SMILE System for 2D/3D DSMC Computations

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Abstract. This paper presents the software system SMILE for 2D/3D direct statistical simulation of rarefied flows. The system is designed for parallel computations on multiprocessor computers, is equipped by a user-friendly graphical interface, and includes sophisticated models of real gas effects. A generic description of the system structure and approaches implemented is given. Results illustrating the possibilities of the SMILE code are presented.

Keywords: DSMC, computation code, real-gas effects.
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INTRODUCTION

A wide range of problems in both science and industry, starting from micronozzles and extending to large aerodynamic configurations and complex fundamental investigations of rarefied flows, have been solved using the Direct Simulation Monte Carlo (DSMC) method [1, 2]**.** Thus, the-ever growing need for a robust, reliable, easy-to-use, and well-validated code for DSMC computations is clearly seen. Such a code should be well-documented and suitable for users without specialized training in DSMC techniques. There exist a number of both freeware and commercial packages that address these needs for numerically and ergonomically efficient DSMC systems. These codes include DS2V/3V developed and maintained by G.A.Bird [3], MONACO developed by Iain D. Boyd [4], and DAC developed in Johnson Space Center [5]. According to [3] the DAC system is 'evidently available for restricted distribution'.

The Laboratory of Computational Aerodynamics from the Khristianovich Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences has more than decade-long experience in the development of the DSMC method. The result of these efforts is a computational package called SMILE (Statistical Modeling In Low-Density Environment) capable of solving a very wide range of basic and applied problems. The SMILE system provides a complete lifecycle of computations starting from a geometry model, pre-processing, going through the computation proper, and finishing with post-processing and presentation of results. All SMILE subsystems have a Graphic User Interface (GUI), which makes them user-friendly and easy to use. The SMILE core code is written in FORTRAN90 and has no memory limitations specific to static FORTRAN programs. The user interface of the system is written in C++ and uses a free cross-platform wxWidgets GUI library.

DESCRIPTION OF THE SMILE SYSTEM

Operating conditions. SMILE is capable of handling a wide range of operating conditions. It can compute external flows, such as flows around models of space vehicles, internal flows for normal-size and microscale nozzles, and plumes expanding from the chamber into a rarefied medium. These flows can be computed for two-dimensional, axisymmetric, and three-dimensional geometry configurations. For external flows, the angle of attack may be varied from -180° to 180°, and the sideslip angle may lie between -90° and 90°. The molecular composition of the free stream or plume may contain N_2, O_2, N, O, CO_2, Ar, He, H_2O, H_2, CO, H, OH, O, and other elements. The SMILE system includes an extendable chemical database (Fig. 1) containing the properties of the above-listed elements and their collision parameters necessary for DSMC computations.

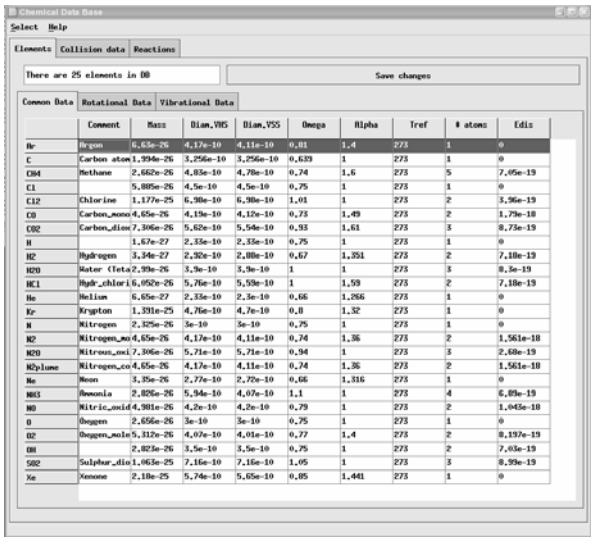

Fig. 1. Extendable chemical database

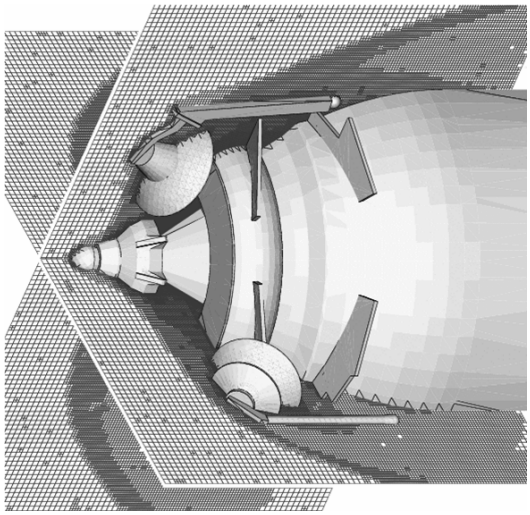

Fig. 2. Collision grid adaptation

Numerical techniques. The SMILE system is based on the majorant collision frequency (MCF) scheme [2] of the DSMC method. SMILE uses a two-layer rectilinear adaptive grid for collision modeling in 2D, axisymmetric, and 3D computations. The major layer, the so-called "background cells layer," stores parameters needed for DSMC computations, such as the maximum value of relative velocity for calculating the majorant collision frequency and the distance to the body surface for particle tracing. In the lower layer or "collision cells layer," collisions between modeling particles are performed. The latter grid uses much less of the memory than the background grid does. Grid adaptation is performed at the collision cells level. The size of the collision cell may be changed automatically depending on the density gradient and local mean free path (see Fig. 2). The level of cell division (or the number of collision cells per background cell) may also be defined manually at the stage of initial data preparation. A separate grid is used for sampling and averaging the molecular properties to compute the flow macroparameters, such as pressure, density, temperature, etc. This grid may also be adapted automatically or manually in the same manner as the collision grid. This multigrid approach allows one to have an extremely fine grid for modeling of collisions and provides a reasonable space resolution for macroparameters without a great memory overhead.

Real gas effects. An extremely important aspect of the DSMC code is the models of interaction of molecules during collisions. SMILE employs both conventional collision models of the DSMC method, which are standard for DSMC codes, and new effective models developed at the Computational Aerodynamics Laboratory of ITAM. The models used in the SMILE system to describe elastic and inelastic collisions are listed below.

A Variable Hard Sphere (VSH) model [1] and a Variable Soft Sphere (VSS) model [6] are used in SMILE to describe elastic collisions. These models are conventional for the DSMC method and are used in the overwhelming majority of researches.

A Larsen-Borgnakke (LB) model [7] is used to model inelastic collisions with translation-rotation (TR) and translation-vibration (TV) energy transfer. Two different types of the LB model are implemented in SMILE: a standard LB model with continuous representation of internal energies and a modification of the LB model for discrete (quantum) representation of internal energies [8]. Either constant or temperature-dependent relaxation numbers can be used in the models. For rotational relaxation, the temperature dependence is described by the relation derived in [9]; vibrational relaxation involves a dependence based on experimental data of Millikan and White [10] with a high-temperature correction of Park [11].

A Total Collision Energy (TCE) model is used in the SMILE system for modeling chemical reactions. The model has two options: standard (for continuous internal energies) [1] and modified (for discrete internal energies) [12]. For discrete internal energies, it is also possible to use a model based on two-temperature kinetics [13]. These models allow modeling bimolecular reactions of dissociation and exchange.

The chemical database contains the parameters of all models listed above for more than 30 mono-, di-, and polyatomic chemical species.

The gas-surface interaction modeling procedure uses a Maxwell model or a multiparametric Nocilla model. The definition of parameters in each model is provided and described for different conditions.

Subsystems. The SMILE computation system contains several subsystems providing a full computation life cycle. The main GUI shell glues all individual subsystems together, thus, significantly reducing the computation set-up time. The first subsystem is an interactive GUI pre-processing system designed to set up a new computation from the very beginning or start from an already existing computation. At the first step, this subsystem allows the user to define a set of chemical elements (atoms and molecules) and their properties, and also choose the chemical reaction set for modeling the reacting flow. The pre-processing subsystem allows the user to define a geometry model for the computation and select a gas-surface interaction model. For a 2D case, it can create the geometry configuration from scratch or load an already created geometry model. For 3D computations, the geometry model should be prepared elsewhere as a set of triangles in a predefined format and then loaded through the pre-processing subsystem. The pre-processing subsystem also defines the parameters of the incoming flow and of the numerical method. The pre-processing system has an interface for multistage DSMC computations and for coupling DSMC and Navier-Stokes computations. This functionality is implemented through intermediary files containing the distribution of required parameters along 2D curves or 3D surfaces called starting surfaces. The pre-processing system can extract/load these starting surfaces from/to DSMC computations. This functionality allows the researcher to perform comprehensive multizone computations without significant efforts.

The high-performance computation subsystem of SMILE, the core of the DSMC computation, has two- and three-dimensional versions. Both versions can run in single-processor or multiprocessor modes. The multiprocessing functionality is realized through an MPI interface and is capable of running on multiprocessor SMP machines with shared memory and HPC clusters with distributed memory. The computation subsystem is written in Fortran90 and uses the main features of dynamic memory allocation. This subsystem was successfully tested on a wide range of processors families (both 32-bit and 64-bit) and Fortran compilers. The dynamic load balancing algorithms realized inside the computation code allow one to achieve high speedups and efficiency even on a large number of processors (up to 256 and more). A separate interactive GUI monitoring tool written in C++ is a part of the computation system. It can monitor the current status of the computation (total number of iterations, current iteration) and stop the computation without the main GUI shell.

The SMILE computation system has an interactive GUI post-processing subsystem designed to process and visualize computation results and thus, complete the computation life cycle. This subsystem is capable of extracting flowfields from the files generated by the DSMC computation code and building three-dimensional and two-dimensional plots. The post-processing subsystem can work in a single-processor mode or in a multiprocessor mode if required. This subsystem allows the researcher to analyze the results obtained during the computation very rapidly and easily. The post-processing subsystem extracts the main gas dynamic parameters, such as pressure, density, temperature, velocity, and molecular fractions, as well as surface properties, such as distributions of pressure, friction, heat flux etc., and integrated aerodynamic characteristics as drag, lift and heat-transfer coefficients. The gas dynamic parameters may be presented as two-dimensional color flowfields, iso-contours, streamlines, etc. The post-processing system can also export flowfields and surface properties to the Tecplot visualization program to provide print-quality plots.

EXAMPLES

Flow over the "Progress" spacecraft. To demonstrate that SMILE is capable of computing complex external flows, three-dimensional computations of the flow around the "Progress" space vehicle are shown and compared with the in-flight results. DSMC computations were performed for p_∞ = 0.313 Pa, M_∞ = 8.06, T_∞ = 173 K, Re_∞ = 2455, Kn_∞=0.004, and T_w= 300K. Two pressure sensors were mounted on the front side of the vehicle, and their values were recorded during the in-flight test. At the first stage, a three-dimensional flow pattern was computed for a simplified geometry model of "Progress." Fig. 3 confirms good agreement between the numerical and experimental results for bow shock position. Then the computation was repeated for the geometry model containing the main superstructures of "Progress." These results are shown in Fig. 4. It can be seen from the figure that the flow near the pressure sensors is highly affected by external superstructures. At the third stage, the flow parameters obtained at the second stage were used as input conditions for computing the flow inside the pressure sensor. The good agreement between the in-flight and computation results shown in Fig. 5 confirms the applicability of the SMILE system for complex three-dimensional computations.

Fig. 3. Simplified geometry model.

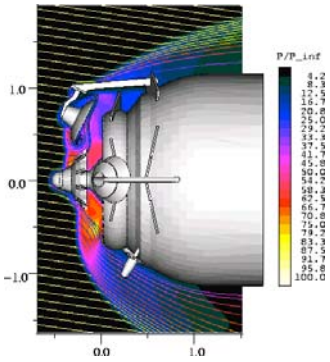

Fig. 4. Three-dimensional computation of the geometry model with superstructures at an angle of incidence equal to 8.5°.

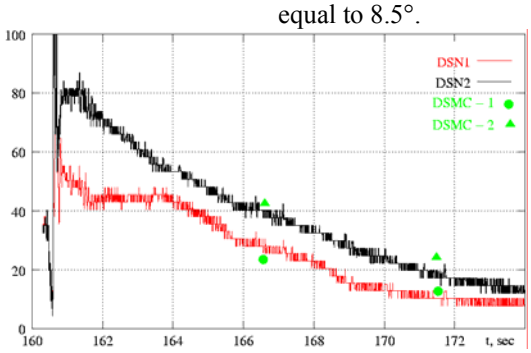

Fig. 5. Comparison with in-flight experiments. Launch date is January 24, 2001.

Investigation of the plume escaping into vacuum (spacecraft contamination). At the present time, the estimation of contamination of the spacecraft surface by orientation thrusters is a very important task for designers of long-life space vehicles. The X-Ray Observatory (XRO), also known as XEUS (X-Ray Evolving-Universe Spectroscopy), is one of the potential future missions belonging to this type of vehicles (Fig. 6). To maintain Xeus orientation, actuators and propulsions are required. The preliminarily selected thrusters will use hydrazine as a propellant. A major concern in exhausting hydrazine is the contamination by these relatively heavy molecules of the Xeus surface outside, but especially inside, where the scientific payload might lose its efficiency. A preliminary study is performed to investigate which chemical species might contaminate the payload.

The flow inside the thruster was first computed by the LORA Navier-Stokes solver, and flow parameters in the nozzle exit plane were used as a starting surface for 3D DSMC computations. The following species were taken into account: H_2, N_2, CO_2, H_2O, NH_3, and N_2H_4. The computational domain (see Fig. 8) was divided into three zones (zones 2, 3, and 4), and flow parameters at the exit of each zone were used as input data for the next zone. The mass flux distribution in Fig. 7 (total flux on the left and H_2 flux on the right) shows that the main contribution to contamination is made by H_2. The results presented show the applicability of the SMILE system for complex multistage computations, which are highly demanded by modern space industry.

Real gas effects on shock detachment. Presently, one of the most challenging problems in terms of the DSMC method development and improvement is related to the need to effectively and reliably simulate processes of energy transfer between internal and translational modes and chemical reactions. The real gas effects such as the excitation of internal degrees of freedom and chemical reactions in the gas phase considerably change flow properties and surface parameters. An example of the scarce data suitable for validation of real gas effect models of the DSMC method is the data presented in [14].

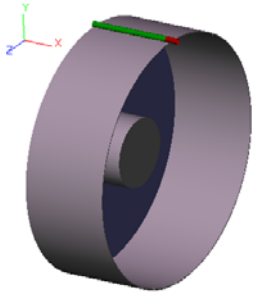

Fig. 6. Three-dimensional view of the Xeus satellite and computational zones. The green and red areas are the second and third zones, respectively.

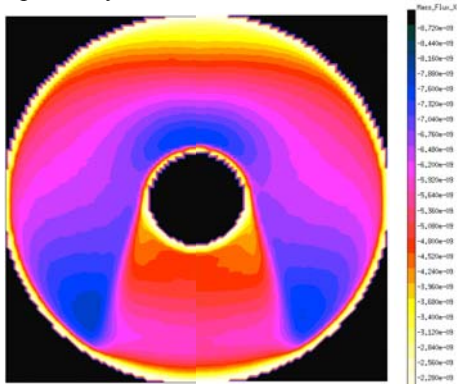

Fig. 7. Mass flux distribution on Xeus's inside zone. Total mass flux on the left and H_2 mass flux on the right.

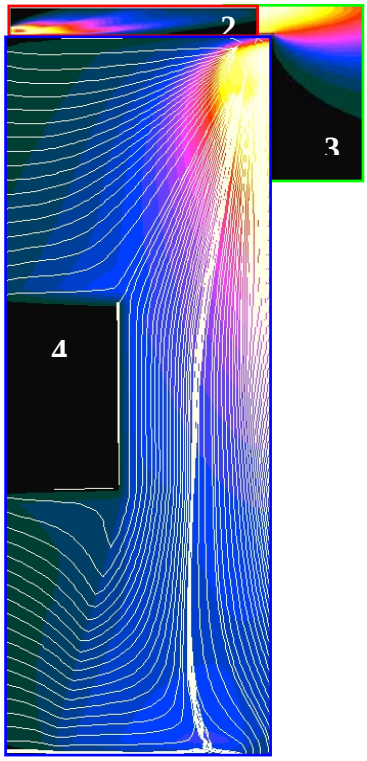

Fig. 8. All DSMC zones. Number density flowfields and streamlines (zone 4). Color scales are different in all zones.

The results of computations of the dissociating nitrogen flow about a wedge and comparisons with the data [14] are shown in Figs. 8 and 9. The flow conditions were: T_∞=940.3 K, M_∞=7.7, and $Kn_\infty=6.52\cdot10^{-4}$. The following flow composition was used: N_2=31.9 and N=7.7 mole/kg. Figure 9 shows the DSMC computations by the SMILE system for reacting and nonreacting cases (the TCE model was used). Owing to allowance for chemical reactions, the stand-off distance of the bow shock wave is almost halved, and the temperature becomes substantially lower. The standoff distance is plotted in Fig. 10 as a function of the wedge angle. Computations with ignored chemical reactions predict a linear dependence of the standoff distance on the wedge angle. Allowance for chemical reactions in computations yields a nonlinear behavior of the standoff distance versus the wedge angle, which is in qualitative agreement with experimental data. Note that the use of a new model of high-temperature dissociation [13] increases the standoff distance and improves the agreement with experimental data.

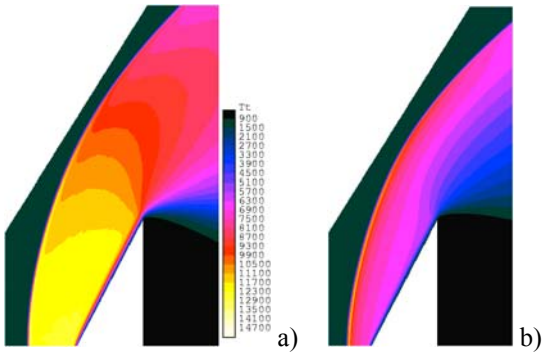

Fig. 9. Distribution of translational temperature. Wedge angle δ_w=62.5°. a) nonreacting nitrogen; b) reacting nitrogen.

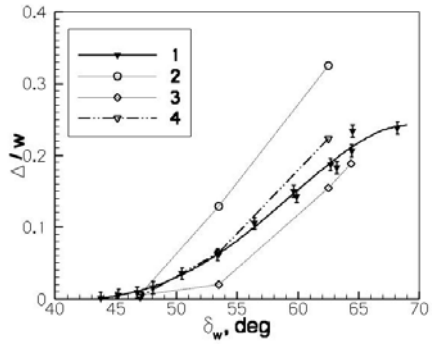

Fig. 10. Shock standoff distance. ***1*** – experiment, ***2*** - DSMC (nonreacting flow) ***3*** - DSMC (reacting flow) with the TCE model ***4*** - DSMC (reacting flow) with the high-temperature dissociation model

CONCLUSIONS

The examples presented above show the good potential of the SMILE computation system for basic research in a wide range of flow conditions from free-molecular to transitional regimes. These investigations may significantly improve our understanding of the nature of rarefied flows and help designers to create safe and effective vehicles and devices.

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