

A scale invariance criterion for LES parametrizations

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Abstract

Turbulent kinetic energy cascades in fluid dynamical systems are usually characterized by scale invariance. However, representations of subgrid scales in large eddy simulations do not necessarily fulfill this constraint. So far, scale invariance has been considered in the context of isotropic, incompressible, and three-dimensional turbulence. In the present paper, the theory is extended to compressible flows that obey the hydrostatic approximation, as well as to corresponding subgrid-scale parametrizations. A criterion is presented to check if the symmetries of the governing equations are correctly translated into the equations used in numerical models. By applying scaling transformations to the model equations, relations between the scaling factors are obtained by demanding that the mathematical structure of the equations does not change.

The criterion is validated by recovering the breakdown of scale invariance in the classical Smagorinsky model and confirming scale invariance for the Dynamic Smagorinsky Model. The criterion also shows that the compressible continuity equation is intrinsically scale-invariant. The criterion also proves that a scale-invariant turbulent kinetic energy equation or a scale-invariant equation of motion for a passive tracer is obtained only with a dynamic mixing length. For large-scale atmospheric flows governed by the hydrostatic balance the energy cascade is due to horizontal advection and the vertical length scale exhibits a scaling behaviour that is different from that derived for horizontal length scales.

Keywords: General fluid dynamics, Atmospheric physics; Scale invariance, GCMs, LES parametrizations

1 Introduction

To investigate the dynamics of fluids by means of numerical models, it is of paramount importance that the model applied for a particular purpose is physically and mathematically consistent (DALY and HARLOW, 1970; OBERLACK, 1997; GASSMANN, 2011). When ignoring this aspect, numerical models can nevertheless be applied with success as long as the limits of such a model are taken into account (cf. PETRIK et al., 2011). However, it can not be excluded that some unphysical model behaviour arises that questions the validity of the results obtained.

Physical and mathematical consistency means, among other things, that conservation laws, mathematically described by corresponding symmetries and invariances of the governing equations, must be taken into account. For instance, conservation of energy is connected to an invariance of the equations of motion with respect to a translation in time; spatial translational invariance is linked to the conservation of momentum, and rotational invariance is reflected by the conservation of angular momentum. These conservation laws are universally valid and independent from the effective length scale of the processes considered. In contrast to the conservation laws, scale invariance does not hold for the whole spectral range of scales and a conserved quantity corresponding to scale invariance that is valid for all scales does not exist. Nevertheless, by applying the Lagrangian formalism and Noether's theorem to scaling transformations of the effective Lagrangian, one may obtain under certain constraints a conserved quantity associated with scale invariance (FORGER and RÖMER, 2004). A profound discussion of the consistent treatment of scale invariance in geophysical fluid dynamics has not been done so far. In the present paper we make an attempt into this direction.

The Euler equations for constant density possess ten infinitesimal invariances or symmetries (OBERLACK, 2000): one in time, two for scales, three for translation (generalized Galileian), three for rotation, and one for pressure. When applying the Euler equations to the atmosphere and focusing on large scales, most of these symmetries are broken. In particular, the pressure invariance and the accelerated Galilei transformation (not the classical Galilei transformation for constant velocities), which are a direct consequence of incompressibility (OBERLACK, 2000), do not hold due to compressibility. Furthermore, for a shallow atmosphere the rotational invariance approximately holds only in the horizontal plane for subsynoptic and smaller scales. Finally, temporal scale invariance is explicitly broken for time scales \gg 1 hour mainly due to the diurnal cycle.

When looking at the turbulent kinetic energy cascade in the atmosphere, there is no single scale-invariant subrange covering the whole spectral range from planetary scales to the microscales where viscosity becomes important. Instead, the energy spectrum is piecewise governed by subranges where different terms of the gov-

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Figure 1: Schematic of the theoretical horizontal kinetic energy spectrum for the atmosphere (solid), and air-borne measurements after NASTROM and GAGE (1985, dotted).

erning equations become dominant. This is illustrated schematically in Fig. 1 for a horizontal kinetic energy spectrum typical for the upper troposphere. For example, the regime of isotropic turbulence (isotropic inertial subrange in Fig. 1), Kolmogorov's spectral theory (see, e.g., VALLIS (2006), chapter 8) assumes a broad inertial range between injection of kinetic energy and dissipation (by molecular friction). Between these scales, the kinetic energy is conservatively transferred to smaller and smaller scales. This picture holds only if we have self-similarity within the inertial range; that is, the Navier-Stokes equations (hereafter: NSE) are only scale-invariant as long as external forcing and internal friction are negligible for the scales that govern the inertial range. For isotropic turbulence, we find this behaviour between the outer or Ozmidov scale (where the transition to isotropic three-dimensional turbulence occurs) and the inner or Kolmogorov scale (where viscosity becomes relevant). The explanation of the mesoscale regime (anisotropic inertial subrange in Fig. 1) in the horizontal wavenumber spectrum is more complicated. A transition from a -3 to the -5/3 power law emerges, according to the observations of NASTROM and GAGE (1985), at scales of about 400 km.

For scales usually resolved in General Circulation Models (GCMs), the Primitive Equations (PE) can be used to describe the fluid. Here, the hydrostatic approximation only allows for a horizontal energy cascade. The assumption of an equipartition of the cascades of kinetic and (available) potential energy then leads to an aspect ratio of horizontal and vertical scales that approaches unity at the Ozmidov scale (see discussion of Stratified Turbulence by, e.g., LINDBORG, 2006; ; BRUNE and BECKER, 2013; ; AUGIER and LINDBORG, 2013). However, there remain still open questions concerning this concept. In contrast, the synoptic subrange is governed by quasi-geostrophic theory and is well understood as a result of a forward enstrophy cascade (e.g., BURROWS, 1976; BOER and SHEPHERD, 1983).

Due to the huge variety of physical processes at different scales, numerical models cannot resolve certain parts of the motion and subgrid-scale parameterizations are needed. It is trivial that GCMs, as an example of Large Eddy Simulations (hereafter: LES), do not simulate molecular friction explicitly. Thus, to obtain the energy cascade that maintains the Lorenz energy cycle (LORENZ, 1967), appropriate parameterizations of subgrid-scale processes are required. This is true also for regional numerical simulations (WILBY and WIGLEY, 1997; HAMILTON and OHFUCHI, 2008). On the other hand, microphysical simulations, e.g. of precipitation processes, have to incorporate molecular friction explicitly, whereas the Coriolis force is irrelevant in this case. Since numerical models are expected to represent the physical processes relevant at the scales resolved, the model equations (including parametrizations) should preserve the same properties as the governing equations at these scales (STULL, 1988; POPOVYCH and BIHLO, 2012).

To resolve part of the mesoscale horizontal energy cascade in a PE model, scale invariance of the applied subgrid-scale parametrization is necessary. In particular, a dissipation mechanism that covers both horizontal and vertical turbulent diffusion above the boundary layer is needed in order to mimic the transfer of energy from resolved to unresolved scales within the mesoscale anisotropic inertial range. A variety of approaches for turbulence parametrizations is known from the literature: the Eddy viscosity or Smagorinsky model (SMAGORINSKY, 1963; SMAGORINSKY, 1993), the nonlinear or gradient model (CLARK et al., 1979), the similarity model (BARDINA et al., 1980), the Dynamic Smagorinsky Model (hereafter: DSM, GERMANO et al., 1991), and the deconvolution method (STOLZ and ADAMS, 1999). Other new approaches make use of concepts that were initially developed in fields other than fluid dynamics and describe the turbulent diffusion and dissipation by scattering and annihilation processes of quasi-particles (called vorticons, BAUMERT, 2009) or they apply a renormalization group analysis approach well known from quantum field theory (YAKHOT and ORSZAG, 1986; BARBI and MÜNSTER, 2010). However, not all of these parametrizations ensure scale invariance. The widelyused classical Smagorinsky model does not ensure scale invariance, while the DSM is scale-invariant (OBER-LACK, 1997).

To demonstrate the importance of scale invariance for the closure used in atmospheric circulation models, Fig. 2 shows the horizontal kinetic energy spectrum for the upper troposphere from three different simulations with the *Kühlungsborn Mechanistic General Circulation Model* (KMCM, see BECKER and BURKHARDT (2007)). The model is applied here with very high resolution as in BRUNE and BECKER (2013). The only difference between the simulations is the formulation of horizontal diffusion. A classical Smagorinsky model using a con-



Figure 2: Kinetic energy spectrum in the upper troposphere from KMCM simulations. Dashed: constant mixing length $l_h = 11.6$ km; dotted: constant mixing length $l_h = 23.2$ km; solid: dynamic mixing length. The classical Smagorinsky model is not sufficient to simulate a reasonable KE spectrum for all resolved wavenumbers, while the simulation using a Dynamic Smagorinsky Model indicates a transition to a shallower slope from wavenumber 120. The thin dashed lines indicate k^{-3} and $k^{-5/3}$ power laws.

stant horizontal mixing length ($l_h = 11.6$ km, dashed line in Fig. 2) results in a reasonable spectrum only for the synoptic subrange with wavenumbers smaller than 100, while a clear -5/3 power law as expected for the mesoscales is not simulated. If we increase the mixing length to $l_h = 23.2$ km in order to reduce the energy at high wavenumbers, the slope of the spectrum becomes too steep at synoptic scales (dotted line in Fig. 2). In contrast, the spectrum obtained when using the DSM for horizontal diffusion (SCHAEFER-ROLFFS and BECKER, 2013) looks reasonable for both the synoptic scales and the mesoscales with the indication of a transition to a -5/3 power law in the mesoscales. Note that in other spectral models such a behaviour is obtained only by means of an unphysical hyperdiffusion.

The present paper is organized as follows: In Section 2 we discuss some general considerations about scale invariance. Section 3 provides a mathematical criterion that allows to check the consistency of the model equations, followed by the application to isotropic turbulence in Section 4. A discussion of the implications of the criterion for LES of atmospheric flows using the PE is given in Section 5. We close our investigation with some general remarks in Section 6.

2 General considerations about scale invariance

Consider a flow and its relevant variables such as fluid velocity or tracer concentration. We call the power spectrum of these variables scale-invariant if the two-point correlation function in wavenumber space obeys a cascade over a large wavenumber regime. For example, an energy cascade is present whenever energy is conservatively transferred over a finite range in wavenumber space (inertial range) from a well defined injection scale to a dissipation scale. The intermediate range is called inertial range and a necessary prerequisite is that the transfer rate or spectral flux, ϵ , is constant. The energy inertial range can develop only if the governing equations, for instance the NSE, exhibit the mathematical property that they can be rescaled without changing the mathematical structure of the equations (OBERLACK, 1997).

Hereafter, the scaling transformation of a variable a is defined as $a^* = e^{c_a}a$, with c_a denoting the scaling factor. We emphasize that this scaling has to be clearly distinguished from non-dimensionalizations. In the latter, we introduce characteristic lengths, times, and other quantities to obtain a non-dimensional version of the original equation. This often leads to dimensionless numbers such as the Reynolds number. Conversely, when rescaled, the variables only change their value, but keep their units. A scaling with the exponent of the scaling factor indicates the relationship of the procedure to the more general Weyl transformation.

It is known that the constraint of a constant spectral energy flux yields a fixed relation between the spatial and temporal scaling factors, $c_t = \frac{2}{3}c_x$, cf. Section 3. In the Euler equations, spatial and temporal scale invariance can independently hold or be broken. In contrast, for the NSE, where friction cannot be neglected, there exists only a combined scale invariance for the spatial and temporal dimensions, leading to a second competing relation between c_x and c_t in contradiction to Kolmogorov's theory: Let us consider a fluid with characteristic length scale \mathcal{L} , velocity scale \mathcal{U} , and (advective) time scale $\mathcal{T} = \mathcal{L}/\mathcal{U}$; then, to retain the same behaviour of the flow at different scales, one has to modify both \mathcal{L} and \mathcal{T} simultaneously such that the Reynolds number $Re = \mathcal{U}\mathcal{L}/\nu$ (where ν is the constant kinematic viscosity) is constant, cf. OBERLACK and ROSTECK (2010). The exclusion of a Kolmogorov regime at scales where molecular viscosity becomes relevant can easily be illustrated: Assume that the viscosity is constant. Dividing the spatial scale \mathcal{L} by a factor of 2, the velocity $\mathcal{U} = \mathcal{L}/\mathcal{T}$ must be multiplied by a factor of 2 to preserve the flow behaviour characterized by Re = const. In other words, the fluid has to move faster, and this is equivalent to shorten the advective time scale \mathcal{T} quadratically, i.e. in this particular case by a factor of four, due to $Re = \mathcal{L}^2 / \mathcal{T} v$. (As in real experiments the velocity often cannot be tuned to a predefined magnitude, a constant Reynolds number is often realized by using a different fluid with a lower viscosity.) Thus, assuming a constant viscosity leads to the second relation, $c_t = 2c_x$ which contradicts scale invariance (the only solution that fulfills both constraints is the trivial solution $c_t = c_x = 0$). However, if molecular friction can be neglected for a range of scales, Kolmogorov's theory can be applied and

3 The invariance criterion

To give a general overview, we start with partial differential equations derived from first principles, e.g. the NSE in the notation of OBERLACK (1999)

$$\mathbf{F}(\mathbf{y}, \mathbf{z}, \mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \dots) = 0.$$
 (3.1)

Here y and z are the independent and dependent variables, respectively and $z^{(n)}$ refers to the *n*th-order derivatives of z with respect to y. The transformation

$$\mathbf{y} = \phi(\mathbf{y}^*, \mathbf{z}^*), \quad \mathbf{z} = \psi(\mathbf{y}^*, \mathbf{z}^*) \tag{3.2}$$

is a symmetry transformation if the following equivalence holds

$$F(y, z, z(1), z(2), ...) = 0$$

⇔ **F**(**y**^{*}, **z**^{*}, **z**^{*(1)}, **z**^{*(2)}, ...) = 0. (3.3)

In other words, the transformation (3.2) substituted into Eq. (3.1) does not change the mathematical structure of Eq. (3.1) when it is written in the new variables y^* and z^* . We suppose that the spatially averaged version of Eq. (3.1), hereafter denoted as *model equations*, which are appropriate for discretization in numerical models, describes the system under consideration reasonably down to a prescribed length scale $\overline{\Delta}$ (that can be interpreted as a cut-off or resolution scale when discretized). Scales smaller than Δ are averaged out, and their impact on larger scales is described only by so-called subscale terms in the averaged equations. Regarding physical consistency, the symmetry related to the transformation (3.2) shall be preserved even if parametrizations of sub-scale terms are included (OBERLACK, 1997), i.e., the model equations have to satisfy

$$\overline{\mathbf{F}}(\mathbf{y}, \mathbf{z}, \mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \dots) = 0$$

$$\Leftrightarrow \quad \overline{\mathbf{F}}(\mathbf{y}^*, \mathbf{z}^*, \mathbf{z}^{*(1)}, \mathbf{z}^{*(2)}, \dots) = 0.$$
(3.4)

Here, averaging over the scale $\overline{\Delta}$ is indicated by an overbar. Specifically, consider a scalar variable *a* that obeys the equation of motion

$$\partial_t a + (\mathbf{v} \cdot \nabla) a = \mathcal{F}_a(t, x_i, a, b_1, b_2, \dots).$$
 (3.5)

Here, \mathcal{F}_a represents sources and sinks for *a* and will henceforth be denoted as source function. The b_l denote additional dependent variables such as pressure, *etc.*

Note that Eq. (3.5) can be regarded as a tracer equation. The transformed equation

$$\partial_{t^*}a^* + (\mathbf{v}^* \cdot \nabla^*)a^* = \mathcal{F}_a(t^*, x_i^*, a^*, b_l^*)$$
(3.6)

must hold if the applied transformation (3.2) is a symmetry. This definition of a symmetry allows us to derive a criterion to validate the consistency of any sub-scale parametrization included in \mathcal{F} with respect to the formal transformation (3.2).

As mentioned in the introduction, symmetries of the NSE have extensively been discussed in the literature (BYTEV, 1972; GUSYANTNIKOVA and YUMAGUZHIN, 1989; OBERLACK, 1997; RAZAFINDRALANDY et al., 2007). Here, we focus on the implications of the less known scale invariance constraint. In contrast to global symmetries, scale invariance is valid only within an inertial subrange; an example is the inertial range corresponding to isotropic three-dimensional turbulence (KOLMOGOROV, 1941).

Let us assume that a rescaled version of Eq. (3.5) can be obtained using the scaling transformations defined for the inertial range where isotropic Kolmogorov-like $k^{-5/3}$ turbulence occurs (for details see OBERLACK (2000))

$$t^{*} = e^{c_{t}}t,$$

$$x_{i}^{*} = e^{c_{x}}x_{i},$$

$$v_{i}^{*} = e^{c_{x}-c_{t}}v_{i},$$

$$a^{*} = e^{c_{a}}a,$$

$$b_{l}^{*} = e^{c_{b_{l}}}b_{l}.$$
(3.7)

With these definitions, a scale invariance criterion can be formulated as following:

Scale invariance of the model equations within a finite range of scales is preserved if the source function fulfills

$$e^{\frac{2}{3}c_x - c_a} \mathcal{F}_a(e^{\frac{2}{3}c_x}t, e^{c_x}x_i, e^{c_a}a, e^{c_b}b_l) = \mathcal{F}_a(t, x_i, a, b_l).$$
(3.8)

Hence, a specific relation between the scaling factors exists in the regime of scale invariance.

Derivation: Assume a constant spectral energy flux $\epsilon^* = \epsilon = \text{const.}$ Since $\epsilon \sim \mathcal{L}^2/\mathcal{T}^3$, we have $0 = c_{\epsilon} = 2c_x - 3c_t$, and the temporal scaling is related to spatial scaling according to

$$c_t = \frac{2}{3}c_x,\tag{3.9}$$

as was already mentioned in Section 2. Inserting this relationship into the ansatz (3.7), we find

$$t^{*} = e^{\frac{4}{5}c_{x}}t,$$

$$x_{i}^{*} = e^{c_{x}}x_{i},$$

$$v_{i}^{*} = e^{\frac{1}{3}c_{x}}v_{i},$$

$$a^{*} = e^{c_{a}}a,$$

$$b_{l}^{*} = e^{c_{b_{l}}}b_{l},$$
(3.10)

which is the well-known scaling behaviour of a Kolmogorov-like turbulent flow (cf. VALLIS (2006), chapter 8.2.3). With the transformation (3.10) the rescaled equation (3.6) can be written as

$$e^{c_a - c_t} \partial_t a + e^{c_a - c_t} (\mathbf{v} \cdot \nabla) a = \mathcal{F}_a(e^{c_t} t, e^{c_x} x_i, e^{c_a} a, e^{c_{b_l}} b_l)$$
(3.11)

or

$$\partial_t a + (\mathbf{v} \cdot \nabla) a = e^{\frac{2}{3}c_x - c_a} \mathcal{F}_a(e^{\frac{2}{3}c_x}t, e^{c_x}x_i, e^{c_a}a, e^{c_b}b_l)$$
$$\stackrel{!}{=} \mathcal{F}_a(t, x_i, a, b_l). \tag{3.12}$$

Hence, scale invariance is preserved if the source function $\mathcal{F}_a(t, x_i, a, b_l)$ fulfills the relation (3.8). Hereafter, we use the abbreviation

$$\mathcal{G}_{a}(t, x_{i}, a, b_{l}) \equiv e^{\frac{2}{3}c_{x}-c_{a}}\mathcal{F}_{a}(e^{\frac{2}{3}c_{x}}t, e^{c_{x}}x_{i}, e^{c_{a}}a, e^{c_{b_{l}}}b_{l})$$
(3.13)

to formulate the criterion concisely as $\mathcal{G}_a \stackrel{!}{=} \mathcal{F}_a$, which is similar to the model analysis of scaling transformations in RAZAFINDRALANDY et al. (2007). Because the scaling transformation (3.10) is linear and multiplicative, it is possible to independently check each summand in the source term for scale invariance.

4 Application of the criterion to isotropic flows

We first verify our criterion by applying it to fluid dynamical equations in the isotropic case for which the results are already known. We begin with the Euler equations, procede with the NSE by incorporating molecular friction, and then consider LES with turbulence parametrization, i.e. the averaged NSE with parameterized turbulent instead of molecular friction.

4.1 Euler equations with constant density

The Euler equations with constant density are given by

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho}; \quad \nabla \cdot \mathbf{v} = 0$$
(4.1)

The continuity equation is trivially fulfilled for any value of the scaling parameter c_x ,

$$\nabla^* \cdot \mathbf{v}^* = e^{-\frac{2}{3}c_x} \nabla \cdot \mathbf{v} = 0. \tag{4.2}$$

Applying the scaling transformation (3.10) to the pressure gradient term leads to

$$\mathcal{G}_{\mathbf{v}} = -e^{\frac{1}{3}c_x} \frac{\nabla^* p^*}{\rho^*} = -e^{-\frac{2}{3}c_x + c_p - c_\rho} \frac{\nabla p}{\rho}.$$
 (4.3)

(Note that throughout this paper, c_p denotes the scaling factor of the pressure and not the specific heat capacity.) From Eq. (4.3) one can see that Eq. (4.1) allows for scale invariance if $c_p - c_\rho = \frac{2}{3}c_x$ such that

$$\mathcal{G}_{\mathbf{v}} = -\frac{\nabla p}{\rho} = \mathcal{F}_{\mathbf{v}}.\tag{4.4}$$

This result agrees with OBERLACK (1999); OBERLACK (2000). Due to the linearity of the criterion we are allowed to skip the pressure gradient term in the subsequent discussions of fluid dynamical equations of motion.

4.2 Navier-Stokes equations (NSE) and turbulent friction

We now consider the NSE for constant density,

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{v}, \quad \nabla \cdot \mathbf{v} = 0.$$
 (4.5)

The second term on the right-hand side of the momentum equation leads to the transformed source term

$$\mathcal{G}_{\mathbf{v},2} = e^{\frac{1}{3}c_x} v^* (\nabla^*)^2 \mathbf{v}^*$$

= $e^{-\frac{4}{3}c_x + c_y} v \nabla^2 \mathbf{v}.$ (4.6)

Here, we assume that the viscosity ν is a material constant that does not scale such that $\nu^* = \nu$ or $c_{\nu} = 0$. This is in contrast to OBERLACK (1999) who includes the molecular viscosity formally as an additional independent variable of the system. Since ν is constant in our consideration, we can write

$$\mathcal{G}_{\mathbf{v},2} = e^{-\frac{4}{3}c_x} v \nabla^2 \mathbf{v} \stackrel{!}{=} \mathcal{F}_{\mathbf{v},2}.$$
 (4.7)

Thus, $G_{v,2}$ is independent of the scaling factor only for $c_x = 0$. This is a consequence of introducing a constant viscosity: The viscous term in the NSE breaks the scale invariance and does not allow for a -5/3 power law at scales where viscous effects are relevant (e.g. the viscous subrange), as expected. Consequently, a simple turbulent diffusion scheme with constant turbulent viscosity is also subject to the constraint (4.7) and cannot ensure scale invariance.

Therefore, we now consider a non-constant turbulent viscosity. Usually, the turbulent stress is assumed to be proportional to the wind shear,

$$\rho \overline{v'_i v'_j} = -KS_{ij}, \qquad (4.8)$$

where *K* is the turbulent analogue of a molecular diffusion coefficient and $S_{ij} = (\partial_i v_j + \partial_j v_i)/2$ are the components of the shear tensor **S**. The Reynolds-averaged NSE with the corresponding parametrization of turbulent friction are

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho} + \nabla (K\mathbf{S}); \quad \nabla \cdot \mathbf{v} = 0.$$
 (4.9)

The transformed momentum diffusion term reads with $c_{\mathbf{S}} = -c_t = -\frac{2}{3}c_x$ and c_K ,

$$\mathcal{G}_{\mathbf{v},2} = e^{\frac{1}{3}c_x} \nabla^* (K^* \mathbf{S}^*) = e^{c_K - \frac{4}{3}c_x} \nabla (K \mathbf{S}) \stackrel{!}{=} \mathcal{F}_{\mathbf{v},2}. \quad (4.10)$$

Thus the scaling factor for the diffusion coefficient has to obey the relation $c_K = \frac{4}{3}c_x$ to ensure scale invariance.

In other words, if we combine molecular and turbulent diffusion as

$$K_{\text{tot}} = K + \nu, \tag{4.11}$$

scale invariance is only possible for $K \gg v$, i.e. at scales where molecular friction is negligible. The limit $K \sim v$ would correspond to the transition in wavenumber space from the inertial to the viscous subrange at the inner scale, see Fig. 1.

4.3 Classical Smagorinsky model

According of Smagorinsky's generalized mixing length concept, the diffusion coefficient is given by

$$K = l^2 |\mathbf{S}|. \tag{4.12}$$

This model has widely been used in LES (c.f., e.g., chapter 13 in: POPE, 2000). For this approach the scaling factor of the diffusion coefficient can be written as

$$c_K = 2c_l - \frac{2}{3}c_x. \tag{4.13}$$

In the classical Smagorinsky model, the mixing length is assumed to be a prescribed parameter. Hence, l is constant such that $l^* = l$ (thus $c_l = 0$) which leads to the following transformed source term corresponding to turbulent momentum diffusion

$$\mathcal{G}_{\mathbf{v},2} = e^{-2c_x} l^2 \nabla(|\mathbf{S}|\mathbf{S}) \stackrel{!}{=} \mathcal{F}_{\mathbf{v},2}. \tag{4.14}$$

According to our criterion (3.8), scale invariance can be achieved only by setting $c_x = 0$ which means that no scale transformation at all can be applied to Eq. (4.9). This is a characteristic result of a prescribed mixing length as assumed by the classical Smagorinsky model as was already pointed out by OBERLACK (1997).

4.4 Dynamic Smagorinsky Model (DSM)

The Dynamic Smagorinsky Model (DSM, GERMANO et al., 1991; MENEVEAU and KATZ, 2000) is a method to calculate the mixing length locally from the resolved scales, using the approach $l = C_S \overline{\Delta}$, where $\overline{\Delta}$ is the prescribed resolution scale and C_S the variable Smagorinsky parameter. Hence, the variability and the scaling behaviour of l is described by C_S . Note that the exact definition of C_S varies due to different solutions of the basic tensor equation in the literature (LILLY, 1992; SCHAEFER-ROLFFS and BECKER, 2013), but the scaling behaviour can satisfactorily be described for all solutions by $l^2 \sim C_S^2 \sim O[\mathbf{v}^2/|\mathbf{S}|^2]$. Thus, $l^* \neq l$ and a closer examination of the scaling properties of the mixing length in this case gives

$$c_l = c_x. \tag{4.15}$$

Instead of Eq. (4.14) we now have the transformed turbulent diffusion term

$$\mathcal{G}_{\mathbf{v},2} = e^{-2c_x} \nabla \left[(e^{c_x} l)^2 \, |\mathbf{S}| \mathbf{S} \right] \tag{4.16}$$

which finally results in

$$\mathcal{G}_{\mathbf{v},2} = \nabla(l^2 |\mathbf{S}|\mathbf{S}) = \mathcal{F}_{\mathbf{v},2}.$$
 (4.17)

According to our criterion (3.8), the averaged NSE together with the DSM to parameterize unresolved turbulent scales are scale-invariant (cf. OBERLACK, 1997). The DSM therefore provides the correct scaling properties to allow for a turbulent energy cascade from the resolved to unresolved scales, as is required in LES.

As mentioned in the introduction, there exist a variety of subgrid-scale models other than the DSM in the literature. The similarity model (BARDINA et al., 1980) assumes that the subgrid-scale momentum flux $(\propto O[\mathbf{v}^{\prime 2}])$ is directly proportional to that of the resolved flow ($\propto O[\mathbf{v}^2]$), thus scale invariance is *a priori* assumed here in a literal sense. Though physical consistency easily is achieved in these models, as the proportionality parameter can be held constant, the dissipation is too weak when this approach is used in simulations. A different, so-called gradient model was proposed by CLARK et al. (1979), where the form of the shear tensor is slightly different from S_{ii} . Nevertheless, the scaling properties are the same as for the Smagorinsky ansatz. Hence, to fulfill scale invariance of the gradient model, one has to introduce a dynamical mixing length in analogy to the DSM.

4.5 Compressible Euler equations

Let us consider the Euler momentum equation

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho}$$
 (4.18)

together with the compressible continuity equation and the thermodynamic equation in terms of enthalpy h for isentropic flow,

$$\partial_t \rho + (\mathbf{v} \cdot \nabla) \rho = -\rho \nabla \cdot \mathbf{v}, \qquad (4.19)$$

$$\partial_t h + (\mathbf{v} \cdot \nabla)h = \frac{(\partial_t + \mathbf{v} \cdot \nabla)p}{\rho}.$$
 (4.20)

In this case, the source term of the rescaled continuity equation (4.19) reads

$$\mathcal{G}_{\rho} = -e^{\frac{2}{3}c_{x}-c_{\rho}}\rho^{*}\nabla^{*}\cdot\mathbf{v}^{*} = -\rho\nabla\cdot\mathbf{v} = \mathcal{F}_{\rho} \qquad (4.21)$$

and scale invariance is automatically fulfilled for any value of the scaling parameter of the density, c_{ρ} . This justifies to skip the continuity equation from the scaling analysis also in the compressible case. The scaling of the pressure gradient term in the thermodynamic equation (4.19) yields

$$\mathcal{G}_{h} = -e^{\frac{2}{3}c_{x}-c_{h}}\frac{\partial_{t^{*}}p^{*} + (\mathbf{v}^{*}\cdot\nabla^{*})p^{*}}{\rho^{*}}$$
$$= -e^{-c_{h}+c_{p}-c_{\rho}}\frac{\partial_{t}p + (\mathbf{v}\cdot\nabla)p}{\rho} \stackrel{!}{=} \mathcal{F}_{h}.$$
(4.22)

Since we know from Section 4.1 that $c_p - c_\rho = \frac{2}{3}c_x$, the thermodynamic equation is scale-invariant if the enthalpy scaling factor satisfy $c_h = \frac{2}{3}c_x$. This is in accordance with the scaling factor for the kinetic energy, $c_{\mathbf{v}^2} = 2c_{\mathbf{v}} = \frac{2}{3}c_x$.

4.6 The TKE closure

A slightly more sophisticated description of turbulent flows includes a prognostic equation to describe the evolution of the turbulent kinetic energy (TKE), $\overline{k} = \overline{v'^2}/2$. The equations describing this so-called *k*-model are given by VAN MIEGHEM (1973) or BECKER (2003). In the absense of gravity we have

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho} + \frac{1}{\rho} \nabla (\rho K \mathbf{S}), \qquad (4.23)$$

$$\partial_t h + (\mathbf{v} \cdot \nabla)h = \frac{(\partial_t + \mathbf{v} \cdot \nabla)p}{\rho} - \overline{d_t k} + \frac{1}{\rho} \nabla \left(\rho h K \frac{\nabla \Theta}{\Theta}\right) + K |\mathbf{S}|^2, \quad (4.24)$$

$$d_{t}k = \partial_{t}k + (\mathbf{v} \cdot \nabla)k + \frac{1}{\rho}\nabla(\rho K \nabla k)$$
$$= K(\mathbf{S}\nabla)\mathbf{v} - \epsilon \qquad (4.25)$$

$$= K(\mathbf{SV})\mathbf{v} - \boldsymbol{\epsilon}, \tag{4.25}$$

$$\partial_t \rho + (\mathbf{v} \cdot \nabla) \rho = -\rho \nabla \cdot \mathbf{v}. \tag{4.26}$$

Here, Θ is potential temperature, $K = l_k \sqrt{k}$, $\epsilon = \overline{k}^{3/2}/l_k$, and l_k the mixing length of the k-model. Since ϵ does not scale, $c_{\epsilon} = 0$. Thus, due to $c_k = \frac{2}{3}c_{l_k} = 2c_{v'}$, we have $c_{v'} = \frac{1}{3}c_{l_k}$. The assumption of a constant l_k leads to $c_{v'} = c_{l_k} = 0$ and the turbulent velocities do not scale, unlike the resolved velocities (which scale as $c_v = \frac{1}{3}c_x$). Therefore, an inertial range for the turbulent scales is not consistent with the assumption of a constant mixing length, in analogy to what we have seen for the classical Smagorinsky model (Section 4.3). Alternatively, there exist approaches for a dynamical mixing length in a kmodel. Applying for instance the formulation of Wong (1992), we get $l_k \propto O[\mathbf{v}^2/(k^{1/2}|\mathbf{S}|)]$. This leads to

$$c_k = \frac{2}{3}c_{l_k},$$
 (4.27)

$$c_{l_k} = 2c_v - \frac{1}{2}c_k - c_{\mathbf{S}} \tag{4.28}$$

with the solution $c_{l_k} = c_x$ (in analogy to the DSM) and $c_k = \frac{2}{3}c_x$. Furthermore, we have $c_{v'} = \frac{1}{3}c_x = c_v$ and $c_K = c_{l_k}c_k/2 = \frac{4}{3}c_x$ such that the application of the transformation (3.10) converts the source terms of the momentum, enthalpy, and TKE equations to

$$\mathcal{G}_{\mathbf{v},2} = e^{\frac{1}{3}c_x} \nabla^* (K^* \mathbf{S}^*) = \nabla (K \mathbf{S}) = \mathcal{F}_{\mathbf{v},2}, \qquad (4.29)$$

$$\begin{aligned} \mathcal{G}_{h,2,3,4} &= e^{0 \cdot c_x} \left[-\left[\partial_{t^*} + (\mathbf{v}^* \cdot \nabla^*)\right] k^* \right. \\ &+ \frac{1}{\rho^*} \nabla \left(\rho^* h^* K^* \frac{\nabla^* \Theta^*}{\Theta^*} \right) + K^* |\mathbf{S}^*|^2 \right] \\ &= -\left[\partial_t + (\mathbf{v} \cdot \nabla)\right] k + \frac{1}{\rho} \nabla \left(\rho h K \frac{\nabla \Theta}{\Theta} \right) \\ &+ K |\mathbf{S}|^2 = \mathcal{F}_{h,2,3,4} \end{aligned}$$
(4.30)
$$\begin{aligned} \mathcal{G}_k &= e^{0 \cdot c_x} [\nabla^* (K^* \nabla^* k^*) + K^* (\mathbf{S}^* \nabla^*) \mathbf{v}^* - \epsilon^*] \\ &= \nabla (K \nabla k) - K (\mathbf{S} \nabla) \mathbf{v} - \epsilon = \mathcal{F}_k. \end{aligned}$$
(4.31)

Hence, only a dynamical mixing length, as formulated by Wong (1992) for instance, ensures scale invariance of the TKE closure.

4.7 The Tracer equation

In the cases considered so far only the equations of motion for a homogenous fluid were investigated. However, the basic equation (3.5) can be applied also to a tracer subject to isotropic turbulent diffusion. Here, we focus on the inertial range for the tracer variance. For the sake of simplicity we restrict ourselves to a fluid with constant density. The corresponding tracer equation is given by

$$\partial_t C + (\mathbf{v} \cdot \nabla) C = \nabla (K_C \nabla C), \qquad (4.32)$$

with some diffusion coefficient K_C . The right-hand side of the rescaled Eq. (4.32) reads

$$\mathcal{G}_C = e^{\frac{2}{3}c_x - c_C} \nabla^* (K_C^* \nabla^* C^*)$$
$$= e^{-\frac{4}{3}c_x + c_{K_C}} \nabla (K_C \nabla C) \stackrel{!}{=} \mathcal{F}_C.$$
(4.33)

For a constant diffusivity K_C (similar to the case of molecular friction), we have the same situation as for the corresponding momentum diffusion, namely that scale invariance is violated. Thus, if experiments show an inertial range in the atmospheric power spectrum of some tracer concentration, we postulate that a constant turbulent diffusivity is not physically consistent. Rather, a dynamic diffusion coefficient $K_C \propto l_C^2 |\mathbf{S}|$ (where l_C is a dynamical mixing length) obeying the relation $c_K = \frac{4}{3}c_x$ (which is identical to the relation in the DSM) must be applied to ensure scale invariance. Note that due to this constraint the tracer mixing length must show the same scaling behaviour as that for momentum, although both mixing lengths are most likely different. A dynamical approach similar to the DSM yields

$$l_C^2 \propto O[(C|\mathbf{v}|)/(|\mathbf{S}||\nabla C|)]$$
(4.34)

which ensures scale invariance.

5 Application to large-scale atmospheric flows

Up to now we have considered only isotropic turbulence without external forces. Apparently, these assumptions are not valid for large-scale flows in the atmosphere. Hence, we now investigate the more complex cases of large-scale stratified flow.

5.1 Large-scale stratified flow

To describe atmospheric flows, we have to take gravity and the apparent separation of horizontal and vertical scales into account as manifested by hydrostatic balance. In general, the appropriate system of equations are the Primitive Equations (cf. PICHLER, 1997),

$$\partial_t \mathbf{u} = \mathbf{u} \times (f + \xi) \mathbf{e}_z - \nabla \frac{\mathbf{u}^2}{2} - w \partial_z \mathbf{u} - \frac{\nabla p}{\rho} + \mathbf{R}$$
 (5.1)

$$\partial_z p = -\rho g, \tag{5.2}$$

$$d_t h = \frac{d_t p}{\rho} + Q + \epsilon, \qquad (5.3)$$

$$0 = \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) + \partial_z (\rho w), \qquad (5.4)$$

where **u** and *w* are the horizontal and vertical velocity, ∇ is the horizontal gradient operator, $\xi = \mathbf{e}_z \cdot (\nabla \times \mathbf{u})$ is the horizontal vorticity, *f* and *g* are the Coriolis parameter and the acceleration due to gravity, and **R**, *Q*, and ϵ are turbulent friction, differential heating, and dissipation respectively. We consider the anisotropic (but horizontally isotropic) inertial range in the mesoscales (see Fig. 1) where Stratified Turbulence is supposed to exist, i.e. a horizontal energy cascade with a -5/3 power law with respect to the horizontal wavenumber (LIND-BORG, 2006). Within this range, we assume that nonconservative terms and the Coriolis force are negligible. The rearranged Primitive Equations are¹

$$\partial_t \mathbf{u} - \mathbf{u} \times \xi \mathbf{e}_z + \nabla \frac{\mathbf{u}^2}{2} + w \partial_z \mathbf{u} = -\frac{\nabla p}{\rho}$$
(5.5)

$$= -\frac{\sigma_z p}{\rho},\tag{5.6}$$

$$(\partial_t + \mathbf{u} \cdot \nabla + w\partial_z)h = \frac{(\partial_t + \mathbf{u} \cdot \nabla + w\partial_z)p}{\rho},$$
 (5.7)

g

$$(\partial_t + \mathbf{u} \cdot \nabla + w \partial_z) \rho = \rho (\nabla \cdot \mathbf{u} + \partial_z w).$$
 (5.8)

It is easy to verify that with respect to the scaling transformation (3.10) the vertical advection terms show the same scaling behaviour as the horizontal advection terms. By applying the scaling transformation from Section 4.1 to the horizontal momentum equation (5.5) we obtain the relation $c_p - c_\rho = \frac{2}{3}c_x$. Applying the scaling

transformation to the hydrostatic equation (5.5) leads to

$$g = -\frac{d_{z^*}p^*}{\rho^*} = -e^{c_p - c_\rho - c_z} \frac{d_z p}{\rho}.$$
 (5.9)

From this we see that scale invariance holds if the vertical scaling relation $c_p - c_\rho = c_z$ is fulfilled. Thus, the intuitive relation $c_z = c_x$ is no longer valid; rather, the horizontal and vertical scaling relations are linked according to

$$c_z = \frac{2}{3}c_x.$$
 (5.10)

Hence, scale invariance is still possible for a hydrostatic (i.e. stratified) flow, but with a different vertical scaling behaviour than in the isotropic case without gravity.

This result can be compared with the aspect ratio from Stratified turbulence (LINDBORG, 2006),

$$Z/X \sim \epsilon^{1/3} X^{-2/3} / N,$$
 (5.11)

where *X* and *Z* are horizontal and vertical length scales. If we acknowledge that the buoyancy frequency *N* is scale dependent, $N^2 = g\partial_z \Theta / \Theta$ yields a scaling factor $c_N = -c_x/3$. Then, we find a scaling relation from the aspect ratio (5.11)

$$c_z - c_x = c_\epsilon - \frac{2}{3}c_x - c_N = -\frac{1}{3}c_x$$
 (5.12)

which is identical to Eq. (5.10). However, the mean buoyancy frequency is usually considered to be constant such that the scaling ratio according to (5.11) would rather yield

$$c_z = \frac{1}{3}c_x.$$
 (5.13)

The question remain how to reconcile the two scale relations (5.10) and (5.13).

5.2 The primitive equations with non-isotropic turbulent diffusion

In large-scale flows as described above the horizontal and vertical length scales are several orders of magnitude larger than the viscous scales. When applying the Primitive Equations to these flows, they have to be closed by a turbulent diffusion scheme in order to balance the energy cascade that correspond to the irreversible branch of the Lorenz energy cycle (LORENZ, 1967). Assuming that the numerical resolution covers a good part of the mesoscales, we can apply the results of Section 4 to the horizontally isotropic horizontal energy cascade and parameterize the non-resolved scales by a corresponding DSM (SCHAEFER-ROLFFS and BECKER, 2013). However, we have to take into account that also a vertical diffusion term of the form $\rho^{-1}\partial_z(\rho K_z \partial_z \mathbf{u})$ is part of the horizontal momentum equation (5.5). In order to

¹Note that $-\mathbf{u} \times \xi \mathbf{e}_z + \nabla \frac{\mathbf{u}^2}{2}$ is subject to the same scaling behaviour as $(\mathbf{u} \cdot \nabla)\mathbf{u}$, but the latter is not correct in spherical coordinates.

check the scale invariance criterion for this term, we apply the transformation (3.10) along with $c_z = \frac{2}{3}c_x$. This yields the transformed source term

$$\mathcal{G}_{\mathbf{u}} = e^{\frac{1}{3}c_x} \frac{1}{\rho^*} \partial_{z^*} (\rho^* K_z^* \partial_{z^*} \mathbf{u}^*)$$

= $e^{-\frac{2}{3}c_x + c_{K_z}} \frac{1}{\rho} \partial_z (\rho K_z \partial_z \mathbf{u}) \stackrel{!}{=} \mathcal{F}_{\mathbf{u}}.$ (5.14)

Thus, the vertical diffusion coefficient has to scale as

$$c_{K_z} = \frac{2}{3} c_x \tag{5.15}$$

to preserve scale invariance. Assuming a simple mixing length ansatz, $K_z = l_z^2 |\partial_z \mathbf{u}|$, where l_z is the vertical mixing length, we obtain

$$c_{K_z} = 2c_{l_z} - \frac{1}{3}c_x \tag{5.16}$$

for the scaling factors and

$$c_{l_z} = \frac{c_x}{2}.$$
 (5.17)

for the vertical mixing length. The latter scales differently from both the horizontal mixing length ($c_{l_h} = c_x$, see Eq. (4.15)) and the vertical length scale $c_z = 2c_x/3$. It is shown in the Appendix that this is a general property of the vertical mixing length, regardless of the parameterized turbulent variable.

As far as we know, an approach to compute dynamically the vertical mixing length such as to preserve scale invariance associated with a forward horizontal energy cascade in the mesoscales has not been discussed in the literature yet. The relation (5.17) suggests the following formulation for the dynamic vertical mixing length,

$$l_z = \sqrt{l_0 l_h},\tag{5.18}$$

where l_0 is a constant and l_h is the dynamic horizontal mixing length given by the DSM. Equation (5.18) represents the dynamic vertical mixing length in the free troposphere when the truncation scale lies within the mesoscales.

6 Summary and conclusions

In this paper we have derived a criterion to check scale invariance for subgrid-scale parametrizations applied in fluid dynamical equations of motion used for LES. The criterion is inspired by the work of OBERLACK (2000) and based on the testing of how the source terms of the model equations transform under a symmetry transformation. The derivation can be summarized as follows: We start by applying the scaling transformation $a^* = e^{c_a}a$ to the equation of motion for some flow variable *a*. Scale invariance implies that the mathematical structure of the equation of motion does not change under the transformation; i.e., the sum of all scaling factors in the exponent must be zero. To check this we rearrange the transformed equation such that the material time derivative is written on the left-hand side whereas all other terms appear on the right-hand side. The sum of these source terms is denoted in the function \mathcal{G}_a ; and each individual term in \mathcal{G}_a can be considered separately. This method is summarized in our criterion (3.8).

The governing equations of motions that describe a system within an inertial range, e.g., the compressible Euler equations without apparent forces and other source terms, are scale-invariant per se and thus fulfill the criterion automatically. However, equations of motions for numerical simulations are usually modified by employing parametrizations of unresolved processes. These parametrizations are part of the inertial range but do not necessarily preserve scale invariance. Hence, the proposed criterion can check the physical consistency of the subgrid-scale parametrizations. As a test of the criterion, we have applied our method to the Euler and Navier-Stokes equations (NSE). We have recovered the result of OBERLACK (2000) that only in absence of molecular viscosity scale invariance is fulfilled for all scales. Because numerical simulations of largescale flow require LES, we extended our investigations to turbulence parametrizations. We have confirmed that the classical Smagorinsky model (which assumes a constant mixing length) does not preserve scale invariance, while the Dynamic Smagorinsky Model (DSM, GER-MANO et al., 1991) does. We have shown that the compressible version of the continuity equation as well as the enthalpy equation in the regime of isentropic flow are scale-invariant. Considering the TKE closure, we have shown that scale invariance holds for a dynamic mixing length according to WONG (1992). Finally, we have proven for the equation for a tracer that a constant tracer diffusion coefficient violates the assumption of scale invariance. Rather, a dynamically calculated tracer diffusivity, showing the same scaling behaviour as the diffusion coefficient for momentum according to the DSM ensures scale invariance. All these results confirm the statement of OBERLACK (1997) that "the dynamic procedure [...] restores scale invariance, which may be violated by certain base [turbulence] models."

In order to apply our criterion to the atmosphere, we investigated the more complex case of large-scale flows. We have seen that in the Primitive Equations, where due to the hydrostatic approximation only a horizontal energy cascade by the resolved flow is allowed, a scale-invariant formulation of the horizontal momentum equation is still possible, as was already shown for strongly stratified flows (BILLANT and CHOMAZ, 2001). According to the proposed criterion, the ratio of vertical and horizontal length scales is $c_z = 2c_x/3$. The corresponding aspect ratio can only be reconciled with the concept of Stratified Turbulence if we allow the buoyancy frequency to be scale dependent. A scale-invariant horizontal momentum equation further leads to the constraint

that the scaling factor of the vertical mixing length is different from both the horizontal mixing length and the vertical scale. We have proposed a formula for the vertical mixing length, $l_z = \sqrt{l_0 l_h}$, where l_0 is a constant factor and l_h is the horizontal mixing length determined by the DSM as given in SCHAEFER-ROLFFS and BECKER (2013).

Summarizing, our criterion to test scale invariance for any subgrid-scale models in LES is easy to apply. From the examples considered in this study it is evident that any turbulent diffusion coefficient has to be calculated dynamically to ensure scale invariance, regardless of the specific flow variable considered. In a more general sense, modelers who need to parameterize subgridscale processes may check their formulation and eventually obtain modifications that ensure scale invariance.

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Appendix

Here we want so show that for hydrostatic flow, a vertical mixing length approach always leads to a scale ratio as given by Eq. (5.17). The basic assumptions are that the turbulent variables scale analogously to their large-scale counterparts and that the vertical wind behaves like

$$w \sim |\mathbf{u}| \frac{Z}{X},$$

where **u** and *w* are horizontal and vertical winds, and *X* and *Z* are horizontal and vertical scales. Thus, $c_w = c_u + c_z - c_x$. Since the mixing length approach for a variable *a* is given by

$$\overline{a'w'} \sim -l_z^2 |\partial_z \mathbf{u}| \partial_z a, \qquad (6.1)$$

we get

$$c_a + c_w = 2c_{l_z} + (c_u - c_z) + (c_a - c_z).$$
(6.2)

The scaling factor c_a cancels, and c_{l_z} can be written as

$$c_{l_z} = \frac{c_w - c_u + 2c_z}{2} = \frac{3c_z - c_x}{2}.$$

Making use of Eq. (5.10) then leads to

$$c_{l_z}=\frac{c_x}{2},$$

which is identical to Eq. (5.17).

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