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Modeling of plume impingement by a hybrid FP–DSMC method

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Abstract

In this work we present a numerical analysis of a nitrogen plume impinging on a flat plat via the Direct Simulation Monte Carlo (DSMC), Fokker–Planck (FP), as well as hybrid FP–DSMC methods. We show that the hybrid–FP approach can produce numerical results very close to the DSMC solution while having a computational cost close to that of a FP only simulation. In the hybrid simulation the maximal deviation to DSMC results in the temperature plume center line profile is reduced from 49.1 % to 7.3 % while the deviation in the surface heat flux could be reduced from 14.2 % to 3.9 % when compared to an FP only simulation. This was achieved with a minimal increase of computational time of 13.4 % when compared to pure FP simulation. The hybrid simulation only took 16.1 % of computational time when compared to DSMC simulation showing that hybrid–FP simulation can be qualitatively high with a relatively low computational cost for certain test cases. These results could be achieved without additional speed up measures like variable particle weights, model specific grid refinement or local time stepping.

Keywords: *kinetic methods, Fokker–Planck, DSMC, hybrid*

Nomenclature

Latin
c – Vibrational relaxation parameter
C – Thermal molecule velocity
d – Diameter
f – Velocity distribution function
L – Distance plate–orifice
m – Mass
n – Number density
p – Pressure
r – Radius
t – Time
T – Temperature
U – Hydrodynamic velocity
V – Molecule velocity
$\dot{q}$ – Heat flux

Greek
β – Plume angle
θ – Characteristic temperature
λ – Mean free path
ω – VHS parameter
Superscripts
$*$ – Orifice property
Subscripts
0 – Plenum property
comp – Computational
k – Facility property
ref – Reference
rot – Rotational
vib – Vibrational
w – Wall property

1. Introduction

During space craft operations a thruster plume can reach and impinge neighboring surfaces due to its spread in high vacuum. This can produce undesired forces or heat loads on especially large areas like solar arrays. Additionally plume impingement can negatively impacting sensitive surfaces like optical

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diagnostics [1]. Degradation of critical surfaces as well as correction burns which use up valuable propellant can greatly reduce the spacecraft's life time. Reliable and accurate modeling of plume impingement effects is therefore an important factor in the design process of spacecraft [2, 3]. Leading to impingement the flow exiting a nozzle goes through a wide range of Knudsen numbers as it expands into vacuum and compresses again due to interactions with the surface [1]. These effects can be described by the Boltzmann equation. A common approach to numerically solve it is the Direct Simulation Monte-Carlo (DSMC) method pioneered by Bird [4]. The method is very efficient for high Knudsen numbers but becomes increasingly computationally intensive when approaching the continuum limit. In this flow regime computational fluid dynamics (CFD) methods are normally used as they provide a high level of maturity and efficiency. As problems like plume impingement require the simulation of a wide range of Knudsen numbers a coupled approach using DSMC and CFD methods can be employed [5]. However, this leads to many issues when two way coupling is required, stemming among others from noise produced by DSMC especially at low Mach numbers [6]. Another way to model the flow in the continuum limit is the kinetic Fokker-Planck (FP) method [7] which, like DSMC, relies on simulated particles to transport mass, momentum and energy through the flow domain, but does not resolve individual collisions which leads to the computational time being independent from the Knudsen number. Both DSMC and FP use particles for the discretization of the velocity distribution function. When applying a coherent position integration scheme in the push step, the models can be coupled leading to an efficient simulation method which solves many of the issues one faces when coupling DSMC to classical CFD methods [8].

In a previous study nitrogen plume impingement experiments were analysed via the FP as well as the DSMC methods [9]. It was found that FP simulations provided a large performance gain and were able to predict surface pressure and shear stress very well when compared to the DSMC model. However, larger differences between the two models were observed in the plume flow fields as well as in the surface heat flux. The goal of this study is to analyze and quantify those differences and use the knowledge gained to select a switching criterion such that a hybrid DSMC–FP simulation can be carried out, generating numerical results comparable to the DSMC model while imposing minimal strain on computational performance. All DSMC simulations are carried out using the code SPARTA [10], while the FP model is implemented as an extension of the same framework.

This paper is structured as follows: in section 2 we provide a short overview over the DSMC as well as the FP models and the FP–DSMC hybrid approach. In section 3 we explain the experimental setup on which the simulations are based and lay our our approach for the numerical analysis. We discuss the simulation results and analyse differences of the hybrid approach when compared to the pure FP model as well its impart on performance. Finally we provide a summary of the work in section 4 and give an outlook to future work.

2. Methods

2.1. Direct Simulation Monte Carlo Method

The idea behind the DSMC method is to "directly" model particle motion and interactions by the use of numeric particles [4]. Each particle represents a large number of real molecules and carries information about its position, velocity, internal energy state, as well as species properties. It can be rigorously proven that the DSMC approach provides a solution to the Boltzmann equation for monoatomic gas [11]. Additionally comparison to experiments strong points to the fact that DSMC is also able to accurately model gases and gas mixtures of molecules with internal energy states [12, 13] as well as chemically reacting gases [14]. This method has become the working horse for the modelling of non-equilibrium gas flows in the rarefied regime. However, there are two major reasons for the restriction of the DSMC methods to this regime. One is the assumption behind DSMC of splitting of particle movement and particle–particle as well as particle–wall interactions. It is done by the use of distinct free flight phases with constant velocity and collision phases in which particles change their velocities and potential internal energy states. This imposes temporal and spatial restrictions on the model which are in the order the collision frequency and the mean free path respectively. The second restriction comes from the need to resolve particle interactions which would require the testing of all particle pairs in a given volume cell for collisions. Several methods were developed to minimize the number of tested pairs. The one used for this work is the No Time Counter (NTC) introduced by Bird [4] which uses cell averaged properties of the particles to estimate the number of pairs being tested. While this greatly reduces computation cost the number of collisions still becomes significant, sometimes prohibitively so, for large local densities like those encounters in nozzle and plume impingement flows.

2.2. Kinetic Fokker–Planck Method

Like DSMC, FP has the goal to solve the Boltzmann equation which describes the evolution of a scalar distribution function f in flows in a wide range of regimes:

$$\frac{\mathrm{D}f}{\mathrm{D}t} = S_{\mathrm{Boltz}} \,, \tag{1}$$

where t is time and S_{Boltz} is the Boltzmann collision integral. The FP approach to make the integro-differential Eq. (1) more manageable is to approximate S_{Boltz} by a Fokker-Planck collision operator S_{FP}:

$$S_{\mathrm{Boltz}} \approx S_{\mathrm{FP}} = -\frac{\partial}{\partial V_i}(A_i f) + \frac{\partial^2}{\partial V_j \partial V_j}\left(\frac{D^2}{2} f\right) \,, \tag{2}$$

where $\mathbf{V}$ is the molecule velocity with indices given in the Einstein notation. Eq. (2) can be solved using a particle method similar to the DSMC approach, but with the collision step being replaced by a velocity update of the particles which does not rely on collision pairs, thus making the computational cost of the FP method become independent of the Kn number. The drift coefficient A_i and the diffusion coefficient D of Eq. (2) are model parameters chosen in such a way that production terms calculated using the Boltzmann collision operator are reproduced by the production terms using the FP collision operator [7]

$$P_{\mathrm{Boltz}} \stackrel{!}{=} P_{\mathrm{FP}}. \tag{3}$$

For the simulations presented in this paper we use the FP cubic model [15], which uses a polynomial ansatz for the drift coefficient. The coefficients of the polynomial are fitted by calculating the set of production terms defined as

$$P(X) = \int SX \mathrm{d}\mathbf{C}, \quad X \in \{C_i,\, C_iC_i,\, C_{<i}C_{j>}C_iC_jC_j\} \tag{4}$$

where $\mathbf{C} = \mathbf{V} - \mathbf{U}$ is the thermal molecule velocity and $\mathbf{U}$ the macroscopic gas velocity. Here $C_{<i}C_{j>}$ refers to the deviatoric part of the tensor C_iC_j. Equality of production terms of the same order between two kinetic models shows that these models display equal behaviour in the continuum limit [16]. Therefore, choosing this set ensures that velocity moments up to the heat flux are correctly reproduced by FP model. Over the last years our FP implementation has been extended to model internal degrees of freedom using the Master Equation Ansatz for diatomic [17] and polyatomic molecules [18, 19] as well as mixtures [20, 21]. Lately an approach to model chemical reactions has been introduced in the FP framework [22].

2.3. Hybrid FP–DSMC Method

As discussed earlier the DSMC model faces strong computational costs due to the modelling of individual collisions inside the cell. The FP model provides a significant speed up compared to DSMC for areas with large local densities and therefore a large number of collisions per time step. However, it is technically only valid for modelling flows close to equilibrium and therefore only for low to moderate Knudsen numbers. This is also the area where FP shows the largest computational advantages when compared to DSMC. FP can be easily hybridized with DSMC on a cell by cell basis by changing only the collision step based on some decision criteria. Several continuum break down criteria where investigated over the years for the purpose of creating a hybrid DSMC approach coupled to other methods [23, 24, 25, 26]. For this study the criteria introduced by Boyd [27], Kn_Q as defined in equation 5 is used:

$$\mathrm{Kn}_Q \equiv \frac{\lambda}{Q}\|\nabla Q\|, \quad Q \in \{T, \rho, U\}. \tag{5}$$

It has the advantage of not being defined for only specific types of flows and is easily evaluated during run time and in post processing. For the following study a critical values of $\max(\mathrm{Kn}_Q) = 0.04$ was chosen which was found to provide a good balance between performance and quality increase of the simulation results.

3. Numerical Analysis of Plume Impingement

3.1. Experimental Setup

The basis of the presented numerical analysis is formed by a test campaign carried out by Doering [28] to investigate surface heat flux in a nitrogen plume impinging on a flat plate. The experiments were conducted at the German Test and Research Institute for Aviation and Space Flight (DFVLR), now named German Aerospace Center (DLR). The experimental setup can be seen in Fig. 1 were p_0 and T_0 are stagnation values inside the plenum and p_k and T_k are the facility background pressure and temperature respectively. The heat flux was evaluated by the rate of change of surface temperature

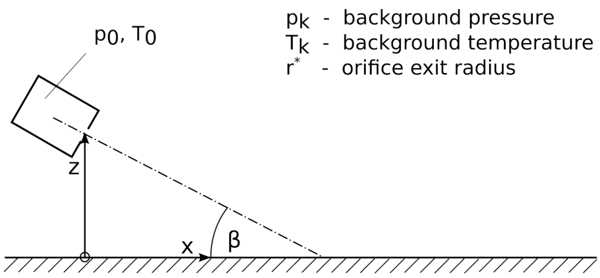


Fig 1. Experimental setup

which was measured using thermocouples. The measurements were performed on the surface along a line coplanar with the plume axis. The plume was generated using nitrogen gas flowing through a circular orifice with a radius of $r^* = 1\,\mathrm{mm}$. The unheated flow ($T_0 = 300\,\mathrm{K}$) expands from a stagnation pressure of $p_0 = 1000\,\mathrm{Pa}$. The flow is sonic at the exit. The relevant physical data is summed up in Tab. 1. Here

Table 1. Experimental parameters

$p_0\,/\,\mathrm{Pa}$	$p_k\,/\,p_0$	$r^*\,/\,\mathrm{mm}$	$L\,/\,r^*$	$\beta\,/\,°$
1000	9×10^{-5}	1	40	90

L refers to the distance from the orifice to the flat plate. During the experimental campaign the angle between the plume centerline and the plate β was varied. For the presented study the perpendicular case of of $\beta = 90°$ was chosen to exploit symmetry. Numerical analysis comparing DSMC and FP simulations to experimental results can be found in [9].

3.2. Simulation Setup

Three simulations where carried out. A DSMC, a FP, and a hybrid DSMC–FP simulation. All three used the same simulation setup of a 3D quarter domain box with its corner centered at the center of the orifice as seen in figure 2. The walls representing symmetry planes were modeled using specular reflection while the boundary condition for the flat plate was chosen to be diffusively reflecting with an accommodation coefficient of 1 and a surface temperature of $T_\mathrm{w} = 300\,\mathrm{K}$. The orifice was assigned the inflow boundary condition while all other surfaces had the background condition assigned. Numeric values for those conditions are summarized in Tab. 2. All simulations used the Variable Hard Sphere

Table 2. Simulation parameters

	$n\,/\,\mathrm{m}^{-3}$	$T\,/\,\mathrm{K}$	$u\,/\,\mathrm{m\,s^{-1}}$
Inflow	1.531×10^{23}	250	322.366
Background	2.173×10^{19}	300	—

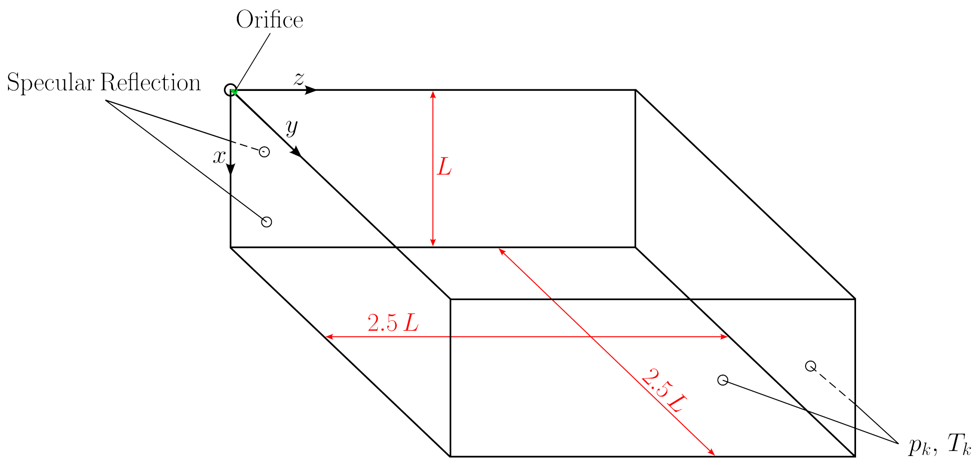


Fig 2. Numerical setup

(VHS) type gas model with a variable collision number to model relaxation of rational and vibraitonal degrees of freedom as defined by Bird [4]. For the FP simulations the internal energy states are modeled via the Master Equation ansatz introduced by Hepp et al. [17]. The model parameters can be found in Tab. 3. All simulations used a time step of $\Delta t = 1 \times 10^{-6}$ s and where run for 8000 steps to reach steady

Table 3. N_2 model parameters

$m\,/\,\text{kg}$	$d_{\text{ref}}\,/\,\text{m}$	ω	$T_{\text{ref}}\,/\,\text{K}$	Z_{rot}^{∞}	$T^*\,/\,\text{K}$	$\theta_{\text{vib}}\,/\,\text{K}$	$c_1\,/\,\text{K}$	$c_2\,/\,\text{K}^{-3}$
4.65×10^{-26}	4.07×10^{-10}	0.74	273.15	18.1	91.5	3371.0	9.1	220.0

state before sampling the results for another 2000 steps. A constant particle weight of $w = 2 \times 10^8$ was used.

For the hybrid simulation a switching criterion of $\max(\text{Kn}_Q) = 0.04$ was chosen which was found to provide a good balance between performance and quality increase of the simulation results. For the given plume impingement test case this value can be mapped to a number density iso-surface of $n_{\text{crit}} = 2 \times 10^{22}\,\text{m}^{-3}$. This isosurface was used as the switching point between DSMC and FP where the DSMC model was applied for $n < n_{\text{crit}}$ after a FP simulation has reached steady. The now hybrid simulation was then given another 100 steps to reach equilibrium before the start of the sampling process.

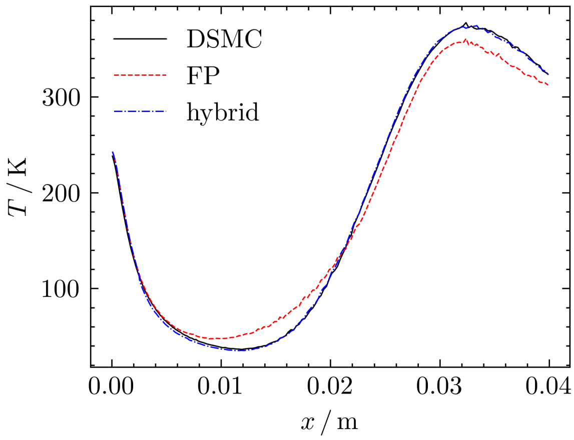
3.3. Results and Discussion

The simulations were carried out on a single node of the DLRs own high performance computing cluster CARO (Computer for Advanced Research in Aerospace) [29]. The FP simulation provides a significant speed up compared to DSMC. The computational time required by the FP model for the 2000 sampling steps was only 14.2 % of the used by DSMC. The hybrid simulation was only insignificantly slower, taking 16.1 % of the DSMC computational time. However, looking at deviations between the models it is clear that the hybrid model far better reproduced the pure DSMC results. Simulation results plotted over the center line of the plume a visualized in Fig. 3 where the deviations, given a quantity Q, to the DSMC model is defined as

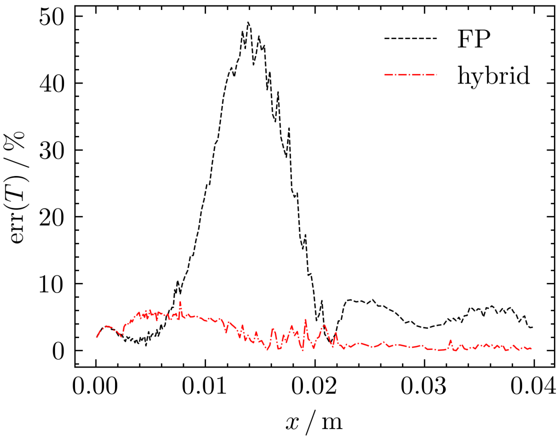
$$\text{err}(Q) \equiv \frac{\left|Q - Q^{\text{DSMC}}\right|}{Q^{\text{DSMC}}}. \tag{6}$$

Especially the temperature profile shown in figures 3 has very large deviations (figure 3b) when compared to the DSMC simulation of up to 49.1 % compared to the maximum 7.3 % deviation seen in the hybrid results. While not as extreme, there is a clear improvement of the maximal error for the number density from 9.1 % to 2.3 % as well as in the velocity from 9.2 % to 4.3 %.

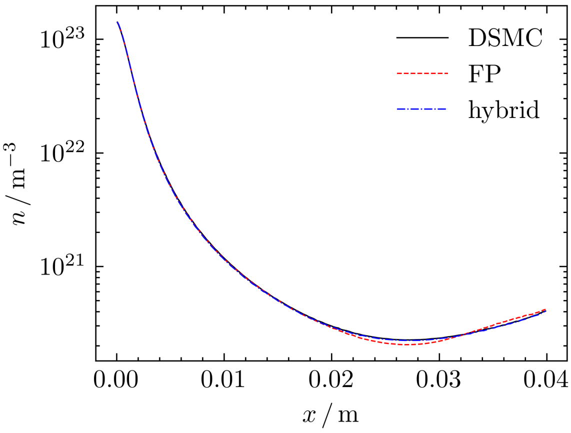
As expected, the deviations in the temperature profile propagate themselves to the surface heat flux.



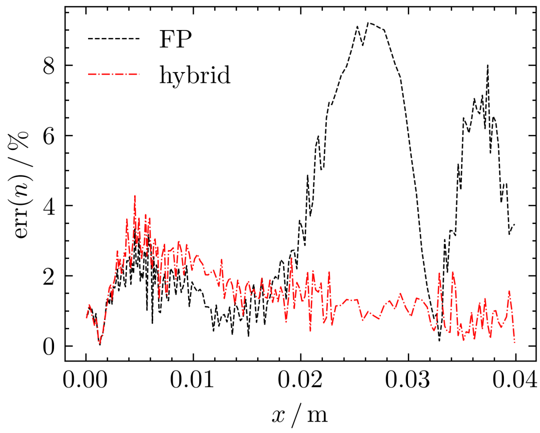
(a) Temperature



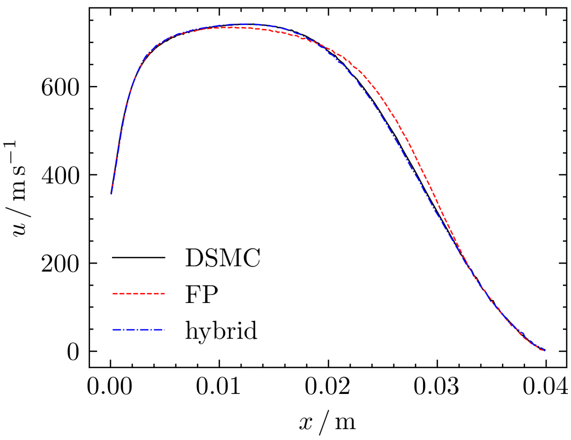
(b) Temperature deviations



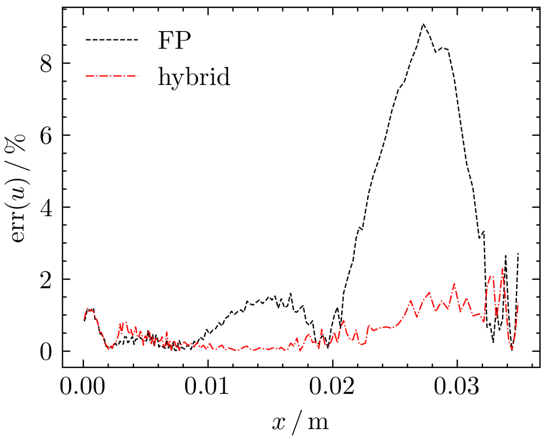
(c) Number density



(d) Number density deviations

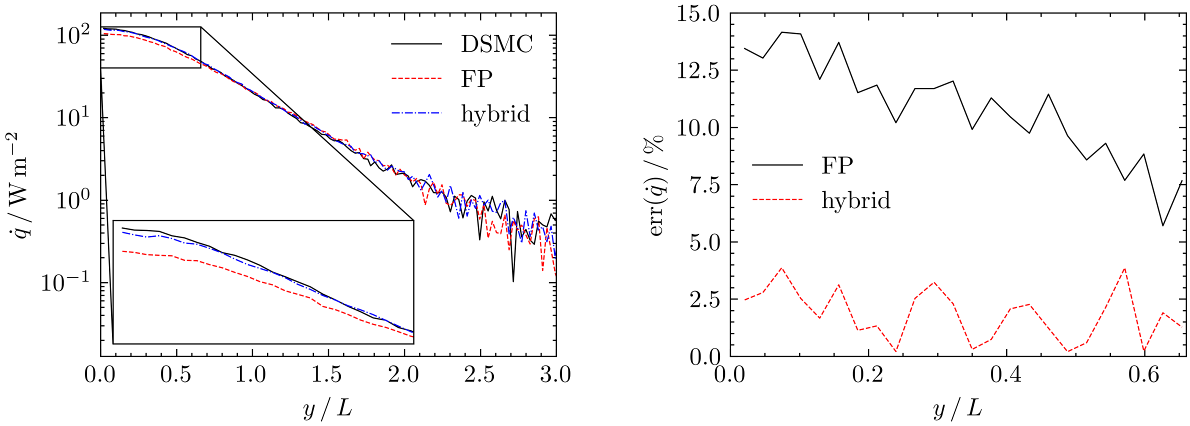


(e) Velocity



(f) Velocity deviations

Fig 3. Hydrodynamic values and their deviations between the models over the plum cetner line



(a) Surface heat flux

(b) Relative error in surface heat flux

Fig 4. Surface heat flux in radial direction

Surface heat flux and associated deviations plotted along die diagonal are displayed in figures 4a and 4b respectively. Here the maximal deviation could be reduced from 14.2 % to 3.9 % showing again the potential of the hybrid approach.

Maximal deviations of FP and the hybrid approach to DSMC as well as the comparisons of computational times are summarized in Tab. 4.

Table 4. Maximal FP to DSMC deviations and comparison of computational times

	FP	**Hybrid**
$t_{\text{comp}} \,/\, t_{\text{comp}}^{\text{DSMC}}$ / %	14.2	16.1
err(T) / %	49.1	7.3
err(u) / %	9.2	4.3
err(n) / %	9.1	2.3
err($\dot{q}$) / %	14.2	3.9

4. Conclusion and Outlook

A large reduction of deviation to numeric DSCM results was achieved by employing a hybrid-FP simulation when compared to FP only simulations. The maximal deviation in the temperature profile center line was reduced from 49.1 % to 7.3 % while the deviation in the surface heat flux was reduced from 14.2 % to 3.9 %. This was achieved with a minimal increase of computational time of 13.4 % when compared to pure FP simulation. The hybrid simulation only took 16.1 % of computational time when compared to DSMC showing that the hybrid–FP approach can produce numerical results very close to DSMC fidelity while being comparatively cheap in terms of computational cost for certain test cases. These results was achieved without additional speed up measures like variable particle weights, model specific grid refinement or local time stepping.

Next steps in the development of the hybrid approach will put a strong focus on the switching criteria which are very import in achieving a good balance between quality of the results and computational time. A general quantitative relation between numeric values of the broad selection of continuum break down criteria and computational time and quality gain is not available. While this will not be easily achieved, a case–specific data base can be created taking a first step towards hybrid automation.

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