White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	***July 23, 2015***

Indicate the primary area this white paper addresses by placing "P" in right column.
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	"P", "S"
• Plasma Atomic physics and the interface with chemistry and biology	
• Turbulence and transport	
• Interactions of plasmas and waves	
• Plasma self-organization	
• Statistical mechanics of plasmas	P

Indicate type of presentation desired at Town Hall Meeting.

	"X"
Oral	
Poster	
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Title:	Kinetic theory to support modeling of dense plasmas in experiments and astrophysics
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**(Limit text to 3-pages including this form. Font Times Roman size 11.
1 page of references and 1 page of figures may also be included. *Submit in PDF format.*)**

- ***Describe the research frontier* and importance of the scientific challenge.**

High energy density plasmas, including warm dense matter, arise in several frontier research fields. These include major experiments in inertial confinement fusion (ICF), including NIF, OMEGA EP and the Z Pulsed Power Facility, as well as experiments exploring materials in extreme conditions, such as LCLS and high-power laser facilities. Dense plasmas are also common in astrophysical objects, including white dwarf stars and giant planet interiors. The design and interpretation of experiments, as well as accurate modeling of the astrophysical objects, depends on an accurate hydrodynamic or magnetohydrodynamic description of the macroscopic behavior of these plasmas. This requires a validated kinetic theory of the microscopic physics that can be used to determine self-consistently the transport and equation of state properties required for the fluid descriptions. *Developing and validating such a theoretical description of this novel state of matter is a research frontier requiring advances in, and coordination between, theory, experiment and simulation.*

Traditional plasma physics has advanced based on a solid foundation of Landau kinetic theory [1], Braginskii transport theory [2], and critically it's validation under applicable conditions. This forms a basis from which more complicated scenarios, such as turbulence, can be addressed. The theoretical

foundation of high energy density plasma has not yet been developed. This is critical for the field to progress.

This is a challenging frontier because several physical effects simultaneously influence high energy density plasmas. It is sometimes described as the intersection of plasma and condensed matter physics, where approximations that are justified in the density and temperature regimes traditional to each subject break down. In particular, ions can range from weak to strong coupling and typically obey a classical statistical mechanics, while electrons range from weak to moderate coupling and range from classical to quantum statistical regimes. Mixtures of ionic species, with varying coupling strengths, are common. The systems are often far from equilibrium, where electron and ion temperatures can greatly differ. Furthermore, very strong magnetic fields arise in many of the applications that are capable of magnetizing one or more of the species.

Despite the complications, progress in this area is critical. The design of experiments, and interpretation of many measurements, relies on accurate descriptions of the macroscopic fluid behavior – which in turn rely on an accurate description of the microphysics. Astrophysical applications, such as stellar evolution, have similar research needs. Progress on this frontier will have impacts across physics, astrophysics and applications such as fusion energy research.

- ***Describe the approach to advancing the frontier and indicate if new research tools or capabilities are required.***

Theory: A theoretical frontier is to develop, to the extent possible, a systematic kinetic theory describing the microscopic dynamics of HED plasmas, as well as a solution of the resulting kinetic equations that describes the macroscopic fluid behavior. It is particularly important to determine the extent to which the traditional forms of hydrodynamic and magnetohydrodynamic equations can accurately describe these systems. Current theories have largely focused on ad hoc extensions of plasma kinetic theories, such as mean field theories [3] or Boltzmann-based approaches [4], to model the transport coefficients arising in traditional fluid equations. Similarly, equilibrium statistical methods, such as hypernetted chain [5] and average atom methods [6], have been used to address the equation of state term. These approaches have succeeded in extending plasma theory, but typically break down when the coupling strength is sufficiently high. A systematic kinetic theory would address several issues: (1) provide a means of quantifying the error in the theory, (2) determine if the general form of magnetohydrodynamics as currently written holds in HEDP conditions, (3) address parameter regimes where the current ad-hoc extensions fail. This will require not only great advances in the kinetic theory, but also the solutions necessary to address fluid behavior (i.e., the appropriate analog to the Chapman-Enskog or Grad solutions of weakly coupled theory). Including magnetization in the kinetic or fluid theories under HEDP conditions is essentially unexplored [7].

Experiment: It is critical that theory be validated with experiments. The only way to truly do so is to make measurements at the specific plasma parameters of interest. This necessarily requires HEDP experiments, which are big-science facilities such as NIF, Omega EP or LCLS [8]. These are critical, but expensive. In addition, a rigorous program of smaller-scale laboratory experiments should be run in parallel. Although these cannot obtain the specific HED parameters of ultimate interest, they can access regimes where different physical aspects that are novel in HEDP (such as strong coupling or degeneracy) arise in isolation. For example, dusty plasmas have long addressed strong coupling physics [9]. These are capable of reaching regimes in which the liquid-solid phase transitions can be measured. Dust in these experiments is well diagnosed optically, which provides a clean testbed for validating aspects of classical transport theory at strong coupling. Similarly, nonneutral plasmas can reach very strong coupling and are well diagnosed optically [10]. A more recent track is ultracold neutral plasmas, which can reach states in which both electrons and ions are moderate to strongly coupled [11]. These are particularly well

diagnosed, especially with regard to ion dynamics ,which can be measured using laser induced fluorescence. It has recently been shown that sonolumenscing microbubble experiments provide a table-top method that may be capable of accessing strong coupling and features of dense electron physics simultaneously [12]. Furthermore, plasmas in each of these experiments are much easier to magnetize than at HEDP conditions.

Simulation: Simulations are essential tools to aid in validating theory and to give insights into the microphysical mechanisms that should be included in a kinetic theory. Classical and quantum molecular dynamics are the prevailing methods in use today to model HEDP conditions. Their successes notwithstanding, those methods present a number of limitations that are both of fundamental and numerical nature. For instance, they are unable to deal with truly non-equilibrium, dynamical conditions such as arising in experiments, which necessitate solving the coupled time-dependent evolution of both quantum electrons and classical ions. As another instance, the current equilibrium quantum molecular dynamics simulations are limited in the physical conditions, system sizes and time-scales it can reach (temperatures up to a few tens of thousands kelvins, for a typical sample size of a few hundred atoms and a few thousand time steps), due to the costly nature of the method based on quantum orbitals. Advances in the fundamental and numerical components of simulation methods should be made to go beyond these limitations, including the development of accurate orbital-free quantum molecular dynamics methods [13], the numerical implementation of hybrid classical and quantum kinetic equations, the development of advanced real-space algorithms (e.g., multigrid) that are more amenable to large grids and parallelization than the usual three dimensional Fast-Fourier transforms, the development of time-dependent density-functional theory to deal with non-equilibrium conditions.

- ***Describe the impact of this research on plasma science and related disciplines and any potential for societal benefit***.

This is a critical frontier that will aid progress in ICF research, potentially contributing to the ultimate goal of fusion energy reactors for electricity production. Aside from this, HED plasmas are a medium that is only beginning to be explored. The history of physics has shown that exploration of new parameter regimes (in time, space, density, temperature, etc) often lead to unexpected discoveries that fuel innovation. HEDP is such an unexplored area. Outside of terrestrial applications, progress on this frontier will contribute directly to astrophysics – particularly in the areas of stellar evolution modeling [14] and the modeling of giant planet formation and evolution. This provides a rich area where plasma physics can make significant contributions to other disciplines.

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