# Modelling of transport phenomena *ab initio*

Felix Sharipov

*Departamento de Física, Universidade Federal do Paraná*

All kinds of calculation of gas flows use some potential of intermolecular interaction. The widely used phenomenological potentials such as hard spheres, Lennard-Jones, Stochmayer, etc., contain several fitting parameters usually extracted from experimental data on transport coefficients (viscosity, thermal conductivity, diffusion) or from virial coefficients. Recently, the potentials for many gases and their mixtures have been calculated from main physical principals applying quantum-mechanical calculations. The group “Rarefied gas dynamics” at Physics Department of UFPR implemented these potentials to solve the Boltzmann equation, see e.g. the works [1,2], and to apply the direct simulation Monte Carlo method, see e.g. papers [3-5]. These results showed that some phenomena like mass flow rate, shear stress and heat flux in a single gas with a small temperature variation are not sensitive to the potential so that the simplest potential like the hard sphere model can be successfully used if the molecular diameter is well adjusted. However, some phenomena in gaseous mixtures like diffusion and thermodiffusion are strongly sensitive to the potential and should be modeled applying *ab initio* potentials when available. In the presentation, recent results on gas flows based on *ab initio* potentials will be reviewed.

**References**

1. F. Sharipov and V.J. Benites, Transport coefficients of helium-argon mixture based on *ab initio* potential. *J. Chem. Phys.* **143**, 154104 (2015).
2. F. Sharipov and V.J. Benites, Transport coefficients of helium-neon mixtures at low density computed from *ab initio* potentials. *J. Chem. Phys.* **147**, 224302 (2017)
3. J.L. Strapasson and F. Sharipov, *Ab initio* simulation of heat transfer through a mixture of rarefied gases. *Int. J. Heat Mass Transfer* **71**, 91-97 (2014).
4. F. Sharipov and J.L. Strapasson, *Ab initio* simulation of rarefied gas flow through a thin orifice. *Vacuum.* **109**, 246-252 (2014)
5. F. Sharipov and F.C. Dias, *Ab Initio* simulation of planar shock waves. *Computers and Fluids* **150**, 115-122 (2017).