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On the Finite Differences Used in Reacting Flow Simulations

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Abstract. There exist many spatial discretization schemes that are well able to provide accurate and stable approximations for isothermal turbulent flows. Comparatively little analysis has been made of the performance of these schemes in the presence of temperature gradients driven by combustion. In this paper, the effects of temperature gradients on numerical stability are explored. A surprising result is that temperature gradients in the flow have a tendency to impinge on *left half plane* (LHP) stability of the spatial discretization scheme. Reasons for this tendency are explored and two remedies are proposed: one based on the particular class of finite difference schemes, and one based on an alternative method of boundary condition specification.

AMS subject classifications: 76M20

Key words: Numerical methods, combustion, stability.

1 Introduction

1.1 Motivation

In a number of works on the Direct Numerical Simulation (DNS) of turbulent flows, observations have been made regarding the spurious generation of unphysical high frequency waves. For non-reacting flows, the origin of the spurious modes is thought to lie in the application of inexact time dependent boundary conditions leading to reflection [16]. A similar line of reasoning for reacting flows identifies leading order effects from viscous boundary conditions as providing additional channels for spurious modes [22]. The high order schemes typically used in DNS have low dissipation and thus the spurious modes may be long lasting, with an associated reduction in the fidelity of the simulation. Depending on the flow regime studied (i.e. low Reynolds number flow), the growth of the modes may be controlled to some extent by naturally dissipative

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processes (such as through viscosity or other transport phenomena) but, in general, best practise should not rely on physical processes to dissipate numerical artifacts. A number of high order filters have been designed explicitly with this problem in mind [13].

The widespread appearance of spurious modes in high fidelity DNS (whether caused by boundary conditions, under-resolution or some other agency) may be inferred by the prevalence of filtering in the literature, both in cold flow simulations (i.e. sponge layers both to absorb physical phenomena and—potentially—spurious artifacts [7]) and reacting flow studies, where filters are explicitly used during the simulation procedure [6, 11, 22, 27]. The role of the differencing schemes in the emergence, growth or propagation of these spurious modes is relatively unexplored in the context of computational combustion; the current work is motivated principally by this observation.

Fig. 1 shows a laminar flame solution for a single step chemical reaction mechanism with unit Lewis number, in which the thermochemical state of the gas is characterized by a *progress variable* (a normalized product mass fraction). The reaction rate has been adjusted to give a laminar flame speed of 30cm/s, a value typical of many hydrocarbon reactions. The mean flow is from left to right, counter to the flame's direction of propagation; by balancing the mean flow speed against the laminar flame speed, the flame is brought to rest relative to the computational domain. This specification gives a simulation Mach number of $\mathcal{O}\left(10^{-3}\right)$ based on the laminar flame speed. The simulation was performed using a mesh of 64 grid points. Profiles are given for temperature, density, velocity and pressure. The boundary conditions for this calculation use Navier-Stokes

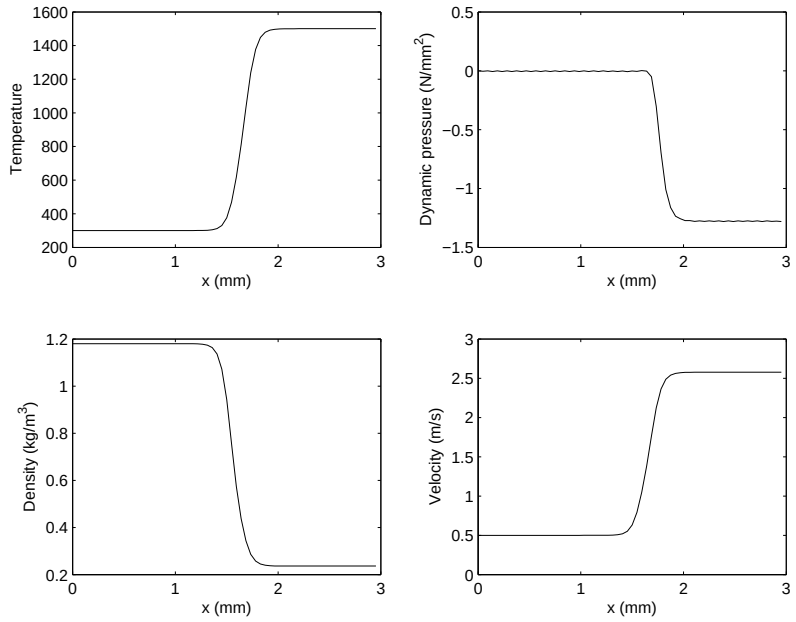

Figure 1: Example laminar flame solution for single step chemistry $R \to P$. Solution obtained using 4th order differences satisfying a *restricted norm* [21].