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MICRO-SCALE CAVITIES IN THE SLIP- AND TRANSITION-FLOW REGIMES

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Abstract. *Differences between Navier-Stokes-Fourier (NSF) slip/jump solutions and direct simulation Monte-Carlo (DSMC) computations are highlighted for a micro lid-driven cavity problem. The results indicate a need for better modelling techniques which at the same time retain low computational cost of NSF models. We also highlight the fact that many micro-flows that have been considered are simple planar flows and typical classification systems are defined on such flows. We show that for complex flows, such as the driven cavity, non-equilibrium effects are more appreciable and their onset occurs at lower Knudsen numbers than expected.*

1 INTRODUCTION

Micro-electro-mechanical systems (MEMS) are being developed in many application areas, including industrial engineering, bio-medical devices, environmental control devices, micro-processor cooling and high-precision printing. Micro-ducts, micro-heat-exchangers, micro-pumps and micro-air-vehicles [1] are now terms commonly used in such fields. One particular area where the research community is particularly active, is the understanding of gas dynamics occurring in micron or sub-micron sized domains. The general characteristics of gaseous flows observed in macro-domains are not always applicable for flows in micro-sized domains. Thus the commonly used Navier-Stokes-Fourier (NSF) equations

with conventional no-slip boundary conditions are no longer considered to be valid when the characteristic length is within the micron range [2].

The inadequacy of the NSF equations to represent gas dynamics in micro-domains can be explained by the fact that they are only able to describe flows which are close to equilibrium. However, non-equilibrium effects are observed in gas flows at small scales. Collisions between gas molecules are the only medium for an ideal gas to achieve equilibrium conditions. Hence, if a gas is too rarefied or confined to micro-geometries, the number of collisions is reduced drastically inducing non-equilibrium effects. A good measure of the degree of rarefaction is the Knudsen number, which is defined as $Kn = \lambda/L$, where λ is the mean free path of the gas (i.e. the mean distance traversed between successive particle collisions) and H is the characteristic length scale of the domain.

2 MODELLING TECHNIQUES

The Boltzmann equation is considered to be the fundamental governing equation of any dilute gas characterized by binary collisions. This integro-differential equation is able to describe gases which are in equilibrium and non-equilibrium alike; however, its solution is a non-trivial task. The basic form of the Boltzmann equation is

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + a_i \frac{\partial f}{\partial c_i} = \left.\frac{\partial f}{\partial t}\right|_C , \tag{1}$$

where f is the particle distribution function (PDF) which is a function of time, t, the position vector, x_i, and the molecular velocity vector, c_i. The term, $\left.\frac{\partial f}{\partial t}\right|_C$ is a production term for f as a result of binary collisions and is often referred to as the collision operator.

Various methods have been used in order to obtain a simpler approximation of Eqn. (1), yet each method attempts to retain acceptable accuracy in order to describe the fundamental gas dynamics occurring in such domains. These methods can be divided into two main approaches.

Discrete molecular modelling is one method, whereby the fluid is modelled using a microscopic formalism, i.e. as a collection of moving molecules which interact through collisions or very close proximity potentials bringing about the exchange of energy and momentum. Such modelling can be performed using either statistical ensemble averages e.g. direct simulation Monte Carlo (DSMC) [3] or deterministic methods e.g. molecular dynamics (MD) [4]. Though such methods achieve a realistic picture, their application has been restricted to simplified flows due to the computationally intensive nature of discrete methods [5].

Continuum modelling is another approach for achieving simpler representations of the Boltzmann equation. The fluid is assumed continuous and infinitely divisible whereby it is possible to define velocity, density, pressure and other properties at any point in space and time. This modelling class can be further divided into two sub-classes. Extended hydrodynamic continuum model approximations of Eqn. (1) is one sub-class which can

be derived by either perturbation methods, commonly known as the Chapman-Enskog expansion [6], or moment methods [7, 8]. The conservation equations with the NSF constitutive relations can be derived by the use of each method [9]. Another sub-class of continuum modelling is the use of simple governing formulations such as the conservation equations with phenomenological extensions in order to capture non-equilibrium effects. Such techniques include the application of velocity slip [10] and temperature jump [11] boundary conditions and constitutive law re-scaling in the form of wall function methods [12].

3 FLOW REGIMES

Four distinct regimes are generally identified to characterise the extent of non-equilibrium and rarefaction effects in a particular flow [2];

- *No-slip (Continuum) Regime* - The conventional no-slip boundary condition combined with either the Euler or NSF equations are considered to be valid for $Kn < 0.001$, since the continuum and thermodynamic equilibrium assumptions are appropriate.

- *Slip Flow Regime* - In the range $0.001 < Kn < 0.1$, the slip-flow regime is applicable and the NSF equations are still considered appropriate, provided wall boundary conditions take into account the effect of velocity slip and temperature jump, resulting from the solid-gas interface and non-equilibrium effects occurring in the proximity of solid walls.

- *Transition Regime* - For $0.1 < Kn < 10$, the flow is said to be in the transition regime and the NSF equations become questionable. Alternative modelling approaches are needed in this regime using either discrete or continuum modelling or a combination of both.

- *Free-Molecular Flow* - For $Kn > 10$, the mean free path is very large compared to the characteristic length scale and the collision frequency is very low. A collisionless form of the Boltzmann equation is deemed to be appropriate to solve such flows.

4 THE 2D MICRO CAVITY PROBLEM

Many investigations presented in the literature on gaseous flows in micron-sized domains have been carried out for 2D-channels. The regimes listed in section 3 have been mainly characterised using simple 2D flows. Such problems generally have a "prevalent" dimension along which the fields have more predominant gradients e.g. Couette flow or Poiseuille flow.

Cavities, steps and cut-outs occur frequently in many engineering designs. Such configurations generate sharp changes in the flow field variables and their gradients. At

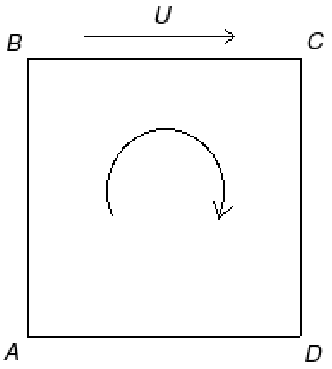

Figure 1: Schematic diagram of the driven cavity problem.

the macro-scale, modelling flow phenomena associated with cavities is challenging, particularly at high subsonic and supersonic Mach numbers. However, at the micro-scale, additional problems can arise due to rarefaction and non-equilibrium effects.

The lid-driven cavity problem has been extensively investigated in a completely different context. This problem is often used for the validation of numerical codes. As a result of its simplicity the cavity geometry has been investigated using a wide range of numerical methods. Its implementation is easy, yet the flow field is rich in flow physics within the recirculating regions. Many of the studies in the literature are presented in a Navier-Stokes incompressible framework which are either solved numerically by a pressure-velocity coupling method or a streamfunction-vorticity formulation [13, 14]. Generally the ultimate objective of such studies is to study the effectiveness of convective numerical schemes over a wide range of Reynolds numbers.

In the present paper we investigate a micro-scale lid-driven cavity. Very few studies are available in the literature in the context of micro or rarefied flow fields. Su *et al.* [15] presented various solutions using the Bhatangar-Gross-Krook (BGK) formulation of the Boltzmann equation whilst Jiang *et al.* [16] compared the DSMC and Information-Preservation (IP) methods. In particular Jiang *et al.* were interested in the validity of the IP method in the limit of low-speed flows. Naris and Valougeorgis [17] conducted a comprehensive study of the driven cavity over the whole Knudsen number range using a discrete velocity method to solve a linearised form of the Boltzmann equation. They showed that as the Knudsen number increased the number of counter-circulating vortices decrease. They also show that for very small speeds, the perturbation in temperature is small justifying the utilisation of the BGK linearisation.

The present paper focuses on the non-equilibrium physics and its effect on the flow field. In particular we shall identify the various shortcomings of the NSF model in both the slip and early transition regimes. In the absence of experimental data we compare the NSF results to DSMC simulations which have been carried out for the various regimes.

5 DIRECT SIMULATION MONTE CARLO

The DSMC technique used in this paper follows the scheme proposed by Bird [3]. In particular, we use a stochastic formulation where a number of real molecules is represented by a smaller number of "stochastic" particles. The algorithm is split into two main stages i.e. translational movement and binary collisions of particles within each kinetic time step. Solid-wall boundaries are accounted for within the translational stage of the algorithm and a special recursive treatment is implemented in the proximity of the cavity corners. A Maxwellian scattering kernel with perfect accommodation is assumed at the walls. The "no time counter" method is used to simulate the collision interactions.

At this stage we are interested in the steady-state solution. Since DSMC is strictly based on a kinetic formulation, (i.e. dependent on time, molecular velocity and position), time-averaged moments over a number of kinetic time steps are computed to yield a number of "macro" variables that can be used to compare the DSMC simulations to the continuum solution. The moments are averaged in space within the cell volumes. In particular, the moments computed are m, $m\bar{c_i}$, $\frac{m\overline{c_i c_i}}{2}$, $m\overline{C_i C_j}$ and $\frac{m\overline{C_i C_i C_j}}{2}$. These averages would respectively yield moments corresponding to density, bulk velocity, internal energy, viscous stress and heat flux where C_i is the peculiar velocity defined as the deviation of the molecular velocity, c_i, from the average velocity u_i i.e. $C_i = c_i - u_i$. The overbar indicates time-averaged values whereas repeated indices represent the Einstein convention of tensor summation.

6 NUMERICAL DISCRETISATION OF NAVIER-STOKES-FOURIER EQUATIONS

The NSF equations are solved using a pressure-velocity-density coupling technique as suggested by Demirdzic *et al.* [18]. A finite-volume collocated node formulation is used to discretise the equations. A central-difference numerical scheme is used for both the convective and diffusive fluxes at the cell boundaries. Source terms are computed at the central nodes. The central-difference scheme was chosen since the Reynolds numbers for the flows considered are relatively small and the scheme achieves accurate results even on coarser grids as suggested by Ferziger and Peric [19]. A grid-independence study was carried out in order to marginalise numerical errors as much as possible. The grid sizes utilised were 40×40, 80×80 and 160×160 cells. In all test cases considered, the results were numerically equivalent for the 80×80 and the 160×160 grids. We present here only the grid-independent results.

Velocity Slip and Temperature Jump Boundary Conditions

Applying velocity slip and temperature jump boundary conditions are simplified phenomenological approaches to represent both non-equilibrium and gas-surface interaction effects occurring near solid walls. These boundary conditions were first suggested by Maxwell [10] and von Smoluchowski [11] respectively. Using Grad's closure approxima-

tion for the PDF, f, the boundary conditions accounting for velocity slip and temperature jump are of the form [9],

$$v_{i_{slip}} = v_{i_{gas}} - v_{i_{wall}} = \frac{-\frac{2-\sigma}{\sigma}\sqrt{\frac{\pi}{2}}\sqrt{RT}\left(\alpha_1\tau_{ij}n_j - n_i\tau_{jk}n_jn_k\right) - \frac{1}{5}\left(\alpha_2 q_i - n_i q_k n_k\right)}{\rho RT + \frac{1}{2}\tau_{jk}n_jn_k}, \quad (2)$$

and

$$\frac{T_{wall}}{T} - 1 = \frac{\frac{2-\sigma_T}{\sigma_T}\sqrt{\frac{\pi}{2RT}}\frac{1}{2}\beta_1 q_k n_k + \frac{1}{4}\tau_{jk}n_jn_k}{p + \frac{1}{2}\tau_{jk}n_jn_k} - \frac{v_{i_{slip}}v_{i_{slip}}}{4RT} \quad (3)$$

respectively. The term, $v_{i_{slip}}$, represents the amount of slip at the wall defined as the difference between the bulk gas velocity at the wall, $v_{i_{gas}}$ and the solid wall velocity, $v_{i_{wall}}$. In a similar fashion, T is the gas temperature at the wall and T_{wall} is the isothermal solid wall temperature. The terms σ and σ_T represent the tangential momentum and energy accommodation coefficients respectively and τ_{ij} and q_i are the viscous stresses and the heat flux. The term, n_i represents the normal vector to the wall, p is the pressure and R is the specific gas constant. α_1, α_2 and β_1 are Knudsen layer correction coefficients. In order to account for the Knudsen layer the correction coefficients are set to $\alpha_1 = 1.114, \alpha_2 = 1.34533$ and $\beta_1 = 1.127$ [9]. Numerically, a second-order one-sided difference was implemented to determine any gradients required for the boundary conditions.

Both models have been extensively used in the slip flow regime i.e. $0.001 < Kn < 0.1$ [2] in combination with the NSF equations. We shall use this combination to investigate flows that fall within the slip and transition regimes and investigate the validity of such a combination for the micro-cavity problem.

7 RESULTS AND DISCUSSION

The results are presented in normalised form. In particular,

$$X = \frac{x_1}{L}, \quad Y = \frac{x_2}{L}, \quad \overline{S} = \frac{s}{L}, \quad \overline{P} = \frac{p}{P_o}, \quad U = \frac{v_1}{\overline{U}} \quad \text{and} \quad V = \frac{v_2}{\overline{U}}. \quad (4)$$

X and Y are the dimensionless horizontal and vertical distances normalised with respect to the cavity length, L. S is the normalised distance along the surface walls progressing in a clockwise fashion, starting from A (as shown in Figure 1). P is the normalised pressure with respect to the initial pressure, $P_o = 101135$ Pa. U and V are the velocity vector components normalised with respect to the lid-speed $\overline{U}$.

These dimensionless parameters are complimented by a number of additional non-dimensional parameters whereby $a = H/L$ is the aspect ratio, $Ma = \overline{U}/\sqrt{2RT_o}$ is the Mach number and $Kn = \lambda/L$ is the Knudsen number.

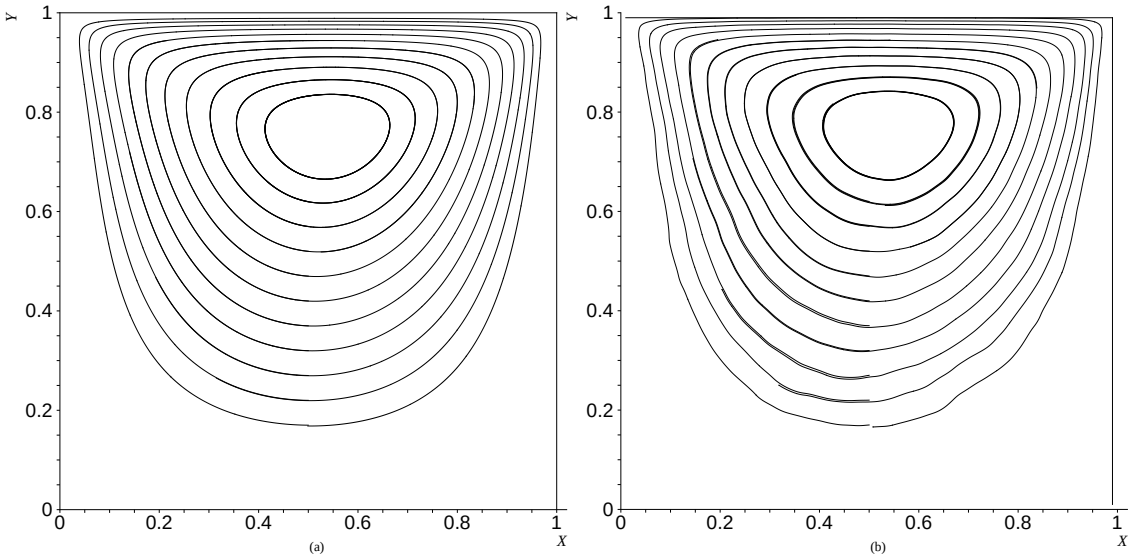

Figure 2: Velocity streamlines for $Kn = 0.005$ – (a) NSF slip/jump solution and (b) DSMC data.

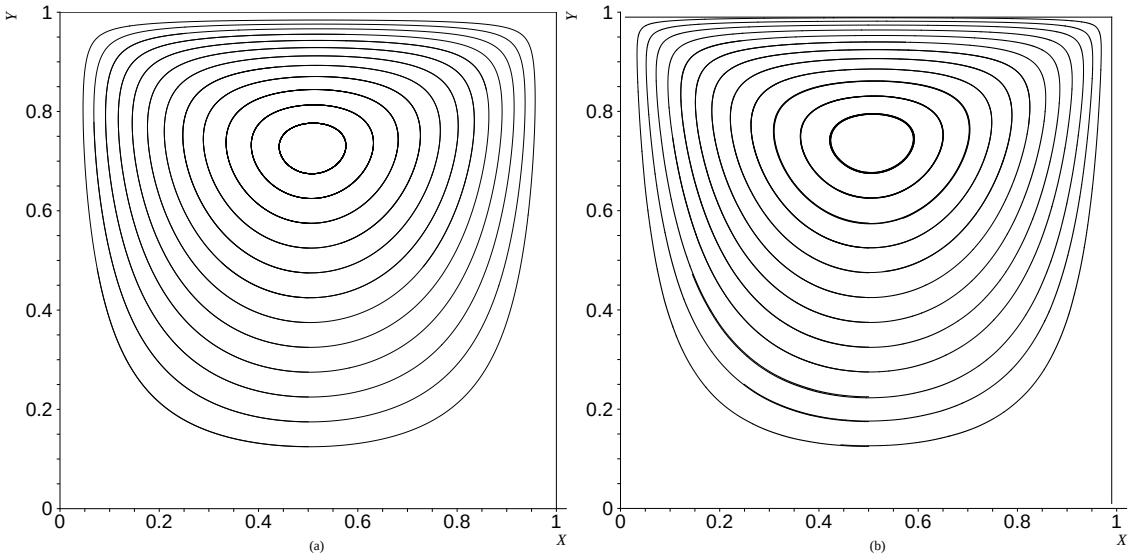

Figure 3: Velocity streamlines for $Kn = 0.1$ – (a) NSF slip/jump solution and (b) DSMC data.

The results shown in the present paper are for an early slip regime ($Kn = 0.005$) and late slip/early transition regime ($Kn = 0.1$) with constant $Ma = 0.09$ and $a = 1$. Figures 2 and 3 show the normalised velocity streamlines for both regimes. The streamlines are in close agreement for $Kn = 0.005$ whereas differences can be observed for $Kn = 0.1$ especially in close proximity to the top corners. These differences can be attributed to the lack of effectiveness of the NSF equations to represent non-equilibrium phenomena.

Figure 4 shows the normalised pressure distribution along the surface S. Here it can be seen that there is good agreement between the DSMC data and the NSF solution for $Kn = 0.005$. For $Kn = 0.1$, there is qualitative agreement but there seems to be a quantitative disparity between the two solution techniques. These results bear a strong resemblance to those obtained by Jiang *et al.* [16] for the pressure distribution along the surface.

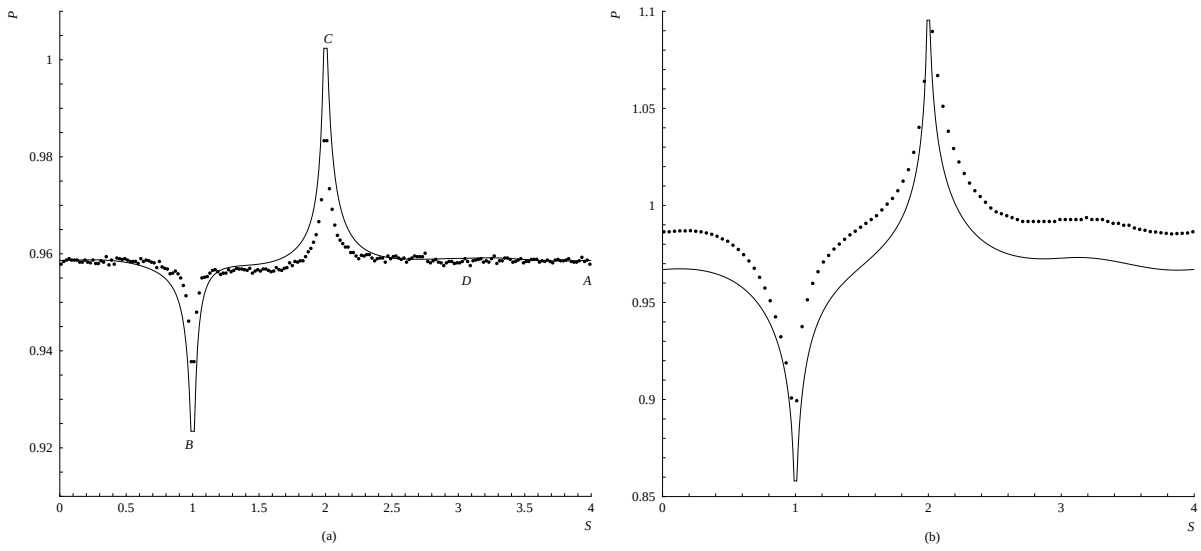

Figure 4: Pressure distribution along the cavity walls – (a) $Kn = 0.005$ and (b) $Kn = 0.1$. Legend DSMC data (•) and NSF Solution (—).

8 CONCLUSIONS

A comparison between Navier-Stokes-Fourier (NSF) slip/jump solutions and direct simulation Monte-Carlo simulations has been carried out for a driven micro-cavity problem. In particular it can be shown that the onset of strong non-equilibrium effects is observed at Knudsen numbers typically falling within the late slip regime. The NSF equations are often considered valid up to a Knudsen number of 0.1. This does not seem to be the case for this particular problem. Non-equilibrium effects are particularly strong in the

proximity of solid walls which in turn affect the structure of the entire flow. The corners of the cavity provide many of the non-equilibrium effects since the local Knudsen number in these regions is particularly large. The results demonstrate that there is a requirement for alternative modelling techniques that provide an efficient and computationally cheap tool to simulate micro-gas dynamics for such problems.

REFERENCES

[1] R. Wootton. From Insects to Microvehicles. *Nature*, January 2000.

[2] M. Gad-el Hak. The Fluid Mechanics of Microdevices - The Freeman Scholar Lecture. *ASME Journal of Fluids Engineering*, 121(403):5–33, March 1999.

[3] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon Press, Oxford, 1995.

[4] D. C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge, UK, 2004.

[5] C. K. Oh E. S. Oran and B. Z. Cybyk. Direct Simulation Monte-Carlo: Recent Advances and Applications. *Annual Review of Fluid Mechanics*, 30(1):403–441, 1998.

[6] S. Chapman and T. G. Cowling. *The Mathematical Theory of Non-uniform Gases*. Cambridge University Press, Cambridge, UK, 1990.

[7] H. Grad. On The Kinetic Theory of Rarefied Gases. *Commun. Pure Appl. Math.*, 2:331–407, 1949.

[8] M. N. Kogan. *Rarefied Gas Dynamics*. Plenum Press, New York, 1969.

[9] H. Struchtrup. *Macroscopic Transport Equation for Rarefied Gas Flows*. Springer, Germany, 2005.

[10] J. C. Maxwell. On Stresses in Rarefied Gases Arising from Temprature Inequalities. *Philos. Trans. R. Soc. London*, 170:231–256, 1879.

[11] M. von Smoluchowski. Über wärmeleitung in verdünnten gasen. *Annalen der Physik und Chemie*, 64:101–130, 1898.

[12] D A. Lockerby, J. M. Reese, and M. A. Gallis. Capturing the Knudsen layer in continuum-fluid models of non-equilibrium gas flows. *AIAA JOURNAL*, 43(6):1391–1393, 2005.

[13] E. Erturk, T.C. Corke, and C. Gökcöl. Numerical Solutions of 2-D Steady Incompressible Driven Cavity Flow at High Reynolds Numbers. *Int. J. Numer. Meth. Fluids*, 48:747–774, 2005.

[14] P. N. Shankar and M. D. Deshpande. Fluid Mechanics in the Driven Cavity. *Annual Review of Fluid Mechanics*, 32(1):93–136, 2000.

[15] M. Su, K. Xu, and M. S. Ghidaoui. Low-Speed Flow Simulation by the Gas-Kinetic Scheme. *Journal of Computational Physics*, 150:17–39, March 1999.

[16] J. Jiang, J. Fan, and C. Shen. Statistical Simulation of Micro-Cavity Flows. In *AIP Conference Proceedings – Rarefied Gas Dynamics: 23rd International Symposium*, volume 663, pages 784–791, May 2003.

[17] S. Naris and D. Valougeorgis. The Driven Cavity Flow Over the Whole Range of the Knudsen Number. *Physics of Fluids*, 17(9):097106, 2005.

[18] I. Demirdzic, Z. Lilek, and M. Peric. A Colocated Finite Volume Method for Predicting Flows at all Speeds. *Int. J. Numer. Meth. Fluids*, 16:1029–1050, 1993.

[19] J.H. Ferziger and M. Peric. *Computational Methods for Fluid Dynamics*. Springer-Verlag, Germany, 1995.