Numerical simulation of low Mach number reacting flows

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Abstract. Using examples from active research areas in combustion and astrophysics, we demonstrate a computationally efficient numerical approach for simulating multiscale low Mach number reacting flows. The method enables simulations that incorporate an unprecedented range of temporal and spatial scales, while at the same time, allows an extremely high degree of reaction fidelity. Sample applications demonstrate the efficiency of the approach with respect to a traditional time-explicit integration method, and the utility of the methodology for studying the interaction of turbulence with terrestrial and astrophysical flame structures.

1. Introduction

The dynamics of reacting flows in a turbulent environment play an important role in a number of areas of science and engineering. High-fidelity simulations are necessary to explore these systems in detail, but require simultaneous numerical resolution of chemical or nuclear reactions, diffusive transport and turbulent fluid mechanics. The combination makes these simulations some of the most demanding in all of computational fluid dynamics. The problem is particularly acute in the deflagration regime where the burning speed and associated velocity scales are much smaller than the speed of sound in the fluid. Low Mach number models exploit the inherent separation of scales in such systems by analytically eliminating acoustic wave propagation entirely from the dynamics, while preserving the important compressibility effects arising from reactions and transport. Low Mach number models were first introduced by Rehm and Baum [1], and were later derived systematically using asymptotics in Mach number by Majda and Sethian [2]. Bell et al. [3] generalized the low Mach number formulation to non-ideal gases for the simulation of stellar material. In this paper, we present the application of a low Mach number model in the context of very large scale parallel adaptive simulations of low speed reacting flow. Example systems from stellar and terrestrial flame applications demonstrate the extent to which modifications in the local structures of propagating flames can have a significant impact on the global flame propagation characteristics. Such detailed studies are not possible without the efficiencies associated with the low Mach number model, and so underscore the importance of advanced algorithm development in tandem with enhancements to raw computing power.

2. Numerical methodology

The low Mach number model is derived from the compressible flow equations based on asymptotic analysis in the Mach number $|U|/c$, where U is the fluid velocity and c is the

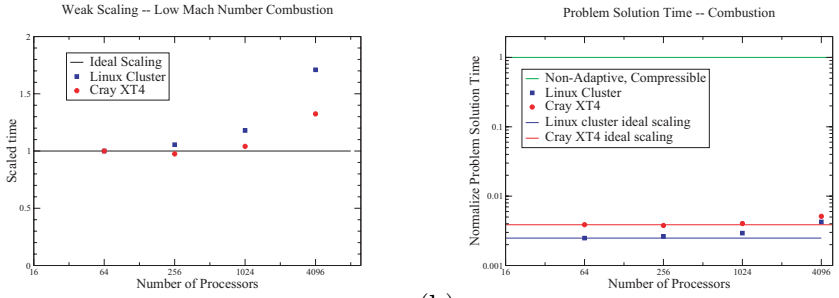
sound speed. This analysis leads to a decomposition of the pressure, $p(x,t) = p_0(t) + \pi(x,t)$, where $\pi/p_0 = O(M^2)$, and the dynamic pressure, π is decoupled from the equation of state for the thermodynamic pressure, $p_0 = p(\rho, T, Y_k)$. In this limit, the equations that express mass, momentum and energy conservation are as follows:

$$\begin{aligned} \frac{\partial \rho U}{\partial t} + \nabla \cdot \rho UU + \nabla \pi &= \nabla \cdot \tau + \rho F, \\ \frac{\partial \rho Y_k}{\partial t} + \nabla \cdot \rho UY_k &= \rho \dot{\omega}_k + \nabla \cdot D_k, \\ \frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho Uh) - \frac{dp_0}{dt} &= \nabla \cdot q. \end{aligned}$$

Here, ρ, U and h are the density, velocity and enthalpy, respectively, and Y_k is the mass fraction of species k. D_k, τ and q are the diffusive fluxes of species, momentum and energy and F represents an external force. In this system, acoustic waves, and the need to resolve them numerically, has been completely removed; the equation of state constrains the evolution.

The basic discretization combines a symmetric operator-split treatment of chemistry and transport with a density-weighted approximate projection method to impose the evolution constraint. The resulting integration proceeds on the time scale of the relatively slow advective transport. Faster diffusion and chemistry processes are treated implicitly in time. This integration scheme is embedded in an adaptive mesh refinement algorithm based on a hierarchical system of rectangular grid patches. The data and work are apportioned over a parallel computing system using a coarse-grained distribution strategy to balance the load and minimize communication costs. Options for data distribution include a knapsack algorithm [4], with an additional step to balance communications, and Morton-ordering space-filling curves. The complete integration algorithm is second-order accurate in space and time, and discretely conserves species mass and enthalpy. The reader is referred to [5] for details of the low Mach number model and its numerical implementation for an ideal gas equation of state and [3] for the extension of the methodology for stellar media.

Compared to a traditional explicit numerical integration of the compressible reacting flow equations, the methodology we have outlined above is enormously complex. The integration algorithm is a multi-stage procedure involving a number of elliptic/parabolic solves each time step. Dynamic regridding operations track developing features in the flow, and require frequent redistribution of the data and workload, and the workload itself is non-uniform due to the inhomogeneous nature of the reaction chemistry. It is of paramount importance to gauge the effectiveness of the low Mach number algorithm with respect to time-explicit simulation approaches, which historically have shown ideal scaling behavior up to tens of thousands of processors. The weak-scaling study we use here for this purpose is based on the propagation of a doubly-periodic wrinkled terrestrial flame in three dimensions using the GRI-Mech 3.0 [6] chemical mechanism for methane combustion. By replicating the problem in the periodic directions, we are able to scale the problem size without modifying the problem characteristics. Computational times versus number of processors is presented in Figure 1(a). This figure shows a modest increase in execution time as we increase the number of processors from 64 to 4096. (With ideal scaling, the execution time would remain constant in a weak scaling study.) A more detailed analysis of the results indicates that performance of the elliptic solvers is the dominant factor in the increased execution time. We also note that the scaling behavior is better on an XT4 type architecture than on a Linux cluster. We speculate that this is a consequence of the relative speed of the communications network to the processor speed. A more relevant metric than simple scalability is the relative performance of the low Mach number methodology to that of a time-explicit scheme. Figure 1(b) shows the *time-to-solution* for the same range of processor counts, using our low Mach number algorithm and a more traditional compressible reacting flow



(a) (b)

Figure 1. Parallel performance of the low Mach number adaptive algorithm: (a) Weak scaling behavior of the adaptive low Mach number algorithm. (b) Scaling of time-to-solution, relative to a compressible solver.

solver [7]. Note that for this study, we did not run the compressible code at all of the resolutions; we simply extrapolated the performance from 64 processors assuming ideal scaling. The figure shows that the low Mach number methodology is more than two orders of magnitude faster.

3. Results

The low Mach number algorithm discussed above is currently being used in a number of ongoing turbulent flame studies. In this paper, we present two examples of work in progress that focus on flame microphysics in the presence of fluid turbulence. The cases are similar, in that they are set in a rectangular domain that is periodic in the x and y directions. Low z is a solid wall, with outflow at the top of the domain. The domains are initialized with homogeneous isotropic turbulence throughout, with a superimposed flat flame near the top of the domain propagating downward. A time-dependent forcing term composed of a superposition of low-wavenumber Fourier modes maintains the turbulence in statistical equilibrium. One study considers the simulation of a lean premixed hydrogen flame. The fuel is a mixture of ideal gases, and the reactions are based on a 27-step fundamental kinetic mechanism. The second study considers the propagation of a nuclear flame characteristic of a type Ia supernova. For the stellar conditions considered here, the pressure contains contributions from ions, radiation and electrons. Although the ionic component has a form associated with an ideal gas the electron pressure is due to fermions and is nearly degenerate. The reaction network for the stellar case simply converts carbon-12 to magnesium-24, but the rate function is a strong function of temperature ($\sim T^9$). The terrestrial and stellar cases are nevertheless similar in as much as the local structure of the flame is modified significantly in the presence of flame curvature and fluid strain associated with turbulence. The two cases represent opposite limiting cases of premixed flame whose dynamics are controlled by extreme differences in the rate of heat and mass diffusion.

The first case we consider is a lean hydrogen flame at $\phi = 0.37$. In a flat-flame configuration, this fuel has a laminar burning speed of approximately 15.2 cm/sec. However, it is highly unstable to perturbations in flame morphology, and spontaneously rolls up into cellular burning structures in virtually any physically realizable configuration. Though these cellular structures have been observed experimentally for decades, it is interesting to investigate the detailed transport of fuel and heat in the presence of turbulent strain fields. Specifically, we wish to understand the impact of turbulence on the effective fuel consumption rate over the "flame brush" (the time-averaged flame location), the formation and stability of cells, the fate of unburned fuel and the generation of nitrogen-based pollutants in the product stream.

In Figure 2(a) we show a volume rendering of the fuel consumption for a snapshot of the computed turbulent hydrogen-air flame. The image shows regions of intense burning separated by localized regions in which the flame has been extinguished. To examine the interplay of

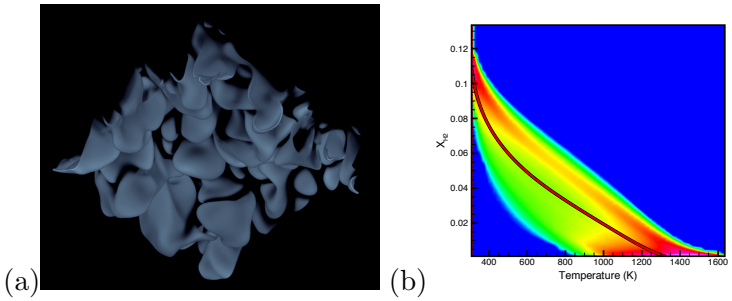


Figure 2. (a) Volume rendering of local fuel consumption of a lean premixed turbulent H_2-air flame. (b) Probability density plot of temperature vs. fuel concentration, overlayed with the laminar flame solution (red line).

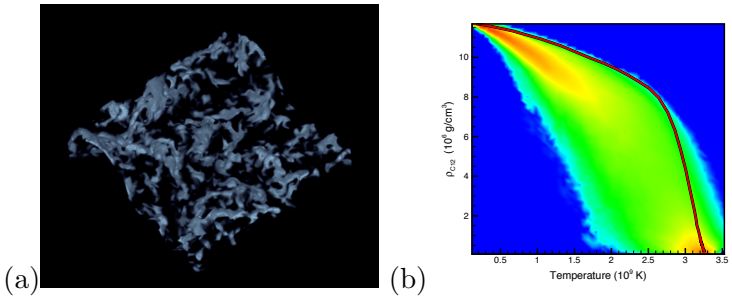


Figure 3. (a) Volume rendering of local fuel consumption for a turbulent type Ia supernova flame. (b) Joint PDF of temperature and fuel mass density. Overlay curve corresponds to the flat laminar flame solution.

the fluid mechanics with the flame chemistry, we plot, in Figure 2(b), a joint PDF of fuel (H_2) concentration and temperature with an overlay of the corresponding correlation from the flat laminar flame solution. In the turbulent case, the peak of the distribution forms a ridge that is significantly shifted from that of the laminar flame, indicating that most of the burning is occurring in regions that are richer in fuel than the original premixture. When the flame surface is not orthogonal to the flow direction, highly mobile H_2 molecules diffuse into regions of active burning, enriching the local flame. O_2 molecules diffuse toward the flame more slowly and are advected further downstream. This preferential separation of fuel and oxidizer results in intense burning regions that are characterized by having their local centers of curvature lie on the product side of the flame (defined to be positive curvature). The mean burning rate, or turbulent burning speed, represents the weighted average of the increased fuel consumption in regions of positive curvature, and extinguished regions with negative curvature. For this case, the turbulent burning speed appears to be approximately 13 times the flat laminar value.

Next, we consider the corresponding turbulent supernova flame. In addition to the non-ideal equation of state issues, the other distinguishing feature of nuclear flames is that they are extremely high Lewis number flames – that is, species diffusion is orders of magnitude smaller than thermal diffusion. A volume rendering of the local nuclear consumption rate of the carbon-12 mass density is shown in Figure 3(a). As in the hydrogen case, the flame surface is highly distorted with regions of dramatically reduced reactivity. In this case, however, the reactions are reduced in regions of positive curvature. In contrast with hydrogen case, the stellar flame appears to extinguish in regions of positive curvature due to a local defocusing, or divergence, of heat flux. Due to the sensitive dependence of the nuclear reactions on temperature, local consumption rate increases in regions of high negative curvature to values as high as 10-15 times that of the corresponding flat flame value.

We plot, in Figure 3(b), the joint PDF of temperature and carbon (fuel) density for the nuclear flame. As in the hydrogen case, we also superimpose the laminar flame solution onto the figure. In this case however, the turbulent flame data tends to be shifted below the curve of the flat flame. We see that the dominant behavior is distinctly different than the laminar flame with the carbon density decreasing more rapidly than in the flat laminar flame. The PDF suggests that fuel has a considerably shorter residence time in the preheat zone in front of the burning regions. This is consistent with the observation that while the zones of significant reactions are extremely intense, they are highly localized, producing localized pockets of intense heating of unburned fuel. The net result is that the effective turbulent flame speed is somewhat lower than the laminar flame speed. Although there are regions of intense burning the overall disruption of the flame reduces the net rate of fuel consumption.

4. Conclusions

In this paper, we have discussed implementation of a parallel adaptive low Mach number simulation capability for modeling reacting flows. We have shown that the resulting methodology scales well up to several thousand processors and is considerably more efficient for solving an important class of reacting flow problems than approaches based on explicit methods for integrating the compressible flow equations. We have demonstrated the methodology by applying it to the study of two turbulent reacting flow simulations, one focused on burning hydrogen at lean conditions and the other on nuclear burning in type Ia supernovae. We show that the detailed structure of the flame may be highly sensitive to the turbulent fluctuations, and that resulting modifications to the reaction processes can have a significant and complex impact on the global propagation speed of the turbulent flame brush. In both the terrestrial and stellar applications, considerably more research will be necessary to understand the relationships between temporal and spatial scales of the turbulence, diffusion and reaction processes. However, for the foreseeable future, such research is accessible only through the symbiotic development of advanced algorithms and large-scale computing platforms.

Acknowledgments

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