PSAAP-III Center

Integrated Simulations using Exascale Multiphysics Ensembles (INSIEME)

"Laser-based ignition of rocket engines: A short description of the Center's overarching problem and solution approach"

Prepared by: Javier Urzay and Gianluca Iaccarino

The overarching problem of the PSAAP-III INSIEME Center is the prediction of reliability of in-space ignition of cryogenic propellants (gaseous methane and liquid oxygen) in a model rocket combustor (see Figure 1). The problem involves a broad set of physical phenomena, such as multi-phase compressible fluid dynamics, thermodynamics, turbulent mixing, laser-induced ignition, and combustion. In the initial stage at near-vacuum pressures, the rocket combustion chamber is primed with one of the propellants. Once the pressure has reached a sufficiently high value suitable for chemical reactions to occur, a non-resonant laser triggers ignition of the cryogenic propellants and gives rise to a secondary stage that includes flame propagation and stabilization in the combustor. The ignition process is fast (of order miliseconds), but is nonetheless crucial for the success of flight missions in real space engineering applications.

Achieving ignition in a rocket combustor using lasers relies on the appropriate timing and location of the laser energy deposition. Important quantities influencing the ignition process that make it highly stochastic in practical combustor flow environments are the local fluctuations of pressure, temperature and equivalence ratio, as well as the turbulent intensities. These quantities are sensitive to aerodynamic effects induced by shock waves, turbulence in shear layers, liquid-gas interface motion, spray droplets, flash vaporization, primary and secondary atomization, and mixing of chemical reactants. In addition, uncertainties in the characterization of the propellants at injection, including their mass flow rates, temperatures, and composition, along with the uncertainties in thermomechanical laser parameters, play an important role in augmenting the unpredictability of the system. These effects lead to significant challenges for assessing the reliability of the ignition sequence.

The Center's simulation strategy is based on the construction of a large ensemble (millions) of simulations with different levels of physical fidelity that will be run on Exascale-class machines. Task-based programming will be at the core of the computational developments using the language Regent in combination with a software compiler and runtime system called Legion — both of which were developed at Stanford — to achieve more seamless performance from next-generation supercomputers. By taking advantage of task concurrency, hardware mapping, and statistical correlations, the technical breakthrough pursued here is to combine all these multi-fidelity simulations to predict the reliability of laser-induced ignition in realistic operating conditions using a single ensemble run. The

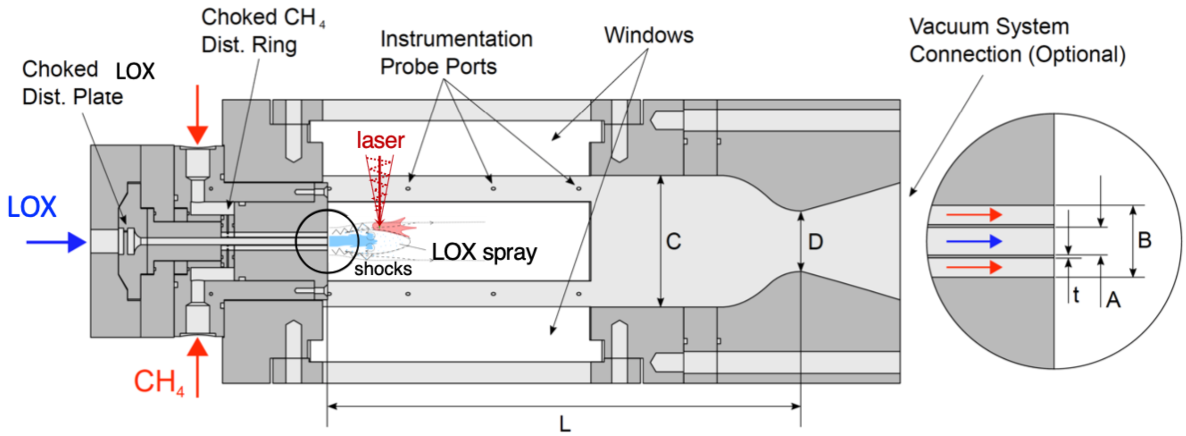

Figure 1: CAD of the INSIEME experimental rocket-combustor geometry (courtesy of Carson Slabaugh, Purdue University).

ensemble infrastructure is also used to enable distributed software verification, shared linear solver preconditioning, and general coupling techniques that will steer and adapt the sampling of new ensemble members. The simulations will be validated by a tailored experimental campaign in world-class rocket-testing facilities at Purdue University.

This project will expand the current state-of-the-art in the computational physics of fluid mechanics for rocket propulsion. For instance, fully resolved simulations of the combustor will push the boundary of available computing resources as a result of the wide range of spatiotemporal scales. Representation of the system dynamics at Kolmogorov scales will require up to one trillion grid points and millions of time steps. Furthermore, uncertainties in the system will require a large number of simulations to construct ignition probability maps. Critical elements that will be investigated to overcome these hurdles are (a) adaptivity in space and time, and (b) multi-fidelity ensemble computations. Different strategies involving physical, numerical, and data-driven formulations will enable a companion effort at University of Colorado at Boulder as part of this PSAAP-III Center to introduce hundreds of low-cost low-fidelity surrogate simulations as part of the ensembles. These will be executed in concert with high-fidelity simulations within the Legion Exascale runtime environment to enable the determination of the ignition success statistics.

Stanford, California
October 2020