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A computational approach to flame hole dynamics using an embedded manifold approach

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ABSTRACT

We present a new numerical algorithm for tracking the evolution of flame holes in diffusion flames. The key element is the solution of an evolution equation for a flame state field defined on a complex moving surface. The surface itself can evolve in time and is defined implicitly as a level set of an associated Cartesian scalar field. The surface coordinates, or parameterization, do not need to be determined explicitly. Instead, the numerical method employs an embedding technique where the evolution equation is extended to the Cartesian space. In our application, the flame state field represents the chemical activity state of a diffusion flame; i.e. quenched and burning regions of the flame surface. We present a formulation that describes the formation, propagation, and growth of flame holes using edge-flame modeling in laminar and turbulent diffusion flames. The evolution equation is solved using a high-order finite-volume WENO method and a new extension algorithm defined in terms of propagation PDEs. The complete algorithm is demonstrated by tracking the dynamics of flame holes in a turbulent reacting shear layer and its applicability is also demonstrated in a turbulent reacting lifted jet simulation.

1. Introduction

The numerical solution of partial differential equations on surfaces is an area of research with a variety of applications such as image processing, geometry, physiology, solidification, gravitation, and fluid mechanics (see Ratz and Voigt [1]). The problem of evolution of a field constrained to a surface can be described in terms of surface differential operators (gradient, divergence, etc.) if a parametric description of the surface (e.g., $\mathbf{z} = (z_1, z_2)$) is available. Unfortunately, it is difficult and computationally expensive to employ this approach for a general surface, where even creating a clean surface mesh might be difficult [1]. Additionally, frequent re-meshing may be needed if the surface evolves in time, and particularly if the surface can develop topological changes. An alternative approach to solving PDEs on surfaces using the parametric coordinates is to embed the surface in the three-dimensional Cartesian space. This requires a transformation of the surface PDE to an equivalent volumetric PDE that allows one to solve the latter using customary Cartesian operators.

The heart of an embedding method is an extension operator by which the surface field is extended smoothly throughout the Cartesian space. Surface data is propagated normal to isosurfaces of an embedding function that implicitly defines the surface. These methods can be classified into geometrical and differential equation-based methods. Introduced by Bertalmıo et al. [2], differential equation-based methods construct a PDE defining the extension operation in the embedding space. The solution of this equation has the property that the extended surface data in the Cartesian domain is normal to the

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isosurfaces of the embedding function. Cartesian discretizations can then be applied in the embedding space to solve the surface PDE on the implicit surface. This method has been applied to a wide variety of problems [1–3] and has been used for solving surface advection problems on evolving surfaces [4,5]. The Cartesian space data structures (rather than the intrinsic coordinates of the complex surface) result generally in faster execution. In addition, to minimize computational cost, the embedding PDE is typically only solved in a narrow band around the surface. However, solving the embedding PDE requires the imposition of artificial boundary conditions at the boundary of the band in which the embedding PDE is solved [3]. If instead we seek to solve the embedding PDE in a much larger band around the surface, the artificial imposition of boundary conditions is not an issue and this type of method does not have difficulty with extending surface data far away from the surface. In the geometrical "closest point method" [6–8], surface data is propagated along the local normal direction by use of a closest point extension. Values of the extended surface field at grid points in the embedding Cartesian space are set to be equal to the value of the surface field evaluated at the point on the surface that is closest to the Cartesian grid point. This is implemented by determining the closest point on the surface relative to a grid point through a closest point transform and then interpolating the value of the variable at that point from the data in the Cartesian grid surrounding it. The closest point extension has the desired property that the intrinsic surface gradient operator (and divergence operator) is the same as the Cartesian gradient of the extended field when evaluated at the surface and does not require the imposition of artificial boundary conditions. The method can also be constructed to be high-order accurate. For instance, the orthogonal gradient radial basis function method of Piret [9] uses a closest point representation with the surface approximated using a radial basis function approach to obtain spectral accuracy. It has been successful in solving diffusion and advection equations [7] and has been modified to efficiently solve problems on a moving surface by Leung et al. [10]. The grid-based particle method by Leung et al. [10] reconstructs the interface through a local least squares approximation. This allows the computation of the closest point transform, which is used to apply the closest point extension. The method tracks the interface motion by using a Lagrangian particle tracking method, using the movement of the surface to update the closest point extension. This type of method allows for the efficient computation of the closest point method for the case of an evolving surface. Finding the closest point to a surface, however, becomes increasingly difficult as the distance from the surface increases. The closest point function can be costly to compute and multivalued. As previously stated, PDE-based methods do not have problematic behavior far from the surface.

The main contribution of the present paper is the development of a hybrid closest point and PDE-based Cartesian embedding method applied to a moving surface to model a dynamically-complex turbulent combustion problem. Turbulent diffusion flames experience velocity gradients (strain rate) that vary in space and time, increasing in magnitude with increasing Reynolds number. Since the combustion conversion rate is limited by the fixed chemical time scales of the elementary reactions that describe the combustion of each fuel-oxidizer mixture, eventually combustion is unable to adjust to fast flow time scales and the reaction is partially and locally quenched. The quenching or extinction process starts at those locations where the rate of heat release, which sustains the high temperature of the combustion, is unable to balance the rate at which the flow extracts heat from the reaction zone [11,12]. The flame ceases to exist once the temperature drops sufficiently bellow the extinction temperature of the flame (all remnant temperature and chemical products diffuse quickly away and radicals recombine into stable, practically inert, species). If the Reynolds number keeps increasing, for example by increasing the velocity in a jet flame, extinction will propagate and quench the flame globally (not just locally or transitorily). The process by which high strain rates quench the flame is called extinction while the healing of a quenched zone, by advection or heating to more favorable regions is termed reignition. These locally quenched regions of a flame are called here "flame holes"; although the extinction zones can have arbitrary shapes even resembling strips or islands [13,14]. After the development of the flame hole, the quenched region grows, shrinks, merges, splits, and changes shape depending on the evolution of the flame rim.

Computationally modeling all these flow/chemistry interactions at high Reynolds numbers is prohibitively expensive using first-principle methods, i.e. resolving all fields. The transport and reaction of each chemical species needs to be computed and the number of species is large, ranging from tens to hundreds of species in reduced and full chemical mechanisms, respectively. More importantly, in turbulent reacting flows of interest for flame hole dynamics, the reaction zone thickness is typically many times smaller than that required to resolve the turbulence [15]. In the absence of extinction, one well-established modeling approach is to represent the mixture as an ensemble of thin reaction zones called flamelets [16–18]. The reaction takes place near the stoichiometric surface, where fuel and oxidizer meet in stoichiometric proportions. Flamelets are based on an asymptotic analysis technique (not based on ad-hoc modeling concepts). The procedure consists in identifying the small flame thickness δ over which all reactions take place and separating the internal layer where these reactions are important, which is governed by

$$-\frac{\partial}{\partial \eta}\left(\rho D_i \frac{\partial Y_i}{\partial \eta}\right) = \omega_i(\vec{Y}, T), \tag{1}$$

where Y_i denotes the species mass fractions, T the temperature, ω_i the reaction rates of species i, and η is an inner spatial coordinate in the reaction zone along the normal coordinate to the flame sheet (from the perspective of the outer non-reactive solution). The technical procedure is quite complicated and can be found in [19] with full details. A predecessor of the formal complete asymptotic theory is due to Peters [17], who identified a simplification to the governing equations