**Background**

Computational Fluid Dynamics (CFD) methods that solve the Navier-Stokes equations are widely utilized by industry and academia to investigate gas flow phenomena. However, these methods reach their limit for complex flow phenomena, which occur under extreme environmental conditions such as in the vacuum of space and under the influence of electromagnetic forces. Numerical particle methods developed at the University of Stuttgart model fluid flows using simulation particles, which represent real gas molecules. Despite the high numerical effort compared to conventional CFD methods, the advent of high-performance computing and sophisticated parallel computing standards enabled the application of particle methods to industrial problems.

**PICLas**

PICLas is a software for simulating gas and plasma flows with particle methods and is cooperatively developed by the Institute of Space Systems (IRS) and Institute of Aerodynamics and Gas Dynamics (IAG) at the University of Stuttgart. PICLas includes the Particle-in-Cell (PIC) method, which models collisionless interaction between charged particles (ions and electrons) and electromagnetic (or electrostatic) fields. The Direct Simulation Monte Carlo (DSMC) method utilizes a microscopic approach that simulates particle trajectories as well as intermolecular and particle-wall collisions. The DSMC method is commonly utilized to simulate non-equilibrium gas flows that typically occur in atmospheric entry applications or micro-electro-mechanical systems (MEMS). The novel combination of both methods in PICLas enables the simulation of reactive plasma flows.
Field-driven Plasma Expansion

**Electric Propulsion**

PICLas enables 3D high-fidelity simulations of electric propulsion systems by using highly efficient and parallelized discontinuous Galerkin methods. In the shown ion thruster, the gas is ionized in the discharge chamber, the plasma is accelerated through the two grid system and a propulsive force is generated. The thruster was simulated using 90758 mesh cells with a spatial order of 4 to resolve the necessary physical phenomena like plasma oscillations and Debye lengths. The electron back streaming effect could be shown in the simulations, which is a common failure mode for ion thrusters. Furthermore, experimental measurements of the back streaming electron current agree well with the simulation results.¹

**Laser Ablation**

Laser ablation is gaining an important role in solid-state physics and material processing. Numerical simulations in the past were restricted to direct interactions and the effects on the solid body for which Molecular Dynamics simulations were applied. The expansion of the plasma, which is created directly after the laser pulse impacts onto the surface, is also of importance due to subsequent events, e.g., laser-plasma interaction. The mesoscalic simulations allow for an analysis of the plasma plume expansion after a laser impact and can therefore be used for the investigation of the subsequent plasma-laser interaction. To gain insight into the laser-driven plasma expansion coupled PIC-DSMC simulations were performed with PICLas.²

¹ Binder et al., “High-Fidelity Particle-In-Cell Simulations of Ion Thruster Optics”, IEPC-2017-451
Electromagnetic Interaction

**Gyrotron**

Gyrotrons are high-power microwave generators for different purposes, e.g., the electromagnetic heating of plasma in fusion reactors like the Wendelstein 7-X. The figure shows a simulation of electrons that are injected in form of a hollow beam into a resonant cavity, where electromagnetic modes are excited by draining the kinetic energy of the electrons. PICLas is able to capture complex physical phenomena within gyrotrot devices by modeling the Maxwell-Vlasov equation system. Recent improvements in PICLas include high-order geometry approximation using curvilinear body-fitted and non-conforming interfaces.¹

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**Streamer Discharge / Spark Plug**

Important physical effects in plasma flows are often triggered by chemical reactions such as ionization and/or charge exchange reactions. Examples are ion thruster systems, where charge exchange reactions significantly influence the produced thrust and vapor deposition processes like sputtering, where ionization effects directly affect the deposition rate. Another application driven by ionization is the streamer discharge. PICLas is able to handle chemical reactions as well as ionization reactions in the plasma, which is exemplary shown for a spark plug simulation. Here, a few electrons are placed in a neutral gas and accelerated by an external electric field. As a result, a plasma is produced by the electron avalanche.²

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¹ Copplestone et al., “Simulation of gyrotrons using the high-order particle-in-cell code PICLas”, Strong Microwaves and Terahertz Waves: Sources and Applications, EPJ Web of Conferences 149, 04019
² Pfeiffer et al., “Two statistical particle merge and split methods for Particle-In-Cell codes”, Computer Physics Communications 191
Rarefied Gas Flows

Atmospheric Entry Maneuvers

During the deceleration of spacecraft through the atmosphere of planetary bodies, the hot gas flow is dominated by chemical reactions and non-equilibrium effects. For the design of the thermal protection system, which allows for a safe descent to the surface, numerical simulations are utilized. Sophisticated methods are required to simulate the rarefied, non-equilibrium gas flow around the spacecraft. For this purpose, the particle method Direct Simulation Monte Carlo is utilized. The high-fidelity simulations results strengthen the confidence in the design of spacecraft and increase the mass available for scientific instrumentation that will facilitate scientific discoveries.5,6

5 Nizenkov et al., “Modeling of chemical reactions between polyatomic molecules for atmospheric entry simulations with direct simulation Monte Carlo”, Physics of Fluids 29(7), 077104.
6 Nizenkov et al., “Verification and validation of a parallel 3D direct simulation Monte Carlo solver for atmospheric entry applications”, CEAS Space Journal 9(1), 127-137.

Features Summary

- Particle methods for non-equilibrium, microscopic fluid modeling
- Coupled or stand-alone Particle-in-Cell and Direct Simulation Monte Carlo modules
- High-order discontinuous Galerkin solver for electromagnetic interaction
- Efficient parallelization concept through Message Passaging Interface
- On-the-fly mesh refinement through octree sorting algorithm
- Broad range of available species from electrons to polyatomic molecules
- Treatment of chemical reactions and ionization processes
- Continuous development supported by the Deutsche Forschungsgemeinschaft (DFG) and industry partners

The code is available upon request.

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