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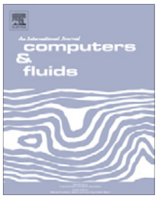

Impact of computational physics on multi-scale CFD and related numerical algorithms

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ABSTRACT

Development of accurate computational methods for the constitutive relation that plays a role as the bridge between microscopic and macroscopic physics becomes a key issue in a continuum approach for describing rarefied and micro-scale gas flows. The mathematical form of the constitutive relation dictates the resulting computational methods and related algorithms. It is, therefore, vital to develop proper computational models on the basis of a correct understanding of the multi-scale physics inherent in non-equilibrium gases. In this study the computational issue is discussed by considering two benchmark multi-scale problems: the compression-dominated shock structure and velocity shear-dominated gas flows. Special emphasis is placed on efficient CFD algorithms within the finite volume formulation. In addition, the verification and validation issue of the multi-scale methods is discussed and a simple verification method based on basic physical laws is proposed.

1. Introduction

The study of the behavior of rarefied and micro-scale gases is not only a fundamentally challenging subject, but also has emerged as a significant technical issue [1–4]. It is generally believed, however, that owing to formidable challenges in theoretical and computational aspects associated with the multi-scale nature of the problem, our understanding of the fundamental physics that lies behind this subject is limited. Also, the computational physics, which concerns the study of computational models for a given physical problem as opposed to the analysis of numerical methods for a given computational model, becomes a key issue during the initial phase of the study of CFD algorithms for rarefied and micro-scale gases. It is, therefore, vital to first develop proper computational models based on a correct understanding of the multi-scale aspects of gases.

There exist various computational methods [5–16] for the multi-scale modeling of gas flows: the molecular approach, the continuum approach, and the hybrid method. In particular, the continuum approach based on conservation laws, which had been initially considered inadequate for high non-equilibrium gas flows, has been studied actively in recent years. The success of the continuum approach depends on the so-called constitutive relation that represents the relationship between the microscopic and macroscopic physics of a specific substance of interest. It is the only ingredient that appears in the continuum mechanics intended to bridge two distinctive worlds (macroscopic and microscopic). For this reason, the mathematical form of the constitutive relation dictates the resulting computational methods and related algorithms [4]. It is also well-known that the verification and validation of computational models for rarefied and micro-scale gases is extremely difficult due to the lack of experimental data. In particular, flows involving solid surfaces are considered most challenging owing to the complexity associated with the gas-surface molecular interaction.

In this study, these computational issues are discussed by considering two benchmark problems: the compression-dominated shock structure and velocity shear-dominated gas flows, which highlight the essence of rarefied and micro-scale gases. Special emphasis is placed on efficient gas-kinetic theory based computational models and CFD methods to bridge the gap between microscopic and macroscopic theory. As an example, a finite volume formulation based on the nonlinear coupled constitutive relation (hereafter called NCCR [4]) is developed and its applications to benchmark problems are described. Finally, the verification and validation issue of the multi-scale methods is discussed and a simple verification method based on basic physical laws is proposed.

2. Computational methods for the multi-scale gas flows

The approach to develop the computational models can be, in general, classified into three categories: molecular, continuum, and hybrid.

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