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Transport in non-ideal, multi-species plasmas

Liam G. Stanton

San Jose State University, liam.stanton@sjsu.edu

Scott D. Bergeson

Brigham Young University

Michael S. Murillo

Michigan State University

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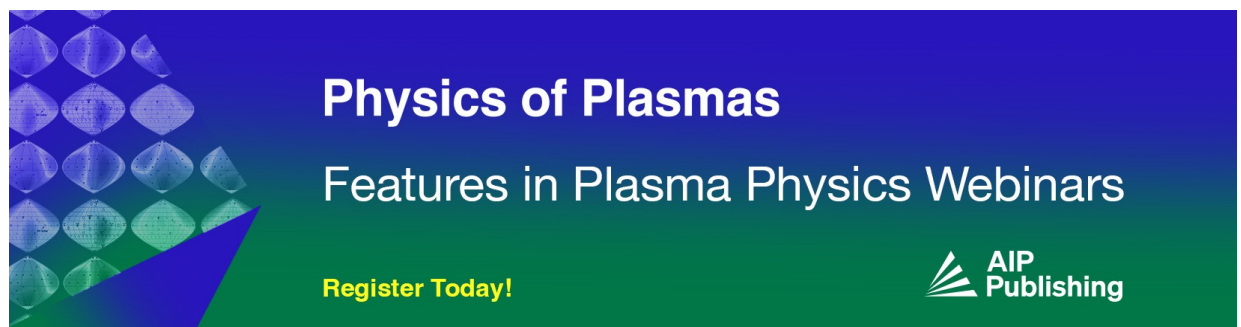
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Liam G. Stanton,^{1,a)}  Scott D. Bergeson,^{2,b)}  and Michael S. Murillo^{3,c)} 

AFFILIATIONS

¹Department of Mathematics and Statistics, San José State University, San José, California 95192, USA

²Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA

³Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, Michigan 48824, USA

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^{a)} Author to whom correspondence should be addressed: liam.stanton@sjsu.edu

^{b)} Electronic mail: scott_bergeson@byu.edu

^{c)} Electronic mail: murillom@msu.edu

ABSTRACT

Charged particle transport plays a critical role in the evolution of high energy-density plasmas. As high-fidelity plasma models continue to incorporate new micro-physics, understanding multi-species plasma transport becomes increasingly important. We briefly outline theoretical challenges of going beyond single-component systems and binary mixtures as well as emphasize the roles experiment, simulation, theory, and modeling can play in advancing this field. The 2020 Division of Plasma Physics mini-conference on transport in Transport in Non-Ideal, Multi-Species Plasmas was organized to bring together a broad community focused on modeling plasmas with many species. This special topics issue of Physics of Plasmas touches on aspects of ion transport presented at that mini-conference. This special topics issue will provide some context for future growth in this field.

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I. INTRODUCTION

Charged particle transport, both ionic and electronic, plays a critical role in the evolution of high energy-density (HED) plasmas. For example, the symmetry of laser-driven implosions relies on controlling ionic transport and eliminating instabilities,¹ and transport is crucial in species mixing and persistent separation as well.^{2,3} This is particularly important for understanding the effect of impurities⁴ or target structure⁵ on plasma performance. As plasma models continue to incorporate new microphysics, a detailed understanding of ion transport becomes an increasingly important priority.^{6–12} Ionic and electronic transport is an active and ongoing area of high interest and importance in HED science.^{13–18} As shown in Fig. 1, the number of citations to research papers in plasma transport now reaches a few tens of thousands per year.

Broadly speaking, transport is determined by three different mechanisms: (1) advection, in which the particles stream freely at their current velocity; (2) forces, which change the velocities on those trajectories; and (3) collisions, which act to impede the fluxes in the presence of gradients in the thermodynamic variables such as pressure, temperature, or density. Depending on the driving fields and physical conditions, collisions shape the time-evolving distribution functions; their relative strength can, for example, determine the growth rate of

instabilities. A simple way to quantify the effects of transport is through the Knudsen number, which is defined as the ratio of the mean free path of particles to the characteristic length scale (L) of a given system. The larger the Knudsen number, the more the assumptions of hydrodynamic models break down, as collisionality can no longer be taken as instantaneous. An approximate formula for the Knudsen number is given by

$$\text{Kn} = \frac{v_{\text{th}}\tau_{ii}}{L} = \frac{\sqrt{2\pi}a_i}{\lambda L\Gamma^2}, \quad (1)$$

where $v_{\text{th}} = \sqrt{2T/m}$ is the thermal velocity, τ_{ii} is the collision time, a_i is the typical inter-particle spacing, Γ is the Coulomb coupling parameter, and λ is the Coulomb logarithm. Furthermore, we have chosen $\lambda = 4K_{11}(g)$, where $K_{11}(g)$ is the dimensionless collision integral taken from Ref. 19. Ranges of Kn are shown in Fig. 2 for typical parameter values of warm dense matter (WDM), inertial confined fusion (ICF), solar atmospheres and the ions and electrons of ultracold neutral plasmas (UNP). It can be seen that the selected plasmas span nearly *ten* orders of magnitude in the Knudsen number, which illustrates the complexity of transport in these systems.

A goal of experiments is to provide information on transport, often in the form of numerical values of the transport coefficients.

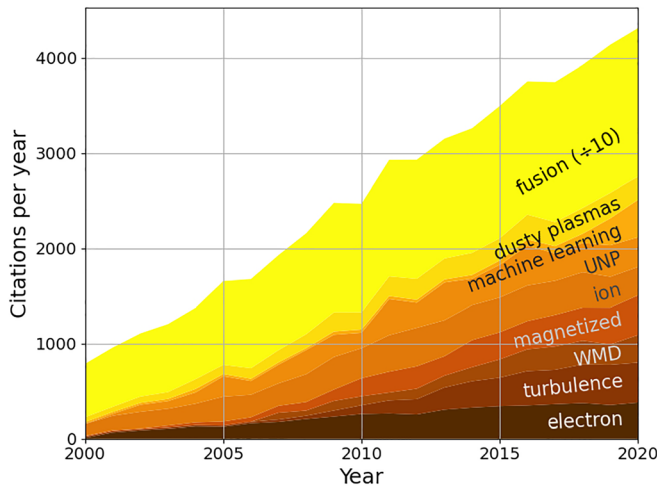


FIG. 1. Citations to plasma transport papers per year, broken out by a few subcategories. The data were obtained by searching Web of Science by topic using the labeled text ended with “transport,” “plasma,” and/or “physics.” The exception is ultracold neutral plasmas (UNP), which shows all citations in that field. WMD = warm dense matter. The number of citations per year for fusion transport has been divided by 10 for convenience of viewing on this plot.

Doing so requires establishing well-controlled gradients in some variables and not others, a very challenging task. Even if the desired initial conditions can be established, one still requires very challenging measurements of small plasma regions on fast time scales.^{20–25} If the experiment cannot resolve the relevant fluxes and associated gradients, plasma models and modeling codes are needed to interpret the measurements.^{26–29} In recent years, the experimental situation has improved with the application of emission spectroscopy of photons and particles^{30–32} and Thomson scattering^{33–36} for higher resolution.

Including detailed transport microphysics in radiation–hydrodynamics codes faces roughly three different kinds of challenges. The

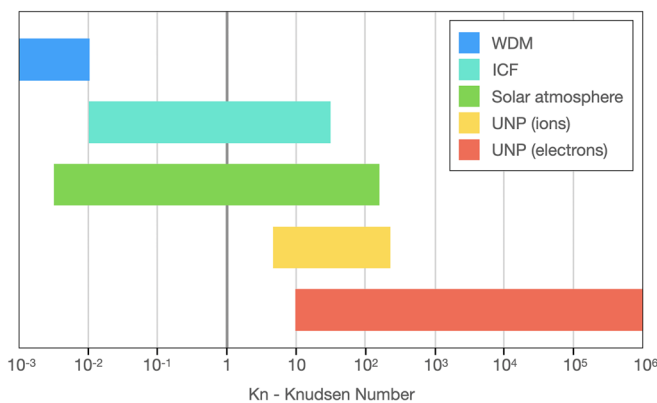


FIG. 2. Range of Knudsen numbers for warm dense matter (WDM), inertial confined fusion (ICF), solar atmospheres, and the ions and electrons of ultracold neutral plasmas (UNP). The Knudsen number is defined as $Kn = \lambda_{mfp}/L$, where λ_{mfp} is the mean free path determined from Eq. (1), and the characteristic length scale of the system was chosen as $L = 1 \mu\text{m}$ for all cases except for solar atmospheres in which $L = 1 \text{ km}$.

first is the overwhelming complexity of writing density, momentum, and energy equations for all of the different species in their various ionization states.^{37,38} The number of equations scales as N^2 for N species, and more importantly, there can be ambiguity as to which gradients should be included, where expansions can be truncated and which terms can be combined (e.g., velocity and temperature fields are often assumed to be locked, but this approximation might be invalid for HED plasmas³⁹) The second challenge is understanding appropriate physics models that can be implemented across the plasma temperature and density ranges as the system evolves; many plasma experiments span the cold, warm, and hot dense matter regimes. The third is knowing the appropriate transport coefficients (or equivalent representations) within the contexts of those models.^{18,19,40} This last challenge can be acute in non-ideal plasmas.^{41–44}

II. PLASMA MIXTURES

In plasma mixtures, kinetic equations can be used to describe the evolution of each single-species distribution function under the influence of the other distribution functions associated with all other species. In particular, the multispecies Boltzmann equation is appropriate for dense plasmas in which collisions are characterized by strong binary scattering events. In this section, we sketch an approach for deriving transport coefficients within this framework.

A. The multispecies Boltzmann equation

The multispecies Boltzmann equation for a mixture of N species can be written as³⁸

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i + \mathbf{a}_i \cdot \nabla_{\mathbf{v}} f_i = \sum_{j=1}^N Q_{ij}[f_i, f_j]. \quad (2)$$

Here, $f_i(\mathbf{x}, \mathbf{v}, t)$ is the single-species distribution function of species i at position \mathbf{x} and velocity \mathbf{v} at time t , and \mathbf{a}_i is the particle acceleration of that species due to both internal and external driving fields. The Boltzmann collision operator $Q_{ij}[f_i, f_j]$ between particles of species i and j is given by

$$Q_{ij}[f_i, f_j] = \int (f_i(\mathbf{v}')f_j(\mathbf{v}'_*) - f_i(\mathbf{v})f_j(\mathbf{v}_*))g\sigma_{ij}d\Omega d\mathbf{v}_*, \quad (3)$$

where $g = |\mathbf{g}| = |\mathbf{v} - \mathbf{v}_*|$ is the relative velocity of the two particles, σ_{ij} is the differential cross section, and Ω is the unit vector in the scattering direction $\mathbf{v}' - \mathbf{v}'_*$. Finally, the velocities in Eq. (3) are coupled and conserve momentum and energy according to

$$m_i\mathbf{v} + m_j\mathbf{v}_* = m_i\mathbf{v}' + m_j\mathbf{v}'_*, \quad (4)$$

$$\frac{m_i}{2}|\mathbf{v}|^2 + \frac{m_j}{2}|\mathbf{v}_*|^2 = \frac{m_i}{2}|\mathbf{v}'|^2 + \frac{m_j}{2}|\mathbf{v}'_*|^2. \quad (5)$$

Numerical solutions of the Boltzmann equations remain prohibitively expensive: N coupled integrodifferential equations need to be solved each in a six-dimensional phase space. This computational issue is partly mitigated by exploiting the collisionality that maintains the plasma close to equilibrium.

B. Hydrodynamic equations

Hydrodynamic equations based on velocity moments of an underlying kinetic equation (such as the Boltzmann equation) reduces the dimensionality from six to three. Furthermore, for collisional

plasmas that are close to equilibrium, only the first few moments are needed for an accurate description. We sketch the derivation of such hydrodynamic models by first multiplying Eq. (2) by the mass m_i of species i and integrating over \mathbf{v} to give the continuity equation,

$$\frac{\partial \rho_i}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{U}_i) = 0, \quad (6)$$

where ρ_i is the mass density of species i . The species diffusion velocity \mathbf{U}_i is given by

$$\mathbf{U}_i = \frac{1}{n_i} \int (\mathbf{v} - \mathbf{u}) f_i d\mathbf{v} = \mathbf{u}_i - \mathbf{u}, \quad (7)$$

where the bulk velocity of species i is $\mathbf{u}_i(\mathbf{x}, t)$, and $\mathbf{u}(\mathbf{x}, t)$ is the center of mass velocity defined as

$$\mathbf{u} = \frac{1}{\rho} \sum_{i=1}^N \rho_i \mathbf{u}_i, \quad \rho = \sum_{i=1}^N \rho_i. \quad (8)$$

Next, the total momentum equation can be determined by multiplying Eq. (2) by $m_i(\mathbf{v} - \mathbf{u})$, integrating over velocity, and summing over all species to give

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = \sum_{i=1}^N \rho_i \mathbf{a}_i, \quad (9)$$

where \otimes denotes an outer product, and the total stress tensor $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = \sum_{i=1}^N \int m_i (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) f_i d\mathbf{v} = \sum_{i=1}^N \boldsymbol{\sigma}_i. \quad (10)$$

Similarly, multiplying Eq. (2) by $m_i |\mathbf{v} - \mathbf{u}|^2/2$, integrating over velocity, and summing over species gives the (kinetic) energy equation,

$$\frac{3}{2} \left(\frac{\partial(nT)}{\partial t} + \nabla_{\mathbf{x}} \cdot (nT\mathbf{u}) \right) + \nabla_{\mathbf{x}} \cdot \mathbf{q} + \boldsymbol{\sigma} : \nabla_{\mathbf{x}} \mathbf{u} = \sum_{i=1}^N \rho_i \mathbf{U}_i \cdot \mathbf{a}_i, \quad (11)$$

where the n is the total number density, the colon ($:$) denotes a tensor contraction over the indices, and the total heat flux \mathbf{q} is given by

$$\mathbf{q} = \sum_{i=1}^N \int \frac{m_i}{2} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) f_i(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = \sum_{i=1}^N \mathbf{q}_i. \quad (12)$$

As the number of species increases, there will be an equation like Eq. (6) for each species. However, hydrodynamic coupling between the species occurs through equations like Eqs. (11) and (12).

C. Transport coefficients

In highly collisional plasmas, the distribution functions are nearly Maxwellian, a fact that hydrodynamics exploits and one we can exploit to model the Boltzmann collision operator. Near equilibrium, we can employ the approximation of Bhatnagar, Gross, and Krook (BGK) for the collision operator of Eq. (3) with the form

$$Q_{ij}^{\text{BGK}} = \nu_{ij} (M_{ij} - f_i), \quad (13)$$

where M_{ij} is a Maxwellian distribution at a pair temperature T_{ij} and velocity \mathbf{v}_{ij} , and ν_{ij} is a collision rate.⁴⁵ The collision frequencies are determined by matching the momentum relaxation rate or

temperature relaxation rate of a plasma mixture in the BGK approximation to the Boltzmann equation.⁴⁶ These rates then connect to the Boltzmann equation through the momentum transfer cross section $\sigma_{ij}^{(\ell)}$, and collision integrals of the form¹⁹

$$\Omega^{(\ell, m)} \sim \int_0^\infty w^{2m+3} \sigma_{ij}^{(\ell)}(w) e^{-w^2} dw \quad (14)$$

can be calculated. Transport coefficients are proportional to these integrals, which then enables the calculation diffusion coefficients, viscosity, temperature relaxation rates, and thermal and electrical conductivity. Collision integrals that have been verified by molecular dynamics (MD) simulations and fit to simple functional forms have been published for binary mixtures.¹⁹

D. Beyond binary mixtures

A binary mixture could be characterized by a seven-dimensional parameter space: $Z_1, Z_2, m_1, m_2, n_1, n_2$, and T , which corresponds to the charge numbers, masses, number densities, and temperature, respectively. While certain symmetries present in the system can allow some of these dimensions to be combined, any model-dependent parameters would further increase the dimensionality. If an experimental or simulation program was designed to (sparsely) explore this parameter space by choosing three points along each dimension, then $3^7 = 2187$ different plasma systems would need to be explored. Taking this idea to the general case of mixtures with N species, the parameter space might be characterized by a $3N + 1$ dimensional space, thus requiring 3^{3N+1} experiments or simulations for this sparse sampling. This scaling is an example of the so-called ‘‘curse of dimensionality,’’ which worsens considerably in the more realistic scenario that more than three points would be needed to appropriately sample a given dimension.

Furthermore, when extending hydrodynamic models to plasma mixtures with more species, the complexity increases rapidly in ways that are fundamentally different from a one-component or binary plasma due to the breakdown of symmetries between species. For example, for three or more species, the number of transport coefficients increases quadratically, and their calculation requires full matrix inversions.^{37,47} Simplifying approximations are often made, such as locking the velocity and temperature fields of each species together; however, it has been found that this unrealistic in non-equilibrium plasmas.³⁹

III. DPP MINI-CONFERENCE ON TRANSPORT IN NON-IDEAL, MULTI-SPECIES PLASMAS

Because of the importance of this complex problem, a miniconference was organized to bring together a broad community focused on modeling plasmas with many species. In this Special Topics issue on Transport in Non-Ideal, Multi-Species Plasmas, contributors from the 2020 DPP mini-conference on this topic present their state-of-the-art research in transport physics. Topics included transport in the solar atmosphere, diffusion in monolayers in dusty plasmas,⁴⁸ electron and ion transport in ultracold neutral plasmas,^{49–51} and MD simulations along with theoretical treatments of pair potentials, electronic transport, transport coefficients in a conservative BGK model, model verification, and using machine learning to extend the applicability of MD data.

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DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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