List of desirable and minimum quantities to be entered into the KB Wiki

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1 Introduction

This document presents and discusses the data that should be collected during DNS simulations and was prepared for use in the EU project HiFi Turb. The document is split up in a main section and appendices. The main body details the mandatory and hence minimum data to be acquired and entered into the KB Wiki, and consists of

- Section 2 briefly introduces the notations which will be used;
- Section 3 details the mandatory data sets consisting of mean-flow quantities and single-point correlations in the volume appearing in the averaged Navier-Stokes equations and the Reynolds stress equations, as well as some additional quantities of interest to practitioners.
- Section 4 gives a list of mandatory statistical data to be computed on solid surfaces;
- Section 5 discusses the computation of the turbulent integral time scales.
- Section 6 provides guidelines for the acquisition of time series of instantaneous data in the boundary-layer region of the flow;

The appendices provide supplementary information including guidelines for acquiring the statistical data, baseline datasets to be stored at checkpoints for reconstructing the former, and further background information on the Reynolds stress equations with additional variants and optional terms appearing in these.

- Appendix A derives and discusses the variants of the Reynolds-stress equations found in the literature, highlighting the differences.
  - Appendix A.1 details the Reynolds averaged Navier-Stokes equations;
  - Appendix A.2 derives and presents the different variants of the compressible Reynolds-stress equations;
  - Appendix A.3 presents the incompressible Reynolds stress equations and introduces the correction terms needed if these equations are computed using a compressible solver.
  - Appendix A.4 discusses the non-equivalence of certain terms in the chosen compressible and incompressible forms of the Reynolds stress equations for constant-density flows.
- Appendix B provides the guidelines for the acquisition of statistical data;
  - Appendix B.1 discusses the computation of single-point correlations;
  - Appendix B.2 provides minimal data sets that should be stored in the computation checkpoints to support the adequate computation of the terms listed in section 3;

  - Appendix B.3 discusses the computation of the integral time scales.

- Appendix C lists a small number of additional quantities for optional storage which complete the variants of the Reynolds stress equations detailed in Appendices A.2 and A.3, but were not covered in the main document.

2 Conventions

2.1 Notation

- vectors $\mathbf{u}$ and tensors $\boldsymbol{\tau}$ are indicated in boldface, whereas scalars as well as vectors and tensor components are noted in regular face.
- Cartesian components are indicated with indices i, j or k; *e.g.* the velocity components are denoted as u_i;
- near walls, n indicates the wall normal component, whereas s, t indicate wall tangential components in the streamwise and transversal direction. For instance, the streamwise and transverse components of the wall shear stress are denoted τ_{ns} and τ_{nt};
- the derivatives of first and second order are respectively noted as

$$a_{,i} \hat{=} \frac{\partial a}{\partial x_i} \qquad\qquad a_{,ij} \hat{=} \frac{\partial^2 a}{\partial x_i \partial x_j}$$

- Einstein notation is used throughout the text, entailing summation on repeated indices

$$a_i b_i \hat{=} \sum_{i=1}^{3} a_i b_i = \mathbf{a} \cdot \mathbf{b} \qquad\qquad a_{i,i} \hat{=} \sum_{i=1}^{3} a_{i,i} = \nabla \cdot \mathbf{a}$$

2.2 Governing equations

We use the following conventions for the flow variables

- density ρ, pressure p, velocity $\mathbf{u}$ and temperature T which
  - satisfy the ideal gas relation $p = \rho \mathcal{R} T$ for compressible flow computations;
  - feature a strictly constant density ρ for incompressible flow computations.
- kinetic energy $\mathcal{K} = \frac{1}{2} u_i u_i$
- internal energy $e = \mathcal{C}_v T$ and enthalpy $h = e + p/\rho$. For a compressible flow computation $h = (\mathcal{C}_v + \mathcal{R})T = \mathcal{C}_p T$.
- stagnation internal energy $\mathcal{E} = e + \mathcal{K}$ and enthalpy $\mathcal{H} = h + \mathcal{K}$
- strain rate $\mathcal{S}_{ij}$ and rotation tensor Ω_{ij}

$$\mathcal{S}_{ij} = \frac{1}{2}\left(u_{j,i} + u_{i,j}\right) \qquad\qquad \Omega_{ij} = \frac{1}{2}\left(u_{j,i} - u_{i,j}\right)$$

- viscous stress tensor $\boldsymbol{\tau}$ and heat flux $\boldsymbol{q}$

$$\tau_{ij} = 2\mu\left(\mathcal{S}_{ij} - \frac{1}{3}u_{k,k}\delta_{ij}\right) \qquad\qquad q_i = -\kappa\; T_{,i}$$

We impose that constant values are taken for gas constant $\mathcal{R}$, heat capacities $\mathcal{C}_v$, $\mathcal{C}_p = \mathcal{C}_v + \mathcal{R}$, dynamic viscosity μ, and conductivity κ since otherwise the averaged equations become even more involved.

With these conventions, the Navier-Stokes equations are

$$\begin{aligned} \rho_{,t} + (\rho u_i)_{,i} &= 0 \\ (\rho u_i)_{,t} + (\rho u_i u_j)_{,j} + p_{,i} &= \tau_{ij,j} \\ (\rho\mathcal{E})_{,t} + (\rho\mathcal{H}u_i)_{,i} &= (u_i\tau_{ij})_{,j} + q_{i,i} \end{aligned} \tag{1}$$

For incompressible constant density flows we have

$$\begin{aligned} u_{i,i} &= 0 \\ \rho u_{i,t} + \rho(u_i u_j)_{,j} + p_{,i} &= \tau_{ij,j} \\ \rho\mathcal{E}_{,t} + \rho(\mathcal{H}u_i)_{,i} &= (u_i\tau_{ij})_{,j} + q_{i,i} \end{aligned} \tag{2}$$

Note that the density is still present for dimensional coherence.

Multiplying the momentum equation with velocity, we obtain the Bernoulli equation:

$$(\rho\mathcal{K})_{,t} + (\rho\mathcal{K}u_i)_{,i} + (pu_i)_{,i} - pu_{i,i} = (u_i\tau_{ij})_{,j} - \tau_{ij}\mathcal{S}_{ij} \tag{3}$$

Combining this equation with the energy equation, and using the symmetry of the shear stress tensor $\boldsymbol{\tau}$, we obtain an equation for internal energy e

$$(\rho e)_{,t} + (\rho e u_i)_{,i} + pu_{i,i} = \tau_{ij}\mathcal{S}_{ij} + q_{i,i} \tag{4}$$

For incompressible flows, this form of the energy equation is often used as an alternative to the total energy equation in the general Navier-Stokes equations. As temperature has no impact on the momentum equations, this equation may even not be solved.

2.3 Averages and fluctuations

The *Reynolds average* and its associated *fluctuation* result from the ensemble average

$$\overline{q}(x,y,z,t) = \frac{1}{N}\sum_{l=1}^{N} q_l(x,y,z,t) \tag{5}$$

$$q'(x,y,z,t) = q(x,y,z,t) - \overline{q}(x,y,z,t) \tag{6}$$

with the index l running on the N realizations of the flow field. For statistically stationary flows, l will correspond to a snapshot in a time series. The *Favre average* is based upon the density weighted ensemble average and the associated fluctuations

$$\widetilde{q} = \frac{\overline{\rho q}}{\overline{\rho}} \tag{7}$$

$$q''(x, y, z, t) = q(x, y, z, t) - \widetilde{q}(x, y, z, t) \tag{8}$$

Obviously the *corresponding* averages for both types of fluctuations are zero:

$$\overline{a'} = 0 \qquad \widetilde{a''} = \overline{\rho a''} = 0 \qquad \overline{a''} \neq 0 \qquad \widetilde{a'} = \overline{\rho a'} \neq 0$$

Any average can be taken out of the average of a product:

$$\overline{\overline{a}\, b} = \overline{a}\, \overline{b} \qquad \overline{\widetilde{a}\, b} = \widetilde{a}\, \overline{b} \qquad \widetilde{\overline{a}\, b} = \overline{a}\, \widetilde{b} \qquad \widetilde{\widetilde{a}\, b} = \widetilde{a}\, \widetilde{b}$$

Averages and derivatives commute

$$\overline{\frac{\partial a}{\partial t}} = \frac{\partial \overline{a}}{\partial t} \qquad \widetilde{\frac{\partial a}{\partial t}} = \frac{\partial \widetilde{a}}{\partial t} \qquad \ldots$$

3 Required statistical data in the volume

The data are organized in 2 levels essentially following the level of closure in turbulence modelling. Typically, as the level increases, the order of correlations increases as well as the importance of fine scales. This means the statistical convergence as well as the required resolutions are more difficult to achieve.

The two levels are

1. level 1 corresponds to the quantities appearing in the averaged Navier-Stokes equations, discussed in appendix A.1;

2. level 2 corresponds to the quantities appearing in the transport equations for the turbulent fluxes. More specifically only the Reynolds stress equation, discussed in appendix A.2 is retained, while at this stage the turbulent heat flux equation is not. Different formulations are available in literature for compressible flows, which are discussed appendices A.2 and A.3. For compressible flow solvers, the formulation of Gerolymos and Vallet [3], described in A.2.3.1, is chosen as mandatory. For incompressible flow solvers the standard incompressible variant described in A.3.2 will be used;

3. originally a third level was planned based on the transport equation for the rate of dissipation ϵ of the turbulent kinetic energy. The terms in this equation are attainable only

by DNS at extremely high resolution, and for compressible flows there are still uncertainties about which formulation to choose. Further, in the turbulence modelling community there are doubts about the usefulness of the exact epsilon equation for modelling purposes. Hence level 3 was not pursued.

3.1 Exact averaged equations

The equations, and later in section 3.3 the data to be stored, are given separately for the use of compressible and incompressible codes.

3.1.1 Compressible codes

The compressible codes need to be able to provide all terms appearing in the exact averaged equations:

- Level 1: the Favre averaged Navier-Stokes equations following Knight [7]:

$$\begin{aligned} \overline{\rho}_{,t} + (\overline{\rho}\widetilde{u}_k)_{,k} &= 0 \\ (\overline{\rho}\widetilde{u}_i)_{,t} + (\overline{\rho}\widetilde{u}_i\widetilde{u}_j)_{,j} + \overline{p_{,i}} &= \left(\overline{\tau_{ij}} - \mathcal{R}_{ij}\right)_{,j} \\ (\overline{\rho}\widetilde{\mathcal{E}})_{,t} + (\overline{\rho}\widetilde{\mathcal{H}}\widetilde{u}_j)_{,j} &= \widetilde{u}_i\left(\overline{\tau_{ij}} - \mathcal{R}_{ij}\right)_{,j} + \left(\overline{q_j} - \mathcal{Q}_j\right)_{,j} + \left(\overline{u_i''\tau_{ij}} - \frac{1}{2}\overline{\rho\left(u_k''u_k''\right)u_j''}\right)_{,j} \end{aligned} \tag{9}$$

with the turbulent fluxes, namely the Reynolds stress and the turbulent heat flux

$$\mathcal{R}_{ij} = \overline{\rho u_i'' u_j''} = \overline{\rho}\ \widetilde{u_i'' u_j''} \tag{10}$$

$$\mathcal{Q}_i = \overline{\rho u_i'' h''} = \overline{\rho}\ \widetilde{u_i'' h''} \tag{11}$$

and modified constitutive relations

$$\overline{p} = \overline{\rho}\mathcal{R}\widetilde{T} \qquad \widetilde{e} = \mathcal{C}_v\widetilde{T} \qquad \overline{\rho}\widetilde{h} = \overline{\rho}\widetilde{e} + \overline{p} = \overline{\rho}\mathcal{C}_p\widetilde{T}$$

$$\overline{\rho}\widetilde{\mathcal{E}} = \overline{\rho}\widetilde{e} + \overline{\rho}\widetilde{\mathcal{K}} + \overline{\rho}\mathcal{K}_t \qquad \overline{\rho}\widetilde{\mathcal{H}} = \overline{\rho}\widetilde{h} + \overline{\rho}\widetilde{\mathcal{K}} + \overline{\rho}\mathcal{K}_t$$

$$\overline{\rho}\mathcal{K}_t = \frac{1}{2}\overline{\rho u_k'' u_k''} = \frac{1}{2}\overline{\rho}\widetilde{u_k'' u_k''} \qquad \overline{\rho}\widetilde{\mathcal{K}} = \frac{1}{2}\overline{\rho}\widetilde{u}_k\widetilde{u}_k$$

- the Reynolds stress equation following Gerolymos and Vallet [3]:

$$\mathcal{R}_{ij,t} + \left(\mathcal{R}_{ij}\widetilde{u}_k\right)_{,k} = P_{ij} + D_{ij} + \Phi_{ij} + \Phi'_{ij} - \epsilon_{ij} + K_{ij} \tag{12}$$

with

– the production term

$$P_{ij} = -\mathcal{R}_{ik}\widetilde{u}_{j,k} - \mathcal{R}_{jk}\widetilde{u}_{i,k} \tag{13}$$

– the turbulent diffusion

$$D^1_{ij} = -\left(\overline{\rho u''_i u''_j u''_k}\right)_{,k} \tag{14}$$

– the pressure diffusion

$$D^2_{ij} = -\left(\overline{p'(u''_i \delta_{jk} + u''_j \delta_{ik})}\right)_{,k} \tag{15}$$

– the viscous diffusion

$$D^3_{ij} = \left(\overline{u''_i \tau'_{jk} + u''_j \tau'_{ik}}\right)_{,k} \tag{16}$$

– the pressure strain term

$$\Phi_{ij} = \overline{p'(u''_{i,j} + u''_{j,i} - \frac{2}{3}u''_{k,k}\delta_{ij})} \tag{17}$$

– the pressure-dilatation term

$$\Phi'_{ij} = \frac{2}{3}\overline{p' u''_{k,k}\delta_{ij}} \tag{18}$$

– the viscous dissipation

$$\epsilon_{ij} = \overline{\tau'_{jk}u''_{i,k} + \tau'_{ik}u''_{j,k}} \tag{19}$$

– the density fluctuation effects

$$K_{ij} = -u''_i \; (\overline{p_{,j}} - \overline{\tau_{jk,k}}) - u''_j \; (\overline{p_{,i}} - \overline{\tau_{ik,k}}) \tag{20}$$

Note that K_{ij} is usually neglected in the modeled $\mathcal{R}_{ij}$ equations, but should be retained in order to obtain a zero residual.

- the equation for the turbulent kinetic energy is found by computing the trace of all the terms in the Reynolds stress equations and are therefore not stored separately. For instance, the kinetic energy dissipation is found from the correlation between stress and velocity gradient

$$\epsilon = 2\overline{\tau'_{ij}u''_{i,j}}$$

We should remark that although the formulation of Gerolymos and Vallet is very similar to the incompressible formulation discussed in the next section, the equations do not correspond on a term by term basis as $u''_i \to u'_i$. More specifically the viscous diffusion term D^3_{ij} and the dissipation term ϵ_{ij} are not exactly the same as the incompressible counterparts as discussed in section 3.1.2 and more in detail in appendix A.4.

3.1.2 Incompressible codes

For incompressible codes, the stored data should contain all terms in

- Level 1: the Reynolds averaged Navier-Stokes equations

$$\overline{u}_{k,k} = 0$$
$$\rho\overline{u}_{i,t} + \rho(\overline{u}_i\overline{u}_j)_{,j} + \overline{p_{,i}} = \left(\overline{\tau_{ij}} - \mathcal{R}^*_{ij}\right)_{,j} \tag{21}$$
$$\rho\mathcal{C}_v\overline{T}_{,t} + \rho\mathcal{C}_v\left(\overline{T}\overline{u}_j\right)_{,j} = \overline{\tau}_{ij}\overline{\mathcal{S}}_{ij} + \overline{\tau'_{ij}\mathcal{S}'_{ij}} + (q_i - \mathcal{Q}^*_i)_{,i}$$

  with the Reynolds stress and turbulent heat flux

$$\mathcal{R}^*_{ij} = \rho\overline{u'_i u'_j} \tag{22}$$
$$\mathcal{Q}^* = \rho\mathcal{C}_v\overline{u'_i T'} \tag{23}$$

- Level 2: the Reynolds stress equations

$$\mathcal{R}^*_{ij,t} + \left(\mathcal{R}^*_{ij}\overline{u}_k\right)_{,k} = P^*_{ij} + D^{*,1}_{ij} + D^{*,2}_{ij} + D^{*,3}_{ij} + \Phi^*_{ij} - \epsilon^*_{ij} \tag{24}$$

  with the following terms

  – production

$$P^*_{ij} = -\left(\mathcal{R}^*_{ik}\overline{u}_{j,k} + \mathcal{R}^*_{jk}\overline{u}_{i,k}\right) \tag{25}$$

  – turbulent diffusion

$$D^{*,1}_{ij} = -\left(\overline{\rho u'_i u'_j u'_k}\right)_{,k} \tag{26}$$

  – pressure diffusion

$$D^{*,2}_{ij} = -\left(\overline{p'\left(u'_i\delta_{jk} + u'_j\delta_{ik}\right)}\right)_{,k} \tag{27}$$

  – viscous diffusion

$$D^{*,3}_{ij} = \frac{\mu}{\rho}\mathcal{R}^*_{ij,kk} \tag{28}$$

  – pressure strain correlation

$$\Phi^*_{ij} = \overline{p'\left(u'_{i,j} + u'_{j,i}\right)} = 2\overline{p'\mathcal{S}'_{ij}} \tag{29}$$

  – dissipation

$$\epsilon^*_{ij} = 2\mu\,\overline{u'_{i,k}u'_{j,k}} \tag{30}$$

- the equations for the turbulent kinetic energy are found by computing the trace of all the terms in the Reynolds stress equations and are therefore not stored separately.

Note that when in the compressible formulation of Gerolymos and Vallet for incompressible flows u_i'' is replaced by u_i', a different splitting up of the viscous terms into diffusion and dissipation results, as discussed in the appendix A.4. Hence these terms are not equivalent in the above compressible and incompressible Reynolds stress equations, but their sum is. The alternative splitting, *i.e.* by Gerolymos and Vallet, is sometimes used in the fundamental literature, and corresponds to the dissipation ϵ of the turbulent kinetic energy (see Batchelor [2], Tennekes and Lumley [11] or Pope [9])

$$\epsilon = \frac{1}{2}\epsilon_{ii} = 2\mu\overline{\mathcal{S}'_{ij}\mathcal{S}'_{ij}}$$

whereas the half of the trace of ϵ^* does not.

3.2 Additional quantities of interest

The following fundamental scales are of interest in view of verifying the adequacy of the spatial and temporal resolution:

- the Taylor microscale (adapted from Batchelor [2], eq. 3.4.8)

$$\eta_T = \sqrt{10\frac{\mu\mathcal{K}_t}{\overline{\rho}^2\overline{\epsilon}}} = \sqrt{5\frac{\mu\overline{\mathcal{R}_{ii}}}{\overline{\rho}\overline{\tau'_{ij}\mathcal{S}''_{ij}}}} \tag{31}$$

- the Kolmogorov length scale, approximated in compressible flow as

$$\eta_K = \sqrt[4]{\frac{\overline{\rho}\nu^3}{\overline{\epsilon}}} \approx \sqrt[4]{\frac{\mu^3/\overline{\rho}^2}{\overline{\tau'_{ij}\mathcal{S}''_{ij}}}} \tag{32}$$

- the Kolmogorov time scale;

$$\tau_K = \sqrt{\frac{\nu}{\epsilon}} \approx \sqrt{\frac{\mu}{\overline{\tau'_{ij}\mathcal{S}''_{ij}}}} \tag{33}$$

Some additional quantities are of interest to verify hypotheses both on a numerical (Morkovin's hypothesis) as on an experimental level (*e.g.* hotwire measurements).

- pressure autocorrelation $\overline{p'p'}$
- density autocorrelation $\overline{\rho'\rho'}$;
- temperature autocorrelations $\overline{T'T'}$

3.3 Mandatory statistical data

As stated in the previous sections, the equations of interest are the averaged Navier-Stokes equations (level 1) and the Reynolds stress equations (level 2). These are listed in the tables together with a number of additional quantities of interest. Separate tables are foreseen for the compressible and the incompressible solvers.

3.3.1 Compressible codes

Table 1 resumes the data that should be accumulated by compressible codes.

Quantity		**#**
Level 1 - averaged Navier-Stokes equations		
Averaged density	$\overline{\rho}$	1
Averaged pressure	$\overline{p}$	1
Favre averaged velocity	$\widetilde{u}_i$	3
Favre averaged temperature	$\widetilde{T}$	1
Averaged shear stress	$\overline{\tau_{ij}}$	6
Averaged heat flux	$\overline{q_i}$	3
Reynolds stress $\mathcal{R}_{ij}$	$\overline{\rho u''_i u''_j}$	6
Turbulent heat flux $\mathcal{Q}_i$	$\overline{\rho h'' u''_i}$	3
Turbulent shear work	$\overline{u''_i \tau_{ij}}$	3
Turbulent kinetic energy flux	$-\overline{\rho \frac{1}{2} u''_k u''_k u''_i}$	3
Cumulative total		**30**
Level 1 - additional quantities		
Averaged velocity	$\overline{u}_i$	3
Averaged temperature	$\overline{T}$	1
Density autocorrelation	$\overline{\rho' \rho'}$	1
Pressure autocorrelation	$\overline{p' p'}$	1
Temperature autocorrelation	$\overline{T' T'}$	1
Taylor microscale η_T	$\sqrt{5 \frac{\mu}{\rho} \frac{\mathcal{R}_{ii}}{\overline{\tau'_{ij} \mathcal{S}''_{ij}}}}$	1
Kolmogorov length scale η_K	$\sqrt[4]{\frac{\mu^3 / \overline{\rho}^2}{\overline{\tau'_{ij} \mathcal{S}''_{ij}}}}$	1
Kolmogorov time scale τ_K	$\sqrt{\frac{\mu}{\overline{\tau'_{ij} \mathcal{S}''_{ij}}}}$	1
Cumulative total		**40**
Level 2 - Reynolds stress equations		
Favre triple velocity correlation	$\overline{\rho u''_i u''_j u''_k}$	10
Pressure velocity correlation	$\overline{p' u''_i}$	3
Shear stress-velocity correlation	$\overline{\tau'_{ij} u''_k}$	18

Difference of the Reynolds and Favre averages	$\overline{u}_i - \widetilde{u}_i = \overline{u_i''}$	3
Cumulative total		**74**
Level 2 - Reynolds stress equations budget terms		
Convection C_{ij}	$\left(\mathcal{R}_{ij}\widetilde{u}_k\right)_{,k}$	6
Production P_{ij}	$-(\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k})$	6
Diffusion D^1_{ij}	$-\left(\overline{\rho u_i'' u_j'' u_k''}\right)_{,k}$	6
Diffusion D^2_{ij}	$-\left(\overline{p'(u_i''\delta_{jk} + u_j''\delta_{ik})}\right)_{,k}$	6
Diffusion D^3_{ij}	$\left(\overline{u_i''\tau_{jk}' + u_j''\tau_{ik}'}\right)_{,k}$	6
Redistribution/Pressure strain Φ_{ij}	$\overline{p'(u''_{i,j} + u''_{j,i} - \frac{2}{3}u''_{k,k}\delta_{ij})}$	6
Pressure dilatation Φ'_{ij}	$\frac{2}{3}\overline{p' u''_{k,k}\delta_{ij}}$	6
Dissipation ϵ_{ij}	$\overline{\tau'_{ik}u''_{j,k} + \tau'_{jk}u''_{i,k}}$	6
Density fluctuation effects K_{ij}	$-\overline{u_i''}\,(\overline{p_{,j}} - \overline{\tau_{jk,k}}) - \overline{u_j''}\,(\overline{p_{,i}} - \overline{\tau_{ik,k}})$	6
Cumulative total		**128**

Table 1: List of volume statistical quantities for compressible codes. For level 1, this concerns the Reynolds averaged Navier-Stokes equations (9) following Knight [7] and additional data for verifying resolution or of interest to experimentalists. In level 2 includes the terms in the compressible Reynolds equation (12) following Gerolymos and Vallet [3].

3.3.2 Incompressible codes

Table 2 lists the quantities that should be accumulated by incompressible flow codes.

Quantity		**#**
Level 1 - averaged Navier-Stokes equations		
Averaged pressure	$\overline{p}$	1
Averaged velocity	$\overline{u}_i$	3
Averaged temperature	$\overline{T}$	1
Averaged shear stress	$\overline{\tau_{ij}}$	6
Averaged heat flux	$\overline{q_i}$	3
Reynolds stress $\mathcal{R}^*_{ij}$	$\rho\overline{u_i' u_j'}$	6
Turbulent heat flux $\mathcal{Q}_i$	$\rho\overline{e' u_i'}$	3
Cumulative total		**23**
Level 1 - additional quantities		
Pressure autocorrelation	$\overline{p'p'}$	1
Temperature autocorrelation	$\overline{T'T'}$	1
Taylor microscale η_T	$\approx \sqrt{5\frac{\mu}{\rho}\frac{\mathcal{R}^*_{ii}}{\overline{\tau'_{ij}S'_{ij}}}}$	1
Kolmogorov length scale η_K	$\approx \sqrt[4]{\frac{\mu^3/\rho^2}{\overline{\tau'_{ij}S'_{ij}}}}$	1

Kolmogorov time scale τ_K	$\approx \sqrt{\frac{\mu}{\overline{\tau'_{ij} S'_{ij}}}}$	1
Cumulative total		**28**
Level 2 - Reynolds stress equations budget terms		
Convection C^*_{ij}	$\left(\mathcal{R}^*_{ij}\overline{u}_k\right)_{,k}$	6
Production P^*_{ij}	$-\left(\mathcal{R}^*_{ik}\overline{u}_{j,k} + \mathcal{R}^*_{jk}\overline{u}_{i,k}\right)$	6
Turbulent diffusion D^{1*}_{ij}	$-\rho\left(\overline{u'_i u'_j u'_k}\right)_{,k}$	6
Turbulent diffusion D^{2*}_{ij}	$-\left(\overline{p'\left(u'_i\delta_{jk} + u'_j\delta_{ik}\right)}\right)_{,k}$	6
Molecular diffusion D^{3*}_{ij}	$\mu\left(\overline{u'_i u'_j}\right)_{,kk}$	6
Pressure strain Φ^*_{ij}	$\overline{p'\left(u'_{i,j} + u'_{j,i}\right)}$	6
Dissipation ϵ^*_{ij}	$2\mu\overline{u'_{i,k}u'_{j,k}}$	6
Cumulative total		**70**
Level 2 - Reynolds stress equations - separate terms		
Triple velocity correlation	$\rho\overline{u'_i u'_j u'_k}$	10
Pressure velocity correlation	$\overline{p' u'_i}$	3
Cumulative total		**83**

Table 2: List of volume statistical quantities for incompressible codes. For level 1, this concerns equation (21) and additional data for verifying resolution or of interest to experimentalists. In level 2, we included the terms in the incompressible Reynolds stress equation (24).

3.4 Recommendations

- The accumulated data should be stored at the full resolution and native representation of the solver, throughout the whole volume;
- However, if the flow has homogeneous directions, an average over these is expected, and the statistics can then be stored as surface data on one of the periodic planes;
- The computation and checkpointing of the statistical data should follow the approach described in the appendices B.1 and B.2;
- A distinction is made between the data sets as a function of the *type of code (compressible/incompressible)* that was used for the computation, not in function of the test case.

4 Required statistical data on solid boundaries

On solid surfaces the statistical data listed in table 3 should be gathered

Quantity	#

pressure average	$\overline{p}$	1
pressure autocorrelation	$\overline{p'p'}$	1
temperature average	$\overline{T}$	1
temperature autocorrelation	$\overline{T'T'}$	1
shear stress average	$\overline{\tau_{ni}}$	3
shear stress autocorrelation	$\overline{\tau'_{ni}\tau'_{nj}}$	6
heat flux average	$\overline{q_n}$	1
heat flux autocorrelation	$\overline{q'_n q'_n}$	1
Total		**15**

Table 3: List of surface statistic data. n indicates the normal direction, whereas i indicates a Cartesian component.

5 Integral time scales

In order to validate the acquisition times for both statistical data as well as the time series in the boundary layer, it is proposed to compare these times to the integral time scales. This quantity, in particular for velocity components, is also relevant for turbulence modeling.

For any quantity a, the *correlation time* or *integral time scale* is computed from two-point correlations in time. Considering a statistically steady flow, we define the two-point time correlation in function of the delay τ as

$$\mathcal{C}_a(\tau) = \lim_{T\to\infty} \frac{1}{T} \int_0^T a'(t)\; a'(t+\tau)\; dt = \lim_{T\to\infty} \frac{1}{T} \int_0^T a(t)\; a(t+\tau)\; dt - \overline{a}\;\overline{a} \tag{34}$$

The correlation function $\mathcal{C}'_a$ is the time correlation non-dimensionalised by the autocorrelation, *i.e.* the value for $\tau = 0$:

$$C'_a(\tau) = \frac{\mathcal{C}_a(\tau)}{\mathcal{C}_a(0)} \tag{35}$$

The integral time scale is then defined as:

$$\tau_a = \int_0^\infty \mathcal{C}'_a(\tau) d\tau \tag{36}$$

The integral time scale should be stored for the three components of the velocity separately as well as for the pressure and density. The computation procedure is discussed in appendix B.3.

6 Instantaneous data in boundary layers

Within the boundary layer, the time series of the solution, in the native representation of the solver, should be stored for a representative amount of time; this time can be estimated on the basis of the volume statistics, in particular with respect to the integral time scale, described in section 5. There are a number of contradictory requirements

- the temporal resolution should be lower than the integral time scales in order to train or calibrate unsteady models;
- the period of acquisition should be much larger than the largest integral time scales in order to allow a good convergence of the statistical data;
- the data should be acquired over a height h that includes the inner part of the boundary layer. It is proposed to guarantee at least $h^+ > 100$ in the developed regions of the boundary layer.

In practice these specifications will have to be defined on a case by case basis, in a uniform manner for all computations. This means that the corresponding values will be based upon global quantities, such as chord, velocity scale, ... The definition of the acquisition domain should be specified geometrically identically for all computations, *i.e.* independent of the results of the computation itself. This does not preclude the definition on the basis of a preliminary or reference computation.

Appendices

A Overview of the averaged equations

A.1 Level 1 - Averaged Navier-Stokes equations

The most basic level concerns the *ensemble*-averaged Navier-Stokes equations and the corresponding flow field. After averaging the Navier-Stokes equations (1), using Favre averages, these read for compressible flows (see Knight [7]):

$$\begin{aligned} \overline{\rho}_{,t} + (\overline{\rho}\widetilde{u}_k)_{,k} &= 0 \\ (\overline{\rho}\widetilde{u}_i)_{,t} + (\overline{\rho}\widetilde{u}_i\widetilde{u}_j)_{,j} + \overline{p_{,i}} &= \left(\overline{\tau_{ij}} - \mathcal{R}_{ij}\right)_{,j} \\ (\overline{\rho}\widetilde{\mathcal{E}})_{,t} + (\overline{\rho}\widetilde{\mathcal{H}}\widetilde{u}_j)_{,j} &= \widetilde{u}_i\left(\overline{\tau_{ij}} - \mathcal{R}_{ij}\right)_{,j} + \left(\overline{q_j} - \mathcal{Q}_j\right)_{,j} + \left(\overline{u_i''\tau_{ij}} - \frac{1}{2}\overline{\rho\left(u_k''u_k''\right)u_j''}\right)_{,j} \end{aligned} \tag{37}$$

complemented by adapted versions of the constitutive equations for the *total energy* $\widetilde{\mathcal{E}}$ and *enthalpy* $\widetilde{\mathcal{H}}$ as functions of the Favre averages of internal energy $\widetilde{e}$, enthalpy $\widetilde{h}$ and velocity $\widetilde{\mathbf{u}}$, the Reynolds average of pressure $\overline{p}$ and the turbulent kinetic energy $\mathcal{K}_t$:

$$\begin{aligned} &\overline{p} = \overline{\rho}\mathcal{R}\widetilde{T} && \widetilde{e} = \mathcal{C}_v\widetilde{T} && \overline{\rho}\widetilde{h} = \overline{\rho}\widetilde{e} + \overline{p} = \overline{\rho}\mathcal{C}_p\widetilde{T} \\ &\overline{\rho}\widetilde{\mathcal{E}} = \overline{\rho}\widetilde{e} + \frac{1}{2}\,\overline{\rho}\widetilde{u}_k\widetilde{u}_k + \overline{\rho}\mathcal{K}_t && \overline{\rho}\widetilde{\mathcal{H}} = \overline{\rho}\widetilde{h} + \frac{1}{2}\,\overline{\rho}\widetilde{u}_k\widetilde{u}_k + \overline{\rho}\mathcal{K}_t && \overline{\rho}\mathcal{K}_t = \frac{1}{2}\overline{\rho u_k''u_k''} = \frac{1}{2}\overline{\rho}\widetilde{u_k''u_k''} \end{aligned}$$

The turbulent transport terms, including Reynolds stress $\mathcal{R}_{ij}$ and turbulent heat flux $\mathcal{Q}_i$, are defined as

$$\mathcal{R}_{ij} = \overline{\rho u_i''u_j''} = \overline{\rho}\;\widetilde{u_i''u_j''} \tag{38}$$

$$\mathcal{Q}_i = \overline{\rho u_i''h''} = \overline{\rho}\;\widetilde{u_i''h''} \tag{39}$$

The average of equation (4) then reads

$$(\overline{\rho}\widetilde{e})_{,t} + (\overline{\rho}\widetilde{e}\widetilde{u}_k)_{,k} + \overline{p}\overline{u}_{k,k} + \overline{p'u_{k,k}'} = \overline{\tau}_{ij}\overline{\mathcal{S}}_{ij} + \overline{\tau_{ij}'\mathcal{S}_{ij}'} + \overline{q}_{k,k} \tag{40}$$

A.1.1 Expressions for the molecular transport terms

Due to the unavailability of the Reynolds averages of velocity and temperature, RANS modeling approaches usually approximate the averaged molecular transport terms using the respective Favre averages that result from the computation, *i.e.* :

$$\overline{\tau_{ij}} = \mu\left(\overline{u}_{i,j} + \overline{u}_{j,i} - \frac{2}{3}\overline{u}_{k,k}\;\delta_{ij}\right) \approx \mu\left(\widetilde{u}_{i,j} + \widetilde{u}_{j,i} - \frac{2}{3}\widetilde{u}_{k,k}\;\delta_{ij}\right) \tag{41}$$

$$\overline{q_i} = \kappa\;\overline{T_{,i}} \approx \kappa\;\nabla\widetilde{T_{,i}} \tag{42}$$

This approximation is inconsistent with a strict averaging of the Navier-Stokes equations; this approximation may be worth checking for strongly compressible flows.

In order to solve the inconsistency in the preceding formulations, Grigoriev *et al.*[4] define additional transport equations for the difference between the Reynolds and Favre average of the velocity and temperature

$$\mathring{u}_i = \widetilde{u}_i - \overline{u}_i = -\overline{u_i''} \tag{43}$$

$$\mathring{T} = \widetilde{T} - \overline{T} \tag{44}$$

With the help of $\mathring{\mathbf{u}}$ and $\mathring{T}$ the constitutive equations can be correctly computed:

$$\overline{\tau_{ij}} = \mu \left((\widetilde{u}_i - \mathring{u}_i)_{,j} + (\widetilde{u}_j - \mathring{u}_j)_{,i} - \frac{2}{3}(\widetilde{u}_k - \mathring{u}_k)_{,k}\ \delta_{ij} \right) \tag{45}$$

$$\overline{q_i} = \kappa\ (\widetilde{T} - \mathring{T})_{,i} \tag{46}$$

Alternatively, $\mathring{u}_i$ can be used to write the averaged Navier-Stokes in terms of $\overline{u}_i$ and $\mathcal{R}^*_{ij}$:

$$\begin{aligned} \overline{\rho}_{,t} + (\overline{\rho}\ \overline{u}_i)_{,i} &= -(\overline{\rho}\mathring{u}_i)_{,i} \\ (\overline{\rho}\ \overline{u}_i)_{,t} + (\overline{\rho}\ \overline{u}_i\overline{u}_j)_{,j} + \overline{p}_{,i} &= \left(\overline{\tau}_{ij} - \mathcal{R}^*_{ij}\right)_{,j} - (\overline{\rho}\ \mathring{u}_i)_{,t} + (\overline{\rho}(\mathring{u}_i\overline{u}_j + \overline{u}_i\mathring{u}_j))_{,j} \end{aligned} \tag{47}$$

with the incompressible Reynolds stress defined as $\mathcal{R}^*_{ij} = \overline{\rho u_i' u_j'}$.

A.2 Level 2 - Compressible Reynolds stress equations

The second level of volume data concerns the Reynolds stress equations. For compressible flows, several variants have been proposed in the literature, depending on how pressure and stress components are decomposed (or not) into mean and fluctuating components.

In the following we will use the short hand notation $(mom)_i$ for the instantaneous i-th component of the momentum equations. The Reynolds stress equations are given by

$$\overline{u_i''\ (mom)_j + u_j''\ (mom)_i} = 0$$

By rearranging we find

$$\underbrace{\overline{u_i''\frac{\partial \rho u_j}{\partial t} + u_j''\frac{\partial \rho u_i}{\partial t}}}_{\mathcal{R}_t} + \underbrace{\overline{u_i''(\rho u_j u_k)_{,k} + u_j''(\rho u_i u_k)_{,k}}}_{\mathcal{R}_c} = -\underbrace{\overline{u_i'' p_{,j} + u_j'' p_{,i}}}_{\mathcal{R}_p} + \underbrace{\overline{u_i''\tau_{jk,k} + u_j''\tau_{ik,k}}}_{\mathcal{R}_{\boldsymbol{\tau}}} \tag{48}$$

The terms $\mathcal{R}_t$ and $\mathcal{R}_c$ are treated similarly by all authors, whereas the treatment of the terms $\mathcal{R}_p$ and $\mathcal{R}_{\mathcal{S}}$ differs in how (or even whether) the pressure p and shear stress $\boldsymbol{\tau}$ are decomposed in fluctuating and average parts and then recombined with the higher order correlations stemming from $\mathcal{R}_c$.

A.2.1 General formulation

In this section, the common treatment of the terms $\mathcal{R}_t$ and $\mathcal{R}_c$ is outlined, leading to the convection term and two contributions to the source terms. In the subsequent sections, different groupings of the right-hand-side terms are discussed. The final section discusses a common storage for all of the different formulations.

The contributions corresponding to the time derivatives in (48) can be rearranged as

$$\mathcal{R}_t = \overline{u_i''\frac{\partial \rho u_j}{\partial t} + u_j''\frac{\partial \rho u_i}{\partial t}} = \underbrace{\overline{u_i''\frac{\partial \rho u_j''}{\partial t} + u_j''\frac{\partial \rho u_i''}{\partial t}}}_{\mathcal{R}_{t1}} + \underbrace{\overline{u_i''\frac{\partial \rho \widetilde{u}_j}{\partial t} + u_i''\frac{\partial \rho \widetilde{u}_j}{\partial t}}}_{\mathcal{R}_{t2}}$$

Developing the first contribution, we have

$$\begin{aligned}\mathcal{R}_{t1} &= 2\overline{\frac{\partial \rho u_i'' u_j''}{\partial t}} - \overline{\rho u_j''\frac{\partial u_i''}{\partial t} + \rho u_i''\frac{\partial u_j''}{\partial t}} = 2\frac{\partial \mathcal{R}_{ij}}{\partial t} - \rho\overline{\frac{\partial u_i'' u_j''}{\partial t}} \\ &= \frac{\partial \mathcal{R}_{ij}}{\partial t} + \overline{u_i'' u_j''\frac{\partial \rho}{\partial t}}\end{aligned}$$

The second contribution is then

$$\begin{aligned}\mathcal{R}_{t2} &= \overline{\cancel{\frac{\partial}{\partial t}\rho\widetilde{u}_j u_i''} + \frac{\partial}{\partial t}\rho\widetilde{u}_i u_j''} - \overline{\rho\widetilde{u}_j\frac{\partial u_i''}{\partial t} - \rho\widetilde{u}_i\frac{\partial u_j''}{\partial t}} \\ &= \cancel{\overline{-\widetilde{u}_j\frac{\partial \rho u_i''}{\partial t} - \widetilde{u}_i\frac{\partial \rho u_j''}{\partial t}}} + \overline{(u_i''\widetilde{u}_j + u_j''\widetilde{u}_i)\frac{\partial \rho}{\partial t}}\end{aligned}$$

The correlations resulting from the transport terms $\mathcal{R}_c$ can then be rearranged as follows

$$\mathcal{R}_c = \overline{u_i''(\rho u_j u_k)_{,k} + u_j''(\rho u_i u_k)_{,k}} = \underbrace{\overline{u_i''(\rho u_j'' u_k)_{,k} + u_j''(\rho u_i'' u_k)_{,k}}}_{\mathcal{R}_{c1}} + \underbrace{\overline{u_i''(\rho\widetilde{u}_j u_k)_{,k} + u_j''(\rho\widetilde{u}_i u_k)_{,k}}}_{\mathcal{R}_{c2}}$$

Developing $\mathcal{R}_{c1}$ and $\mathcal{R}_{c2}$ we find

$$\begin{aligned}\mathcal{R}_{c1} &= 2\overline{u_i'' u_j''(\rho u_k)_{,k}} + \overline{\rho u_k(u_i'' u_j'')_{,k}} = \overline{u_i'' u_j''(\rho u_k)_{,k}} + \overline{(\rho u_i'' u_j'' u_k)_{,k}} \\ &= \overline{u_i'' u_j''(\rho u_k)_{,k}} + \overline{(\rho u_i'' u_j''\widetilde{u}_k)_{,k}} + \overline{(\rho u_i'' u_j'' u_k'')_{,k}} \\ &= (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} + \overline{(\rho u_i'' u_j'' u_k'')_{,k}} + \overline{u_i'' u_j''(\rho u_k)_{,k}} \\ \mathcal{R}_{c2} &= \overline{u_i''\widetilde{u}_j(\rho u_k)_{,k} + u_j''\widetilde{u}_i(\rho u_k)_{,k}} + \overline{\rho u_i'' u_k(\widetilde{u}_j)_{,k} + \rho u_j'' u_k(\widetilde{u}_i)_{,k}} \\ &= \overline{(u_i''\widetilde{u}_j + u_j''\widetilde{u}_i)(\rho u_k)_{,k}} + \overline{\rho u_i'' u_k''\widetilde{u}_{j,k} + \rho u_j'' u_k''\widetilde{u}_{i,k}} + \cancel{\overline{\rho u_i''\widetilde{u}_k(\widetilde{u}_j)_{,k} + \rho u_j''\widetilde{u}_k(\widetilde{u}_i)_{,k}}} \\ &= \mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k} + \overline{(u_i''\widetilde{u}_j + u_j''\widetilde{u}_i)(\rho u_k)_{,k}}\end{aligned}$$

Collecting the left-hand-side we find the general formulation of the Reynolds stress equations:

$$\mathcal{R}_t + \mathcal{R}_c = \frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} + (\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) + \overline{(\rho u''_i u''_j u''_k)_{,k}} + \cancel{\overline{(u''_i u''_j + u''_i \widetilde{u}_j + u''_j \widetilde{u}_i)\left(\frac{\partial \rho}{\partial t} + (\rho u_k)_{,k}\right)}}$$

$$= \frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} + (\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) + \overline{(\rho u''_i u''_j u''_k)_{,k}}$$

and therefore the Reynolds stress equations are given by

$$\frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} = \mathcal{R}_p + \mathcal{R}_{\boldsymbol{\tau}} - (\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) - \overline{(\rho u''_i u''_j u''_k)_{,k}} \tag{49}$$

The triple velocity correlation is usually combined with others, but sometimes written explicitly. It can be found as the combination

$$\overline{\rho u''_i u''_j u''_k} = \overline{\rho u_i u_j u_k} - \overline{\rho u_j u_k}\widetilde{u}_i - \overline{\rho u_k u_i}\widetilde{u}_j - \overline{\rho u_i u_j}\widetilde{u}_k + 2\overline{\rho}\widetilde{u}_i\widetilde{u}_j\widetilde{u}_k$$

A.2.2 Formulation using instantaneous values of molecular stresses

In his contribution [7] in the AGARD R817 report [8], Knight uses the instantaneous values of the pressure p and molecular stress $\boldsymbol{\tau}$ rather than their fluctuations, so that the Reynolds stress equation reads:

$$\frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} = A_{ij} + B_{ij} + C_{ij} - D_{ij} \tag{50}$$

The *production* term A_{ij} is the third term on the right-hand-side of (49)

$$A_{ij} = -(\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) \tag{51}$$

To find the other terms, the correlations between the stress divergence terms and the velocity fluctuations are first converted as follows

$$\mathcal{R}_p = \overline{u''_i p_{,j} + u''_j p_{,i}} = \overline{(p u''_i \delta_{jk} + p u''_j \delta_{ik})_{,k}} - \overline{p(u''_{i,j} + u''_{j,i})}$$

$$\mathcal{R}_{\boldsymbol{\tau}} = \overline{u''_i \tau_{jk,k} + u''_j \tau_{ik,k}} = \overline{(u''_i \tau_{jk} + u''_j \tau_{ik})_{,k}} - \overline{\tau_{jk} u''_{i,k} + \tau_{ik} u''_{j,k}}$$

The first terms of both $\mathcal{R}_p$ and $\mathcal{R}_{\boldsymbol{\tau}}$ are combined with the last term in (49) to form the *diffusion* term

$$B_{ij} = \left\{ -\overline{\rho u''_i u''_j u''_k} + \overline{u''_j \tau_{ik}} + \overline{u''_i \tau_{jk}} - \overline{p u''_i}\delta_{jk} - \overline{p u''_j}\delta_{ik} \right\}_{,k} \tag{52}$$

The remaining terms are then grouped in two stress-velocity gradient correlation terms, respectively the *pressure-strain* C_{ij} and *dissipation* D_{ij}

$$C_{ij} = \overline{p u''_{i,j} + p u''_{j,i}} \tag{53}$$

$$D_{ij} = \overline{\tau_{ik} u''_{j,k} + \tau_{jk} u''_{i,k}} \tag{54}$$

Notice that this form does not revert directly to the standard incompressible formulation.

A.2.3 Formulations using Reynolds averaged fluctuations of pressure and viscous stresses

A second possibility is to split the pressure and stress into their *Reynolds averages* and corresponding *fluctuations*

$$p = \overline{p} + p' \qquad\qquad \boldsymbol{\tau} = \overline{\boldsymbol{\tau}} + \boldsymbol{\tau}'$$

Since the stress contributions in the Favre-averaged Navier-Stokes equations appear through Reynolds rather than Favre averages, this choice is logical. Moreover, this choice is consistent with incompressible formulations, as illustrated in section A.3.

A.2.3.1 Gerolymos and Vallet [3] as well as Sarkar *et al.*[10] provide similar formulations for the Reynolds stress equations, using this approach, whereas Huang *et al.* [5] use a similar decomposition for the turbulent kinetic energy equation. The correlations between the instantaneous stress divergence and the velocity fluctuations are decomposed as follows:

$$\begin{aligned}
\mathcal{R}_p &= \overline{u_i''\overline{p_{,j}} + u_j''\overline{p_{,i}}} + \overline{u_i''p'_{,j} + u_j''p'_{,i}} \\
&= (\overline{u_i''}\ \overline{p_{,j}} + \overline{u_j''}\ \overline{p_{,i}}) + \overline{(p'u_i''\delta_{jk} + p'u_j''\delta_{ik})_{,k}} - \overline{p'(u''_{i,j} + u''_{j,i})} \\
\mathcal{R}_{\boldsymbol{\tau}} &= \overline{u_i''\overline{\tau_{jk,k}} + u_j''\overline{\tau_{ik,k}}} + \overline{u_i''\tau'_{jk,k} + u_j''\tau'_{ik,k}} \\
&= (\overline{u_i''}\ \overline{\tau_{jk,k}} + \overline{u_j''}\ \overline{\tau_{ik,k}}) + \overline{(u_i''\tau'_{jk} + u_j''\tau'_{ik})_{,k}} - \overline{\tau'_{jk}u''_{i,k} + \tau'_{ik}u''_{j,k}}
\end{aligned}$$

Notice that the first terms, involving the averaged values of p and $\boldsymbol{\tau}$, disappear for incompressible flow since $\overline{\mathbf{u'}} = 0$. However, Favre fluctuations are used and therefore $\overline{\mathbf{u''}} \neq 0$. This then leads to the following formulation, following Gerolymos and Vallet [3][1]:

$$\frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} = P_{ij} + D_{ij} + \Phi_{ij} - \epsilon_{ij} + \frac{2}{3}\overline{p'u''_{k,k}\delta_{ij}} + K_{ij} \tag{55}$$

The terms in (55) are defined as follows :

- the *production* term is the same as A in section A.2.2

$$P_{ij} = -(\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) \tag{56}$$

- the *diffusion*

$$D_{ij} = T_{ijk,k} = \left(-\overline{\rho u_i''u_j''u_k''} - \overline{p'u_i''\delta_{jk} + p'u_j''\delta_{ik}} + \overline{u_i''\tau'_{jk} + u_j''\tau'_{ik}}\right)_{,k} \tag{57}$$

[1] The notation is not fully consistent with [3] due to the definition $\mathcal{R}_{ij} = \overline{\rho u_i''u_j''}$, and the conversion to the Favre average was not always explicitly used, for instance $\overline{\rho u_i''u_j''u_k''}$ is retained instead of $\overline{\rho}\widetilde{u_i''u_j''u_k''}$.

- correlations between fluctuating pressure and strain are split into the *redistribution* term

$$\Phi_{ij} = \Pi_{ij} = \overline{p'(u''_{i,j} + u''_{j,i} - \frac{2}{3}u''_{k,k}\delta_{ij})} \tag{58}$$

and the *pressure-dilatation* term

$$\frac{2}{3}\overline{p' u''_{k,k}\delta_{ij}} \tag{59}$$

- the correlations between fluctuating stress and strain then result in the *dissipation*

$$\epsilon_{ij} = \overline{\tau'_{jk}u''_{i,k} + \tau'_{ik}u''_{j,k}} \tag{60}$$

- finally, the remaining terms are grouped in the *density fluctuation effects*

$$K_{ij} = -u''_i\left(\overline{p_{,j}} - \overline{\tau_{jk,k}}\right) - u''_j\left(\overline{p_{,i}} - \overline{\tau_{ik,k}}\right) \tag{61}$$

Note that Gerolymos and Vallet consider K_{ij} to be negligible in their model development. For verifying the residual of the exact equations, this term should however be included.

A.2.3.2 Grigoriev *et al.* [4] use the same stress decomposition for the compressible Reynolds stress equation, but a different organisation of the terms

$$\begin{aligned}\frac{\partial \mathcal{R}_{ij}}{\partial t} + \left(\mathcal{R}_{ij}\widetilde{u}_k\right)_{,k} + \left(\overline{\rho u''_i u''_j u''_k}\right)_{,k} = &- \left(\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}\right) \\ &- \overline{u''_i\left(p'_{,j} - \tau'_{jk,k}\right)} - \overline{u''_j\left(p'_{,i} - \tau'_{ik,k}\right)} \\ &+ \mathring{u}_i\left(\overline{p}_{,j} - \overline{\tau}_{jk,k}\right) + \mathring{u}_j\left(\overline{p}_{,i} - \overline{\tau}_{ik,k}\right)\end{aligned} \tag{62}$$

where $\mathring{u}_i$ was defined in equation 44 in section A.1.1.

A.2.4 Formulation using mixed fluctuations of molecular stresses

Finally a hybrid decomposition of the pressure and viscous stresses can be used:

$$p = \overline{p} + p' \qquad\qquad \boldsymbol{\tau} = \widetilde{\boldsymbol{\tau}} + \boldsymbol{\tau}''$$

This decomposition is only superficially more consistent than that in section A.2.3. The use of the Favre average of the stress is consistent with its computation from the Favre averages of velocity in (41), but the stress appearing in the averaged momentum and energy equation is still Reynolds averaged.

This decomposition is used by Khlifi and Lili [6][2] as well as Adumitroaie *et al.* [1]. Following Khlifi and Lili, the Reynolds stress equation becomes:

$$\frac{\partial \mathcal{R}_{ij}}{\partial t} + (\mathcal{R}_{ij}\widetilde{u}_k)_{,k} = P_{ij} + D_{ij} + \phi_{ij} - \epsilon_{ij} + T_{ij} \tag{63}$$

The terms appearing in (63) are

- production

$$P_{ij} = -(\mathcal{R}_{ik}\widetilde{u}_{j,k} + \mathcal{R}_{jk}\widetilde{u}_{i,k}) \tag{64}$$

- diffusion

$$D_{ij} = \left(-\overline{\rho u_i'' u_j'' u_k''} - \overline{p' u_i'' \delta_{jk} + p' u_j'' \delta_{ik}} + \overline{u_i'' \tau_{jk}'' + u_j'' \tau_{ik}''}\right)_{,k} \tag{65}$$

- correlations between fluctuating pressure and velocity gradient resulting in the *redistribution* term

$$\phi_{ij} = \overline{p'(u_{i,j}'' + u_{j,i}'')} \tag{66}$$

- the correlations between fluctuating stress and velocity gradient resulting in the *dissipation*

$$\epsilon_{ij} = \overline{\tau_{jk}'' u_{i,k}'' + \tau_{ik}'' u_{j,k}''} \tag{67}$$

- finally, the remaining terms are grouped in

$$T_{ij} = -\overline{u_i''}\ \overline{p_{,j}} - \overline{u_j''}\ \overline{p_{,i}} + \overline{u_i''}\ \widetilde{\tau_{jk,k}} + +\overline{u_j''}\ \widetilde{\tau_{ik,k}} \tag{68}$$

A.3 Level 2 - Incompressible Reynolds stress equation

By "incompressible Reynolds stress equations" we mean an equation that describes the evolution of the Reynolds stress $\mathcal{R}^*_{ij} = \overline{\rho u_i' u_j'}$ involving Reynolds fluctuations[3].

A.3.1 Formulation when using compressible codes

Next to the compressible Reynolds stress equation (62) mentioned previously, Grigoriev *et al.* [4] derived a consistent equation for the incompressible Reynolds stress equation (*i.e.* involving Reynolds fluctuations of the velocity) which is also valid in case of compressible flows:

$$\begin{aligned}\frac{\partial \mathcal{R}^*_{ij}}{\partial t} + \left(\mathcal{R}^*_{ij}\overline{u}_k\right)_{,k} + \left(\overline{\rho u_i' u_j' u_k'}\right)_{,k} = &- \left(\mathcal{R}^*_{ik}\overline{u}_{j,k} + \mathcal{R}^*_{jk}\overline{u}_{i,k}\right) \\ &- \left(\overline{u_i'\left(p'_{,j} - \tau'_{jk,k}\right)} + \overline{u_j'\left(p'_{,i} - \tau'_{ik,k}\right)}\right) \\ &- \overline{\rho}\left(\mathring{u}_i D_t u_j + \mathring{u}_j D_t u_i\right)\end{aligned} \tag{69}$$

[2] The paper of Khlifi and Lili [6] has a typo: the divergence in the dissipation term d_{ij} was forgotten in (15).
[3] Note that the density is inside the average.

with

$$D_t u_i = -\overline{u_k' u_{i,k}'} - \overline{\left(\frac{p_{,j} - \tau_{jk,k}}{\rho}\right)}$$

A.3.2 Standard incompressible formulation

For incompressible flows, the Reynolds stress equation is usually written as

$$\frac{\partial \mathcal{R}_{ij}^*}{\partial t} + \left(\mathcal{R}_{ij}^* \overline{u}_k\right)_{,k} = P_{ij}^* + \Phi_{ij}^* + D_{ij}^{*,1} + D_{ij}^{*,2} + D_{ij}^{*,3} - \epsilon_{ij}^* \quad (70)$$

with

$$P_{ij}^* = -\left(\mathcal{R}_{ik}^* \overline{u}_{j,k} + \mathcal{R}_{jk}^* \overline{u}_{i,k}\right) \qquad \Phi_{ij}^* = \overline{p' \left(u_{i,j}' + u_{j,i}'\right)} \qquad \epsilon_{ij} = 2\mu \, \overline{u_{i,k}' u_{j,k}'}$$

$$D_{ij}^{*,1} = -\left(\overline{\rho u_i' u_j' u_k'}\right)_{,k} \qquad D_{ij}^{*,2} = -\left(\overline{p' \left(u_i' \delta_{jk} + u_j' \delta_{ik}\right)}\right)_{,k} \qquad D_{ij}^{*,3} = \mu \left(\overline{u_i' u_j'}\right)_{,kk} = \nu \mathcal{R}_{ij,kk}^*$$

For flows with compressibility effects, equation (70) is equivalent to (69), when the following correction terms are added

$$-\overline{\rho} \left(\mathring{u}_i D_t u_j + \mathring{u}_j D_t u_i\right) + \frac{\mu}{3} \, \overline{u_i' u_{k,kj}' + u_j' u_{k,ki}'} \quad (71)$$

A.4 Level 2 - Check of the equivalence of the incompressible and the compressible form of the Reynolds stress equations following Gerolymos and Vallet

We will check the equivalence of the compressible form of Gerolymos and Vallet and the standard incompressible Reynolds stress equations. The Reynolds stress equation following Gerolymos *et al.* reads

$$\mathcal{R}_{ij,t} + \left(\mathcal{R}_{ij} \widetilde{u}_k\right)_{,k} = P_{ij} + D_{ij} + \Phi_{ij} + \Phi_{ij}' - \epsilon_{ij} + K_{ij}$$

with the viscous diffusion and dissipation terms

$$D_{ij}^3 = \left(\overline{u_i'' \tau_{jk}' + u_j'' \tau_{ik}'}\right)_{,k} \qquad \epsilon_{ij} = \overline{\tau_{jk}' u_{i,k}'' + \tau_{ik}' u_{j,k}''}$$

and the incompressible form

$$\mathcal{R}_{ij,t}^* + \left(\mathcal{R}_{ij}^* \overline{u}_k\right)_{,k} = P_{ij}^* + D_{ij}^{*,1} + D_{ij}^{*,2} + D_{ij}^{*,3} + \Phi_{ij}^* - \epsilon_{ij}^*$$

with the viscous diffusion and dissipation terms

$$D_{ij}^{*,3} = \nu \mathcal{R}_{ij,kk}^* \qquad \epsilon_{ij}^* = 2\mu \, \overline{u_{i,k}' u_{j,k}'}$$

We will now check the equivalence for the case where the flow is incompressible, *i.e.*

$$u''_i = u'_i \qquad u'_{i,i} = 0 \qquad \tau'_{ij} = \mu\left(u'_{i,j} + u'_{j,i}\right)$$

In these conditions, the dissipation following Gerolymos and Vallet can be developed as

$$\begin{aligned}
\epsilon_{ij} &= \left(\overline{u'_i\tau'_{jk} + u'_j\tau'_{ik}}\right)_{,k} \\
&= \mu\overline{\left(\left(u'_{j,k} + u'_{k,j}\right)u'_{i,k} + \left(u'_{i,k} + u'_{k,i}\right)u'_{j,k}\right)} \\
&= 2\mu\overline{u'_{i,k}u'_{j,k}} + \mu\overline{u'_{k,j}u'_{i,k} + u'_{k,i}u'_{j,k}} \\
&= \epsilon^*_{ij} + \mu\overline{u'_{k,j}u'_{i,k} + u'_{k,i}u'_{j,k}}
\end{aligned} \tag{72}$$

The incompressible viscous diffusion term can be developed as

$$D^{*,3}_{ij} = \nu\mathcal{R}^*_{ij,kk} = \mu\left(u'_iu'_j\right)_{,kk} = \mu\ \overline{u'_{i,kk}u'_j + 2u'_{i,k}u'_{j,k} + u'_iu'_{j,kk}} \tag{73}$$

while from the compressible equations the viscous diffusion is

$$\begin{aligned}
D^3_{ij} &= \left(\overline{u'_i\tau'_{jk} + u'_j\tau'_{ik}}\right)_{,k} \\
&= \mu\overline{u'_i\left(u'_{j,k} + u'_{k,j}\right) + u'_j\left(u'_{i,k} + u'_{k,i}\right)}_{,k} \\
&= \mu\overline{u'_{i,kk}u'_j + 2u'_{i,k}u'_{j,k} + u'_iu'_{j,kk}} + \mu\overline{u'_{i,k}u'_{k,j} + u'_{k,i}u'_{j,k}} + \cancel{\mu\overline{u'_iu'_{k,jk} + u'_ju'_{k,ik}}} \\
&= D^{*,3}_{ij} + \mu\overline{u'_{i,k}u'_{k,j} + u'_{k,i}u'_{j,k}}
\end{aligned} \tag{74}$$

The compressible form of the dissipation terms is the closest to a componentwise decomposition of the dissipation of the mechanical/kinetic energy $\epsilon = 2\tau_{ij}\mathcal{S}_{ij}$ while the reorganisation of the incompressible form seems targeted to obtain a straightforward diffusion of the Reynolds stress itself (see Batchelor [2], Tennekes and Lumley [11] or Pope [9]). We see therefore that even when $u''_i = u'_i$, the incompressible and compressible versions of neither the viscous diffusion nor the dissipation are fully equivalent but their sum is. This means one has to take care when using these terms for model development.

B Guidelines for the acquisition of statistics

B.1 One-point correlations

B.1.1 Simple averages

We start with the accumulation of direct averages, for instance of the density velocity correlation. Obviously, the most straightforward approximation of the average after n time steps is

$$\overline{\rho u_i} \approx \overline{\rho u_i}^n = \frac{1}{n}\sum_{t=1}^{n} \rho^t u_i^t \tag{75}$$

with ρ^l, u_j^l the instantaneous values at time t. This average is computed through the recurrence

$$\overline{\rho u_i}^n = \frac{(n-1)\overline{\rho u_j}^{n-1} + \rho^n u_j^n}{n} \tag{76}$$

The approximation to the Favre average of the velocity is simply found as

$$\widetilde{u}_i \approx \widetilde{u}_i^n = \frac{\overline{\rho u_i}^n}{\overline{\rho}^n} \tag{77}$$

B.1.2 Correlations between fluctuations

Some care has to be taken when considering fluctuations, since they are supposed to be computed *with respect to a converged average.* This means that correlations between fluctuations can not be accumulated in the same way as a direct average. Take for instance the Reynolds stress. The latter is computed as

$$\mathcal{R}_{ij} = \overline{\rho u_i'' u_j''} = \overline{\rho(u_i - \widetilde{u}_i)(u_j - \widetilde{u}_j)} \approx \mathcal{R}_{ij}^n = \frac{1}{n}\sum_{t=1}^{n} \rho^t (u_i^t - \widetilde{u}_i)(u_j^t - \widetilde{u}_j) \tag{78}$$

Note that $\widetilde{u}_i$ is supposed to be the *exact* Favre average of the velocity. This seems to imply we need to converge the Favre average first before starting the accumulation of the Reynolds stress. This is undesirable since it has profound implications both on the quality and computational cost of the accumulation procedure:

- the samples used for the average are not used for the accumulation of the Reynolds stress, thus reducing the statistical convergence of the latter;
- conversely, none of the samples used for the Reynolds stress are used for the averages;
- the approximation of the Reynolds stress depends on the quality of the average *which is no longer improved.*

Fortunately, this prior convergence is not necessary and both averages $\overline{\rho}$ and $\widetilde{u}_i$ as well as the Reynolds stress $\mathcal{R}_{ij}$ can (and should) be accumulated at the same time. At each time step, the accumulated correlations should be computed using the latest average available *for each sample in the series*, leading to

$$\mathcal{R}_{ij} \approx \mathcal{R}_{ij}^n = \overline{\rho u_i'' u_j''}^n = \frac{1}{n} \sum_{t=1}^{n} \overline{\rho^t (u_i^t - \widetilde{u}_i^n)(u_j^t - \widetilde{u}_j^n)} \tag{79}$$

Notice the difference in superscript indices for the instantaneous and averaged quantities. The most straightforward way, which also is the least sensitive to round-off error, is to accumulate simple "baseline" correlations between the velocities and density

$$\overline{\rho u_i u_j} \approx \overline{\rho u_i u_j}^n = \frac{1}{n} \sum_{t=1}^{n} \rho^t u_i^t u_j^t \tag{80}$$

and only compute the Reynolds stress when needed (*e.g.* for exporting to disk), as a post-processing step:

$$\mathcal{R}_{ij}^n = \overline{\rho u_i u_j}^n - \overline{\rho}^n \widetilde{u}_i^n \widetilde{u}_j^n \tag{81}$$

Other correlations can be constructed in a similar way. For instance, the approximation of the triple velocity correlation then reads

$$\begin{aligned} \overline{\rho u_i'' u_j'' u_k''} &= \overline{\rho u_i u_j u_k} - \overline{\rho u_i u_j} \widetilde{u}_k - \overline{\rho u_j u_k} \widetilde{u}_i - \overline{\rho u_k u_i} \widetilde{u}_j + 2 \overline{\rho} \widetilde{u}_i \widetilde{u}_j \widetilde{u}_k \\ &\approx \overline{\rho u_i u_j u_k}^n - \overline{\rho u_i u_j}^n \ \widetilde{u}_k^n - \overline{\rho u_j u_k}^n \ \widetilde{u}_i^n - \overline{\rho u_k u_i}^n \ \widetilde{u}_j^n + 2 \overline{\rho}^n \widetilde{u}_i^n \widetilde{u}_j^n \widetilde{u}_k^n \end{aligned} \tag{82}$$

Accumulating the final correlations directly would not only increase the "on-board" storage, but render the accumulation much more complicated and even require the storage of additional auxiliary quantities.

B.1.3 Partitioning of the averaging window

It is difficult to verify during the run when exactly the stationary regime is obtained. Therefore, it is recommended to keep regular checkpoints such that the actual averaging window can still be corrected. We propose that a checkpoint at time t^n contains the averages and baseline correlations over the full history from the start of the statistics acquisition - supposedly at t^0 - up to t^n.

Say we find that the regime is finally achieved at t^m, then we can compose the approximation of the average of $\overline{a}$ or baseline correlation $\overline{a\ b}$ as

$$\overline{a}^{m:n} = \frac{1}{n-m} \left(n\ \overline{a}^n - m\ \overline{a}^m \right) \tag{83}$$

$$\overline{ab}^{m:n} = \frac{1}{n-m} \left(n\ \overline{ab}^n - m\ \overline{ab}^m \right) \tag{84}$$

where $\overline{a}^n$ denotes the average up to t^n and $\overline{a}^{n:m}$ indicates the average between t^n and t^m.

During the computation, the code then merely has to read the checkpoint at t^m and then perform this recombination of the baseline correlations, before computing and exporting the actual correlations. Note that storing the final correlations in the checkpoint would render this operation much more complex.

Alternatively the checkpoint could store the average t^n over the window between the current and the previous checkpoint, however this would require storing (and reading) all checkpoints over a given interval to compute the average over this interval.

B.1.4 Recommendations

- for the reasons outlined in sections B.1.1, B.1.2 and B.1.3, only direct averages and baseline correlations should be stored in the checkpoint, whereas the actual correlations between fluctuations will be computed via post-processing. Lists of averages and baseline correlations needed for reconstructing the data sets are provided in appendix B.2;

- in principle statistics can be accumulated only if the flow has reached statistic stationarity. Since the latter is hard to prove / estimate, one should partition the averaging time in several windows. This then allows to correct the average a posteriori. Using checkpoint data with direct averages up to the current time step, one then decides a posteriori which intervals to keep in the average following the approach discussed in B.1.3;

- if the flow possesses homogeneous directions, the averaging procedure can include a spatial average over these directions; the result may then be stored on the associated periodic plane. This however does not imply any simplification (*i.e.* reduction of indices) of the resulting correlations.

B.2 Minimum required volumetric data in checkpoints

B.2.1 Compressible codes

Table 4 lists a minimal set of averages that allow to reconstruct all of the quantities of interest in table 1 using the accumulation approach (81). This is the minimal set of data which should be accumulated during the computation and therefore stored in the checkpoint/restart files.

Quantity		**#**
Level 1 - averaged Navier-Stokes equations		
Averaged density	$\overline{\rho}$	1
Averaged pressure	$\overline{p}$	1
Density - velocity correlation	$\overline{\rho u_i}$	3

Density - temperature correlation	$\overline{\rho T}$	1
Averaged shear stress	$\overline{\tau_{ij}}$	6
Averaged heat flux	$\overline{q_i}$	3
Density weighted velocity autocorrelation	$\overline{\rho u_i u_j}$	6
Density weighted temperature - velocity correlation	$\overline{\rho T u_i}$	3
Velocity - shear stress correlation	$\overline{u_i \tau_{jk}}$	18
Density - velocity triple correlation	$\overline{\rho u_i u_j u_k}$	10
Cumulative total		**52**
Level 1 - additional quantities		
Averaged velocity	$\overline{u_i}$	3
Averaged temperature	$\overline{T}$	1
Velocity autocorrelation	$\overline{u_i u_j}$	6
Temperature - velocity correlation	$\overline{T u_i}$	3
Density autocorrelation	$\overline{\rho\rho}$	1
Pressure autocorrelation	$\overline{pp}$	1
Temperature autocorrelation	$\overline{TT}$	1
Cumulative total		**68**
Level 2 - Reynolds stress equations		
Pressure - velocity correlation	$\overline{p u_i}$	3
Pressure - strain rate correlation	$\overline{p(u_{i,j} + u_{j,i})}$	6
Shear stress - velocity gradient correlation	$\overline{\tau_{ik} u_{j,k} + \tau_{jk} u_{i,k}}$	6
Velocity gradient autocorrelation	$\overline{u_{i,k} u_{j,k}}$	6
Averaged specific stress resultant	$\overline{(p_{,i} - \tau_{jk,k})/\rho}$	3
Velocity - velocity divergence gradient correlation	$\overline{u_i u_{k,kj} + u_j u_{k,ki}}$	6
Cumulative total		**98**

Table 4: List of baseline quantities, required to reconstruct the quantities of interest of table 1. These terms are also sufficient to reconstruct all terms in table 6.

B.2.2 Incompressible codes

Table 5 lists a minimal set of averages that allow to reconstruct all of the quantities of interest in table 2 using the accumulation approach (81). This is the minimal set of data which should be accumulated during the computation and therefore present in a checkpoint/restart file.

Quantity		#
Level 1 - averaged Navier-Stokes equations		
Averaged pressure	$\overline{p}$	1
Averaged velocity	$\overline{u_i}$	3

Averaged temperature	$\overline{T}$	1
Velocity autocorrelation	$\overline{u_i u_j}$	6
Temperature - velocity correlation	$\overline{T u_i}$	3
Pressure - velocity correlation	$\overline{p u_i}$	3
Cumulative total		**17**
Level 1 - additional quantities		
Pressure autocorrelation	$\overline{pp}$	1
Temperature autocorrelation	$\overline{TT}$	1
Cumulative total		**19**
Level 2 - Reynolds stress equations		
Triple velocity correlation	$\overline{u_i u_j u_k}$	10
Velocity - velocity gradient correlation	$\overline{u_k u_{i,k}}$	3
Velocity gradient autocorrelation	$\overline{u_{i,k} u_{j,k}}$	6
Pressure - strain rate correlation	$\overline{p(u_{i,j} + u_{j,i})}$	6
Shear stress - velocity correlation	$\overline{\tau_{ij} u_k}$	18
Cumulative total		**62**

Table 5: List of baseline quantities, required to reconstruct the quantities of interest in table 2.

B.3 Integral time scales

B.3.1 Procedure

In practice, the time correlation $\mathcal{C}_a(\tau)$ can only be known at discrete values of τ, with a resolution corresponding to a multiple of the computation time step $N\Delta t$. Since we need to store previous snapshots, this integral can therefore only be accumulated at time steps $t_n = nN\Delta t$, $n = 1 \ldots \infty$, for discrete values of the time separation $\tau_k = kN\Delta t$, $k = 0 \ldots K$. The accumulation procedure therefore should construct the time correlation between the full values

$$\tilde{\mathcal{C}}_a^n(\tau_k) \hat{=} \frac{\left((n-1)\left(\mathcal{C}_a^{n-1}(kN\Delta t) + \overline{a}^{n-1}\overline{a}^{n-1}\right) + a((n-k)N\Delta t)\ a(nN\Delta t)\right)}{n} \tag{85}$$

Only at the time of the export, these values are post-processed, *e.g.* using the trapezoid rule

$$\tau_a^n \hat{=} \frac{N\Delta t}{\mathcal{C}_a^n(0) - \overline{a}^n\overline{a}^n} \left(\left(\sum_{k=0}^{K-1} \frac{\mathcal{C}_a^n(\tau_k) + \mathcal{C}_a^n(\tau_{k+1})}{2}\right) - K\ \overline{a}^n\overline{a}^n\right) \tag{86}$$

B.3.2 Recommendations

- During the computation and in the checkpoints, the code should store the time correlations between the full values, not between the fluctuations for the same reasons mentioned for the one-point correlations: *i.e.* simplifying accumulation and restart and enable the recombination of several acquisition windows.

- The computation and storage cost depends on the number of values K for which the correlation is computed. This depends in turn on the resolution in time $N\Delta t$, as well as well as the maximum value of τ. The truncation of the series should satisfy the following criteria
  - the resolution $N\Delta t$ should be at least 20 times smaller than τ_a;
  - the maximum time length should be larger than τ_a;
  - the statistics should also be partitioned.

  This means that at any time during the acquisition of statistics, the computation should keep track of 20 solution snapshots. The actual value of $N\Delta t$ unfortunately has to be assessed during the computation, and its ideal value may vary over the domain.

C Optional data sets for compressible flow solvers

Table 6 provides an optional list of data for compressible flow solvers, which allow to obtain the compressible Reynolds stress equations proposed by Knight (50), Khlifi *et al.* (63) and Grigoriev *et al.* (62), as well as the incompressible Reynolds stress equation proposed by Grigoriev *et al.* (69). Note that similar correlations appear as in table 1 with different combinations of instantaneous values as well as Reynolds and Favre fluctuations; some of these are effectively the same as in the terms used in the Gerolymos formulation and therefore not repeated here.

Quantity		**#**
Level 2 - Reynolds stress equations		
Pressure - velocity correlation	$\overline{pu_i''}$	3
Pressure - strain rate correlation	$\overline{p(u_{i,j}'' + u_{j,i}'')}$	6
Velocity - pressure gradient correlation	$\overline{u_i'p_{,j}' + p_{,i}'u_j'}$	6
Shear stress - velocity gradient correlation	$\overline{\tau_{ik}u_{j,k}'' + \tau_{jk}u_{i,k}''}$	6
Shear stress - velocity gradient correlation	$\overline{\tau_{ik}''u_{j,k}'' + \tau_{jk}''u_{i,k}''}$	6
Velocity - shear stress divergence correlation	$\overline{u_i'\tau_{jk,k}' + u_j'\tau_{ik,k}'}$	6
Cumulative total		**33**
Level 2 - incompressible Reynolds stress equations		
Triple velocity correlation	$\overline{\rho u_i'u_j'u_k'}$	10
Velocity - velocity gradient correlation	$\overline{u_i'u_{j,i}'}$	3
Specific stress resultant	$\overline{(p_{,i} - \tau_{ik,k})/\rho}$	3
Velocity - velocity divergence gradient	$\overline{u_i'u_{k,kj}' + u_j'u_{k,ki}'}$	6

Level 2 - Incompressible Reynolds stress equations budget terms		
Convection C^*_{ij}	$\left(\mathcal{R}^*_{ij}\overline{u}_k\right)_{,k}$	6
Production P^*_{ij}	$-\left(\mathcal{R}^*_{ik}\overline{u}_{j,k} + \mathcal{R}^*_{jk}\overline{u}_{i,k}\right)$	6
Turbulent diffusion D^{1*}_{ij}	$-\left(\overline{\rho u'_i u'_j u'_k}\right)_{,k}$	6
Turbulent diffusion D^{2*}_{ij}	$-\left(\overline{p'\left(u'_i\delta_{jk} + u'_j\delta_{ik}\right)}\right)_{,k}$	6
Molecular diffusion D^{3*}_{ij}	$\mu\left(\overline{u'_i u'_j}\right)_{,kk}$	6
Pressure strain Φ^*_{ij}	$\overline{p'\left(u'_{i,j} + u'_{j,i}\right)}$	6
Dissipation ϵ^*_{ij}	$2\mu\overline{u'_{i,k}u'_{j,k}}$	6
Correction term	$-\overline{\rho}\left(\mathring{u}_i D_t u_j + \mathring{u}_j D_t u_i\right) + \frac{\mu}{3}\ \overline{u'_i u'_{k,kj} + u'_j u'_{k,ki}}$	6
Cumulative total		**103**

Table 6: List of additional volume statistical quantities, including the missing terms† of the compressible formulations of equations (50), (63) and (62); and those* in equation (70).

With

$$D_t u_i = -\,\overline{u'_k u'_{i,k}} - \overline{\left(\frac{p_{,j} - \tau_{jk,k}}{\rho}\right)}$$

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