

# Balance Equations in Finite-Volume Large-Eddy Simulations

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## Abstract

Rigorous methods are presented for the derivation of all terms in the equations for the Reynolds stresses and dissipation components, from finite-volume large-eddy simulations of turbulence performed on staggered meshes. The methods are designed to produce exact balance to machine accuracy in the computed budgets, and yield a single term representing the statistical convergence error for each computed budget. Aspects of these budgets are presented for boundary-layer simulations, demonstrating the utility of the method.

## 1 Introduction

### 1.1 Finite-volume large-eddy simulations

The use of the finite-volume method for large-eddy simulations goes back as far as the original simulations of Smagorinsky (1963). The methods were formalised by Arakawa (1963), Lilly (1965) and Bryan (1966), and taken up by Deardorff (1970) and Schumann (1975) in early large-eddy simulation studies, but fell into disfavour as the spectral approach of Orszag (1971) appeared more accurate for fundamental studies and direct numerical simulations. Finite-volume methods continued to be used in Europe up to the present for large-eddy simulation, and are currently returning to favour as a flexible and economic means of simulating flows in complex

industrial and environmental geometries. The strongly conservative nature of the discretisation is supported by findings in dynamical systems simulation, where the embedding of analytic conservation properties in the numerical algorithms is frequently found to be more important than formal accuracy for veracity in predicting the statistical properties of chaotic attractors.

The present paper focusses on the popular linear finite-volume method on a staggered mesh, for incompressible simulations. The method conserves momentum to machine accuracy volume by volume, and conserves mass to a level determined by the pressure solution accuracy — in the optimal case of a well-conditioned pressure problem solved by a direct algorithm, to the same accuracy as the momentum. Using the interpolation formulae of Bryan (1966) in the advection term, the method also conserves each component ( $u^2$ ,  $v^2$  and  $w^2$ ) of kinetic energy and hence also the total flow kinetic energy to the same accuracy in this term, thus ensuring that the removal of energy from the simulation takes place via the discrete approximation to the viscous term. This mimics a fundamental property of the analytic Navier-Stokes equations.

## 1.2 Computing budgets

Large-eddy simulations (LES) and direct numerical simulations (DNS) are increasingly being used as sources of information for the calibration, analysis and reconstruction of closure models of turbulent and transitional flows. This activity is becoming an important justification for performing LES and DNS as industry moves towards second-moment closures as the standard design and research tool in turbulence. Vital as physical experiments are, they usually cannot provide any information on the crucial pressure-velocity correlations, and the use of a validated LES or DNS is a most powerful weapon in creating closures, either at the eddy-viscosity or second-moment levels, that are firmly rooted in the physics of the flows.

The majority of the current work in deriving budgets from simulations has utilised spectral simulations (Mansour *et al.* 1989; Rodi and Mansour, 1993; Kessler, 1993) in which the accuracy of the spectral approximations for derivatives are relied upon to provide the terms in the budget equations. Very little work has been done along these lines using finite-volume methods; it is the purpose of the present paper to give in full for the first time methods for the derivation of rigorous budgets for Reynolds stress,  $k$  and  $\epsilon$ , from staggered-mesh finite-volume simulations.

Simulations carried out on staggered meshes have the disadvantage that computations of many higher-order statistical quantities are at best ambiguous, and at worst may be misleading. Each velocity component is defined as a volume or surface aver-

age on a different face of the mesh, while the pressure is a volume average at the cell centre, Figure 1. Cross-products of the velocity components or of velocity with the pressure are not straightforward to define. To make matters worse, simple analytic identities fail to carry over into the finite-volume discretisation, so that even the definitions of certain terms becomes ambiguous. The time discretisation necessary for carrying out a time-dependent simulation of turbulence also creates a similar problem.

The remainder of this paper presents an approach to the resolution of these problems. A rigorous method for the definition of a statistically convergent budget is presented, followed by the discrete equations that may be used to deal consistently and unambiguously with the spatial interpolations and differencing.

## 2 Analytical Budgets

### 2.1 Notation

The incompressible Navier-Stokes equations are written

$$\begin{aligned} \partial_i U_i + \partial_k U_k U_i + \partial_i P - \nu \partial_k S_{ik} &= 0 \\ \partial_i U_i &= 0, \end{aligned} \tag{1}$$

where the summation convention is assumed,  $\partial$  represents a partial derivative,  $P$  is the physical pressure divided by density, and  $S_{ik}$  is the strain rate (with no factor of 1/2),

$$S_{ik} = \partial_i U_k + \partial_k U_i. \tag{2}$$

In this paper capitals are used for the total instantaneous quantities, lower case symbols for fluctuating parts of the dynamical variables and overbars for the time-average values:

$$U_i = \overline{U}_i + u_i. \tag{3}$$

In this notation the fluctuating Reynolds stress is written  $\overline{u_i u_j}$ .

The addition of the symmetrising term obtained by exchanging  $i$  and  $j$  subscripts is a common feature affecting every term in the budget equations. It is denoted  $+i \leftrightarrow j$ , which means that to the preceding term or terms is added a similar term or terms with  $i$  and  $j$  subscripts interchanged.

## 2.2 The Reynolds stress budget

We shall review the familiar process by which the budget equation for the fluctuating Reynolds stress is derived, focussing on those aspects which are of special concern in this study. We take the incompressible Navier-Stokes equations (1) and write down equations for the time average immediately:

$$\begin{aligned}\partial_t \overline{U}_i + \partial_k \overline{U}_i \overline{U}_k + \partial_i \overline{P} - \nu \partial_k \overline{S}_{ik} &= 0. \\ \partial_i \overline{U}_i &= 0\end{aligned}\tag{4}$$

The equations for the fluctuations  $u_i$  are found by subtraction:

$$\begin{aligned}\partial_t u_i + \partial_k (U_i U_k - \overline{U}_i \overline{U}_k) + \partial_i p - \nu \partial_k s_{ik} &= 0 \\ \partial_i u_i &= 0\end{aligned}\tag{5}$$

The fundamental principle allowing precisely balanced budgets to be derived from numerical simulations of turbulence is that every budget is based on the equations (5). The simulation itself must advance in time using some discrete analogue of (1), and the steps leading to (5) must remain valid for the time-averaging procedure used. Subsequent operations leading to a budget, whether of Reynolds stress, kinetic energy or a dissipation component, must be such as to preserve the zero sum on the right hand side of (5), guaranteeing a budget balanced to machine accuracy.

The equation for the fluctuating stress is derived by multiplying the above momentum equation for  $u_i$  by  $u_j$ . To this is added  $u_i$  times a corresponding equation for  $u_j$ , giving an equation for the evolution of  $u_i u_j$  that is symmetric in  $i$  and  $j$ . For instance for the time derivative term itself,

$$u_i \partial_t u_j + u_j \partial_t u_i = \partial_t (u_i u_j).\tag{7}$$

By definition of a time average, this term tends to zero in the mean of a statistically stationary process,

$$\overline{\partial_t (u_i u_j)} \rightarrow 0,\tag{8}$$

as the number of samples tends to infinity. A finite sample will always be used in a real simulation, so we can at best expect the average of this term to reduce as we increase the sample size, and its magnitude is used as a measure of the convergence of the statistics. However, all the other steps used above to derive equations for the average and fluctuating parts are valid even when the sample size is finite.

We now proceed as outlined, multiplying by  $u_j$  and symmetrising the indices  $i$  and  $j$ , to obtain

$$u_j \partial_t u_i + u_j \partial_k (U_i U_k - \overline{U}_i \overline{U}_k) + u_j \partial_i p - \nu u_j \partial_k s_{ik} + i \leftrightarrow j = 0.\tag{9}$$

Time averaging this equation yields the budget for the fluctuating Reynolds stress. In the following sections the overbar indicating the accumulation of this final time average is omitted, the equations being given for the terms that contribute to the sum. Nevertheless, terms that are precisely zero in a full average, such as  $\overline{U}_i u_j$ , are dropped from the budget.

The terms in equation (9) are normally rearranged to obtain a form in which each term has a straightforward physical interpretation in the time average. Using the definition (3) we expand the nonlinear term in (9). Making use of the incompressible continuity relation for both  $u_k$  and  $\overline{U}_k$ , and dropping the term in  $\overline{U}_i \overline{U}_k$  which does not contribute to the time average even for a finite sample size, we obtain

$$u_j \partial_k (\overline{U}_i u_k + u_i \overline{U}_k + u_i u_k) + i \leftrightarrow j = u_j u_k \partial_k \overline{U}_i + i \leftrightarrow j + \overline{U}_k \partial_k (u_i u_j) + \partial_k (u_i u_j u_k). \quad (10)$$

These are the familiar production, convection and turbulent transport terms for the fluctuating Reynolds stress. In deriving the terms on the right hand side it is most important to note the frequent use of the continuity condition and the identity for the derivative of a product, for these very natural analytic procedures do not generalise to the finite-volume form of the equations.

The pressure term is normally rearranged as

$$u_j \partial_i p + i \leftrightarrow j = \partial_i (u_j p) + i \leftrightarrow j - p s_{ij}, \quad (11)$$

once more using the identity for the derivative of a product. The first term is called the pressure diffusion, the second is the pressure strain. The viscous term is similarly rearranged as

$$\begin{aligned} -\nu u_j \partial_k s_{ik} + i \leftrightarrow j &= -\nu u_j \partial^2 u_i + i \leftrightarrow j \\ &= -\nu \partial_k (u_j \partial_k u_i) + i \leftrightarrow j + 2\nu \partial_k u_j \partial_k u_i \\ &= -\nu \partial^2 (u_i u_j) + 2\nu \partial_k u_i \partial_k u_j. \end{aligned} \quad (12)$$

The first of these terms is the viscous diffusion of stress; the second is the viscous dissipation tensor,  $\epsilon_{ij}$ .

The terms contributing to the fluctuating Reynolds stress budget are:

Production	$u_j u_k \partial_k \overline{U}_i + i \leftrightarrow j$
Convection	$\overline{U}_k \partial_k (u_i u_j)$
Turbulent transport	$\partial_k (u_i u_j u_k)$
Pressure diffusion	$\partial_i (u_j p) + i \leftrightarrow j$
Pressure strain	$-p s_{ij}$
Viscous diffusion	$-\nu \partial^2 (u_i u_j)$
Viscous dissipation	$2\nu \partial_k u_i \partial_k u_j$
Residual error	$\partial_t (u_i u_j)$

The budget for the dissipation rate tensor is derived in a similar manner, but since no additional principles are involved for our purposes the reader is referred to standard texts for details.

## 2.3 The kinetic energy budget

The turbulence kinetic energy  $k$  is  $u_i u_i / 2$ , with summation over  $i$ , often denoted  $u^2 / 2$ . The individual contributions  $u_1^2$ ,  $u_2^2$  and  $u_3^2$  to  $k$  are called the turbulence intensities and their time averages are the diagonal components of the fluctuating Reynolds stress tensor.

Individual budgets for each diagonal stress therefore exist and are obtained by setting  $i = j$  in the corresponding term of the Reynolds stress budget. The terms when accumulated in a time average give the budget for individual intensities if *not* summed over  $i$ . (There is summation over  $k$ ). With summation over  $i$  also, and dividing each term by 2, we get the terms of the budget of  $k$ . In the latter case the pressure strain obviously vanishes by continuity. Note that the expression  $u^2 = u_i u_i$  (summed) is only equal to  $2k$  in the average in the convection term. The turbulence transport involves triple products of fluctuations. The viscous dissipation of  $k$  is

$$\epsilon = \epsilon_{ii} / 2 = \nu (\partial_k u_i)^2 \quad (13)$$

which is positive definite and represents a drain of energy.

## 3 The Triple-Step Method

### 3.1 Principles

The attainment of a balance of terms in budgets for Reynolds stress, energy and dissipation depends on the fundamental identity, used in equation (7):

$$a \partial_t b + b \partial_t a = \partial_t (ab). \quad (14)$$

Unfortunately this elementary piece of mathematics fails to generalise to discretised time,

$$\begin{aligned} a \delta_t b + b \delta_t a &= a \frac{b^{n+1} - b^n}{\Delta t} + b \frac{a^{n+1} - a^n}{\Delta t} \\ &\neq \delta_t (ab) = \frac{a^{n+1} b^{n+1} - a^n b^n}{\Delta t}, \end{aligned} \quad (15)$$

unless the undefined  $a$  and  $b$  factors are replaced by

$$\begin{aligned} a^C &= \frac{a^{n+1} + a^n}{2} \\ b^C &= \frac{b^{n+1} + b^n}{2}. \end{aligned} \quad (16)$$

The  $n$  and  $n+1$  superscripts index the time step. The method uniquely re-establishes the identity (14) in the form

$$a^C \delta_t b + b^C \delta_t a = \delta_t(ab). \quad (17)$$

The average of this quantity will tend towards zero with increasing number of statistical samples  $N$  of a stationary process.

We can now create budgets of Reynolds stress, turbulence energy and dissipation rate from the simulation variables that are strictly analogous to those derived analytically. For instance, consider the simplest example of the budget for  $u_i^2$ . We take the time-discrete equation for the fluctuation velocity  $u_i$ ,

$$\delta_t u_i = -\partial_i p - \partial_k (U_k U_i - \overline{U_k U_i})^X + \nu \partial_k s_{ik}^X \quad (18)$$

No superscript is used for the pressure since it is treated by the method of Gavrilakis (1992) in our simulations, though the principles outlined here extend straightforwardly to other pressure treatments, for instance Crank-Nicolson. The remaining terms take an  $X$  superscript indicating the explicit formula used for their time advancement. The equation is multiplied by  $u_i^C$  (with no summation over  $i$ ):

$$u_i^C \delta_t u_i = \delta_t u_i^2 = -u_i^C [-\partial_i p - \partial_k (U_k U_i - \overline{U_k U_i})^X + \nu \partial_k s_{ik}^X] \quad (19)$$

The accumulated time average of this combination must tend toward zero because the time average of

$$\delta_t u_i^2 = \frac{(u_i^{n+1})^2 - (u_i^n)^2}{\Delta t} \quad (20)$$

tends to zero, provided  $u_i^2$  in the simulation does not drift systematically over the period the statistics are accumulated: that is, provided the simulation is statistically stationary.

To compute the terms on the right hand side, it is necessary to reconstruct the individual acceleration terms at all the time steps involved in the explicit formulae and multiply them by  $u_i^C$ , which requires  $u_i$  at steps  $n$  and  $n+1$ . For example, for a second order explicit formula, it should be evident that we need (i) average velocity components and pressure (and temperature in the case of a thermal simulation); (ii) fluctuating velocities (and temperatures) at steps  $n-1$ ,  $n$  and  $n+1$ ; (iii) the

fluctuating pressure  $p$  used in moving from step  $n$  to step  $n + 1$ . The velocities (and temperature) are therefore stored at three adjacent time steps and the pressure at one for each of the  $N$  samples. The averages of the  $N$  samples are found first and stored. The data is then scanned, the average being subtracted to get the fluctuating parts, and the term that is sought is constructed as the product of a  $C$ -superscript variable with an  $X$ -superscript combination representing part of the acceleration. This technique has been dubbed the triple-step method for computing terms in budgets.

### 3.2 The Reynolds stress budget

We give the explicit form of the above ideas for the budget of  $u_i u_j$ . Overbars for the final averaging are omitted.

$$\begin{aligned}\delta_t(u_i u_j) &= u_i^C \delta_t u_j + i \leftrightarrow j \\ &= u_i^C (-\partial_j p - \partial_k (U_k U_j - \overline{U_k U_j})^X + \nu \partial_k s_{jk}^X) + i \leftrightarrow j.\end{aligned}\quad (21)$$

Both sides of this equation tend to zero in the limit of sufficiently extended samples of a statistically stationary simulation. Exactly as in the analytic derivation of budgets, the time average of the term

$$u_i^C \partial_k \overline{U_k U_j}^X \quad (22)$$

is identically zero, as is the part

$$u_i^C \partial_k \overline{U_k}^X \overline{U_j}^X \quad (23)$$

of the triple term, because  $u_i^C$  is calculated in such a way that its average is zero. The remaining nonzero terms are:

Production	$u_i^C \partial_k (u_k \overline{U_j})^X + i \leftrightarrow j$
Convection	$u_i^C \partial_k (\overline{U_k} u_j)^X + i \leftrightarrow j$
Turbulent transport	$u_i^C \partial_k (u_k u_j)^X + i \leftrightarrow j$
Pressure work	$u_i^C \partial_j p + i \leftrightarrow j$
Viscous work	$-\nu u_i^C \partial_k s_{jk}^X + i \leftrightarrow j$
Residual error	$\delta_t(u_i u_j)$

Note that the pressure and viscous terms are not separated into the standard forms used in the analytic budget, since the discrete spatial differentiation can make such manipulations approximate. For similar reasons, the production, mean convection



and turbulent transport terms are not rearranged in any way using the continuity equation.

To summarise, the time-discrete budgets are computed by the use of a triple-step database obtained from a simulation that is second-order accurate in time. The database consists of a sequence of fields at steps  $n - 1, n$  and  $n + 1$ , allowing the subsequent recomputation of the accelerations used to advance the velocities, and the products of these terms with the combination

$$u_i^C = (u_i^{n+1} + u_i^n)/2. \quad (24)$$

In order to extract the standard production, convection, and turbulent transport terms, we recompute the nonlinear terms in three parts, with the velocities being split into mean and fluctuating parts.

### 3.3 Interpolation and differencing

The triple-step method for budgets deals with those problems arising from time-stepping in defining a proper balance. It says nothing about the space discretisation, but does imply that the precise forms of spatial interpolation and differencing used to compute accelerations during the simulation should also be used when computing the  $X$ -superscript terms for the budgets.

The general form of a term in a discrete budget equation using the triple-step method is

$$u_i^C a_j + i \leftrightarrow j, \quad (25)$$

where  $a_j$  is an acceleration term derived exactly as it was during the simulation. For instance in the transport term

$$u_i^C \partial_k (u_k u_j)^X + i \leftrightarrow j, \quad (26)$$

the second factor must be computed by the same explicit scheme is used in the simulation, and the interpolations of  $u_k$  and  $u_j$  must be exactly the same as those used for  $U_k$  and  $U_j$  in the simulation.  $\partial_k$  must also be replaced by the difference operation  $\delta_k$  used in the simulation. The separation of mean and fluctuating velocity components makes no difference to these requirements. From this point, the notation  $\delta_k$  is used for the appropriate difference operation rather than the analytic derivative.

### 3.4 Interpolation of stresses

For the three cases where  $i = j$ , the velocity  $u_i^C$  and the acceleration  $a_i$  are defined at the same point on the staggered mesh (the  $i$  face) and the product will naturally be computed there. Thus we compute the budget terms for the diagonal stresses at the same position on the mesh as the diagonal stresses themselves —  $u_i^2$  on the  $i$  face and similarly for the other two components.

For the off-diagonal stresses, the velocity factor  $u_i^C$  and the acceleration terms  $a_j$  are defined at different points on the staggered mesh. In spite of this, the balance will be exactly obtained in the limit of a large enough sample when the two factors are interpolated to a common edge, Figure 2, in a consistent way before being multiplied together.

Suppose we interpolate the velocities  $u_i^C$  in the  $j$  direction to obtain interpolated velocities denoted  $v_i^C$ , and all the acceleration terms  $a_j$  consistently in the  $i$  direction to obtain interpolated accelerations denoted by  $b_j$ . Since the  $b$  terms are simple linear combinations of the accelerations actually used in the simulation, they are equal to the time rate of change of the corresponding velocity component  $u_j$ , interpolated in the same way in the  $j$  direction, denoted  $w_j$ .

Thus the sum of all the products will be

$$v_i^C \delta_t b_j = (v_i^{n+1} + v_i^n)(w_j^{n+1} - w_j^n)/2\Delta t . \quad (27)$$

We now must add the symmetrising term denoted by  $i \leftrightarrow j$ . However, the  $u_i$  component will still be interpolated in the  $j$  direction to obtain  $v_i$ , and the  $u_j$  component interpolated in the  $i$  direction to obtain  $w_j$ ; thus the symmetrised expression computed must be

$$\begin{aligned} v_i^C \delta_t b_j + i \leftrightarrow j &= [(v_i^{n+1} + v_i^n)(w_j^{n+1} - w_j^n) + (w_j^{n+1} + w_j^n)(v_i^{n+1} - v_i^n)]/2\Delta t \\ &= (v_i^{n+1} w_j^{n+1} - v_i^n w_j^n)/\Delta t \\ &= \delta_t(v_i w_j) . \end{aligned} \quad (28)$$

This is exactly what we require: the time rate of change of an off-diagonal stress interpolated to the  $ij$  cell edge in any way we choose. Clearly, for consistency with the computed mean off-diagonal stresses and with the simulation dynamics, the interpolation method should be exactly that used for the velocities in the simulation when computing the nonlinear stress terms.

### 3.5 Splitting the pressure term

The separation of the pressure work into pressure diffusion and pressure strain (and the similar separation of the viscous work into viscous diffusion and dissipation) is rather more tricky. The analytic separation,

$$u_i \partial_j p + i \leftrightarrow j = \partial_j(u_i p) + i \leftrightarrow j - p s_{ij} , \quad (29)$$

does not generalise straightforwardly to the discrete representation on a staggered mesh. To do so,  $u_i$  and  $p$  would have to be defined at the same points in the first term on the right hand side, while  $u_i$  on the left hand side (and  $p$  in the other term likewise) have to be special unweighted interpolations of these for the identity to hold. None of these requirements can be met easily on a staggered mesh.

To retain the discretised stress balance, it is vital that the left-hand-side product is computed exactly as the triple-step method demands, namely

$$u_i^C \delta_j p + i \leftrightarrow j . \quad (30)$$

The two terms which we wish to extract must sum to give the pressure work in precisely this form, otherwise the stress budget will no longer balance. The only way to do this is to compute the pressure work in the way demanded by the triple-step method to give the stress balance, compute separately the pressure strain in a sensible manner at the same point of the staggered mesh, and add the two to obtain the pressure diffusion term.

The computation proceeds as follows. For the diagonal terms,  $u_i^C \delta_i p$  is computed at the  $i$  face. The pressure strain  $-ps_{ii}^C$  is computed at the cell centre (guaranteeing that the summation over  $i$  will be zero by continuity) and is then interpolated in any way that is convenient to the  $i$  face. The diagonal diffusion terms are then computed as

$$2\delta_i(u_i p) = 2u_i^C \delta_i p + ps_{ii}^C . \quad (31)$$

The off-diagonal terms  $i \neq j$  must be interpolated like the velocities in the nonlinear terms in the simulation, as explained in the previous section, if they are to combine with all the other terms interpolated in the same way to give a stress balance. We proceed as in the previous section to obtain

$$u_i^C \delta_j p + i \leftrightarrow j \quad (32)$$

at the  $ij$  cell edge. The fluctuating strain rate  $s_{ij}$  is also naturally computed at the  $ij$  edge. The pressure is interpolated from the centre to this edge in any way we choose, to give the pressure strain  $-ps_{ij}$ , and the off-diagonal diffusion is finally computed as

$$\delta_j(u_i p) + i \leftrightarrow j = u_i^C \delta_j p + i \leftrightarrow j + ps_{ij}^C . \quad (33)$$

### 3.6 Splitting the viscous term

The analytic splitting of the viscous work,

$$-\nu u_i \partial_k s_{jk} + i \leftrightarrow j = -\nu u_i \partial^2 u_j + i \leftrightarrow j = -\nu \partial^2 (u_i u_j) + 2\nu \partial_k u_i \partial_k u_j, \quad (34)$$

is not easily reproduced on a discrete mesh, for reasons similar to those presented in the case of the pressure rearrangement. Once more, we seek a simple way to ensure that the terms finally output as representing the viscous diffusion and dissipation sum to the expression

$$-\nu u_i^C \delta_k s_{jk}^X + i \leftrightarrow j, \quad (35)$$

which must be interpolated in the way described in the preceding sections in order to guarantee the proper contribution to the overall stress balance. Each diagonal term must be computed on the correct face, and each off-diagonal term at the correct edge.

By analogy with the method proposed for the pressure terms, the sum should be computed in the manner described, with the acceleration  $\delta_k s_{jk}^X$  naturally being on the  $j$  face, as for the computation of the viscous terms in the simulation.  $u_i^C$  is computed on the  $i$  face. For the off-diagonal terms the interpolation of the two factors to the  $ij$  edge must be done consistently with all the other terms.

The following approach has been found in the analysis of real boundary layer simulations to give the most convincing dissipation profiles. The viscous diffusion terms for the diagonal stresses are computed using the discrete Laplacian  $\delta^2 u_i^2$  of each squared velocity fluctuation, on its own face. The viscous work is then subtracted to obtain the estimate for the diagonal components of the dissipation tensor:

$$\nu \delta^2 (u_i^2) - 2\nu u_i \delta_k s_{ik} = \epsilon_{ii}. \quad (36)$$

This method is successful in producing credible profiles of  $\epsilon$ , which is computed by interpolating the three diagonal dissipation components  $\epsilon_{ii}$  to the cell centre and summing. The method is extended to the off-diagonal components, with all interpolations being carried out in the standard manner:

$$\nu \delta^2 (u_i u_j) - (\nu u_i \delta_k s_{jk} + i \leftrightarrow j) = \epsilon_{ij}. \quad (37)$$

To keep strictly to the philosophy of the triple-step method, the viscous diffusion term should be computed as

$$\nu \delta_k (u_j^C \delta_k u_i^X + i \leftrightarrow j). \quad (38)$$

This represents an impossible complication on the staggered mesh, however, and since the splitting of the viscous work is necessarily spatially approximated, the term is simply computed as

$$\nu \delta^2 (u_i^n u_j^n), \quad (39)$$

using values at time step  $n$ .

### 3.7 The subgrid fluctuation term

The previous section has given an analysis of the work done by the constant molecular viscosity, and its splitting into viscous dissipation and diffusion terms. In a large-eddy simulation there is also a subgrid eddy-viscosity, whose contributions to the budget are similar to those given in the previous section. However, because an eddy-viscosity varies in magnitude in time and space, there is an additional small term whose computation must be included if a strictly balanced budget, to machine accuracy, is to be obtained. The analysis is given in terms of the simplest Smagorinsky (1963) model, though it applies equally well for the dynamic subgrid model of Germano *et al.* (1991) based on a Smagorinsky eddy-viscosity, or (with two sets of such terms) for a split eddy viscosity model like that of Schumann (1975).

The subgrid stress is normally computed as

$$\tau_{jk} = \tilde{\nu}_s S_{jk} , \quad (40)$$

where the eddy-viscosity  $\tilde{\nu}_s$  is spatially and temporally varying. The term appears in the momentum equation as

$$\delta_k \tau_{jk} = \delta_k (\tilde{\nu}_s S_{jk}) , \quad (41)$$

and hence in the fluctuating Reynolds stress budget in the form

$$u_i \delta_k (\overline{\nu}_s s_{jk}) + U_i \delta_k (\nu_s S_{jk}) + i \leftrightarrow j . \quad (42)$$

Note that we have split the total time-dependent eddy-viscosity  $\tilde{\nu}_s$  into its time average  $\overline{\nu}_s$  and fluctuating part  $\nu_s$ . The first term in the above equation mimics almost precisely the form for the molecular viscous work, the only difference being that since  $\overline{\nu}_s$  varies in space it cannot be extracted from the spatial difference. The term is split into subgrid diffusion and subgrid drain (the model dissipation) in much the same way as the molecular viscous work is split into diffusion and dissipation.

The second term in (42) is new, and arises because the eddy-viscosity has a fluctuating part  $\nu_s$ . It does not correspond to any term in the molecular viscous work, and is called the subgrid fluctuation term. The term could be further analysed into separate parts as

$$\overline{U}_i \delta_k (\nu_s s_{jk}) + u_i \delta_k (\nu_s \overline{S}_{jk}) + u_i \delta_k (\nu_s s_{jk}) + i \leftrightarrow j . \quad (43)$$

We do not distinguish these parts separately since the total term is very small in simulations at low Reynolds numbers; nevertheless it must be included in the budget if a machine-accurate balance is required.

In summary, the complete set of tensor terms computed by these methods from the analysis of a large-eddy simulation are as follows:

Production	$u_i^C \delta_k (u_k \overline{U}_j)^X + i \leftrightarrow j$
Convection	$u_i^C \delta_k (\overline{U}_k u_j)^X + i \leftrightarrow j$
Turbulent transport	$u_i^C \delta_k (u_k u_j)^X + i \leftrightarrow j$
Pressure diffusion	$u_i^C \delta_j p + i \leftrightarrow j + p s_{ij}^C$
Pressure strain	$-p s_{ij}^C$
Viscous diffusion	$-\nu \delta^2 (u_i^n u_j^n)$
Viscous dissipation	$\nu \delta^2 (u_i^n u_j^n) - (\nu u_i^C \delta_k s_{jk}^X + i \leftrightarrow j)$
Subgrid diffusion	$-\overline{\nu}_s \delta^2 (u_i^n u_j^n)$
Subgrid drain	$\overline{\nu}_s \delta^2 (u_i^n u_j^n) - (u_i^C \delta_k (\overline{\nu}_s s_{jk})^X + i \leftrightarrow j)$
Subgrid fluctuation	$U_i^C \delta_k (\nu_s S_{jk})^X + i \leftrightarrow j$
Residual error	$\delta_t (u_i u_j)$

### 3.8 The dissipation budget

The analytic dissipation budget is derived in a manner formally similar to that used for the fluctuating stress budget. The definition of the dissipation tensor,

$$\epsilon_{ij} = 2\nu \delta_k u_i \delta_k u_j , \quad (44)$$

invites us to compute the budget in the form

$$\delta_t \epsilon_{ij} = \nu (\delta_k u_i^C \delta_k \delta_t u_j) + i \leftrightarrow j . \quad (45)$$

As noted, we do not compute the dissipation tensor in this way in the stress budget since the expression is difficult to compute on a staggered mesh, but as the difference between the viscous diffusion and the viscous work:

$$\nu \delta^2 (u_i^n u_j^n) - (\nu u_i^C \delta_k s_{jk}^X + i \leftrightarrow j) . \quad (46)$$

For subsequent developments, we need to use the discrete continuity condition on the fluctuating velocity

$$\delta_k u_k = 0 , \quad (47)$$

which is enforced on the flow fields to high accuracy at each timestep, to rewrite the viscous work using

$$\delta_k s_{jk}^X = \delta_k (\delta_j u_k + \delta_k u_j) = \delta^2 u_j \quad (48)$$

In the case of a large-eddy simulation, we wish to include the mean subgrid drain as part of the total dissipation budget, and therefore include the mean eddy-viscosity thus:

$$\nu_t \delta^2 (u_i^n u_j^n) - [u_i^C (\nu_t \delta^2 u_j)^X + i \leftrightarrow j] , \quad (49)$$

where

$$\nu_t = \nu + \overline{\nu}_s , \quad (50)$$

and no contribution to the dissipation is included from the subgrid eddy-viscosity variation in time or space.

For consistency, therefore, we derive a budget for the dissipation tensor as a difference between the budget for the viscous diffusion and that for the viscous work. The terms in the budget for the viscous diffusion are very simple to define since they are proportional to the discrete Laplacian of the corresponding terms in the stress budget:

$$\delta_t \nu_t \delta^2(u_i^n u_j^n) = \nu_t \delta^2(u_i^C \delta_t u_j + i \leftrightarrow j). \quad (51)$$

The acceleration  $\delta_t u_j$  is then replaced by each of the separate terms in the evolution equation for the velocity fluctuation to obtain the full budget.

The terms in the budget for the viscous work are hardly more difficult. We take the discrete rate of change of an instantaneous estimate for the viscous work,  $u_i^n (\nu_t \delta^2 u_j)^n + i \leftrightarrow j$  and write

$$\begin{aligned} \delta_t(u_i \nu_t \delta^2 u_j) + i \leftrightarrow j &= u_i^C \nu_t \delta^2 \delta_t u_j + \nu_t \delta^2 u_j^C \delta_t u_i + i \leftrightarrow j \\ &= u_i^C \nu_t \delta^2 \delta_t u_j + \nu_t \delta^2 u_i^C \delta_t u_j + i \leftrightarrow j. \end{aligned} \quad (52)$$

It is then straightforward to substitute the terms contributing to  $\delta_t u_i$ , as in the fluctuating stress balance, with terms contributing to the acceleration  $a_j$ .

To give the complete budget for the dissipation it is convenient to define an operator  $\mathcal{D}_2$  which operates on a pair of fluctuating fields, the first being a velocity  $u_i$  and the second an acceleration  $a_j$ , to yield a component part of the dissipation tensor  $\epsilon_{ij}$  computed as in (46), thus:

$$\begin{aligned} \mathcal{D}_2[u_i, a_j] &\equiv \nu_t [\delta^2(u_i^C a_j^X) - u_i^C \delta^2 a_j^X - \delta^2 u_i^C a_j^X] + i \leftrightarrow j \\ &\approx \nu_t \delta_k u_i^C \delta_k a_j^X + i \leftrightarrow j \end{aligned} \quad (53)$$

The dissipation budget may then be summarised very concisely (omitting the symmetrising terms denoted  $i \leftrightarrow j$  for convenience):

Creation terms:	$\mathcal{D}_2[u_i^C, \delta_k(u_k \bar{U}_j)^X]$
Mean flow terms:	$\mathcal{D}_2[u_i^C, \delta_k(\bar{U}_k u_j)^X]$
Turbulence terms:	$\mathcal{D}_2[u_i^C, \delta_k(u_k u_j)^X]$
Pressure terms :	$\mathcal{D}_2[u_i^C, \delta_j p]$
Viscous terms:	$-\nu \mathcal{D}_2[u_i^C, \delta_k s_{jk}^X]$
Subgrid terms:	$-\mathcal{D}_2[u_i^C, \delta_k(\bar{\nu}_s s_{jk}^X)]$
Subgrid fluctuation:	$-\mathcal{D}_2[U_i^C, \delta_k(\nu_s S_{jk}^X)]$
Residual error:	$\delta_t \mathcal{D}_2[u_i, u_j]$

The description of the dissipation budget above is formally similar to that for the stress budget, with each term  $u_i^C a_j^X$  in the stress budget being replaced by a corresponding term  $\mathcal{D}_2[u_i^C, a_j^X]$  in the dissipation budget. The computation of the terms in the budget for a dissipation component  $\epsilon_{ij}$  is therefore easily effected by means of a subprogram that is passed  $u_i^C$  and  $a_j^X$  and computes the  $\mathcal{D}_2$  function. The terms listed often need to be split further, in order to bring the budget into the exact form derived from the analytical equations. The term denoted ‘creation’ above can be split into the so-called mixed production and part of the mean gradient production:

$$\mathcal{D}_2[u_i^C, \delta_k(u_k \bar{U}_j)^X] \approx \mathcal{D}_2[u_i^C, u_k^X] \delta_k \bar{U}_j^X + \mathcal{D}_2[u_i^C, \delta_k \bar{U}_j^X] u_k^X . \quad (54)$$

The ‘mean flow terms’ are the sum of the remaining production from the mean gradient and the mean convection of  $\epsilon_{ij}$ :

$$\mathcal{D}_2[u_i^C, \delta_k(\bar{U}_k u_j)^X] \approx \mathcal{D}_2[u_i^C, \bar{U}_k^X] \delta_k u_j^X + \mathcal{D}_2[u_i^C, \delta_k u_j^X] \bar{U}_k^X . \quad (55)$$

The ‘turbulence terms’ contain the turbulent production of  $\epsilon_{ij}$  and the turbulent transport:

$$\mathcal{D}_2[u_i^C, \delta_k(u_k u_j)^X] \approx \mathcal{D}_2[u_i^C, u_k^X] \delta_k u_j^X + \mathcal{D}_2[u_i^C, \delta_k u_j^X] u_k^X \quad (56)$$

The ‘pressure terms’ can be split into pressure strain and pressure diffusion:

$$\mathcal{D}_2[u_i^C, \delta_j p] \approx \delta_j \mathcal{D}_2[u_i^C, p] - \mathcal{D}_2[\delta_j u_i^C, p] , \quad (57)$$

and the ‘viscous terms’ into viscous diffusion and viscous decay of  $\epsilon_{ij}$ , using approximations identical to those used originally to separate  $\epsilon_{ij}$  itself in the stress budget:

$$-\nu \mathcal{D}_2[u_i^C, \delta_k s_{jk}^X] + i \leftrightarrow j \approx -\nu \delta^2 (\mathcal{D}_2[u_i^n, u_j^n]) + 2\nu \mathcal{D}_2[\delta_k u_i, \delta_k u_j] . \quad (58)$$

The various subgrid terms are not normally split, though further analysis is possible, and there is no splitting of the residual error. For all the terms in which further splitting is required, the left hand side representing the total term contributing to the budget is computed, guaranteeing the precise machine-accurate balance. The first term on the right hand side is then computed in the given form, and subtracted from the total term to give an approximation for the second term on the right.

We compute the diagonal components of  $\epsilon_{ij}$  at the velocity points on the cell faces. To find the budget of the scalar dissipation rate  $\epsilon = \epsilon_{ii}/2$ , the three diagonal components of every term in the budgets for  $\epsilon_{ii}$  are interpolated to the cell centre and added, in line with the method used for computing the terms in the  $k$  balance.



## 4 Application to Boundary Layers

### 4.1 Bypass transition

We show selected results from simulations which have been analysed using the methods of this paper. Elsewhere we have reported on the simulation of the pseudo-laminar boundary layer and bypass transition provoked by high levels of free stream turbulence (Yang and Voke, 1993; Voke and Yang, 1993) One simulation has been analysed in detail at four streamwise stations,  $Re_x = 16600, 29800, 62900,$  and  $129100$ , to extract the fluctuating stress budgets from 800 equally spaced triple-step samples gathered over a time period of  $12000\nu/u_\tau^2$ .

Figure 3 shows the balance of  $u'^2$  at the station  $Re_x = 129100$ . The residual error term  $\overline{\partial_i(u'v')}$ , arising from lack of statistical convergence, is indistinguishable from zero on the scale of the graph, its maximum value being 2% of the maximum of the production. The error term is more significant at some stations, but in these cases is clearly associated with an equal and opposite deviation in the convection term. One of the worst cases is shown in Figure 4. Even without the evidence of the error term, one would suspect poor statistical convergence of the convection term, owing to its deviation from expected physical behaviour. Since the error term clearly points to its lack of convergence, it is possible to combine these terms, giving a balance instead for the combination

$$u_i\delta_k(\overline{U_k u_j}) + i \leftrightarrow j + \delta_i(u_i u_j) , \quad (59)$$

which may be taken to represent the average of the material derivative of the fluctuating stress,

$$\frac{Du_i u_j}{Dt} . \quad (60)$$

The resulting budget is shown in Figure 5. The slow convergence of the convection term in comparison with other terms in the stress budget is assumed to arise from the non-Gaussian nature of its distribution.

In other equations where the error term was non-negligible (it is generally much smaller than in the case in Figure 4) an association with a deviation of the convection term from expectations is also suspected: we therefore combine the error term into the convection for all data from this simulation. Other terms arising from the subgrid eddy-viscosity in this simulation are so much smaller than those shown that they are safely omitted from the figures.

## 4.2 A tripped boundary-layer

One of us has simulated a boundary layer forced rapidly into turbulence by a solid physical trip at  $Re_x = 33000$  closely similar to those used by experimentalists. The resulting large-eddy simulation is compared with a parallel experiment of an identical boundary layer conducted in conjunction with the computation, and extending into the near wake of the 1mm thick plate. Details of the methods and results will be reported elsewhere; here we focus on the budgets extracted from the simulation.

Budgets at six stations in the boundary layer downstream of the trip have been obtained using the methods of this paper. The budgets are based on 400 samples extending over  $0.8\delta/u_\tau$ , which is found to be sufficient time to obtain very convincing intensity and kinetic energy budgets. Figure 6 shows the budget of  $k$  at  $Re_x = 172000$ . The statistical error is very small for this budget. It is found that the budget of  $\epsilon$  remains poorly converged with this number of samples, indicating that a much longer sampling time may be required to obtain a good dissipation budget. As before, the convection term clearly contains most of the statistical error, but the combination of the error with the convection term results in an unconvincingly large net convection owing to residual statistical error from other terms in the dissipation budget. Budgets of intensities, Reynolds stresses and kinetic energy have also been computed at five other stations in the boundary layer, and at four stations in the symmetric wake. These results will be reported elsewhere.

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# Figure Captions

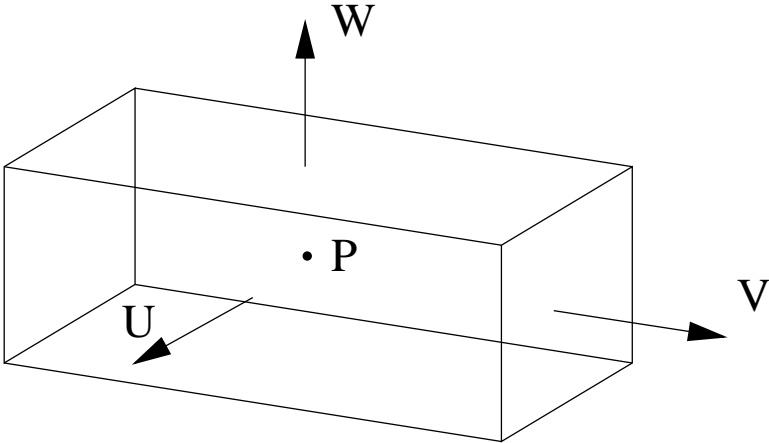


Figure 1. Geometry of a staggered mesh control volume.

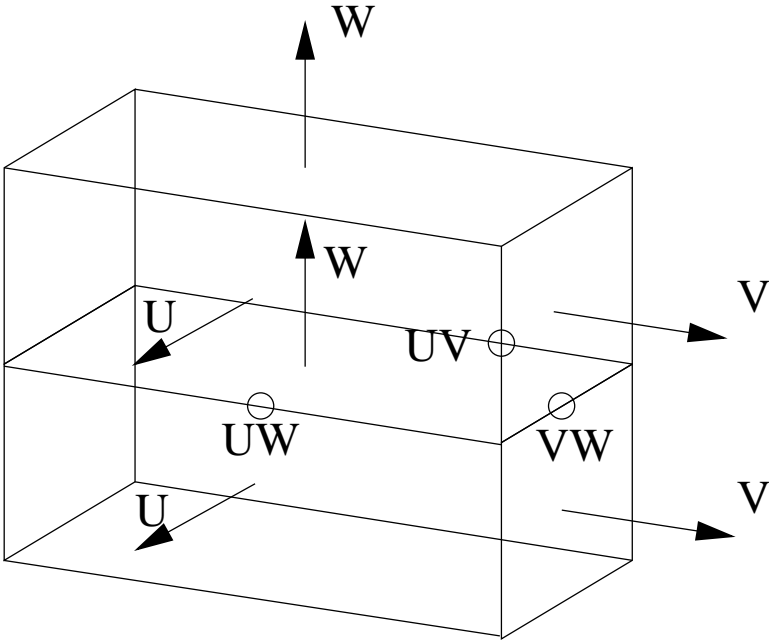


Figure 2. Interpolation of off-diagonal stresses to cell edges.

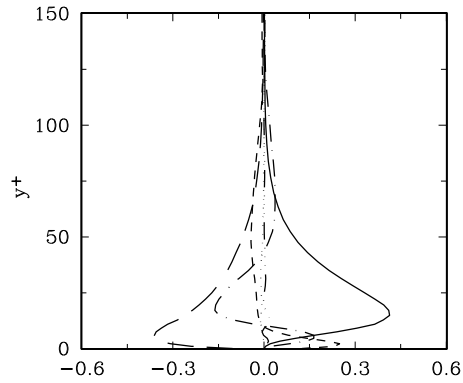


Figure 3. Balance of  $\overline{u'^2}$  for bypass transition at  $Re_x = 129100$  in units of  $u_\tau^4/\nu$ , the viscous units being defined at  $Re_x = 112200$ . Solid line, production; dotted line, mean convection; dot-dash, turbulent transport; dashed, pressure work; long dashes, viscous work; triple-dot-dash, residual error.

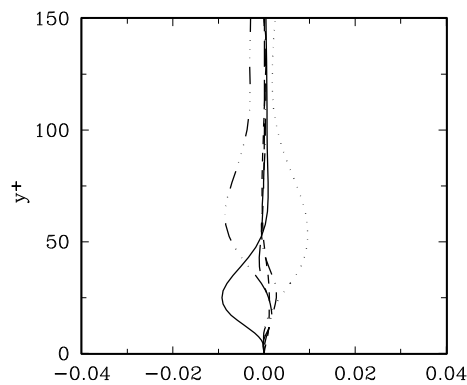


Figure 4. Balance of  $\overline{u'v'}$  for bypass transition at  $Re_x = 29800$ . As Figure 3.

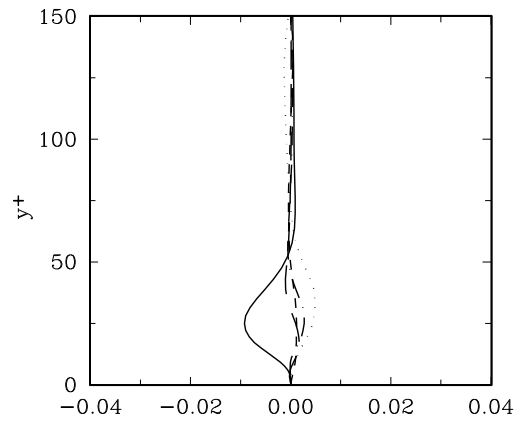


Figure 5. Balance of  $\overline{u'v'}$  for bypass transition at  $Re_x = 29800$ . As Figure 4, but the mean convection includes the residual error term.

Figure 6. Balance of  $k$  for the tripped boundary layer, at  $Re_x = 172000$  in units of  $u_\tau^4/\nu$ , the viscous units being defined at the same position. As Figure 3.