Direct numerical simulations of turbulent reacting flows with embedded solid boundaries

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Abstract

The immersed boundary method (IBM) is developed and implemented into direct numerical simulation (DNS) of turbulent reacting flows in complex geometries. While the method has been available for some time, their application to a system with a large number of reactive scalars requires additional considerations and modifications in order to ensure robust and accurate description of physical behavior. The present study provides an improved IBM application by incorporating detailed diffusive flux conditions for multi-component systems. The developed method is validated using DNS of propagation of a premixed hydrogen/air flame around a backward-facing step, which represents a canonical configuration of realistic combustion devices. In addition, DNS of reacting and non-reacting flows around a bluff body cylinder are also performed and the vortex-shedding frequency of the non-reacting flow is compared with experimental results. Results demonstrate that the improved IBM can be successfully implemented to combustion DNS in more complex geometries without loss of fidelity.

1. Introduction

Direct numerical simulation (DNS) has become an invaluable tool in fundamental studies of turbulent combustion by providing temporally and spatially resolved solution fields at high fidelity. Recent advances in high performance computing has allowed DNS of small-scale laboratory turbulent flames at significantly large Reynolds numbers [1]. Considering that the characteristic time scales of detailed chemistry is comparable with acoustic time scales, many current approaches to combustion DNS utilize compressible flow formulation in favor of the simplicity in time integration. One of the computational difficulties in the compressible flow formulation is to implement physically correct and numerically robust boundary conditions, since the domain size of a typical combustion DNS is limited due to the cost constraints. A study by Sutherland and Kennedy [2] expanded on the Navier-Stokes Characteristic Boundary Conditions by deriving the necessary boundary conditions for reacting flows and open boundaries. Yoo et al. [3,4] further determined that for cases where there are large transverse gradients at inflows and flows which would occur in the presence of turbulence, an improper accounting for these transverse terms lead to severe and unphysical pressure increase in the computation domain corrupting the validity of reacting flows that include pressure sensitive reactions. These advances have been useful in generating some of the largest datasets of combustion phenomena, such as the auto ignition stabilized hydrogen jet flame by Lignell, Chen, and Yoo [5].

As the application of DNS is being extended to realistic combustion systems, there are increasing needs to simulate reacting flows in the presence of complex solid boundaries, as would be encountered in bluff-body combustor as an example. Previous computational fluid dynamic simulations with complex geometries have been attempted for turbulent flows; however, they have often been accomplished by utilizing grid stretching and mapping, and as such are limited to solid bodies attached to the boundary of the computational domain, and often require significant code rewrite. Mittal and Iaccarino [6] extensively reviewed various methods that have been used to simulate solid geometries in fluids. Fadlun et al. [7] used a direct imposition/linear interpolation method of the solution variables in order to simulate solid geometries for non-reacting incompressible flows, and showed that it is possible to use different schemes to interpolate and impose a solution on the grid above a ghost plane, albeit with the limitation that the grids near the immersed wall must fully resolve the boundary layer .

Despite the extensive development and implementation of various numerical methods for solid body representation in the flow field, most of these approaches have been limited to nonreactive flows. In the present study, a robust, accurate, and efficient method to incorporate geometry into combustion codes is described. First attempts are done on simple geometries and non-reactive cases. These cases are compared to experimental data to validate our methods. Simple reactive flow cases with immersed boundary walls are compared to hard walls and shown to be an effective method to simulate boundaries. Finally, a reactive backward facing step is simulated in order to demonstrate the capability of generating real world combustor geometries.

2. Code Development

The code employed in the present study is named S3D, developed by the authors in collaboration with a number of researchers over the past decades. It utilizes high-order spatial derivatives and high order Runge-Kutta time integrator. Highly portable, it has been utilized for basic combustion research on a multitude of platforms, including various Cray XT systems at DOE National Laboratory supercomputers, showing near-linear scalability with more than 10,000 cores. Multi-physics modules have been incorporated for radiation, soot formation, and particle-in-cell spray.

Two methods are utilized to represent solid boundaries in the computational domain. The first method is to directly impose immersed boundary conditions on actual grid points when the solid boundary aligns with the grid lines. The second method is to indirectly impose the solution on the grid where the actual solid boundary is located between grid points. The latter is important when the solid body has inherent curvature, such as a cylinder. Since we are interested in the behavior of the fluid interaction with the solid boundaries, it is not necessary to define material properties for the solid. Therefore, it is sufficient to simply isolate the derivative and filter modules for the flow domain from the predefined interior of the embedded boundary. This requires that additional logic conditions be prescribed in order to impose one-sided derivatives on the solid boundary, thereby effectively isolating the fluid from the arbitrary conditions in the interior of the solid object.

To prescribe the solution on the grid points above the ghost plane, 3rd order Hermite interpolation scheme was used [8]. The interpolation scheme mitigates the effects of polynomial interpolation errors known as the Runge phenomenon. Attempts at using linear interpolation to impose the solution on the grids above the ghost plane failed due to interpolation errors at the flame location on the wall. A simpler linear interpolation adopted by other researchers [7] cannot be used for the present reacting flow simulations as it cannot satisfy the additional constraints related to the reactive scalar variables or compressibility.

3. Results and Discussion

Case 1. Flame propagation in a channel

As a first test validation of the immersed boundary method, a 2D premixed hydrogen-air flame propagating between parallel solid walls was simulated, first by imposing solid-wall characteristic boundary conditions at the top and bottom boundaries. Adiabatic conditions were prescribed at the channel walls, and the inflow and outflow were imposed at the inflow and outflow boundaries, respectively. Then the simulation was repeated by including the top and bottom solid walls into the computational domain and the immersed boundary treatment was imposed accordingly. For both cases, a 1D solution of a premixed stoichiometric hydrogen-air flame, obtained from the PREMIX package in CHEMKIN, was mapped into the 2D domain as the initial condition, and the simulations were run until a steady state was reached. The same uniform grid size of 5 μm was used and the differences between the two solutions were assessed by the L2-error norm defined as:

$$L2 = \int |\varphi|^2 dxdydz$$

Such that the normalized L2 –norm is defined as:

$$\ll L2 \gg_{\emptyset} = \frac{L2_{\emptyset} - L2_{5\mu m}}{L2_{5\mu m}}$$

where ∅ indicates the grid resolution.

Figure 1 shows the heat release rate profiles. Both hard inflow and immersed boundary channel walls show visually identical solutions. The magnified view clearly shows that the immersed boundary method properly represents a solid wall imbedded into the domain, without interfering with the fidelity of the gas-phase reacting flow solutions. Figure 2 demonstrate that the L2-norms of pressure for 3 resolution; 20 μm, 16 μm, and 5 μm. Figure 3 further shows that the normalized pressure L2-norms for the reference and the IBM solutions not only agree with each other but the value decreases as the grid resolution is increased.

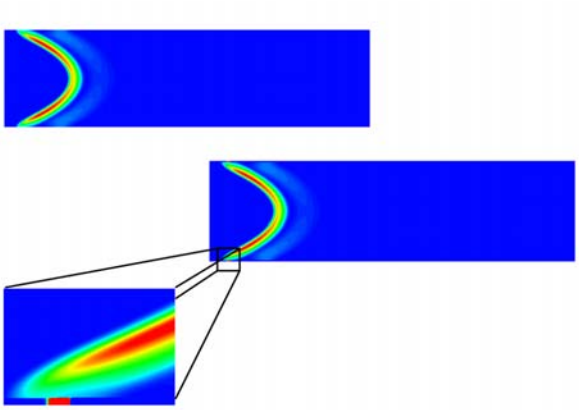

Figure 1: Heat release rate iso-contours of premixed hydrogen-air flame propagating in a channel. Top is the solution with hard solid wall channel, and the bottom is the solution using the immersed boundary method, where the magnified view clearly shows that the interior of the immersed solid does not interact with the gas-phase interior flow.

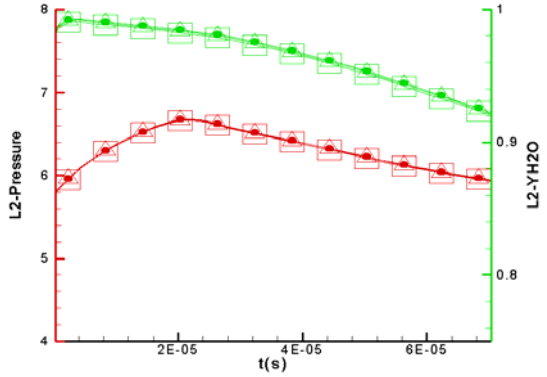

Figure 2: L2-norms of pressure (red) and Y_{H2O} (green) for the immersed boundary channel. 20, 16 and 5 μm resolutions are represented by circles, triangles, and square, respectively.

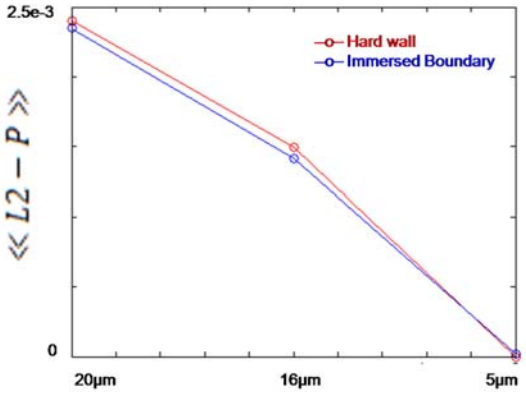

Figure 3: Normalized L2-norm of Pressure, taken at t = 2e-5 s.

Case 2. Nonreactive flows around a cylinder

As the next step of validation, the IBM approach is employed in non-reactive flows with an embedded solid cylinder. The challenge of imposing the prescribed solution on geometries with curvature is that the boundary of the solid is largely between the grid points. Figure 4 illustrates how points on the outside of the boundary of the embedded surface must be interpolated from data between the prescribed physical boundary condition and a point at a uniform distance from normal to the boundary. The point at a distance r away from the intended physical boundary, where $\epsilon\sqrt{\Delta x^2 + \Delta y^2} <$ r and ϵ is a value slightly larger than 1.0, is used as the outer bound for the interpolation onto the point just outside the physical boundary (Fig. 5) . This algorithm ensures that the outer point is entirely extracted from data updated by the computational method of the code.

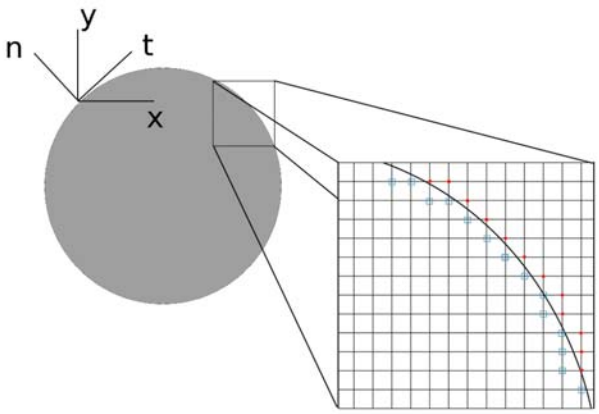

Figure 4: Curved surface of sphere is inevitably between grids. Rotations of vectors defined in X and Y coordinates must be translated to n and t coordinates.

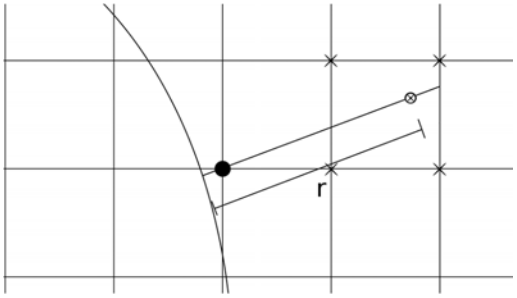

Figure 5. The grid point with the solid circle is the point where the scalars are interpolated, based on intended values and the extracted data point, designated by an circumscribed x at a distance r. The value of the scalar is extracted using linear interpolation, which is then used as a boundary point for the Hermite interpolation onto the grid point with solid circle.

The configuration tested in this study was an immersed cylinder of 0.2 cm in diameter, with a domain size of 5.4cm x 2cm. Figure 6 shows the time evolution of vorticity around the cylinder. Vortex shedding occurs after t = 0.46 ms, and Strouhal number of 0.21 matches with experimental results for the Reynolds number of 1500.

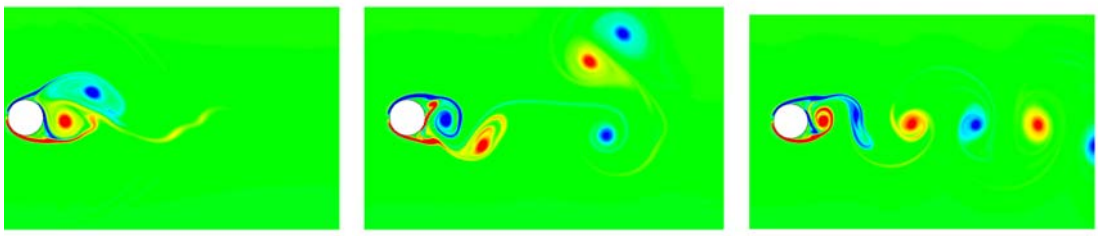

Figure 6: Flow around a cylinder simulated using the IBM approach. Vorticity contours for t= 0.5, 0.8, and 1.6 ms. Under moderate to high Reynolds numbers, von Karman vortex street begins to manifest behind any bluff body.

Case 3. Reacting flows around a backward- facing step

As a final test case to demonstrate the capabilities of the IBM approach for reacting flows, a simulation was conducted for hydrogen/air premixed flames around a backward-facing step as shown in Figure 7. The geometry represents a canonical configuration for practical combustion systems, such as sudden-expansion lean-burn methane burners [9]. The inflow velocity is set to be higher than the laminar burning velocity of the stoichiometric hydrogen-air flame, allowing for blow-off from the choked region to the expanded area.

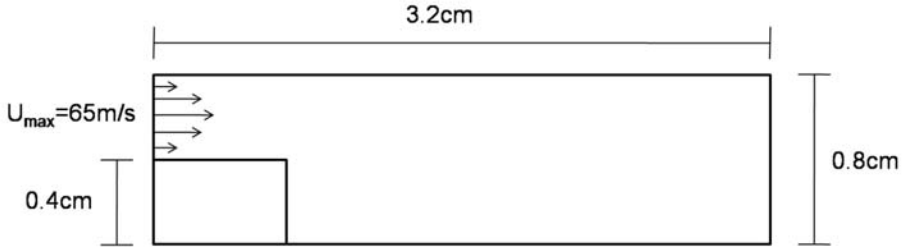

Figure 7: Backward facing step configuration. This experiment is scaled down version of industrial combustors utilizing both methane and higher carbon fuels.

Figure 8 shows the temporal evolution of heat release isocontours. As expected, a recirculation zone appears behind the backward facing step, providing a stabilization mechanism for the anchored flame. Due to fast inflow velocity, the upper branch of the flame is blown out of the domain, leaving just the recirculation stabilized lower branch. Using our method of rotations for points along the surface of a cylinder, we correctly impose the boundary conditions for heat and diffusive flux at both the top and bottom corners of the backward step.

3. Conclusions

An immersed boundary method was incorporated into the Cartesian grid system used in direct numerical simulation of reacting flows with detailed chemistry. The method was validated with three configurations that cover a wide range of geometric complexity, advancing the capabilities of DNS, and extending it from a tool to study fundamental interactions to one that can simulate practical devices. The validity and accuracy of the 3rd order Hermite interpolation method is confirmed both qualitatively and quantitatively using the channel configuration and our method of imposing adiabatic and non-normal-diffusive conditions is confirmed to be both necessary and valid for combustion problems. The interpolation/imposition method described is used to generate the first ever complex geometric flow and combustion problems using S3D, showing correct behavior of vortex shedding for a cylinder. A small scale test of a backward-facing step combustor is used to demonstrate the applicability of our method to practical combustion systems, and in the future, will allow for DNS to directly contribute to detailed description of practical combustion systems.

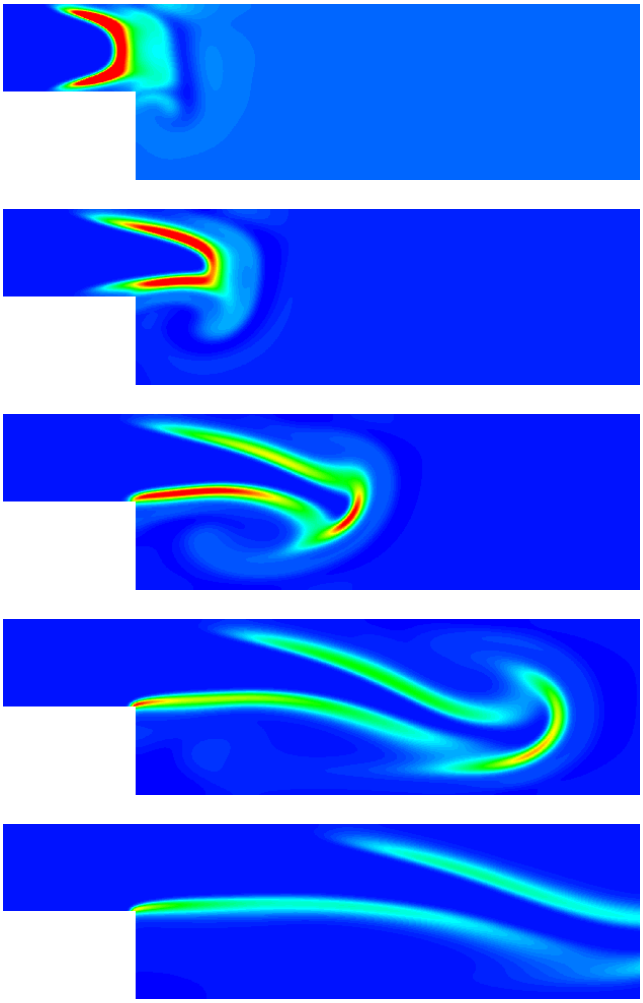

Figure 7: Heat release evolution of backward facing step for t = 0.085, 0.16, 0.30, 0.52, and 0.95 ms. Backward step induces a recirculation zone, stabilizing part of the flame at the step corner, as the rest of the flame is blown out of the domain.

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