LARGE-SCALE NUMERICAL SIMULATIONS:
PRESENT AND FUTURE ROLE IN FUNDAMENTAL AND APPLIED COMBUSTION RESEARCH

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Abstract

In thermal systems for transportation and power generation *turbulence and combustion* are ubiquitous and very often inextricably coupled processes, down to the smallest scales of continuum mechanics in non-linear fashion. Unfortunately for our environment, sub-optimal technological design together with intrinsic process and equipment limitations cause these widely used thermal systems to waste much of the fuel's chemical energy (effective efficiencies are often well below 50%) simultaneously releasing nearly all of the atmospheric pollutants generated by mankind. Even considering future scenarios where Renewable Energy Sources (RES) and electric transportation will cover an increasing share of needs, combustion-based electricity generation by clean, efficient and flexible power plants will retain a central role due to electric grid stability requirements. Therefore, novel approaches to improve the present design of thermal machines are needed in order to meet increasingly strict emissions regulations, while maintaining a robust and fuel-efficient performance, and bring this technology beyond the state-of-the-art. Highly resolved large-scale numerical simulations, Direct Numerical Simulation (DNS) and Large Eddy Simulations (LES), can today be paired with increasingly affordable (and accessible!) high-performance computational resources and this combination has the potential to fill knowledge and methodology gaps, still present in such mature combustion technologies, to achieve the needed improvements and breakthroughs. We will illustrate that DNS is able to provide an unprecedented level of insight and detail to isolate and understand the mechanistic causality between turbulence, mixing and chemical reactions. These first principles DNS are well-suited to provide the underlying science base and verification data required to develop vastly more accurate predictive models needed by LES. Once its fundamental assumptions are finely-tuned and verified against DNS and experimental data, LES has the potential to be the ultimate design tool within applied combustion research and development. Exascale computing, to be deployed throughout Europe, the USA and Asia in the early 2020s, will *theoretically* enable combustion simulations, both DNS and LES, in parameter regimes still inaccessible today. However, making the transition to exascale poses a number of algorithmic, software and technological challenges. As Moore's Law and Dennard scaling come to an end exascale computing will be achieved only through massive concurrency. Addressing issues of data movement, power consumption, memory capacity, interconnection bandwidth, programmability, node failure and scaling is critical to ensure that future combustion simulations can take advantage of the computer architectures of the future.