Adaptive Finite Element Methods for Turbulent and Reactive Flow

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We have ongoing efforts to provide accurate solutions for time-dependent (unsteady) heat transfer [1], geophysical modeling (including atmospheric transport processes), indoor environmental transport [2], and, most recently, multiphase reactive flow using adaptive Finite Element Methods (FEM). For the last item, a method particularly well suited to combustion simulation is being developed in both 2D and 3D.

The fundamental mathematical model for a fluid momentum solution is based on predictor-corrector equation splitting. By using the pressure (density) solution, the predicted velocity or momentum is projected to the correct state. Solutions to energy and turbulent closure models are performed by scalar transport equations. The time-dependent solution is currently evolved by a backward Euler method, although second-order-in-time evolutions are possible. The resulting system of equations, particularly the Poisson equation for pressure or density, is solved with a preconditioned conjugate-gradient (PCG) solver package [3] where matrix preconditioning comes from in situ stationary methods [4].

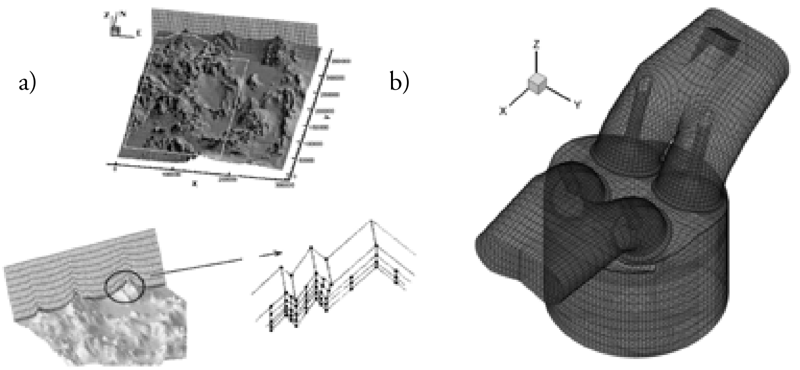

Fig. 1. a) Initial grids for atmospheric boundary layer [5], and b) unstructured grid for internal combustion engine for KIVA-4mpi simulation [6].

Grids and Automatic Mesh Refinement. Simulation is accomplished by representing a domain in a discrete manner. FEM allows for the use of nonorthogonal or unstructured grids. A complex domain is represented with various discrete type elements, typically hexahedrals and trapezoids in 3D models. Grids for complex domains such as atmospheric boundary layers and internal combustion engines are shown in Fig.1.

The use of *h*-adaptation, or mesh refinement, yields accurate solutions and rapid convergence rates. Exponential convergence occurs when higher order interpolation is employed, creating a hp-adaptive method [7]. The idea of using self-adaptive grids became apparent around 1970 – practically solving large-scale problems requires an optimal grid. The goal of adaptation is to achieve the proper mesh, one that significantly improves the computational speed and resolution, and reduces error. Embedding elements within the existing grid is a form of *h*-adaptation, a quickly processed procedure. There are many error estimators that can be used to control the adaptive process, e.g., the element-residual method, interpolation methods, and stress-error methods. The use of a simple residual-error estimator as described by Ainsworth and Oden [8] is used in the examples below.

For turbulent incompressible flows, an Euler-Lagrange variational formulation is developed resulting in a fractional-step method [9]. This method is applicable to the turbulent heat transfer of incompressible flows, atmospheric dispersion modeling, indoor air pollution modeling, solidification, and non-Newtonian incompressible flows. The model is also well suited for determining the wind's power over complex terrain – useful for precisely locating wind turbines.

For turbulent combustion modeling a characteristic-based split (CBS) is developed as described by Zienkiewicz and Codina [10]. The model spans all flow regimes and is applicable to the above-mentioned modeling areas in addition to compressible flow in the subsonic, transonic, and supersonic regimes. A second-gradient shock capturing scheme is employed along with *h*-adaptation to capture shocks – the specifics of the general method can be found in a recent report [11].

The backward-facing step is a benchmark problem indicative of how implemented algorithms/models will perform for many important aspects of flow. Study of flow and heat transfer over a backward-facing step with its richness of physics and availability of experimental data provides a rigorous test of the code. Flow phenomena

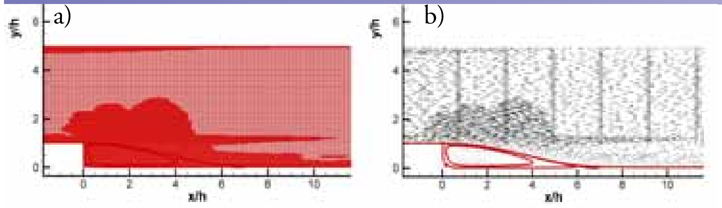

Fig 2. a) Two levels of mesh enrichment, and b) vectors and streamlines on refined grid.

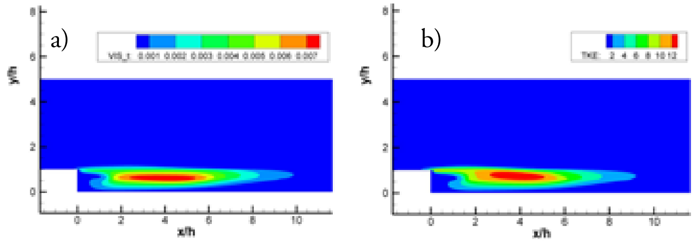

Fig. 3. a) Effective viscosity behind step, and b) turbulent kinetic energy behind step.

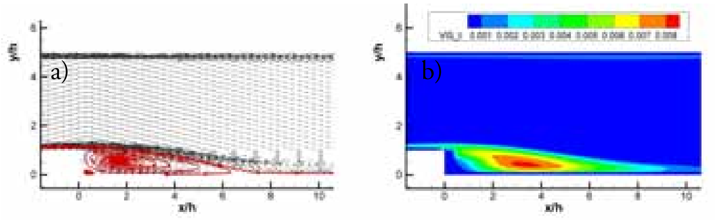

Fig. 4. a) Vectors and streamlines on refined grid, and b) effective viscosity behind step.

include unsteady behavior, separation, recirculation, and reattachment. Vogel and Eaton's experiments [12] provide experimental data for convective turbulent flow over a backward-facing step having an expansion ratio of 1.25.

Shown in Fig. 2 are results from a k-ω turbulence closure model using the projection method for the experimental setup of Vogel and Eaton with a Reynolds number (Re) = 28,000 [13]. Figure 2a shows the final grid, where the initial grid was enriched once nearly everywhere. More cell enrichment was needed as determined by a residual-error estimator in the boundary layer and near the expansion. Figure 2b shows the velocity vectors and streamlines behind the expansion. The recirculation region size matches experimental results, at 6.4 h, where h is the step height.

Figure 3 depicts the effective viscosity and turbulent kinetic energy behind the step, respectively. The contours are in general agreement with other results. The results compare favorably with Vogel and Eaton's findings.

Turbulent Reactive Flow – Combustion Modeling. Resolution ushers in a need for greater computational power – a need for parallel processing. But solving the resolved problem with more computing power alone is not the only development required for achieving a desired accuracy. There are limits to what can be efficiently achieved by decomposing domains with moving parts and distributing the processing. It is generally better to have algorithms that are more accurate and also provide for higher resolution and accuracy only where and when it is required in the simulation process.

The KIVA team is facilitating combustion engine modeling by improving accuracy and robustness of the algorithms. To address the needs of the combustion engine community, including universities and industry, we recently began developing the CBS method. The method, combined with higher-order polynomial approximation (*p*-adaption) and *h*-adaption to form an *hp*-adaptive method, is being developed to provide for accurate and robust solutions in the next generation of KIVA software [11]. Shown in Fig. 4 is a solution using the CBS FEM method for the Vogel and Eaton experiment previously described. At Re=28,000 the inflow is 17m/s (Mach number ~0.05), and the results compare favorably with other solutions and data. This is near the flow velocity at a cylinder's intake for a typical internal combustion engine running at 1000 rpm.

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