White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	23 June 2015

Indicate the primary area this white paper addresses by placing "P" in right column.
Indicate secondary area or areas by placing "S" in right column

	"P", "S"
• Plasma Atomic physics and the interface with chemistry and biology	
• Turbulence and transport	P
• 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	
Either Oral or Poster	X
Will not attend	

Title:	Exa-scale computing; The new computational frontier for solving kinetic equations
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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.**

The regime of plasma physics called high energy density physics (HEDP) is rich in complex phenomena, spanning warm dense mater, through inertial confinement fusion (ICF) plasmas to supernova progenitors and gamma-ray bursts. Of particular interest to this paper is those plasmas characteristic of ICF implosions and explosions. The computational workhorse for HED continues to be continuum radiation-hydrodynamic codes. These codes are massively-parallel, 3D and millions of lines long. With the advent of new computational GPU architectures, and the possibility of exa-scale computing, a great deal of effort of the scientific community is going into developing new efficient numerical algorithms for the set of radiation-hydrodynamic equations. However, with the advent of the new powerful computers, the time is ripe to go beyond the continuum radiation-hydrodynamic description to the more fundamental kinetic description of HEDP matter. The timeliness of moving to numerically solving the kinetic equations for HEDP matter seems obvious when coupled with the fact that recent observations on OEMGA and NIF point to large kinetic effects in ICF implosions. These effects are not captured in our simulations and it is clear that a more fundamental treatment is needed. The time is ripe to consider another axis on the exa-scale challenges axis. Instead of thinking about making the algorithms for the existing equations faster, we should also consider solving the full phase space distribution function in a thermos-nuclear burning, radiative environment and for multiple species. In other words, exa-scale is

now opening up the possibility that we can numerically solve the kinetic equations for a macroscopic ICF implosions and explosions in two and three spatial dimensions and two and three momentum dimensions and for the first time, capture the detailed transport physics in a fundamental way.

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

The Department of Energy (DOE) will be investing $325 million in a pair of computers that set the stage for exa-scale computing. The recent efforts in moving the ICF design codes to advanced architectures have focused on improved algorithms for the existing equations. It is important to simultaneously advance the frontier along another axis; improved physics fidelity for HEDP matter. Ultimately, we would like to solve the kinetic equation in 3 spatial and 3 momentum coordinates along with having it coupled to thermonuclear burn and radiation transport. This requires a tremendous amount of computer memory along with a large number of floating-point operations (FLOPs). The new computer architectures are dictating the types of algorithms we must employ; intensive local computing coupled with minimizing data passing and global memory storage. The characteristic which has wholly changed is that data motion becomes the computationally limiting factor not processing power.

The path forward is to explore the algorithms that are suitable on the new architectures by experimenting on the simplest non-trivial kinetic equations. The Vlasov-Fokker-Planck equation will act as a testing ground for more complex equations. Therefore, we first consider the Vlasov-Fokker-Planck equation in 1 spatial dimension and 2 momentum dimensions (1D-2P). The recent work of Luis Chacon and his team [1-2] who have developed iFP: an optimal, fully conservative, fully implicit, 1D-2P Vlasov-Fokker-Planck solver for ICF capsule simulations, is demonstrating the possibility of using advanced algorithms to solve kinetic equations for real world simulations. The path forward is to use high-order, computationally intensive numerical schemes to difference the equations on the phase space mesh. These algorithms create a high resolution solution of the particle distribution function. Algorithms that take advantage of dense matrix systems will be utilized. The next steps are based on two branches. One branch is to keep the Vlasov-Fokker-Planck form of the kinetic equation but to go to 3D-3P and develop exa-scale capable algorithms. The other branch is to go to higher-physics fidelity collision operators. Of particular interest is the quantum Lenard-Balescu (QLB) equation which is finite with no Coulomb logarithms. New spectral methods are showing promise for solving the 1P QLB equation. These methods would have to be applied to the Vlasov-QLB equation in 1D-2P. They need to be tested on advanced architecture machines but they show promise since they exactly conserve particle number, momentum and energy and they are computationally intensive.

The next step is to adopt the algorithms developed for the Vlasov-Fokker-Planck test bed to higher physics fidelity kinetic equations that possess more realistic equations of state (EOS). Of particular interest is to write down the first order equation in the BBGKY hierarchy, keeping the pair correlation function. This function would be computed using either molecular dynamics (MD) or hyper-netted chain equations. The computational challenges would be tremendous. What are the exa-scale algorithms needed to bride the time and length multi-scale problem of MD and kinetic theory?

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

This impact to the HEDP community would be significant. Current simulations of ICF implosions on exploding pusher experiments are showing an inconsistency between data and simulation [3]. Solving the kinetic equations for ICF applications would capture the various transport effects such as kinetic effects due to pressure, species and thermal gradients in a natural way. These codes would be multi-species and

multi-velocity which the ICF design codes typically are not. These kinetic equation codes would underwrite the predictive capability of the continuum radiation-hydrodynamic codes and they would allow researchers to understand the bound of validity of the models used in the continuum ICF design codes.

References (Maximum 1 page)

1. W. Taitano et al, *J. Comput. Phys.*, submitted (2014)
2. L. Chac´on et al, *J. Comput. Phys.*, **157**, 654-682 (2000)
3. P. Amendt, et al., Phys. Rev. Lett., 105, 115005(1)-115005(2) (2010)