Using MAPLE for the analysis of bifurcation phenomena in gas combustion

A. El Hamidi\textsuperscript{a,\ast}, M. Garbey\textsuperscript{b}

\textsuperscript{a}Département de Mathématiques, Université de La Rochelle, Avenue Marillac, F-17042 La Rochelle Cedex, France
\textsuperscript{b}CDCSP et Laboratoire d'Analyse Numérique, Université Claude Bernard Lyon I, 43 Bd 11 Novembre 1918, F-69622 Villeurbanne Cedex, France

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{align}
L_\mu[u] &= 0, \quad z \neq \Phi(t, r, \psi), \\
[u]_{z=\Phi(t, r, \psi)} &= f, \\
\lim_{z \to \mp \infty} u &= u_t/r, \quad \text{when} \quad z \to \pm \infty,
\end{align}

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, \((z, r, \psi)\) are the cylindrical coordinates, \(L\) is a nonlinear time-dependant partial differential operator, \(\mu\) is a bifurcation parameter and \([\cdot]_{z=\Phi(t, r, \psi)}\) denotes the jump of \(u\) at \(z = \Phi(t, r, \psi)\). We suppose that (1) admits some
known travelling wave solution $u_0(z - \lambda t)$, of speed $\lambda$, and that the so called "basic solution" $u_0$ loses stability at some critical value $\mu_0$ of $\mu$. 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, $\Phi$ 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 unstability 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 $\mu$ close to $\mu_0$ 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 \((r', \psi, x_3)\) is given by \(x_3 = \Phi(t, r', \psi)\), where \(\Phi\) is to be determined. The burner is located at \(x_3 = 0\). Introducing a coordinate system \((r, \psi, \xi)\) attached to the flame front where \(\xi = x_3 - \Phi(t, r, \psi)\) and \(r = r'/a\).

The equations satisfied by the temperature \(\Theta\), the concentration \(S\) and \(\Phi\) are

\[
\begin{align*}
\frac{\partial \Theta}{\partial t} + \left( m - \frac{\partial \Phi}{\partial t} \right) \frac{\partial \Theta}{\partial \xi} - \Delta \Theta &= 0, \quad \xi \neq 0, \\
\frac{\partial S}{\partial t} + \left( m - \frac{\partial \Phi}{\partial t} \right) \frac{\partial S}{\partial \xi} - \Delta S - \beta \Delta \Theta &= 0, \quad \xi \neq 0, -\Phi,
\end{align*}
\]  

(2.1) (2.2)

with the jump conditions

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

(2.3)

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

(2.4)

\[
\left[ \frac{\partial S}{\partial \xi} \right]_{\xi=-\Phi} - \left\{ 1 + \frac{|
abla \Phi|^2}{a^2} \right\}^{-1} \kappa \Theta|_{\xi=-\Phi} = 0,
\]

(2.5)

\([S]_{\xi=-\Phi} = 0\)

(2.6)

and the boundary conditions

\[
\frac{\partial \Theta}{\partial \xi} \to 0, \quad \frac{\partial S}{\partial \xi} \to 0 \text{ as } \xi \to +\infty \quad \text{and} \quad \Theta \to 0, \quad S \to 0 \text{ as } \xi \to -\infty,
\]

(2.7)

\[
\frac{\partial \Theta}{\partial r} - \frac{\partial \Phi}{\partial r} \frac{\partial \Theta}{\partial \xi} = 0 \quad \text{and} \quad \frac{\partial S}{\partial r} - \frac{\partial \Phi}{\partial r} \frac{\partial S}{\partial \xi} = 0 \text{ on } r = 1,
\]

(2.8)

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

(2.9)

where \(\delta\) is the Dirac function, \(m\) is the flow rate and \(\Delta\) 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

\[
\begin{align*}
\hat{\Theta}(\xi) &= \begin{cases} 
1 & \text{if } \xi > 0, \\
\mathrm{e}^{m\xi} & \text{if } \xi < 0,
\end{cases} \\
\hat{S}(\xi) &= \begin{cases} 
B & \text{if } \xi > 0, \\
B - \beta \mathrm{e}^{m\xi} & \text{if } -h < \xi < 0, \quad \hat{\Phi} = h, \\
B \mathrm{e}^{m(\xi+h)} - \beta m \xi \mathrm{e}^{m\xi} & \text{if } \xi < -h,
\end{cases}
\end{align*}
\]
where \( B = 2 \log m \) and \( h = \log \left( -K/(Bm) \right)/m \). This basic solution represents a stationary planar flame located at \( x_3 = h \). Let us define the following perturbations of the basic solution:

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

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

\[
\begin{pmatrix}
[2.11] \frac{w}{z}
\end{pmatrix} = RJ_n(k_{n,s}r)e^{i\xi + i\mu}(W/Z) + c.c.,
\]

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:

\[
2l(1 - p)^2 + \beta m(l^2 - k_{n,s}^2/a^2) + Km(l - p)e^{i(l - p)} = 0. \tag{2.12}
\]

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

\[
\beta = -2\alpha^2/m^2 + \frac{2Kx\hbar}{m(m - \alpha)} \quad \text{where} \quad \alpha^2 = m^2 + 4k_{n,s}^2/a^2. \tag{2.13}
\]

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 \( \beta \) is a double eigenvalue. We study bifurcation in a neighborhood of such a double eigenvalue, so
we consider two closely spaced eigenvalues which coalesce to a double eigenvalue \((\beta_0, a_0)\). We employ a perturbation analysis in a neighborhood of \((\beta_0, a_0)\) as follows:

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

The definition of the expansion parameter \(\varepsilon\) will be given later, the values of \(\beta_0\) 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:

\[
\phi = \Phi - \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \cdots, \quad w = \Theta - \varepsilon \Theta + \varepsilon^2 \Theta + \cdots, \tag{3.2}
\]

\[
z = S - \varepsilon \tilde{S} + \varepsilon \tilde{S}_0 + \varepsilon^2 \tilde{S}_1 + \varepsilon^3 \tilde{S}_2 + \cdots. \tag{3.3}
\]

Upon formal substitution and expansion, we equate coefficients of like powers of \(\varepsilon\) and obtain a sequence of problems for the recursive determination of \(w_j, z_j\) and \(\phi_j\).

\[
m \frac{\partial w_j}{\partial \xi} - \frac{1}{a_0^2} \nabla^2 w_j - \frac{\partial^2 w_j}{\partial \xi^2} = \zeta_j, \quad \xi \neq 0, \tag{3.4}
\]

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

with the jump conditions

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

\[
\left[ \frac{\partial z_j}{\partial \xi} \right]_0 + \beta_0 \left[ \frac{\partial w_j}{\partial \xi} \right]_0 + \beta_0 m[w_j]_0 = \rho_{j2}, \tag{3.7}
\]
and the boundary conditions
\[
\frac{\partial w_j}{\partial \zeta} \to 0 \quad \text{and} \quad \frac{\partial z_j}{\partial \zeta} \to 0 \quad \text{as} \quad \zeta \to +\infty, \quad w_j \to 0 \quad \text{and} \quad z_j \to 0 \quad \text{as} \quad \zeta \to -\infty,
\]
(3.10)
\[
\frac{\partial w_j}{\partial r} = \frac{\partial z_j}{\partial r} = 0 \quad \text{on} \quad r = 1 \quad \text{and} \quad w_j \text{ and } z_j \text{ are } 2\pi\text{-periodic in } \psi.
\]
(3.11)

The nonhomogeneous terms \(\zeta_j, \zeta_j, \rho_j, \rho_2, \rho_3, \text{ and } \rho_4\) for \(j \geq 2\) depend on the \(w_i, z_i\) and \(\phi_i\), for \(i = 1, 2, \ldots, j - 1\). 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
\[
\begin{pmatrix}
&w_1 \\
z_1 \\
\phi_1
\end{pmatrix}
= \left[ R_1 e^{\text{i}\psi} + \bar{R}_1 e^{-\text{i}\psi} \right] J_n(k_{n_1}, r)
\begin{pmatrix}
W_1(\zeta) \\
Z_1(\zeta)
\end{pmatrix}
+ \left[ R_2 e^{\text{i}\psi} + \bar{R}_2 e^{-\text{i}\psi} \right] J_n(k_{n_2}, r)
\begin{pmatrix}
W_2(\zeta) \\
Z_2(\zeta)
\end{pmatrix}
\]
(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
\[
L(w_j, z_j) = (\chi_j, \tilde{\chi}_j), \quad j \geq 2.
\]
(3.13)

We define the inner product \(\langle ; \rangle\):
\[
\langle (f_1, f_2), (g_1, g_2) \rangle = \int_0^{2\pi} \int_0^1 \int_{-\infty}^{+\infty} (f_1 \tilde{g}_1 + f_2 \tilde{g}_2) r \, dr \, d\zeta \, d\psi.
\]
(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,
\[
\langle L(w_j, z_j), (w^*, z^*) \rangle = 0, \quad \forall (w^*, z^*) \in \text{Ker}(L^*).
\]
(3.15)

Thus, the nonhomogeneous problem (3.4)–(3.11) is solvable iff
\[
\langle (\zeta_{j1}, \zeta_{j2}), (w^*, z^*) \rangle = \langle (\rho_1, \rho_2); (w^*(0), z^*(0)) \rangle + \left( \langle \rho_3, \rho_4; \left( -mz^*(-h) - \frac{\partial z^*}{\partial \zeta} \bigg|_{\zeta = -h^+}, z^*(-h) \right) \rangle \right)
\]
\[
\forall (w^*, z^*) \in \text{Ker}(L^*),
\]
(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

\[ j \rightarrow j + 1, \]

solve (3.13) subject to (3.20),

\[ L(w_j, z_j) = (\tilde{Z}_j, \tilde{Z}_j), \]

\[ ((w_1, z_1), (w_i^*, z_i^*)) = C_i, \quad i = 1, 2. \]

apply (3.15) to (3.17),

\[ ((x_{j+1}, \tilde{z}_{j+1}), (w_i^*, z_i^*)) = 0, \quad i = 1, 2. \]

Enddo

where

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

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

\[ \left( \begin{array}{c} w_i^* \\ z_i^* \end{array} \right) = J_{n_i}(k n_i, r) e^{\pm in_i \psi} \left( \begin{array}{c} W_i^* \\ Z_i^* \end{array} \right), \quad i = 1, 2, \quad (3.17) \]

where \( W_i^* \) and \( Z_i^* \) are found explicitly.

3.3. Normalization

At this point, we define the expansion parameter \( \varepsilon \) by the relation

\[ \langle (w, z), (w_i^*, z_i^*) \rangle = C_i \varepsilon, \quad i = 1, 2. \quad (3.18) \]

The relation (3.18) imply simultaneously that

\[ \langle (w_1, z_1), (w_i^*, z_i^*) \rangle = C_i, \quad i = 1, 2, \quad (3.19) \]

\[ \langle (w_j, z_j), (w_i^*, z_i^*) \rangle = 0, \quad i = 1, 2, \quad j \geq 2. \quad (3.20) \]

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 \( \tau_1 \)-scale. Then one solves (3.13) for \( j = 2 \) subject to the condition (3.20). At the
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 \( \tau_z \)-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 \( \tau_m \)-scale of the form

\[
\frac{\partial R_1}{\partial \tau_m} = D_1(R_1, R_2),
\]

\[
\frac{\partial R_2}{\partial \tau_m} = D_2(R_1, R_2),
\]

(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 \( \xi \). For this purpose we analyze the structure of the functions \( w_j \), \( z_j \) and \( \phi_j \) in some detail. In this section we examine the case \( n_2 = 2n_1 \). We begin by introducing the abbreviation

\[ F = e^{	ext{i} n_1 \psi}. \]  

(4.2)

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

\[ w_1 = w_1^F F + w_1^{-1} F^{-1} + w_1^2 F^2 + w_1^{-2} F^{-2}, \]

\[ z_1 = z_1^F F + z_1^{-1} F^{-1} + z_1^2 F^2 + z_1^{-2} F^{-2}. \]

(4.3)

(4.4)

The coefficients \( w_1^q \) and \( z_1^q \) are functions of \( r, \xi \) and the slow time variables. Since the vectors \( \chi_2 \) and \( \tilde{\chi}_2 \) on the right-hand side of (3.13) depend quadratically on \( w_1 \) and \( z_1 \), \( \chi_2 \) 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 \( \chi_3 \) and \( \tilde{\chi}_3 \) are polynomials of degree eight in \( F \) and its inverse. In general, we have

\[ \zeta_{j_1} = \sum_{q=-n(j)}^{n(j)} f_{j_1, j}(r) \mathcal{F}_{j_1, j}(\xi) \mathcal{A}_{j_1, q}(R_1, R_2) F^q \]

and

\[ \zeta_{j_2} = \sum_{q=-n(j)}^{n(j)} g_{j_2, j}(r) \mathcal{G}_{j_2, j}(\xi) \mathcal{B}_{j_2, q}(R_1, R_2) F^q, \]

(4.5)

where \( n(j) = 2^{(j-1)} \), \( \mathcal{A}_{j_1, q}(R_1, R_2) \) and \( \mathcal{B}_{j_2, q}(R_1, R_2) \) are linear differential operators in \( R_1 \) and \( R_2 \) on the \( \tau_k \)-time-scale, \( k \leq j - 1 \), and \( f_{j_1, q}(r) \) and \( g_{j_2, q}(r) \) 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 \( f_{j_1, q}(r) \) and \( g_{j_2, q}(r) \) in Dini series as

\[ f_{j_1, q}(r) = \sum_{s \geq 1} a_{q, s}^j J_q(k_{q, s} r) \]

and

\[ g_{j_2, q}(r) = \sum_{s \geq 1} b_{q, s}^j J_q(k_{q, s} r), \]

(4.6)
where \(a^j_{q,s}\) and \(b^j_{q,s}\) are known real constants. Thus, we can write
\[
\omega_j = \omega_j^{(h)} + \omega_j^{(p)} \quad \text{and} \quad \omega_j = \omega_j^{(h)} + \omega_j^{(p)},
\]
where \(\omega_j^{(h)}\) and \(\omega_j^{(p)}\) (resp. \(\omega_j^{(l)}\) and \(\omega_j^{(p)}\)) are the complementary (resp. particular) solutions of the problem (3.13). We choose
\[
\omega_j^{(p)} = \sum_{q=-m(j)}^{m(j)} \left\{ \sum_{s=1}^{\infty} a^j_{q,s} J_q(k_q,s r) W^j_{q,s} \right\} F^q
\]
and
\[
\omega_j^{(p)} = \sum_{q=-m(j)}^{m(j)} \left\{ \sum_{s=1}^{\infty} b^j_{q,s} J_q(k_q,s r) Z^j_{q,s} \right\} F^q,
\]
where \(W^j_{q,s}(\xi)\) and \(Z^j_{q,s}(\xi)\) are the solutions of the system of ordinary differential equations
\[
-\frac{d^2 W^j_{q,s}(\xi)}{d \xi^2} + m \frac{d W^j_{q,s}(\xi)}{d \xi} + \frac{k^2_{q,s}}{a_0^2} W^j_{q,s} = \mathcal{F}_{j,q}(\xi), \quad \xi \neq 0,
\]
\[
-\frac{d^2 Z^j_{q,s}(\xi)}{d \xi^2} + m \frac{d Z^j_{q,s}(\xi)}{d \xi} + \frac{k^2_{q,s}}{a_0^2} Z^j_{q,s} = \hat{\mathcal{F}}_{j,q}(\xi), \quad \xi \neq -h, 0
\]
subject to the jump conditions
\[
\left[ W^j_{q,s}(\xi) \right]_0^{\xi_0} = 0, \quad \left[ Z^j_{q,s}(\xi) \right]_0^{\xi_0} = 0,
\]
\[
\left[ \frac{d W^j_{q,s}(\xi)}{d \xi} \right]_0^{\xi_0} = m \left[ W^j_{q,s}(\xi) \right]_0^{\xi_0} = \rho^q_{j1},
\]
\[
\left[ \frac{d Z^j_{q,s}(\xi)}{d \xi} \right]_0^{\xi_0} = \rho^q_{j2},
\]
\[
\left[ \frac{d Z^j_{q,s}(\xi)}{d \xi} \right]_{-h} = \rho^q_{j3},
\]
\[
\left[ \frac{d Z^j_{q,s}(\xi)}{d \xi} \right]_{-h} = K W^j_{q,s}(\xi) |_{\xi=-h} = \rho^q_{j4},
\]
and the boundary conditions
\[
\frac{d W^j_{q,s}(\xi)}{d \xi} \to 0, \quad \frac{d Z^j_{q,s}(\xi)}{d \xi} \to 0 \quad \text{as} \quad \xi \to +\infty,
\]
\[
W^j_{q,s}(\xi) \to 0, \quad Z^j_{q,s}(\xi) \to 0 \quad \text{as} \quad \xi \to -\infty.
\]
where \(\rho^q_{ji}\) is the coefficient of \(F^q\) in \(\rho_{ji}\), \(i=1,2,3,4\), i.e.,
\[
\rho_{ji} = \sum_{q=-m(j)}^{m(j)} \rho^q_{ji} F^q,
\]
The general solution of (4.9)–(4.10) is

\[
W_{q,s}^{j}(\xi) = \begin{cases} 
(W_{q,s}^{j}(\xi))^{\text{hom}}_{\text{part}} + a^{-}((T_{1},T_{2},\ldots))(W_{q,s}^{j}(\xi))^{+}_{\text{hom}} & \text{if } \xi < 0, \\
(W_{q,s}^{j}(\xi))^{\text{part}} + a^{+}((T_{1},T_{2},\ldots)) & \text{if } \xi > 0,
\end{cases}
\]

(4.20)

\[
Z_{q,s}^{j}(\xi) = \begin{cases} 
(Z_{q,s}^{j}(\xi))^{\text{hom}}^{\text{part}} + b^{-}((T_{1},T_{2},\ldots))(Z_{q,s}^{j}(\xi))^{+}_{\text{hom}} & \xi < -h, \\
(W_{q,s}^{j}(\xi))^{\text{part}} + b^{+}((T_{1},T_{2},\ldots)) & -h < \xi < 0,
\end{cases}
\]

(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,

\[
Mx = b.
\]

(4.22)

\(M\) is a matrix whose coefficients depend on \(T_{1}\) and \(T_{2}, x\) is the vector such that \(x^{t} = (a^{-}, a^{+}, b^{-}, b^{+})\), and \(b\) is the vector with \(b^{t} = (0, \rho_{j}^{q}, \rho_{j}^{q}, \rho_{j}^{q}, \rho_{q}^{q})\), 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:

\[
\int_{0}^{1} \int_{-\infty}^{+\infty} \left( \zeta_{j2}^{q} w_{*} + \zeta_{j2}^{q} z_{*} \right) r \, dr \, d\xi
= \int_{0}^{1} \left( \rho_{j1}^{q} w_{*} |_{\xi = 0^{-}} + \rho_{j2}^{q} z_{*} |_{\xi = 0^{+}} \right) r \, dr
+ \int_{0}^{1} \left\{ \rho_{j3}^{q} \left( -mz_{*} - \frac{\partial z_{*}}{\partial \xi} \right) |_{\xi = -h} + \rho_{q4}^{q} z_{*} |_{\xi = -h} \right\} r \, dr,
\]

(4.23)

where \(\zeta_{j}^{q}\) is the coefficient of \(F_{q}\) in \(\zeta_{j}\), \(i = 1,2,3,4\), 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)

\[
\int_{0}^{1} \int_{-\infty}^{+\infty} J_{i}(k_{i},s_{i}) r(W_{i,s}^{j} w_{*}^{i} + Z_{i,s}^{j} z_{*}^{i}) r \, dr \, d\xi = 0, \quad i = 1,2, \quad j \geq 2.
\]

(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

\[
\begin{align*}
&\text{For } q \text{ from } 0 \text{ to } n(j) \text{ do} \\
&\quad \text{for } s \text{ from } 1 \text{ to } +\infty \text{ do} \\
&\quad\quad \text{solve the ordinary differential system (4.9)--(4.10),} \\
&\quad\quad \text{solve the five-by-five linear algebraic system (4.22),} \\
&\quad\quad \text{enddo} \\
&\quad \text{enddo} \\
&\text{for } (q,s) \in \{(1,s_1),(2,s_2)\} \text{ do} \\
&\quad \text{solve the three quadratures (4.23) and (4.24).} \\
&\quad \text{enddo}
\end{align*}
\]

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, \(\phi_j\) 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 \(\chi_j\) 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 \texttt{\LaTeX}-convention (\textit{Theta} for $\Theta$, etc.), to simply attach sub- and superscripts to the names of variables ($\phi_1$ for $\phi_1$, etc.), and use a shorthand notation for derivatives if they are not evaluated explicitly ($\partial \psi / \partial z$, etc.). However, in the following discussion we will maintain the mathematical notation for convenience.

\textit{MAINalg} takes the nonlinear equations satisfied by the quantities $\Theta$, $S$ and $\Phi$ and computes the right-hand sides $\zeta_1$, $\zeta_2$, $\rho_1$, $\rho_2$, $\rho_3$ and $\rho_4$ in (3.4)–(3.9) in the form (4.5) and (4.18). It consists of three procedures.

- \textit{MainA} computes the polynomials $\zeta_1$, $\zeta_2$, $\rho_1$, $\rho_2$, $\rho_3$ and $\rho_4$ as functions of $w_i$, $z_i$ and $\phi_i$, and their derivatives for $i = 1, 2, \ldots, j - 1$ as follows: One substitutes the expansions (3.2)–(3.3) of $\Theta$, $S$ and $\Phi$ and their formal derivatives into the Eqs. (2.1) and (2.2), expands everything in powers of $\varepsilon$, and identifies the coefficients of like powers of $\varepsilon$.

- \textit{MainB} generates the expansions of $w_j$, $z_j$ and $\phi_j$ in terms of $F$. One computes the actual expressions for the derivatives of $w_j$, $z_j$ and $\phi_j$ with respect to $r$ and $\psi$, but not those with respect to $\xi$ and $\tau_1$, $\tau_2$, $\ldots$, which are introduced by name according to the shorthand notation described above.

- \textit{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 $\phi_j$ and their derivatives in the expressions for $\zeta_1$, $\zeta_2$, $\rho_1$, $\rho_2$, $\rho_3$ and $\rho_4$ obtained by \textit{MainA}.

The end products of \textit{MAINalg} are polynomial functions which depend only on the spatial variables $r$ and $\xi$ and the slow time variables $\tau_1$, $\tau_2$, $\ldots$. These polynomials are the input for \textit{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 \textit{MAINalg} easy to read. This is an important advantage, because each element of the vectors $\chi_j$ and $\tilde{\chi}_j$ in (3.13) may have around thousand of terms once $j$ is three or more.

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

- \textit{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 $\zeta_{j1}$ and $\zeta_{j2}$ in Dini series as (4.6).

The algorithm proceeds from the computation of the homogeneous solutions $(W_{q,s}(\xi))_{\text{hom}}^\pm$ and a particular solution $(W_{q,s}(\xi))_{\text{part}}^\pm$ of (4.9) to the computation of the homogeneous solutions $(Z_{q,s}(\xi))_{\text{hom}}^\pm$, $(Z_{q,s}(\xi))_{\text{hom}}^{++}$ and a particular solution $(Z_{q,s}(\xi))_{\text{part}}^\pm$, $(Z_{q,s}(\xi))_{\text{part}}^{++}$ 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 $j$ ($j = 1, \ldots, m$). 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.
References


