A Spectral Framework for Solving the Nonlinear Boltzmann Equation

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Direct numerical solution of the nonlinear Boltzmann transport equation remains elusive nearly 150 years after its discovery. Appropriate approximations continue to serve as the foundation of aerodynamics and plasma physics. However, some important problems in fusion don't lend themselves to such approximations, such as runaway electron avalanche and regimes of dense neutral populations in scrape-off layers. Routine and robust solution of the nonlinear Boltzmann equation will be needed to close these gaps in computational capability.

Several approaches have been successfully developed throughout the 20th century to numerically solve the Boltzmann equation in various limits, particularly in the case of linear collision operators. These include the Monte Carlo technique used in EIRENE and DEGAS2, and the weakly-anisotropic expansion used in BOLSIG+. Advances in applied mathematics now make routine numerical solution of the nonlinear equation feasible. For example, a Fourier representation has been recently applied to find new fluid closures using machine learning [1].

This talk focuses on a new computational framework (LightningBoltz), which is based on a generalization of the conservative spectral method of Gamba, Rjasanow, and Keßler [2][3]. This framework takes ample advantage of pre-computing the discrete collision operator in a distributed computing system. Depending on the demands of the specific problem, this capability allows the full bilinear Boltzmann operator to be calculated in fractions of a millisecond on a laptop, while time-dependent and spatially-inhomogeneous kinetic problems can be readily solved on a workstation or small cluster. Other features include: force-field acceleration, implicit time-stepping, and arbitrary cross sections read from atomic physics databases.

LightningBoltz has been verified against constructed analytic solutions to the Boltzmann equation and against the Chapman-Cowling expansion at low Knudsen number. Cross-verification with the DEGAS2, Gkeyll, and BOLSIG+ codes is presented. A proof-of-principle for a one-dimensional model of a tokamak scrape-off layer is shown, which includes rigorous treatment of elastic scattering: a unique capability. The spectral technique is also being applied to the coupling between DEGAS2 and the gyrokinetic edge code XGC to rigorously account for elastic scattering and enforce conservation in charge-exchange interactions [4]. Runaway electron distributions pose unique challenges due to the disparate velocity scales, and potential paths to tackling the nonlinear kinetic avalanche problem will be discussed.

[1] J. Han, et al. *Proceedings of the National Academy of Sciences* **116**:21983 (2019)
[2] I. Gamba & S. Rjasanow. *Journal of Computational Physics* **366**:341 (2018)
[3] T. Keßler & S. Rjasanow. *Kinetic and Related Models* **12**:507 (2019)
[4] D. Stotler, et al. *Computational Science and Discovery* **6**:015006 (2013)