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Short note

Suitable initial conditions

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Abstract

The aim of this note is to draw attention on a computational problem related to the (initial) simulation of very large time-dependant systems. The underlying theoretical problem has been the object of many relevant works in theoretical mathematical, and in the applied literature as well, but it seems that its computational implications are not familiar to many; we hope that this Note will help.

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1. Introduction

Recent discussions with distinguished specialists of numerical fluid mechanics have shown that it would be useful to write a physicist friendly version of the article [14], and this is the aim of this note.

Consider a very simple problem, namely the heat equation in space dimension one:

$$\begin{cases} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f, \quad 0 < x < 1, \ \ t > 0, \\ u(0,t) = u(1,t) = 0, \\ u(x,0) = u_0(x). \end{cases} \tag{1}$$

For u_0 and f given sufficiently regular, "explicit" forms of the solution u of (1) are available using the Green function of the heat equation [2]. Also mathematical results of existence and uniqueness of solutions of (1) are available when f and u_0 are just square integrable, or even less regular [12]. The issues discussed in [14] do not relate to unsmooth data but rather to smooth ones. Assume for instance that $f \equiv 0$, and $u_0(x) = 1$, $\forall x \in (0, 1)$. The existence and uniqueness of solution of (1) is then guaranteed by many theorems, and the solution will be $\mathscr{C}^\infty$ except near $t = 0$. The existence of a discontinuity near $t = 0$ can be seen by just observing that, for f and u_0 as above, $u(0, t) = 0$, for all $t > 0$, whereas $u(0, 0) = u_0(0) = 1$. In fact, assuming that f and u_0 are $\mathscr{C}^\infty$, the

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solution u of (1) will not, in general, be smooth near $t = 0$. It will be so only if (when) u_0 and f satisfy a sequence of conditions called the *compatibility conditions*, the level of regularity near $t = 0$ depending on the number of compatibility conditions that are satisfied. In Section 2 we describe the first and second compatibility conditions (CC) for (1), as well as for the convection and wave equations in space dimension one (the first one for (1) being $u_0(0) = u_0(1) = 0$). As another illustration of the results in [14] we present in Section 3, the substantially more complex case of the Navier–Stokes equations.

The problem of the compatibility conditions has been known and addressed in the mathematical literature for a long time; see e.g. [13] and the references in [14]. The novelty in [14] was to derive *all* the necessary and sufficient conditions for the solutions of certain classes of parabolic equations to be $\mathscr{C}^\infty$ near $t = 0$, and especially the incompressible Navier–Stokes equations.

How this issue relates to computation? From the physical (and somehow ''philosophical'') point of view, except when considering ab initium problems, any phenomenon considered for $t > 0$ will just be the continuation of a phenomenon which pre-existed, so that we should in principle be able to solve the problem under consideration *backward in time*.[1] Now, for an equation like (1), given f smooth for all $t \in \mathbb{R}$, the u_0 for which (1) can be solved backward are relatively very rare and, for this to be true some (but not all) of the requirements on u_0 are precisely the compatibility conditions. Hence solving (1) with an u_0 which is not physically suitable in this sense, means, despite the beautiful mathematical theorems, that we are trying to solve this problem with a non-physical initial data. There is likely a computational price to pay for that, which is negligible for (1), but is not for more complex equations. For instance those practicing large simulations for the Navier–Stokes equations or geophysical flows, know very well that they have to ''prepare'' their initial data before launching the actual computations. One may wonder if this ''preparation'' is not related to making the initial data ''suitable'' in the sense above. This article does not provide any recipe but, hopefully, by shedding some light on this difficulty, may help the practitioner.

The problem of the choice of initial (and boundary) data has been discussed from many angles, in the applied and computational literature, the compatibility conditions being implicitly or explicitly mentioned. For the Navier–Stokes equations (NSE) the problem of the first and second compatibility conditions has been addressed e.g. by Heywood [9], and Heywood and Rannacher [10]; in [10] the authors emphasize the computational relevance of the compatibility conditions. In his nice book [3], Gallavotti mentions the numerical difficulty caused by an inconsistency in the initial conditions for the NS equations; this difficulty relates to the second compatibility condition (19) below, although the compatibility conditions are not alluded to. See also the book of Kreisz and Lorenz [11] who address related issues (in particular in Chapter 10, Section 10.3.2) in the context of the initialization by ''the bounded derivative principle''. Several articles of Gresho alone or with co-authors address the initial and boundary conditions issues; see e.g. [4] where the first and second compatibility conditions appear; see also the review articles [5,6]. These issues appear also explicitly in work by Boyd and Flyer [1], Flyer and Fernberg [7], and Flyer and Swarztrauber [8]; see also the references in these articles. These articles emphasize the computational impact of the CC and propose a number of remedies (in particular computing analytically the singularities near $t = 0$, and ''removing'' them from the solutions).

2. One-dimensional equations

As indicated before we now describe the first and second compatibility conditions for three very simple equations in space dimension one, the first ones being that the initial data satisfies the boundary conditions of the problem, as we already observed in the case of the heat equation.

2.1. Heat equation

As indicated before, u_0 and f are smooth, so that the solution u of (1) is smooth for $t > 0$. We infer from the boundary condition at $x = 0$ that

[1] We realize that this factual remark somehow contradicts the irreversible nature of certain phenomenas, e.g. those described by parabolic equations. Irreversibility reappears however in the fact that one can solve initial boundary value problems for parabolic equations with initial data which *are not* the final value of an anterior phenomenon.