - \Delta r \left([\Phi_2(0, y)]U_o''(x, u_*^k) + \partial_x\phi_2 \right) \\ + \left(\Phi_2 + [\Phi_2(0, y)]U_o'(x, u_*^k) \right) \left(\partial_x r + [r(0, y)]U_o''(x, u_*^k) \right) \\ - \Delta[\Phi_2(0, y)] \left([r(0, y)]U_o''(x, u_*^k) + \partial_x r \right) \\ - \frac{U_o'(x, u_*^k)}{2u_\infty} \int_{-1}^1 \partial_y[\Phi_2(0, y)] \partial_y[r(0, y)] dy \\ + \left(r + [r(0, y)]U_o'(x, u_*^k) \right) \left(\partial_x\Phi_2 + [\Phi_2(0, y)]U_o''(x, u_*^k) \right), \\ \quad x \neq 0, y \in [-1, 1], \\ 0, y \in [-1, 1], \\ -\partial_y[\Phi_2(0, y)] \partial_y[r(0, y)], y \in [-1, 1]. \end{cases}$$

Finally $\mathcal{Q}_2(\tilde{F}_{ww}(0,0)(\Phi_2, \ddot{w}(0)))$ may be approximated by a numerical $2D$ integration. Summing up, we are able to compute numerically $\mu_k(0)$, at least for small values of k , see Figure 3 below. In fact, we find an increasing sequence of values, starting at 5.94 for $k = 1$. □

4. NUMERICAL APPROXIMATION

This section, dedicated to the numerics, is divided into three subsections: the first one deals with the numerical approximation of problem (2.2) for w . In the second one we take the continuation into account, and we introduce a relevant ordering of both unknowns and equations. Finally, numerical results are presented in the third part.

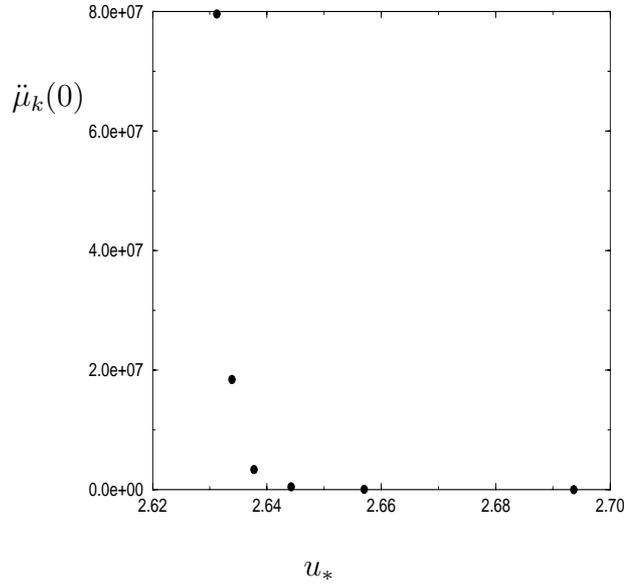


FIGURE 3. Computed values of $\ddot{\mu}_k(0)$ vs. u_*^k , $k = 1, \dots, 6$.

4.1. A numerical scheme for the w -problem

Several difficulties have to be taken into account: although U is continuous at the origin, w is not because of the splitting (2.1), which requires $w(0^+, y)$ and $w(0^-, y)$ to be defined separately. The problem is set on an unbounded domain, and it contains nonlocal terms. The fully nonlinear nature of the problem leads to complex discrete formulae, most of them being skipped hereafter (see [1] for details). A further simplification of (2.2) is that, for large x , the influence of the front is rather weak, therefore derivatives w.r.t. y may be neglected between $\pm\infty$ and $\pm X_{\max}$. The latter can be rigorously established as in [2], where a mollifier is introduced in the splitting defining w . This enables us to derive boundary conditions at an “artificial boundary” $\Gamma_{\pm M}$, see below (4.2).

Let $X_{\max} > 0$. From now on we will work on the bounded domain $[-X_{\max}, X_{\max}] \times [-1, 1]$, on which problem (2.2) reads:

$$\left\{ \begin{array}{l} (c - c_0)(U'_0 + [w]U''_0 + w_x) = \mathcal{L}w + \mathcal{F}(w), \quad -X_{\max} < x < X_{\max}, \quad x \neq 0, \\ Bw(0, y) = 0, \quad y \in [-1, 1], \\ Cw - \mathcal{G}(w)(y) = 0, \quad y \in [-1, 1], \\ \partial_y w(x, \pm 1) = 0, \quad x \neq 0, \\ a_-(w(-X_{\max}, y)) = a_+(w(X_{\max}, y)) = 0, \quad y \in [-1, 1], \\ \partial_y [w(0, \pm 1)] = 0, \end{array} \right. \tag{4.1}$$

together with

$$\begin{cases} \Gamma_{-M} = \{(-X_{\max}, y), y \in [-1, 1]\}, \Gamma_M = \{(X_{\max}, y), y \in [-1, 1]\}, \\ a_-(w) = (c - c_0)U_0 - \partial_x w - \frac{1}{2}w^2 + w(c - U_0) = 0 \text{ on } \Gamma_{-M}, \\ a_+(w) = (c - c_0)(u_\infty - U_0) + \partial_x w - \frac{1}{2}w^2 + w(U_0 - c) = 0 \text{ on } \Gamma_M. \end{cases} \quad (4.2)$$

We introduce some notation. The rectangular domain $R_- = [-X_{\max}, 0] \times [-1, 1]$ is discretized by a regular mesh of $(N_x + 2)(N_y + 2)$ points with step h . A nodal point of R_- is denoted by (x_i, y_j) , $i = 0, \dots, N_x + 1$, $j = 0, \dots, N_y + 1$. The discrete values of w in R_- are denoted by $w_{i,j}^-$. The other rectangular domain $R_+ = [0, X_{\max}] \times [-1, 1]$ is approximated similarly, the values of w being denoted by $w_{i,j}^+$.

At the front, the left values $w(0^-, y_j)$ are approximated by l_j , the right values by r_j , $j = 0, \dots, N_y + 1$. This allows us to express the discrete front as

$$s(y_j) = [w(0, y_j)] = r_j - l_j. \quad (4.3)$$

Via a centered finite-difference approximation, we have at an inner point of R_+ :

$$\begin{aligned} Fw_{i,j}^+ = & -(c - c_0)_h \left(U'_{0i} + (r_j - l_j)U''_{0i} + \frac{1}{2h}(w_{i+1,j}^+ - w_{i-1,j}^+) \right) \\ & + \frac{1}{h^2}(w_{i+1,j}^+ + w_{i-1,j}^+ + w_{i,j-1}^+ + w_{i,j+1}^+ - 4w_{i,j}^+) + \frac{U_{0i} - c_0}{2h}(w_{i+1,j}^+ - w_{i-1,j}^+) \\ & + \frac{\theta(j)}{4h^2} \left(-U''_{0i} + U_{0i}^{(3)}(r_j - l_j) + \frac{1}{h^2}(w_{i+1,j}^+ + w_{i-1,j}^+ - 2w_{i,j}^+) \right) \\ & - \frac{\beta(j)}{4h^3}(w_{i+1,j+1}^+ - w_{i+1,j-1}^+ - w_{i-1,j+1}^+ + w_{i-1,j-1}^+) + U'_{0i}w_{i,j}^+ \\ & - \frac{\gamma(j)}{h^2} \left(U''_{0i}(r_j - l_j) + \frac{1}{2h}(w_{i+1,j}^+ - w_{i-1,j}^+) \right) \\ & + \left(w_{i,j}^+ + (r_j - l_j)U'_{0i} \right) \left(\frac{1}{2h}(w_{i+1,j}^+ - w_{i-1,j}^+) + (r_j - l_j)U''_{0i} \right), \end{aligned} \quad (4.4)$$

where

$$\begin{aligned} \beta(j) &= (r_{j+1} - l_{j+1} - r_{j-1} + l_{j-1}), \quad \theta(j) = \beta(j)^2, \\ \gamma(j) &= (r_{j+1} - l_{j+1} + r_{j-1} - l_{j-1} - 2r_j + 2l_j). \end{aligned}$$

A similar discrete equation is written at an inner point $w_{i,j}^-$ of R_- .

An important term is $(c - c_0)_h$ which approximates (2.13). It depends upon all the discrete unknowns between $x = -2h$ and $x = 2h$. It also involves the approximation of the boundary operators at the interface $\{0\} \times [-1, 1]$. Since $(c - c_0)_h$ appears at any inner point (see (4.4)), the unknowns defining it have clearly a big impact on the final linear system. We call them *global unknowns*, versus the other variables which are called *local unknowns*.

While it is not difficult to approximate the operators \mathcal{B} and \mathcal{G} :

$$(\mathcal{B}w)_j \simeq l_j(U_o^+)'_0 - r_j(U_o^-)'_{N_x+1}, \quad (4.5)$$

$$\mathcal{G}(w)_j \simeq 1 - \left(1 + \frac{\theta(j)}{4h^2} \right)^{-\frac{1}{2}}, \quad (4.6)$$

an additional difficulty arises with the approximation of the linear operator \mathcal{C} . Due to the discontinuity of $\partial_x w(0, y)$, it is impossible to use a centered approximation. To get the same accuracy, we approximate $\partial_x w(0^+, y)$ and $\partial_x w(0^-, y)$ by a non-centered formula with a three points stencil. It yields the discrete formula for the operator \mathcal{C} at a point $(0, y_j), 0 \leq j \leq N_y + 1$, of the interface

$$(\mathcal{C}w)_j \simeq -\frac{3}{2h}(r_j + l_j) + \frac{2}{h}(w_{1,j}^+ + w_{N_x,j}^-) - \frac{1}{2h}(w_{2,j}^+ + w_{N_x-1,j}^-) + (u_* - c_o)(r_j - l_j). \tag{4.7}$$

Thanks to (4.5, 4.6) and (4.7), the discrete formulae at the interface are

$$(\mathcal{B}w)_j = 0, \quad 0 \leq j \leq N_y + 1, \tag{4.8}$$

$$(\mathcal{C}w)_j = \mathcal{G}(w)_j, \quad 0 \leq j \leq N_y + 1. \tag{4.9}$$

Afterwards, we express $(c - c_o)_h$ as

$$(c - c_o)_h = \frac{1}{2u_\infty} \sum_{k=0}^{k=N_y+1} d_k f_k, \tag{4.10}$$

where $d_o = d_{N_y+1} = \frac{h}{3}$, $d_{2i} = \frac{2h}{3}$, $d_{2i+1} = \frac{4h}{3}$, and $f_k = \frac{\theta(k)}{4h^2} \left\{ 1 - (\mathcal{C}w)_k \right\} - 1 + \left(1 + \frac{\theta(k)}{4h^2} \right)^{-\frac{1}{2}}$.

As far as the boundary conditions are concerned, we use the standard technique of fictitious points to take into account Neumann conditions at $y = \pm 1$. On the other hand, introducing the fictitious points $w_{-1,j}^-$ and $w_{N_x+2,j}^+, 1 \leq j \leq N_y + 1$ at the artificial boundary $\Gamma_{\pm M}$, the mixed boundary conditions (4.2) are approximated by:

$$w_{-1,j}^- = w_{1,j}^- + 2h \left(-\frac{(w_{o,j}^-)^2}{2} + (c - c_o)_h U_{oo}^- + w_{o,j}^- ((c - c_o)_h + c_o - U_{oo}^-) \right),$$

$$w_{N_x+2,j}^+ = w_{N_x,j}^+ + 2h \left(\frac{(w_{N_x+1,j}^+)^2}{2} - (c - c_o)_h (u_\infty - U_{o,N_x+1}^+ - w_{N_x+1,j}^+ (U_{o,N_x+1}^+ - (c - c_o)_h - c_o)) \right).$$

Moreover, the fictitious point for the front at $x = 0$ yields $r_1 - l_1 = r_{-1} - l_{-1}$. Note that r_j and l_j are always coupled.

Remark 4.1. For $i = 1$ (resp. for $i = N_x$), the discrete formula (4.4) in R_+ (resp. R_-) involves only global unknowns.

4.2. Continuation method, final system

The final step of the discretization is to introduce the continuation constraint. We recall in a few words the spirit of continuation techniques. Consider, to fix ideas, the nonlinear problem $f(u, \lambda) = 0$. Arc length continuation consists in adding a parameter σ and in coupling the nonlinear equation with a *normal parametrization*

$$\begin{cases} f(u(\sigma), \lambda(\sigma)) = 0, \\ N(u(\sigma), \lambda(\sigma), \sigma) = \|\partial_\sigma u\|^2 + \|\partial_\sigma \lambda\|^2 - 1 = 0. \end{cases} \tag{4.11}$$

We have chosen to track bifurcated branches *via* a discrete continuation. We write the nonlinear system coming from the approximation of (4.4) as

$$F_h(Y, u_*) = 0.$$

Here Y is the set of all the global and local unknowns, and has $N = 2(N_x + 2)(N_y + 2)$ components. F_h is the set of all the discrete nonlinear formulae (4.4), plus the two conditions at the interface (4.8, 4.9).

We emphasize that u_* is now an additional unknown of the problem, therefore we set

$$X = Y \cup \{u_*\}.$$

The discrete continuation equation for the unknown X reads

$$\sum_{i=1}^{N+1} \left(X_i^{n+1} - X_i^n, \frac{X_i^n - X_i^{n-1}}{\Delta\sigma} \right) - \Delta\sigma = 0, \quad (4.12)$$

where n is the index of the continuation method, and $\Delta\sigma$ is the arc length step. Therefore the system becomes

$$J_h(X) = 0 \quad (4.13)$$

where J_h takes into account F_h and the continuation equation (4.12). We solve the nonlinear problem (4.13) by a standard Newton method in \mathbb{R}^{N+1} .

However, the normal parametrization may lead to a full Jacobian matrix. To avoid this inconvenience, we carefully arrange the unknowns and the equations. Another problem arises with the fill-in of the matrix during the resolution of the linear system. To avoid this phenomenon, the idea is to work with sparse matrices having an increasing profile. One can also take advantage of the latter properties to save memory and to reduce CPU time by storing only the upper part of the profile and by using an adequate method of trangularization of the matrix.

Thanks to a convenient ordering, we are able to get a bloc tridiagonal matrix. Let us give some insight: the trick is to number the local unknowns at first. Therefore, the contributions of the global unknowns will appear in the upper triangular part of the matrix throughout the process. In the same spirit, the first line of the Jacobian matrix represents the continuation equation. We then order the equations coming from the discretization of (4.1) at an inner points $w_{i,j}^-$ $0 \leq i \leq N_x - 1$, $0 \leq j \leq N_y + 1$ (see the remark in the previous subsection). Next come the equations written at an inner point $w_{i,j}^+$, $2 \leq i \leq N_x + 1$, $0 \leq j \leq N_y + 1$. Finally, the last lines of the matrix are for the equations with *global unknowns* only. This arrangement of the equations is really the key to get a matrix with increasing profile, see Figure 4.

4.3. Numerical results

The numerical results presented hereafter are obtained with a value of $X_{\max} = 10$. The meshes R_- and R_+ are defined by $N_x = 199$ and $N_y = 39$. Also, the continuation step is $\Delta\sigma = 5 \times 10^{-2}$.

We need to initialize the continuation method. X^0 is 0 except $u_* = u_*^k$. We look for the next iterate X^1 , at σ small, by mean of the Crandall-Rabinowitz expansion (3.1, 3.2), up to the *2nd*-order terms. This has to be matched with the continuation equation (4.12) for $n = 0$, namely,

$$\sum_{i=1}^{N+1} \left(X_i^1 - X_i^0, \dot{X}_i^0 \right) = \Delta\sigma.$$

Knowing both X^0 and X^1 , we can launch the continuation process. In the sequel we present some numerical results obtained *via* the above method. A nice representation of the bifurcated branches is provided by the evolution of the speed increase $c - c_0$ of the non planar travelling waves. A special emphasize will be put on the first branch, see Figures 7 to 9.

From Figure 5, we see that the bifurcated branches are unbounded, with a vertical asymptote. The corresponding computed values of the asymptotes are graphed in the next Figure 6.

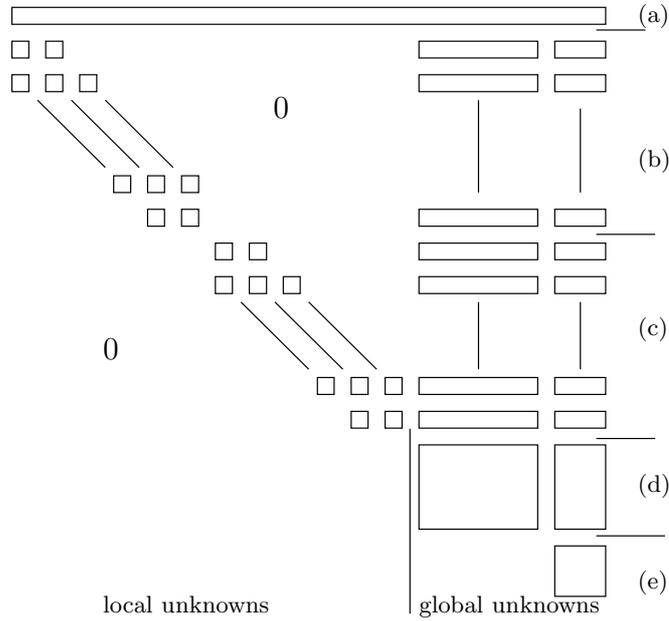


FIGURE 4. Structure of the Jacobian matrix with: (a) continuation equation, (b) equations in R_- , (c) equations in R_+ , (d) equations with global unknowns only and equations for $(C)_j$, (e) equations for $(B)_j$. Note the increasing profile of this sparse matrix.

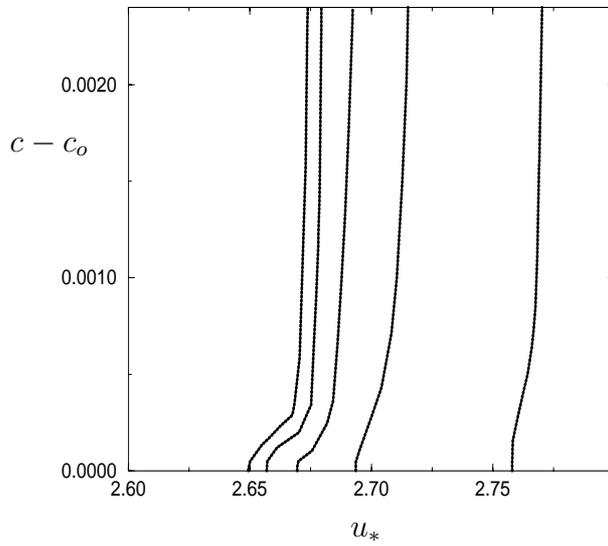


FIGURE 5. Bifurcation diagram for the first $2D$ branches, $k = 1, \dots, 5$.

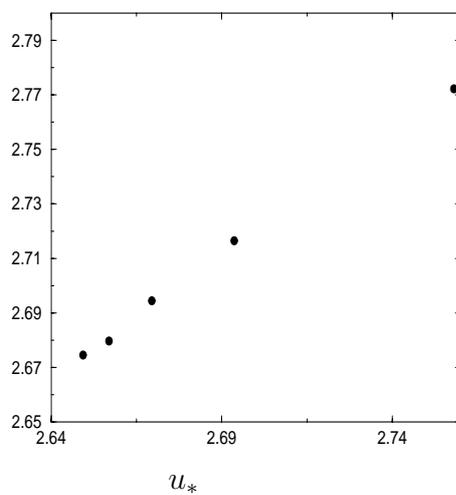


FIGURE 6. Computed values of the vertical asymptote *vs.* u_*^k , $k = 1, \dots, 5$.

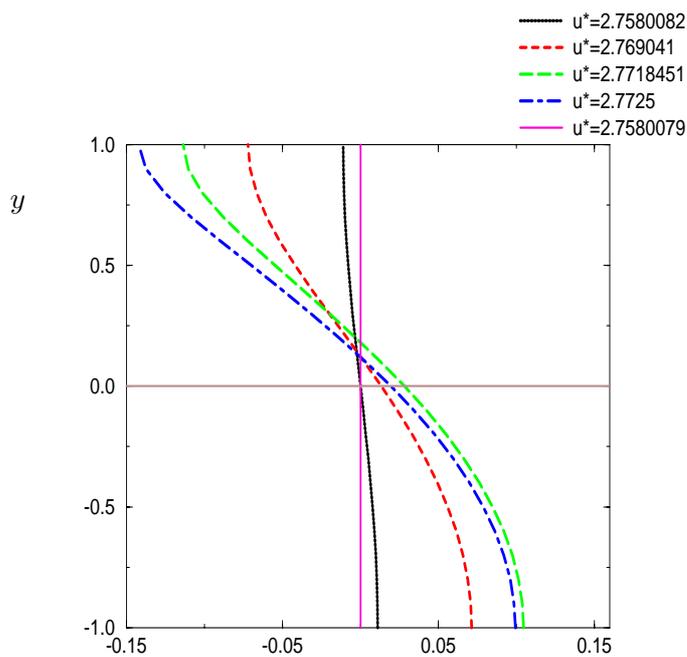
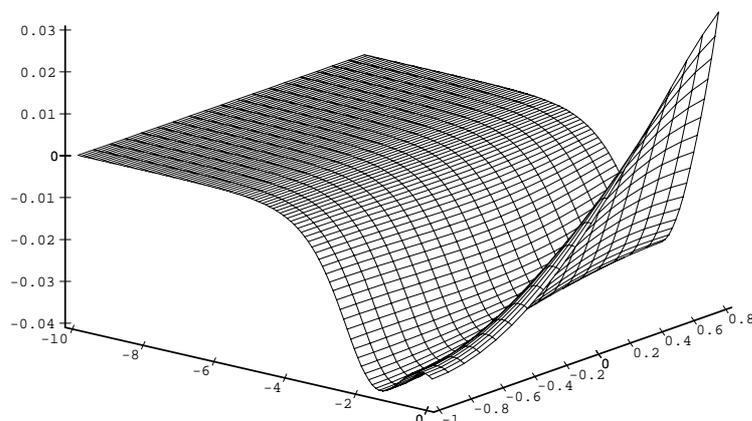
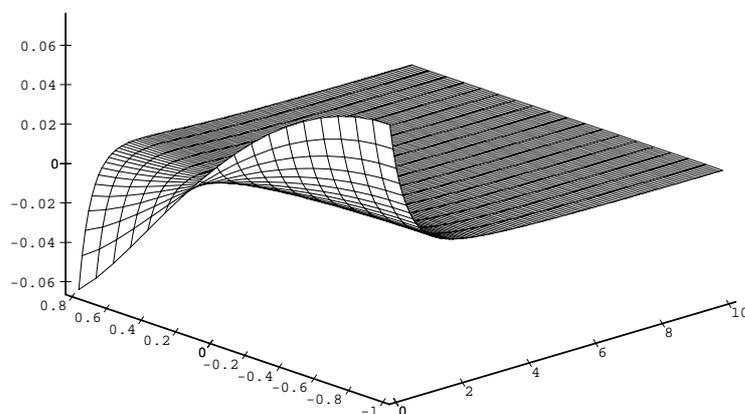


FIGURE 7. Profile of the front $s(y)$ for different values of u_* on the first bifurcated branch. Note the symmetry breaking in the direction $y > 0$.

FIGURE 8. Profile of w for $x < 0$ on the first bifurcated branch.FIGURE 9. Profile of w for $x > 0$ on the first bifurcated branch.

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