AMD-IDDES Theories

1. Framework

A universal form of eddy viscosity is

$$\nu_t = C^2 F\left(u_i, \Delta_i\right) \tag{0.1}$$

where $F_m\left(u_i, \Delta_i\right)$ has the same dimension as ν_t. For isotropic models,

$$F\left(u_i, \Delta_i\right) = \Delta^2 D\left(u_i\right) \tag{0.2}$$

where $D\left(u_i\right)$ is a differential operator, homogeneous to a frequency and acting on the resolved velocity field. In DES, assuming an equilibrium in subgrid turburence, i.e. $P_k = D_k$ and $P_\omega = D_\omega$, the LES model in DES is

$$\nu_t = \left(\frac{\beta}{\gamma}\right)^{\frac{3}{2}} l_{LES}^2 S_{LES} \tag{0.3}$$

Note that $P_k = \nu_t S^2$ is assumed in Eq. (0.3). In order to make a DES model mimic a given SGS model in the form of Eq. (0.1), the first way is to change the destruction term

$$l_{LES} = C\left(\frac{\gamma}{\beta}\right)^{\frac{3}{4}} \left(\frac{F\left(u_i, \Delta_i\right)}{S_{RANS}}\right)^{\frac{1}{2}} \tag{0.4}$$

For isotropic models, Eq. (0.4) becomes

$$l_{LES} = C\left(\frac{\gamma}{\beta}\right)^{\frac{3}{4}} \left(\frac{D\left(u_i\right)}{S_{RANS}}\right)^{\frac{1}{2}} \Delta \tag{0.5}$$

The second way is to change the production term

$$S_{LES} = C^2 \left(\frac{\gamma}{\beta}\right)^{\frac{3}{2}} \frac{D\left(u_i, \Delta_i\right)}{l_{RANS}^2} \tag{0.6}$$

For isotropic models, Eq. (0.6) becomes

$$S_{LES} = C^2 \left(\frac{\gamma}{\beta}\right)^{\frac{3}{2}} \left(\frac{\Delta}{l_{RANS}}\right)^2 D\left(u_i\right) \tag{0.7}$$

The third way is to change both the production and destruction term. This way is equibvalent to the first or second way for anisotropic models since $F_m(u_i, \Delta_i)$ is an integral, which cannot be spitted into the form of Eq. (0.2). For isotropic models, the third way is

$$S_{LES} = D(u_i) \tag{0.8}$$

$$l_{LES} = C\left(\frac{\gamma}{\beta}\right)^{\frac{3}{4}}\Delta \tag{0.9}$$

In Smagorinsky model, $C = 0.165$ leads to $C_{DES}^{SMG} = 0.74$ for $k-\omega$ and $C_{DES}^{SMG} = 0.58$ for $k-\varepsilon$. Since it is the $k-\varepsilon$ branch that works in the LES region, we set $C_{DES}^{SMG} = 0.61$ (from DIT) in the CFL3D implementation. Mockett et al. adopted the third way for sigma-DES and WALE-DES, and standard DES uses the first way. In AMD-IDDES, we employed the first way, i.e. Eq. (0.4).

2. Basic model

The major idea of AMD-IDDES is to make full use of the favorable properties of the AMD model proposed by Rozema et al. (2015). The most attracting behavir is that it gives good results on anisotropic grids (Haering et al., 2019) in the DIT case. It locally approximates the exact dissipation, and consistent with the nonlinear gradient model. Its eddy visocisy is required for scale separation. It is stable as indicated by Moser et al. (2021), although the calculated viscosity is not as smooth as other models, such as Smagorinsky, WALE, and sigma, but the irregular property is due to the exact form of eddy dissipation. The most important aspect may not be instantaneous eddy viscosity and dissipation, but time-averaged values. It seems in the LES community, they hardly pay attention to instantaneous eddy viscosity. The AMD model is

$$\nu_t = C_{\mathrm{A}}^2 \frac{-\Delta_k^2 g_{ik} g_{jk} S_{ij}}{g_{ml} g_{ml}} \tag{0.10}$$

where $g_{ij} = \frac{\partial u_i}{\partial x_j}$. Note that C_{A}^2 is used in Eq. (0.10) to be consistent with commonly used SGS models and Eq. (0.1). Hence, $C_{\mathrm{A}}^2 = 0.30$ for a second-order central scheme and

$C_{\mathrm{A}}^2 = 0.21$ for a fourth-order central sceme. The LES length scale of AMD-IDDES is expressed in the form of Eq. (0.4) as

$$l_{LES} = C_{\mathrm{A}} \left(\frac{\gamma}{\beta} \right)^{\frac{3}{4}} \left(\frac{-\Delta_k^2 g_{ik} g_{jk} S_{ij}}{g_{ml} g_{ml} S} \right)^{\frac{1}{2}} \tag{0.11}$$

In fact, the part in the square root is indeed a representation of cell size. This can be seen more clearly from its isotropic version,

$$l_{LES} = C_{\mathrm{A}} \left(\frac{\gamma}{\beta} \right)^{\frac{3}{4}} \left(\frac{-g_{ik} g_{jk} S_{ij}}{g_{ml} g_{ml} S} \right)^{\frac{1}{2}} \Delta \tag{0.12}$$

The denominater is exactly the product of the magnitudes of the three factors in the numerator. Hence, a different interpretation of the AMD-IDDES model is that we are trying to develop a length scale from the Poincaré inequality or the exact eddy dissipation or the minimum dissipation theory. Finally, Eq. (0.11) can be rewritten as

$$l_{LES} = C_{\mathrm{DES}}^{\mathrm{AMD}} \Delta_{\mathrm{AMD}} \tag{0.13}$$

$$C_{\mathrm{DES}}^{\mathrm{AMD}} = C_{\mathrm{A}} \left(\frac{\gamma}{\beta} \right)^{\frac{3}{4}} \tag{0.14}$$

$$\Delta_{\mathrm{AMD}} = \left(\frac{-\Delta_k^2 g_{ik} g_{jk} S_{ij}}{g_{ml} g_{ml} S} \right)^{\frac{1}{2}} \tag{0.15}$$

where $C_{\mathrm{DES}}^{\mathrm{AMD}} = 1.92$. In CFL3D, we set $C_{\mathrm{DES}}^{\mathrm{AMD}} = 2.40$ from DIT at present. The value of $C_{\mathrm{DES}}^{\mathrm{AMD}}$ surely depends on the constraints mentioned below, so it needs to be recalibrated if extra constraints are included. A recalibration is necessary especially if the value of $C_{\mathrm{DES}}^{\mathrm{AMD}}$ given by DIT based on Eq. (0.15) is significantly different from 1.92 It should be noted that Eq. (0.15) is not in tensorial form, which makes it useless in most circumstances. Eq. (0.15) should be expressed as the following tensorial form as in the appendix of Haering et al., 2019,

$$\Delta_{\mathrm{AMD}} = \left(\frac{-R_{ij} S_{ij}}{g_{ml} g_{ml} S} \right)^{\frac{1}{2}} \tag{0.16}$$

$$R_{ij} = M_{km} g_{im} M_{kn} g_{jn} \tag{0.17}$$

where M is a second-order grid resolution tensor, whose eigenvalues and eigenvectors are the edge lengths and edge directions of a rectangular cell. It is a symmetric, positive-definite tensor representing a rectangular cell. In a finite volume framework, it is computed using $M = A\Lambda A^T$, where A is composed of eigenvectors in column (opposite/positive eigenvector signs yield the same matrix M), and Λ is the eigenvectors. The interpretation is that the three normalized edges are the principal axes of M. Note that A is not a tensor, though M is a tensor. In a finite difference framework, it is computed via $M = \left(JJ^T\right)^{\frac{1}{2}}$, where J is the Jacobian matrix from the computational space to physical space (not from physical to computational). We have $J = A\Lambda$, which leads to $\left(JJ^T\right)^{\frac{1}{2}} = A\left(\Lambda^2\right)^{\frac{1}{2}} A^{-1} = A\Lambda A^T$. Common cell measures are invariants or eigenvalues of M. For instance, the cell volume is $\lambda_1\lambda_2\lambda_3 = III_M$ and body diagonal is $\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2\right)^{\frac{1}{2}} = \left(M_{ij}M_{ji}\right)^{\frac{1}{2}}$. Also, the wall-normal cell size can be evaluated by $\Delta_{\mathrm{wn}} = \left|M_{ij}n_j\right|$ and the wall-normal direction $n_j = \dfrac{\partial d}{\partial x_j} \Bigg/ \sqrt{\dfrac{\partial d}{\partial x_k}\dfrac{\partial d}{\partial x_k}}$. Note that Eq. (0.16) is rotationally and reflectionally invariant, because "any scalar obtained from a tensor is call an invariant, because its value is the same in any coordinate system" (Pope, 2000)

$$R_{ij}S_{ij} = M_{km}g_{im}M_{kn}g_{jn}S_{ij} = \hat{M}_{km}\hat{g}_{im}\hat{M}_{kn}\hat{g}_{in}\hat{S}_{ij} \tag{0.18}$$

where $\hat{M} = \Lambda$ and the upper hat denotes a local coordinate system parallel to the three cell edges. Note that Eq. (0.15) must be used in the local coordinate system, but Eq. (0.16) can be computed in any coordinate systems. Hence, Eq. (0.16) should be preferred in the implementation of the AMD length scale. Note that the form of Eq. (0.17) should also be used in Vreman's model.

3. Constraints

Like many SGS models (e.g. dynamic models, gradient models), we introduce some constraits to make the length scale Eq. (0.12) usable and robust. A literature review shows that typical treatments can include

1) Setting a lower limit (cliping);
2) Spatial averaging (averaging).

For instance, both (1) and (2) are applied by Shur et al. because their formulations have $F_{KH}^{\min} = 0.1$ and $\langle VTM \rangle$. Also, both the constraits were used by Yin et al. (2015) by setting $C_{\lim}$ as the lower limit of C_{dyn} and performing spatial averaging on C_{dyn}. Similarly, He et al. (2017) and Sohankar et al. (2000) used both clipping and spatial averaging. In AMD-IDDES, constraint (1) is a necessity for robustness because the AMD model the numerator of Eq. (0.10), i.e., exact eddy dissipation, is negative in the case of energy backscatter. Rozema et al. (2015) clipped the numerator by zero, and Verstappen (2011) uses the absolute value of the numerator to closes the interaction of resolved and sub-filter scales in both directions (private communications with Wybe Rozema). Here, we set a lower limit to Eq. (0.11) and the threshold is positive as in the models of Shur et al. and Yin et al. for better robustness considering that DES applications cover a wide range of Mach numbers and configuration complexity. Specifically, we employ

$$l_{LES} = \left(C_{\mathrm{A}} \left(\frac{\gamma}{\beta} \right)^{\frac{3}{4}} \left(\frac{\max\left(-\Delta_k^2 g_{ik} g_{jk} S_{ij}, 0 \right)}{g_{ml} g_{ml} S} \right)^{\frac{1}{2}}, C_{\lim} V^{\frac{1}{3}} \right) \tag{0.19}$$

This is equivalent to a limitation on the eddy viscosity of Eq. (0.10) by

$$\nu_t = \left(\frac{\beta}{\gamma} \right)^{\frac{3}{2}} \left(\frac{C_{\lim}}{C_s} \right)^2 \left(C_s V^{\frac{1}{3}} \right)^2 S \tag{0.20}$$

where $C_{\lim} = 0.15$ and $C_s = 0.165$ yields $\left(\frac{\beta}{\gamma} \right)^{\frac{3}{2}} \left(\frac{C_{\lim}}{C_s} \right)^2 = 0.067$ with other coefficients from $k-\varepsilon$. Note that $C_{\lim} V^{\frac{1}{3}}$ has been applied, rather than $C_{\lim}\Delta_{\max}$ to retain small l_{LES} values in the "grey area". We have not applied constraint (2), i.e., averaging, to Eq. (0.12) because we have not encountered numerical instability. However, it would be incorporated in the future if the required $C_{\mathrm{DES}}^{\mathrm{AMD}}$ is much higher than 1.92 ($C_{\mathrm{DES}}^{\mathrm{AMD}} = 2.40$ currently) in the simulation of DIT. Shur et al, 2015 mentioned that averaging does benefit to correct spectra in DIT. In contrast to pure LES models, DES typically introduces special treatments to the

LES length scale in the RANS modeled boundary layers and in the farfield. In AMD-IDDES, we use

$$l_{LES} = \begin{cases} C_{\mathrm{DES}}^{\mathrm{AMD}} \Delta_{\mathrm{AMD}}, \, f_p < 0.01 \\ C_{\mathrm{DES}}^{\mathrm{SMG}} \Delta_{\max}, \, f_p \geq 0.01 \end{cases} \tag{0.21}$$

where $f_p \approx 1.0$ in the RANS modeled boundary layers alleviate MSD in the outer part and in the inviscid regions to increase numerical stability considering possible oscillations of Eq. (0.19) in the edge of turbulent regions. In other words, the AMD length scale only works in the resolved turbulent regions. It can also be interpreted as a blending of two LES length scales (LES models). This aspect can be better shown with a picture. The expression for f_p is

$$f_p = \max\left(f_d, f_f \right) \tag{0.22}$$

$$f_d = \max\left(1 - f_{dt}, f_b\right) \tag{0.23}$$

$$f_f = \tanh\left(\left(\frac{0.2\nu}{\max\left(\nu_t - \nu_{t,\infty}, 10^{-6}\nu_{t,\infty}\right)} \right)^3 \right) \tag{0.24}$$

Note that f_f is not as necessary as it is in Shur et al. 2015 in which the wavering of VTM is indeed strong, as shown in our jet case. Also, it is unjustifiable to increase the length scale/eddy viscosity in the inviscid regions because they are negligible even in RANS. **Thus, it is possible to completely remove f_p as long as f_d is reliable enough.** We have also considered using Ω/S to detect the irrotational farfield, but it was defeated by its small values within shocks, which means it has to be coupled with a shock detector. Finally, Eq. (0.19), (0.21), (0.22), (0.23) and (0.24) constitutes the LES length scale of AMD-IDDES.

3. Enhancements

We may adopt the following enhancements in the future development of AMD-IDDES.

The **first** enhancement is to develop a better shielding function to cover the outer layer of turbulent boundary layers. The shielding function is expected to be simple, robust and does not affect the "grey area" mitigation. In fact, $C_{dt1} > 20$ should be allowed in AMD-IDDES since the “grey area” has been significantly alleviated. We may finally set $C_{dt1} = 28$ based on mixing layer test. Anyway, a more effective shielding function inevitably causes thicker RANS models in separated and reattached regions with resolved turbulence. One idea is to introduce a function differetiating 2D/3D turbulence. The simplest and most natural way is

$$f_{\mathrm{AMD}} = \frac{|g_{ik} g_{jk} S_{ij}|}{g_{ml} g_{ml} S} \tag{0.25}$$

The added computaional cost of Eq. (0.25) is negligible because only the term $g_{ik} g_{jk} S_{ij}$ needs to be calculated, since the denominator has been calculated in Eq. (0.19). Other methods can include

$$\mathrm{VSM} = \frac{|S\omega|}{|S||\omega|} \tag{0.26}$$

$$\mathrm{VTM} = \frac{|(S \cdot \omega) \times \omega|}{|\omega| \sqrt{-Q_{\tilde{S}}}} \tag{0.27}$$

$$f_\sigma = \frac{\sigma_3 (\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^3} \tag{0.28}$$

A simple modified shielding function can be

$$f_{dt} = 1 - \tanh\left(C_{dt1} r_{dt}\right)^{C_{dt2}} \tag{0.29}$$

$$r_{dt} = \frac{\nu_t}{\kappa^2 d^2 \sqrt{S^2 + \Omega^2}} \left(1 - f_{\mathrm{3D}}\right) \tag{0.30}$$

where f_{3D} can be f_{AMD}, VSM, VTM, σ_3/σ_1, etc. It should be remained that we can not use f_{3D} to completely replace f_{dt}, because all the f_{3D} formulations do not distinguish wall-bounded shear layers from free shear layers. For instance, f_{dt} would cover all regions in a RANS-modeled mixing layer if the quantities are used, which makes the simulation impossible to switching to LES in the free mixing layer. The root reason may be that are insensitive to wall distance. On the contrary, f_{dt} is sensitive to wall distance. For wall-bounded shear layers, integral turbulent scales are proportional to wall distance, but for free shear layers, they are proportional to their thickness which is smaller than wall distance. Hence, f_{dt} is able to distinguish wall bounded shear layers from free shear layers. Alternative solutions may be derived after the ideas of Deck et al. 2019.

The **second** enhancemnt is to introduce an extra detection function of 2D/2C turbulence to reduce the length scale if Eq. (0.19) is not small enough in the grey area because its value is dependent of the grid cell orientation relative to the local velocity gradient tensor. The AMD model yields different values if an anisotropic grid cell is rotated by a centain angle, although this is not a problem for an isotropic grid cell. The dependence on cell orientation is reasonable for 3D turbulence, but may not for 2D flows, where it should always predict zero eddy viscosity with no relation to the oritation of a grid cell. Table 1 shows that although problematic in pure shear, the AMD model always yields zero eddy viscosity for solid rotation and simple shear. Hence, the AMD model gives zero in the very initial simple shear layer. However, it is nonzero when a simple shear is superimposed by solid body rotation. Note that rotation of a cell is achieved by RMR^T, where R is extrinsic rotation matrix given in https://en.wikipedia.org/wiki/Rotation_matrix.

Table 1 Dependence of AMD eddy viscosity on the relative positions between stretched grid cells and local flow directions. Cell size is $(\mathrm{d}x, \mathrm{d}y, \mathrm{dz}) = (1.0, 2.0, 4.0)$ at $\gamma = 0$ deg. C_{A}^2 is left out in Eq. (0.10) in tensorial form

Angle γ	0 deg	30 deg	60 deg	90 deg	Arbitrary α, β, γ
Pure shear	0	1.30	1.30	0	+/-
Solid rotation	0	0	0	0	0
Simple shear	0	0	0	0	0
Solid+simple	0	-0.52	-0.52	0	+/-
Axismmetric	-2	-0.88	1.38	2.5	+/-
Isotropic	-7	-7	-7	-7	-7

Pure shear, $g_{12} = 1$ and $g_{21} = 1$;

Solid/pure rotation, $g_{12} = -1$ and $g_{21} = 1$;

Simple shear, $g_{12} = 1$;

Pure axisymmetric expansion (contraction), $g_{11} = -2$, $g_{22} = 1$ and $g_{33} = 1$;

Isotropic expansion (contraction), $g_{11} = 1$, $g_{22} = 1$ and $g_{33} = 1$.

Solid+simple (2D K-H instability), $g_{12} = 1 + 1$, $g_{21} = -1$

More practically, one can use Eq. (0.25), Eq. (0.26), Eq. (0.27) or Eq. (0.28) coupled with a simple gradient weigthed length scale (proposed by Haering et al.)

$$\Delta = \left(\frac{\Delta_k^2 g_{ik} g_{ik}}{g_{ml} g_{ml}} \right)^{\frac{1}{2}} = \left(\frac{R_{ii}}{g_{ml} g_{ml}} \right)^{\frac{1}{2}} \tag{0.31}$$

where the definition of R_{ij} is Eq. (0.17). Note that Eq. (0.31) is always positive, nothing to do with zero eddy viscosity. This definition is similar to Δ_ω, but is better in at least three ways. First, it takes velocity gradients into consideration. For instance, given a cell of $(\mathrm{d}x, \mathrm{d}y, \mathrm{d}z) = (1.0, 2.0, 4.0)$, Eq. (0.31) is equal to $\Delta = \sqrt{\frac{(\mathrm{d}x)^2 + 4(\mathrm{d}y)^2}{5}}$ for a 2D roller $g_{12} = -2$ and $g_{21} = 1$, but $\Delta_\omega = \sqrt{\frac{(\mathrm{d}x)^2 + (\mathrm{d}y)^2}{2}}$ with no relation to the gradient. Second, it incorporates all cell sizes, but Δ_ω only incorporates the cell size in the vorticity direction, which is surely unreasonable in 3D turbulence. Third, Eq. (0.31) always gives edge length for isotropic cells, but Δ_ω does not. In fact, a small modification of Δ_ω would make it always equal to cell edge length for isotropic cells. The modified definition is $\Delta_\omega = M \frac{\omega}{|\omega|}$.

Anyway, the framework (Eq.(0.31) coupled with $f_{3\mathrm{D}}$ function) is similar to the shear-layer-adapted length scale. We believe that it is more tenable theoretically to be based on anisotropic minimum dissipation for applicability on anisotropic grids and mitigation of "grey area". Thus, it is good to name "AMD-IDDES" even with future enhancements.

The **third** enhancement is to actively introduce turbulent fluctuations. The turbulence generation method is supposed to be simple, robust and friendly to complex configurations, such as aircraft and engines.

4. Comparison

This setion compares the AMD model with popular LES models in several aspects. Some notes on Table *2*.

1) $\tau_{ij}-\frac{1}{3}\tau_{kk}\delta_{ij}=-2\nu_t S_{ij}$, so the anisotropic part is zero for solid body rotation ($S_{ij}=0$) even if the eddy viscosity is nonzero;
2) The near-wall symptotic behavior is easily obtained using MATLAB and the paper of Nicoud et al. (2011).

Table 2 Properties of SGS models

	AMD	σ	Vreman	Smagorinsky
Model constant	$C_{\mathrm{A}}=0.55$	$C_\sigma=1.35$	$C_v=0.26$	$C_s=0.165$
Asymptotic	$O\left(y^1\right)$	$O\left(y^3\right)$	$O\left(y\right)$	$O\left(y^0\right)$
Pure shear	0	0	$0.71C_v^2$ (0.048)	$2C_s^2$ (0.054)
Solid rotation	0	0	$0.71C_v^2$ (0.048)	0
Simple shear	0	0	0	C_s^2 (0.027)
2D	0	0	N	0
2C	N	0	N	0
Axismmetric	C_{A}^2 (0.30)	0	$1.22C_v^2$ (0.083)	$3.46C_s^2$ (0.094)
Isotropic	$-C_{\mathrm{A}}^2$ (-0.30)	0	C_v^2 (0.068)	$2.45C_s^2$ (0.067)
Backscatter	Y	N	N	N

Smagorinsky model

$$\nu_t=\left(C_s\Delta\right)^2 S \tag{0.32}$$

σ model

$$\nu_t=\left(C_\sigma\Delta\right)^2\frac{\sigma_3\left(\sigma_1-\sigma_2\right)\left(\sigma_2-\sigma_3\right)}{\sigma_1^2} \tag{0.33}$$

Vreman model

$$\nu_t=C_v^2\sqrt{\frac{\beta_{11}\beta_{22}-\beta_{12}^2+\beta_{11}\beta_{33}-\beta_{13}^2+\beta_{22}\beta_{33}-\beta_{23}^2}{g_{ij}g_{ij}}} \tag{0.34}$$

$$\beta_{ij}=\Delta_m^2 g_{im}g_{jm} \tag{0.35}$$

Its isotropic form is

$$\nu_t = \left(C_v \Delta\right)^2 \sqrt{\frac{Q_{gg^T}}{P_{gg^T}}} \tag{0.36}$$

AMD model

$$\nu_t = \left(C_{\mathrm{A}} \Delta\right)^2 \frac{-g_{ik} g_{jk} S_{ij}}{g_{ml} g_{ml}} \tag{0.37}$$