

Using MAPLE for the analysis of bifurcation phenomena in gas combustion

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Abstract

We consider a three-dimensional thermal-diffusion model for a premixed burner flame. Many experimental and theoretical works in condensed-phase and gas combustion show that the flame front may propagate in a number of different ways. The structure and stability properties of the front depend essentially on the physical parameters of the model. This article describes the use of the symbolic manipulation language MAPLE for the analysis of bifurcation phenomena in gas combustion. It shows how symbolic manipulation languages can be combined effectively with analysis and numerical computations for this type of investigation.

1. Introduction

In this article, we describe a symbolic manipulation program that implements the bifurcation analysis of a three-dimensional gas combustion problem. The present work is a generalization to three space dimensions of our former work on surface solid combustion [6, 7]. Let us describe briefly the class of model problem in combustion for which our approach is relevant. It can be described formally as follows:

$$\begin{aligned}L_\mu[u] &= 0, & z &\neq \Phi(t, r, \psi), \\ [u]_{z=\Phi(t, r, \psi)} &= f, & & (1) \\ u &\rightarrow u_{l/r}, & \text{when } z &\rightarrow \mp \infty,\end{aligned}$$

where the unknowns are the vectorial function $u(t, z, r, \psi)$ and the free boundary $\Phi(t, r, \psi)$. In this system, t is the time variable, (z, r, ψ) are the cylindrical coordinates, L is a nonlinear time-dependant partial differential operator, μ is a bifurcation parameter and $[]_{z=\Phi(t, r, \psi)}$ denotes the jump of u at $z = \Phi(t, r, \psi)$. We suppose that (1) admits some

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known travelling wave solution $u_0(z - \lambda t)$, of speed λ , and that the so called “basic solution” u_0 loses stability at some critical value μ_0 of μ . Such a model problem occurs in solid combustion, as well as gas combustion; it is also common to other problems as frontal polymerization in chemical reactors, or solidification processes [6, 5, 11, 15]. Typically, the model corresponds to the conservation of the physical quantities. For the example under investigation in this article, Φ is the location of the flame front and u_0 is a steady planar flame front attached to the burner.

The goal of our asymptotic analysis is to investigate the mechanism of instability of such flame front as a function of the many physical parameters involved in the model, (flow rate, radius of the burner, heat loss, Lewis number), and to obtain the type of new solutions that appear when u_0 is no longer stable. Our analysis describes, in particular, the appearance of the so-called polyhedral flame [4, 8, 12–14], and, for example, the phenomenon of burst that has been observed in a similar problem [7]. Direct numerical simulations starting from the asymptotic result are then used to extend our weakly nonlinear investigation to strong nonlinear regime away from the domain of validity of the asymptotic.

Because our computation of possible bifurcation is based on a perturbation analysis for μ close to μ_0 and u close to u_0 in some sense, we make extensive use of asymptotic expansions. The result of the computation is a dynamical system, called “*normal set*”, satisfied by the amplitude of the bifurcated solutions. We know in advance the form of the dynamical system using some symmetry argument [1], but more difficult is the actual computation of its coefficients as a function of the many physical parameters involved in the physical model. Although the steps of the analysis follow a well-determined pattern, their complexity make *a manual treatment utterly impractical*. We refer to the companion paper [9] for the details of the results of our analysis.

This article is focused on the method that we have developed to implement the analysis with a MAPLE code. The plan of the paper is as follows. In Section 2 we present the mathematical model, the basic solution which represents a plane circular front attached to the burner and its linear stability. In Section 3 we present the algorithm for the weakly nonlinear analysis. In Section 4 we describe the salient feature of the implementation of this algorithm. In section 5, we conclude our paper with a few observations about the validation of the MAPLE code and some remarks on the execution in parallel of the code on a network of workstations.

2. Statement of the problem

2.1. Mathematical model

We consider a premixed flame anchored on a flat cylindrical burner of radius a [10, 12]. We scale the Lewis number L and the heat-loss coefficient H as $L = 1 + \beta/M$ and $H = K/M$, where $M \gg 1$ is proportional to the activation energy. In the limit of large activation energy, the reaction zone becomes a thin sheet of flame whose location in

nondimensional coordinates (r', ψ, x_3) is given by $x_3 = \Phi(t, r', \psi)$, where Φ is to be determined. The burner is located at $x_3 = 0$. Introducing a coordinate system (r, ψ, ξ) attached to the flame front where $\xi = x_3 - \Phi(t, r, \psi)$ and $r = r'/a$.

The equations satisfied by the temperature Θ , the concentration S and Φ are

$$\frac{\partial \Theta}{\partial t} + \left(m - \frac{\partial \Phi}{\partial t} \right) \frac{\partial \Theta}{\partial \xi} - \Delta \Theta = 0, \quad \xi \neq 0, \tag{2.1}$$

$$\frac{\partial S}{\partial t} + \left(m - \frac{\partial \Phi}{\partial t} \right) \frac{\partial S}{\partial \xi} - \Delta S - \beta \Delta \Theta = 0, \quad \xi \neq 0, -\Phi, \tag{2.2}$$

with the jump conditions

$$\left[\frac{\partial \Theta}{\partial \xi} \right]_{\xi=0} + \left\{ 1 + \frac{|\nabla \Phi|^2}{a^2} \right\}^{-1/2} \exp \left(\frac{S|_{\xi=0}}{2} \right) = 0, \tag{2.3}$$

$$\left[\frac{\partial S}{\partial \xi} \right]_{\xi=0} + \beta \left[\frac{\partial \Theta}{\partial \xi} \right]_{\xi=0} = 0, \tag{2.4}$$

$$\left[\frac{\partial S}{\partial \xi} \right]_{\xi=-\Phi} - \left\{ 1 + \frac{|\nabla \Phi|^2}{a^2} \right\}^{-1} K \Theta|_{\xi=-\Phi} = 0, \tag{2.5}$$

$$[S]_{\xi=-\Phi} = 0 \tag{2.6}$$

and the boundary conditions

$$\frac{\partial \Theta}{\partial \xi} \rightarrow 0, \quad \frac{\partial S}{\partial \xi} \rightarrow 0 \text{ as } \xi \rightarrow +\infty \quad \text{and} \quad \Theta \rightarrow 0, \quad S \rightarrow 0 \text{ as } \xi \rightarrow -\infty, \tag{2.7}$$

$$\frac{\partial \Theta}{\partial r} - \frac{\partial \Phi}{\partial r} \frac{\partial \Theta}{\partial \xi} = 0 \quad \text{and} \quad \frac{\partial S}{\partial r} - \frac{\partial \Phi}{\partial r} \frac{\partial S}{\partial \xi} = 0 \text{ on } r = 1, \tag{2.8}$$

$$\Theta = 1 \text{ at } \xi = 0 \quad \text{and} \quad \Theta, S \text{ are } 2\pi\text{-periodic in } \psi, \tag{2.9}$$

where δ is the Dirac function, m is the flow rate and Δ is the Laplacian in the moving coordinate system.

2.2. Basic solution and its linear stability

The system of Eqs. (2.1)–(2.9) admits a stationary solution of the form

$$\hat{\Theta}(\xi) = \begin{cases} 1 & \text{if } \xi > 0, \\ e^{m\xi} & \text{if } \xi < 0, \end{cases}$$

$$\hat{S}(\xi) = \begin{cases} B & \text{if } \xi > 0, \\ B - \beta m \xi e^{m\xi} & \text{if } -h < \xi < 0, \quad \hat{\Phi} = h, \\ B e^{m(\xi+h)} - \beta m \xi e^{m\xi} & \text{if } \xi < -h, \end{cases}$$

where $B = 2 \log m$ and $h = \log(-K/(Bm))/m$. This basic solution represents a stationary planar flame located at $x_3 = h$. Let us define the following perturbations of the basic solution:

$$\phi = \Phi - \hat{\Phi}, \quad w = \Theta - \hat{\Theta}(\xi) - \phi \frac{d\hat{\Theta}}{d\xi} \quad \text{and} \quad z = S - \hat{S}(\xi) - \phi \frac{d\hat{S}}{d\xi}. \quad (2.10)$$

From (2.10) we have $\phi = [w]_0/m$ and $[z]_0 + \beta[w]_0 = 0$. Substituting (2.10) into (2.1)–(2.9), we linearize the operator about $\phi = w = z = 0$. The linearized problem has normal mode solutions of the form

$$\begin{pmatrix} w \\ z \end{pmatrix} = R J_n(k_{n,s} r) e^{i\omega t + i n \psi} \begin{pmatrix} W \\ Z \end{pmatrix} + \text{c.c.}, \quad (2.11)$$

where R is a complex constant, J_n is the Bessel function of the first kind of order n , $k_{n,s}$ is the s th root of the equation $J'_n(x) = 0$, and c.c. denotes the complex conjugate of the first term. The functions W and Z are found explicitly. The solution (2.11) is nontrivial if and only if the following dispersion relation is satisfied:

$$2l(l - p)^2 + \beta m(l^2 - k_{n,s}^2/a^2) + Km(l - p)e^{h(l-p)} = 0. \quad (2.12)$$

The basic solution is stable (respectively, unstable) if $\mathcal{R}(\omega) < 0$ ($\mathcal{R}(\omega) > 0$). Eq. (2.12) possesses two stability boundaries on which $\mathcal{R}(\omega) = 0$ (Fig. 1). The cellular boundary is given explicitly by

$$\beta = -2 \frac{\alpha^2}{m^2} + \frac{2K\alpha e^{-h\alpha}}{m(m - \alpha)} \quad \text{where} \quad \alpha^2 = m^2 + 4k_{n,s}^2/a^2. \quad (2.13)$$

3. Nonlinear analysis

We are going to construct formally the algorithm of computation of the normal set.

3.1. Perturbation expansion

In this section, we carry out a nonlinear analysis to determine bifurcations from the basic solution. In some nondegenerate cases, hand computations are sufficient to determine these bifurcations [4]. To capture with our local analysis more interesting physical phenomena and further steps of transition to turbulence, we need to study degenerated cases. A higher-order analysis is necessary and the hand computation is very tedious and practically intractable. For these reasons we have chosen to use a symbolic manipulation language. Let us restrict ourselves to the case where two modes (n_1, s_1) and (n_2, s_2) interact. Thus, we confine our attention to the lower part of the stability diagram, i.e., cellular stability with a Lewis number $L < 1$ (Fig. 1). By choosing the radius a appropriately, we can make any two successive wave numbers, say k_{n_1, s_1} and k_{n_2, s_2} , the first unstable modes so that the corresponding value of β is a double eigenvalue. We study bifurcation in a neighborhood of such a double eigenvalue, so

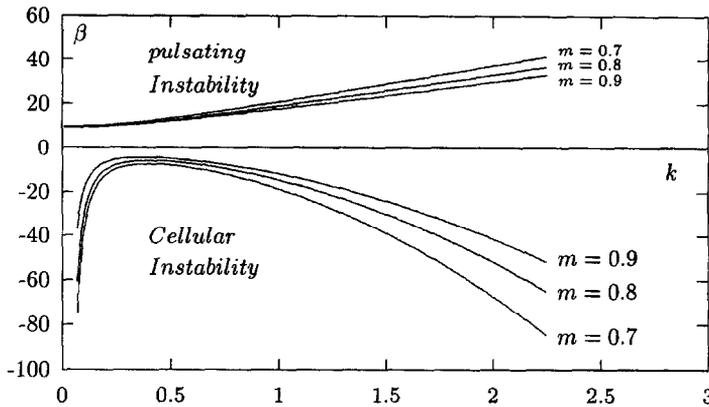


Fig. 1. Neutral stability curve.

we consider two closely spaced eigenvalues which coalesce to a double eigenvalue (β_0, a_0) . We employ a perturbation analysis in a neighborhood of (β_0, a_0) as follows:

$$\beta = \beta_0(1 + \mu_1 \varepsilon + \mu_2 \varepsilon^2 + \dots) \quad \text{and} \quad a = a_0 + \sigma_1 \varepsilon + \sigma_2 \varepsilon^2 + \dots \tag{3.1}$$

The definition of the expansion parameter ε will be given later, the values of β_0 and a_0 , which depend on the parameters m and K as well as on the mode indices, are found numerically. We introduce the slow time-scales $\tau_i = \varepsilon^i t$ for i integer and expand each unknown as follows:

$$\phi = \Phi - h \sim \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \dots, \quad w = \Theta - \hat{\Theta} - \phi d\hat{\Theta}/d\xi \sim \varepsilon w_1 + \varepsilon^2 w_2 + \dots, \tag{3.2}$$

$$z = S - \hat{S} - \phi d\hat{S}_0/d\xi \sim \varepsilon z_1 + \varepsilon^2 z_2 + \dots, \quad \hat{S} \sim \hat{S}_0 + \varepsilon \hat{S}_1 + \varepsilon^2 \hat{S}_2 + \dots \tag{3.3}$$

Upon formal substitution and expansion, we equate coefficients of like powers of ε and obtain a sequence of problems for the recursive determination of w_j, z_j and ϕ_j .

$$m \frac{\partial w_j}{\partial \xi} - \frac{1}{a_0^2} \nabla^2 w_j - \frac{\partial^2 w_j}{\partial \xi^2} = \zeta_{j1}, \quad \xi \neq 0, \tag{3.4}$$

$$m \frac{\partial z_j}{\partial \xi} - \left(\frac{\nabla^2}{a_0^2} + \frac{\partial^2}{\partial \xi^2} \right) (z_j + \beta_0 w_j) = \zeta_{j2}, \quad \xi \neq 0, -h \tag{3.5}$$

with the jump conditions

$$\left[\frac{\partial w_j}{\partial \xi} \right]_0 - m[w_j]_0 + \frac{m}{2} z_j|_{\xi=0^+} = \rho_{j1}, \tag{3.6}$$

$$\left[\frac{\partial z_j}{\partial \xi} \right]_0 + \beta_0 \left[\frac{\partial w_j}{\partial \xi} \right]_0 + \beta_0 m[w_j]_0 = \rho_{j2}, \tag{3.7}$$

$$[z_j]_{-h} = \rho_{j3}, \tag{3.8}$$

$$\left[\frac{\partial z_j}{\partial \xi} \right]_{-h} - Kw_j|_{\xi=-h} = \rho_{j4}; \tag{3.9}$$

and the boundary conditions

$$\frac{\partial w_j}{\partial \xi} \rightarrow 0 \quad \text{and} \quad \frac{\partial z_j}{\partial \xi} \rightarrow 0 \quad \text{as} \quad \xi \rightarrow +\infty, \quad w_j \rightarrow 0 \quad \text{and} \quad z_j \rightarrow 0 \quad \text{as} \quad \xi \rightarrow -\infty, \tag{3.10}$$

$$\frac{\partial w_j}{\partial r} = \frac{\partial z_j}{\partial r} = 0 \quad \text{on} \quad r = 1 \quad \text{and} \quad w_j \quad \text{and} \quad z_j \quad \text{are} \quad 2\pi\text{-periodic} \quad \text{in} \quad \psi. \tag{3.11}$$

The nonhomogeneous terms $\zeta_{j1}, \zeta_{j2}, \rho_{j1}, \rho_{j2}, \rho_{j3}$ and ρ_{j4} for $j \geq 2$ depend on the w_i, z_i and ϕ_i , for $i = 1, 2, \dots, j - 1$. For $j = 1$ these quantities are all zero and (3.4)–(3.11) is a homogeneous linear problem whose general long-time solution is given by

$$\begin{aligned} \begin{pmatrix} w_1 \\ z_1 \\ \phi_1 \end{pmatrix} &= [R_1 e^{in_1 \psi} + \bar{R}_1 e^{-in_1 \psi}] J_{n_1}(k_{n_1, s_1} r) \begin{pmatrix} W_1(\xi) \\ Z_1(\xi) \\ 1/m \end{pmatrix} \\ &+ [R_2 e^{in_2 \psi} + \bar{R}_2 e^{-in_2 \psi}] J_{n_2}(k_{n_2, s_2} r) \begin{pmatrix} W_2(\xi) \\ Z_2(\xi) \\ 1/m \end{pmatrix}. \end{aligned} \tag{3.12}$$

The problems (3.4)–(3.11) with $j \geq 2$ are nonhomogeneous forms of the problem with $j = 1$ and are, in general, not solvable unless solvability conditions are satisfied.

3.2. Solvability conditions

Let us summarize the linear problem (3.4)–(3.11) as

$$L(w_j, z_j) = (\chi_j, \tilde{\chi}_j), \quad j \geq 2. \tag{3.13}$$

We define the inner product $\langle ; ; \rangle$:

$$\langle (f_1, f_2), (g_1, g_2) \rangle = \int_0^{2\pi} \int_0^1 \int_{-\infty}^{+\infty} (f_1 \bar{g}_1 + f_2 \bar{g}_2) r \, dr \, d\xi \, d\psi. \tag{3.14}$$

Let L^* be the adjoint of L with respect to the inner product (3.14). The Eq. (3.13) is solvable iff the vector on the right-hand side is orthogonal to the kernel of L^* , that is,

$$\langle L(w_j, z_j), (w^*, z^*) \rangle = 0, \quad \forall (w^*, z^*) \in \text{Ker}(L^*). \tag{3.15}$$

Thus, the nonhomogeneous problem (3.4)–(3.11) is solvable iff

$$\begin{aligned} \langle (\zeta_{j1}, \zeta_{j2}); (w^*, z^*) \rangle &= \langle (\rho_{j1}, \rho_{j2}); (w^*(0), z^*(0)) \rangle_1 \\ &+ \left\langle (\rho_{j3}, \rho_{j4}); \left(-mz^*(-h) - \frac{\partial z^*}{\partial \xi} \Big|_{\xi=-h^+}, z^*(-h) \right) \right\rangle_1 \\ &\quad \forall (w^*, z^*) \in \text{Ker}(L^*), \end{aligned} \tag{3.16}$$

Table 1
Derivation of the dynamical system

$j = 1.$
 While $R_1(\tau_1, \tau_2)$ and $R_2(\tau_1, \tau_2)$ are unknown, Do
 $j \leftarrow j + 1,$
 solve (3.13) subject to (3.20),
 $L(w_j, z_j) = (\chi_j, \tilde{\chi}_j),$
 $\langle (w_1, z_1), (w_i^*, z_i^*) \rangle = C_i, \quad i = 1, 2.$
 apply (3.15) to (3.17),
 $\langle (\chi_{j+1}, \tilde{\chi}_{j+1}), (w_i^*, z_i^*) \rangle = 0, \quad i = 1, 2.$
 Enddo

where

$$\langle (f_1, f_2), (g_1, g_2) \rangle_1 = \int_0^1 \int_0^{2\pi} (f_1 \bar{g}_1 + f_2 \bar{g}_2) r \, dr \, d\psi.$$

The null space of the adjoint operator is spanned by the functions

$$\begin{pmatrix} w_i^* \\ z_i^* \end{pmatrix} = J_n(k_{n_i, s_i}, r) e^{\pm i n_i \psi} \begin{pmatrix} W_i^* \\ Z_i^* \end{pmatrix} \quad i = 1, 2, \tag{3.17}$$

where W_i^* and Z_i^* are found explicitly.

3.3. Normalization

At this point, we define the expansion parameter ε by the relation

$$\langle (w, z), (w_i^*, z_i^*) \rangle = C_i \varepsilon, \quad i = 1, 2. \tag{3.18}$$

The relation (3.18) imply simultaneously that

$$\langle (w_1, z_1), (w_i^*, z_i^*) \rangle = C_i, \quad i = 1, 2, \tag{3.19}$$

$$\langle (w_j, z_j), (w_i^*, z_i^*) \rangle = 0, \quad i = 1, 2, \quad j \geq 2. \tag{3.20}$$

The solution of (3.13) is thus uniquely determined. We conclude that the construction of the formal asymptotic expansion follows from the algorithm summarized in Table 1.

4. Toward automation

4.1. The dynamical system

The computation of the coefficients w_j and z_j in the expansions (3.2) and (3.3) proceeds sequentially. First, one applies the solvability conditions (3.16) for $j = 2$, which gives a system of equations for the evolution of the amplitudes R_1 and R_2 on the τ_1 -scale. Then one solves (3.13) for $j = 2$ subject to the condition (3.20). At the

next step, one applies the solvability conditions (3.16) for $j = 3$ to obtain a system of equations for the evolution of R_1 and R_2 on the τ_2 -scale. One continues this procedure until a closed problem for w_1 and z_1 is obtained. The procedure is summarized in Table 1. If the index of the last relevant term in the expansion (3.2) and (3.3) is m , one obtains a system of differential equations for the evolution of the amplitudes R_1 and R_2 on the τ_m -scale of the form

$$\begin{aligned} \partial R_1 / \partial \tau_m &= D_1(R_1, R_2), \\ \partial R_2 / \partial \tau_m &= D_2(R_1, R_2), \end{aligned} \tag{4.1}$$

where D_1 and D_2 are polynomials of degree $m + 1$ in R_1 and R_2 .

4.2. Reduction to ordinary differential equations

To actually carry out the computation outlined in the previous section it is necessary to first reduce the linear system of PDEs (3.13) to a system of ordinary differential equations involving only the variables ξ . For this purpose we analyze the structure of the functions w_j , z_j and ϕ_j in some detail. In this section we examine the case $n_2 = 2n_1$. We begin by introducing the abbreviation

$$F = e^{in_1 \psi}. \tag{4.2}$$

The functions w_1 and z_1 are polynomials in F and its inverse:

$$w_1 = w_1^1 F + w_1^{-1} F^{-1} + w_1^2 F^2 + w_1^{-2} F^{-2}, \tag{4.3}$$

$$z_1 = z_1^1 F + z_1^{-1} F^{-1} + z_1^2 F^2 + z_1^{-2} F^{-2}. \tag{4.4}$$

The coefficients w_1^q and z_1^q are functions of r, ξ and the slow time variables. Since the vectors χ_2 and $\tilde{\chi}_2$ on the right-hand side of (3.13) depend quadratically on w_1 and z_1 , χ_2 and $\tilde{\chi}_2$ are polynomials of degree four in F and its inverse. Next, when we solve the boundary value problem (3.13) for $j = 2$, we find that w_2 and z_2 and, consequently, the vectors χ_3 and $\tilde{\chi}_3$ are polynomials of degree eight in F and its inverse. In general, we have

$$\begin{aligned} \zeta_{j_1} &= \sum_{q=-n(j)}^{n(j)} f_{j,q}(r) \mathcal{F}_{j,q}(\xi) \mathcal{A}_{j,q}(R_1, R_2) F^q \quad \text{and} \\ \zeta_{j_2} &= \sum_{q=-n(j)}^{n(j)} g_{j,q}(r) \mathcal{G}_{j,q}(\xi) \mathcal{B}_{j,q}(R_1, R_2) F^q, \end{aligned} \tag{4.5}$$

where $n(j) = 2^{(j-1)}$, $\mathcal{A}_{j,q}(R_1, R_2)$ and $\mathcal{B}_{j,q}(R_1, R_2)$ are linear differential operators in R_1 and R_2 on the τ_k -time-scale, $k \leq j - 1$, and $f_{j,q}(r)$ and $g_{j,q}(r)$ are summations of products of Bessel functions. To find a particular solution of the problem (3.13), one must develop each product of Bessel functions appearing in $f_{j,q}(r)$ and $g_{j,q}(r)$ in Dini series as

$$f_{j,q}(r) = \sum_{s \geq 1} a_{q,s}^j J_q(k_{q,s} r) \quad \text{and} \quad g_{j,q}(r) = \sum_{s \geq 1} b_{q,s}^j J_q(k_{q,s} r), \tag{4.6}$$

where $a_{q,s}^j$ and $b_{q,s}^j$ are known real constants. Thus, we can write

$$w_j = w_j^{(h)} + w_j^{(p)} \quad \text{and} \quad z_j = z_j^{(h)} + z_j^{(p)}, \tag{4.7}$$

where $w_j^{(h)}$ and $z_j^{(h)}$ (resp^t $w_j^{(p)}$ and $z_j^{(p)}$) are the complementary (resp^t particular) solutions of the problem (3.13). We choose

$$w_j^{(p)} = \sum_{q=-n(j)}^{n(j)} \left\{ \sum_{s=1}^{\infty} a_{q,s}^j J_q(k_{q,s}r) W_{q,s}^j \right\} F^q \quad \text{and}$$

$$z_j^{(p)} = \sum_{q=-n(j)}^{n(j)} \left\{ \sum_{s=1}^{\infty} c_{q,s}^j J_q(k_{q,s}r) Z_{q,s}^j \right\} F^q, \tag{4.8}$$

where $W_{q,s}^j(\xi)$ and $Z_{q,s}^j(\xi)$ are the solutions of the system of ordinary differential equations

$$-\frac{d^2 W_{q,s}^j(\xi)}{d\xi^2} + m \frac{dW_{q,s}^j(\xi)}{d\xi} + \frac{k_{q,s}^2}{a_0^2} W_{q,s}^j = \mathcal{F}_{j,q}(\xi), \quad \xi \neq 0, \tag{4.9}$$

$$-\frac{d^2 Z_{q,s}^j(\xi)}{d\xi^2} + m \frac{dZ_{q,s}^j(\xi)}{d\xi} + \frac{k_{q,s}^2}{a_0^2} Z_{q,s}^j = \tilde{\mathcal{G}}_{j,q}(\xi), \quad \xi \neq -h, 0 \tag{4.10}$$

subject to the jump conditions

$$[Z_{q,s}^j(\xi)]_0 + \beta_0 [W_{q,s}^j(\xi)]_0 = 0, \tag{4.11}$$

$$\left[\frac{W_{q,s}^j(\xi)}{d\xi} \right]_0 - m [W_{q,s}^j(\xi)]_0 + \frac{m}{2} Z_{q,s}^j(\xi)|_{\xi=0^+} = \rho_{j1}^q, \tag{4.12}$$

$$\left[\frac{Z_{q,s}^j(\xi)}{d\xi} \right]_0 + \beta_0 m [W_{q,s}^j(\xi)]_0 + \beta_0 \left[\frac{W_{q,s}^j(\xi)}{d\xi} \right]_0 = \rho_{j2}^q, \tag{4.13}$$

$$\left[\frac{Z_{q,s}^j(\xi)}{d\xi} \right]_{-h} = \rho_{j3}^q, \tag{4.14}$$

$$\left[\frac{Z_{q,s}^j(\xi)}{d\xi} \right]_{-h} - K W_{q,s}^j(\xi)|_{\xi=-h} = \rho_{j4}^q, \tag{4.15}$$

and the boundary conditions

$$\frac{dW_{q,s}^j(\xi)}{d\xi} \rightarrow 0, \quad \frac{dZ_{q,s}^j(\xi)}{d\xi} \rightarrow 0 \quad \text{as } \xi \rightarrow +\infty, \tag{4.16}$$

$$W_{q,s}^j(\xi) \rightarrow 0, \quad Z_{q,s}^j(\xi) \rightarrow 0 \quad \text{as } \xi \rightarrow -\infty, \tag{4.17}$$

where ρ_{ji}^q is the coefficient of F^q in ρ_{ji} , $i = 1, 2, 3, 4$, i.e.,

$$\rho_{ji} = \sum_{q=-n(j)}^{n(j)} \rho_{ji}^q F^q, \tag{4.18}$$

and

$$\zeta_{j2} + \beta_0 \left(\frac{1}{a_0^2} \nabla^2 w_j + \frac{\partial^2 w_j}{\partial \xi^2} \right) = \sum_{q=-n(j)}^{n(j)} \left\{ \sum_{s=1}^{\infty} c_{q,s}^j J_q(k_{q,s} r) \tilde{\mathcal{G}}_{j,q}(\xi) \right\} F^q. \tag{4.19}$$

The general solution of (4.9)–(4.10) is

$$W_{q,s}^j(\xi) = \begin{cases} (W_{q,s}^j(\xi))_{\text{part}}^- + a^-(\tau_1, \tau_2, \dots)(W_{q,s}^j(\xi))_{\text{hom}}^- & \text{if } \xi < 0, \\ (W_{q,s}^j(\xi))_{\text{part}}^+ + a^+(\tau_1, \tau_2, \dots)(W_{q,s}^j(\xi))_{\text{hom}}^+ & \text{if } \xi > 0, \end{cases} \tag{4.20}$$

$$Z_{q,s}^j(\xi) = \begin{cases} (Z_{q,s}^j(\xi))_{\text{part}}^- + b^-(\tau_1, \tau_2, \dots)(Z_{q,s}^j(\xi))_{\text{hom}}^-, & \xi < -h, \\ (W_{q,s}^j(\xi))_{\text{part}}^+ + b^{-+}(\tau_1, \tau_2, \dots)(Z_{q,s}^j(\xi))_{\text{hom}}^{-+}, & -h < \xi < 0, \\ (Z_{q,s}^j(\xi))_{\text{part}}^+ + b^+(\tau_1, \tau_2, \dots)(Z_{q,s}^j(\xi))_{\text{hom}}^+, & \xi > 0, \end{cases} \tag{4.21}$$

where hom (*resp.* part) for the homogeneous (*resp.* particular) solution. The unknown coefficients a^- , a^+ , b^- , b^{-+} and b^+ are determined by the jump conditions (4.11)–(4.15), which yield a five-by-five system of linear algebraic equations,

$$Mx = b. \tag{4.22}$$

M is a matrix whose coefficients depend on τ_1 and τ_2 , x is the vector such that $x^t = (a^-, a^+, b^-, b^{-+}, b^+)$, and b is the vector with $b^t = (0, \rho_{j1}^q, \rho_{j2}^q, \rho_{j3}^q, \rho_{j4}^q)$, where x^t and b^t denote the transposed vectors to x and b , respectively. The linear system is singular when $(n_1 \times q, s) = (n_1, s_1)$ or $(n_1 \times q, s) = (n_2, s_2)$, i.e., when $(q, s) = (i, s_i)$, $i = 1, 2$, because $n_2 = 2n_1$. However, if the solvability condition is satisfied, the system has infinitely many solutions. The expression for the solvability condition, using the polynomial structure of the expansions, can be written as follows:

$$\begin{aligned} & \int_0^1 \int_{-\infty}^{+\infty} (\zeta_{j1}^q w^* + \zeta_{j2}^q z^*) r \, dr \, d\xi \\ &= \int_0^1 (\rho_{j1}^q w^* |_{\xi=0^-} + \rho_{j2}^q z^* |_{\xi=0^+}) r \, dr \\ &+ \int_0^1 \left\{ \rho_{j3}^q \left(-mz^* - \frac{\partial z^*}{\partial \xi} \right) |_{\xi=-h} + \rho_{j4}^q z^* |_{\xi=-h} \right\} r \, dr, \end{aligned} \tag{4.23}$$

where ζ_{ji}^q is the coefficient of F^q in ζ_{ji} , $i = 1, 2, 3, 4$, and w^* and z^* will be chosen as in (3.17). In the case where the system (4.22) is singular, i.e., $(q, s) = (i, s_i)$ for $i = 1, 2$, the free constant is determined by the polynomial form of the normalization condition (3.20)

$$\int_0^1 \int_{-\infty}^{+\infty} J_i(k_{i,s_i} r) (W_{i,s_i}^j w_i^* + Z_{i,s_i}^j z_i^*) r \, dr \, d\xi = 0, \quad i = 1, 2, \quad j \geq 2. \tag{4.24}$$

Thus, we have reduced the solution of the boundary value problem (3.13) to the integration of a sequence of ordinary differential system (4.9)–(4.10), the resolution of

Table 2
Construction of w_j and z_j for j given

```

For  $q$  from 0 to  $n(j)$  do
  for  $s$  from 1 to  $+\infty$  do
    solve the ordinary differential system (4.9)–(4.10),
    solve the five-by-five linear algebraic system (4.22),
  enddo
enddo
for  $(q, s) \in \{(1, s_1), (2, s_2)\}$  do
  solve the three quadratures (4.23) and (4.24).
enddo

```

a five-by-five linear algebraic system (4.22), and the three quadratures (4.23) and (4.24). We recall that, once w_j is known, ϕ_j follows from the identity $\phi_j = [w_j]_0/m$.

Table 2 summarizes the construction of each (w_j, z_j) in the asymptotic expansions (3.2) and (3.3).

4.3. Structure of the computation

The computation presented in the previous sections can be implemented in a number of different ways. The choice is first of all dictated by the requirement that the computation time and memory allocation be minimized. Another constraint is imposed by the fact that one does not know a priori the order to which the expansion (3.2) and (3.3) needs to be carried out, or which are the relevant time scales in the analysis.

To select the relevant scales in the asymptotic analysis, to determine the impact of particular scaling choices, to understand the data dependency and eliminate redundant variables, and to determine the order of approximation necessary to obtain a closed problem for w_1 and z_1 , it generally suffices to know only the algebraic structure of the solvability condition that yields the dynamical system for the amplitudes R_1 and R_2 . This structure can be determined by a preliminary computation of the inhomogeneous terms χ_j and $\tilde{\chi}_j$ in (3.13). The computation can be done entirely symbolically, using only the polynomial capabilities of MAPLE. This task is performed by the so-called program MAINalg.

Once the algebraic structure of the inhomogeneous terms is known and each product of Bessel functions appearing in it is developed in Dini series, the remaining task consists of the integration of the system of ordinary differential Eqs. (4.9)–(4.10). The relevant program DYNcomp yields the dynamical system (4.1). Let us proceed with a brief description of the MAPLE code.

MAINalg. The program *MAINalg* enables us to explore the algebraic structure of the inhomogeneous terms in the differential Eq. (3.13). It uses only the polynomial capabilities of MAPLE.

Since MAPLE recognizes only strings of alphanumeric characters and we preferred to keep the notation in the program as close as possible to the mathematical notation,

we adopted the convention to spell the Greek letters throughout, following the \LaTeX -convention (*Theta* for Θ , etc.), to simply attach sub- and superscripts to the names of variables (*phi1* for ϕ_1 , etc.), and use a shorthand notation for derivatives if they are not evaluated explicitly (*w1psiz* for $\partial^2 w_1 / \partial \psi \partial z$, etc.). However, in the following discussion we will maintain the mathematical notation for convenience.

MAINalg takes the nonlinear equations satisfied by the quantities Θ , S and Φ and computes the right-hand sides ζ_{j1} , ζ_{j2} , ρ_{j1} , ρ_{j2} , ρ_{j3} and ρ_{j4} in (3.4)–(3.9) in the form (4.5) and (4.18). It consists of three procedures.

- *MainA* computes the polynomials ζ_{j1} , ζ_{j2} , ρ_{j1} , ρ_{j2} , ρ_{j3} and ρ_{j4} as functions of w_i , z_i and ϕ_i , and their derivatives for $i=1, 2, \dots, j-1$ as follows: One substitutes the expansions (3.2)–(3.3) of Θ , S and Φ and their formal derivatives into the Eqs. (2.1) and (2.2), expands everything in powers of ε , and identifies the coefficients of like powers of ε .
- *MainB* generates the expansions of w_j , z_j and ϕ_j in terms of F . One computes the actual expressions for the derivatives of w_j , z_j and ϕ_j with respect to r and ψ , but not those with respect to ξ and τ_1, τ_2, \dots , which are introduced by name according to the shorthand notation described above.
- *MainC* yields the coefficients in the expansions (4.5) and (4.18). They are found upon substitution of the polynomial expressions for w_j , z_j and ϕ_j and their derivatives in the expressions for ζ_{j1} , ζ_{j2} , ρ_{j1} , ρ_{j2} , ρ_{j3} and ρ_{j4} obtained by *MainA*.

The end products of *MAINalg* are polynomial functions which depend only on the spatial variables r and ξ and the slow time variables τ_1, τ_2, \dots . These polynomials are the input for *DYNcomp* which computes the coefficients of the dynamical system.

We notice that the process of formal differentiation, where we simply add a suffix to the name of the differentiated variable, may create a large number of variables. However, it makes the results of *MAINalg* easy to read. This is an important advantage, because each element of the vectors χ_j and $\tilde{\chi}_j$ in (3.13) may have around thousand of terms once j is three or more.

DYNcomp. The program *DYNcomp* generates the dynamical system (4.1). *DYNcomp* uses as input the data produced by *MAINalg*. It consists of two procedures.

- *INHOMcomp* computes w_j and z_j from (3.13), subject to the constraint (3.20). To find a particular solution of the problem (3.13), one must extract and develop each product of Bessel functions appearing in ζ_{j1} and ζ_{j2} in Dini series as (4.6). The algorithm proceeds from the computation of the homogeneous solutions $(W_{q,s}^j(\xi))_{\text{hom}}^{\pm}$ and a particular solution $(W_{q,s}^j(\xi))_{\text{part}}^{\pm}$ of (4.9) to the computation of the homogeneous solutions $(Z_{q,s}^j(\xi))_{\text{hom}}^{\pm}$, $(Z_{q,s}^j(\xi))_{\text{hom}}^{-+}$ and a particular solution $(Z_{q,s}^j(\xi))_{\text{part}}^{\pm}$, $(Z_{q,s}^j(\xi))_{\text{part}}^{-+}$ of (4.10). Next, it computes the constants a^{\pm} , b^{\pm} and b^{-+} either by solving the five-by-five system of linear algebraic equations (4.22) directly (if it is nonsingular) or by solving the system subject to the orthogonality condition (4.24) (if the system is singular). Thus, we obtain the coefficients $W_{q,s}^j$ and $Z_{q,s}^j$ for each value of j ($j=1, \dots, m$). We then combine these coefficients in the sums (4.8) to obtain $w_j^{(p)}$ and $z_j^{(p)}$, and, consequently, w_j and z_j .

We remark that we do not use the ODE solver of MAPLE to obtain the particular solutions of (4.9) and (4.10). As we deal with very simple ODEs, the computation is much faster with a procedure specifically designed for this particular problem.

- *SOLVcomp* handles the computations involved in the solvability condition. It evaluates the integral identities (4.23), solves the equations obtained, and gives the explicit formulae for the dynamical system.

5. Implementation

We wish to comment first on the computational cost and memory requirement of our symbolic computation. In the first loop of Table 2, we restrict q from 0 to $n(j)$ rather than $-n(j)$ to $n(j)$, because the solution at the term q is the conjugate of the corresponding solution of the term $-q$. The second loop is executed until numerical convergence of the values of the coefficients in the dynamical system (4.1) is attained. In practice, s from 1 to 5 gives satisfactory results.

We recall that, for each order in the Dini series, each pair (w_j, z_j) requires the solution of 2^j differential equations, 2^{j-1} five-by-five linear algebraic systems, and 6 quadratures. The first-order computation is straightforward and can be done easily on a workstation. We found that the second-order computation was intractable on a workstation, because the memory requirement is very high. We have therefore done the computations with specific numerical values of the parameters m and K and for a given interaction (n_1, s_1) and (n_2, s_2) , combining symbolic manipulation and evaluation of the coefficients in the Dini series to reduce the memory requirement. However, the tables and arrays generated by MAPLE are still of the order of 100 MB.

We observe that the computation of the ordinary differential equations is inherently parallel. By splitting the computation on a network of workstations, we roughly divide the size of the tables and arrays by the number of workstations, thus reducing disc access, and obtain superlinear speedup.

The most costly part of the computation is the symbolic integration of left-hand side of (4.23). When $q=2$ ($q=4$) the integration is a sum of approximately 1200 terms (1600 terms). This integration was done on a network of 7 workstations (DN 3500) and required about 10 h. The right-hand side of (4.23) can be computed in about 3 h on a single HP 400 workstation. The overall code takes about 16 h to compute the numerical values of the coefficients in the dynamical system (4.1) for a given set of parameters m and K and a given interaction (n_1, s_1) , (n_2, s_2) .

The validation of the MAPLE code is nontrivial. We have made extensive use of the redundancy between (4.24) and the solvability condition for the linear algebraic system (4.22). The validation of the numerical part of the code was done by comparing the results using different numbers of digits in the computations.

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