LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-TR-414246

A General Realizability Method for the Reynolds Stress for 2-Equation RANS Models

M. Ulitsky

June 26, 2009

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Contents

1 Introduction

In two equation RANS (Reynolds Averaged Navier-Stokes) modeling, it is common for one of the two transported turbulent quantities to be the turbulent kinetic energy per unit mass (k). The other transported variable is usually a turbulent length scale (L) or dissipation per unit mass (ϵ), although there are other possible choices as well (like Ω, which is an inverse time scale). For variable density turbulence, k is directly related to the trace of a more general second order tensor correlation known as the Reynolds stress, which is given by:

$$R_{ij} \equiv \overline{\rho u_i'' u_j''}, \tag{1}$$

where ρ is the fluid density, u_i'' is the i^{th}-component of the Favre fluctuating velocity, and the overbar represents an ensemble average or a spatial average over the homogeneous direction(s). The trace of the stress is simply

$$R_{ii} \equiv \overline{\rho u_i'' u_i''} \;\; = \;\; 2\overline{\rho} k \;\; .$$

For readers unfamiliar with Favre (density weighting) averaging, assume we have a state variable X, which could represent a velocity component, mass or volume fraction fraction, or some other field. The Favre average of that field is then defined as

$$\tilde{X} \equiv \frac{\overline{\rho X}}{\overline{\rho}} \; .$$

Fluctuations from the mean, X'', are then computed by

$$X'' = X - \tilde{X} \; .$$

What can be a bit confusing to those accustomed to Reynolds (unweighted) averaging, is that the ensemble average of a Favre fluctuating quantity is non-zero. It is the ensemble average of the density weighted fluctuation that vanishes. This means,

$$\begin{aligned} \overline{X''} &\neq 0 \, , \\ \overline{\rho X''} &= 0 \, . \end{aligned}$$

Some RANS models have a transport equation for the full Reynolds stress, (6 scalar components in 3D since $\mathbf{R}$ is a symmetric tensor) rather than for just its trace. The advantage of this approach is that one is better able to handle anisotropy. The disadvantage, however, is that the Favre averaged equation for the variable density Reynolds stress contains significantly more terms (as well as more complicated terms) that require model closure than the corresponding k-equation. There is also the extra computational exprense of transporting six scalars rather than just one. Finally, even if one decides to transport the full tensor, there is no guarantee that after closing the various unclosed terms that the 6 scalar components will satisfy the necessary tensor constraints. That is, our closure model could (and almost certainly will in some cases) violate realizability. For this reason, some modelers prefer to work with stochastic differential equations (like Langevin equations), since any moments that are computed from a stochastic process are by construction fully realizable. In any case, having a simple, robust method that can ensure realizability for the stress tensor under all conditions will be extremely useful.

2 Realizability

In turbulence models where we are transporting k, there is a shear term on the right hand side of the k-eqn that accounts for turbulence production due to the Kelvin-Helmholz instability. This term has the form of $\mathbf{R} : \mathbf{S}$, where $\mathbf{S}$ is the mean strain rate tensor (the symmetric part of the mean velocity gradient tensor). To conserve total energy, the momentum equation will have a term of the form $\nabla \cdot \mathbf{R}$. Therefore, we need a closed form expression for $\mathbf{R}$ that is consistent with the positive semi-definiteness implied by eqn. 1. A typical model for $\mathbf{R}$ is given by the Boussinesq approximation and takes the form of

$$R_{ij} = \frac{2}{3}\overline{\rho} k \delta_{ij} - D_{ij} \ , \tag{2}$$

where δ_{ij} is the Kronecker delta tensor and D_{ij} is the following traceless, deviatoric tensor

$$D_{ij} = 2\mu_t \left(S_{ij} - \frac{1}{3} \nabla \cdot \tilde{\mathbf{u}} \, \delta_{ij} \right) \ . \tag{3}$$

Here, μ_t, the turbulent viscosity is given by $C_\mu \overline{\rho} k^2/\epsilon$ for a $k - \epsilon$ model and by $C_\mu \overline{\rho} \sqrt{k} L$ for a $k - L$ model. The main point is that while R_{ij} is by definition a symmetric positive semi-definite tensor, the model for R_{ij} given in eqs. 2–3 may not always satisfy the realizability properties required by a symmetric positive semi-definite tensor.

At this point let's digress for a moment and review some basic tensor theory relevant for second order tensors that can be found in any good applied math or continuum mechanics book. All second order tensors have 3 eigenvalues which are directly related to the 3 principal invariants. The first invariant of a second order tensor $\mathbf{A}$ is I_A, which is just the trace of the tensor. That is,

$$I_A = A_{ii} \ .$$

The second invariant is related to the square of $\mathbf{A}$ and is given by the following

$$II_A = \frac{1}{2} \left(A_{ii} A_{jj} - A_{ij} A_{ji} \right) \ .$$

The third invariant is just the determinant of $\mathbf{A}$ and is therefore related to the cube of the tensor. It is given by

$$III_A = \frac{1}{6} \left[A_{ii} A_{jj} A_{kk} + 2 A_{ik} A_{km} A_{mi} - 3 A_{ik} A_{ki} A_{jj} \right] \ .$$

It can be shown that if $\mathbf{A}$ is a symmetric tensor, then the three eigenvalues of $\mathbf{A}$ (denoted by λ_1, λ_2, and λ_3) are real and are related to the principal invariants by

$$\begin{aligned} I_A &= \lambda_1 + \lambda_2 + \lambda_3 \\ II_A &= \lambda_1 \lambda_2 + \lambda_1 \lambda_3 + \lambda_2 \lambda_3 \\ III_A &= \lambda_1 \lambda_2 \lambda_3 \ . \end{aligned}$$

The requirements on the eigenvalues for a symmetric positive semi-definite tensor are even more strict. Here, not only must the eigenvalues be real, but they must be positive semi-definite or non-negative definite (that is, $\lambda_i \geq 0$). In deriving the conditions on the elements of $\mathbf{R}$ that must be satisfied, we are led to the following independent constraints

$$\begin{aligned} 0 &\leq R_{\beta\beta} \leq R_{ii} \ , \\ R_{\beta\gamma}^2 &\leq R_{\beta\beta} R_{\gamma\gamma} \quad \text{for} \ \ \beta \neq \gamma \ , \\ \det(\mathbf{R}) &\geq 0 \ , \end{aligned}$$

where there is no implied summation when Greek indices are used.

The first inequality shall be referred to as the linear or diagonal constraint. Basically, since $\overline{\rho\left(u''_{\beta}\right)^2}$ is positive semi-definite, we must have the diagonal elements greater than or equal to zero. Also, each diagonal element must be smaller than or equal to the trace of the tensor. If this were not the case, then one of the diagonal elements would have to be negative. The second inequality will be referred to as the quadratic constraint or Cauchy-Schwarz inequality. This condition essentially states that a covariance squared must be less than or equal to the product of its variances. Even with the linear and quadratic constraints satisfied, it is still possible for one of the eigenvalues to be negative. The cubic constraint or determinant condition given by the last inequality ensures that all the eigenvalues will be positive semi-definite.

Since the Cauchy-Schwarz condition is quite prevalent in applied mathematics, we will give a rigorous derivation here. Assume we have an orthonormal set of basis vectors in $3D$ Euclidean space denoted by $\mathbf{e}_\beta$. Then $\mathbf{R}$ can be expressed as

$$\mathbf{R} = R_{ij}\mathbf{e}_i\mathbf{e}_j \ .$$

The condition that $\mathbf{R}$ is positive semi-definite can also be represented by the requirement that

$$\mathbf{v}\cdot\mathbf{R}\cdot\mathbf{v} \geq 0 \ ,$$

for any vector $\mathbf{v}$. If we let $\mathbf{v} = \mathbf{e}_\beta$, we arrive at the first inequality or linear constriant. If we let $\mathbf{v} = c\mathbf{e}_\beta + \mathbf{e}_\gamma$, where $\beta \neq \gamma$, then we end up with the condition

$$c^2 R_{\beta\beta} + 2cR_{\beta\gamma} + R_{\gamma\gamma} \geq 0 \ \text{ for all } \ c \ . \tag{4}$$

The parabola on the left hand side of eq. 4 has a minimum for its vertex since c^2 is positive. Therefore, as long as the vertex is above (or just touching) the c-axis, the inequality (equality) will be satisfied. To ensure that there are not multiple points of intersection with the c-axis, we require that the discriminant of the quadratic equation be less than or equal to zero. This means that $R^2_{\beta\gamma} \leq R_{\beta\beta}R_{\gamma\gamma}$, which is precisely the quadratic constraint listed above.

3 Ensuring Realizability

Given a modeled expression for a positive semi-definite symmetric second rank tensor, there are several ways that one can envision modifying the tensor to satisfy realizability. The approach described in this report is a result of some unpublished notes by Chuck Cranfill (formerly with group X-3 at LANL) from 1991 that I have expanded upon. Chuck's rather elegant idea was to identify a single constant (or scale factor) c^{-1} that would only be applied to the deviatoric part of the stress. This would ensure that the trace of the stress would remain unchanged (since the deviatoric stress is traceless) and also provide a *single* constant that could restore realizability if it were ever violated (rather than having multiple constants for different components of the tensor).

For the problem of interest, we can express the stress tensor as

$$R_{ij} = \alpha\delta_{ij} - \frac{1}{c}D_{ij} \ , \tag{5}$$

where c is a constant that satisfies $c \geq 1$, $\alpha \equiv 2\overline{\rho}k/3$, and D_{ij} is given by eq. 3. Thus, the method used to ensure realizability will be to assume initially that $c = 1$. We will then test the stress tensor to verify it satisfies the linear, quadratic, and cubic constraints. If it does, then no action is taken. If one of the constraints is violated, however, then we will determine the largest value for c that satisfies all of the constraints. Effectively, this means that when realizability is violated, it can be viewed as the viscosity being too large. We are therefore scaling down (or renormalizing) the viscosity to make sure the stress tensor is mathematically well-behaved.

To make these ideas more explicit, let's consider the case of using the turbulence model to investigate a shock tube (with constant planar cross-section) that is oriented in the x-direction. Since we can assume the turbulence is homogeneous in the spanwise directions, all of our correlations will only be functions of the inhomogeneous direction and time. We will also assume that $c = 1$ and then show that even for this simple problem, realizability cannot be guaranteed. Since S_{ij} is defined as

$$S_{ij} \equiv \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) ,$$

and the mean flow velocity is only in the x-direction, then the only non-zero component of S_{ij} is S_{xx}. We also have the simplification that $\nabla \cdot \tilde{\mathbf{u}} = \partial \tilde{u}_x / \partial x$. This leads to three non-zero components for R_{ij}, which are as follows

$$\begin{aligned} R_{xx} = \alpha - D_{xx} &= \alpha - \frac{4}{3}\mu_t \frac{\partial \tilde{u}_x}{\partial x} , \\ R_{yy} = \alpha - D_{yy} &= \alpha + \frac{2}{3}\mu_t \frac{\partial \tilde{u}_x}{\partial x} , \\ R_{zz} = \alpha - D_{zz} &= \alpha + \frac{2}{3}\mu_t \frac{\partial \tilde{u}_x}{\partial x} . \end{aligned}$$

If we have a strong expansion or rarefaction, then D_{xx} could overwhelm α and drive R_{xx} negative. On the other hand, a strong compression could make D_{yy} or D_{zz} overwhelm α and drive R_{yy} and R_{zz} below zero. Clearly, if c is allowed to be greater than unity, we can always prevent the diagonal components of R_{ij} from going negative.

4 The General Procedure

In this section, we will consider the most general case for a problem in an XYZ-geometry. Assume we have a second order symmetric tensor $\mathbf{R}$ of the form

$$R_{ij} = \alpha \delta_{ij} - \frac{1}{c} D_{ij} , \tag{6}$$

where $\alpha > 0$, $c \geq 1$, and $D_{ii} = 0$. We start by finding a value for c that will satisfy the linear constraint. This value shall be referred to by c_{diag}. Since we know the values for α and the components of $\mathbf{D}$, we can compute c_{diag} by

$$c_{\text{diag}} = \text{ Max } \left[1, \frac{D_{xx}}{\alpha}, \frac{D_{yy}}{\alpha}, \frac{D_{zz}}{\alpha}\right] . \tag{7}$$

If all the diagonal elements are already well-behaved, then c_{diag} will equal unity. Otherwise, c_{diag} will be larger than unity.

Now we consider the implications of the quadratic constraints. For the xy Cauchy-Schwarz condition we have

$$\begin{aligned} R_{xx} &= \alpha - \frac{1}{c} D_{xx} , \\ R_{yy} &= \alpha - \frac{1}{c} D_{yy} , \\ R_{xy} &= -\frac{1}{c} D_{xy} . \end{aligned}$$

The relation $R_{xx}R_{yy} - R_{xy}^2 \geq 0$ is equivalent to

$$\alpha^2 - \frac{\alpha}{c}\left(D_{xx} + D_{yy}\right) + \frac{1}{c^2}\left(D_{xx}D_{yy} - D_{xy}\right) \geq 0 \; .$$

Since c^2 is positive, we can multiply through by c^2 to obtain

$$\alpha^2 c^2 - \alpha c\left(D_{xx} + D_{yy}\right) + \left(D_{xx}D_{yy} - D_{xy}\right) \geq 0 \; . \tag{8}$$

With a little algebra, it can be shown that the roots to the above quadratic are

$$c_{\pm} = \frac{1}{\alpha}\left[\frac{D_{xx} + D_{yy}}{2} \pm \sqrt{\frac{\left(D_{xx} - D_{yy}\right)^2}{4} + D_{xy}^2}\,\right] \; . \tag{9}$$

Thus the parabola has two real roots in general and has a vertex that is a minimum. The solutions to the inequality therefore are given by values of c that satisfy $c \geq c_+$ or $c \leq c_-$.

As $\mathbf{D}$ is traceless, we can also express the solutions by

$$c_{\pm} = \frac{1}{\alpha}\left[\frac{-D_{zz}}{2} \pm \sqrt{\frac{\left(D_{xx} - D_{yy}\right)^2}{4} + D_{xy}^2}\,\right] \; . \tag{10}$$

If we recall that one part of the linear constraint is that we must have $R_{\beta\beta} \leq R_{ii}$, then this translates to

$$c \geq \frac{-D_{\beta\beta}}{2\alpha} \; .$$

Therefore, only values of c greater than or equal to c_+ can be a solution. Since the xz and yz Cauchy-Schwarz conditions are completely analagous to the xy case, we can summarize the Cauchy-Schwarz solutions as

$$\begin{aligned}
c_{xy} &= \frac{1}{\alpha}\left[\frac{-D_{zz}}{2} + \sqrt{\frac{\left(D_{xx} - D_{yy}\right)^2}{4} + D_{xy}^2}\,\right] \; , \\
c_{xz} &= \frac{1}{\alpha}\left[\frac{-D_{yy}}{2} + \sqrt{\frac{\left(D_{xx} - D_{zz}\right)^2}{4} + D_{xz}^2}\,\right] \; , \\
c_{yz} &= \frac{1}{\alpha}\left[\frac{-D_{xx}}{2} + \sqrt{\frac{\left(D_{yy} - D_{zz}\right)^2}{4} + D_{yz}^2}\,\right] \; , \\
c_{\text{CS}} &\equiv \text{Max}\;\left[1, c_{xy}, c_{xz}, c_{yz}\right] \; ,
\end{aligned}$$

where c_{CS} is the value of c that will satisfy all of the Cauchy-Schwarz conditions.

If we stop here and simply define our final c value to be the maximum of c_{diag} and c_{CS}, then it is still possible for the determinant or cubic constraint to be violated. The determinant of $\mathbf{R}$ can be expressed as

$$\begin{aligned}
\begin{vmatrix} R_{xx} & R_{xy} & R_{xz} \\ R_{xy} & R_{yy} & R_{yz} \\ R_{xz} & R_{yz} & R_{zz} \end{vmatrix} &= R_{xx}\begin{vmatrix} R_{yy} & R_{yz} \\ R_{yz} & R_{zz} \end{vmatrix} - R_{xy}\begin{vmatrix} R_{xy} & R_{yz} \\ R_{xz} & R_{zz} \end{vmatrix} + R_{xz}\begin{vmatrix} R_{xy} & R_{yy} \\ R_{xz} & R_{yz} \end{vmatrix} \\
&= R_{xx}R_{yy}R_{zz} + 2R_{xy}R_{xz}R_{yz} - R_{xx}R_{yz}^2 - R_{yy}R_{xz}^2 - R_{zz}R_{xy}^2 \; .
\end{aligned} \tag{11}$$

If we substitute in the relations that

$$\begin{aligned} R_{\beta\beta} &= \alpha - \frac{1}{c} D_{\beta\beta} \\ R_{\beta\gamma} &= -\frac{1}{c} D_{\beta\gamma} \, , \end{aligned}$$

use a little algebra and the fact that $D_{ii} = 0$, we can show that the cubic constraint becomes

$$x^3 - xp + q \geq 0 \, , \tag{12}$$

where p, q, and x are defined as

$$\begin{aligned} p &= \left[D_{yy}^2 + D_{zz}^2 + D_{yy} D_{zz} + D_{xy}^2 + D_{xz}^2 + D_{yz}^2 \right] \\ q &= \left[D_{xx} D_{yz}^2 + D_{yy} D_{xz}^2 + D_{zz} D_{xy}^2 - D_{xx} D_{yy} D_{zz} - 2 D_{xy} D_{xz} D_{yz} \right] \\ x &= \alpha c \, . \end{aligned}$$

The three roots to the cubic, which we will denote by x_0, x_+ and x_- can be calculated by

$$x_0 = S_+ + S_- \tag{13}$$

$$x_\pm = -\left[\frac{1}{2} x_0 \pm i \frac{\sqrt{3}}{2} (S_+ - S_-) \right] \, . \tag{14}$$

To determine the values for $S_\pm$, we first need to compute the quantities ϕ, and d^2 given by

$$\begin{aligned} \phi &\equiv \frac{1}{4} q^2 - \frac{1}{27} p^3 \\ d^2 &= |\phi| \, . \end{aligned}$$

If $\phi \geq 0$, then $S_\pm$ is straightforward and is given by

$$S_\pm = \sqrt[3]{-\frac{q}{2} \pm d} \, ,$$

and the root of interest is x_0. The expression for x_0 takes the form of

$$x_0 = \sqrt[3]{-\frac{q}{2} + d} + \sqrt[3]{-\frac{q}{2} - d} \, . \tag{15}$$

If $\phi < 0$, then the roots are all real, but $S_\pm$ is complex and is given by

$$\begin{aligned} S_\pm &= \sqrt{\frac{p}{3}} \, e^{i\theta} \\ \theta &= \frac{1}{3} \arctan \frac{-2d}{q} \, . \end{aligned}$$

Now that we have $S_\pm$, some algebra will give the three roots as

$$x_0 = 2 \sqrt{\frac{p}{3}} \, \cos\theta \tag{16}$$

$$x_\pm = \sqrt{\frac{p}{3}} \, \left(-\cos\theta \pm \sqrt{3} \sin\theta \right) \, . \tag{17}$$

To see which of the three roots is the largest, we can set 3θ equal to 0, $\pi/2$, and π respectively. The solutions are

$$
\begin{aligned}
x_0 &= \sqrt{\frac{p}{3}}\left(2, \sqrt{3}, 1\right) \\
x_+ &= \sqrt{\frac{p}{3}}\left(-1, 0, 1\right) \\
x_- &= \sqrt{\frac{p}{3}}\left(-1, -\sqrt{3}, -2\right) .
\end{aligned}
$$

Therefore, whether ϕ is positive or negative, the only root that needs to be tested is x_0. If we let c_{cubic} denote the constant that comes from the cubic constraint, then we have

$$
c_{\text{cubic}} = \text{Max}\left[1, \frac{x_0}{\alpha}\right] . \tag{18}
$$

Finally, the value for c that will satisfy all the constraints is given by

$$
c = \text{Max}\left[c_{\text{diag}}, c_{\text{cs}}, c_{\text{cubic}}\right] . \tag{19}
$$

5 Examples

In this section we give some examples of tensors that violate one or more of the constraints needed for positive semi-definiteness and show what the values are for c_{diag}, c_{cs}, and c_{cubic}. For all the examples given, we will keep $R_{ii} = 60$. Consider the stress tensor given by

$$
\begin{aligned}
R_{xx} &= -10 \\
R_{yy} &= 30 \\
R_{zz} &= 40 \\
R_{xy} &= R_{xz} = R_{yz} = 0 .
\end{aligned}
$$

For this relatively simple tensor, the only constraint that needs to be tested is the linear one, since all of the off-diagonal terms are zero. The value for c_{diag} is 1.5 and thus the viscosity will be multiplied by $c^{-1} = .667$.

Now consider the more complicated tensor given by

$$
\begin{aligned}
R_{xx} &= -10 \\
R_{yy} &= 30 \\
R_{zz} &= 40 \\
R_{xy} &= 2\sqrt{R_{xx}R_{yy}} \\
R_{xz} &= -\sqrt{10 R_{xx}R_{zz}} \\
R_{yz} &= .3\sqrt{R_{yy}R_{zz}} .
\end{aligned}
$$

Here, multiple tensor constraints are violated. The c values are found to be as follows

$$
\begin{aligned}
c_{\text{diag}} &= 1.5 \\
c_{\text{cs}} &= 3.65 \\
c_{\text{cubic}} &= 4.28 .
\end{aligned}
$$

Therefore, for this tensor, the c value is 4.28 and the viscosity would need to be multiplied by $c^{-1} = .234$ in order to guarantee realizability.

As a third example, consider the tensor

$$\begin{aligned} R_{xx} &= 10 \\ R_{yy} &= 30 \\ R_{zz} &= 20 \\ R_{xy} &= .9\sqrt{R_{xx}R_{yy}} \\ R_{xz} &= -\sqrt{10R_{xx}R_{zz}} \\ R_{yz} &= .3\sqrt{R_{yy}R_{zz}}\ . \end{aligned}$$

Here the diagonal elements are well behaved, but the xz Cauchy-Schwarz and cubic constraints are violated. The calculated c values are

$$\begin{aligned} c_{\text{diag}} &= 1 \\ c_{\text{cs}} &= 2.5 \\ c_{\text{cubic}} &= 2.71\ . \end{aligned}$$

Therefore, the c value is 2.71, and the viscosity should be multiplied by $c^{-1} = .369$.

In all the examples given, we have observed that

$$c_{\text{diag}} \leq c_{\text{cs}} \leq c_{\text{cubic}}\ .$$

Since the diagonal constraint only involves the diagonal elements of the tensor (while the Cauchy-Schwarz constraint involves both diagonal and off-diagonal elements), it should not be too surprising that the Cauchy-Schwarz constraint is more restrictive. In fact, it is assumed when looking at Cauchy-Schwarz that the diagonals satisfy $R_{\beta\beta} \geq 0$. As for the cubic constraint, consider the expression for the determinant of the stress given by eq. 11. If we add and subtract $2R_{xx}R_{yy}R_{zz}$, we can express the determinant ($|\mathbf{R}|$) as

$$\begin{aligned} |\mathbf{R}| &= R_{xx}\left(R_{yy}R_{zz} - R_{yz}^2\right) + R_{yy}\left(R_{xx}R_{zz} - R_{xz}^2\right) + R_{zz}\left(R_{xx}R_{yy} - R_{xy}^2\right) \\ &+ 2\left(R_{xy}R_{xz}R_{yz} - R_{xx}R_{yy}R_{zz}\right)\ . \end{aligned} \tag{20}$$

Thus, from the first 3 terms on the right hand side of eqn. 20, we observe that it is not sufficient to satisfy just the diagonal and the quadratic constraints. That is, there are still additional terms in the determinant that must be considered to satisfy the cubic constraint.

6 Simplifications for RZ Problems

Although we have considered how to guarantee realizability of the stress tensor for a general XYZ-geometry, we sometimes work in a 2D RZ-geometry where the velocity in the θ-direction is zero. Basically, this means that $R_{r\theta}$ and $R_{\theta z}$ are both identically zero. Be careful not to set the $\theta\theta$-component of the strain rate tensor to zero, as this component can be shown to depend on the radial velocity.

For an RZ-geometry, the linear constraint becomes

$$c_{\text{diag}} = \text{Max}\left[1, \frac{D_{rr}}{\alpha}, \frac{D_{\theta\theta}}{\alpha}, \frac{D_{zz}}{\alpha}\right]\ . \tag{21}$$

The Cauchy-Schwarz constraint becomes

$$c_{rz} = \frac{1}{\alpha}\left[\frac{-D_{\theta\theta}}{2} + \sqrt{\frac{(D_{rr}-D_{zz})^2}{4} + D_{rz}^2}\right] , \quad (22)$$

$$c_{\text{cs}} \equiv \text{Max } [1, c_{rz}] . \quad (23)$$

Finally, the cubic constraint becomes

$$x^3 - xp + q \geq 0 ,$$

where p, q, and x are defined as

$$\begin{aligned} p &= \left[D_{\theta\theta}^2 + D_{zz}^2 + D_{\theta\theta}D_{zz} + D_{rz}^2\right] \\ q &= \left[D_{\theta\theta}D_{rz}^2 - D_{rr}D_{\theta\theta}D_{zz}\right] \\ x &= \alpha c . \end{aligned}$$

The largest root, x_0 is calculated by

$$x_0 = S_+ + S_- , \quad (24)$$

where to calculate $S_\pm$, we must first compute ϕ and d^2. These quantities are determined by

$$\begin{aligned} \phi &\equiv \frac{1}{4}q^2 - \frac{1}{27}p^3 \\ d^2 &= |\phi| . \end{aligned}$$

If $\phi \geq 0$, then $S_\pm$ is straightforward and is given by

$$S_\pm = \sqrt[3]{-\frac{q}{2} \pm d} .$$

This leads to the root of interest as

$$x_0 = \sqrt[3]{-\frac{q}{2} + d} + \sqrt[3]{-\frac{q}{2} - d} . \quad (25)$$

If $\phi < 0$, then we compute $S_\pm$ by

$$\begin{aligned} S_\pm &= \sqrt{\frac{p}{3}}\ \exp i\theta \\ \theta &= \frac{1}{3}\arctan\frac{-2d}{q} , \end{aligned}$$

which leads to the root x_0 of

$$x_0 = 2\sqrt{\frac{p}{3}}\ \cos\theta . \quad (26)$$

Thus, the constant required to satisfy the cubic constraint is

$$c_{\text{cubic}} = \text{Max } \left[1, \frac{x_0}{\alpha}\right] . \quad (27)$$

Finally, the value for c that will satisfy all the constraints is given by

$$c = \text{Max } \left[c_{\text{diag}}, c_{\text{cs}}, c_{\text{cubic}}\right] . \quad (28)$$

7 Conclusions

This report has described a general, robust method due to Chuck Cranfill for ensuring that the Boussinesq model for the turbulent variable density Reynolds stress tensor is always positive semi-definite (non-negative definite). The method uses a single constant or scale factor to keep the deviatoric part of the stress tensor well behaved, without changing the turbulent pressure part of the tensor. It should be kept in mind that this method does not address the accuracy or appropriateness of the Boussinesq approximation in the first place. That topic can be addressed by comparing components of the modeled tensor to the analagous stress correlations that come from high quality 3D DNS or experimental data.

This report is really dealing with the fact that while the prevalent Boussinesq model for the stress tensor in the literature is symmetric, it does not guarantee (even for statistically 1D problems) that the 3 eigenvalues associated with the stress tensor will remain greater than or equal to zero as the turbulent flow evolves. When there are regions of the flow that contain strong compressions or rarefactions (or noisy velocity gradients), it is more likely for the tensor to suffer from realizability problems.