

# Comparison Between the Kinetic Fokker-Planck and TAU Navier-Stokes Simulations of Hypersonic Air Flow Around the the RFZ-ST2 Upper Stage



Moritz Ertl and Leo Basov

**Abstract** We are developing a kinetic Fokker-Planck (FP) method to complement our existing computational fluid dynamics (CFD) code for aerodynamic and aerothermal simulations of space applications. The FP method is capable of simulating problems at low atmospheric densities, where the continuum assumptions of the CFD lose their validity. The FP method solves the Boltzmann equation and has the additional benefit of being computationally effective for low Knudsen numbers when compared to the Direct Simulation Monte Carlo method (DSMC). The FP method has been extended to model internal degrees of freedom using the Master Equation Ansatz for diatomic molecules as well as mixtures. In order to validate the new FP implementations and to better understand the limits of CFD and FP, we are simulating an upper stage, as a large test case. In this work we continue previous investigation with CFD and FP of upper stages, by expanding the modelling from single species diatomic  $N_2$  gas to representing air as a gas mixture. We introduce the underlying simulation methods and explain the relevant differences. We compare the resulting flow fields.

**Keywords** CFD · Particle method · Fokker-Planck · Aerodynamics · Aerothermodynamics · Hypersonic flow · Upper stage

## 1 Introduction

Predictions of the flow around a vehicle play an important role in the development of space applications. Simulations can support the design process in many ways, from performance analysis, over load predictions to control system design. Computational fluid dynamics (CFD) are well established and well suited for applications in denser atmospheres, such as airplanes or first stages or reusable vertical takeoff

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landing (VTVL) stages [8]. However, the underlying continuum assumptions lose their validity for higher Knudsen numbers, which are the typical regime for upper stages at higher altitudes and lower atmospheric densities. In these higher Knudsen (Kn) number regimes the flow can be described by the Boltzmann equation. Our approach is to numerically solve the Boltzmann equation using the kinetic Fokker-Planck (FP) method [9]. It fulfills our requirement of being computationally efficient both for high Knudsen numbers and when approaching the continuum limit.

In order to validate the new FP implementations, to better understand the limits of CFD and FP and to investigate the differences, our team is currently looking into several test cases. One of the more applied and large cases we selected is the simulation of an upper stage. The aim is to validate the methodologies, to gain insights into their limitations and to establish best practices on where and how to apply each method for large scale engineering applications. For the CFD simulations the DLR TAU code is used. It is well established for the simulation of space applications [10]. For the FP simulations a DLR in-house development of the method has been implemented using the DSMC code SPARTA [16] developed at the Sandia National laboratories. The FP method has been extended to model internal degrees of freedom using the Master Equation Ansatz for diatomic [13] and polyatomic molecules [2] as well as mixtures [12, 13]. For the upper stage simulation, the second stage of the RFZ model was selected. The RFZ model is an initiative of the Spacecraft department of the Institute of Aerodynamics and Flow Technology at the German Aerospace Center in Göttingen, and aims to provide an open source, common research model for reusable launch vehicles [6]. The specifics of the upper stage are presented in ref [7]. In this work we continue our previous investigation with CFD and FP of the upper stage [1], by expanding the modelling from considering only single species diatomic  $N_2$  gas to representing air as a gas mixture. First we shortly introduce the underlying simulation methods and explain the relevant differences. We then compare the resulting flow fields and pressure distribution and discuss relevant differences.

## 2 Numerical Methods

The governing equation used to describe flows in a wide range range of regimes is the Boltzmann equation:

$$\frac{Df}{Dt} = S_{\text{Boltz}}, \quad (1)$$

where  $f$  is the scalar velocity distribution function,  $t$  is time, and  $S_{\text{Boltz}}$  is the Boltzmann collision integral. A common approach to numerically solve Eq. (1) is the DSMC method proposed by Bird [3] which is a stochastic model that solves the spatial and temporal evolution of simulation particles, each of which represents a large number of real molecules. The interactions between particles are assumed to be binary collisions with instantaneous changes of velocity. These assumptions require grouping of particles in cells with a size in the order of the mean free path and time

steps in the order of the collision frequency. The DSMC method has become very mature over the last decades and was shown to be applicable for complex problems with thermal and chemical non-equilibrium. However, applying the model in a flow regime close to continuum makes it prohibitively expensive due the aforementioned resolution criteria (see [4, 14] and references therein).

One approach to make Eq. (1) more manageable is to approximate the collision operator  $S_{\text{Boltz}}$  by a Fokker-Planck collision operator  $S_{\text{FP}}$ :

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

where  $V$  is the molecule velocity with indices given in the Einstein notation. Equation (2) can be reformulated as stochastic differential equation which in turn can be solved using a particle method similar to the DSMC approach. The collision step is then replaced by a velocity update of the particles which does not rely on the building of collision pairs 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 [15] with the extension for diatomic gas mixtures based on the master equation ansatz [11]. For the simulations presented in this paper we use the FP cubic model [9].

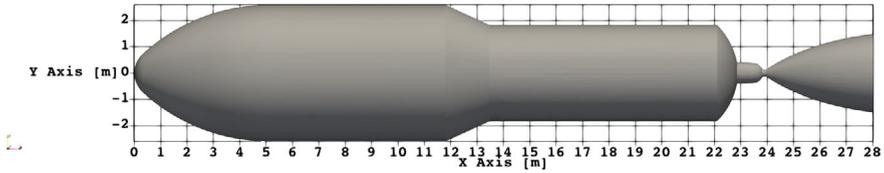
The CFD simulations are done using the well established DLR TAU code [17] with the spacecraft extensions [10]. TAU solves the compressible Navier-Stokes equations on finite volumes. We use a AUSMDV upwinding with a carbuncle fix combined with least squares gradient reconstruction and a 3-stage explicit Runge-Kutta scheme to achieve second order accuracy in space and time.

### 3 Numerical Setup and Geometry

#### 3.1 Definition of the Rocket Geometry and the Simulation Grids

The RFZ-ST2 model is a generic model of an upper stage for a VTVL reusable launch vehicle which is shown in Fig. 1. It is part of the RFZ model suite of open source rocket models created to provide a common research geometry for simulating VTVL reusable launch vehicles. The geometry sources and trajectory data are freely available at [5].

Both simulations are exploiting the rotational symmetry of the configuration by reducing the computational domain to a 2D axi-symmetric mesh. The CFD mesh is a body fitted triangular mesh with rectangular sublayer. The FP uses a cartesian hirachichaly refine mesh with the geometry represented as per cell surface elements.



**Fig. 1** Visualisation of the RFZ-ST2 upper stage geometry

The mesh refinement functionality of TAU and SPARTA are used to obtain well resolved grids. The final mesh used in this work consists of  $1.15 \times 10^6$  grid points. The FP simulation domain is a rectangular box with dimensions  $L_x = 41$  m,  $L_y = 12$  m, and  $L_z = 1$  m in  $x$ ,  $y$ , and  $z$  direction respectively. The volume grid was generated containing  $820 \times 240 \times 1$  cells and was locally adapted during a pre-run using SPARTA's build in grid adaptation method until each cell contained at least 10 numerical particles for a total of  $21 \times 10^6$  volume cells. The surface mesh contains 3192 faces.

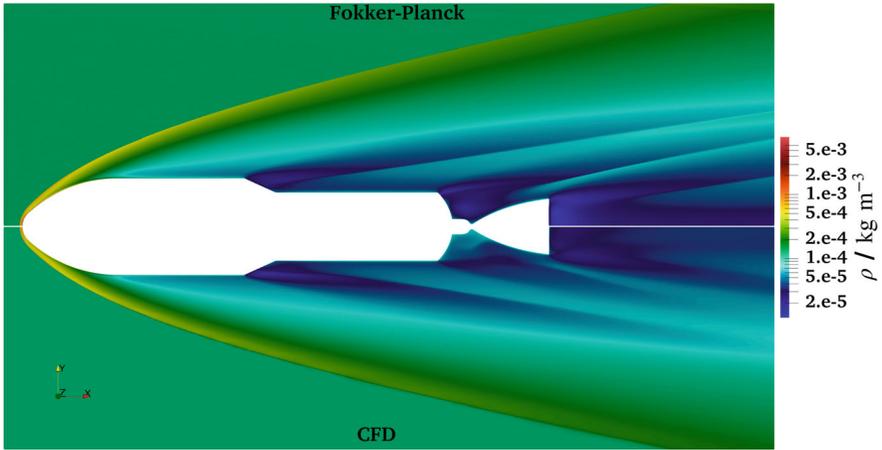
### 3.2 Settings and Boundary Conditions

A trajectory point within the applicable region of the CFD method is selected from [5] for an altitude of  $h = 70$  km. The trajectory point is used to define the farfield boundary condition for both simulations with a velocity in  $x$ -direction  $v_\infty = 2249.72$  m s<sup>-1</sup>, a density  $\rho_\infty = 1.2 \times 10^{-4}$  kgm<sup>-3</sup> and a temperature  $T_\infty = 226.9$  K. The gas is a mixture of diatomic nitrogen  $N_2$  and oxygen  $O_2$  with a mass fraction ratio of  $x_{N_2} : x_{O_2} = 0.767 : 0.233$ . A Knudsen number of  $Kn = 2.0 \times 10^{-4}$  was calculated for this flight regime using the largest diameter of the rocket  $L_{ref} = D_{fairing} = 2.6$  m as the reference length with the mean free path being calculated using the VHS model with parameters taken from [3].

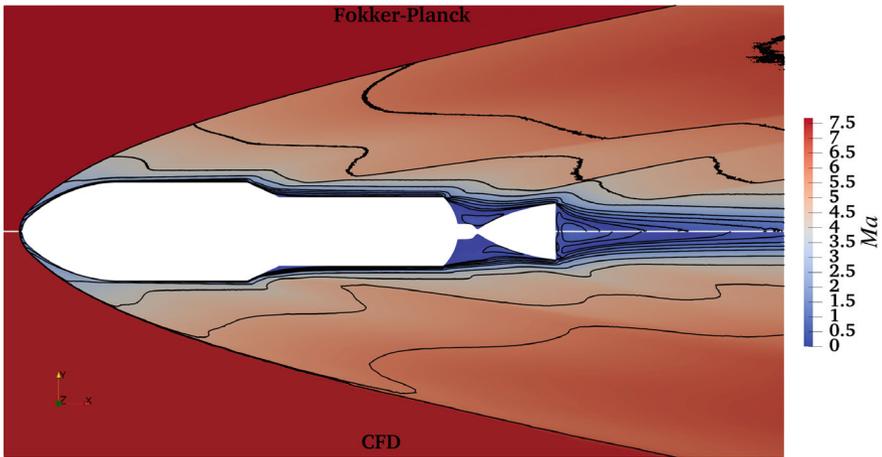
For the CFD the boundary condition for surfaces of the upper stage are set as isothermal viscous walls. The FP simulation uses a diffuse boundary condition for the surface with an accommodation coefficient of 1.0. Both simulations use a wall temperature  $T_w = 300$  K. The FP simulation was performed using a time step of  $\Delta t = 1 \times 10^{-6}$  s with a particle weight of  $w = 2 \times 10^{15}$ . The particle weight was chosen so that a minimum of 8 particles are present in each FP cell.

## 4 Results

The comparison of the flow fields is visualised as a  $x$ - $y$ -slice with the FP results displayed in the upper half and the CFD in the lower half. The density distribution is given in Fig. 2 with a logarithmic scale and the Mach number distribution show in Fig. 3.

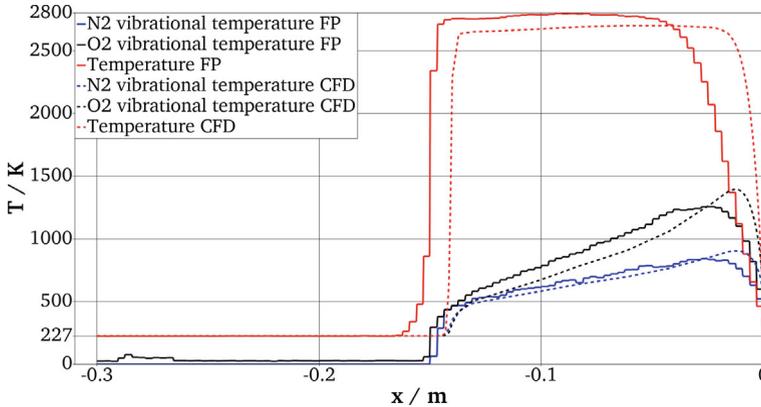


**Fig. 2** Comparative visualisation of the RFZ-ST2 upper stage density  $\rho$  distribution on a logarithmic scale for the Fokker-Planck simulation (upper half) and the CFD simulation (lower half)



**Fig. 3** Comparative visualisation of the RFZ-ST2 upper stage velocity  $Ma$  distribution for the Fokker-Planck simulation (upper half) and the CFD simulation (lower half)

The flow field visualisations exhibit a good agreement between the two methods. The structures and angles of shocks in the density visualisation show a good match, as do the the boundary layers and wake regions in the Mach number visualisation. The contour lines in the Mach plot reveal some differences especially in the wake region behind the vehicle. Here, the CFD struggles to resolve the weak shocks in the rarefied regions as sharply as the FP simulation. A difference can be observed in the shock stand-off distance and in the density behind the base plate. A plot of the translational temperature for the mixture and of the vibrational temperatures for both



**Fig. 4** Comparative Plot of the RFZ-ST2 upper stage temperature  $T$  distribution along a center line to the stagnation point for the Fokker-Planck simulation and the CFD simulation

$N_2$  and  $O_2$  over a center line along the  $x$ -axis into the stagnation point is provided in Fig. 4. The steps in the FP results are due to the grid.

The vibrational temperatures of the CFD converge by methodical construction towards an equilibrium with the translational temperature, leading to a value of  $T_{trans} = T_{vib} = T_{\infty} = 227$  K in the free stream. In the FP model the vibrational energies are modeled as discrete level. The probability of a particle changing its vibrational energy level is a function of the translational temperature. Hence the vibrational temperatures tends towards zero in the free stream, due to the low probability of a vibrational mode being excited. The difference in shock stand-off distance is visible in the translational temperature jump with FP predicting the shock at  $x_{S,FP} \approx 0.15$  m and CFD predicting it at  $x_{S,CFD} \approx 0.14$  m. This difference is assumed to be due to the modelling of the species mixtures in the FP method. The shock prediction of the DLR TAU is well established and validated and the authors have shown in [1] that the shock stand-off distance matches very well for FP and CFD for a single species free stream. The maximum temperatures of both translational and vibrational temperatures compare well. The relaxation also starts slightly sooner in the FP simulations.

## 5 Conclusions

We compared simulations of the open source generic upper stage RFZ-ST2 with a  $N_2$  and  $O_2$  species mixture free stream for a trajectory point at 70 km altitude. We simulated using the DLR CFD code TAU and our implementation of the kinetic Fokker-Planck particle method in the open source code SPARTA. The goal is to validate our FP method for use with industrial size cases of space vehicles at high

altitudes. Our results showed a general good agreement between the flow fields, with shock positions and angles comparing very well. Small differences were observed in the shock stand-off distance, which we attribute to the difference in Prandtl number from the current FP implementation. Other possible sources for the differences are the resolution in time and space as given by the cell size and the time step size, as well as the number of simulation particles given by the particle weight. Over all the study shows, that we have a first working implementation of a usable tool for simulating real scale upper stages in high atmospheres, while also pointing out some areas of possible improvements. One of our next steps is the development of a polyatomic model for FP which reproduces a correct Prandtl number for single species gases as well as mixtures. Additionally we are looking into increasing the complexity of our simulations by investigating upper stages with engine plumes.

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