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The velocity slip problem: Accurate solutions of the BGK model integral equation

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ABSTRACT

The velocity slip problem (also known as the Kramers problem) in the kinetic theory has been solved by a variety of techniques, and some accurate numerical as well as general variational results are available for both simple gases and gas mixtures. For the model equations, reasonably accurate solutions (within about 1% of the exact results) have been obtained by solving the related integral equations, but such techniques have not previously been pushed far enough to explore the possibilities of obtaining benchmark solutions. Some of the reasons for not further pursuing these techniques were limitations on the efficiencies and accuracies of the computer routines that could be constructed for the needed Abramowitz functions and limitations in terms of computational resources with respect to available precision and storage capabilities. These limitations have now effectively been removed with modern advances in computer technology and the computational tools that have become available, and it is the purpose of the present paper to report on our explorations in this regard within the specific context of the velocity slip problem as based on the BGK model which we have approached using the singularity subtraction technique in conjunction with numerical quadratures.

1. Introduction

The velocity slip problem in the kinetic theory has been solved by a variety of techniques, and some accurate numerical as well as general variational results are available for both simple gases and gas mixtures [1–5]. For the model equations, reasonably accurate solutions (within about 1% of the exact results) have been obtained by solving the related integral equations [1,6–9], but such techniques have not previously been pushed far enough to explore the possibilities of obtaining benchmark solutions. Some of the reasons for not further pursuing these techniques were limitations on the efficiencies and accuracies of the computer routines that could be constructed for the needed Abramowitz functions and limitations in terms of computational resources with respect to available precision and storage capabilities. These limitations have now effectively been removed with modern advances in computer technology and the computational tools that have become available.

We note that despite the substantial progress of the last many years towards solving the Boltzmann equation, the model equations remain of interest in a variety of situations for both external and internal flows in arbitrary geometries [10–21] and, thus, our explorations here would have wider implications in the field than may be apparent from just the solution of the present problem.

2. The integral equation and its solution

The integral equation corresponding to the velocity slip problem for the BGK model (and diffuse reflection) is given as [2]:

$$q(x) - \frac{1}{\pi^{1/2}} \int_0^\infty T_{-1}\left(|x - x'|\right) q(x')\, dx' = \frac{1}{\pi^{1/2}} T_1(x) \tag{1}$$

Here, the normalized velocity parallel to a plate in a semi-infinite expanse of gas is, $x + q(x)$, where x is the non-dimensionalized, perpendicular distance from the plate, and the Abramowitz functions, $T_n(x)$, are defined by:

$$T_n(x) = \int_0^\infty t^n \exp\left[-t^2 - x/t\right] dt \tag{2}$$

The velocity slip coefficient, A, is determined from:

$$A = \frac{1}{\pi^{1/2}} + \frac{2}{\pi^{1/2}} \int_0^\infty q(x) T_1(x)\, dx \tag{3}$$

Eq. (1) is of the form of a Fredholm integral equation of the second kind, i.e.:

$$\phi(x) - \int_a^b K(x, x')\phi(x')\, dx' = S(x); \quad x \in (a, b) \tag{4}$$

where the kernel $K(x, x')$ has a singularity at $x = x'$. In the singularity subtraction technique, one converts such an equation to:

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$$g(x)\phi(x) - \int_a^b K(x,x')\big[\phi(x') - \phi(x)\big]\,dx' = S(x) \tag{5}$$

where:

$$g(x) = 1 - \int_a^b K(x,x')\,dx' \tag{6}$$

Eq. (5) can be approximated by a simple system of algebraic equations:

$$\sum_{j=1}^{N} A_{ij}\phi_j = S_i; \quad i = 1, 2, 3, \ldots, N \tag{7}$$

where:

$$A_{ij} = \begin{cases} -\beta_{ij}; & i \neq j \\ g_i + \sum_{\substack{k=1 \\ k\neq i}}^{N} \beta_{ik}; & i = j \end{cases} \tag{8}$$

and:

$$\beta_{ij} = w_j K(x_i, x_j) \tag{9}$$

Here, x_i and w_i are the nodes and weights of some suitable quadrature. Using this scheme, Eq. (7) can easily be solved to determine the ϕ_j by using either Gaussian quadratures or the more accurate Gauss–Kronrod quadratures [22] with the accuracy of the method for any given type of quadrature being dependent upon the order of the quadrature used, N.

We have solved Eq. (7) numerically to determine the velocity and, hence, the velocity slip using *Mathematica*®. Note that:

$$K(x,x') = \frac{1}{\pi^{1/2}} T_{-1}\big(|x - x'|\big) \tag{10}$$

and:

$$g(x) \equiv 1 - \frac{1}{\pi^{1/2}} \int_0^\infty T_{-1}\big(|x - x'|\big)\,dx' = \frac{1}{\pi^{1/2}} T_0(x) \tag{11}$$

Thus, this integral need not be evaluated from a quadrature but, rather, can be evaluated directly. For purposes of evaluating the $T_i(x)$ directly with *Mathematica*®, we note that the Abramowitz functions can be expressed in terms of the Meijer-G functions [23, 24]:

$$\begin{aligned} G_{p,q}^{m,n}\left(x \,\middle|\, \begin{matrix} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{matrix}\right) &\equiv \frac{1}{2\pi i} \int_{\gamma_L} \frac{\prod_{j=1}^{m}\Gamma(b_j - s)\prod_{j=1}^{n}\Gamma(1 - a_j + s)}{\prod_{j=n+1}^{p}\Gamma(a_j - s)\prod_{j=m+1}^{q}\Gamma(1 - b_j + s)} x^s\,ds \\ &= \frac{1}{2\pi i} \int_{\gamma_L} \frac{\prod_{j=1}^{m}\Gamma(b_j + s)\prod_{j=1}^{n}\Gamma(1 - a_j - s)}{\prod_{j=n+1}^{p}\Gamma(a_j + s)\prod_{j=m+1}^{q}\Gamma(1 - b_j - s)} x^{-s}\,ds \end{aligned} \tag{12}$$

which are sometimes expressed in a more general 2-argument form as:

$$G_{p,q}^{m,n}\left(x, r \,\middle|\, \begin{matrix} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{matrix}\right) \equiv \frac{1}{2\pi i} \int_{\gamma_L} \frac{\prod_{j=1}^{m}\Gamma(b_j + s)\prod_{j=1}^{n}\Gamma(1 - a_j - s)}{\prod_{j=n+1}^{p}\Gamma(a_j + s)\prod_{j=m+1}^{q}\Gamma(1 - b_j - s)} x^{-s/r}\,ds \tag{13}$$

In these definitions, the contour of integration, γ_L, lies between the poles of $\Gamma(1 - a_i - s)$ and $\Gamma(b_i + s)$. Thus, in terms of the basic Meijer-G functions one has that:

Table 1
Values of the velocity slip coefficient, A, as a function of quadrature order, N

N	Velocity slip coefficient, A
41	1.016194
82	1.0161920
164	1.01619149
328	1.016191428
656	1.0161914195
1312	1.01619141848
Exact	1.016191418323...

$$T_{-1}(x) = \frac{1}{2\sqrt{\pi}} G_{0,3}^{3,0}\left(\tfrac{1}{4}x^2 \,\middle|\, \begin{matrix} - \\ 0, 0, \tfrac{1}{2} \end{matrix}\right) \tag{14}$$

$$T_0(x) = \frac{x}{4\sqrt{\pi}} G_{0,3}^{3,0}\left(\tfrac{1}{4}x^2 \,\middle|\, \begin{matrix} - \\ -\tfrac{1}{2}, 0, 0 \end{matrix}\right) \tag{15}$$

$$T_1(x) = \frac{1}{2\sqrt{\pi}} G_{0,3}^{3,0}\left(\tfrac{1}{4}x^2 \,\middle|\, \begin{matrix} - \\ 0, \tfrac{1}{2}, 1 \end{matrix}\right) \tag{16}$$

and so forth for other $T_i(x)$. As such, these can be evaluated to arbitrary accuracy in *Mathematica*®.

Further in our work, to transform the range from $x \in (0, \infty)$ to $\xi \in (0, 1)$, we have considered use of the transformation:

$$\xi = 1 - e^{-(x)^{1/n}}; \quad n = (1, 2, \ldots) \tag{17}$$

which gives:

$$x = \big[-\ln(1 - \xi)\big]^n \tag{18}$$

and:

$$dx = \frac{n[-\ln(1 - \xi)]^{n-1}}{1 - \xi}\,d\xi \tag{19}$$

We have numerically explored the use of various values of n in conjunction with this transformation and have found that $n = 2$ is generally a good choice from the point of view of economy in quadratures.

We have employed Gauss–Kronrod quadratures starting with 41 points in the interval $(0, 1)$ with a precision of 60 digits. Larger successive quadrature sets are generated by dividing the interval into 2, 4, 8, 16, and 32 equal segments and using a 41 point quadrature set for each segment. This results in quadrature orders for this work of 41, 82, 164, 328, 656, and 1312, respectively.

3. The results

Our results for the slip coefficient, A, are reported in Table 1. The exact value of A is known for this special case from the relationship:

$$A = \pi^{1/2} \int_0^\infty \frac{w \exp(w^2)}{p^2(w) + \pi^2 w^2}\,dw \tag{20}$$

in which:

$$p(u) = \pi^{1/2}\left(\exp(u^2) - 2u \int_0^u \exp(t^2)\,dt\right) \tag{21}$$

and, to several digits, has the value $A = 1.016191418323352759\ldots$. Thus, it is possible for us to assess the accuracy of the subtraction technique that we have used for any given order of the quadrature. This comparison allows one to have confidence in the subtraction technique to a comparable degree of precision in problems where an exact solution is unavailable. We note that the results in Table 1 improve remarkably as the quadrature order is increased and the highest order quadrature used in the present work gives $A = 1.01619141848$.

Table 2
Velocity profiles near a planar surface, $x+q(x)$, as a function of quadrature order, N

x	Order of the numerical Gauss–Kronrod quadrature used, N					
	41	82	164	328	656	1312
0	0.7071044	0.70710647	0.70710675	0.707106781	0.707106782	0.707106781
1/20	0.7215083	0.72153084	0.72153589	0.721535760	0.721535743	0.721535744
1/10	0.8879188	0.88791790	0.88791845	0.887918576	0.887918600	0.887918605
1/5	1.0274136	1.0274142	1.02741490	1.0274150828	1.027415072	1.027415068
2/5	1.2761521	1.2761609	1.27616135	1.2761613235	1.276161300	1.276161305
3/5	1.5068858	1.5069006	1.50690290	1.5069033561	1.506903449	1.506903441
4/5	1.7284599	1.7284590	1.72846276	1.7284633521	1.728463307	1.728463321
1	1.9444456	1.9444404	1.94444461	1.9444448290	1.944444913	1.944444935
2	2.9855789	2.9855586	2.98555806	2.9855584571	2.985558568	2.985558600
3	4.0012951	4.00122577	4.00121270	4.0012137505	4.001213542	4.001213584
4	5.0084699	5.00835017	5.00832079	5.0083195860	5.008319103	5.008319011
5	6.0120596	6.01190363	6.01186079	6.0118543446	6.011854323	6.011854342
7	8.0150607	8.01483607	8.01476337	8.0147470324	8.014745878	8.014745607
10	11.016260	11.01599887	11.01590086	11.0158732619	11.015868237	11.015867934
20	21.016656	21.01635567	21.01623838	21.0161994274	21.016189434	21.016187450

We have also reported values of the velocity profile in Table 2. The accuracy of our results increases systematically as the order of the quadrature, N, is increased and the values that we have obtained agree with the ones reported through use of the singular eigenfunction expansion technique [7] to the digits quoted (the results are also in agreement with those reported more recently [21]). Thus, the present technique can be used to obtain results of benchmark accuracy for integral transport equations in the kinetic theory corresponding to both internal and external flow problems, and domains that extend to infinity. Note that in many instances, the kinetic models of the Boltzmann equation provide good descriptions of real flows (at least for the macroscopic hydrodynamic quantities) and, thus, it remains of interest to explore these models more as well as techniques for obtaining increasingly accurate results when using them.

We wish to emphasize that the present paper provides a benchmark verification of the technique against known exact solutions for a well studied case, for which in the past it had not been possible to obtain results of such accuracy by direct solutions of the integral equation of the type often encountered in kinetic theory (the precision of the Abramowitz functions, the size of the quadratures and numerical precision of computation, and semi-infinite range of the interval all had been issues; and these all have been successfully addressed in this paper). While it has been previously possible to obtain benchmark accuracy for planar problems, most of the techniques used for such purposes [7,17,21], were limited in their applicability to just the planar problems. In contrast, the present technique applies directly to non-planar problems also, and it provides a means for obtaining benchmark results for a host of non-planar problems against which results obtained from approximate methods can be verified, and thus improved. The computational time required for the technique is machine dependent, and for the present problem it was sufficiently low that it is does not warrant a discussion. We have, however explored application of this technique for a non-planar problem (condensation on a spherical particle in the BGK model framework) and since in this case numerical integrations on the Abramowitz functions are needed (integrals corresponding to Eq. (6) cannot be carried out analytically as was possible in the present case), the computational time does become an issue if some parametric studies (like Knudsen number, role of different boundary conditions, etc.) are also to be conducted. We have been able to address this issue successfully, however, by using parallel computations (we have used an 8 node processor), as the technique is simply and directly parallelizable. We will be reporting some of these results in the near future together with computational times needed, but based on the present work and the explorations we have mentioned, it can be stated with confidence that the technique will provide much needed benchmarks for many problems in the kinetic theory where such results have previously not been available.

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