DEGAS 2 Verification Test with Fluid Neutral Momentum Transport Reference Problem

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1 Background

The "Fluid Neutral Momentum Transport Reference Problem" [1] was used to verify the original DEGAS [2] Monte Carlo neutral transport code. The resulting benchmark was subsequently employed in the development of DEGAS 2 [3]. The practical conclusions of these exercises were published in Ref. [4]; the principal requirement is that the computational mesh has to be fine enough for the Monte Carlo neutrals to experience the temperature gradient associated with the thermal force.

A uniform mesh was chosen (neither the codes nor the model require one) for the comparison to facilitate characterization of the simulation's spatial resolution. The initial set of simulations performed with DEGAS also utilized several different plasma profiles in addition to the one described above.

These simulations agreed with the second of the two model solutions, $N_2(x)/N(0)$ in [1], when $\max(l/L) \leq 0.1$ (i.e., maximum value of l/L in the plasma), where l is the charge exchange mean free path, and $\min(l/\Delta) \geq 0.5$, where Δ is the mesh spacing. The former criterion renders the fluid approximation valid; the latter ensures that the atoms "see" enough of the temperature gradient to reproduce the thermal force. Note that l varies with x; only by using the min and max values in this way were the results with different plasma profiles (not discussed in [1]) unified. Figure 1 demonstrates the latter inequality with four runs, all with $\max(l/L) = 0.1$, and $\min(l/\Delta) = 0.04$, 0.1, 0.5, and 1. In particular, the $\min(l/\Delta) = 1$ curve here corresponds to the DEGAS 2 (version 3.3) `Analytic_fluid_bench` example with 6400 flights; we will refer to this as the "baseline" case throughout this document. The other three curves were obtained by reducing the number of grid points by the appropriate factor.
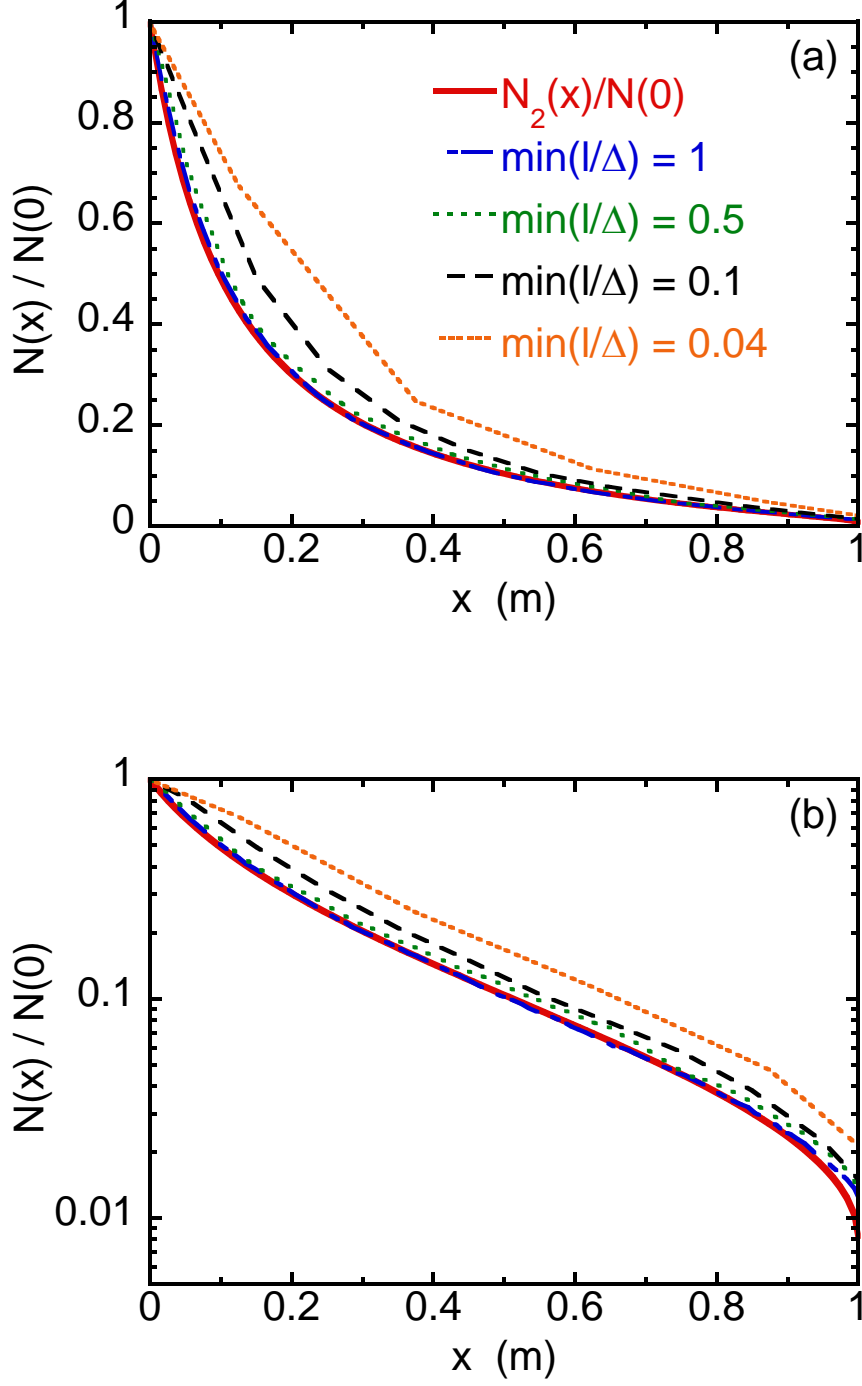
Figure 1: Normalized neutral density profiles on linear (a) and semi-log (b) scales for the second solution of [1] and four DEGAS 2 runs with varying amounts of spatial resolution. In particular, these runs utilized 100 [$\min(l/\Delta) = 1$], 50, 10, and 4 grid points.

2 Detailed Investigation

In this document, we revisit the comparisons described above and in [4] in the interest of making them more objective and rigorous. In particular, "agreement" in [4] and the precursor DEGAS simulations was qualitatively established. Here, we will use the error estimates described in [1] and those associated with the DEGAS 2 simulations to establish a firmer, quantitative basis for the original conclusions. To do this, we first need to estimate the errors in the DEGAS 2 results.

2.1 Error Estimates for Simulated Results

For the purposes of this comparison, we will assume that the dominant source of error [beyond that associated with the dimensionless parameters $\max(l/L)$ and $\min(l/\Delta)$ of Sec. 1] in the simulated results is that due to the Monte Carlo statistics. These errors are, of course, randomly distributed. There may be other, perhaps systematic errors, in the problem that remain to be investigated. The effects due to deviations of the actual charge exchange cross section [5] from the $\sigma_{\mathrm{cx}} = 4 \times 10^{-19}$ m^2 value used in [1] in particular need to be examined (see Sec. 2.3).

The output from most Monte Carlo simulations, including DEGAS 2, consists of the mean value for the quantity of interest (here, the neutral density at a point in the problem space), as well as its standard deviation. As noted in the previous paragraph, we will set the error bars for our simulated results equal to this standard deviation.

As a check on the processing of the DEGAS 2 statistics, we show that this standard deviation has the expected scaling. Namely, it should vary as $1/\sqrt{N}$, where N is the number of Monte Carlo particles or "flights" used in the simulation. The baseline simulation utilizes 6400 flights. As shown in Table 2.1, the average (over all "zones" in the simulation) relative standard deviation σ/μ (ratio of the standard deviation to the mean) follows the expected scaling as the number of flights is increased and decreased by a factor of two.

2.2 Effect of Varying Spatial Resolution

The comparison documented in [4] focused on the spatial resolution required to adequately simulate the thermal force. We now repeat this exercise, but

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Flights	$\langle \sigma/\mu \rangle$
1600	2.9×10^{-2}
6400	1.5×10^{-2}
25,600	7.4×10^{-3}

Table 1: Variation of relative standard deviation with number of flights.

replace the qualitative assessment of agreement made there with one based on a quantitative error analysis.

The data presented in [4] are reproduced in Fig. 1 (the results differ in subtle ways from those in [4] due to intervening modifications to DEGAS 2). For the reasons described in [1], the DEGAS 2 results have been rescaled to match the semi-analytic solution $N_2(x)/N(0)$ at the first grid point.

The errors associated with the baseline simulated, $N_D/N(0)$ (standard deviation σ_D), and semi-analytic, $N_2/N(0)$ (standard deviation σ_2), results are plotted in Fig. 2. Comparing the density profiles amounts to examining the difference, $|N_D/N(0) - N_2/N(0)|$. By propagation of errors, the expected standard deviation in this quantity is $\sigma_{\text{eff}} = \sqrt{\sigma_D^2 + \sigma_2^2}$; its variation with x in the baseline case is also shown in Fig. 2.

We can then use the relative difference $|N_D/N(0) - N_2/N(0)|/\sigma_{\text{eff}}$ to determine which of the DEGAS 2 solutions match the semi-analytic result (Fig. 3). Not surprisingly, the relative differences are largest for the $\min(l/\Delta) = 0.04$ case and smallest for the $\min(l/\Delta) = 1$ run. The average of the relative differences for the $\min(l/\Delta) = 1$ run is 0.57, i.e., < 1, allowing us to conclude that the two results match to within the estimated errors; This is also true for the $\min(l/\Delta) = 0.5$ case in which the average relative difference is 0.86, confirming the spatial resolution criterion quoted in [4], $\min(l/\Delta) \leq 0.5$. What went unnoticed in [4], however, was that the quality of the agreement in the two cases satisfying this restriction was poorer for $x < 0.2$ than elsewhere, with relative differences there well in excess of 1, suggesting that there may be some persistent systematic error. Additional investigation would be required to determine the cause of this apparent discrepancy.

2.3   Effect of Varying Plasma-Neutral Coupling

The simulations described above all have $\max(l/L) = 0.1$. We now examine the effect of varying l on the level of agreement between the simulated and
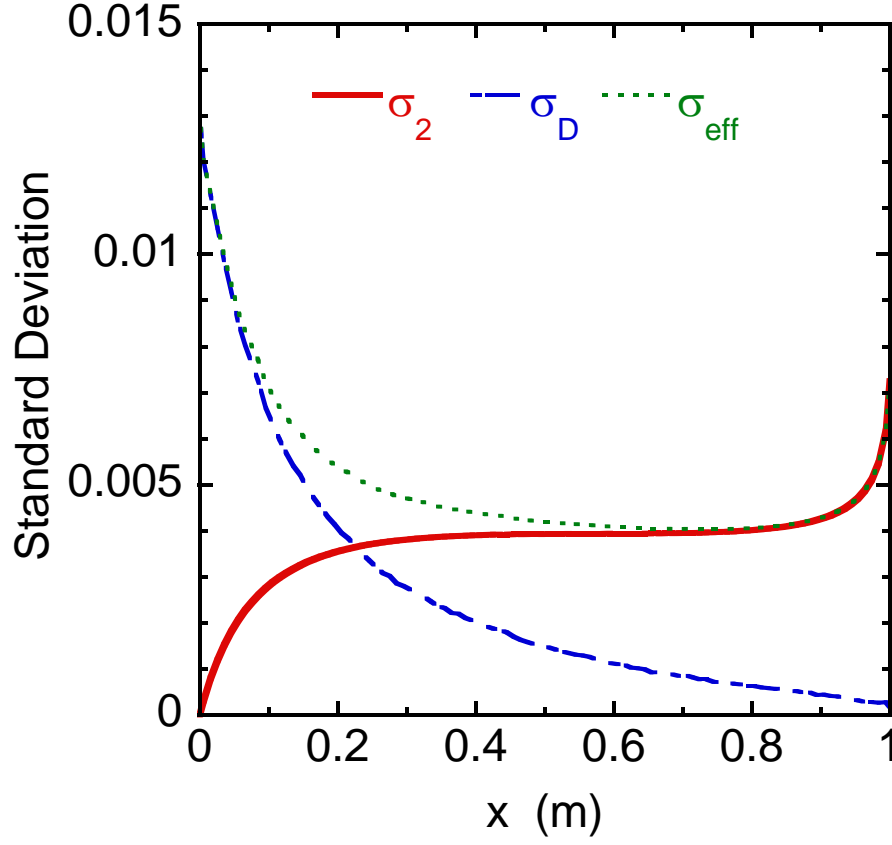
Figure 2: Standard deviation associated with the semi-analytic solution, σ_2, the baseline $[\min(l/\Delta) = 1]$ DEGAS 2 result, σ_D, and the expected standard deviation in the difference between the semi-analytic and simulated density profiles, σ_{eff}.
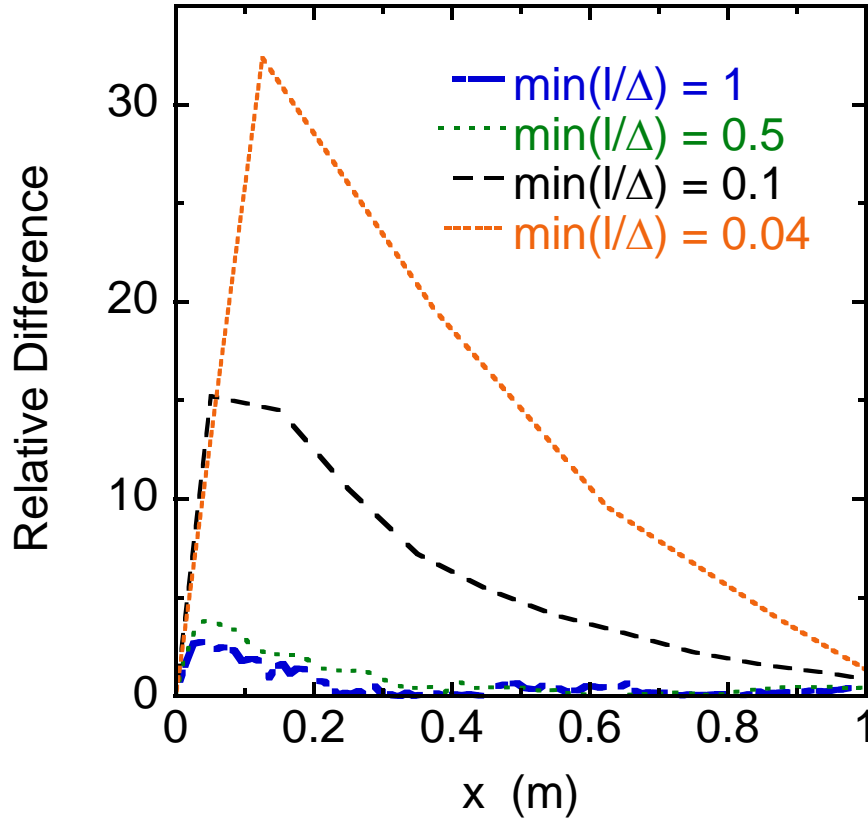
Figure 3: Relative differences $|N_D/N(0) - N_2/N(0)|/\sigma_{\text{eff}}$ between the four DEGAS 2 runs shown in Fig. 1 and the semi-analytic result.

$\min(n_i)$ (m^{-3})	$\max(l/L)$	# Grid Points
1.7×10^{18}	0.5	20
8.5×10^{18}	0.1	100
4.25×10^{19}	0.02	500

Table 2: parameters used in varying neutral mean free path.

semi-analytic density profiles. We do this by altering the plasma ion density. But, to keep the value of $\min(l/\Delta)$ unchanged, we make corresponding changes to the number of grid points in the simulation. The parameters for the three simulations to be considered here are provided in Table 2.3. Again, the middle case with $\max(l/L) = 0.1$ corresponds to the baseline simulation of the previous sections.

The degree of plasma-neutral coupling in the three cases is illustrated by the temperature profiles in Fig. 4. The simplest approach to computing the temperature from the DEGAS 2 output is to divide the neutral pressure (2/3 of the total neutral energy density) by the neutral density. But, the temperature appearing in the equations associated with the reference problem [1, 6] is evaluated relative to the frame of the neutral flow,

$$T_n = \frac{P}{N} - \frac{1}{2}mv^2. \tag{1}$$

As expected, the larger the value of $\max(l/L)$, the greater the deviation between T_i and T_n. Moreover, since the mean free path varies inversely with the ion density, the coupling is poorest near the exit where the density is lowest.

The resulting neutral density profiles and corresponding semi-analytic results are shown in Fig. 5(a). Note that unlike the variants shown in Fig. 1, the semi-analytic solution depends on the value $\max(l/L)$ so that each simulation has a corresponding semi-analytic profile. Not surprisingly, the DEGAS 2 simulation with the largest $\max(l/L)$ clearly deviates from its semi-analytic solution. The case with $\max(l/L) = 0.1$ is the same as in previous sections and constitutes acceptable agreement.

These qualitative assessments are confirmed by the relative differences shown in Fig. 5(b). The errors in the simulated and semi-analytic solutions were estimated in the manner described in [1] and in Secs. 2.1 and 2.2. Based on the various simulations leading up to [4], we would expect the case with
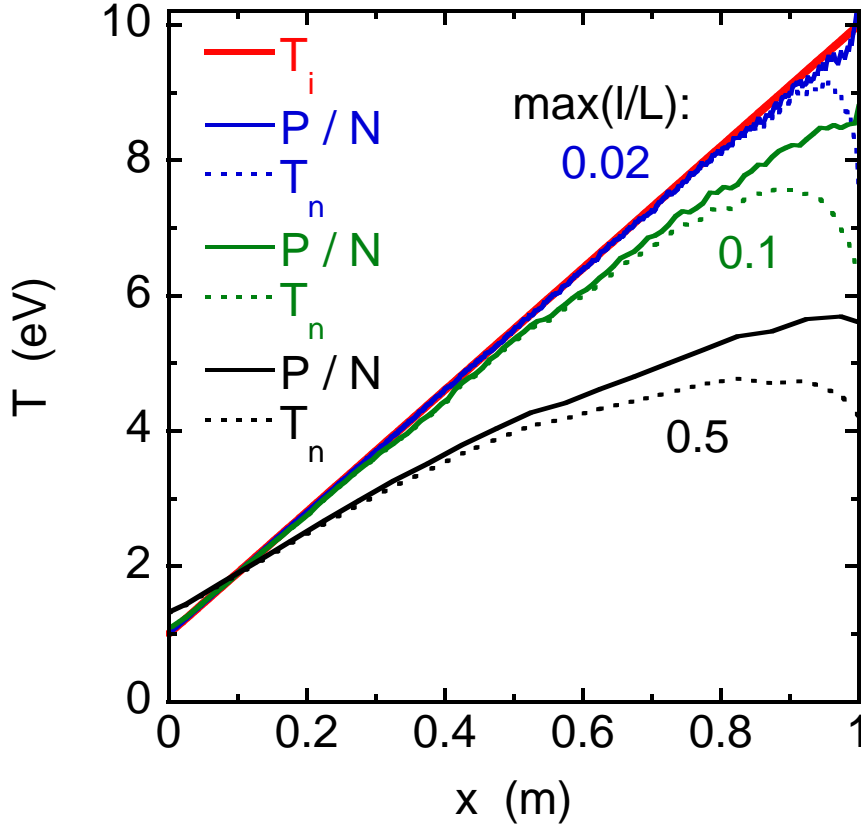
Figure 4: Temperature profiles for the plasma ions and three DEGAS 2 runs with different values of max(l/L). For each of the two simulations, the "total" temperature (computed by dividing the neutral density into the neutral pressure) and the thermal temperature (subtracting the drift energy) are plotted.
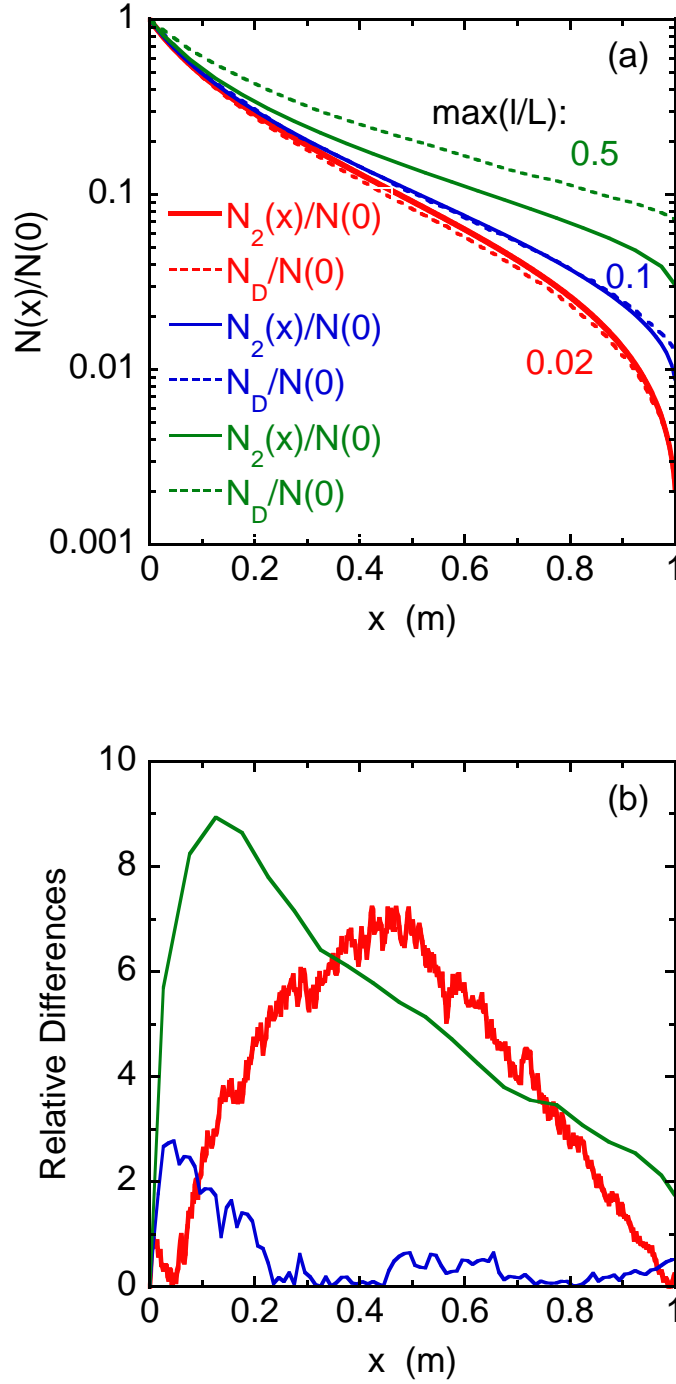
Figure 5: (a) Normalized neutral density profiles from three DEGAS 2 simulations and the corresponding semi-analytic profiles for different values of $\max(l/L)$. (b) The absolute differences between the simulated and semi-analytic neutral densities relative to the effective standard deviation.

$\max(l/L) = 0.02$ to agree *better* with the semi-analytic result than the baseline $\max(l/L) = 0.1$ case. However, the relative difference shown in Fig. 5(b) implies that this is not the case! The interesting contrast is that whereas all of the other simulations deviated from the semi-analytic result either near the entrance ($x = 0$) or the exit ($x = L$), the $\max(l/L) = 0.02$ differs most in the middle of the box. This suggests that the mechanism responsible for this discrepancy is distinct from that indicated in Sec. 2.2. Possible explanations include that the value of $1/\gamma$ appearing in the semi-analytic solution [1] needs to be > 2 in this case or that there are enough collisions in this simulation that the deviations of the charge exchange cross section from the constant value used in the semi-analytic solution are significant [1, 5].

3   Conclusions

Code verification is an ongoing process. The comparisons of both DEGAS and DEGAS 2 against this reference problem have been continuing for over 10 years with an ever increasing level of detail and scrutiny. As is clear from the unresolved discrepancies noted above, this process is not yet complete. This conclusion highlights a recurring characteristic of verification: that the tests are never as simple as they seem. New knowledge about the problem at hand and the code being verified will always be uncovered. This is even truer for the task of validation.

References

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