Analytical and Computational Problems in Kinetic Collisional Transport Theory

Lecturers:

Armando Majorana, University of Catania -Italy- (1st week) Irene M. Gamba, University of Texas at Austin -USA- (2nd week)

Motivations

The classical theory of continuum, or macroscopic regimes, given by Navier Stokes type models applies in the dynamical description of a dense gas particles or charged electrons transport regime, in a given volume, when the averaged scaled mean free path is negligibly small. However, it is well know that as particle interactions become rarefied, the averaged scaled mean free path is of order one unity and such macro models of continuum fluid dynamics do not hold any longer. As the degree of rarefaction increases, statistical model corrections become necessary. These observation was introduced by L. Boltzmann given raise in late nineteenth century to an statistical description of thermodynamics, in which the Navier-Stokes systems of equations for a few thermodynamic variables in three dimensions needs to be replaced by the dynamics of the Boltzmann collisional equation posed in six dimensions. This is a non-linear integro-differential equation, whose analytical and computational methods have been developed since just a few decades. At the same time collisonal kinetic equations have introduced and studies in different contexts, such as hot electron transport semiconductor devices, micro or nano-dimensional material in two dimensional dimensional for electron transport in graphene, structures, binary gas mixtures and multi-energy level gases and the grazing approximation from Boltzmann to Fokker Planck Landau models. In these lectures we will introduced and discuss the analytical properties, approximations and computational techniques that solve, both, scalar and systems of Boltzmann type equations under neutral or charged transport regimes. We will also focus on new developments ranging from the existence theory, tail formation and trends to equilibrium as well as detailed numerical approximations as much as error estimates associated to the aforementioned problems.

Part I: The Boltzmann Collisional Models - Elementary properties and Approximations

During the first six lectures, we will introduce the probabilistic properties of the Boltzmann collisonal operator, both for the classical monoatomic perfect gas and for charged particles in the semiclassic limit. We will discuss the Runge-Kutta discontinuous Galerkin (RKDG) method, which is a class of finite element methods originally devised to solve hyperbolic conservation laws. This method was employed and was fully validated for solving the Boltzmann transport equation accurately. Using a completely discontinuous polynomial space for both the test and trial functions in the phase-space variables, coupled with explicit and nonlinearly stable high order Runge-Kutta time discretization, the method has the nice advantage of flexibility for arbitrarily unstructured meshes. We will show some applications to different kinetic equations. I will also show some applications to the transport of electrons in graphene and to the system of BTEs for hole-electron interactions.

Part II: Boltzmann gas mixtures, grazing limit to the Landau equation - Numerical approximations and simulations

During the second six lectures, we will first focus on a unified approach of existence and

uniqueness theory to the Boltzmann equation for hard potentials, including tail formation and decay rate of equilibrium and extend these analytical issues to collisional gas mixtures that applies to the classical billiard model for elastic interactions and extends to mixtures and polytropic gas models. In addition we will discuss the grazing collision limit for Coulomb interactions for the Boltzmann problem that results in the Fokker Plank Landau model.

Following the themes from the first six lectures from A. Majorana, in the last lectures we will discuss hybrid computational solvers of two kinds: conservative spectral based and Finite Element Method (FEM) based for the Boltzmann equation binary interactions. We will show error estimates and convergence to statistical equilibrium results for the discuss the conservative spectral method and discuss a new fast solver based on a Petrov-Galerkin FEM approach.

We will discuss several recent numerical example that include

- 1. Gas mixtures and a multi-energy level gas models.
- 2. An anisotropic gas model for grazing collision form and its approximations to the Landau transport flow.
- 3. A hybrid DG/conservative spectral solver for Vlasov Poisson Landau system for electron transport Validation of the scheme confirming the predicted degenerate decay rate to equilibrium.
- 4. The global effect of rough boundary conditions on insulating boundaries for hot electron transport at nano-scale and the lack of suitable macroscopic approximations.

Tentative Bibliography

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