White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	***23July2015***

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	S

Indicate type of presentation desired at Town Hall Meeting.

	"X"
Oral	X
Poster	
Either Oral or Poster	
Will not attend	

Title:	Structure Preserving Numerical Algorithms
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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 long-term accuracy and fidelity of numerical algorithms is essential for describing the nonlinear behavior of plasmas. Because it is not feasible to solve the parent equations we would like, various reductions are made and it is often the case that geometrical structure of the parent equations is lost. Retention of structure in reductions and eventual numerical algorithms, such as phase space or energy conservation, is the frontier.

The 1980s experienced rapid development of symplectic integration techniques (e.g. [1]) for ordinary differential equations. The success of these techniques for accurately representing solutions is based on the idea that the numerical method for a Hamiltonian system should advance in time via a canonical transformation, thereby preserving phase space invariants. Since the Hamiltonian part of dissipative system is often the most difficult to accurately solve, this technique can be used effectively in split-step methods. Similarly, conservative integration techniques (e.g. [2]) that exactly preserve invariants may be useful for systems where the long time state depends, e.g., critically on conservation of energy.

However, computational plasma science requires the solution of difficult partial differential equations, and for these the area of structure preserving algorithm development is a rapidly expanding field. Such

algorithms allow accurate delineation of numerical and real dissipation. In the plasma physics community, there has been a burst of such activity and interest in the last few years. This is because the accuracy rendered by the geometric algorithms fits exactly the need of modern large-scale computer simulations of the multi-scale, complex dynamics of both laboratory fusion plasmas and astrophysical plasmas.

Symplectic (e.g. [3]) and energy conserving (e.g. [4]) algorithms have been developed for partial differential equations. Yet, variational integration techniques for plasma kinetic theories have recently receive much attention. For example, low noise variational PIC codes have been developed (e.g. [5,6]), as well as Vlasov solvers (e.g. [7]) that use underlying variational structure. And similar techniques are also workable for MHD models (e.g. [8]). However, because of the curse of dimensionality, Vlasov codes cannot describe important geometries of interest. This leads to the challenge.

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

The present method for overcoming the difficulty of understanding strongly magnetized plasmas is via gyrokinetic theory. We propose a general approach for addressing this challenge, as demonstrated by the following example: First, return to the derivation of gyrokinetics or whatever equation is believed to contain the essential approximatins. In [9] this was done for gyrokinetics and a new form of these equations that has both variational and Hamiltonian structure was obtained. The new form overcomes the difficulty of the elliptic solve that is usual in gyrokinetics by replacing it by hyperbolic propagation in a slow pseudo-vacuum, the gyrokinetic vacuum, which circumvents the elliptic solve. Next, the new form of the equations is amenable to variational or symplectic methods. This is merely and example, but it shows how algorithm development should not be separated from systematic structure preserving approximation.

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

The analytical and computational tools developed will have application to any field interested in transport, including e.g. astrophysics, fluid mechanics, atmospheric science, climate science, and oceanography. The potential for societal benefit goes without saying.

References (Maximum 1 page)

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