A SYSTEMATIC FORMULATION OF MULTIPHYSICS SYSTEMS AND ITS APPLICATIONS TO BOUNDARY LAYERS AND SHOCK PROFILES

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There are two approaches to multiscale modeling: information passing and concurrent, and the latter one is further divided into overlapping and non-overlapping. This paper presents a general and systematic method for treating concurrent non-overlapping approaches to multiscale modeling that can be applied whenever both the coarse and fine resolutions belong to the realm of continuum mechanics. These results are derived from an axiomatic formulation of the mathematical models of continuum mechanics previously introduced by the author. Applications of such a method to local events yield a bi-physical approach to them, which in turn permits deriving a new procedure for treating boundary-layers and shock profiles associated with singular perturbations of partial differential equations. Some advantages of the new procedure over standard methods are indicated in the paper.

KEY WORDS: *multiscale modeling, concurrent approaches, multiphysics, boundary layers, asymptotic expansions*

1. INTRODUCTION

Scientific behavior-prediction of nature and other systems of human interest is carried out by means of physicomathematical and computational models. In the case of macroscopical physical systems of engineering and science, up to now, such models have been based on continuum mechanics, which adopts a macroscopical point of view to treat physical systems. However, as Paul Dirac recognized when quantum mechanics was born (Dirac, 1929), The Schroedinger equation is the ultimate basis of scientific prediction of nature-behavior and, therefore, continuum mechanics is only an approximation in which the quantic response of the ultra-microscopic constituents of matter is incorporated in the models by means of empirical constitutive equations. Although thus far this approach has been very successful, unsurmountable barriers have been found for extending it to many other, more complex systems and at present intensive international scientific research is being carried out on *multiscale-modeling* (Fish, 2013; Galvanetto and Aliabadi, 2009; Weinan, 2011), whose purpose is to establish procedures capable of incorporating the microscopic information into the macroscopic models in a more effective manner than the *constitutive-equations approach*. Multiscale modeling represents a fundamental change in the manner of making science, whose effectiveness recently received a recognition of first order; namely, the Nobel Chemistry Prize 2013 (Karplus, 2014).

In his 2013 Nobel Lecture (Karplus, 2014), Martin Karplus, referring to Paul Dirac's 1929 statement (Dirac, 1929): The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations that are much too complicated to be soluble, pointed out that a less familiar part of Dirac's remark states that It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much

computation. And this latter statement is what he considers the *leitmotif* of the work that led him to obtain the 2013 Nobel Prize in Chemistry.

Therefore, we may say that Karplus' *laureate* work was in response to Dirac's 1929 invitation to search for simplifying quantum mechanical approaches and furthermore, paraphrasing him, we can also say that such a Dirac's invitation is the *leitmotif* of much of the multiscale-modeling research effort that is being carried out. This assertion is more transparent when multiscale models are set in a hierarchical order, starting with *quantum mechanics* (The Schroedinger equation) at the bottom and finishing with *continuum mechanics* at the top; albeit, it should be noticed that at the continuum mechanics level itself there is also a hierarchy of models.

In spite of the significant progress already achieved in multiscale modeling, many questions are still opened and this paper is intended as a contribution to that international scientific-research effort. According to Fish (2013), there are two categories of multiscale approaches: information-passing (or hierarchical), and concurrent. In Fish's terms: *In the information-passing multiscale approach, the fine-scale response is idealized (approximated or unresolved) and its overall (average) response is infused into the coarse scale. In the concurrent approaches, fine and coarse-scale resolutions are simultaneously employed in different portions of the problem domain, and the exchange of information occurs through the interface. The subdomains where different scale resolutions are employed can be either disjoint or overlapping. In this paper a general class of concurrent non-overlapping approaches is addressed, such that both the fine and coarse-scale resolutions belong to the realm of continuum mechanics. For concurrent multiscale approaches of that class, an axiomatic formulation is developed that reduces their treatment to <i>initial-boundary value problems with prescribed jumps (bvpj)* of the type discussed by the author in Herrera (2007), which are explicitly given (i.e., the basic system of *differential equations* and *jump conditions*) by the general axiomatic mathematical-model previously introduced (Herrera and Pinder, 2012).

Axiomatic formulations are very effective for achieving three fundamental paradigms of mathematical thinking: generality, clarity, and simplicity (Herrera and Pinder, 2012). Generality yields an enormous economy of effort in the study and discussion of many subjects; in research, it is invaluable because models possessing it anticipate results for many unforeseen situations. Clarity yields certainty of knowledge. As for simplicity: simplifying ideas permit transforming complicated systems and phenomena into simple ones, which in turn upgrades efficiency and the level of complexity of systems amenable to treatment. Of course, the beneficial and powerful properties of axiomatic approaches are not exhausted by the brief enumeration made above; the interested reader is referred to Herrera and Pinder (2012) for a more extended discussion of that topic.

It is well known that the groundwork for establishing axiomatic approaches to continuum mechanics was done in the second half of the 20th Century by a group of scholars and researchers, some of whose most conspicuous leaders were C. Truesdell and W. Noll (Truesdell and Noll, 1965; Truesdell and Toupin, 1960). The author had the privilege of participating in some of such developments; see Coleman et al. (1965). A fundamental stone of the theory of mathematical models of continuous systems are the balance conditions for *extensive properties*; or, equivalently, for *intensive properties* (Herrera and Pinder, 2012). For the axiomatic formulation referred to above, such balance conditions—constituted by *differential equations* and *jump conditions*—appeared in a general and rigorous form in Allen et al. (1988). Based on such results I. Herrera developed a very general mathematical model for continuous systems that has been applied as an effective tool in research (Herrera, 1996; Herrera and Camacho, 1997; Herrera and Herrera, 2011) and teaching (Herrera and Pinder, 2012).

The general axiomatic model provides a systematic yet simple procedure for constructing the mathematical model (i.e., the basic system of *differential equations* and *jump conditions*) of any macroscopic continuous system. This paper constitutes a further application of it, besides those already mentioned. Indeed, the results here presented stem from the application of such an axiomatic mathematical model for continuous systems to *concurrent approaches* with disjoint subdomains, and it always yields *initial-boundary value problems with prescribed jumps (bvpj)* of the type discussed by the author in Herrera (2007).

After having developed the theory in the first part of the paper, in its second part the axiomatic formulation is applied to treat *boundary and internal layers*, obtaining in this manner a new method for treating them. Specifically, the examples treated of *boundary layers* refer to some that occur in advection-dominated transport and also some that occur in incompressible-slightly viscous fluids, while those of *internal layers* correspond to shock profiles.

2. THE GENERAL MATHEMATICAL MODEL OF MACROSCOPIC SYSTEMS

When models are built with the purpose of mimicking specific physical systems, probably due to this fact, the distinction between physical reality and such models is frequently blurred. However, in many instances it is healthier to clearly distinguish between the physical objects and the mathematical models. This is what is done in this section, using for this purpose the *axiomatic approach* referred to in the Introduction.

An essential assumption (or, axiom) of this *axiomatic approach* is that each physical system is characterized by a finite set of *extensive properties* (whose cardinality will be represented by **N**); or, equivalently, a finite set of *intensive properties*, because with every *extensive property* there is associated uniquely an *intensive property*. Furthermore, a fundamental stone of mathematical models of continuous systems are the *balance conditions*, which have to be satisfied by every *extensive property* of that set, or its corresponding *intensive property*. Then the governing equations of each physical system is a set of **N** pairs, each one constituted by a *differential equation* and a *jump equation*, which are the expressions in terms of the *intensive properties* of such balances.

Therefore, the basic mathematical model is given by the following system of differential equations:

$$\frac{\partial \Psi^{\alpha}}{\partial t} + \nabla \cdot (\Psi^{\alpha} \underline{v}^{\alpha}) = g^{\alpha} + \nabla \cdot \underline{\tau}^{\alpha}, \quad \alpha = 1, \dots, N$$
(2.1)

together with the system of *jump conditions*:

$$\left[\left[\Psi^{\alpha}(\underline{v}^{\alpha}-\underline{v}_{\Sigma})-\underline{\tau}^{\alpha}\right]\right]\cdot\underline{\mathbf{n}}=0; \quad \alpha=1,\ldots,N; \quad \text{on} \quad \Sigma(t)$$
(2.2)

Here, the square bracket stands for the jump of the function inside it [the reader is referred to Herrera and Pinder (2012) for additional notation]. The problem consists of finding a finite sequence of functions $\{\Psi^1, \ldots, \Psi^N\}$ and a surface $\Sigma(t)$, for each t, which satisfy Eqs. (2.1) and (2.2) together with suitable boundary conditions. In what follows, we will use the notation

$$\underline{\Psi} \equiv (\Psi^1, \dots, \Psi^N) \tag{2.3}$$

Above,

$$\underline{v}^{\alpha} \equiv \underline{v}^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi}), \quad g^{\alpha} \equiv g^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi}) \quad \text{and} \quad \underline{\tau}^{\alpha} \equiv \underline{\tau}^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi})$$
(2.4)

are given functions; such relations frequently are referred to as *constitutive equations*. As for \underline{v}_{Σ} , it is the velocity of the surface $\Sigma(t)$, which is defined on $\Sigma(t)$, exclusively. In general, this system of equations when complemented with suitable boundary and, possibly, initial conditions yields a well-posed *bvpj* of the kind discussed in Herrera (2007).

The following nomenclature will be used: \underline{v}^{α} is the *phase velocity*, g^{α} is the *external supply*, and $\underline{\tau}^{\alpha}$ is the *flux* (Herrera and Pinder, 2012). When a system of partial differential equations can be written in the form of Eq. (2.1), for some $\underline{v}^{\alpha} \equiv \underline{v}^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi})$, $g^{\alpha} \equiv g^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi})$ and $\underline{\tau}^{\alpha} \equiv \underline{\tau}^{\alpha}(\underline{x}, t, \underline{\Psi}, \nabla \underline{\Psi})$ we refer to Eq. (2.1) as the "canonical form" of such a system and Eq. (2.2) are the concomitant jump conditions. In the following developments, it is assumed that the canonical differential equations together with the concomitant jump conditions, when subjected to suitable boundary conditions yield a well-posed boundary-value problem with prescribed jumps (bvpj); see Herrera (2007).

Remark: Here we have assumed that for each \underline{x} and t, \underline{v}^{α} , g^{α} , and $\underline{\tau}^{\alpha}$ are functions of $\underline{\Psi}$ and $\nabla \underline{\Psi}$ only. Such an assumption may be changed and more general models can be obtained by doing so.

In relation with these latter conditions, the *concomitant jump conditions*, some facts that are relevant for the discussions of the following sections should be made. Firstly, when the functions \underline{v}^{α} , g^{α} , and $\underline{\tau}^{\alpha}$ together with their derivatives occurring in Eq. (2.2) are continuous, the *concomitant jump conditions* are satisfied at any surface $\Sigma(t)$ whenever the functions $\{\Psi^1, \ldots, \Psi^N\}$ together with their derivatives occurring in Eq. (2.2) are continuous. Thus, when the functions \underline{v}^{α} , g^{α} , and $\underline{\tau}^{\alpha}$ are sufficiently regular in a domain, one only has to apply the system of differential equations of Eq. (2.1) when looking for solutions in a space of functions whose members are sufficiently regular. When the functions \underline{v}^{α} , g^{α} and $\underline{\tau}^{\alpha}$ have jump discontinuities on a surface $\Sigma(t)$ and the set of functions $\{\Psi^1, \ldots, \Psi^N\}$ satisfies the *concomitant jump conditions*, then at least one of the functions of such a set has non-vanishing jumps at $\Sigma(t)$.

Remark: In previous work, unified formulations of EOR (enhaced oil recovery) models have been introduced (Herrera and Herrera, 2011) and a general class of shocks (shocks with double discontinuities) that occur in petroleum reservoirs was discovered (Herrera, 1996; Herrera and Camacho, 1997). To treat such shocks it was necessary to introduce a more general form of jump conditions, in which the right-hand side of Eq. (2.2) is different than zero. However, Eq. (2.2) as it stands here is sufficiently general for the purposes of this paper.

3. AXIOMATIC FORMULATION OF MULTIPHYSICAL MACROSCOPIC MODELS

Consider a multiphysical macroscopic system such that its physical characteristics (or, properties) are piecewisedefined; i.e., the domain occupied by the physical system is decomposed into a finite set of subdomains and the system physical properties are defined separately at each one of such subdomains. Generally, for such a system the physical properties change abruptly from one to another subdomain and the *intensive properties* associated with the system are discontinuous across the boundaries that separate the subdomains from each other. When the physics at each one of the subdomains belongs to the realm of continuum mechanics, the general axiomatic mathematical model for continuous systems of Section 2 is applicable. In particular, its mathematical model is constituted by the system of *partial differential equations* of Eq. (2.1), to be satisfied at each subdomain, and the *jump conditions* of Eq. (2.2) to be fulfilled at the common boundaries that separate the subdomains from each other. Generally, Σ in Eq. (2.2) is the union of the common boundaries.

3.1 Axiomatic Formulation of Multiscale Concurrent Approaches

Clearly, multiscale *concurrent approaches* of the class introduced in the Section 1 are characterized by: the *fine* and *coarse resolutions* belong to the realm of continuum mechanics and the subdomains, where the different scale resolutions are employed, are disjoint. In such cases, the mathematical model is constituted by the *differential equations* of Eq. (2.1) and the *jump conditions* of Eq. (2.2).

A type of problem that has received considerable attention in multiscale studies and research are called *local* events. They correspond to cases in the subdomain where *coarse-scale resolution* applies covers most of the domain while that corresponding to the *fine-scale* is small. This kind of problems is suitable to applying a bi-physical model (i.e, only two subdomains in the multiphysical model) and in what follows we present a general procedure for *resolving local events* for the case when both physics, the *fine-scale* one—governing the *local-event*– and the *coarse-scale* physics—which governs the remaining space—belong to the realm of continuum mechanics.

3.2 The Multiphysical Model in 1D

Several of the examples that will be discussed in what follows are formulated in a one-dimensional (1D) space. For the sake of clarity, in this subsection we give explicitly the form that Eqs. (2.1) and (2.2) adopt when the physical space is one-dimensional. Then, Eq. (2.1) becomes

$$\frac{\partial \Psi^{\alpha}}{\partial t} + \frac{\partial \Psi^{\alpha} v^{\alpha}}{\partial x} = g^{\alpha} + \frac{\partial \tau^{\alpha}}{\partial x}, \quad \alpha = 1, \dots, N$$
(3.1)

while the jump conditions of Eq. (2.2) are (for 1D problems, $\Sigma(t)$ consists of only one point: $x_{\Sigma}(t)$):

$$\left[\left[\Psi^{\alpha}(v^{\alpha}-v_{\Sigma})-\tau^{\alpha}\right]\right]=0, \quad \alpha=1,\ldots,N; \quad \text{at} \quad x_{\Sigma}(t)$$
(3.2)

When deriving Eqs. (3.1) and (3.2) from Eqs. (2.1) and (2.2), we made use of the fact that in 1D problems the vector $\underline{\mathbf{n}}$ is a scalar that can take the values -1 and +1, exclusively, and the value +1 was chosen. This implies that the positive side of $x_{\Sigma}(t)$ is the right-hand side of it.

4. A BI-PHYSICAL APPROACH TO SINGULAR PERTURBATIONS

Generally, the solutions of perturbed partial differential equations, and systems of such equations, when the perturbation is sufficiently small can be approximated adequately by means of the solutions of the unperturbed equations. This, however, does not happen when the perturbation is a "*singular perturbation*" (Kevorkian and Cole, 1981); in such a case the convergence as the perturbation goes to zero is not uniform and boundary layers occur in which such an approximation is unsatisfactory.

Standard approaches used to treat such boundary layers are matched asymptotic expansions and some other similar procedures [see Cousteix and Mauss (2007); Cousteix (2005); Kevorkian and Cole (1981); Weinan (2011)]. In them the domain of definition of the problem is decomposed into two subdomains, the *inner domain* where the perturbed equation has to be satisfied and the *outer domain* in which the unperturbed equation prevails. In each one of such subdomains an asymptotic expansion is carried out and afterward they are matched, applying suitable criteria for that purpose. Thereby, we mention that it is in the choice of such a criteria where different approaches of this general framework differ most and it is also where the foundations of such procedures are less satisfactory (Cousteix and Mauss, 2007; Cousteix, 2005; Kevorkian and Cole, 1981).

Here, these problems are treated as *local events* using the general framework of *multiscale modeling*. In this manner we are led to propose an alternative bi-physical approach to *boundary and inner-layers*, which among some other attractive features overcomes the weaknesses just mentioned of the matched-asymptotic-expansions methodology. The basic idea of this bi-physical approach is to associate with such a problem, which is governed by a *singularly perturbed differential equation* throughout the whole domain, a *surrogate local-event problem* for which the *fine physics* is governed by the perturbed differential equation while the *coarse physics* corresponds to the unperturbed one. It should be mentioned that, as it will be seen through the examples here discussed, the solution of such a *surrogate* problem satisfies a well-posed *boundary-value problem with prescribed jumps (bvpj)* of the type discussed in Herrera (2007).

5. ADVECTION-DOMINATED TRANSPORT: THE STEADY-STATE

As a first illustration, here we study the steady state of advection-dominated transport in 1D. This example has been chosen mainly because of its simplicity, which permits analyzing it thoroughly with insignificant effort. The differential equations to be discussed depend on only one independent variable denoted by x. However, the problems also depend on a parameter, ε , and a significant part of our discussion objectives is to analyze the behavior of the problems solutions when ε varies. Therefore, the problem solutions are written explicitly as functions that depend on both x and ε whenever necessary for clarity.

Remark: If asymptotic expansion methods are applied to study the problem of this section—the boundary layer that occurs in steady state of advection dominated transport—it yields nothing [see, for example Weinan (2011)]. However, when the bi-physical approach here proposed is applied to it the boundary layer can be effectively treated.

5.1 The Singular Perturbation

Consider the equation

$$\frac{\partial c}{\partial x} = \varepsilon \frac{\partial^2 c}{\partial x^2}; \quad \text{with} \quad \varepsilon > 0 \tag{5.1}$$

which is a normalized form of the equation governing the steady state of diffusive transport, since its transport velocity is one. Furthermore, we impose the following boundary conditions:

$$c(0,\varepsilon) = 1 \quad \text{and} \quad c(1,\varepsilon) = 0 \tag{5.2}$$

This defines a well-posed boundary-value problem, whose exact solution is

$$c(x,\varepsilon) = \frac{1 - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}} = 1 + \frac{e^{-1/\varepsilon} - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}}$$
(5.3)

5.2 Some Features Characteristic of Singular Perturbations

When $\varepsilon \ll 1$, Eq. (5.1) is a *singular perturbation* of the equation:

$$\frac{\partial c}{\partial x} = 0 \tag{5.4}$$

We observe that the solution $c(x, \varepsilon)$, as given by Eq. (5.3) converges in the interval [0,1] as $\varepsilon \to 0$ but its convergence is not *uniform* in the semi-open subinterval [0,1). In the closed interval [0,1], it converges to the discontinuous function:

$$c(x,0) = \begin{cases} 1, & 0 \le x < 1\\ 0, & x = 1 \end{cases}$$
(5.5)

However, its convergence to the identically one constant function is *uniform* in any closed subinterval of [0, 1). Furthermore, such a limit function fulfills Eq. (5.4), which is the unperturbed form of the differential equation we are considering.

From the above discussion, we can draw the following conclusion: If x^* is a real number such that $0 < x^* < 1$ then c(x, 0) is the unique solution of the boundary-value problem, posed in the closed-interval $[0, x^*]$ and defined by the unperturbed differential equation together with the boundary condition

$$c(0,0) = 1 \tag{5.6}$$

5.3 The Bi-Physical Approximation

Motivated by the above discussion, we adopt the following bi-physical model. We divide the whole domain (i.e., the unit interval [0, 1]) into two subdomains: the *coarse-model domain* and the *fine-model domain*. To this end we choose a real number x^* such that $0 < x^* < 1$; then we define $[0, x^*)$ to be the *coarse-model domain*, while $(x^*, 1]$ will be the *fine-model domain*. The physics of the *coarse-model-domain* is *non-diffusive*, while at the *fine-model domain* is *diffusive*, with $0 < \varepsilon \ll 1$. In both of such domains Eq. (5.1) prevails, except that ε jumps from zero to non-zero when x^* is crossed. In conclusion, the *bi-physical model* we have just introduced is governed by a differential equation with discontinuous coefficients and the theories of Sections 3 and 4 are applicable to them.

Comparing Eq. (5.1) with the *canonical form* of Eq. (3.1), it is seen that one obtains the former from the latter when

$$1 \leftarrow N, \quad c \leftarrow \Psi, \quad 0 \leftarrow g, \quad \varepsilon \frac{\partial c}{\partial x} \leftarrow \tau$$
 (5.7)

The physics occurring in these two subdomains are matched, at their common boundary: $x = x^*$ by the jump conditions of Eq. (3.2), which for this case reduce to

$$\left[\left[c_{BP}(1 - v_{\Sigma}) - \varepsilon \frac{\partial c_{BP}}{\partial x} \right] \right] = 0, \quad \text{at} \quad x = x^*$$
(5.8)

The use of the sub-indexes, here as in what follows, is:

- i. c_{BP} , is the *bi-physical* solution, defined in the whole domain;
- ii. c_{BPC} , is the *coarse-model* solution, defined in the *coase-model-domain*; and
- iii. c_{BPf} , is the *fine-model* solution, defined in the *fine-model-domain*.

Furthermore, in Eq. (5.8) $v_{\Sigma} = 0$ since x^* is time-independent. Using this fact, we get

$$\left[\left[c_{BP} - \varepsilon \frac{\partial c_{BP}}{\partial x} \right] \right] = 0, \quad \text{at} \quad x^*$$
(5.9)

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Equations (5.1) and (5.9), together with the boundary conditions:

$$c_{BP}(0) = 1$$
 and $c_{BP}(1) = 0$ (5.10)

define a well-posed *boundary-value problem with prescribed jumps (bvpj)*, which governs the *surrogate bi-physical system*.

5.4 The Solution at the Coarse-Model Domain

The boundary condition:

$$c_{BP}(0) = 1 \tag{5.11}$$

together with the differential Eq. (5.4) define a well-posed problem in the closed-interval $[0, x^*]$, whose solution yields

$$c_{BP}(x) = 1, \quad \text{for} \quad 0 \le x < x^*$$
(5.12)

5.5 The Solution at the Fine-Model Domain

The latter equation, together with the jump conditions of Eq. (5.9), imply

$$\left(c_{BPf} - \frac{\partial c_{BPf}}{\partial x}\right)(x_{+}^{*}) = c_{BPC}(x_{-}^{*}) = 1$$
(5.13)

Here, the notations x_{+}^{*} and x_{-}^{*} refer to the limit from the right and from the left, respectively, at $x = x^{*}$. Equation (5.13) yields a left-hand boundary condition for the *fine-scale* physical model, which together with the equation

$$c_{BPf}(1) = 0 (5.14)$$

defines a well-posed boundary-value problem for $c_{BPf}(x)$, whose exact solution is

$$c_{BPf}(x) = \frac{1 - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}} = 1 + \frac{e^{-1/\varepsilon} - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}}, \quad \text{at} \quad x^* < x \le 1$$
(5.15)

5.6 The Solution of the Bi-Physical Model

In summary, putting together the results for the *coarse-scale* and *fine-scale domains* the solution of the *bvpj* in the whole domain [0, 1] is obtained:

$$c_{BP}(x) = \begin{cases} 1 & , \quad 0 \le x < x^* \\ \\ \frac{1 - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}} = 1 + \frac{e^{-1/\varepsilon} - e^{(1-x)/\varepsilon}}{1 - e^{1/\varepsilon}} & , \quad x^* < x \le 1 \end{cases}$$
(5.16)

5.7 Error of the Surrogate Model

Comparing Eqs. (5.3) and (5.16) an interesting property becomes apparent: *the solutions of the original problem and surrogate problem coincide, in the fine-scale subdomain.* The error associated with the bi-physical model is

$$E(x) = |c(x) - c_{BP}(x)| = \begin{cases} \frac{e^{-(1-x)/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}} & , & 0 \le x < x^* \\ 0 & , & x^* < x \le 1 \end{cases}$$
(5.17)

The maximum error occurs at the *coarse-model domain* side of x^* ; i.e., the point that separates it from the *fine-model domain*. Its value is

$$E_{max} = \frac{e^{-(1-x^*)/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}}$$
(5.18)

Notice that $1 - x^* \equiv \delta$ is the thickness of the *fine-model domain*; i.e., the *boundary layer*. In terms of δ , E_{max} is given by:

$$E_{max} = \frac{e^{\delta/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}} = \frac{e^{\delta/\varepsilon} \left(1 - e^{\delta-1/\varepsilon}\right)}{1 - e^{-1/\varepsilon}}$$
(5.19)

Assume that the "admissible error" h is a real number such that 0 < h < 1, while $0 < \varepsilon < 1$. Then, it can be seen that the condition $E_{max} \leq h$ is granted when

$$\delta \ge -\varepsilon log(2h) \tag{5.20}$$

This exhibits a condition that the *bi-physical surrogate model* needs to satisfy in order for the error introduced by its use be bounded by h. Thereby, we see that another necessary condition (although weaker) is that

$$\delta = O(\varepsilon) \tag{5.21}$$

6. ADVECTION-DOMINATED TRANSPORT: THE TRANSIENT-STATE

As a further example, in this section we extend the previous analysis to the time-dependent *1D advection-dominated transport*. As the physical space we keep the unit interval of the real line. To avoid complicating unnecessarily the notation, we will drop any reference to the parameter ε except in cases when such a reference is essential.

The example here considered was taken from Weinan (2011). In particular, we consider the differential equation

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = \varepsilon \frac{\partial^2 c}{\partial x^2} \tag{6.1}$$

subjected to the boundary conditions:

$$c(x,0) = c_0(t)$$
 and $c(1,t) = c_1(t), -\infty < t < \infty$ (6.2)

6.1 The Bi-Physical Model

The case of *advection-dominated transport* constitutes a *singular perturbation* of Eq. (6.1) around the value $\varepsilon = 0$, in which a *boundary layer* occurs at the right-hand-side boundary of the physical domain, since the velocity, +1, is positive. For this problem the *coarse-model physics* corresponds to *non-diffusive transport*, while the *fine-model physics* is *diffusive transport*. Both of these physics are governed by Eq. (6.1) with $\varepsilon = 0$ and $\varepsilon > 0$, respectively. Therefore, this is a problem governed by a differential equation with discontinuous coefficients whose systematic formulation was presented in Section 4.

6.2 The Concomitant Jump Conditions

The bi-physical formulation is similar to the steady-state case. In general, for a time-dependent problem one can choose x^* , the point where the physical model exhibits an abrupt jump of the physical properties, to be also time-dependent. However, here x^* will be time-independent. Thereby, we notice that for the application of the results of Section 3, $x_{\Sigma} = x^*$.

In order to identify the canonical form of Eq. (6.1), and through it obtain the *jump conditions* required to formulate the bi-physical model, we notice that such equation is obtained from Eq. (3.1) when the following replacements are made: $1 \leftarrow N$, $1 \leftarrow v^1$, $0 \leftarrow g^1$, $\varepsilon(\partial c/\partial x) \leftarrow \tau^1$ and $c \leftarrow \Psi^1$. Therefore, applying Eq. (3.2) it seen that the *concomitant jump conditions* of Eq. (6.1) are

$$\left[\left[c_{BP} - \varepsilon \frac{\partial c_{BP}}{\partial x} \right] \right] = 0, \quad \text{at} \quad x = x^*$$
(6.3)

In conclusion, the exact solution of the *bi-physical model* is determined by a well-posed boundary-value problem with prescribed jumps [*bvpw*, see Herrera (2007)] defined by Eqs. (6.1) to (6.3).

The jump conditions of Eq. (6.3) are tantamount to

$$c_{BPf} - \varepsilon \frac{\partial c_{BPf}}{\partial x} = c_{BPC}, \quad \text{at} \quad x = x^*$$
(6.4)

Here, it is recalled that the notations c_{BP} , c_{BPC} , c_{BPf} were introduced in Section 6; c_{BP} is the *bi-physical* solution, defined in the whole domain; c_{BPC} is the *coarse-model* solution, defined in the *coarse-model domain*; and c_{BPf} is the *fine-model* solution, defined in the *fine-model domain*.

6.3 The bvpwj

In summary, we can say that the *bi-physical regularization method* transforms the original singular boundary-value problem into a *boundary-value problem with prescribed jumps (bvpwj)*. In the case that we are treating, the solution of this bvpwj is facilitated because it can be obtained by solving successively two boundary-value problems, the first one in the *coarse-model domain*, and the second one in the *fine-model domain*. The procedure consists of firstly defining the boundary-value problem satisfied by c_{BPC} in $[0, x^*)$ and, afterward, the boundary-value problem satisfied by c_{BPf} in $(x^*, 1]$.

6.4 The Boundary-Value Problem in the Coarse-Model Domain

The function c_{BPC} is determinated by the differencial equation

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = 0, \quad \text{in} \quad [0, x^*) \quad \text{and} \quad -\infty < t < \infty$$
(6.5)

and only one boundary condition (the condition at the left-hand side of the coarse-model domain):

$$c(0,t) = c_0(t), \quad -\infty < t < \infty$$
 (6.6)

In particular, for such a boundary condition the solution is

$$c_{BPC}(x,t) = c_0(t-x)$$
 (6.7)

6.5 The Boundary-Value Problem in the Fine-Model Domain

As for the function c_{BFf} , it is determined by a parabolic boundary-value problem formulated in the *fine-model do*main. Since $\varepsilon > 0$, the equation

$$\frac{\partial c_{BPf}}{\partial t} + \frac{\partial c_{BPf}}{\partial x} = \varepsilon \frac{\partial^2 c_{BPf}}{\partial x^2}, \quad \text{in} \quad (x^*, 1] \quad \text{and} \quad -\infty < t < \infty$$
(6.8)

is a parabolic equation. The boundary conditions in the interval $(x^*, 1]$ are

$$c_{BPf}(x^*,t) - \varepsilon \frac{\partial c_{BPf}}{\partial x}(x^*,t) = c_0(t-x^*)$$

$$c_{BPf}(1,t) = c_1(t)$$

$$\left. \begin{array}{c} & & \\ & \\ & \\ \end{array} \right\}, \quad -\infty < t < \infty$$

$$(6.9)$$

7. BOUNDARY LAYERS IN INCOMPRESSIBLE FLUIDS

In this section, we consider two-dimensional incompressible flow of a slightly viscous fluid. We write the system of governing Navier–Stokes equations as

$$\frac{\partial u}{\partial t} + \underline{V} \cdot \nabla u + \frac{\partial p}{\partial x} = \varepsilon \nabla^2 u$$

$$\frac{\partial V}{\partial t} + \underline{V} \cdot \nabla V + \frac{\partial p}{\partial y} = \varepsilon \nabla^2 V$$

$$\nabla \cdot \underline{V} = 0$$
(7.1)

where the *dynamic viscosity*, $\varepsilon > 0$, is a constant. In particular, the flow of such a fluid past the half-plane:

$$\Omega = \left\{ \underline{x} = \begin{pmatrix} x \\ y \end{pmatrix} | y \ge 0 \right\}$$
(7.2)

with a no-slip boundary condition will be discussed.

$$\underline{V} = 0, \quad \text{at} \quad y = 0 \tag{7.3}$$

Above, $\underline{V} \equiv \begin{pmatrix} u \\ V \end{pmatrix}$ is the velocity and p is the pressure.

When the fluid is *slightly viscous* (i.e., $0 < \varepsilon \ll 1$) the system of equations (7.1) is a *singular perturbation* of the system of equations that governs the flow of *inviscid fluid*, which is obtained setting $\varepsilon = 0$ in the same system of equations. Due to the no-slip condition, a *boundary layer* occurs next to the horizontal boundary y = 0.

7.1 The Bi-Physical Approach

From the bi-physical framework perspective, the *coarse physics* is non-diffusive while the *fine physics* is diffusive. The treatment of this problem using the *coarse-model physics* is satisfactory everywhere, except at a *local event*: the *boundary layer* that needs to be *resolved* in order to obtain the *boundary-layer profile*. Thus, in what follows we assume that the *fine-model domain*, which corresponds to such a boundary layer, is the subdomain where $0 < y < y_{\Sigma}$, while the *coarse-model domain* is the remaining of the half-plane.

7.2 The Concomitant Jump Conditions

To obtain the system of jump conditions that are *concomitant* with the system of Eq. (7.1), it is necessary to find the *canonical form* of this latter system of partial differential equations. For the sake of clarity, here we write Eq. (2.1) in a more explicit form taking N = 3:

$$\frac{\partial \Psi^{1}}{\partial t} + \nabla \cdot (\Psi^{1} \underline{v}^{1}) = g^{1} + \nabla \cdot \underline{\tau}^{1}$$
(7.4)

This equation becomes the first of Eqs. (7.1) when $\Psi^1 \equiv u$, $\underline{v}^1 \equiv \underline{V}$, $g^1 \equiv 0$, and $\tau^1 \equiv \varepsilon \nabla u - p\underline{e}^1$; here, $\underline{e}^1 \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. The second *canonical equation* is:

$$\frac{\partial \Psi^2}{\partial t} + \nabla \cdot (\Psi^2 \underline{v}^2) = g^2 + \nabla \cdot \underline{\tau}^2$$
(7.5)

It becomes the second of Eqs. (7.1) when $\Psi^2 \equiv V$, $\underline{v}^2 \equiv \underline{V}$, $g^2 \equiv 0$, and $\tau^2 \equiv \varepsilon \nabla V - \underline{p} \underline{e}^2$; here, $\underline{e}^2 \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Finally, we observe that the third *canonical equation*,

$$\frac{\partial \Psi^3}{\partial t} + \nabla \cdot (\Psi^3 \underline{v}^3) = g^3 + \nabla \cdot \underline{\tau}^3 \tag{7.6}$$

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is transformed into the third of Eqs. (7.1) when $\Psi^3 \equiv 0$, $\underline{v}^3 \equiv \underline{V}$, $g^3 \equiv 0$, and $\tau^3 \equiv 0$. Therefore, for this particular case, the *concomitant jump conditions*:

$$[[\Psi^{\alpha}(v^{\alpha} - v_{\Sigma}) - \tau^{\alpha}]] \cdot \underline{n} = 0, \quad \alpha = 1, 2, 3$$
(7.7)

are

$$\underbrace{u\underline{V}}{\cdot \underline{n}} = \left[\left[\varepsilon \frac{\partial u}{\partial n} - p\underline{e}^{1} \cdot \underline{n} \right] \right] \\
 \underbrace{V\underline{V}}{\cdot \underline{n}} = \left[\left[\varepsilon \frac{\partial V}{\partial n} - p\underline{e}^{2} \cdot \underline{n} \right] \right] \\
 \underbrace{V}{\cdot \underline{n}} = 0$$
(7.8)

7.3 The Well-Posed Problem of the Bi-Physical Approximation

The well-posed problem corresponding to this case is constituted by the system of differential equations of Eq. (7.1), where $\varepsilon = 0$, in the *coarse-model domain*, and $\varepsilon > 0$ in the *fine-model domain*, together with the *jump conditions* of Eq. (7.8) and the boundary conditions of the original problem. As for the boundary that separates the *fine-model domain* from the *coarse-model domain*, it is the horizontal line $y = y_{\Sigma}$, where $y_{\Sigma} > 0$, and therefore the unit normal vector pointing upward is given by

$$\underline{n} = \underline{e}^2 = \begin{pmatrix} 0\\1 \end{pmatrix} \tag{7.9}$$

Thus, for this problem $\underline{V} \cdot \underline{n} = \underline{V} \cdot \underline{e}^2 = V$ and the above jump conditions imply that v is continuous across the line $y = y_{\Sigma}$. Using these facts, it can be verified that Eq. (7.8) reduces to

$$\left. \begin{array}{l} u_{f} - \frac{\varepsilon}{V_{f}} \frac{\partial u_{f}}{\partial y} = u_{C} \\ p_{f} - \varepsilon \frac{\partial V_{f}}{\partial y} = p_{C} \\ v_{f} = v_{C} \end{array} \right\} \quad \text{at} \quad y = y_{\Sigma}$$

$$(7.10)$$

These conditions, together with the no-slip condition at the lower boundary of the *fine-model domain*, complete the definition of the well-posed problem. They are

$$\begin{aligned} u_f &= 0\\ v_f &= 0 \end{aligned} \right\} \quad \text{at} \quad y = 0 \tag{7.11}$$

8. THE BI-PHYSICAL SHOCK-PROFILE MODEL

Viscous shock profiles provide simple examples of *internal layers*. The *Burger's equation* is frequently used as a simplified model of compressible flow (Weinan, 2011):

$$\frac{\partial v}{\partial t} + \frac{1}{2} \frac{\partial}{\partial x} (v^2) = \varepsilon \frac{\partial^2 v}{\partial x^2}$$
(8.1)

To illustrate the bi-physical treatment of shocks, we consider *Burger's equation* in the case when $0 < \varepsilon \ll 1$.

8.1 The Well-Posed Boundary-Value Problem with Prescribed Jumps

In standard approaches to this problem, the fluid is treated as inviscid at most of the domain and its viscosity is accounted for in the neighborhood of shocks, exclusively. Thus, when the bi-physical approach is adopted, the domain is divided into two subdomains: the *coarse-model* and the *fine-model domain*, respectively, and the physics in each one of them is governed by a partial differential equation of the form of Eq. (8.1), but $\varepsilon = 0$ in the first one and $\varepsilon > 0$ in the latter one.

Thus, the bi-physical model corresponding to the system so defined is a particular case of the general multiphysical systems explained in Section 4. The *canonical* form corresponding to Eq. (8.1) is obtained making the following substitutions in Eq. (3.1):

$$1 \leftarrow N, \quad v \leftarrow \Psi, \quad v/2 \leftarrow v, \quad 0 \leftarrow g, \quad \varepsilon \frac{\partial v}{\partial x} \leftarrow \tau$$
 (8.2)

In view of Eq. (3.2), this implies that the concomitant jump conditions are

$$\left[\left[v(v/2 - v_{\Sigma}) - \varepsilon \frac{\partial v}{\partial x} \right] \right] = 0$$
(8.3)

In the *bi-physical approach*, the general method to treat shocks consists of a two-step procedure in which we first solve a well-posed bvpj formulated in the *coarse physics* and, afterward, a *well-posed bvpj* that combines both physics is treated. To illustrate such a procedure, in a first instance we consider boundary conditions that are easy to handle. The problem is posed, in the real line, $-\infty < x < +\infty$ and $t \ge 0$. The initial conditions are

$$v(x,0) = \begin{cases} 1 & , -\infty < x < 0 \\ -1 & , \infty > x > 0 \end{cases}$$
(8.4)

This defines an *initial boundary-value problem with prescribed jumps (initial-bvpj)*, which is first solved when the governing physics is the *coarse physics*. For such an *initial-bvpj* the differential equation is obtained setting $\varepsilon = 0$ in Eq. (3.1); that is:

$$\frac{\partial v}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}(v^2) = 0 \tag{8.5}$$

Since $\varepsilon = 0$, the *concomitant jump conditions* of Eq. (8.3), reduce to

$$[[v(v/2 - v_{\Sigma})]] = 0 \tag{8.6}$$

It is a simple exercise to verify that the solution to this *initial-bvpj* is the function

$$v(x,t) = \begin{cases} 1 & , & -\infty < x < 0 \\ & & t \ge 0 \\ -1 & , & \infty > x > 0 \end{cases}$$
(8.7)

Indeed, this function fulfills Eq. (8.5) and exhibits a jump discontinuity for $t \ge 0$, whose position in the physical space, at x = 0, is time-independent. Therefore, $v_{\Sigma} = 0$ and Eq. (8.6) reduces to

$$[[v(v/2 - v_{\Sigma})]] = [[v^2/2]] = 1/2 - 1/2 = 0$$
(8.8)

A jump discontinuity such as that occurring above—which satisfies the jump conditions—is known as a *shock*.

An important piece of information that the solution of *initial-bvpj*, subjected to the *coarse physics* supplies is the location of the shock around which an *internal layer*, similar to a boundary layer, develops. Once the *coarse-physics* solution has been obtained, the goal of the second step of the *bi-physical approach* is to *resolve* the *local event*; i.e., to predict the details of the solution at the *internal layer*. To this end, as was indicated previously, and in a similar

fashion to what is done in the case of *boundary layers*, the domain is divided into two subdomains: the *coarse-model domain* and the *fine-model domain*. This latter domain is defined by

$$D_f \equiv \{(x,t) | -\delta_{-}(t) < x < \delta_{+}(t)\}$$
(8.9)

while the first one, its complementary space, is given by

$$D_C \equiv \{(x,t) | x < -\delta_-(t) \quad \text{or} \quad \delta_+(t) < t\}$$

$$(8.10)$$

Above, $\delta_{-}(t)$ and $\delta_{+}(t)$ are the thicknesses, at time t, to the left and to right, respectively, of the shock profile. The *coarse-model domain* may be decomposed into two disjoint pieces; namely:

$$D_C^- \equiv \{(x,t) | x < -\delta_-(t)\} \quad \text{and} \quad D_C^+ \equiv \{(x,t) | \delta_+(t) < x\}$$
(8.11)

Clearly $D_C = D_C^- \cup D_C^+$. There is considerable freedom for choosing the functions $\delta_-(t)$ and $\delta_+(t)$, albeit they must fulfill some requirements, which are not discussed here. As for the physics involved in *the bi-physical model*, the fluid is *viscous* in D_f , and it is *inviscid* in D_C ; thus Eq. (8.1) applies in both of these subdomains, but $\varepsilon > 0$ in D_f , while $\varepsilon = 0$ in D_C . Therefore, the jumps that occur at the boundary that separates D_f from D_C satisfy Eq. (8.3). We observe that, at every given time, such a boundary is made of two points: one is the point separating D_f from $D_C^$ and the other one separates D_f from D_C^+ . We adopt the notations $x_{\Sigma}^-(t)$ and x_{Σ}^+ for them, respectively.

They satisfy the equation:

$$x_{\Sigma}^{-} = -\delta_{-}(t) \quad \text{and} \quad x_{\Sigma}^{+} = \delta_{+}(t)$$

$$(8.12)$$

Taking all of this into account, Eq. (8.3) becomes

$$\left[\left[v(v/2 - v_{\Sigma}) - \varepsilon \frac{\partial v}{\partial x} \right] \right] = 0, \quad \text{at} \quad x_{\Sigma}^{-} \quad \text{and} \quad x_{\Sigma}^{+}$$
(8.13)

with

$$v_{\Sigma} = -\frac{d\delta_{-}}{dt}$$
 and $v_{\Sigma} = \frac{d\delta_{+}}{dt}$, at $x_{\Sigma}^{-}(t)$ and $x_{\Sigma}^{+}(t)$, respectively (8.14)

Or, in a more explicit form, we have

$$v_C\left(\frac{v_C}{2} - \frac{d\delta_+}{dt}\right) = v_f\left(\frac{v_f}{2} - \frac{d\delta_+}{dt}\right) - \varepsilon \frac{\partial v_f}{\partial x}, \quad \text{at} \quad x = \delta_+(t) \\ v_C\left(\frac{v_C}{2} - \frac{d\delta_-}{dt}\right) = v_f\left(\frac{v_f}{2} - \frac{d\delta_-}{dt}\right) - \varepsilon \frac{\partial v_f}{\partial x}, \quad \text{at} \quad x = -\delta_-(t) \end{cases}$$

$$\left. \begin{cases} t \ge 0 \end{cases} \right.$$

$$(8.15)$$

We recall that the solution in the *coarse-model domain*, which is independent of the *fine-model-domain* solution, has already been obtained and it is given in Eq. (8.7). Furthermore, if we take $\delta_+(t) = \delta_-(t) \equiv \nu t$, where $0 < \nu \ll 1$ then

$$v_R(v_f/2 - \mathbf{v}) - \varepsilon \frac{\partial v_f}{\partial x} = 1/2 + \mathbf{v}, \quad \text{at} \quad x = \mathbf{v}t \\ v_f(v_f/2 + \mathbf{v}) - \varepsilon \frac{\partial v_f}{\partial x} = 1/2 + \mathbf{v}, \quad \text{at} \quad x = -\mathbf{v}t \end{cases}$$

$$t \ge 0$$

$$(8.16)$$

Equation (8.16) supplies boundary conditions, which together with Eq. (8.1) define a well-posed problem in D_f .

9. DISCUSSIONS AND CONCLUSIONS

There are two categories of multiscale approaches: information-passing (or hierarchical), and concurrent. In turn, there are two classes of concurrent approaches: disjoint and overlapping (Fish, 2013). This paper presents a general method

for treating a subclass of disjoint-concurrent multiscale approaches; namely, that for which the *fine* and *coarse resolutions* are in the realm of continuous mechanics. Such a method transforms the problem into an *initial-boundary value problem with prescribed jumps (bvpj)* of the type previously discussed by the author in Herrera (2007). Furthermore, the method supplies a general formula that by mere substitutions yields the explicit expressions of the *differential equations* and *jump conditions* that define the *bvpj* for each case.

In particular, the new method is applicable to *local events* when the *fine* and *coarse resolutions* are in the realm of continuous mechanics. Using this fact, a new methodology is also introduced for treating *boundary* and *internal layers* associated with singular perturbations of partial differential equations. Several typical problems of this kind were discussed and treated in this paper. Although this is a new manner of formulating such problems and it will take some time to evaluate its implications, an advantage that is immediately apparent is that it eliminates some of the most controversial aspects of standard approaches such as matched asymptotic expansions and some other similar procedures (Cousteix and Mauss, 2007; Cousteix, 2005; Kevorkian and Cole, 1981).

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