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Hybrid Quantum-Hydrodynamics/Kinetics Model for Dense Plasma Mixtures

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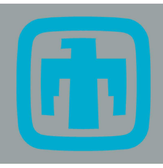

Abstract

Fusion energy promises nearly unlimited, clean energy; one approach to fusion energy production employs lasers to compress fusion fuel to conditions similar to those in the sun. Unfortunately, in the presence of a wide variety of energy loss mechanisms, obtaining a net gain in energy remains a challenge. The mixing of cooler materials into hot regions can spoil the production of fusion energy. Two ways that cooling occurs is from the mixing of two ion species, or by conduction from the electron species. An existing kinetic model for studying the mixing of ions, is the multi-component BGK (McBGK) equation which describes the ionic heat transfer. One way to add the effects of heat conduction from the electrons is by solving a kinetic equation which is not a computationally tractable approach due to the considerable difference in timescales for the electron and ion species. Instead, hydrodynamic equations of motion for the electron species are derived directly from the McBGK equation and are used to determine how the electrons transfer heat to the ion species. We plan to use our model to aid in the design and interpretation of experiments at Sandia National Laboratories that are being performed on the Z Machine, a large pulsed-power facility.

Motivation and Existing Model

Mixing Experiment

Setup of Experiment: Consider a periodic system with two materials separated by interfaces, which can be seen in the figure below. This system is then flash-heated by x-rays to create a two species plasma.

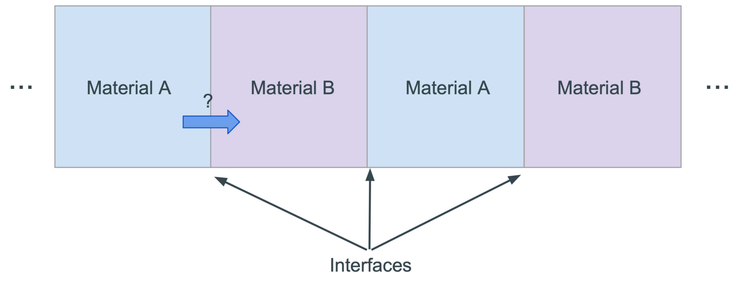

Figure 1: Diagram of a two-material periodic system separated by interfaces.

Goal of Experiment: Measure the the atomic mixing rate for the different materials across the interface after ionization (plasma interdiffusion). This will yield insight on the efficiency of fusion experiments where interface mixing is present (e.g. inertial confinement fusion).

Model and Goal of this Work: A multi-componenet BGK (McBGK) model [2] is currently being used to describe this experiment. The McBGK model is currently purely classical and we aim to generate a set of semi-classical hydrodynamic equations of motion to include effects from the electron species.

Two-Temperature Model (TTM)

In the early stages of this work, we considered using a "two-temperature model"[3] (TTM) to introduce the electron temperature to the McBGK equation. The two-temperature model has the form

$$C_e\frac{\partial}{\partial t}T_e = \nabla_{\mathbf{r}}\cdot\kappa_e\nabla_{\mathbf{r}}T_e + \frac{T_1-T_e}{\tau_{e1}} + \frac{T_2-T_e}{\tau_{e2}} + S_e(\mathbf{r},t), \tag{1}$$

$$C_1\frac{\partial}{\partial t}T_1 = \nabla_{\mathbf{r}}\cdot\kappa_1\nabla_{\mathbf{r}}T_1 + \frac{T_e-T_1}{\tau_{1e}} + \frac{T_2-T_1}{\tau_{21}} + S_1(\mathbf{r},t), \tag{2}$$

$$C_2\frac{\partial}{\partial t}T_2 = \nabla_{\mathbf{r}}\cdot\kappa_2\nabla_{\mathbf{r}}T_2 + \frac{T_2-T_e}{\tau_{2e}} + \frac{T_1-T_2}{\tau_{21}} + S_2(\mathbf{r},t), \tag{3}$$

Where equations (2) and (3) would be replaced by the McBGK kinetic model. The issue with this model is that it has no opinion of the electron density or momentum which is important for our problem. Another choice of model for the electron species is to derive a set of equations directly from the McBGK model to ensure consistency, which we will refer to as the "electron temperature model" (ETM).

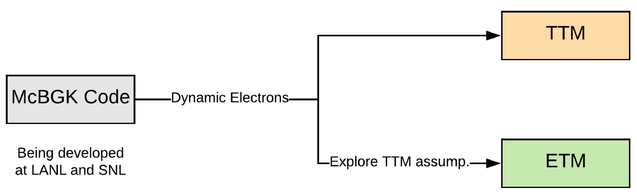

Figure 2: Possible choices for adding dynamic electron effects to existing model.

Electron Temperature Model (ETM)

Multi-component BGK (McBGK) Equation

A model for describing mixing that occurs on this time and length scale is the multi-component BGK model - a kinetic equation of the form

$$\frac{\partial}{\partial t}f_i + \mathbf{v}\cdot\nabla_{\mathbf{r}}f_i + \mathbf{a}_i\cdot\nabla_{\mathbf{v}}f_i = \sum_{j=1}^{N}\frac{M_{ij}-f_i}{\tau_{ij}} \qquad \forall\, j=1,\ldots,N, \tag{4}$$

where $f_i = f_i(\mathbf{r},\mathbf{p},t)$ is a phase-space distribution function for species i, $\mathbf{a}_i = \mathbf{a}_i(\mathbf{r},t)$ is the acceleration of a particle of species i at position $\mathbf{r}$ at time t. Additionally, τ_{ij} is a velocity independent collision rate between species i and j and M_{ij} is a target equilibrium distribution function for species i and j defined as

$$M_{ij} = n_i\left(\frac{m_i}{2\pi T_{ij}}\right)^{3/2}\exp\left(-\frac{m_i(\mathbf{v}-\mathbf{u}_{ij})^2}{2T_{ij}}\right), \tag{5}$$

where $n_i, \mathbf{u}_{ij}$ and T_{ij} are all functions of $\mathbf{r}$ and t. We define the electron kinetic equation as

$$\frac{\partial}{\partial t}f_e + \mathbf{v}\cdot\nabla_{\mathbf{r}}f_e + \mathbf{a}_e\cdot\nabla_{\mathbf{v}}f_e = \sum_{j=1}^{N}\frac{M_{ej}-f_e}{\tau_{ej}}. \tag{6}$$

From this equation we derive hydrodynamic equations of motion for which the solutions will be inputs for the forces acting on the ionic species. Moments of the target equilibrium have the following form

$$\int d\mathbf{v} M_{ij} = n_i, \tag{7}$$

$$\int d\mathbf{v}\mathbf{v} M_{ij} = n_i\mathbf{u}_{ij}, \tag{8}$$

$$\int d\mathbf{v} v^2 M_{ij} = n_i\left(u_{ij}^2 + \frac{3}{m_i}T_{ij}\right). \tag{9}$$

For a single **electron species**, the equilibrium, or target, distribution is given by a Fermi-Dirac distribution given by

$$FD(\mathbf{v}) = \frac{1}{\exp\left(\beta\left(\frac{|\mathbf{v}-\mathbf{u}|}{2}-\mu\right)\right)+1}, \tag{10}$$

where $\beta = 1/k_bT$, and μ is the chemical potential. The $k-th$ order **Fermi-Dirac integrals** are given by

$$\mathcal{I}_k := \int_0^\infty dx \frac{x^k}{\exp(x-\beta\mu)+1}, \tag{11}$$

and are used to determine the moments of the Fermi-Dirac equilibrium distribution (10) similar to the Maxwell-Boltzmann distribtuion. In the above expression x is in energy units.

Classical Euler Hydrodynamics

We define our macroscopic quantities as

$$n_e = \int d\mathbf{v}\, f_e, \tag{12}$$

$$\mathbf{u}_e = \frac{1}{n_e}\int d\mathbf{v}\,\mathbf{v} f_e, \tag{13}$$

$$K_e = \frac{m_e}{2n_e}\int d\mathbf{v}\, v^2 f_e, \tag{14}$$

$$p_e = \int d\mathbf{v}(v-u_e)^2\, f_e, \tag{15}$$

$$\mathbf{q}_e = \frac{m_e}{2n_e}\int d\mathbf{v}\,(v-u_e)^2(\mathbf{v}-\mathbf{u}_e)f_e. \tag{16}$$

Where n_e is the mean density, $\mathbf{u}_e$ is the mean velocity, K_e is the mean kinetic energy density, p_e is the scalar pressure, and $\mathbf{q}_e$ is the relative heat flux vector. Taking moments of equation (6), by multiplying by powers of $\mathbf{v}$ and integrating gives the following set of hydrodynamic equations

$$\frac{\partial}{\partial t}n_e + \nabla_{\mathbf{r}}\cdot(n_e\mathbf{u}_e) = 0, \tag{17}$$

$$n_e\frac{\partial}{\partial t}\mathbf{u}_e + (n_e\mathbf{u}_e\cdot\nabla_{\mathbf{r}})\mathbf{u}_e + \nabla_{\mathbf{r}}(n_eT_e) - \mathbf{a}_en_e = \sum_{j=2}^{N}\frac{n_e}{\tau_{ej}}\left(\mathbf{u}_{ej}-\mathbf{u}_e\right), \tag{18}$$

$$\frac{\partial}{\partial t}(n_eK_e) + \nabla_{\mathbf{r}}\cdot(n_e\mathbf{q}_e) + \frac{m_e}{2}\nabla_{\mathbf{r}}\cdot(n_eT_e\mathbf{u}_e) + \frac{m_e}{2}\nabla_{\mathbf{r}}\cdot(u_e^2\mathbf{u}_en_e) - m_e\mathbf{a}_e\cdot(n_e\mathbf{u}_e) = \sum_{j=2}^{N}\frac{n_e}{\tau_{ej}}\left(\mathbf{u}_{ej}^2 + \frac{3}{m_e}T_{ej} - \frac{2}{m_e}K_e\right), \tag{19}$$

where we have used the classical scalar pressure $p_e = n_eT_e$.

Quantum Euler Hydrodynamics

To include the quantum properties from the electrons (i.e. fermions), we instead consider a Fermi-Dirac equilibrium distribution which will be considered when computing the right hand side of the above equation and in the closures for pressure. Therefore, equations (17) - (19) become

$$\frac{\partial}{\partial t}n_e + \nabla_{\mathbf{r}}\cdot(n_e\mathbf{u}_e) = 0, \tag{20}$$

$$n_e\frac{\partial}{\partial t}\mathbf{u}_e + (n_e\mathbf{u}_e\cdot\nabla_{\mathbf{r}})\mathbf{u}_e + \nabla_{\mathbf{r}}p_e - \mathbf{a}_en_e = \sum_{j=2}^{N}\frac{n_e}{\tau_{ej}}\left(\mathbf{u}_{ej}-\mathbf{u}_e\right), \tag{21}$$

$$\frac{\partial}{\partial t}(n_eK_e) + \nabla_{\mathbf{r}}\cdot(n_e\mathbf{q}_e) + \frac{m_e}{2}\nabla_{\mathbf{r}}\cdot(p_e\mathbf{u}_e) + \frac{m_e}{2}\nabla_{\mathbf{r}}\cdot(u_e^2\mathbf{u}_en_e) - m_e\mathbf{a}_e\cdot(n_e\mathbf{u}_e) = \sum_{j=2}^{N}\frac{n_e}{\tau_{ej}}\left(\mathbf{u}_{ej}^2 + \frac{3}{m_e}T_{ej} - \frac{2}{m_e}K_e\right) \tag{22}$$

The red portions in the above equations indicate where the quantum effects will appear. A Chapman-Enskog expansion will be done to include quantum effects in the transport coefficients.

Quantum Mechanical Opinion of Kinetic Energy

Total Kinetic Energy in a Quantum System

To generate a temperature equation from (22) that has a similar structure to (1) - (3) we require an opinion on the *total kinetic energy* to generate the specific heat, C_e. The total kinetic energy for quantum systems is comprised of two parts. The *ideal* part, denoted K_0 and the *excess* part, denoted K_{ex}. The total kinetic energy has the form

$$K = K_0 + K_{ex}. \tag{23}$$

From [4], K_0 and K_{ex} can be computed via

$$K_0 = \frac{3}{2}nT\theta^{3/2}\mathcal{I}_{3/2}, \quad K_{ex} = -nT\theta\left(\frac{\partial f_{ex}}{\partial\theta}\right)_\Gamma, \tag{24}$$

where

$$\theta := \frac{T}{E_F}, \quad \mu := \mathcal{I}_{-1/2}\left(\frac{2}{3}\theta^{-3/2}\right).$$

Here θ is the degeneracy parameter, E_F is the Fermi energy, f_{ex} is the excess free-energy, and Γ is the coulomb coupling parameter.

Where Do Quantum Effects Matter?

From K_0 in (24) we have a energy-temperature relationship and the following plot highlights the temperature regimes in which quantum mechanical effects are important to consider.

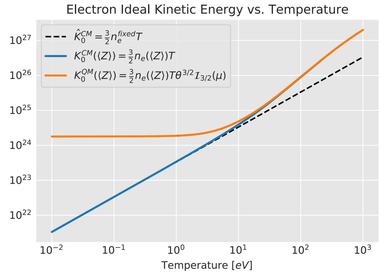

Figure 3: Vanadium ion number density: n_i = 6.48e Quantum effects are important to consid temperatures less than 10 ev. Python pa "fdint" was used to compute Fermi-Dirac in - see [1] for more details on this.

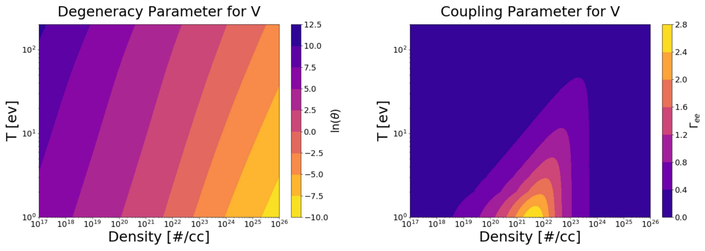

Figure 4: Brighter regions in left figure show where quantum effects are non-negligible. Brighter regions in the right figure show where particles are more strongly coupled.

Bibliography

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