A Marie-Curie-ITN
within H2020

Proceedings of the 2nd MIGRATE Workshop
June 29-30, 2017 – Sofia, Bulgaria

MIGRATE-2017:154154

GENERALIZED BERNOULLI TRIAL COLLISION SCHEME IN DSMC APPLIED TO NANOCAVITY FLOW

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KEYWORDS

Direct Simulation Monte Carlo, Collision model, Generalized Bernoulli Trial (GBT) scheme.

ABSTRACT

The impetus of this paper is to present an evaluation of the performance a newly suggested collision scheme called Generalized Bernoulli Trail (GBT) in the nanocavity test case. The Kac stochastic equation is the starting point of the derivation of the Bernoulli Trail (BT), Balot Box (BB), Simplified Bernoulli Trial (SBT) and GBT schemes [1]. Variants of the Bernoulli Trail (BT) schemes such as BB and SBT reduce the number of selected pairs to check for a possible binary collision while they keep the accuracy of the solution in comparison with the original BT scheme. The number of considered pairs for a possible collision per each cell in the above-mentioned schemes varies between $N(N-1)/2$ in BT, 1 in BB, and (N-1) in SBT, where N is the number of particles per cell. The GBT scheme is aimed to work with any desired number of collision pairs, e.g., $N_{sel}<N-1$. This new collision scheme proposed in [2] further reduces the computational effort of the SBT collision model if the number of simulator particles is not small. In this research, rarefied flow in a lid-driven nanocavity is simulated to evaluate the performance of the GBT scheme using various N_{sel} magnitudes. Our GBT results are compared with the SBT solution in terms of accuracy and computational efficiency.

GBT Scheme

The problem with the SBT scheme is that most of the N-1 selected pairs for a possible collision will not have a significant acceptance chance if a small time step is considered. It is because SBT collision probability directly depends on the time step. In this occasion, it is preferred to reduce the number of selected pairs (N_{sel}) to a lower magnitude but increasing the pair weight and respectively the collision probability such that the collision frequency remains intact. According to [2], the GBT procedure is as follows:

1- Select N_{sel}, i.e., assume N_{sel} is a fraction/function of number of particles in the cell. The following procedure is performed if $N_{sel}<N^{(l)}-1$ in the cell, otherwise, standard SBT scheme is followed [2].
2- Choose N_{sel} random particles from the list of particles in the cell; we assume that the movement step of the DSMC solution made the particle set in a cell randomly ordered,
3- Run the SBT procedure from i=1 to N_{sel}, but modify the collision probability of every pair with the following correction:

$$W_{ij} = \frac{k'k * F_{num} dt \sigma_{ij} g_{ij}}{V^l} \tag{1}$$

, where

$$k'k = \frac{C(N^{(l)},2)}{N_{sel}(2N^{(l)} - N_{sel} - 1)}(N_{sel} - i\,). \qquad (2)$$

$\boldsymbol{C(n,m)}$ is the number of combinations of *m* from *n* elements.

Results and discussion

The square lid-driven nano-cavity of length 90×10^{-9} m containing the argon gas at Kn=0.1 is considered. The lid velocity is set at 1000 *m/s*, and all walls are diffuse reflectors at a constant temperature of 300 K. The GBT scheme was implemented in the DSMC2.FOR code of Bird [3]. The accuracy of GBT scheme in the prediction of the cavity flow is depicted in Fig. 1 where GBT results with different N_{SEL} values is compared with those of SBT with the same number of particles per cell, PPC=10, for all cases. A grid of 200×200 cells was used. In Fig. 1-left, the dimensionless x-velocity, and y-velocity distributions are plotted along the vertical and horizontal centerline of the cavity, respectively. The right frame in this Figure shows the normalized velocity slip and temperature jump. Both frames show excellent agreements between GBT and SBT results in the prediction of velocity and temperature fields. Table 1 compares simulation time of SBT and GBT schemes with various N_{sel}. The table shows that simulation time does not decrease monotonically with reducing N_{sel}.

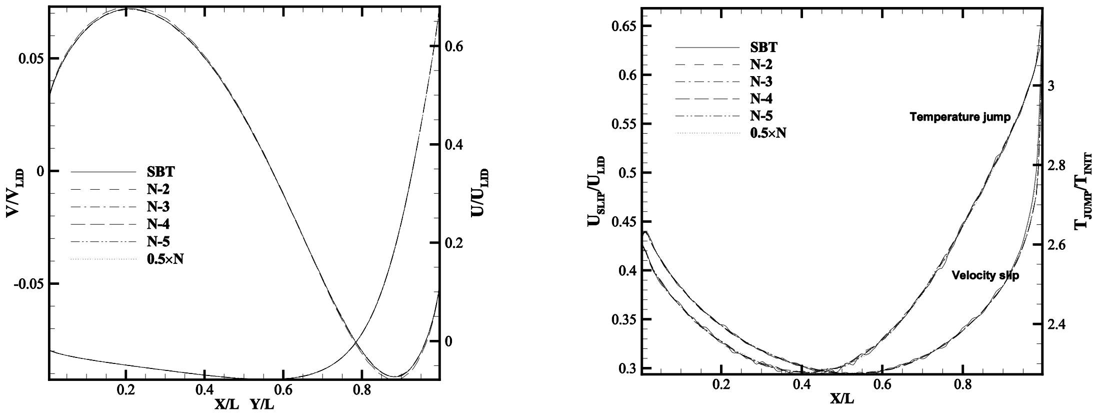

Figure 1: Left: Velocity distribution along the vertical and horizontal centerlines of the cavity, Right: Velocity slip and temperature jump over the lid.

N_{sel}	*N*-1 (SBT)	*N*-2	*N*-4	*N*-5	*N*-6	0.5×*N*
Normalized Simulation time	1	0.96	0.86	0.80	0.71	0.74

Table 1: CPU time of SBT solution and GBT solution with various N_{sel}, *N* is the instantaneous number of particles per cell.

Acknowledgements

This study has received funding from the Horizon 2020 Marie Skłodowska-Curie program under grant agreement MIGRATE No 643095. Two of the authors, E.R and S.S., acknowledge the financial support of the Bulgarian NSF under grant FNI_2016_DH-02-7. E.R also acknowledges supports from Iranian National Science Foundation (INSF) under grant No. 96000742.

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