White Paper for Frontiers of Plasma Science Panel

Date of Submission: 9 June 2015

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Title: Predictive Simulation of Pattern Formation and Self-Organization in Plasmas

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Predictive Simulation of Pattern Formation and Self-Organization in Plasmas

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• Research frontier:

Pattern formation and self-organization are complex and fascinating phenomena common in diverse types of biological, chemical, and physical systems. Their occurrence has been associated to instability, symmetry breaking, bifurcation, and to the formation of dissipative structures. Pattern formation and self-organization are also prevalent in a wide range of plasmas, from low-pressure - high-current vacuum arcs, to low-pressure - low-current glow, streamer, and dielectric barrier (DBD) discharges, to high-pressure - low-current glow, DBD, and arc discharges, and to high-pressure - high-current arc discharges [1-5]. Figure 1 shows representative experimental and computational results of self-organized patterns in different types of plasmas.

The understanding of pattern and self-organization formation in low temperature plasmas is more limited than for other types of physical systems, probably due to the tightly coupled interaction of fluid dynamic, thermal, chemical, and electromagnetic phenomena. This limited understanding is evidenced by often inconsistent or incomplete research findings. The phenomenological behaviors associated to the formation of electrode patterns differ significantly among different types of low temperature plasmas. Particularly, pattern formation is often observed in the regions near the electrodes, as evidenced by current transfer spots [6]. Electrode spots may produce detrimental effects within plasma processing applications or may limit the life of the electrodes. Therefore, pattern formation in low temperature plasmas is of interest not only from a fundamental, but also from practical, point of view.

Despite their prevalence in experimental observations, the capture of pattern formation and self-organization phenomena in general purpose plasma flow simulations has proven exceedingly elusive. Predictive modeling and simulation methodologies and tools are needed that are suitable for fundamental research studies in canonical plasma flows, but also robust and flexible enough to be used for the analysis of practical plasma processes and devices. Such methodologies and tools would advance the level of understanding of pattern formation and self-organization phenomena and lead to more efficient, reliable, and potentially to new plasma systems.

• Approach to advancing the frontier:

To achieve the predictive computational simulation of pattern formation and self-organization in plasma flows, modeling and simulation methodologies and tools with high numerical accuracy (e.g. from second-order or higher to spectral accuracy), commonly found in research problem-specific codes, together with the robustness and flexibility of commercial software, are needed. Such methods and tools should be suitable for the analysis of different types of plasma flow models (e.g. drift-diffusion, reactive, resistive magnetohydrodynamic, thermally-coupled, multi-fluid) in time-dependent three-dimensional configurations, such to capture spatial symmetry-breaking and dynamic behaviors (e.g. self-organization events) of patterns, and in complex geometries, commonly found in industrial plasma sources and processes. Moreover, the methods and tools should lead to grid-independent solutions, which may require Adaptive Mesh Refinement (ARM) strategies, potentially coupled to high-order discretization approaches; and should be able to exploit High Performance Computing (HPC) resources (i.e. massively-parallel simulation runs in heterogeneous computing clusters).

Figure 2 shows results of the spontaneous occurrence of anode spot patterns in arc discharge simulations [7, 8] obtained with a general-purpose plasma flow solver. The simulations used a time-
dependent three-dimensional thermodynamic nonequilibrium monolithic fluid-electromagnetic plasma flow model numerically implemented within a second-order-accurate in space and time Variational Multiscale (VMS) Finite Element Method (FEM) [9]. The results reveal the spontaneous formation of self-organized patterns of anode attachment spots in the free-burning arc, in qualitative agreement with experimental observations [10]. The number of spots, their size, and distribution within the pattern depend on the applied total current and on the level of anode cooling. The results showed that the location and number of spots depend on the resolution of the computational grid. Furthermore, the limited symmetry of some of the obtained patterns, together with their dynamic behavior, suggests that higher than second-order accuracy in space and time is needed. These observations represent limitations that need to be overcome to achieve predictive computational analyses of low temperature plasma systems.

• **Impact on plasma science and potential societal benefits:**

  The predictive simulation of pattern formation and self-organization in plasmas would advance the level of fundamental understanding of such universal phenomena, and have the potential to impact other disciplines such fluid flow stability, flame development, combustion front propagation, and transition to turbulence. Predictive pattern formation and self-organization simulation capabilities can lead to more efficient and reliable plasma systems, with longer electrode life, process uniformity, and energy efficiency; and can potentially lead to novel plasma processes that exploit inherent self-organization and localization, such as surface functionalization and nano-structure syntheses.
References

Figures

Figure 1 – Formation of electrode spot patterns in different types of electrical discharges: experimental results in (left most) a low temperature direct current discharge [2], (second from left) low pressure microdischarges [3], and (second from right) dielectric barrier discharges [4]; and (right most) computational simulation results of cathode spots in a glow discharge [5].

Figure 2 – Formation of anode spot patterns in a direct-current arc discharge: (left-top) depiction of the heavy-species temperature field obtained with a time-dependent three-dimensional thermodynamic non-equilibrium plasma flow model of the free-burning arc with a 10 [mm] inter-electrode spacing operating at atmospheric pressure [8, 10]; (left-bottom) close-up view of the region near the anode; and (right) matrix of the distribution of heavy species temperature along the plane at 0.2 [mm] away from the anode for different values of total arc current and level of cooling of the anode; the obtained attachment spots vary from a single diffuse spot for high currents and/or low cooling, to the spontaneous formation of self-organized static patterns for increasing cooling, and eventually to dynamic patterns for low currents and very high cooling levels.