Run-time channel budgets

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Start from the continuous momentum equation (constant density and viscosity):

$$\partial_t u_i + u_j \partial_j u_i = \nu \partial_j \partial_j u_i - \partial_i p \tag{1}$$

This equation is discretised in your code. Leaving the temporal integration out of consideration:

$$\partial_t u_i = -\Omega^{-1} \left(C(\mathbf{u}_s) + D \right) \mathbf{u}_c - G_c \mathbf{p}_c \tag{2}$$

where $D = -\nu(I_{NDim} \otimes L)$. The temporal derivative of $k = \frac{1}{2}\langle u_i' u_i' \rangle$ can be expressed as:

$$\partial_t k = \langle u_i' \partial_t u_i' \rangle = \langle u_i \partial_t u_i \rangle - \langle u_i \rangle \langle \partial_t u_i \rangle \tag{3}$$

The first set of budget terms, convective, C_k, diffusive, D_k, and pressure diffusion, D_k^p, are then found easily as;

$$C_k = -\overline{\mathbf{u}_c^T \Omega^{-1} C(\mathbf{u}_s) \mathbf{u_c}} + \overline{\mathbf{u}_c^T}\ \overline{\Omega^{-1} C(\mathbf{u}_s) \mathbf{u_c}} \tag{4}$$

$$D_k = -\overline{\mathbf{u}_c^T \Omega^{-1} D \mathbf{u_c}} + \overline{\mathbf{u}_c^T}\ \overline{\Omega^{-1} D \mathbf{u_c}} \tag{5}$$

$$D_k^p = -\overline{\mathbf{u}_c^T G_c \mathbf{p}_c} + \overline{\mathbf{u}_c^T}\ \overline{G_c \mathbf{p}_c} \tag{6}$$

These budget terms can be expressed exactly in the way as your code is discretised.

Usually, we are interested in the transport and production, not just the convective term as a whole. To arrive to those terms, we first rewrite:

$$\begin{aligned} \left(u_j \partial_j u_i \right)' &= u_i \partial_j u_i - \overline{u_j \partial_j u_i} \\ &= \overline{u_j} \partial_j \overline{u_i} + u_j' \partial_j \overline{u_i} + \overline{u_j} \partial_j u_i' + u_j' \partial_j u_i' - \overline{u_j \partial_j u_i} \end{aligned} \tag{7}$$

Which allows us to rewrite the convective budget:

$$-\overline{u_i' \left(u_j \partial_j u_i \right)'} = -\overline{u_i' u_j'} \partial_j \overline{u_i} - \overline{u_j} \partial_j k - \overline{u_i' u_j' \partial_j u_i'} \tag{8}$$

Similarly, the diffusive budget is split up into dissipation and viscous diffusion.

$$\nu\overline{u_i'\partial_j\partial_j u_i'} = \nu\partial_j\partial_j k - \nu\overline{\partial_j u_i'\partial_j u_i'} \tag{9}$$

Rewriting these equations, we arrive to the transport equation of turbulent kinetic energy:

$$\frac{Dk}{Dt} = \partial_t k + \overline{u_j}\partial_j k = -\overline{u_i' u_j'}\partial_j\overline{u_i} - \overline{u_i' u_j'\partial_j u_i'} + \nu\partial_j\partial_j k - \nu\overline{\partial_j u_i'\partial_j u_i'} - \overline{u_i'\partial_i p'} \tag{10}$$

with the terms on the RHS: production, P_k, transport, T_k, viscous diffusion, D_k^ν, dissipation, ϵ and pressure diffusion, D_k^p, respectively. The problem with the splitting of the convective and diffusive term is that they involve the product and chain rule for derivatives. How to do these on a discrete level is not straight-forward and will lead to the necessity of making a choice in the discretisation, whereas the discretisations for $C_k(= P_k^p + T_k^p - \overline{u_j}\partial_j k)$, $D_k(= D_k^\nu + \epsilon)$ and D_k^p follow from the discrete momentum equations.

When rewriting these expressions to avoid the use of fluctuating terms, to allow for averaging during run-time, we find:

$$\begin{aligned}\epsilon &= -\nu\overline{\partial_j u_i'\partial_j u_i'} \\ &= -\nu\overline{\partial_j u_i\partial_j u_i} + \nu\overline{\partial_j u_i}\,\overline{\partial_j u_i}\end{aligned} \tag{11}$$

$$\begin{aligned}D_k^\nu &= \nu\partial_j\partial_j k \\ &= \frac{1}{2}\nu\overline{\partial_j\partial_j u_i u_i} - \frac{1}{2}\nu\partial_j\partial_j\left(\overline{u_i}\,\overline{u_i}\right)\end{aligned} \tag{12}$$

we want to avoid taking derivatives in in the post-process, to reflect the discrete code more accurately. Therefore:

$$\begin{aligned}D_k^\nu &= \frac{1}{2}\nu\overline{\partial_j\partial_j u_i u_i} - \frac{1}{2}\nu\partial_j\partial_j\left(\overline{u_i}\,\overline{u_i}\right) \\ &= \frac{1}{2}\nu\overline{\partial_j\partial_j u_i u_i} - \nu\overline{u_i}\,\overline{\partial_j\partial_j u_i} - \nu\overline{\partial_j u_i}\,\overline{\partial_j u_i}\end{aligned} \tag{13}$$

But this term can then be rewritten to:

$$\begin{aligned}D_k^\nu &= \frac{1}{2}\nu\overline{\partial_j\partial_j u_i u_i} - \nu\overline{u_i}\,\overline{\partial_j\partial_j u_i} - \nu\overline{\partial_j u_i}\,\overline{\partial_j u_i} \\ &= \nu\overline{u_i\partial_j\partial_j u_i} + \nu\overline{\partial_j u_i\partial_j u_i} - \nu\overline{u_i}\,\overline{\partial_j\partial_j u_i} - \nu\overline{\partial_j u_i}\,\overline{\partial_j u_i} \\ &= D_k - \epsilon\end{aligned} \tag{14}$$

Therefore, it seems easiest to express viscous diffusion as the difference between D_k, which is known exactly, and ϵ. This way, only the cell centered derivative of $\mathbf{u}_c$ has to be discretised. The problem of using the chain and product rules in a discrete sense can be seen here. The budget term uses cell-centered gradients, whereas the gradient in the diffusive operator is

a face-gradient. The highest oscillatory modes of velocity are missed by this cell-centered gradient, therefore ϵ might not reflect the exact dissipation of your code.
Similarly, the product budget term is expressed as:

$$\begin{aligned} P_k &= -\overline{u_i' u_j'}\,\overline{\partial_j u_i} \\ &= -\left(\overline{u_i u_j} - \overline{u_i}\,\overline{u_j}\right)\overline{\partial_j u_i} \end{aligned} \tag{15}$$

And finally, the transport term is expressed as:

$$\begin{aligned} T_k &= -\overline{u_i' u_j' \partial_j u_i'} \\ &= -\overline{u_i u_j \partial_j u_i} + \overline{u_i}\,\overline{u_j \partial_j u_i} + \overline{u_j}\,\overline{u_i \partial_j u_i} + \overline{u_i u_j}\,\overline{\partial_j u_i} - 2\overline{u_i}\,\overline{u_j}\,\overline{\partial_j u_i} \end{aligned} \tag{16}$$

Since, in a channel flow, $\overline{u_j}\partial_j k = 0$, and since $\overline{u_i u_j}$ is already averaged to find the Reynolds stresses, it is easiest to express the transport term as:

$$T_k = C_k - P_k \tag{17}$$

In summary:

$$\partial_t k = C_k + D_k + P_k \tag{18}$$

$$\frac{Dk}{Dt} = \partial_t k + \overline{u}\partial_j k = P_k + T_k + D_k^{\nu} + \epsilon + P_k \tag{19}$$

And for a channel flow we calculate these terms as:

$$\begin{aligned} C_k &= -\overline{\mathbf{u}_c^T \Omega^{-1} C(\mathbf{u}_s)\mathbf{u_c}} + \overline{\mathbf{u}_c^T}\;\overline{\Omega^{-1} C(\mathbf{u}_s)\mathbf{u_c}} \\ D_k &= -\overline{\mathbf{u}_c^T \Omega^{-1} D\mathbf{u_c}} + \overline{\mathbf{u}_c^T}\;\overline{\Omega^{-1} D\mathbf{u_c}} \\ D_k^p &= -\overline{\mathbf{u}_c^T G_c \mathbf{p}_c} + \overline{\mathbf{u}_c^T}\;\overline{G_c \mathbf{p}_c} \\ P_k &= -\left(\overline{u_i u_j} - \overline{u_i}\,\overline{u_j}\right)\overline{\partial_j u_i} \\ \epsilon &= -\nu\overline{\partial_j u_i \partial_j u_i} + \nu\overline{\partial_j u_i}\;\overline{\partial_j u_i} \\ T_k &= C_k - P_k \\ D_k^{\nu} &= D_k - \epsilon \end{aligned} \tag{20}$$

This only leaves the discussion of how to take the cell-centered gradient of the velocity.