Numerical simulation has become an important approach to understand combustion processes and to speed up the design and optimization of advanced combustion engines. Chemical kinetics is an integral component of combustion while detailed chemistry of practical fuels can be highly complex and computationally prohibitive. In the last decade, the rapid growth in supercomputing power made it possible to accommodate fairly detailed reaction kinetics in large-scale flame simulations, including state-of-the-art direct numerical simulations (DNS). A new challenge has nevertheless emerged in computational diagnostics of the massive simulation data that can be of petabytes in cleaned form. Such large datasets defy current diagnostic methods that involve empirical criteria selection and/or frequent human interactions. New computational diagnostics are therefore needed to systematically extract salient information from the massive simulation data and to subsequently create models to predict the flame behaviors. In this presentation, our recent effort on mechanism reduction and stiff chemistry integration will be reviewed. A chemical explosive mode analysis (CEMA) will be presented for systematic identification of critical flame features, such as local ignition and extinction, onset of flame instabilities, and premixed reaction fronts from complex flow fields. The use of CEMA as a general-purpose flame diagnostic will be demonstrated with DNS data for different types of turbulent flames.

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