A conservative entropic multispecies BGK model

J. Haack, haack@lanl.gov
C. Hauck, hauckc@ornl.gov
M. Murillo, murillom@msu.edu

We derive a conservative multispecies BGK model that follows the spirit of the original, single species BGK model by making the specific choice to conserve species masses, total momentum, and total kinetic energy and to satisfy Boltzmann's H-Theorem. The derivation emphasizes the connection to the Boltzmann operator which allows for direct inclusion of information from higher-fidelity collision physics models. We also develop a complete hydrodynamic closure via the Chapman-Enskog expansion, including a general procedure to generate symmetric diffusion coefficients based on this model. We numerically investigate velocity and temperature relaxation in dense plasmas and compare the model with previous multispecies BGK models and discuss the trade-offs that are made in defining and using them. In particular, we demonstrate that the BGK model in the NRL plasma formulary does not conserve momentum or energy in general.

Background and Motivation

Kinetic equations describe the evolution of a many-body particle system using a single-particle distribution function and rely on collision operators to approximate the underlying details of the many-body interactions. The most well-known of these operators is the Boltzmann collision operator, which models particle interactions as binary collisions. For a single species of particles, the Boltzmann operator takes the form

$$Q[f](\mathbf{c}) = \int (f(\mathbf{c}')f(\mathbf{c}'_*) - f(\mathbf{c})f(\mathbf{c}_*))g\sigma\, d\Omega d\mathbf{c}_*. \tag{0.1}$$

Unfortunately, the Boltzmann operator is very expensive to compute. Indeed, the five-dimensional integral in (0.1) must be evaluated at each $\mathbf{x}$, $\mathbf{c}$, and t at which the value of f is desired; this integral cannot be evaluated analytically except in the case of Maxwell molecules with carefully prepared initial conditions. As a consequence, computing the collision operator is typically the most expensive part of solving the Boltzmann equation numerically. Due to its simplicity and reduced cost, one of the most widely used approximations of the Boltzmann collision operator is the Bhatnagar-Gross-Krook (BGK) operator [1]. It is a nonlinear relaxation operator of the form

$$Q_{\mathrm{BGK}}[f] = \nu(\mathcal{M}[f] - f), \tag{0.2}$$

where ν is a collision frequency that is independent of velocity and the Maxwellian $\mathcal{M}[f]$ is the local equilibrium state:

$$\mathcal{M}[f] = n\left(\frac{m}{2\pi T}\right)^{3/2} \exp\left(\frac{m(\mathbf{c}-\mathbf{v})^2}{2T}\right). \tag{0.3}$$

This model is defined so as to capture the most fundamental properties of the Boltzmann operator: (i) conservation of the mass, momentum, and energy; (ii) entropy dissipation; and (iii) verification of Boltzmann's $\mathcal{H}$-Theorem (discussed below). The key assumption in deriving the model is that the distribution function is near equilibrium, and thus it performs well for problems close to the hydrodynamic limit.

Generalizing the BGK model to multispecies systems is not straight-forward; in particular, there is some ambiguity in how to set the collision frequencies and the parameters for the Maxwellians in the relaxation operators that model collisions between species. Simply using the moments of the target species as is suggested in the NRL Plasma Formulary [4] results in loss of conservation of momentum and energy. Other multispecies BGK methods [5, 3, 2] enforce conservation and use Boltzmann-derived velocity and temperature relaxation rates as constraints but fail to satisfy the multispecies H-Theorem.

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Description/Impact

We make an ad-hoc derivation of the multi-species version of the BGK operator

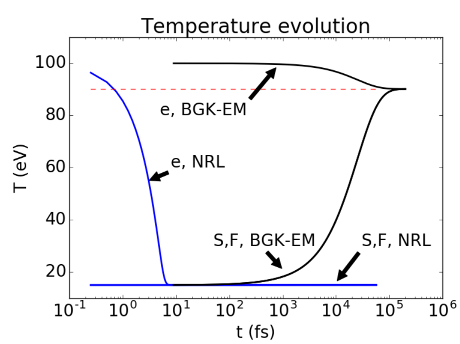
$$Q_{ij}^{\mathrm{BGK}} = \nu_{ij}(\mathcal{M}_{ij} - f_i), \tag{0.4}$$

where ν_{ij} is the collision rate for species i and j. To determine the unknown parameters $\mathbf{v}_{ij}, T_{ij}$ we enforce $\mathbf{v}_{ij} = \mathbf{v}_{ji}$, $T_{ij} = T_{ji}$, which is suggested by the derivation from Boltzmann and guarantees the H-Theorem, and enforce conservation of momentum and kinetic energy across species collision pairs. The collision frequencies ν_{ij} are defined by matching one of the momentum relaxation rate or temperature relaxation rate of a binary mixture in the Boltzmann equation. The rates connect to the Boltzmann equation through the momentum transfer cross section $\sigma_{ij}^{(1)}(g)$ through expressions of the form

$$\int_0^\infty w^5 \sigma_{ij}^{(1)}(w) e^{-w^2} dw. \tag{0.5}$$

Recent work by Stanton and Murillo [6] provides molecular dynamics validated fits for these integrals in the case of dense plasmas.

We derive a full set of macroscopic transport coefficients that correspond to this kinetic model, and perform some temperature relaxation studies. In particular, we note that the BGK model suggested by the NRL Plasma formulary can give catastrophically incorrect results.



Electron-Ion temperature relaxation. dashed line is the correct equilibrium value

Anticipated Impact

This new model provides a tool that allows for practical kinetic theory simulation of matter in warm dense matter to hot dense matter regimes, where many other kinetic models suffer. In these regimes scattering is strong enough that the Fokker Planck model that is typically used for kinetic simulation of plasma does not apply, and the direct computational expense of computing the Boltzmann equation as well as gridding requirements for mixtures of species with significant mass ratios also makes it impractical in these regimes.

Path Forward

In future work, we will use this model to compute numerical solutions for spatially-dependent problems, such as shocks and interfaces in dense plasmas. We also plan to develop new collision rate models for electron interactions based on quantum cross sections and insert them into this model, and from this derive new electron-ion transport coefficients based on this new kinetic model.

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