The Center for Exascale Simulation of Plasma-Coupled Combustion (XPACC)

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The Center for Exascale Simulation of Plasma-Coupled Combustion (XPACC) is a new Predictive Science Academic Alliance Program (PSAAP II) Multidisciplinary Simulation Center at the University of Illinois in its first six months of operation. The Center uses large-scale computing to enable predictive simulation that advances the science and technology of plasmas to initiate and control turbulent combustion. The target application is a gas-phase fuel jet, which requires novel computational approaches that utilize extreme-scale computing. The Center funds 20 PhD-level student projects, most of whom will spend a 10-week internship at an NNSA national laboratory.

"At Illinois, PSAAP II has created a core of activity in computational predictive science, where faculty and students from diverse disciplines pursue joint scientific goals and develop new capabilities in extreme-scale computing," said William Gropp.

Plasmas offer a unique and untapped means of affecting combustion to boost performance and efficiency. Chemistry produced in plasmas can short-circuit the standard reactions; electric fields in the charged gas can undermine the flame stability; and the heating due to resistance of the plasma can impact both the flow and the chemistry. Predictions that include Bayesian-based analysis of the uncertainty in the calculation will maximize the utility of the simulations; low-dimensional, physics-targeted experiments will be used to identify physics and calibrate models for the principal Quantity of Interest: the sustained ignition threshold.

Each of the physical subcomponents of the coupled plasma-combustion system—the flow turbulence, plasma physics, reaction pathways, and electrode aging and electrodynamics—may require petascale computational resources for physics-based predictions. Coupling them across necessary length and time scales to make quality predictions demands the co-development of simulation models with tools to harness the heterogeneous architectures of anticipated exascale computing platforms.

(a) Basic DBD actuator design (b) Plasma off (c) Plasma on

Figure 1. The DBD plasma showing an order-one effect on an H_2 flame in a model, physics-targeted configuration.

The Center builds upon an existing petascale code, PlasComCM, and pursues new programming approaches that provide portable access to better performance and scalability through data structure and code optimizations for memory efficiency, exploitation of high-throughput computing elements, and automatic load balancing. Along with other tools and techniques, these will be designed to work on applications with similar needs, and the Center will actively engage the community to ensure their broad utility.

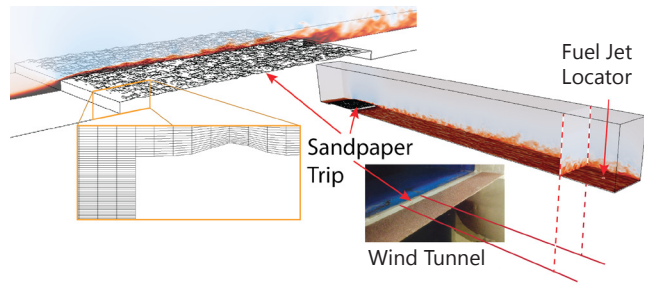

Figure 2. 3D inert turbulence resolved simulation of the wind tunnel, including a geometric realistic representation of the sandpaper turbulence trip. Upper left: cross-section near the inlet that shows the flow crossing over a piece of #40 sandpaper, which is used to initiate turbulence. Image just below: the computational mesh at the beginning of the sandpaper. To the right: a wind tunnel section, starting at the inlet before the sandpaper and ending a little after the location of the fuel jet (which is not used in this simulation). Below that (lower right): photo showing where this cross section sits in the wind tunnel—this shows that the computation (upper right) is for the center of the flow, well away from the sides of the wind tunnel.

A co-designed experiment-simulation plan is a key part of the principal predictive science goal. An annular dielectric barrier discharge (DBD) plasma actuator has been demonstrated to directly influence a hydrogen jet flame in a reduced model configuration (see Figure 1). When placed in a turbulent cross flow, the role of this actuator is to sustain ignition. Similar reduced, physics-targeted configurations have been developed to enable advanced bench-top diagnostics to identify mechanisms and calibrate models. The full system will couple the actuator, a spark ignition system, and the fuel jet into a turbulent boundary layer (see Figure 2).

Simulations are progressing along two paths. A two-dimensional (2D) model has been developed to integrate first-generation models for the plasma, chemical kinetics, and flow. At the same time, a large turbulent 3D boundary layer simulation will match the upstream measurements from the Illinois wind tunnel. Inflow conditions are anticipated to be particularly important, so a realistic sandpaper trip is explicitly represented as shown in Figure 2.

PlasComCM has been subjected to detailed analysis in preparation for the transforms that will enable it to achieve high sustained performance on emerging machines. In addition to an optimization that doubled its performance and improved memory management, it has been analyzed with the Illinois tools VectorSeeker, AMPI (via ROSE), and Triolet. To facilitate analysis and subsequent transforms, representative pieces of the code termed codelets have been developed to highlight key features of the full application—a similar approach to development has been successful at NNSA national laboratories.