Multiscale Modeling in Combustion Simulations

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Detailed numerical simulation is ubiquitous in combustion research. Indeed much of the progresses in combustion science have been brought by the unique tradition within the combustion community to explain combustion phenomena, from homogeneous chemical reactions to turbulent combustion, in as quantitative and predictive a manner as possible. Because even a simplest flame process involves coupled chemical reaction, heat release, and mass and heat transport, combustion simulations are inherently multi-scale and multi-phenomenon. Without a doubt combustion simulation is perhaps one of the most successful stories of multiscale modeling of complex, nonlinear chemical problems, despite the fact that the community rarely labels such approaches as multiscale modeling.

In moving forward, we are keenly aware that the multiscale modeling approach to combustion science is limited by our ability to manage massive quantities of fundamental chemical kinetics and combustion property data, as well as combustion models that built on these data. This limitation also extends to our ability to collaborate across several disciplines, from pure chemistry to fluid mechanics. In the field of combustion kinetics, this limitation is often exemplified by studies that fail to consider all relevant data, or duplicating efforts because of lack of communication. This limitation can be and will have to be resolved by appropriate cyber infrastructure that will enable scientific data organization, interpretation, and communication, as well as efficient uses of computational tools. This talk will review our approaches to combustion simulation as a science of multiscale modeling and how the recent grass-root development of Process Informatics (PrIME) is critical in moving forward.