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Numerical methods for Boltzmann-type equations in cloud and aerosol models

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Clouds are composed of large numbers of (liquid or solid) particles, which in a standard approach are described by distributions of size or mass of particles. Similar concepts are used for aerosols (i.e. liquid or solid particles in air), where particle concentrations exhibit similar variations as in clouds, but where also chemical composition plays an important role. In general, the sought distribution function f depend on time t, on the spatial coordinate x, and on internal coordinates **m** = (m1,...,mN), that is, f = f(t,x,**m**). For instance,ifm1,...,mN correspondtothemassesofdifferenttypesofparticles,fisthe joint density of particles of a given mass at a particular time and spatial location. Its time evolution is described by Boltzmann-type equations of the form

$$\partial_t(\rho f) + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v} f) + \nabla_{\mathbf{m}} \cdot (\rho \mathbf{g} f) = K(f),$$

with the density ρ, the spatial flow field v and the displacements g in the internal coordinates (e.g., due to diffusive growth of particles).

The source term K(f) on the right hand side describes formation and annihilation of particles due to different processes, as e.g. nucleation, evaporation or collision. A special but important case is the exclusive treatment of collision processes, neglecting all other processes, which could contribute to K(f). In case of only one internal coordinate m (that is, N = 1), such as mass or size of one type of particle, one arrives at a classical Smoluchovski coagulation equation, where

$$K(f)(t,\mathbf{x},m) = \frac{1}{2}\int_0^m f(t,\mathbf{x},m')\, f(t,\mathbf{x},m-m')\, C(m,m-m')\, dm' \\ - \int_0^\infty f(t,\mathbf{x},m)\, f(t,\mathbf{x},m')\, C(m,m')\, dm' \quad (*)$$

with a collision kernel function C. Handling this equation numerically including the full spatial and temporal dependence is already a significant challenge, and one typically resorts to spatially homogeneous approximations and to very coarse piecewise constant approximations in m, so-called bin models that amount to considering only transitions between different categories of particles. The problem becomes more complex when several internal coordinates are involved, for instance in models for interaction of cloud droplets and aerosols. An important example is the scavenging of aerosols by cloud particles, which is relevant at very different cloud regimes (e.g. warm liquid clouds or even ice clouds at very high altitudes).

The aim of the present project is to develop efficient numerical methods for problems of this type, starting with the case of (∗). The numerical analysis of this model already poses some interesting challenges, especially due to the interaction of transport terms with a nonlinear integral operator. We will follow two approaches: splitting methods treating the different contributions in an alternating fashion, and unified weak formulations. In both cases, standard discretizations of the integral operator K(f) lead to dense matrices. An efficient treatment can be achieved by sparse approximations with respect to suitable basis functions. For handling a larger number of internal coordinates, special approximation methods for higher-dimensional problems are required.

Progress in this direction will have substantial impact in the numerical modeling of clouds, aerosols, and their interactions. The project offers to the PhD student the opportunity to familiarize themselves with the use of statistical physics concepts in cloud models, and at the same time with modern numerical techniques for higher-dimensional integro-differential equations. Finally, the model can be used for the interpretation of airborne measurements, which are available in collaboration with the “Aerosol and Cloud Physics group” (Prof. Borrmann/Dr. Weigel).