Assessment of a Hybrid Finite Element and Finite Volume Code for Turbulent Incompressible Flows^{*}

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ABSTRACT

Hydra-TH is a hybrid finite-element / finite-volume incompressible / low-Mach flow simulation code based on the Hydra multiphysics toolkit being developed and used for thermal-hydraulics applications. In the present work, a suite of verification and validation (V&V) test problems for Hydra-TH was defined to meet the design requirements of the Consortium for Advanced Simulation of Light Water Reactors (CASL). The intent for this test problem suite is to provide baseline comparison data that demonstrates the performance of the Hydra-TH solution methods. The simulation problems vary in complexity from laminar to turbulent flows. A set of RANS and LES turbulence models were used in the simulation of four classical test problems. Numerical results obtained by Hydra-TH agreed well with either the available analytical solution or experimental data, indicating the verified and validated implementation of these turbulence models in Hydra-TH. Where possible, some form of solution verification has been attempted to identify sensitivities in the solution methods, and suggest best practices when using the Hydra-TH code.

Keywords: incompressible flow; turbulence model; RANS; LES.

1. INTRODUCTION

Hydra-TH [1-9] refers to the hybrid finite-element / finite-volume incompressible / low-Mach flow solver in the Hydra toolkit being used for thermal-hydraulics (“TH”) applications for the Consortium for Advanced Simulation of Light Water Reactors (“CASL”) [10]. Hydra-TH features a recently developed second-order, hybrid finite-element / finite-volume, incremental projection algorithm for time-dependent incompressible viscous flows [11]. The algorithm circumvents the

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usual div-stability constraints, i.e., does not require explicit treatment of troublesome pressure modes using Rhie-Chow interpolation or a pressure-stabilized Petrov-Galerkin formulation. The use of a co-velocity and high-resolution advection scheme with consistent edge-based treatment of viscous/diffusive terms yields a robust algorithm for a broad spectrum of incompressible flows. A detailed description of the numerical algorithms, implementations, and basic verification and validation problems has been presented in the work of Christon et al. [11].

Hydra-TH was built as one of a number of applications using the Hydra multiphysics toolkit. The Hydra toolkit was written in C++, and it provides a rich suite of components that permits rapid application development, supports multiple discretization techniques, and provides I/O interfaces to permit reading/writing multiple file formats for meshes, plot data, time-history, surface-based and restart output. Data registration is used to provide the ability to register variables at appropriate locations (e.g., node, element, dual-edge, etc.), and provides integrated and automatic output and restart capabilities along with memory management. The toolkit also provides run-time parallel domain decomposition with data-migration for both static and dynamic load balancing. Linear algebra is handled through an abstract virtual interface, which makes it possible to use some of the most popular libraries such as PETSc [12] and Trilinos [13]. The use of output delegates provides the ability to develop lightweight physics-specific output kernels with minimal memory overhead that can be tailored to a specific physics, e.g., computation of vorticity, helicity, enstrophy for large-eddy simulations. Verification testing is part of the Hydra software control process and ensures that Hydra-TH is solving problems of interests to the CASL project and meeting design requirements. It is one component of a larger testing infrastructure. This paper is aimed at identifying verification problems and the Hydra-TH solutions to those problems. More test problems will be added to the suite of verification and validation for flow simulation, as the Hydra-TH code will change over time.

The rest of this paper is organized as follows: Section 2 first introduces the baseline numerical method employed by Hydra-TH, and then the Reynolds-averaged Navier-Stokes (“RANS”) and large-eddy simulation (“LES”) turbulence models implemented in the current suite. Section 3 presents four classical test cases computed by Hydra-TH: 1) the steady-state Poiseuille flow; 2) a laminar flow past a flat plate at Reynolds number of $Re = 100,000$, which can be compared with the Blasius solution; 3) a wall-bounded turbulent channel flow at $Re_\tau = 590$, where two RANS turbulence models are verified and validated according to the referenced Direct Numerical Simulation (DNS) data; 4) large-eddy simulation of a lid-driven cavity flow, in which three LES models in Hydra-TH are tested and verified with respect to the referenced experimental data. Section 4 gives a conclusion of the work in this paper, and outlook for future work.

2. NUMERICAL METHOD

Hydra-TH uses a hybrid finite-element / finite-volume discretization for the incompressible/low-Mach Navier-Stokes equations. All the transport variables are cell-centered and treated with a conservative discretization that includes a high-resolution monotonicity-preserving advection algorithm. In Hydra-TH, the spatial discretization is formally derived using a discontinuous Galerkin (“DG”) framework that, in the limit, reduces to a locally conservative finite volume method [11] (also see [14] as an example of high-order DG implementation). In order to provide compatibility with modern piecewise linear interface construction (PLIC) based volume-tracking algorithms that are based on a finite volume formalism, we choose piecewise-constant test functions for the compressible and incompressible flow solvers in the Hydra toolkit. However, it should be noted that this choice does not restrict the current methods or software from extension to include higher-order (higher than linear) reconstruction techniques or the incorporation of higher-order test functions. In addition, this choice simplifies sharing a common discretization for both the compressible and incompressible flow solvers.

In the present work, the high-resolution advection algorithm is designed to permit both implicit and explicit advection with the explicit advection targeted primarily at volume tracking with interface reconstruction. The time-integration methods include backward-Euler and neutrally dissipative trapezoidal method. The implicit advective treatment delivers unconditional stability for the linear scalar transport equations, and conditional stability for the momentum transport equations. A sharp stability estimate for the momentum equations is not available, but operational experience shows that the upper stability range is on the order of $CFL = 20$ to $CFL = 40$ for steady-state problems, and of $CFL = 5$ to $CFL = 10$ for time-accurate problems. Note that for the steady-state problems, the backward-Euler time integration provides an additional damping that, in conjunction with the upper stability range of CFL numbers, provides a computationally efficient solution method. For the Unsteady Reynolds-Averaged Navier-Stokes (“URANS”) and Large-Eddy Simulation (“LES”) computations, the trapezoid rule is neutrally dissipative, and delivers optimal performance for the more stringent CFL requirements for time-accurate flow.

Hydra-TH is designed to incorporate both the well established and state-of-the-art turbulence models, ranging from the traditional RANS, through the LES, to the hybrid RANS/LES models. The following models implemented in Hydra-TH have been used in this work:

- RANS models

- a. The Spalart-Allmaras (“S-A”) one-equation eddy viscosity model developed by Spalart & Allmaras [15]. It is important to include this model besides its reliability in complex flows [16], since the most popular hybrid RANS/LES model (DES) is built around this model. It is important to mention that DES has gained significant attention due to its potential for predicting complex unsteady turbulent flows at low computational cost [17].
- b. The Re-Normalized Group (“RNG”) k - ε two-equation model developed by Yakhot et al. [18], along with the use of a wall function. For the current implementation, the “law-of-the-wall” approach has been used to provide near-wall modeling avoiding the need for highly resolved boundary layer meshes. Due to its limitations in usage, e.g. recirculating flows, the standard law-of-the-wall was modified based on a new scale for the friction velocity following the method proposed by Launder & Spalding [19]. The modified law-of-the-wall reduces to the standard law-of-the-wall under the conditions of uniform wall shear stress and when the generation and dissipation of turbulent kinetic energy are in balance (i.e. when the turbulence structure is in equilibrium). Under such conditions, $u^* \approx u^+$ and thus, $y^* \approx y^+$.

• LES models

- a. The MILES or ILES model [20]. This family of models is obtained using a monotonicity preserving advection treatment (“MILES”) and is also referred to as implicit LES (“ILES”). The representation of the unresolved scales can also be explicit or implicit. Explicit models explicitly add model terms to the filtered continuum equations. An example is to employ the turbulent viscosity hypothesis with the turbulent viscosity computed via the Smagorinsky model, which is analogous to Prandtl’s mixing length model in the Reynolds averaged context. Implicit models rely on the dissipative properties of the applied numerical method, resulting in implicit large eddy simulation, or, if the numerical treatment ensures monotonicity, monotonically integrated implicit LES.
- b. The Smagorinsky model, one of the earliest LES models proposed by Smagorinsky [21]. This model accounts for the unresolved scales via the turbulent viscosity hypothesis and computing the turbulent viscosity by a simple dimensional model. It was implemented in Hydra-TH to serve as a baseline for comparison to other models.
- c. The Wall-Adapted Large Eddy (“WALE”) model [22] computes the unresolved-scale dissipation by employing the turbulent viscosity hypothesis (similar to the Smagorinsky model), but the turbulent viscosity is determined based on both the filtered-scale shear, and the square of filtered-scale velocity gradient. According to Nicoud & Ducros [22], compared to the Smagorinsky model, the WALE model has the following advantages: 1) It accounts for both

local strain and rotation, which has the potential to capture the full production of turbulent kinetic energy in shear-driven flows. 2) The turbulent viscosity approaches zero at the wall, consequently no adjustment of the model constant or damping function is necessary in the vicinity of the wall. Only local information is required to compute the turbulent viscosity. As a consequence, the model is well suited for complex flow geometries. 3) The model is invariant to coordinate translation and rotation. 4) The turbulent viscosity cannot be negative or infinite.

In addition, the use of LES implies a required suit of post-processing tools for extracting useful averages and statistics. Hydra-TH provides an interface for performing windowed time averaging suitable for the runtime estimation of averages, once the simulation reaches a statistically stationary state. All of the statistical measurements of the LES of the turbulent flows presented in this work are based upon the Reynolds average for stationary flows. With the definition of the Reynolds average given above, any variable can be decomposed into its mean and fluctuating component,

$$\text{Equation 1 } \phi(x_i, t) = \langle \phi(x_i) \rangle + \phi'(x_i, t)$$

and will obey the following Reynolds-averaging rules,

$$\text{Equation 2 } \langle \phi' \rangle = 0$$

$$\text{Equation 3 } \langle \langle \phi \rangle \rangle = \langle \phi \rangle$$

$$\text{Equation 4 } \langle \phi \psi \rangle = \langle \phi \rangle \langle \psi \rangle + \langle \phi' \psi' \rangle$$

$$\text{Equation 5 } \langle \phi' \langle \psi \rangle \rangle = \langle \psi' \langle \phi \rangle \rangle = 0$$

The time average is approximated by the discrete summation,

$$\text{Equation 6 } \langle \phi(x_i) \rangle = \lim_{N \rightarrow \infty} \frac{\sum_{n=1}^N \phi(x_i, t_n) \Delta t_n}{\sum_{n=1}^N \Delta t_n}$$

where Δt_n is the time step increment for the n -th time integration step and $t_n = \sum_{m=1}^n \Delta t_m$ is the accumulated time. Let

ϕ represent a scalar quantity, and let v_i , ($i = 1, 2, 3$) represent the i -th Cartesian component of the instantaneous velocity.

The variance of a scalar is

$$\text{Equation 7 } \sigma^2 = \langle (\phi - \langle \phi \rangle)^2 \rangle = \langle \phi^2 \rangle - \langle \phi \rangle^2$$

where σ is the root mean square (RMS). Similarly, the Reynolds stress tensor is

$$\text{Equation 8 } R_{ij} = \langle v'_i v'_j \rangle = \langle v_i v_j \rangle - \langle v_i \rangle \langle v_j \rangle$$

and the turbulent kinetic energy is one half of the trace of the Reynolds stress tensor

$$\text{Equation 9 } q' = \frac{1}{2} \langle v'_k v'_k \rangle = \frac{1}{2} (\langle v_k v_k \rangle - \langle v_k \rangle \langle v_k \rangle)$$

where the repeated indices imply the summation.

3. VERIFICATION PROBLEMS

3.1 Poiseuille Flow

The objective of this numerical experiment is to verify if the spatially second-order finite volume method in Hydra-TH can achieve a theoretical order of convergence rate for incompressible laminar flows. The test problem chosen in this case is the steady Poiseuille flow, which represents an exact solution to the full system of the two-dimensional incompressible Navier-Stokes equations for a laminar flow in a channel. The analytical solution to the velocity distribution at any given streamwise location is a parabolic profile given by

$$\text{Equation 10 } v_{\text{analytical}} = \frac{1}{2\mu} \left(-\frac{dp}{dx} \right) y(L_y - y)$$

where L_y is the width of the channel, μ the dynamic viscosity, and p the fluid pressure. In this experiment, the computational domain is bounded from 0 to 20 in the streamwise x -direction ($L_x = 20$, inflow at the left end, and outflow at the right end), from 0 to 1 in the y -direction ($L_y = 1$), and from 0 to 1 in the spanwise z -direction ($L_z = 1$). The laminar Reynolds number, defined as $Re = \rho v_{\text{ave}} L_y / \mu$, is equal to 100, where the input $\mu = 0.01$, fluid density $\rho = 1$, full-width of the channel $L_y = 1$, and averaged velocity $v_{\text{ave}} = 1$. Consequently, the $dp/dx = -0.12$ is a priori by assuming the length-averaged integration of Equation 10 along L_y equal to 1 (the average velocity). For the boundary conditions, a constant pressure $p = 0$ was imposed at the right outflow boundary, while a parabolic velocity profile given by Equation 10 was imposed at the left inflow boundary. The no-slip and no-penetration conditions were imposed at the top and bottom boundaries. The slip boundary conditions were imposed at the front and back boundaries. Finally, Table 1 shows the $L2$ errors and grid convergence rate obtained from the four grids, indicating that Hydra-TH is spatially second-order accurate in solving the velocity field for the incompressible Navier-Stokes equations.

Table 1: Grid convergence analysis of the steady Poiseuille flow in a channel on four successively refined grids $100 \times 5 \times 1$, $200 \times 10 \times 1$, $400 \times 200 \times 1$, and $800 \times 40 \times 1$.

Cell Size	$\log_{10}(L2)$	Order
0.2	-0.5886	---
0.1	-1.23673	2.152
0.05	-1.81829	1.932
0.025	-2.41830	1.994

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Figure 1: Plot of the converged x-velocity contour obtained on the $100 \times 5 \times 1$ grid.

Figure 2: Plot of the converged x-velocity contour obtained on the $200 \times 10 \times 1$ grid.

Figure 3: Plot of the converged x-velocity contour obtained on the $400 \times 20 \times 1$ grid.

Figure 4: Plot of the converged x-velocity contour obtained on the $800 \times 40 \times 1$ grid.

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Figure 5: The converged x-velocity profile through the outflow boundary cell centers on the $100 \times 5 \times 1$ grid.

Figure 6: The converged x-velocity profile through the outflow boundary cell centers on the $200 \times 10 \times 1$ grid.

Figure 7: The converged x-velocity profile the outflow boundary cell centers on the $400 \times 20 \times 1$ grid.

Figure 8: The converged x-velocity profile the outflow boundary cell centers on the $800 \times 40 \times 1$ grid.

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3.2 Flow Past a Flat Plate

The laminar boundary layer over an adiabatic flat plate is considered in this test case. This problem is chosen to assess the accuracy of the Hydra-TH solution methods for the discretization of the viscous and heat fluxes in the incompressible Navier-Stokes equations, as the Blasius solution can be used to measure the accuracy of the numerical solution. In this experiment, the Reynolds number based on the length of the flat plate is given as $Re = 100,000$. The computational domain is bounded by $x \in [-0.5, 1.0]$, $y \in [0, 1.0]$, and $z \in [0, 0.1]$, and the no-slip surface starts at point $(0, 0, z)$ and extends to $(1, 0, z)$, as shown in Figure 9. The inflow boundary condition when $x = -0.5$ is prescribed with a fixed velocity of $\mathbf{V} = (1, 0, 0)$. The no-slip and no-penetration conditions with $\mathbf{V} = (0, 0, 0)$ are prescribed when $y = 0$ for $x \in [0, 1]$. The slip condition is prescribed along the bottom side of the domain for $x \in [-0.5, 0]$ with $V_y = 0$. The symmetry conditions are prescribed in the one-cell thick region with $V_z = 0$. The pressure at the outflow boundary is prescribed to be $p = 0$ on the top boundary ($y = 1$) and right boundary ($x = 1$).

Figure 9: The schematic for the flow past a flat plate.

The three hexahedral grids used in this computation have the same number of cells $(25+50) \times 30 \times 1$, with $25 \times 30 \times 1$ cells ahead of the flat plate and $50 \times 30 \times 1$ cells for the flat plate. In order to provide an adequate grid resolution for where the numerical solution varies most drastically in space, the grid points are clustered at the vicinity of the leading edge of the flat plate, and in the boundary layer region. The grid-stretching ratio (SR), defined as the ratio of the widths or heights of the two successive elements in the x - or y -directions respectively, is often used to quantify the distribution of the grid points. For the flat plate part, the three grids have the same SR value of 1.05 in the x -direction, but a different SR value in the y -direction, i.e. 1.15, 1.20 and 1.30, respectively. The grids are plotted in Figure 10. The non-dimensional wall distance y^+ is defined as $y^+ = u_* y / \nu$, where $u_* = (\tau_w / \rho)^{1/2}$ is the friction velocity at the nearest wall, $\tau_w = \mu(\nabla u / \nabla y)|_{y=0}$ is the wall shear stress, and y is the distance to the nearest wall (the y coordinate of the cell center of the first layer). A complete

quantitative description is shown in Table 2. For example, in the grid of $SR = 1.15$, the height of the first element is 2.3002×10^{-3} , and it is also characterized with the normalized height of $y^+ = 12.35$. As a result, the grid of $SR = 1.30$ provides the finest grid resolution for the first layer of elements in the boundary layer region. Indeed, many other factors can also affect the overall solution accuracy, e.g. the SR in the x -direction. Nevertheless, this test case is focused on a comparative study among the series of these three grids, as to demonstrate the significant impact on the quality of the solution by solely adjusting the grid-stretching ratio normal to the no-slip surface, which is often an important factor that people are concerned with when having to constrain the total computational costs.

Table 2: Boundary layer of the grid for steady flow past a flat plate at $Re = 100,000$.

Stretching Ratio (SR) in the y -direction	y of the first-layer	y^+ of the first layer
1.15	2.3002×10^{-3}	12.35
1.20	8.4611×10^{-4}	4.542
1.30	1.1455×10^{-4}	0.615

All the plots are computed from the cell-centered solutions at the steady state. Figure 11 shows the time history of the domain-averaged kinetic energy (KE) obtained on the three grids. The domain-averaged KE is computed as

$$\text{Equation 11} \quad KE = \frac{1}{\Omega} \int_{\Omega} \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} d\Omega = \frac{1}{\Omega} \sum_{i=1}^{Nel} \bar{\rho}_i \bar{\mathbf{v}}_i \cdot \bar{\mathbf{v}}_i \Omega_i$$

where i denotes the i -th cell, and the cell-averaged variables are denoted by a bar. The domain-averaged KE computed from the grid of $SR = 1.15$ is about 0.1% smaller than from the other two grids, probably due to the grid dissipation in the boundary layer region. Figure 12 shows the logarithmic plots of the computed skin friction coefficient c_f distributions along the flat plate $x \in [0,1]$. The grid of $SR = 1.30$ provided the best prediction of c_f among the three grids. The grid of $SR = 1.20$ over-predicted the c_f distribution in the region near the leading edge of the plate, due to the insufficient grid resolution. The grid of $SR = 1.15$ resulted in an under-predicted c_f distribution within the first 2% of the plate, and an over-predicted c_f distribution in the first 2% - 20% of the plate, indicating that the boundary layer region was not well-resolved near the leading edge of the plate. Figure 13 and Figure 14 show the plots of the computed V_x and V_y profiles along the cells cut through by plane $x = 0.5$ in the boundary layer region. In comparison, the x -velocity profiles obtained on the three grids all matched well with the Blasius solution; and the y -velocity profiles displayed a best accuracy on the grid of $SR = 1.30$. Above all, this numerical experiment has demonstrated that the numerical methods in Hydra-TH can

1 accurately simulate the laminar boundary layer given the adequate grid resolution, which is an important prerequisite to
 2 proceed to the turbulent boundary layer problems.

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 4 **Figure 10: A series of three hexahedral grids for steady flow past a flat plate at $Re = 100,000$: $SR = 1.15$ (left), $SR =$
 5 1.20 (middle), and $SR = 1.30$ (right).**

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 7 **Figure 11: Plot of time history for the domain-averaged kinetic energy obtained on the three grids.**

Figure 12: Logarithmic plot of the computed skin friction coefficient distribution compared with the analytical solution along the flat plate at $x = [0, 1]$.

Figure 13: Plot of the x -velocity profiles compared with the similarity solutions along the cells cut through by plane $x = 0.5$ in the boundary layer region.

Figure 14: Plot of the y -velocity profiles compared with the similarity solutions along the cells cut through by plane $x = 0.5$ in the boundary layer region.

3.3 Turbulent Channel Flow at $Re_\tau = 590$

The test case chosen in this numerical experiment is a turbulent channel flow at a friction Reynolds number of $Re_\tau = 590$ [18]. The $Re_\tau = u_\tau \delta / \nu$ is based on the friction velocity u_τ (equivalent to the definition of u_* in Section 3.2), the channel half width $\delta = 1/2$, and ν the laminar kinematic viscosity. The S-A model, and RNG $k-\varepsilon$ model with a wall function [19] were used for the RANS simulations in this test case, respectively. This 2-D turbulent flow problem consists of a 2-D duct with a 20:1 aspect ratio. The channel dimensions are 20 units in the x -direction ($L_x = 20$), 1 unit in the y -direction ($L_y = 1$), and 0.05 unit in the z -direction ($L_z = 0.05$), as shown in Figure 15. The laminar Reynolds number Re (as defined in Section 3.1) is equal to 10000 based on the input $\mu = 0.0001$, fluid density $\rho = 1$, full-width of the channel $L_y = 1$, and averaged velocity $v_{ave} = 1$. The streamwise pressure gradient of $\nabla p / \nabla x = -2.785 \times 10^{-2}$ were given so that it resulted in an approximate posteriori $Re_\tau = 590$ by matching the computed u_τ value. In this study, the computation was conducted for each of the turbulence models on a series of three successively refined hexahedral grids, as described in Table 3, respectively. The grids are uniformly distributed in the x -direction.

Figure 15: The bounded domain for simulation of a turbulent channel flow.

In order to represent the constant pressure gradient, an inflow pressure boundary condition of $p = 0.557$ was prescribed at the left boundary of the domain (SideSet 4), and an outflow pressure boundary condition of $p = 0$ was prescribed at the right boundary (SideSet 5). Accordingly, a Neumann velocity boundary condition with $V_y = 0$ and $V_z = 0$ was prescribed at SideSet 4; and the homogeneous Neumann velocity boundary conditions were applied at SideSet 5. In addition, the Neumann boundary conditions for the turbulence model variables, i.e. v_t for the S-A model, and k and ε for the RNG $k-\varepsilon$ model, were applied at SideSet 4 and SideSet 5 in the corresponding turbulent model equations. The no-slip/no-penetration conditions $\mathbf{V} = (0, 0, 0)$ were prescribed along the top (SideSet 6) and bottom (SideSet 2) duct walls, with the additional conditions of $v_t = 0$ for the S-A model. The slip and no-penetration conditions ($V_x = 0$ and $V_y = 0$) were prescribed on the front (SideSet 3) and back (SideSet 1) duct walls. The initial velocity field was at rest with no random perturbations. The initial v_t was equal to 3.1×10^{-4} in the field for the S-A model; and the initial k was equal to 0.015 and ε

was equal to 0.002 in the field for the RNG $k-\varepsilon$ model. The termination time for all the test cases was $t = 500$, when the simulation was fully converged.

Table 3: Grids used for turbulent channel flow, $Re_\tau = 590$.

For the Spalart-Allmaras model		
Gird Size	y of the first layer	y^+ of the first layer
50×101×1	1.162×10^{-3}	1.371
50×201×1	2.823×10^{-4}	0.333
50×401×1	9.343×10^{-5}	0.110
For the RNG k-e model		
Gird Size	y of the first layer	y^+ of the first layer
50×41×1	1.220×10^{-2}	14.39
50×81×1	6.173×10^{-3}	7.284
50×161×1	3.106×10^{-3}	3.665

Figure 16 and Figure 17 show the time history of domain-averaged kinetic energy for the S-A model and RNG $k-\varepsilon$ model, respectively. The cell-centered solution was extracted and plotted versus the normal distance from the bottom wall to the half-width of the channel at $x = 5$ (which corresponds to 3/4 of the channel length) in the following figures: mean streamwise velocity V_x (Figure 18 and Figure 19), turbulent eddy viscosity ν_t (Figure 20 and Figure 21). Wall functions are critically important for accurate prediction of the near wall turbulent behavior. Thanks to the use of damping functions in the S-A model, the turbulent viscosity transport equation is integrated to the wall with $y^+ < 5$ in the first cell adjacent to the wall for accurate results. Thus the grid refinement for the simulations using the S-A model resulted in a good convergence of the ν_t profiles (Figure 20). However, the wall function used in the RNG $k-\varepsilon$ model requires that the first cell has $y^+ > 11.225$ (i.e. above the viscous sub-layer) in order to function properly. Due to the uniform grid refinement in the y -direction where the $y^+ < 11.225$ in the 50×81×1 and 50×161×1 grids, the ν_t profiles were not converging under the grid refinement for the RNG $k-\varepsilon$ model (Figure 21). The non-dimensional velocity profiles in comparison with the DNS result by Moser et al. [23] were shown in Figure 22 and Figure 23, for the S-A and RNG $k-\varepsilon$ models, respectively. The non-dimensional velocity V_x^+ is defined as $V_x^+ = V_x/u_\tau$, where u_τ is the friction velocity. The velocity profiles obtained from the S-A model matched the DNS result quite well in both the log layer and sub-layer regions (Figure 22). The velocity profiles obtained from the RNG $k-\varepsilon$ model indicate a good convergence of solution profiles that agree well with the DNS profiles in the log layer region, but not in the viscous sub-layer (Figure 23), again due to the limitations of the wall functions used in the RNG $k-\varepsilon$ model [19]. In particular, the velocity profile obtained on the 50×161×1 grid deviated from the theoretical law-of-the-wall for $y^+ < 7.5$. But it needs to be pointed out that, this velocity profile predicted on the

50×161×1 grid is not expected to continue to agree with the theoretical law-of-the-wall in the sub-layer region. Otherwise, if the grid were indefinitely refined, the predicted velocity would approach zero when $y^+ \approx 0.1$, which is obviously wrong. Thus the grid resolution in near-wall regions usually needs to be carefully designed in order to guarantee the effectiveness of the turbulence model being applied. Finally, the non-dimensional turbulent kinetic energy k^+ (normalized by u_τ^2) and energy dissipation rate ε of the RNG $k-\varepsilon$ model were plotted against the DNS data in Figure 24 and Figure 25 respectively. The overall trend of k^+ and ε profiles obtained on the 50×81×1 and 50×161×1 grids matched well with the DNS data, despite the already mentioned defect of the present RNG $k-\varepsilon$ model that led to the mispredictions closer to the wall. Above all, the key flow variable profiles obtained from the Hydra-TH simulations agreed well with the DNS results, within the designed capabilities of those two turbulent models.

Figure 16: Time history of domain-averaged kinetic energy for simulation of a turbulent channel flow, $Re_\tau = 590$, Spalart-Allmaras model.

Figure 17: Time history of domain-averaged kinetic energy for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\varepsilon$ model.

Figure 18: V_x versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, Spalart-Allmaras model.

Figure 19: V_x versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\varepsilon$ model.

Figure 20: Turbulent eddy viscosity versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, Spalart-Allmaras model.

Figure 21: Turbulent eddy viscosity versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\epsilon$ model.

Figure 22: V_x^+ versus y^+ from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, Spalart-Allmaras model.

Figure 23: V_x^+ versus y^+ from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\epsilon$ model.

Figure 24: Turbulent kinetic energy versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\epsilon$ model.

Figure 25: Turbulent kinetic energy dissipation versus normal distance from bottom wall for simulation of a turbulent channel flow, $Re_\tau = 590$, RNG $k-\epsilon$ model.

3.4 Large-Eddy Simulation of a Lid-Driven Cavity

This numerical experiment is the LES of a 3-D lid-driven cavity at a Reynolds number of $Re = 10,000$ based on the lid velocity u_b , and lid length L_x . The cavity dimensions are unity in the x - and y -directions, i.e. $L_x = L_y = 1$, and half in the z -direction, i.e. $L_z = 0.5$, as shown in Figure 26. A grid refinement study was performed with three LES turbulence models implemented in Hydra-TH: the ILES model, the WALE subgrid-scale model, and the Smagorinsky subgrid-scale model.

The computations were conducted for each of the turbulence models using a series of three successively refined hexahedral grids, shown in Figure 27. The total numbers of cells are $32 \times 32 \times 16$ for the coarse, $64 \times 64 \times 32$ for the medium, and $128 \times 128 \times 64$ for the fine grid, respectively. The grid is non-uniform in the horizontal x -directions and vertical y -direction, but is uniform in the spanwise z -direction. Grid points are clustered near the walls in the x - and y -directions. The grid spacing is stretched away from the wall, where the minimum edge length is 5×10^{-3} for the coarse and medium grids, and 5×10^{-4} for the fine grid. On the bottom and the four sidewalls (left, right, back, and front), the no-slip/no-penetration boundary conditions were prescribed. Along the top “lid”, a no-penetration boundary condition with a unit lid velocity $u_b = 1$ was prescribed. The velocity field was at rest at $t = 0$ with no random perturbations. Note that in this test case, the grid spacing was non-uniform and mostly clustered near the solid walls, where the boundary layers need to be sufficiently resolved.

Figure 26: Schematic of the 3-D lid-driven cavity.

Figure 27: A series of refined grids, $32 \times 32 \times 16$, $64 \times 64 \times 32$, and $128 \times 128 \times 64$, for the LES of a flow in lid-driven cavity at $Re = 10,000$, x-y plane (top) and x-z plane (bottom).

All the tests in this experiment were run for approximately 500 time units with 20 time planes containing average statistics being written between the 100th and 500th time unit. Figure 29, Figure 30, and Figure 31 show the time histories of the domain-averaged kinetic energy for each turbulence model. The cell-centered solution of the mean velocity vector and Reynolds stress tensor were extracted and plotted along the centerlines on the spanwise mid-plane for a direct comparison with the experimental data published by Prasad & Koseff [24], as shown in Figure 31, Figure 34, and Figure 37 for the ILES model, Figure 32, Figure 35 and Figure 38 for the WALE model, and Figure 33, Figure 36 and Figure 39 for the Smagorinsky model, respectively. The mean velocity in the x -direction, $\langle u \rangle$, was plotted along the vertical centerline, and the mean velocity in the y -direction, $\langle v \rangle$, was plotted along the horizontal centerline as shown in Figure 31, Figure 32, and Figure 33. Improvement of the mean velocities can be clearly observed from the coarse grid to the medium grid for all of the three models. The mean velocities varied only slightly from the medium grid to the fine grid for these models, and both agree quite well with the experimental data. The scaled RMS velocity in the x -direction, $\langle u'u' \rangle$, was plotted along the vertical centerline, and the scaled RMS velocity in the y -direction, $\langle v'v' \rangle$, was plotted along the horizontal centerline, shown in Figure 34, Figure 35 and Figure 36. The scaled Reynolds stress tensor component $\langle u'v' \rangle$ was plotted along the vertical and horizontal centerlines as shown in and Figure 37, Figure 38 and Figure 39. The figures show that the $\langle u'u' \rangle$ and $\langle u'v' \rangle$ profiles were significantly improved from the coarse to the medium grid. Further

1 improvement of the $\langle u'u' \rangle$ and $\langle u'v' \rangle$ profiles was obtained from the medium grid to the fine grid compared to the
2 experimental data. Comparison of the results obtained from three models indicates that the accuracy of the ILES and
3 WALE models is commensurate, while both closer to the experimental data than that of the Smagorinsky model. The
4 differences observed between the Smagorinsky model and the other two are probably due to the absence of wall damping
5 in the standard Smagorinsky model implemented in Hydra-TH. Note that wall damping is typically added to the
6 Smagorinsky model for wall-bounded flows. In addition, the use of the relatively sparse grid distribution in the spanwise
7 z -direction might have damped the w' fluctuations. And due to the process of homogenization of velocity fluctuations in
8 turbulent flows, the statistics of the other two fluctuating velocity components might have been affected as well. Though
9 preferred, a uniform grid spacing and grid refinement in all the three directions that is aimed to better capture the turbulent
10 flow features is prohibitive in terms of both the memory requirement and computing time. Above all, it is suggested that
11 1) the option of wall damping be added to the Smagorinsky model, and 2) the ILES and WALE models undergo further
12 V&V testing that involve more complex geometric configurations.

Figure 28: Time history of domain-averaged kinetic energy on different grids using the ILES model.

Figure 29: Time history of domain-averaged kinetic energy on different grids using the WALE model.

Figure 30: Time history of domain-averaged kinetic energy on different grids using the Smagorinsky model.

Figure 31: Comparison of mean velocity components $\langle u \rangle / u_b$ and $\langle v \rangle / v_b$ in the spanwise mid-plane with experimental data using the ILES model.

Figure 32: Comparison of mean velocity components $\langle u \rangle / u_b$ and $\langle v \rangle / v_b$ in the spanwise mid-plane with experimental data using the WALE model.

Figure 33: Comparison of mean velocity components $\langle u \rangle / u_b$ and $\langle v \rangle / v_b$ in the spanwise mid-plane with experimental data using the Smagorinsky model.

Figure 34: Comparison of the scaled RMS velocity $10\langle u'u' \rangle^{1/2}/u_b$ and $10\langle v'v' \rangle^{1/2}/u_b$ in the spanwise mid-plane with the experimental data, using the ILES model.

Figure 35: Comparison of the scaled RMS velocity $10\langle u'u' \rangle^{1/2}/u_b$ and $10\langle v'v' \rangle^{1/2}/u_b$ in the spanwise mid-plane with the experimental data, using the WALE model.

Figure 36: Comparison of the scaled RMS velocity $10\langle u'u' \rangle^{1/2}/u_b$ and $10\langle v'v' \rangle^{1/2}/u_b$ in the spanwise mid-plane with the experimental data, using the Smagorinsky model.

Figure 37: Comparison of the scaled Reynolds stress tensor component $500\langle u'v' \rangle / u_b^2$ in the spanwise mid-plane with the experimental data, using the ILES model.

Figure 38: Comparison of the scaled Reynolds stress tensor component $500\langle u'v' \rangle / u_b^2$ in the spanwise mid-plane with the experimental data, using the WALE model.

Figure 39: Comparison of the scaled Reynolds stress tensor component $500\langle u'v' \rangle / u_b^2$ in the spanwise mid-plane with the experimental data, using the Smagorinsky model.

CONCLUSIONS

A set of RANS and LES turbulence models, implemented in the flow solver suite Hydra-TH, have been used to compute a series of classical, well-documented incompressible flow problems. The results indicate that the tested turbulence models in Hydra-TH offer a reliable numerical prediction that agree well with either the available analytical solution or experimental data for these cases. Future verification and validation efforts will be focused on flows with more complex geometries and multiple thermodynamic phases.

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REFERENCES

- [1] Christon, M. A. (2011). Hydra-TH Theory Manual, *Tech. Rep., LA-UR-11-05387*, Los Alamos National Laboratories, Los Alamos, New Mexico.
- [2] Christon, M. A., Bakosi, J., and Lowrie, R. B. (2012). Hydra-TH User's Manual, *Tech. Rep., LA-CC-11120*, Los Alamos National Laboratory, Los Alamos, New Mexico.
- [3] Christon, M. A., Bakosi, J., Barnett, N., Francois, M. M., Lowrie, R. B., and Sankaran, R. (2012). Integration of Hydra-TH in VERA, *Tech. Rep., L2 Milestone THM. CFD. P5. 01*, Los Alamos National Laboratory, Los Alamos, New Mexico, 2012.
- [4] Bakosi, J., Christon, M. A., Francois, M. M., Lowrie, R. B., and Nourgaliev, R. (2012). GTRF Calculations Using Hydra-TH, *Tech. Rep., L3 Milestone THM. CFD. P5. 05*, Los Alamos National Laboratory, Los Alamos, New Mexico.
- [5] Bakosi, J., Christon, M. A., Pritchett-Sheats, L., and Nourgaliev, R. (2013). Hydra-TH Advanced Capabilities, *Tech. Rep., L3 Milestone THM. CFD. P6. 01*, Los Alamos National Laboratory, Los Alamos, New Mexico, 2013.
- [6] Bakosi, J., Christon, M. A., Pritchett-Sheats, L., and Nourgaliev, R. (2013). Meshing, GTRF, Hydra-TH Performance, *Tech. Rep.*, Los Alamos National Laboratory, Los Alamos, New Mexico.
- [7] Bakosi, J., Christon, M. A., Francois, M. M., Lowrie, R. B., and Nourgaliev, R. (2012). THM-GTRF: New Spider Meshes, New Hydra-TH Runs, *Tech. Rep.*, Los Alamos National Laboratory, Los Alamos, New Mexico.
- [8] Christon, M. A., Bakosi, J., Francois, M. M., Lowrie, R. B., and Nourgaliev, R. (2012). Multiphase Flow Analysis in Hydra-TH, *Tech. Rep.*, Los Alamos National Laboratory, Los Alamos, New Mexico.

- [9] Christon, M. A. (2013). Thermal Hydraulics Methods and Hydra-TH Development, *Tech. Rep.*, Los Alamos National Laboratory, Los Alamos, New Mexico.
- [10] CASL: the Consortium for Advanced Simulation of Light Water Reactors. 2013. URL <http://www.casl.gov/>.
- [11] Christon, M. A., Bakosi, J., Nadiga, B., Berndt, M., Francois, M. M., Stagg, A. K., Xia, Y., and Luo, H. (2015). A hybrid incremental projection method for thermal-hydraulics applications, *Journal of Computational Physics*, submitted.
- [12] Balay, S., Abhyankar, S., Adams, M., Brown, J., Brune, P., Buschelman, K., and et al. (2014). PETSc Users Manual Revision 3.5 (No. ANL-95/11 Rev. 3.5), Argonne National Laboratory (ANL).
- [13] Heroux, M.A., Bartlett, R.A., Howle, V.E., Hoekstra, R.J., Hu, J.J., Kolda, T.G., et al. (2005) An overview of the Trilinos project. *ACM Transactions on Mathematical Software (TOMS)*, 31(3), 397–423.
- [14] Luo, H., Baum, J. D., and Löhner, R. (2008). A discontinuous Galerkin method based on a Taylor basis for the compressible flows on arbitrary grids. *Journal of Computational Physics*, 227(20), 8875-8893.
- [15] Spalart, P. R. and Allmaras, S. R. (1994). A one-equation turbulence model for aerodynamic flows, *La Recherche Aerospatiale*, 1, 5–21.
- [16] Spalart, P. R. (2000). Strategies for turbulence modeling and simulations. *International Journal of Heat and Fluid Flow*, 21(3), 252-263.
- [17] Spalart, P. R. (2009). Detached-eddy simulation. *Annual Review of Fluid Mechanics*, 41, 181-202.
- [18] Yakhot, V., Orszag, S. A., Thangam, S., Gatski, T. B., and Speziale, C. G. (1992). Development of turbulence models for shear flows by a double expansion technique, *Physics of Fluids A: Fluid Dynamics (1989 – 1993)*, 4(7), 1510–1520.
- [19] Launder, B. E., and Spalding, D. B. (1974). The numerical computation of turbulent flows. *Computer Methods in Applied Mechanics and Engineering*, 3(2), 269-289.
- [20] Grinstein, F.F., Margolin, L.G., and Rider, W.J. (2007). Implicit large eddy simulation: computing turbulent fluid dynamics. Cambridge University Press, New York, USA.
- [21] Smagorinsky, J. (1963). General circulation experiments with the primitive equations. *Monthly Weather Review*, 91(3), 99-164.
- [22] Nicoud, F., and Ducros, F. (1999). Subgrid-scale stress modeling based on the square of the velocity gradient tensor. *Flow, Turbulence and Combustion*, 62(3), 183-200.
- [23] Moser, R. D., Kim, J., and Mansour, N. N. (1999). Direct numerical simulation of turbulent channel flow up to $Re_\tau = 590$, *Physics of Fluids*, 11(4), 943-945.
- [24] Prasad, A. K., and Koseff, J. R. (1989). Reynolds number and end-wall effects on a lid-driven cavity flow, *Physics of Fluids A: Fluid Dynamics (1989-1993)*, 1(2), 208-219.