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Terascale direct numerical simulations of turbulent combustion – fundamental understanding towards predictive models

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Abstract.
Advances in high-performance computational capabilities enable scientific simulations with increasingly realistic physical representations. This situation is especially true of turbulent combustion involving multiscale interactions between turbulent flow, complex chemical reaction, and scalar transport. A fundamental understanding of combustion processes is crucial to the development and optimization of next-generation combustion technologies operating with alternative fuels, at higher pressures, and under less stable operating conditions, such as highly dilute, stratified mixtures. Direct numerical simulations (DNS) of turbulent combustion resolving all flow and chemical features in canonical configurations are used to improve fundamental understanding of complex flow processes and to provide a database for the development and validation of combustion models. A description of the DNS solver and its optimization for use in massively parallel simulations is presented. Recent DNS results from a series of three combustion configurations are presented: soot formation and transport in a nonpremixed ethylene jet flame, the effect of fuel stratification in methane Bunsen flames, and extinction and reignition processes in nonpremixed ethylene jet flames.

1. Introduction
The rapid growth in computational capabilities has presented both opportunities and challenges for high-fidelity simulations of turbulent reacting flows. The advent of terascale computing power made it possible to glean fundamental physical insight into fine-grained aero-thermo-chemical interactions in simple laboratory-scale turbulent flames with detailed chemistry using three-dimensional direct numerical simulations [1–5].

1.1. Direct numerical simulation computational approach
In direct numerical simulation (DNS), the instantaneous governing equations are solved without averaging or filtering; all relevant continuum scales are resolved on the grid with no closure models using accurate numerical methods. Such simulations are costly, requiring several million CPU-hours on a terascale computer, up to a billion grid points, and generating hundreds of terabytes of data. It is anticipated that petascale computing (and beyond) will provide access to directly simulating a larger dynamic range of scales \(O(10^4)\) and the transport of greater...
numbers of species representative of renewable fuels of practical interest, enabling DNS to access relevant parameter regimes.

1.2. Direct numerical simulation of canonical configurations

Next-generation alternative-fuel internal combustion engines and aero-transport and power generation gas turbines will operate in nonconventional, mixed-mode, turbulent combustion under previously unexplored aero-thermo-chemical regimes. Compared to present devices, combustion in next-generation devices is likely to be characterized by higher pressures, lower temperatures, and higher levels of dilution and/or excess air (fuel-lean). Combustion processes in these environments, combined with new physical and chemical fuel properties associated with non-petroleum based-fuels, results in complex interactions that are unknown even at a fundamental level. These unknown processes place new demands on simulation and severely restrict our ability to predict the behavior of these systems from first principles and our ability to optimize them. Therefore, there is an urgent demand for high-fidelity simulation approaches that capture these reacting thermo-fluid interactions and, in particular, capture and discriminate the effects of variations in fuel composition. DNS can uniquely isolate and reveal fundamental causal relationships that are required for physical understanding and to develop predictive models. With petascale computing on the horizon, aero-thermo-chemical interactions are amenable to study by DNS, and here we highlight recent results from terascale DNS focused on soot formation and transport in turbulent ethylene/air jet flames, stratified combustion in turbulent slot jet flames, and extinction and reignition phenomena in turbulent ethylene/air jet flames. For each configuration, a range of physical conditions has been explored. In many instances, the unique simulation benchmarks are being used in a priori development and validation of advanced models for combustion closures used in engineering CFD simulations.

2. DNS performance and nodal optimization

Terascale DNS simulations were performed with the code S3D, which solves the compressible reactive Navier-Stokes, total energy, and species continuity equations for detailed chemistry. Typical DNS currently transport as many as 20–60 species in addition to momentum, energy and density. As such, S3D is data-intensive, and memory constrained on the microprocessor-based supercomputers. S3D is parallelized with a Cartesian domain decomposition, and nearly all the interprocess communication is performed with nearest-neighbor processes. Negligible global communication occurs. As such, weak scaling tests confirm that S3D scales to the full size of current supercomputers, to as many as 30,000 cores on the 250-Tflop Cray XT4 at ORNL. However, it achieves only 10–12% of the peak performance on a nodal basis. A detailed performance analysis of runs on heterogeneous allocations of the Cray XT3 and XT4 at ORNL was performed using TAU [6]. Analysis of execution time of loops and processes distributed among all processes showed performance limitations caused by lower memory bandwidth of the XT3 nodes, causing the faster XT4 nodes to wait in MPI_wait statements.

S3D is a data-intensive code that is limited by memory bandwidth. Without careful optimization, scientific codes often achieve as little as 5–10% of peak performance on microprocessor-based systems. Therefore, careful restructuring of S3D's data-intensive kernels was required to reduce its memory footprint and to boost its overall performance. Collaborating with computer scientists of the Performance Engineering Research Institute (PERI) S3D Tiger Team, S3D was reconfigured to reuse data in memory registers improving nodal performance. Rice University’s HPCToolkit performance tools [7] were used to study single-processor execution of a pressure wave test on a 50^3 domain. The study used a single node of a Cray XD1 with a 2.2 GHz Opteron 275 processor and DDR 400 memory, which provides 6.4 GB/s of memory bandwidth (as on Jaguar’s XT3 nodes). For the model problem S3D achieved 0.305 FLOPs/cycle (15% of peak). The HPCToolkit pinpointed several data-intensive routines in
S3D that did not fully exploit the memory hierarchy. The most important of these was the diffusive flux routine for species, momentum, and energy transport. This routine contains loops over a five-dimensional data structure: three position, one vector direction, and a scalar variable. In the model problem, this loop accounted for 11.3% of the total execution time, and the loop nest achieved only 4% of peak performance. The original code made very poor reuse of data in cache memory. The diffusive flux routine was restructured using Rice University’s LOOPTOOL utility [8], which supports source-to-source restructuring of loop nests written in Fortran. Loop reordering and unrolling performed by LOOPTOOL resulted in a speed increase of 2.94 times over the original code, with a 6.8% overall speedup for this change alone.

Further analysis of S3D’s node performance with HPCTOOLKIT, tuning loops with LOOPTOOL, and some manual adjustment of procedure argument passing conventions to avoid copying four-dimensional slices of a five-dimensional array yielded an aggregate improvement of 12.7% for the 50th problem on the Cray XD1. Future DNS computations will involve increasingly complex combustion chemistry involving up to 60 or more transported species and large numbers of grid points to resolve the turbulence and internal flame structure. Code optimizations will be extended with a focus on efficient evaluation of the chemical reaction source term and spatial transport routines.

3. Turbulent combustion simulations

With the optimized S3D code, we have performed direct numerical simulations of turbulent combustion with detailed chemistry in a wide variety of environments spanning a range of flame regimes and conditions. Here, examples of three configurations are presented:

(i) Soot formation and transport in nonpremixed turbulent ethylene flames
(ii) Fuel/air stratification in methane jet flames
(iii) Flame extinction and reignition in nonpremixed ethylene flames

3.1. Soot formation and transport

Soot formation is an important process in most practical combustion environments. The majority of heat transfer from combustion occurs through radiative emission of soot in the vicinity of high temperature flame zones. Soot is formed on the fuel side of nonpremixed flames as fuel diffuses into the high temperature flame zone where it is pyrolyzed in the absence of oxidizing species. Large molecular weight species are formed which grow by coagulation and chemical reaction to form primary soot particles which further grow by surface reaction and aggregation. Soot emission occurs when the soot is not fully oxidized as it passes through flames during the burnout of the fuel by oxidizer (e.g., air). This is a particular problem in diesel combustion and results in copious quantities of smoke emission in large-scale fires such as wildfires. Soot emission reduces combustion efficiency through unburned hydrocarbon emission. Emission of soot is also a significant source of small particles in the atmosphere (PM 2.5) causing haze and smog. When breathed, these particles are able to penetrate deeply into the lungs, contributing to health problems including asthma, chronic bronchitis, and even premature death.

A fundamental understanding of soot formation and transport processes is important in order to develop and validate combustion models that can be used to perform engineering equipment design and optimization and fire hazard evaluation. While turbulent combustion is a multiscale physical phenomenon, combustion with soot formation is a special challenge. Experimental measurements of soot in turbulent flames are complicated by the difficulty of noninvasive measurement techniques, such as laser diagnostics, due to the optical thickness of soot. Soot exists as a particulate phase with a particle size distribution that must be measured or modeled in order to accurately describe its formation processes. The composition and reactivity...
may depend strongly on the soot size and its age in a flame. The basic chemistry involved in soot formation is complicated by the large number of increasingly high molecular weight species involved in its formation and growth. As a particle phase, soot transport is distinct from the gaseous species comprising the diffusion flame. Soot transport occurs primarily through thermophoretic diffusion (diffusion down temperature gradients) as opposed to any significant soot concentration-based driving force.

While many detailed experimental and numerical studies of laminar flames have been performed, experimental turbulent flame data are limited to providing only mean quantities such as mean soot concentration, without simultaneously resolved instantaneous flow and chemical structure information. Simulations of turbulent sooting flames have been limited to RANS and LES simulations in which only large-scale structures are resolved, with fine-scale turbulence-chemistry interactions accounted for through subgrid modeling approaches. Direct numerical simulations have recently been performed with soot formation that reveal the detailed flow-flame structure of turbulent nonpremixed ethylene flames [5, 9]. The application of DNS to soot formation in turbulent combustion provides fundamental insights that are not otherwise available. These insights and the DNS data obtained may be used to develop and validate subgrid-scale models for practical combustion simulations. Here, DNS simulation results are presented of soot formation in a three dimensional nonpremixed ethylene jet flame.

The simulation is a temporally-evolving planar jet with a central $C_2H_4/N_2$ fuel core with a species mole ratio of 0.342. The fuel core is surrounded by oxidizer with an $O_2/N_2$ mole ratio of 0.359. These streams result in a stoichiometric mixture fraction $\xi_{st}$ of 0.25, where the mixture fraction (mass fraction of fuel stream material) $\xi$ is a flame coordinate and varies from zero in the oxidizer stream to unity in the fuel stream. The fuel and oxidizer streams flow axially in opposite directions. The boundary conditions are periodic in the streamwise (axial) and spanwise directions, and are nonreflecting outflow in the cross-stream direction. The domain size is $28.8 \times 19.8 \times 10.8$ cm in the streamwise, cross-stream, and spanwise directions. The grid size is 30 $\mu$m, resulting in 228 million computational grid points. The initial jet height is 1.8 mm, the velocity difference between the streams is 82 m/s, and the jet evolved for 50 characteristic jet times. The combustion mechanism is a validated reduced mechanism consisting of 19 transported species [9], and the soot model consists of semi-empirical nucleation, growth, oxidation, and coagulation steps, with the particle size distribution represented by transporting the first three mass-moments [5]. The simulation was run on 7920 processors on the Cray Redstorm machine at Sandia National Laboratories at a computational cost of approximately 1.5 million CPU-hours.

Figure 1 shows the OH mass fraction indicative of the flame zone and the soot number density at $41\tau_j$. This figure highlights the qualitative difference between the reactive gaseous species and the soot. The OH mass fraction exists only in the vicinity of the flame zone and has a
Figure 2. Joint PDFs of normal (NDT) and curvature (CT) components of $v_\xi$ on the flame surface at six times.

Relatively high diffusivity, whereas the soot number density, with its low diffusivity, is formed on the fuel side of the flame and convected into the fuel core where it is strained by the turbulence and forms very thin structures.

The transport of soot in the mixture fraction coordinate is of central importance to soot formation in turbulent flames as this dictates the location of the soot relative to the flame zone, hence the temperature, reactivity, radiative emission rate. As soot is a particulate with a low diffusivity, it is primarily convected with the flow and its transport in the mixture fraction (flame) coordinate is determined by the relative velocity between convection and isocontours of the mixture fraction. It was previously shown that this relative flame velocity $v_\xi$ arises from two additive terms: (1) flame curvature, and (2) normal strain [9]:

$$v_\xi = -D_\xi \nabla \cdot n -\frac{D_\xi}{2} \frac{\partial}{\partial \eta} \ln \left( \rho D_\xi \frac{\partial \xi}{\partial \eta} \right).$$

(1)

Here, $D$ is diffusivity, $\rho$ is density, $\eta$ is the flame normal coordinate, and $n$ is the flame normal $\left( \frac{\nabla \xi}{|\nabla \xi|} \right)$. Soot concentrations are higher when $v_\xi$ is positive such that soot is convected into the flame, as happens when the center of flame curvature is in the fuel stream. In addition, normal strain tends to move soot away from the flame zone due to the low $\xi_{st}$ relative to the inflection point in a $\xi$ profile across a flame (i.e., as a nominal S-shape profile of $\xi$ relaxes diffusively, the stoichiometric value moves away from the higher $\xi$ soot formation zone).

The soot transport is quantified by examining the joint PDF of the curvature and normal diffusion components of $v_\xi$. Figure 2 shows this joint PDF at six times during the simulation. The curvature term (CT) and normal diffusion term (NDT) are of similar magnitudes throughout the simulation. At each time, the mean of the CT is centered at zero. Conversely, the NDT is strongly biased to negative values at early times (soot transported away from the flame zone), but by the end of the simulation nearly 50% of the NDT is positive (soot convected towards the flame. This motion of the soot is related to the turbulent transport of soot away from its formation zone, along with the bulk mixing of $\xi$ as the jet evolves. Eventually, the fuel core will burn out completely, and the soot will be forced towards the flame zone where it will either burn or be emitted.

Figure 1 shows evidence of soot-flame breakthrough in regions where soot is on the oxidizer side of $\xi_{st}$. While noticeable levels of soot number density break through the flame, the
corresponding soot mass is very low since the soot is oxidized, but the soot particle number is not. However, it is conceivable that under conditions of higher soot loading, significant levels of soot mass may escape. Soot-flame breakthrough is an important problem in environments such as fires in which soot effectively shields surrounding objects from flame radiation.

The DNS data obtained provide not only fundamental understanding of soot-flame interactions but a database by which new turbulent combustion models may be validated. The transport of soot in the ξ (flame) coordinate is of prime importance in modeling turbulent sooting flames. A new conditional moment closure (CMC) [10] model has been proposed to directly account for the differential transport of soot in the ξ coordinate [11, 12]. Figure 3 shows an a priori comparison of the differential transport term in the CMC equation evaluated in its exact, unclosed form from the DNS data, and a modeled, closed form of the term suitable for subgrid-scale modeling. The agreement between the curves is reasonably good and illustrates the utility of DNS data for directly quantifying such models.

3.2. Stratified methane jet flames

Stratified flames occur in many practical combustion environments. In direct injection engines, fuel is injected directly into the combustion chamber to generate a highly stratified fuel-air mixture prior to ignition. This is done to reduce fuel consumption, particularly at low-speed light-load operation and is of great interest to both spark-ignition gasoline and compression ignition diesel engine manufacturers. In stratified combustion, the fuel and oxidizer are neither completely mixed nor completely segregated prior to combustion, and therefore traditional modeling approaches based on pure premixed or nonpremixed burning modes are inadequate. Another example of stratified combustion is found in aero-gas turbine engines where fuel and secondary air are injected at different spatial locations, resulting in a nonuniform equivalence ratio at the flame front.

Flame response to equivalence ratio gradients has been studied in simulations of laminar premixed flames, [13], and two-dimensional turbulent configurations [14]. Recent developments in experimental diagnostic techniques for stratified flows provide access to fully resolved composition fields at low turbulence levels [15]. A new set of fully resolved three-dimensional direct numerical simulations of turbulent stratified methane Bunsen flames are presented at a jet Reynolds number of 2100. The objective of the study is to determine the combustion efficiency and emissions characteristics (e.g., NO and CO) resulting from a range of initially stratified distributions of fuel and oxidizer. The flame structure and burning velocity under stratified conditions are to be compared to an equivalent uniformly premixed case.

The flame series consists of an existing DNS database of a
Figure 5. $|\nabla c|\delta_L$ conditionally averaged on progress variable $c$ and equivalence ratio $\phi = 0.5$ (left) and $\phi = 0.7$ (right) compared to the laminar flame profile for three simulations at $\frac{1}{2}$ the flame height.

Turbulent premixed combustion is dependent on flame speed, which depends on flame structure. Hence, a fundamental understanding how a turbulent flow field affects local flame structures is important for developing and testing turbulent premixed and stratified premixed combustion models. Characterizing the turbulence by the velocity fluctuations and length scales evaluated at one-quarter of the domain height [16], and evaluating the laminar flame properties for the range of equivalence ratio in each case, provides a range of Karlovitz numbers $(Ka = (\alpha/S_L l_k)^2)$ observed in the simulations. Here, $\alpha$ is the thermal diffusivity, $S_L$ is the laminar flame speed and $l_k$ is the Kolmogorov length scale. $Ka$ is the square of the ratio of the flame thickness to the smallest turbulent eddies. Previous analysis [16] has illustrated that the premixed DNS case, with $Ka = 5.2$, results in turbulent eddies penetrating the flame’s preheat layer, but not the reaction zone, placing that case in the thin reaction zones regime [18]. Scaling the Karlovitz number by the ratio of the full width half maximum heat release thickness $(\delta_H)$ to the flame’s thermal thickness $(\delta_L)$, $Ka^* = Ka \cdot (\delta_H/\delta_L)^2$, gives a value of 1.9 for the premixed case, but a range of 17.7-1.0 for the low stratification case. This suggests that the
highly turbulent flow will perturb the reaction zone itself in the leaner mixtures of the stratified cases leading to combustion in the broken reaction zones regime.

A progress variable $c$ is defined that varies between zero and unity in the unburnt and burnt gases, respectively. Figure 5 compares the normalized mean progress variable gradient versus $c$ at $\phi = 0.5$, and $\phi = 0.7$. Values of $|\nabla c|_{\delta_L} < 1$ indicate flame thickening relative to the laminar flame, where $|\nabla c|^{-1}$ is a measure of the flame thickness. The peak heat release occurs at $c = 0.65$, and low values of $c$ constitute the flame’s preheat zone. Figure 5 shows thickening of the flame’s preheat zone relative to the laminar flame. Near the peak heat release zone and at higher $c$, the turbulence acts to thin the flame $\phi = 0.5$, whereas at $\phi = 0.7$ the turbulent cases are comparable to the laminar flame and to the turbulent premixed flame [16]. These results emphasize the importance of correctly modeling the turbulence-chemistry interactions across the range of equivalence ratios present.

### 3.3. Nonpremixed flame extinction and reignition

Extinction and reignition phenomena are important in nonpremixed flames under high turbulence conditions. Nonpremixed flames occur at the interface between fuel and oxidizer, and turbulence acts to increase flame surface area and scalar gradients, which enhances mixing rates, hence combustion rates. As turbulence increases, finite rate chemical kinetic effects become important, and flame extinction may occur if heat release rates cannot keep up with diffusive heat losses. This is an important problem in modeling and simulation of combustion devices that push the limits of flame stability [18] to improve combustion efficiencies and reduce pollutant emissions. Flame regions that become extinguished continue to mix with fuel, oxidizer, and combustion products, and may reignite. The mechanism and mode of reignition is a subject of ongoing research. Reignition occurs as turbulent strain rates decrease and fluid parcels may reignite through several possible mechanisms. These include autoignition [19, 20], edge flame propagation [21], flame folding/mixing [22], and premixed or partially premixed flame propagation.

A series of three turbulent flame simulations were performed with varying levels of flame extinction. The flow configuration and chemical mechanism is the same as in the sooting simulation described above, that is, a temporally evolving planar nonpremixed ethylene jet flame. In each case, all flow and geometrical parameters were constant, with the differences being the composition of the fuel and oxidizer streams. These stream compositions were varied to yield a factor of two difference between Cases 1 and 3 in the levels of the stoichiometric steady laminar flamelet extinction scalar dissipation rate (i.e., loosely, the imposed flame strain

![Figure 6. Temperature contours with stoichiometric mixture fraction surface at the point of peak extinction.](image)
of one-dimensional opposed jet diffusion flames at extinction). The streamwise and spanwise
domain sizes are 11.5 and 7.7 cm, respectively, while the initial jet width is 0.96 mm. The
stream velocity difference is 196 m/s, giving a Reynolds number of approximately 5000 for the
three cases. In each case $\xi_{st}$ is 0.17, and the jets evolved for 75–140 characteristic jet times. The
cases were run on Jaguar at NCCS at ORNL, and consisted of 270, 308, and 341 million
computational grid cells, the differences being in the cross-stream direction only. The three cases
were run on 10,752, 10,752, and 14,112 processors at computational costs of approximately 0.9,
1.2, and 2 million CPU-hours, respectively.

Figure 6 shows axial cuts of the jet for the three cases. Temperature is shown with the
stoichiometric contour overlaid. The time of each case corresponds to the maximum level of
extinction: 27, 37, 72$\tau_j$, for Cases 1, 2, 3, respectively, for which the degree of extinction
increases dramatically. The level of extinction is important to the development of the jet and the
subsequent reignition of the flame. The presence of a flame reduces the local turbulence intensity
through flow dilatation, as well as the increased kinematic viscosity at higher temperatures.
This results in higher turbulence intensity as the flame extinguishes, which enhances the flame
extinction, and hinders flame reignition. In addition, the total stoichiometric flame surface area
is higher in cases with greater amounts of extinction, resulting in higher rates of total heat
release during reignition.

The degree of extinction of the flame surface also impacts the mode of reignition. High flame
extinction allows significant mixing of fuel and oxidizer in the absence of reaction, allowing
reignition to occur in a mixture of fuel, oxidizer, and combustion products. These reignition
modes blur the lines between premixed, stratified and nonpremixed combustion. Current efforts
are underway to quantify the impact of flame extinction on the jet evolution characteristics,
as well as understand the complex reignition processes occurring in the three cases. These
investigations make use of flame indicies that quantify the mode of reignition through the
alignment of gradients of fuel and oxidizer species. Preliminary results indicate that Case 3
experiences extreme extinction, near the limit of global blowout. This allows significant mixing
of the fuel, oxidizer, and products resulting in near complete reignition in a premixed flame
mode. Hence, an initially nonpremixed flame reignites through premixed flame propagation.
Conversely, Case 1 appears to retain its nonpremixed character through most of the reignition
process.

4. Conclusions
The growth in high-performance computing has allowed the simulation of turbulent combustion
with realistic chemistry and transport on up to 30,000 processors. The performance of the
DNS code S3D has been optimized to make efficient use of available computational resources by
using advanced performance and profiling tools to increase use of memory bandwidth resources.
A series of results from three recent DNS configurations were presented including nonpremixed
flames with soot formation, and extinction and reignition, and stratified methane Bunsen flames.
Soot formation in nonpremixed combustion is important to heat transfer, and as an emitted pollutant. Results show the importance of flame structure on transport of soot into and out of
reaction zones. Stratified combustion is increasingly important to achieving high efficiency and
low pollutant emission. Initial results of the stratified methane Bunsen flames show turbulence-
induced thickening of the preheat layer, impacting flame speed and overall burning rate, with
high stratification possibly leading to broken flames with disruptions in reaction zones. Flame
extinction and reignition phenomena are important in flame stabilization and for flows operating in
high-strain environments which maximize combustion rates through high turbulent mixing.
Results indicate that the extent of extinction has an important effect on the extent of premixing
prior to reignition, hence affecting the reignition mode and flow characteristics.
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