White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	***06/19/2015***

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	P
• Turbulence and transport	S
• Interactions of plasmas and waves	
• Plasma self-organization	
• Statistical mechanics of plasmas	

Indicate type of presentation desired at Town Hall Meeting.

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

Title:	High-Fidelity Numerical Simulations of Atmospheric-Pressure Plasma Jets with Application to Medicine
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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.***

In recent years, low-temperature, atmospheric-pressure plasmas have received tremendous interest, in no small part due to their application in biology and medicine (Laroussi et al., 2009). In practice, plasma-created species can be remotely delivered to the surface to be treated by applying a pulsed electric discharge to a gas flowing through a tube and exiting into the ambient (Lu et al., 2012). Electric fields, photons and charged species thereby produced interact with the biological fluids and tissue, and have been shown to contribute to the treatment via signaling mechanisms, oxygenation and supplying activation energy (Graves, 2012). While atmospheric-pressure plasma jets have been shown to successfully deactivate bacteria (Laroussi et al., 2000), sterilize surfaces (Laroussi et al., 2009), heal wounds (Fridman et al., 2008) and kill cancer cells (Keidar et al., 2013), plasma medicine remains in its infancy. Precise mechanisms are still poorly understood, largely due to the complex multiphysics (electromagnetism, fluid dynamics) nature of processes involving all states of matter (solids, liquids, gases and plasmas) across scales ranging from hundreds of nanometers (subcellular phenomena) to decimeters (jets), from nanoseconds (plasma discharge) to days (tissue healing). Predictive capabilities required to engineer safe and effective technologies that translate from the bench to the bedside are currently lacking. There is thus a critical need to elucidate the fundamental physical, chemical and

biological processes that govern interactions between low-temperature, atmospheric-pressure plasmas and tissue.

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

High-fidelity numerical simulations constitute an ideal tool to advance the field of low-temperature plasmas interacting with biological tissue. Although comprehensive investigations resolving all length and time scales and with full physics, chemistry and biology are infeasible no current computing architectures, simulations can be exploited to isolate specific physical/chemical/biological interactions; the data and knowledge thereby generated can be used to develop and validate reduced-order models to be applied over larger/longer scales. For instance, in early simulations of low-temperature, atmospheric plasma jets interacting with biological tissue, the problem was broken up into a succession of steps by considering a jet into (humid) air with single and multiple pulses (Norberg et al., 2015a), its interaction with dielectric and metallic surfaces (Norberg et al., 2015b), including a water layer (Norberg et al., 2014). While our understanding of the plasma chemistry and dynamics in these processes has improved, the development of medical procedures requires precise control of the species produced during the plasma discharge and their transport to the surface to be treated, for which an accurate representation of the coupling between plasmas and the flow is critical. This coupling gives rise to complex dynamics of plasma jets in laminar and turbulent regimes flow (Iseni et al, 2014). These considerations are critical given the intricacies of turbulent mixing, a truly multiscale process in which turbulence dynamics as well as species transport play important roles (Dimotakis, 2005).

For basic research, established approaches exist for high-fidelity simulations of turbulent flow, such as direct numerical simulations (DNS, Moin & Mahesh, 1998) in which all dynamical scales are resolved, or large-eddy simulation (LES, Meneveau & Katz, 2000) in which large scales are resolved on the grid and small-scale features are represented using physics-based models. High-order accurate numerical methods developed for such purposes undergo careful verification and validation (Roache, 1997), including against experiments, and sophisticated uncertainty quantification techniques (Najm, 2009) can be used to estimate parametric uncertainties. While highly sophisticated plasma chemistry models have been used to simulate atmospheric-pressure plasma jets (Norberg et al., 2015), the numerical methods require extensions (e.g., high-order accuracy, subgrid-scale models) to be capable of conducting accurate simulations of (turbulent) plasma jets at the Reynolds numbers of interest. The merger of these high-order methods for turbulence with sophisticated plasma chemistry models has the potential to significantly advance our understanding of low-temperature plasma jets.

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

Plasma medicine is a field ripe for scientific discovery. Capabilities to predict the interaction of atmospheric-pressure plasmas and biological tissue constitute the first step toward optimization and control of plasma jets. The design and optimization of devices for targeted purposes requires an understanding of the basic physical, chemical and biological understanding. Engineering devices that translate from the bench to bedside necessitates precise control, e.g., to accommodate effects such as varying ambient humidity or jerky movement of the user. Modern high-performance computing paradigms based on verified and validated methods and combined with uncertainty quantification have emerged as essential complements to experimental endeavors.

This research will advance plasma science by providing a greater understanding of complex coupled plasma flows in which chemistry is important. Furthermore, novel computational approaches must be developed to incorporate the multiphysics and multiscale capabilities at the required fidelity. Such research could open paths in biomedical engineering to fabricate such devices and medicine in general through the optimization and use of such devices. Such advances have the potential to transform the treatment of soldiers on the field.

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