Manufactured Solution for the Compressible Navier–Stokes Equations with Large Eddy Simulation models using automatic differentiation

Marc T. Henry de Frahan

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Abstract

In this document, we describe the equations used for the generation of the source terms for the Navier-Stokes with Large Eddy Simulation models. We will use automatic differentiation for the source term derivation.

1 Mathematical Model

The conservation of mass, momentum, and total energy for the Favre-filtered compressible viscous fluid may be written as:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{u}_j\right) = 0, \tag{1}$$

$$\frac{\partial \bar{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{u}_i\widetilde{u}_j + \bar{p}\delta_{ij} - \widetilde{\sigma}_{ji} - \tau_{ji}\right) = 0, \tag{2}$$

$$\frac{\partial \bar{\rho}\widetilde{E}}{\partial t} + \frac{\partial}{\partial x_j}\left(\left(\bar{\rho}\widetilde{E} + \bar{p}\right)\widetilde{u}_j + \widetilde{q}_j + \gamma c_v \mathcal{Q}_j - \widetilde{\sigma}_{ij}\widetilde{u}_i - \mathcal{J}\right) = 0. \tag{3}$$

The resolved variables are denoted by an overbar

$$\bar{f} = \int_D f(\boldsymbol{x'}) G(\boldsymbol{x}, \boldsymbol{x'}; \bar{\Delta})\, \mathrm{d}\boldsymbol{x'} \tag{4}$$

where D is the domain, G is the filter, $\bar{\Delta}$ is the filter width. For compressible flows, we use Favre-filtering, where the variable is $\widetilde{f} = \frac{\overline{\rho f}}{\bar{\rho}}$. Equations (1)–(3) are known as Favre-filtered Navier–Stokes equations and, ρ is the density, $\boldsymbol{u} = (u, v, w)$ is the velocity in x, y or z-direction, respectively, and p is the pressure. For a calorically perfect gas, these equations are closed with two auxiliary relations for energy:

$$E = e + \frac{u_i u_i}{2}, \quad \text{and} \quad e = \frac{1}{\gamma - 1} RT, \tag{5}$$

and with the ideal gas equation of state:

$$p = \rho R T. \tag{6}$$

The diffusive fluxes

$$\widetilde{\sigma}_{ij} = 2\widetilde{\mu}\widetilde{S}_{ij} - \frac{2}{3}\widetilde{\mu}\delta_{ij}\widetilde{S}_{kk}, \tag{7}$$

$$\widetilde{q}_j = -\widetilde{k}\frac{\partial \widetilde{T}}{\partial x_j}, \tag{8}$$

where $\widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right)$ is the strain rate tensor, $\widetilde{\mu}$ and $\widetilde{k}$ are the viscosity and termal conductivity for the filtered temperature $\widetilde{T}$.

The sub-filter terms for the SFS stresses, SFS heat flux, and SFS turbulent diffusion, are

$$\tau_{ij} = \bar{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j\right), \tag{9}$$

$$\mathcal{Q}_j = \bar{\rho}\left(\widetilde{u_j T} - \widetilde{u}_j \widetilde{T}\right), \tag{10}$$

$$\mathcal{J}_j = \bar{\rho}\left(\widetilde{u_j u_k u_k} - \widetilde{u}_j \widetilde{u_k u_k}\right), \tag{11}$$

and need to be modeled. In this work, we choose to model the SFS terms using the standard Smagorinsky model.

The SFS stresses are modeled as

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = 2\mu_t\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right) \tag{12}$$

where $\mu_t = C_s^2 \bar{\Delta}^2 \bar{\rho} |\widetilde{S}|$, $\tau_k k = 2 C_I \bar{\Delta}^2 \bar{\rho} |\widetilde{S}|^2$, and $|\widetilde{S}| = \sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}$.

The SFS heat flux is modeled as

$$\mathcal{Q}_j = -\frac{\mu_t}{Pr_t}\frac{\partial \widetilde{T}}{\partial x_j} \tag{13}$$

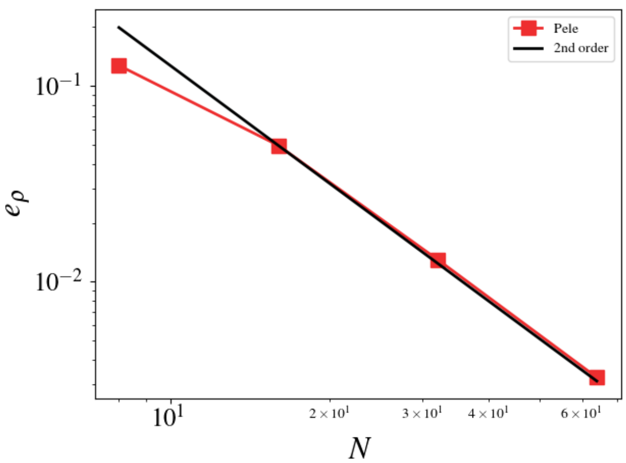
The SFS turbulent diffusion is modeled as

$$\mathcal{J}_j = \widetilde{u}_k \tau_{jk} \tag{14}$$

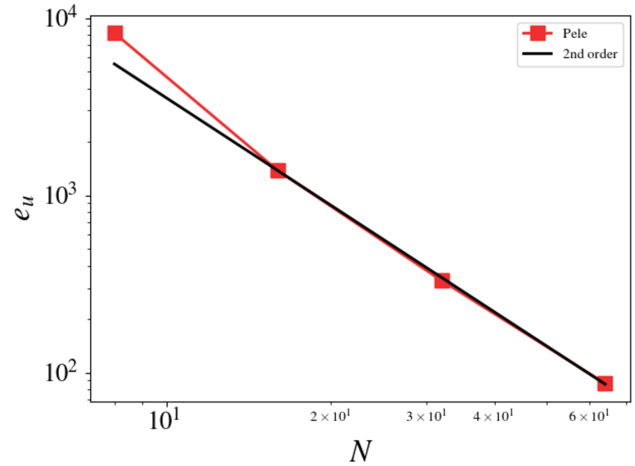
The source terms for these equations are obtained through automatic differentiation as implemented in MASA and METAPHYSICL.

2 Results

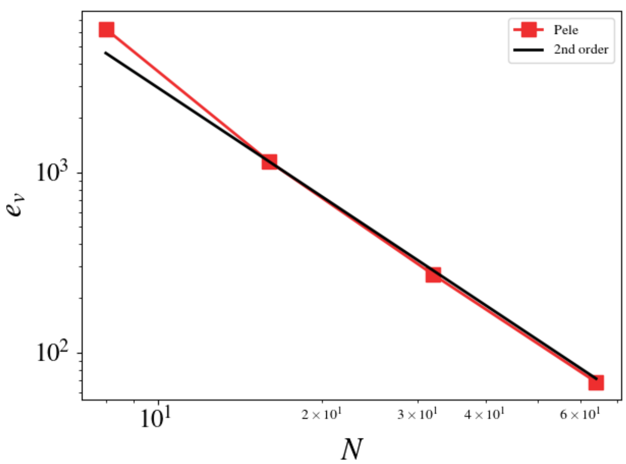
The method of manufactured solutions was used to verify the PeleC code at the National Renewable Energy Laboratory. PeleC is a second order finite volume code used in combustion applications. For these cases, the Reynolds, Mach, and Prandtl numbers were set to 1 to ensure that the different physics were equally important (viscosity, conductivity, and bulk viscosity are non-zero and determined by the appropriate non-dimensional number). The CFL condition was fixed to 0.1 to ensure that the predictor-corrector time stepping method found a solution to the system of equations. The initial solution was initialized to the exact solution. Periodic boundaries are imposed everywhere. The Large Eddy Simulation (LES) constants, C_s and C_I, were chosen such that the turbulent eddy viscosity was comparable to the viscosity, i.e. $\frac{\mu_t}{\mu} = \mathcal{O}(1)$. Since the model scales with the mesh spacing, C_s and C_I were scaled inversely with the mesh spacing for the mesh refinement studies. For example, C_s is set to 2 for the 8^3 mesh and set to 4 for the 16^3 mesh (for C_I, it is 1 and 4, respectively). A convergence study shows second order for Pele's treatment of the compressible Navier-Stokes equations with the constant Smagorinsky Large Eddy Simulation model, Figure 1.



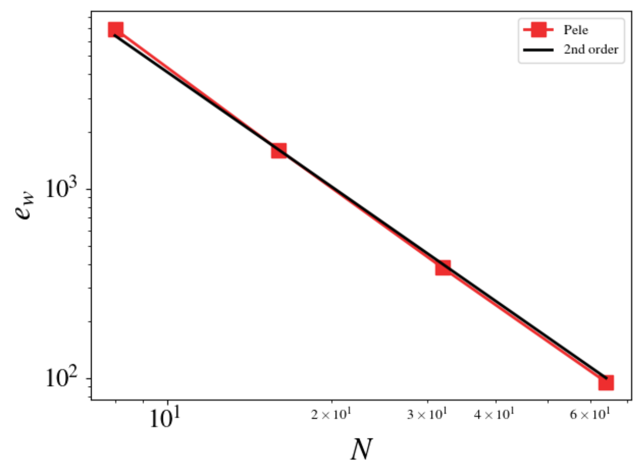
(a) Density.



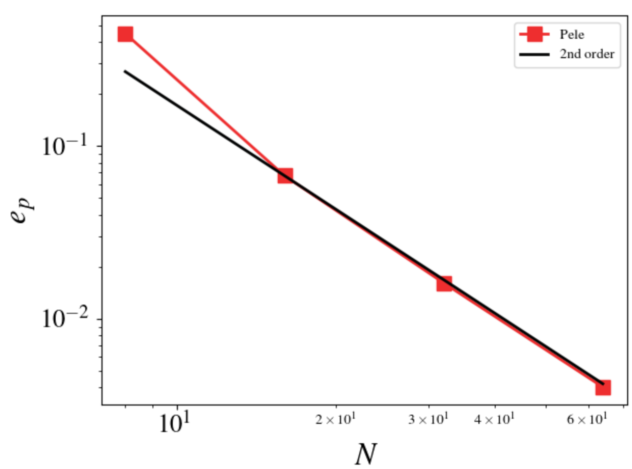
(b) u_1.



(c) u_2.



(d) u_3.



(e) Pressure.

Figure 1: L_2 error as a function of N, the number of elements per side of the cube.