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Extension of a second order velocity slip/temperature jump boundary condition to simulate high speed micro/nanoflows

Seyed Ali Rooholghdos, Ehsan Roohi *

High Performance Computing (HPC) Laboratory, Department of Mechanical Engineering, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran

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ABSTRACT

In the current work, for the first time, we extend the application of a second order slip/jump equations introduced by Karniadakis et al. for the simulation of high speed, high Knudsen (Kn) number flows over a nano-scale flat plate and a micro-scale cylinder. The NS equations subject to a second order slip/jump boundary conditions are solved using the Petrov–Galerkin Finite Element discretization. We compare our numerical solution for flow and thermal field with the solution of the DSMC and Generalized Hydrodynamic (GH) techniques, as well as a recently developed slip/jump boundary condition, i.e., Paterson equation. Current results demonstrate the suitable accuracy of the employed boundary conditions for different set of test cases. Our numerical solutions are obtained with much less numerical costs compared to alternative boundary conditions.

1. Introduction

During the last decades, the use of micro/nano electromechanical systems (MEMS/NEMS) has been significantly increased in various industries [1]. The low-pressure gas flow or small length scale which is present in micro/nanofluidics devices results in flow rarefication. Consequently, the departure from thermodynamic equilibrium due to the rarefication makes the Navier–Stokes (NS) equations invalid. The degree of gas rarefication is determined by the Knudsen number, defined as follows:

$$Kn = \frac{\lambda}{L} \tag{1}$$

where λ and L are the mean free path and characteristic length of the geometry, respectively. With regard to the values of the Knudsen number, the gas flows are classified as the continuum regime ($Kn < 10^{-3}$), slip flow regime ($10^{-3} < Kn < 10^{-1}$), transition regime ($10^{-1} < Kn < 10$), and free molecular flow ($Kn > 10$). The gas flow can be simulated using the Boltzmann equation in all regimes while the NS equations can be used only in continuum regimes. Nevertheless, we can still simulate the rarefied gas flow with the NS equations in the slip flow regime and slightly beyond provided that no-slip boundary conditions are replaced with velocity slip and temperature jump boundary conditions. Alternatively, moment methods have been widely employed for rarefied gas flows [2–4]. The benefit of moment methods is high accuracy and low computational costs [5]. Recently, boundary conditions (BC) for the regularized 13 moments equations were also extended to derive second order BCs for the NS equations [5].

* Corresponding author. Tel.: +98 511 8805136; fax: +98 511 8763304.
E-mail address: e.roohi@ferdowsi.um.ac.ir (E. Roohi).

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Eu [6] demonstrated that the high Mach number effects also contribute in non-equilibrium besides rarefication. He introduced a combined parameter that considers both of the rarefaction and compressibility factors. This parameter is defined as:

$$N_\delta = KnM\sqrt{\frac{2\gamma}{\pi}}. \tag{2}$$

To consider the effects of flow rarefactions near the walls, a first-order accurate velocity slip boundary condition was derived for the first time by Maxwell [7]:

$$U_s - U_w = \left(\frac{2-\sigma_v}{\sigma_v}\right) Kn \frac{\partial U_s}{\partial n} \tag{3}$$

where σ_v and σ_T represent the momentum and thermal accommodation coefficients, respectively. Similarly, Smoluchowski proposed a first-order temperature jump condition with the following equation [8]:

$$T_s - T_w = \left(\frac{2-\sigma_T}{\sigma_T}\right)\left(\frac{2\gamma}{\gamma+1}\right)\frac{Kn}{Pr}\frac{\partial T}{\partial n}. \tag{4}$$

Generally, slip/jump boundary conditions can be classified according to their accuracy and limits of applicability. The first-order slip boundary conditions can be expressed as in the following general form [9]:

$$U_s - U_w = C_1 Kn \left(\frac{\partial U}{\partial n}\right)_s \tag{5}$$

where C_1 represents first-order slip coefficient, i.e., $C_1 = \frac{2-\sigma_v}{\sigma_v}$ in Maxwell's condition. Different values have been proposed for this coefficient based on various analytical, numerical or experimental approaches. For example, see Loyalka et al. [10], Bohukudumbi et al. [11], Karniadakis et al. [12] and Agrawal et al. [13].

When rarefication increases, more accurate boundary conditions are required. Similar to the aforementioned general equation, the following equation can be considered for the second-order slip condition:

$$U_s - U_w = C_1 Kn \left(\frac{\partial U}{\partial n}\right)_s - C_2 Kn^2 \left(\frac{\partial^2 U}{\partial n^2}\right)_s \tag{6}$$

where C_1 and C_2 are the first-order and second-order coefficients. Different magnitudes have been proposed for the following coefficients based on the experimental or theoretical approaches. For example, see Refs. [14–18]. In addition to the following equation, another type of slip/jump boundary condition, Langmuir type, has been presented considering the condensation of gas molecules on the surface. Eu et al. [19] and Myong [20–22] developed this family of boundary conditions.

2. Karniadakis boundary condition

Karniadakis et al. [12] derived a second-order accurate slip/jump boundary condition based on the kinetic theory of gases. They calculated mean tangential velocity of the gas molecules and temperature jump boundary conditions as follows [12]:

$$u_s = \frac{1}{2}\left[u_\lambda + (1-\sigma_v)\, u_\lambda + \sigma_v u_w\right] \tag{7}$$

$$T_s = \left(\frac{(2-\sigma_T)}{Pr}\frac{2\gamma}{(\gamma+1)}T_\lambda + \sigma_T T_w\right) \Big/ \left(\sigma_T + \frac{2\gamma}{(\gamma+1)}\frac{(2-\sigma_T)}{Pr}\right) \tag{8}$$

where the subscripts λ and w denote value of the variables calculated at a distance proportional to the mean-free-path away from the surface and at the surface, respectively. Karniadakis et al. [12] showed that the Taylor expansion of Eq. (7) results in a second order BC in terms of Kn number; therefore, this BC is called the second order in the current paper.

Karniadakis et al. [12] reported that the best agreement with the DSMC solution for micro-channel geometry was obtained if u_λ and T_λ were calculated at a distance equal to one mean free path away from the wall. In the current work, a sensitivity analysis was performed for employment of Eqs. (7)–(8) for external flow geometries. We observed that best agreement with the DSMC solutions for velocity and temperature field is obtained if we calculate u_λ and T_λ at distances equal to λ and 2λ, respectively. σ_v and σ_T are the tangential momentum and energy accommodation coefficients. In addition, all of the variables are non-dimensionalized with the reference quantities in the freestream.

Contrary to most other common slip/jump boundary conditions, these boundary conditions are independent of calculating any velocity or temperature derivatives at the surface. Karniadakis et al. [12] noted that explicit implementation of boundary conditions which needs to calculate velocity or temperature gradients at the surface may result in unstable results. This reason along with high computational cost and numerical difficulties that come from calculating the higher order gradients encourage the researcher to focus on non-gradient slip/jump boundary conditions. In the current work, for the first time, we extend the applicability of Eqs. (7)–(8) for simulation of high speed external rarefied micro/nano flows.