In our research group, we are using the facilities and resources of the Penn State Institute for CyberScience Advanced CyberInfrastructure (ICS-ACI) to address urgent issues related to energy and the environment. Specifically, we are developing predictive computational fluid dynamics (CFD) tools that can be used to design high-efficiency, low emissions combustion systems for propulsion and power generation using conventional (fossil hydrocarbon fuels) and alternative (e.g., bio-derived) fuels. The principal area of application has been advanced reciprocating-piston internal combustion engines. The models account for liquid fuel injection, vaporization and mixing, ignition and turbulent combustion, pollutant formation, and heat transfer. Recent work has emphasized detailed chemical kinetics for real fuels, radiative heat transfer, and soot formation.