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

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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. These equations and source terms are implemented as `ad_cns_3d_les` and `ad_cns_3d_les_sph` (spherical MMS version) in MASA.

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

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

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

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

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 $\mu_t = C_s^2 \bar{\Delta}^2 \bar{\rho}|\widetilde{S}|$, $\tau_k k = 2C_I \bar{\Delta}^2 \bar{\rho}|\widetilde{S}|^2$, 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. These equations and source terms are implemented as `ad_cns_3d_les` and `ad_cns_3d_les_sph` (spherical MMS version) in MASA.

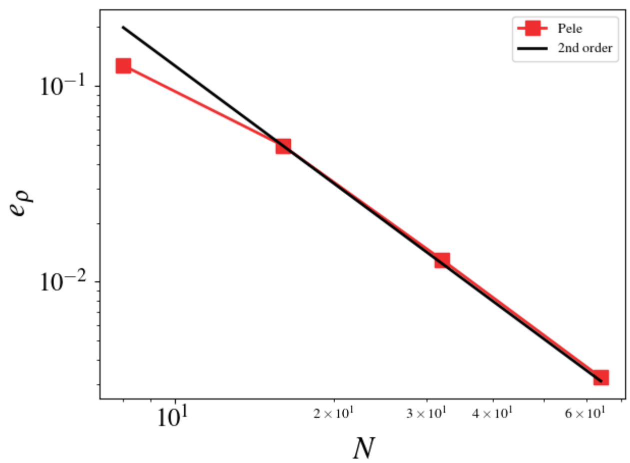
The `ad_cns_3d_les` version uses standard manufactured solutions with sine and cosine fields for use in cartesian simulations. The spherical MMS version (implemented as `ad_cns_3d_les_sph`) was designed to test cartesian simulations that use boundary methods to represent complex boundaries within the domain, e.g. embedded boundary method, immersed boundary method, etc. This implementation can be used to create (in a cartesian simulation) smoothly varying cosine fields that are depended on the radial coordinate. For example, the velocity field, u_i, is defined as:

$$u_i = u_0 + u_r \cos(a_{u_r}\pi r); \tag{15}$$

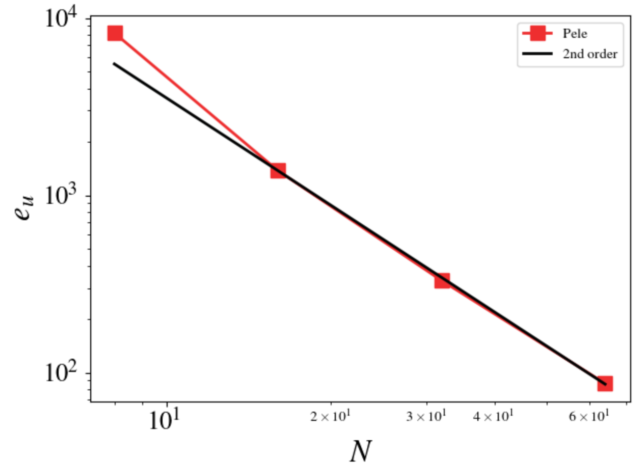
where $r = \sqrt{x^2 + y^2 + z^2}$. The free parameters can be chosen to ensure that the velocities are zero at the boundary of an embedded sphere within the domain.

2 Results

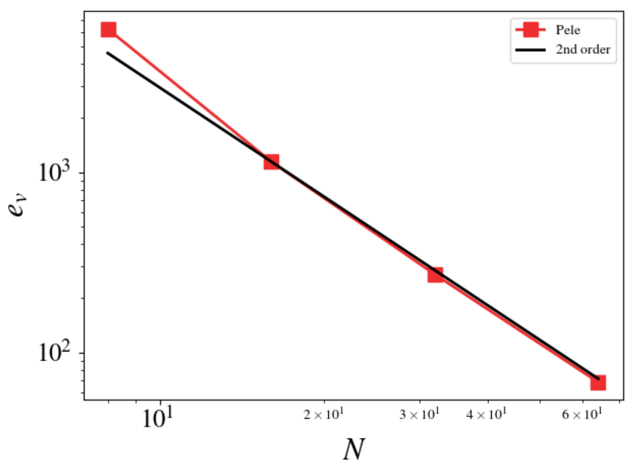
The method of manufactured solutions was used to verify the PeleC code (available at: https://github.com/AMReX-Combustion/PeleC) at the National Renewable Energy Laboratory. PeleC is a second order finite volume code used in combustion applications. For these cases, the Reynolds, Mach, and Prandtl numbers 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.



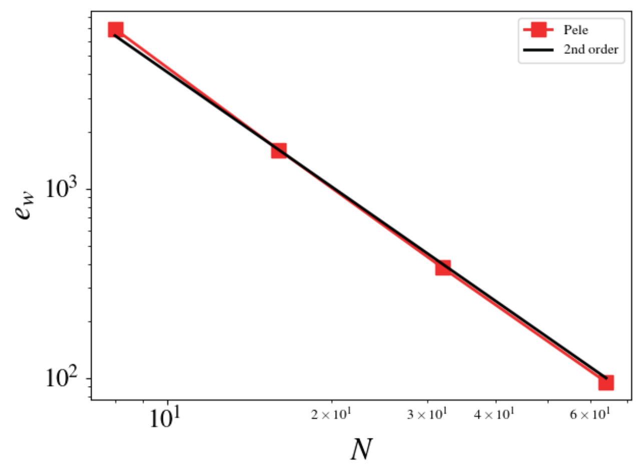
(a) Density.



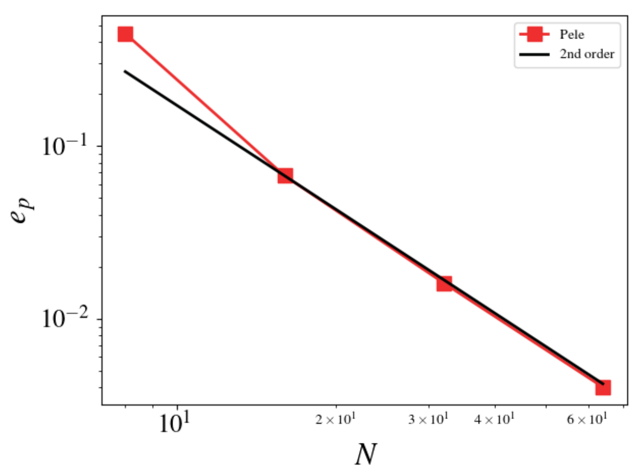
(b) u_1.



(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.