# COMPUTATIONAL SOLUTION OF THE LINEARIZED BOLTZMANN EQUATION WITH AB INITIO POTENTIAL

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**Key words:** Boltzmann equation, Intermolecular potential, HPC, Large-scale simulations, MPI parallel programming, Discrete velocity method.

The Boltzmann equation (BE) is the governing integro-differential equation in the scientific fields of kinetic theory and rarefied gas dynamics and its numerical solution is considered as one of the most computationally demanding tasks (both in CPU time and storage) in computational physics and engineering. The unknown dependent variable in the BE is the velocity distribution function (VDF), which depends, in general, in seven independent variables, namely time, position vector and molecular velocity vector, while the macroscopic quantities of practical interest (bulk velocity, stresses, heat flux, etc.) are obtained as moments of the VDF. The complexity of the BE is due to the five-fold collision integral term describing the effect of the intermolecular collisions in the evolution of the VDF.

Here, by employing the so-called discrete velocity method, the continuum molecular velocity space is replaced by a set of discrete velocities. To sustain accuracy, thousands of discrete velocities are required and massive parallelization in the molecular velocity space with MPI parallel programming is applied. More specifically, the BE is replaced by a system of differential equations (one for each molecular velocity) which is solved by typical finite-volume schemes in the physical space, via a marching scheme. The differential equations are distributed to different CPUs and at the end of the calculations, data are exchanged between CPUs in order to compute the moments of the VDF via Gauss quadratures. The calculations are repeated upon convergence of the macroscopic quantities. Owing that data are exchanged between CPUs one time per iteration of the code and that each CPU can solve independently a number of equations, the algorithm has strong scaling and memory bounded problems can be avoided. Furthermore, it is well-known that the reliable simulation of rarefied gas flows heavily relies on the implemented intermolecular potential (IP). Therefore, the most computationally demanding, ab initio (AI) potential, recently available in the literature, is implemented. Since the BE with AI potential is based on fundamental principles, without any modeling approximations and experimental uncertainties the developed algorithm may be employed in large scale simulations producing benchmark results of high fidelity.