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Verification of RANS Turbulence Model in Eilmer using the Method of Manufactured Solutions

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Abstract

This paper presents the verification study of a Reynolds-Averaged Navier-Stokes (RANS) turbulence model using the Method of Manufactured Solutions (MMS) in a finite volume Computational Fluid Dynamics (CFD) code. The `Eilmer` CFD code is an open-source fluid solver which solves the compressible Navier-Stokes equations to provide time-accurate simulations of compressible flows in two and three dimensions. The turbulence model verified is Wilcox's (2006) $k-\omega$ model. The turbulence model implementation is verified through the order of accuracy test. An expected spatial order of accuracy of 2 is demonstrated with mesh refinement, matching the formal order of `Eilmer` numerics. The verification process significantly facilitated the detection and removal of coding mistakes in our implementation. We also provide discussion of coding mistakes that were identified and corrected as part of our verification exercise.

Introduction

With increased use of simulation for fluid dynamics calculations, the trustworthiness of those results is increasingly important. Defined as "solving the equations right" [1], verification is the process of assessing and ensuring the correctness of the implemented numerical algorithms, as well as the accuracy of the numerical solution. One practice in code verification is the use of exact solutions to the governing equations to compare against the numerical solution. However, traditional exact solutions are usually only available when the governing equations are fairly simple, which is certainly not the case for problems of practical interest. Considering this challenge, an alternative approach, the Method of Manufactured Solutions (MMS), was first proposed by Steinberg and Roache [2] and extended by Roache *et al.* [3]. The detail of how the method works is presented in Section: "Method of Manufactured Solutions". Here, we review where the method has been applied.

In the pioneering work from Steinberg and Roache [2] in 1984, the MMS approach was first applied to verify a code for generation of 3D transformations for elliptic partial differential equations (PDEs). The book by Oberkampf and Roy [4] provides a comprehensive discussion on the use of MMS for code verification along with the order of accuracy test. This method gradually became a general and powerful technique for code verification. Knupp and Salari [5] presented a detailed account of MMS-based code verification for incompressible and compressible Navier-Stokes codes. More recently, Roy and co-workers extended the use of MMS for the verification of various aspects of numerical modelling[6, 7, 8], including turbulence models, boundary conditions and unsteady flows. Based on the verification cases in Roy's paper [6], Gollan and Jacobs [9] have verified `Eilmer` for Euler and laminar Navier-Stokes solutions. Veeraragavan *et al.* [10] used MMS to test the implementation of tightly-coupled conjugate heat transfer solver for gas-solid domain coupling, also in `Eilmer`. In this work, we extend our verification cases to test our implementation of the $k-\omega$ turbulence model.

The use of MMS has not been widely applied for turbulence model verification. Only a handful of researchers have recently begun to address the verification of CFD codes with Reynolds-Averaged Navier-Stokes (RANS) turbulence models. Bond *et al.* [11] developed a general methodology for generating manufactured solutions that satisfy a desired boundary condition and applied it to multiple turbulence models. A new manufactured solution for wall-bounded turbulent flow with the Spalart-Allmaras model [12] was proposed by Oliver [13] and applied to verify the implementation of the FANS-SA equations. Eça and co-researchers [14, 15, 16] developed solutions that are intended to mimic two-dimensional, incompressible, stationary boundary layer flow, and multiple turbulence models including one-equation model and two-equation models were tested. While successful in some cases, their physically realistic solutions often led to numerical instabilities, a reduction in the observed grid convergence rate, or even inconsistency of the numerical scheme. Roy [17] *et al.* tried to use non-physical manufactured solutions for code verification, and successfully applied these manufactured solutions to the verification of a Menter's $k-\omega$ model. The verification case for turbulence modelling presented by Roy [17] is used here to test the implementation of the Wilcox (2006) $k-\omega$ turbulence model [18] in `Eilmer`.

Governing Equations

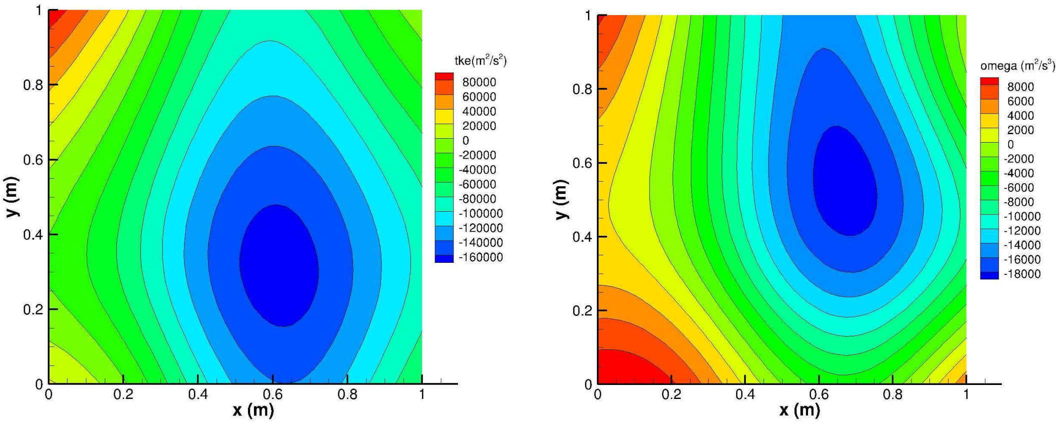
`Eilmer` is an integrated collection of programs that solves the compressible Navier-Stokes equations to provide time-accurate simulations of compressible flows in two and three dimensions [9]. The governing equations are expressed in integral form over cell-centered, finite-volume cells, with the time rate of change of conserved quantities in each cell specified as a summation of the mass, momentum and energy flux through the cell interfaces. In this work, we are interested in verifying the implementation of the the Wilcox (2006) $k-\omega$ model[18]. The Favre-averaged equations for conservation of mass, momentum, energy and the equations defining the $k-\omega$ model are as follows.

Mass Conservation:

$$\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\right)=0 \quad (1)$$

Momentum Conservation:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{u}_i\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{u}_i\right)=-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\bar{t}_{ji}+\bar{\rho}\tau_{ji}\right] \quad (2)$$



(a) (b)

Figure 1: Manufactured solution source terms for turbulence equations: a) k-equation source term, b) ω-equation source term.

Energy Conservation:

$$\frac{\partial}{\partial t}\left[\bar{\rho}\left(\tilde{e}+\frac{\tilde{u}_i\tilde{u}_i}{2}+k\right)\right]+\frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_j\left(\tilde{h}+\frac{\tilde{u}_i\tilde{u}_i}{2}+k\right)\right]$$
$$=\frac{\partial}{\partial x_j}\left[\left(\frac{\mu}{Pr_L}+\frac{\mu_T}{Pr_T}\right)\frac{\partial \tilde{h}}{\partial x_j}+\left(\mu+\sigma^*\frac{\bar{\rho}k}{\omega}\right)\frac{\partial k}{\partial x_j}\right]$$
$$+\frac{\partial}{\partial x_j}\left[\tilde{u}_i\left(\bar{t}_{ij}+\bar{\rho}\tau_{ij}\right)\right] \quad (3)$$

Molecular and Reynolds-Stress Tensors:

$$\bar{t}_{ij}=2\mu\bar{S}_{ij} \qquad \bar{\rho}\tau_{ij}=2\mu_T\bar{S}_{ij}-\frac{2}{3}\bar{\rho}k\delta_{ij} \qquad \bar{S}_{ij}=S_{ij}-\frac{1}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}$$

Eddy Viscosity:

$$\mu_T=\frac{\bar{\rho}k}{\tilde{\omega}} \qquad \tilde{\omega}=\max\left\{\omega,\ C_{lim}\sqrt{\frac{2\bar{S}_{ij}\bar{S}_{ij}}{\beta^*}}\right\} \qquad C_{lim}=\frac{7}{8}$$

Turbulence Kinetic Energy:

$$\frac{\partial}{\partial t}(\bar{\rho}k)+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_jk)=\bar{\rho}\tau_{ij}\frac{\partial \tilde{u}_i}{\partial x_j}-\beta^*\bar{\rho}k\omega$$
$$+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma^*\frac{\bar{\rho}k}{\omega}\right)\frac{\partial k}{\partial x_j}\right] \quad (4)$$

Specific Dissipation Rate:

$$\frac{\partial}{\partial t}(\bar{\rho}\omega)+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\omega)=\alpha\frac{\omega}{k}\bar{\rho}\tau_{ij}\frac{\partial \tilde{u}_i}{\partial x_j}-\beta\bar{\rho}\omega^2+\sigma_d\frac{\bar{\rho}}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}$$
$$+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma\frac{\bar{\rho}k}{\omega}\right)\frac{\partial \omega}{\partial x_j}\right] \quad (5)$$

Closure Coefficients:

$$\alpha=\frac{13}{25} \qquad \beta=\beta_o f_\beta \qquad \beta^*=\frac{9}{100} \qquad \sigma=\frac{1}{2} \qquad \sigma^*=\frac{3}{5} \qquad \sigma_{do}=\frac{1}{8}$$

$$\beta_o=0.0708 \qquad Pr_T=\frac{8}{9} \qquad \sigma_d=\begin{cases}0, & \frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}\le 0\\ \sigma_{do}, & \frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}>0\end{cases}$$

$$f_\beta=\frac{1+85\chi_\omega}{1+100\chi_\omega} \qquad \chi_\omega=\left|\frac{\Omega_{ij}\Omega_{jk}\hat{S}_{ki}}{(\beta^*\omega)^3}\right| \qquad \hat{S}_{ki}=S_{ki}-\frac{1}{2}\frac{\partial \tilde{u}_m}{\partial x_m}\delta_{ki}$$

Method of Manufactured Solutions

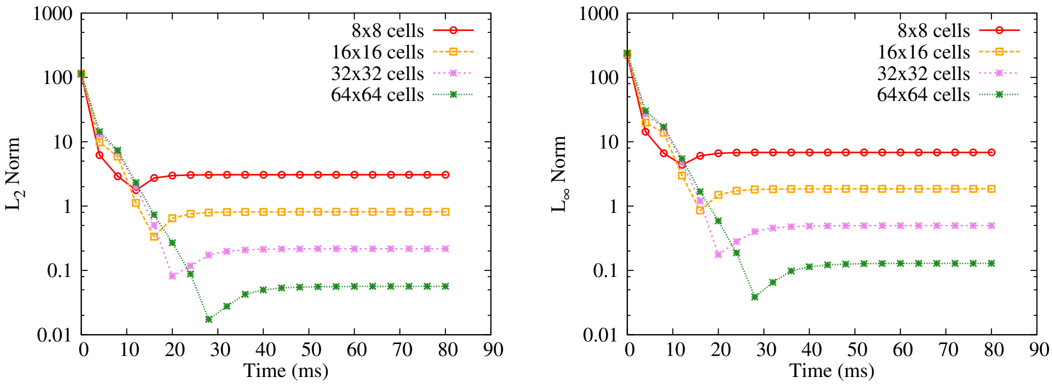
The Method of Manufactured Solutions involves choosing an analytical solution that does not satisfy the governing equations exactly. Then the manufactured solution is passed through the differential operators of the governing equations to generate source terms. These source terms are added to the original governing equations so that the manufactured solution is recovered as a solution to the governing equations plus source terms. Now the manufactured solutions are guaranteed to be the solutions of the "modified" equations. Through the discretization of the "modified" equations, the code should produce a numerical approximation to the manufactured solution, and the difference between the two is defined as the discretization error. The order of accuracy test evaluates discretization error on multiple grid levels, and then determines whether or not the discretized error is reduced at an expected rate given by the formal order of the implemented numerical scheme, in other words, if the observed order of accuracy matches the formal order. Because of this rigor, the test is therefore the recommended acceptance criteria for code verification[4]. Following Roy *et al.*, the manufactured solutions employed here for RANS turbulence model test all take the form:

$$\phi(x,y)=\phi_0+\phi_x f_s\left(\frac{a_{\phi x}\pi x}{L}\right)+\phi_y f_s\left(\frac{a_{\phi y}\pi y}{L}\right)$$
$$+\phi_{xy} f_s\left(\frac{a_{\phi xy}\pi xy}{L^2}\right) \quad (6)$$

where $\phi=[\rho,\ u,\ v,\ p,\ k,\ \omega]^T$ represents any of the primitive variables and the f_s function represents sine or cosine functions. The special values for the constants can be found in Ref. [17]. We used a computer algebra system to generate the source terms. Specifically, we used the Python package SymPy [19]. The produced source terms for the governing equations of turbulence ($k-\omega$) are shown in Figure 1. As can be seen, these source terms exhibit smooth variations in both the x and y directions.

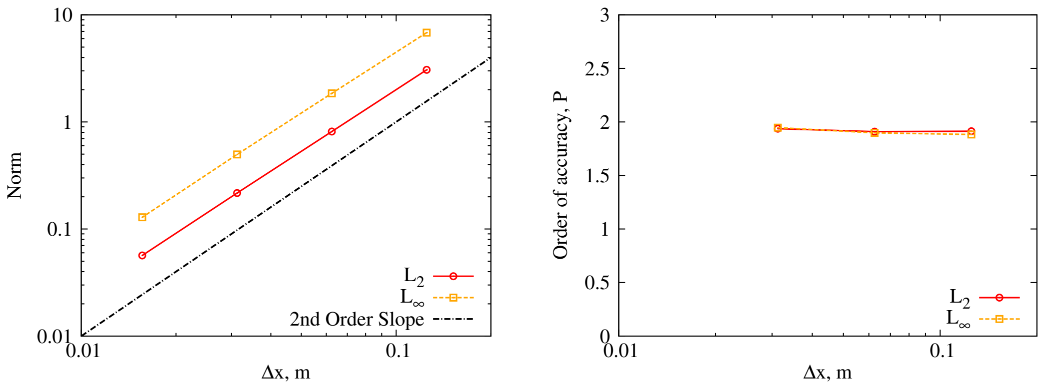
Results and Discussions

Based on the above manufactured solutions, verification of the turbulence model implementation was performed. The square



(a) (b)

Figure 2: Convergence history of norms based on k for different mesh sizes: a) L_2 norms, b) L_∞ norms.



(a) norms (b) observed order of accuracy

Figure 3: Norms and observed order of accuracy.

test domain employed regular structured grids and was initialized by ϕ_0 everywhere in the field. The ideal gas model was selected and Prandtl number had a constant value of $Pr = 1.0$. The viscosity was set to a large value of $\mu = 10Ns/m^2$ to balance the order of magnitude of viscous terms and convection terms, such that error detection in the viscous terms is easier [6]. Exact Dirichlet values given by the manufactured solution are specified at all of the boundaries. In order to determine whether or not the spatial discretization error is diminishing as predicted by the formal order of accuracy, we ran simulation tests on four different levels of grid. The numbers of cells for the meshes in the x and y directions are: 8×8, 16×16, 32×32 and 64×64, respectively. The discretization error is assessed by L_2 and L_∞ norms:

$$L_2 = \left(\frac{\sum_{n=1}^{N} |\phi_n - \phi_{exact}|^2}{N} \right)^{1/2}, \tag{7}$$

and

$$L_\infty = max\,|\phi_n - \phi_{exact}|\,. \tag{8}$$

Figure 2 presents the transient behaviors of the L_2 and L_∞ norms based on turbulence kinetic energy (k) for various mesh sizes. As the simulation proceeds, the norm errors first decrease drastically and then gradually approach the steady state ($\geq 60ms$). For successive grid refinements, the expected trend of a decreasing error is also displayed.

Using the norm values at grid level k and at the coarser grid level $k+1$, the observed order of spatial accuracy can be computed.

$$P_k = \log\left(\frac{L_{k+1}}{L_k}\right) / \log(r) \tag{9}$$

where the r is the grid refinement factor, and equals 2.0 here. Figure 3(a) shows the steady-state error norms for the various meshes plotted as a function of cell size Δx. Also shown is a theoretical slope for 2nd order convergence. The L_2 and L_∞ norms both display second order spatial convergence. This is confirmed in Figure 3(b) where the observed order of accuracy is shown. The observed order of accuracy approaches the formal order of two as the grid density increases. The other primitive variables that are not plotted in this paper, but the results of converging towards second order accuracy were also observed. The formal order of accuracy of `Eilmer` is matched and the implementation of turbulence model is verified successfully.

During code verification studies, the order of accuracy test for turbulence model failed initially. The observed order of accuracy appeared to be first order, and then kept reducing with increased grid resolution. In order to find the reason that caused the reduction in order of accuracy, we devised a code debugging method in which we started only with the inviscid terms in both the numerical solver and the manufactured solution and demonstrated second-order convergence of the errors. We then turned on the turbulence terms associated with the invscid terms, and then the viscous terms and its associated turbulence terms in sequence. By this process we could locate and remove some coding errors when the order of accuracy test failed. Using this process, a bug in the convective flux term in the total energy equation was identified. The turbulent kinetic energy had not been included in the total energy calculation in a consistent manner throughout the code. This bug was corrected. However, the coding bug was undetected during previous validation of the the Wilcox (2006) $k-\omega$ model against experiments performed by Wilson *et al.* [20]. This highlights, therefore, the need for demonstrating the verification of models used in computational solvers as an important and necessary step prior to model validation to ensure that there are no hidden coding errors in the implementation. In this instance, the error was not influential and the results with and without the error were comparable and hence a reasonable validation against experiments occurred. However, in other instances this could be a result of the particular experimental validation dataset not pushing all of the physical effects that the model carries.

Conclusions

The paper presented the verification work for the implementation of Wilcox's (2006) $k-\omega$ model in `Eilmer` using the Method of Manufactured Solutions (MMS). The employed manufactured solutions are smooth, non-physical and exercise all terms in the turbulence equations. Through computing the observed order of accuracy on a series of consistently-refined grids, the implementation has been verified after a bug was identified and corrected. For regular structured grids, the observed order of spatial accuracy matched the formal order of two. The use of MMS on selective parts of the governing equations was an extremely useful way to detect and eliminate coding mistakes in our implementation.

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