An efficient scheme for large eddy simulation of low-Ma combustion in complex configurations

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1. Motivation and objectives

The fractional step method has resulted in very efficient integration schemes for time-dependent incompressible flow solvers. This efficiency comes from the fact that these solvers allow a segregated solution approach without outer iterations in the time step. Because the resulting error (splitting error) is of the same order as the time integration error, there is generally no need to cycle to reduce or eliminate it. This means that the scalar and momentum systems are built and solved only once in the time step, and a constant-coefficient Poisson system is also solved only once.

For problems in low-Ma combustion, variable-density solvers provide a potentially efficient strategy because they formally decouple pressure and density, removing any acoustic restrictions on time step. When integrated using the fractional-step approach, however, variable-density flow solvers typically require outer iterations to achieve accuracy and stability. For the case of an unstructured 2nd-order flow solver like CDP†, the variable-density solver is up to 10 times more expensive per time step than the incompressible flow solver on an identical grid.

The variable-density approach currently implemented in CDP is the method of Pierce & Moin (2004) modified for CDP's node-based collocated discretization. Convergence of the outer iterations is determined by monitoring the maximum change in density between outer iterations and considering the step converged when this value falls below 10^{-3}. Additionally, the maximum number of outer iterations can be limited by some user-specified value, typically 3 to 5. This limit is required because, as described in Shunn & Ham (2006), convergence is not monotonic and local oscillations in density can stall convergence. While the solutions proposed in Shunn & Ham (2006) can help to address this problem, the density relaxation required is case-specific and the higher-order state evaluations are very expensive, particularly if they need to be performed multiple times per time step.

Clearly these case-specific tunings and large residual levels are highly undesirable, and a robust, parameter-free approach for variable density solvers that is stable and accurate without outer iterations would be an important development. This paper describes such a method. This new method moves the evaluation of the equation of state (i.e. density) to the start of the time step based on predicted scalar values, and then introduces an additional Poisson solution to produce an advecting velocity field that discretely satisfies the continuity equation. Details are provided in the following section, and some preliminary results are provided later in the paper. This new method as well as the previous variable density approach with outer iterations are being verified using the method of

† CDP is a set of massively parallel unstructured flow solvers developed specifically for Large Eddy Simulation by Stanford's Center for Integrated Turbulence Simulations as part of the Department of Energy's ASC Alliance Program, see http://cits.stanford.edu.
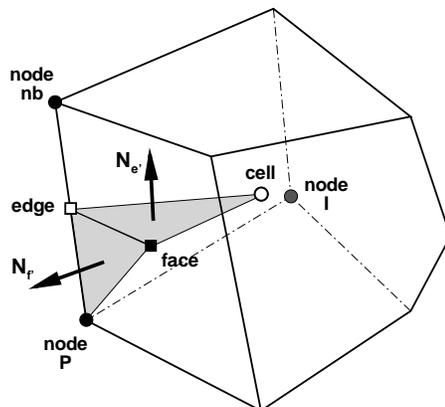
FIGURE 1. Sample sub-edge and sub-face normals for the median dual volume associated with boundary node P. The cell center is located at the simple average of cell nodes, and face center at the simple average of face nodes, making the reconstruction of nodal data at these points by simple averaging linearly exact and 2nd-order accurate.

manufactured solutions, with details reported elsewhere in this volume (Shunn & Ham 2007).

2. Numerical method

The proposed method achieves stability without outer iterations by adding an additional Poisson solve at the start of each time step. While an additional Poisson solve increases the cost of a single iteration, savings is realized because multiple outer iterations are not required. Variable-density solvers with multiple Poisson solutions per time step have been proposed before in the literature. For example, the method of Bell & Marcus (1992) uses an initial Poisson solve to ensure the discrete divergence of the velocity field satisfies a constraint on the divergence extrapolated from previous time steps. This concept of correcting the predicted velocity field to satisfy an extrapolated constraint is also part of the present method, although there are some important differences. In the present method, we write the constraint in terms of the mass fluxes, ρu_i, rather than the velocity. This leads to a constant coefficient Poisson system that will be much more efficient to solve many times over the course of a simulation by an algebraic multigrid method (Falgout & Yang 2002; Henson & Yang 2002) because the coefficient anisotropy is fixed. Consequently the coarse grid operators can be computed once and stored.

Consider an unstructured, node-based, finite-volume discretization of the zero-Ma number variable density Navier-Stokes equations (Mahesh *et al.* 2006). Velocity, density, pressure, and all scalars are collocated in space at the nodes, where each node is associated with a median dual volume as shown in figure 1. An additional set of normal mass-flux velocity components are carried at integration points on the dual volume surfaces referred to as sub-edges or sub-faces on boundary surfaces. In time, scalars and density are staggered relative to velocity to produce a compact, symmetric discretization of the continuity equation (Pierce & Moin 2004). For the case of constant time step Δt the integration proceeds as follows. In all cases, superscripts are used to indicate the

time level. When data is not directly available at the required time level, values are interpolated by simple averages of values at adjacent levels.

(1) Prediction using Adams-Bashforth extrapolation

Predict mass flux velocity components at t^{n+1} and scalar values at time level $t^{n+3/2}$

$$(\widehat{\rho U_n})^{n+1} = 2(\rho U_n)^n - (\rho U_n)^{n-1} \tag{2.1}$$

$$\widehat{\phi}^{n+3/2} = 2\phi^{n+1/2} - \phi^{n-1/2} \tag{2.2}$$

(2) Equation of state

Look up density based on predicted scalar values.

$$\rho^{n+3/2} = f(\widehat{\phi}_1, \widehat{\phi}_2, ...) \tag{2.3}$$

(3) First Poisson solve

Correct the predicted mass flux components by solving a constant coefficient Poisson equation such that the discrete continuity equation is satisfied:

$$V\frac{\rho^{n+3/2} - \rho^{n+1/2}}{\Delta t} + \sum_{se,sf}(\rho U_n)^{n+1}A = 0 \tag{2.4}$$

where se, sf refers to the summation over sub-edges and sub-faces for the dual volume, and a minimal correction is computed using the temporary scalar field ψ as follows:

$$(\rho U_n)^{n+1} = (\widehat{\rho U_n})^{n+1} + \frac{\delta\psi}{\delta n} \tag{2.5}$$

The substitution of equation (2.5) into (2.4) yields a constant coefficient Poisson system that can be solved for temporary scalar field ψ.

At this point we note that, in the limit of constant density, the algorithm yields identical results for the mass flux components as the incompressible case. For the incompressible case, these velocity components are simply produced by Adams-Bashforth extrapolation. Because both of the previous time levels are divergence free, a linear combination of the two levels will also be divergence free. For the present variable density case in the limit of constant density, the predicted mass flux components are similarly produced by Adams-Bashforth extrapolation, and the correction resulting from the Poisson equation will be zero.

(4) Advance scalars using scalar advection diffusion equations

$$V\frac{\rho^{n+3/2}\phi^{n+3/2} - \rho^{n+1/2}\phi^{n+1/2}}{\Delta t} + \sum_{se,sf}(\rho U_n)^{n+1}\overline{\phi}^{n+1}A = ... \tag{2.6}$$

Here for brevity we have not included the diffusive or source terms (if any) in the scalar equation. The overbar operator $\overline{()}$ represents a spatial averaging operator as described in Ham *et al.* (2006).

(5) Advance velocity using momentum equation

$$V\frac{\rho^{n+1}\widehat{u_i}^{n+1} - \rho^n u_i^n}{\Delta t} + \sum_{se,sf} (\rho U_n)^{n+1/2}\overline{u_i}^{n+1/2}A = -V\frac{\delta p}{\delta x_i}^{n-1/2}... \tag{2.7}$$

The densities used in the momentum equations are

(6) Second Poisson solve to correct the velocity and pressure

Interpolate mass fluxes to sub-edges and correct to satisfy the discrete continuity equation. This is done in a way that implicitly adds a 4th-order pressure dissipation term as described in Ham & Iaccarino (2004).

$$V\frac{\rho^{n+1}u_i^* - \rho^{n+1}\widehat{u_i}^{n+1}}{\Delta t} = +V\frac{\delta p}{\delta x_i}^{n-1/2} \tag{2.8}$$

$$(\rho U_n)^* = \overline{(\rho^{n+1}u_i^*)}\,n_{i,se} \tag{2.9}$$

$$\frac{(\rho U_n)^{n+1} - (\rho U_n)^*}{\Delta t} = -\frac{\delta p}{\delta n}^{n+1/2} \tag{2.10}$$

Substitution of equation (2.10) into the continuity equation (2.4) yields a second constant-coefficient Poisson equation for the new pressure $p^{n+1/2}$. The node-based velocity field is finally corrected as follows:

$$\frac{\rho^{n+1}u_i^{n+1} - \rho^{n+1}u_i^*}{\Delta t} = -\frac{\delta p}{\delta x_i}^{n+1/2} \tag{2.11}$$

3. Results

The accuracy of the method in space and time has been tested using the method of manufactured solutions, and is reported elsewhere in this volume (Shunn & Ham 2007). The method has been applied to the reacting jet engine combustor of Pratt & Whitney at cruise conditions where results using the previous variable density solver with outer iterations have been reported elsewhere (Mahesh *et al.* 2006). For this case it was found necessary to use a 1st-order scalar predictor in step (1) to maintain a stable scheme when no outer iterations were performed. The resulting simulation was very stable and efficient, and afforded a detailed investigation of the reacting flow field at two different levels of grid refinement. Figure 2 presents snapshots of instantaneous temperature from this simulation to illustrate the flow structure resolved by the method.

4. Future work

A stable and efficient variable density flow solver has been developed for the large eddy simulation of low-Ma reacting flows on unstructured grids. By performing two Poisson solutions per time step, the segregated equations can be advanced using a fractional step method without outer iterations. Both Poisson solutions involve identical constant coefficient Laplacian operators, and can be solved very efficiently using an algebraic multigrid method where the cost associated with developing the coarse grid hierarchy is incurred only once at the start of the simulation. For the case of realistic density ratios it was found necessary to use a 1st-order scalar predictor before looking up density from the tabulated equation of state to maintain stability. Future work will include investigating
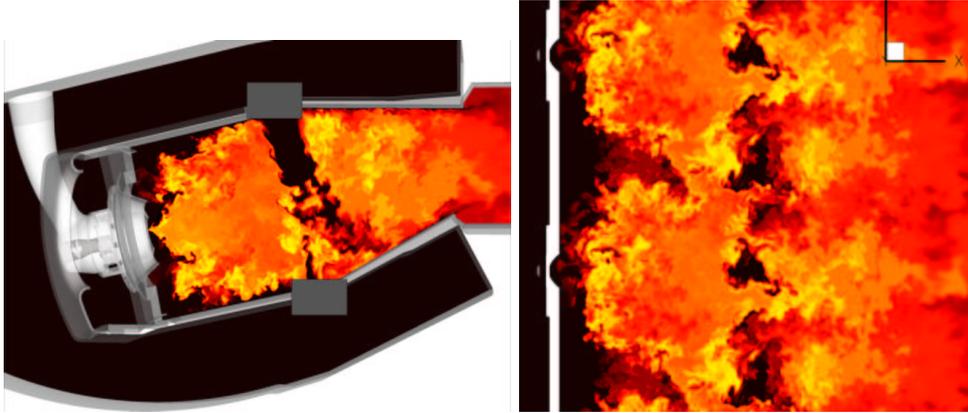
Figure 2. Snapshots of instantaneous temperature from variable-density simulations of the reacting jet engine combustor of Pratt & Whitney at cruise conditions. Left) combustor mid-plane; Right) Cut at a constant radius through the annular combustor centerline.

the source of this instability, as well as the effect of this lower temporal accuracy on the overall accuracy of the turbulent reacting simulation.

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