Self-consistent derivation of subgrid stresses for large-scale fluid equations

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A self-consistent procedure for deriving subgrid scale models for a complex system of equations is presented. When applied to the Navier-Stokes equation for incompressible flow it reproduces the differential version of the stress-similarity model with a correct coefficient. As an example the complete system of equations is derived for an ocean global circulation model.

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I. INTRODUCTION

Numerical simulations of high-Reynolds-number flows usually require one to limit the scales resolved by the numerical scheme to the largest ones, while modeling the effect of the small unresolved scales in the form of subgrid scale stresses (SGSS) acting on the resolved flow. One of the main objectives of this so called large-eddy simulation approach is to model the SGSS in terms of the resolved variables only (see [1] for a recent review). The usual approach to derive SGSS models is to describe the effect of the small scale flow as that of a statistically averaged turbulent flow, whose characteristics are determined by the instantaneous large scale flow (a very clear and self-contained application is given in [2]). This technique allows well developed statistical turbulence theories to be used (see [3] for a theory applicable to complex systems), and it is seen that, under certain conditions [4], it gives correct large-scale flow statistics. Another approach that shows the highest correlations between modeled and real SGSS is given by the similarity models [5], derived not from statistical theories but from the observation (in numerical simulations and experiments) of certain similarities between different scales of the flow (see [6] for a related, alternative approach).

The purpose of the present work is to present a complementary approach, that does not includes neither statistical theories nor scale similarity assumptions, in which the SGSS are derived directly from the flow equations. This is particularly useful in the application to complex systems of fluid equations, such as those appearing in astrophysics and geophysics, for which no statistical theories of turbulence have been yet developed, and/or where no clear evidence of similarity behavior exists.

The two main ingredients are (i) a nonstandard definition of fluctuations (originally developed by Schumann [7]) that avoids the appearance of non-Reynolds-like SGSS, and (ii) the solution of a scaling relation (not necessarily a similarity one) between SGSS, derived from the expression of Germano's identity [8], applied to the SGSS determined by the fluctuations defined in (i).

Approximations enter in the derivation and in the solution of the scaling relation mentioned in (ii), and reduce to assuming that the large scale flow is spatially smooth so that the accuracy of the final expressions can be quantified in terms of the ratio of the smallest resolved scale to the spatial scale of variation of the large-scale flow. At the lowest nontrivial level of approximation the formalism gives a very simple general relation applicable to different systems of equations that, for the case of the Navier-Stokes (NS) equations, reproduces the differential version of the similarity model with a correct numerical coefficient.

II. FORMALISM

To introduce the technique it is convenient to consider a relatively simple system, the NS equations for an isothermal incompressible fluid:

$$\frac{\partial \mathbf{v}}{\partial t}+(\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{v}=-\frac{1}{\rho}\boldsymbol{\nabla}p+\nu\nabla^2\mathbf{v},\quad \boldsymbol{\nabla}\cdot\mathbf{v}=0, \tag{1}$$

where $\mathbf{v}$ is the velocity field, ρ is the mass density, assumed uniform, ν the kinematic viscosity, and p the pressure.

In order to deal with smooth magnitudes and to make explicit the SGSS it is advantageous to filter Eqs. (1) [9]. Among all possible filters it will prove convenient, due to its analytical simplicity, to use a top-hat filter defined by

$$A(\mathbf{X},t)=\langle a(\mathbf{x},t)\rangle_{\mathbf{X}}=\frac{1}{\Delta V}\int a(\mathbf{x},t)dV, \tag{2}$$

where $\mathbf{X}=\langle \mathbf{x}\rangle_{\mathbf{X}}$ denotes the center of the volume ΔV, and $a(\mathbf{x},t)$ is any field variable function of the space coordinate $\mathbf{x}$ and of the time t. Applying the approach of Schumann [7] to avoid the generation of Leonard and cross terms [10], the fluctuations are *defined* as the difference

$$\delta a(\mathbf{X},\mathbf{x},t)=a(\mathbf{x},t)-A(\mathbf{X},t). \tag{3}$$

Note that fluctuations depend on both independent variables $\mathbf{x}$ and $\mathbf{X}$; the usual definition corresponds to $\mathbf{x}=\mathbf{X}$. Taking the derivative of Eq. (2) with respect to $\mathbf{X}$, it is readily seen that

$$\frac{\partial A}{\partial \mathbf{X}}=\left\langle \frac{\partial a}{\partial \mathbf{x}}\right\rangle_{\mathbf{X}}. \tag{4}$$

Moreover, the following relations are immediately seen to hold:

$$\langle A(\mathbf{X})\rangle_{\mathbf{X}}=A(\mathbf{X}),\quad \langle \delta a(\mathbf{X},\mathbf{x},t)A(\mathbf{X})\rangle_{\mathbf{X}}=0. \tag{5}$$

That is, definitions (2) and (3) lead to averages that satisfy Reynolds' postulates, resulting in neither Leonard nor cross terms [10]. The only proviso for this to hold is that the averages in Eq. (5) must be centered at the same point **X** on which the magnitudes to be averaged depend. This is an essential condition that, in the derivations to follow, leads to the particular expressions to be obtained for the SGSS. When a numerical discretization procedure is implemented, points **X** are identified with fixed grid points and the averages are then over volumes fixed in space, which results in the ''*volume based procedure*'' used in [7]. For the purpose of deriving expressions for the SGSS, **X** is considered as a continuous variable independent of **x**, and the condition of averaging around the same **X** on which fluctuations depend must be observed accordingly.

Averaging of Eq. (1) is then very simple and leads to

$$\frac{\partial \mathbf{V}}{\partial t}+(\mathbf{V}\cdot\nabla_{\mathbf{X}})\mathbf{V}=-\frac{1}{\rho}\nabla_{\mathbf{X}}P+\nu\nabla^2_{\mathbf{X}}\mathbf{V}+\nabla_{\mathbf{X}}\cdot\boldsymbol{\tau},$$

$$\nabla_{\mathbf{X}}\cdot\mathbf{V}=0, \tag{6}$$

where capital letters denote averages of the field represented by the corresponding lower-case letters, and spatial derivatives are all with respect to **X**. The SGSS are (time dependence will be henceforth not indicated)

$$\boldsymbol{\tau}(\mathbf{X})=-\langle\delta\mathbf{v}(\mathbf{X},\mathbf{x})\,\delta\mathbf{v}(\mathbf{X},\mathbf{x})\rangle_{\mathbf{X}}. \tag{7}$$

To obtain an equation for $\boldsymbol{\tau}$ we now derive a particular expression of Germano's identity [8] for the filter (2) and fluctuations (3). For this, consider a second average over a larger volume of value $\Delta V'=2^d\Delta V$, where d is the space dimension, obtained by doubling the linear scale of the volume ΔV. The integral over $\Delta V'$ centered at **X** can be decomposed into $N=2^d$ subintegrals over equal volumes ΔV centered at $\mathbf{X}^i\equiv\mathbf{X}+\delta\mathbf{X}^i$, with i running from 1 to N. In this way, denoting with a prime the averages over the volume $\Delta V'$, we can write

$$A'(\mathbf{X})=\frac{1}{\Delta V'}\sum_{i=1}^{N}\Delta V\langle a(\mathbf{x})\rangle_{\mathbf{X}^i}=\frac{1}{N}\sum_{i=1}^{N}A(\mathbf{X}^i).$$

By taking a as any component of **v** we immediately obtain

$$\mathbf{V}'(\mathbf{X})=\frac{1}{N}\sum_{i=1}^{N}\mathbf{V}(\mathbf{X}^i), \tag{8}$$

while if we take as a any component of the tensor $[\mathbf{v}(\mathbf{x})-\mathbf{V}'(\mathbf{X})][\mathbf{v}(\mathbf{x})-\mathbf{V}'(\mathbf{X})]$, and inside each average around $\mathbf{X}^i$ we write the velocity as $\mathbf{v}(\mathbf{x})=\mathbf{V}(\mathbf{X}^i)+\delta\mathbf{v}(\mathbf{X}^i,\mathbf{x})$, the following form of Germano's identity is readily obtained:

$$\boldsymbol{\tau}'(\mathbf{X})=\frac{1}{N}\sum_{i=1}^{N}\{\boldsymbol{\tau}(\mathbf{X}^i)-[\mathbf{V}(\mathbf{X}^i)-\mathbf{V}'(\mathbf{X})][\mathbf{V}(\mathbf{X}^i)-\mathbf{V}'(\mathbf{X})]\}. \tag{9}$$

We now derive approximate differential versions of the exact relations (8) and (9), taking advantage of the smoothness of the averaged fields. Taylor expanding $\boldsymbol{\tau}$ and **V** about their values at $\mathbf{X}^i$ we write (A denotes any component of $\boldsymbol{\tau}$ or **V**)

$$A(\mathbf{X}^i)=A(\mathbf{X})+\frac{\partial A}{\partial X_p}\delta X_p^i+\frac{1}{2}\frac{\partial^2 A}{\partial X_p\partial X_q}\delta X_p^i\delta X_q^i+\cdots, \tag{10}$$

where all derivatives are evaluated at **X**, and summation over repeated subindexes is assumed. In the case that the volumes ΔV and $\Delta V'$ are parallelepipeds with sides parallel to Cartesian axes, the following relations hold:

$$\sum_{i=1}^{N}\delta\mathbf{X}^i=\sum_{i=1}^{N}\delta\mathbf{X}^i\,\delta\mathbf{X}^i\,\delta\mathbf{X}^i=\mathbf{0}, \tag{11a}$$

$$\frac{1}{N}\sum_{i=1}^{N}\delta X_p^i\delta X_q^i=\frac{\Delta_{(p)}^2}{4}\delta_{pq}, \tag{11b}$$

where δ_{pq} is Kronecker's delta, and $\Delta_{(p)}$ is the length of the side parallel to the axis X_p.

Using Eqs. (11a) and (11b) the expression of Eq. (8) is particularly simple for a cubic volume ΔV of side Δ

$$\mathbf{V}'(\mathbf{X})=\mathbf{V}(\mathbf{X})+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}\mathbf{V}+O(\Delta^4). \tag{12}$$

Using Eqs. (10), (11a), (11b), and (12), the identity (9) can be written as

$$\tau'_{lm}=\tau_{lm}+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}\tau_{lm}-\frac{\Delta^2}{4}\frac{\partial V_l}{\partial X_p}\frac{\partial V_m}{\partial X_p}+O(\Delta^4). \tag{13}$$

In these expressions the order Δ of approximation refers actually to Δ/L_X, where L_X is the spatial scale of variation of averaged quantities.

The mathematical form of Eqs. (12) and (13) is rather general. For generic fields denoted by lower-case letters $a(\mathbf{x})$, $b(\mathbf{x})$, etc., with top-hat average (2) about **X** represented by the corresponding upper-case letters $A(\mathbf{X})$, $B(\mathbf{X})$, etc., and fluctuation (3) $\delta a(\mathbf{X},\mathbf{x})$, $\delta b(\mathbf{X},\mathbf{x})$, etc., a derivation completely analogous to that of Eqs. (12) and (13) leads to

$$A'(\mathbf{X})=A(\mathbf{X})+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}A+O(\Delta^4), \tag{14}$$

and, for the average of two fluctuating fields,

$$\langle\delta a(\mathbf{X},\mathbf{x})\,\delta b(\mathbf{X},\mathbf{x})\rangle'_{\mathbf{X}}=\langle\delta a(\mathbf{X},\mathbf{x})\,\delta b(\mathbf{X},\mathbf{x})\rangle_{\mathbf{X}}+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}\langle\delta a(\mathbf{X},\mathbf{x})\,\delta b(\mathbf{X},\mathbf{x})\rangle_{\mathbf{X}}+\frac{\Delta^2}{4}\nabla_{\mathbf{X}}A\cdot\nabla_{\mathbf{X}}B+O(\Delta^4). \tag{15}$$

Analogously, the average of three fluctuating quantities can be calculated to be

$$\langle \delta a\,\delta b\,\delta c\rangle'_{\mathbf{X}}=\langle \delta a\,\delta b\,\delta c\rangle_{\mathbf{X}}+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}\langle \delta a\,\delta b\,\delta c\rangle_{\mathbf{X}}+\frac{\Delta^2}{4}(\nabla_{\mathbf{X}}A\cdot\nabla_{\mathbf{X}}\langle\delta b\,\delta c\rangle_{\mathbf{X}}+\nabla_{\mathbf{X}}B\cdot\nabla_{\mathbf{X}}\langle\delta a\,\delta c\rangle_{\mathbf{X}}+\nabla_{\mathbf{X}}C\cdot\nabla_{\mathbf{X}}\langle\delta a\,\delta b\rangle_{\mathbf{X}})+O(\Delta^4). \tag{16}$$

We then see that in Eqs. (15) and (16) the relation between a fluctuation average f over a cube of side 2Δ and that over a cube of side Δ is

$$f'=f+\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}f+\Delta^2 q+O(\Delta^4), \tag{17}$$

where q is prescribed independently of f.

Finally, to obtain a closed equation for the SGSS, we now propose to solve Eq. (17) approximately considering that f and q are not only functions of $\mathbf{X}$ but also of the scale Δ of the filter.

Since f' corresponds to twice the value of the scale Δ of f, by Taylor expanding f' about Δ we can write

$$f'=f+\Delta\frac{\partial f}{\partial\Delta}+\frac{1}{2}\Delta^2\frac{\partial^2 f}{\partial\Delta^2}+O(\Delta^3), \tag{18}$$

where all derivatives are evaluated at the scale Δ.

In Eq. (18) the expansion is made in terms of Δ/L_λ, where L_λ can be estimated as $1/(\partial \ln f/\partial\lambda)$. In the Appendix it is shown that the order Δ/L_λ of approximation in Eq. (18) coincides with the same order in Δ/L_X; for this reason we will hitherto refer simply with Δ to the Δ/L_X order of approximation.

The idea is now to retain terms only up to order Δ^2 both in Eqs. (17) and (18), and solve the resulting partial differential equation:

$$\Delta\frac{\partial f}{\partial\Delta}+\frac{1}{2}\Delta^2\frac{\partial^2 f}{\partial\Delta^2}=\frac{\Delta^2}{8}\nabla^2_{\mathbf{X}}f+\Delta^2 q(\mathbf{X},\Delta). \tag{19}$$

It is convenient to use a nondimensional variable $\lambda=\Delta/\Delta_0$, with Δ_0 a fixed reference scale, to write Eq. (19) as

$$\frac{\partial^2 f}{\partial\lambda^2}+\frac{2}{\lambda}\frac{\partial f}{\partial\lambda}-\frac{\Delta_0^2}{4}\nabla^2_{\mathbf{X}}f=2\Delta_0^2 q(\mathbf{X},\lambda). \tag{20}$$

Since f is the average of fluctuations, it is easily seen that f tends to zero as the scale of the filter decreases. Fourier transforming with respect to the space coordinate,

$$f(\mathbf{X},\lambda)=\frac{1}{(2\pi)^d}\int e^{i\mathbf{K}\cdot\mathbf{X}}\tilde{f}(\mathbf{K},\lambda)\,d^dK,$$

$$q(\mathbf{X},\lambda)=\frac{1}{(2\pi)^d}\int e^{i\mathbf{K}\cdot\mathbf{X}}\tilde{q}(\mathbf{K},\lambda)\,d^dK,$$

with d the dimensionality of space, the Fourier transform of the exact solution to Eq. (20) that satisfies $f(\mathbf{X},\lambda=0)=0$ is readily found to be

$$\tilde{f}(\mathbf{k},\lambda)=\frac{\Delta_0^2}{\lambda k}\int_0^\lambda \sin[k(\lambda-\lambda')]\lambda'\tilde{q}(\mathbf{k},\lambda')\,d\lambda', \tag{21}$$

where the dimensionless wave vector $\mathbf{k}$ is defined as

$$\mathbf{k}=\frac{\Delta_0}{2}\mathbf{K},\quad k=|\mathbf{k}|.$$

Consider now the "source" $\tilde{q}(\mathbf{k},\lambda')$; it represents the contribution to wave number k of averages over volumes of (dimensionless) scale λ'. Since $\tilde{f}(\mathbf{k},\lambda)$ is the Fourier transform of an average over scales λ, the relevant wave numbers are those smaller than (approximately) λ^{-1}; but for these values of wave numbers an average over scales λ' has approximately the same value for any $\lambda'<\lambda$ (intuitively, the large scale component of a filtered magnitude is not sensitive to the precise scale of the filter if the latter is sufficiently small); that is,

$$\tilde{q}(\mathbf{k},\lambda')\simeq\tilde{q}(\mathbf{k},\lambda). \tag{22}$$

In this way, the large scale solution of Eq. (21) can be approximated by

$$\tilde{f}(\mathbf{k},\lambda)=\frac{\Delta_0^2\tilde{q}(\mathbf{k},\lambda)}{\lambda k}\int_0^\lambda \sin[k(\lambda-\lambda')]\lambda'\,d\lambda'=\frac{\Delta_0^2\tilde{q}(\mathbf{k},\lambda)}{k^2}\left[1-\frac{\sin(k\lambda)}{k\lambda}\right]. \tag{23}$$

The function multiplying $\tilde{q}(\mathbf{k},\lambda)$ in Eq. (23) has a very rapidly convergent series expansion in $k\lambda$:

$$\frac{1}{x^2}\left[1-\frac{\sin(x)}{x}\right]=\frac{1}{6}-\frac{x^2}{120}+\frac{x^4}{5040}+O(x^6),$$

which allows to Fourier transform (23) very easily up to terms consistent with the approximation in Eqs. (17) and (18) to write (using $\lambda\Delta_0=\Delta$)

$$f(\mathbf{X},\lambda)=\frac{\Delta^2}{6}q(\mathbf{X},\lambda)+O(\Delta^3). \tag{24}$$

It is shown in the Appendix that approximation (22) leads to $O(\Delta^4)$ errors in Eq. (24), so that the error in the latter is determined by the accuracy of Eq. (18).

III. APPLICATIONS

For the NS SGSS, comparing Eqs. (13) and (17) the $q(\mathbf{X},\lambda)$ is easily identified, and Eq. (24) gives

$$\tau_{lm}=-\frac{\Delta^2}{24}\frac{\partial V_l}{\partial X_p}\frac{\partial V_m}{\partial X_p}+O(\Delta^3). \tag{25}$$

This expression coincides with a differential version of the stress-similarity model [5], with a value of the model constant $c_L=0.5$ [Δ in Eq. (25) is half of that used in [5]]. The value estimated in the same reference (adjusted in order to obtain the right energy dissipation) is $c_L=0.45\pm0.15$.

As an additional example of the applicability of the formalism we now derive the complete set of large scale equations for a relatively complex fluid system, a global circulation ocean model [11],

$$\frac{\partial}{\partial t}[(h+\zeta)\mathbf{u}]=-\boldsymbol{\nabla}\cdot[(h+\zeta)\mathbf{u}\mathbf{u}]+\boldsymbol{\nabla}\cdot[\nu(h+\zeta)\boldsymbol{\nabla}\mathbf{u}]+\frac{\mathbf{t}}{\rho}-(h+\zeta)[\mathbf{f}\times\mathbf{u}+g\boldsymbol{\nabla}\zeta+\gamma\mathbf{u}], \tag{26a}$$

$$\frac{\partial\zeta}{\partial t}=-\boldsymbol{\nabla}\cdot[(h+\zeta)\mathbf{u}], \tag{26b}$$

where $\mathbf{u}$ is the horizontal two-dimensional velocity, $\boldsymbol{\nabla}$ the two-dimensional gradient operator, h the resting depth of the fluid, ζ the free surface elevation, $\mathbf{f}$ the Coriolis force, g the acceleration of gravity, γ the bottom drag coefficient, ν the lateral viscosity, ρ the density of the fluid, and $\mathbf{t}$ the wind stress acting on the surface. We have chosen this particular system because it is relatively well known, and at the same time sufficiently complex to exemplify many aspects of the application of the formalism. However, its corresponding SGSS is not part of any current research.

Denoting the average (2) and fluctuations (3) of ζ and $\mathbf{u}$ by

$$\zeta(\mathbf{x})=Z(\mathbf{X})+\delta\zeta(\mathbf{X},\mathbf{x}), \tag{27a}$$

$$\mathbf{u}(\mathbf{x})=\mathbf{U}(\mathbf{X})+\delta\mathbf{u}(\mathbf{X},\mathbf{x}), \tag{27b}$$

where $\mathbf{x}$ is the two-dimensional horizontal coordinate and $\mathbf{X}$ the center of the filter volume (surface in this case). After replacing Eqs. (27a) and (27b) in Eqs. (26a) and (26b) and averaging around $\mathbf{X}$ one obtains quite easily, thanks to properties (4) and (5),

$$\frac{\partial}{\partial t}[h+Z)\mathbf{U}]=-\boldsymbol{\nabla}\cdot[(h+Z)\mathbf{U}\mathbf{U}]+\frac{\mathbf{t}}{\rho}-(h+Z)\times[\mathbf{f}\times\mathbf{U}+g\boldsymbol{\nabla}Z+\gamma\mathbf{U}]+\boldsymbol{\nabla}\cdot[\nu(h+Z)\boldsymbol{\nabla}\mathbf{U}]+\mathbf{S}_U, \tag{28a}$$

$$\frac{\partial Z}{\partial t}=-\boldsymbol{\nabla}\cdot[(h+Z)\mathbf{U}]+S_Z, \tag{28b}$$

where the SGSS terms are given by

$$\mathbf{S}_U=-\frac{\partial}{\partial t}\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}-\boldsymbol{\nabla}\cdot[(h+Z)\langle\delta\mathbf{u}\delta\mathbf{u}\rangle_{\mathbf{X}}+\mathbf{U}\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}+\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}\mathbf{U}+\langle\delta\zeta\,\delta\mathbf{u}\delta\mathbf{u}\rangle_{\mathbf{X}}]+\boldsymbol{\nabla}\cdot[\nu\langle\delta\zeta\boldsymbol{\nabla}\,\delta\mathbf{u}\rangle_{\mathbf{X}}]-\mathbf{f}\times\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}-g\langle\delta\zeta\boldsymbol{\nabla}\,\delta\zeta\rangle_{\mathbf{X}}-\gamma\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}, \tag{29a}$$

$$S_Z=-\boldsymbol{\nabla}\cdot\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}, \tag{29b}$$

where the gradient operator acts on the variable $\mathbf{X}$. In the averaging process we have assumed that $\mathbf{f}$, $\mathbf{t}$, γ, ν, ρ, and h are smooth functions of space.

From the general expressions (15) and (16) we immediately identify the source term q in the generic relation (17) for every average of fluctuations appearing in Eqs. (29a) and (29b), and using Eq. (24) write

$$\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}}=\frac{\Delta^2}{24}\boldsymbol{\nabla}Z\cdot\boldsymbol{\nabla}\mathbf{U}+O(\Delta^3),$$

$$\langle\delta\mathbf{u}\delta\mathbf{u}\rangle_{\mathbf{X}}=\frac{\Delta^2}{24}\boldsymbol{\nabla}\mathbf{U}\cdot\boldsymbol{\nabla}\mathbf{U}+O(\Delta^3),$$

$$\langle\delta\zeta\boldsymbol{\nabla}\,\delta\mathbf{u}\rangle_{\mathbf{X}}=\frac{\Delta^2}{24}\boldsymbol{\nabla}Z\cdot\boldsymbol{\nabla}(\boldsymbol{\nabla}\mathbf{U})+O(\Delta^3),$$

$$\langle\delta\zeta\boldsymbol{\nabla}\,\delta\zeta\rangle_{\mathbf{X}}=\frac{\Delta^2}{24}\boldsymbol{\nabla}Z\cdot\boldsymbol{\nabla}(\boldsymbol{\nabla}Z)+O(\Delta^3),$$

$$\langle\delta\zeta\,\delta\mathbf{u}\delta\mathbf{u}\rangle_{\mathbf{X}}=\frac{\Delta^2}{24}(\boldsymbol{\nabla}Z\cdot\nabla\langle\delta\mathbf{u}\delta\mathbf{u}\rangle_{\mathbf{X}}+2\boldsymbol{\nabla}\mathbf{U}\cdot\boldsymbol{\nabla}\langle\delta\zeta\,\delta\mathbf{u}\rangle_{\mathbf{X}})+O(\Delta^3).$$

As indicated explicitly in Eq. (25), the scalar product in the previous expressions corresponds to contracting the indices generated by the gradient operators.

Although exact, the system (28a)–(29b) is of little practical use as it stands due to the many terms involved and the appearance of a time derivative in the right hand side of Eq. (29a), which makes the numerical implementation cumbersome. A more practical system results if one writes Eq. (26a) in nonconservative form

$$\frac{\partial\mathbf{u}}{\partial t}=-\mathbf{u}\cdot\nabla\mathbf{u}-\mathbf{f}\times\mathbf{u}-g\boldsymbol{\nabla}\zeta-\gamma\mathbf{u}+\nabla\cdot(\nu\boldsymbol{\nabla}\mathbf{u})+\nu\boldsymbol{\nabla}\mathbf{u}\cdot\boldsymbol{\nabla}\ln(h+\zeta)+\frac{\mathbf{t}}{\rho(h+\zeta)},$$

and in the last two terms the approximation $|\delta\zeta|\ll h+Z$ is made in the form

$$\frac{1}{h+\zeta}\simeq\frac{1}{h+Z}\left(1-\frac{\delta\zeta}{h+Z}\right).$$

The resulting large scale equation is

$$\frac{\partial\mathbf{U}}{\partial t}=-\mathbf{U}\cdot\nabla\mathbf{U}-\mathbf{f}\times\mathbf{U}-g\boldsymbol{\nabla}Z-\gamma\mathbf{U}+\nabla\cdot(\nu\boldsymbol{\nabla}\mathbf{U})+\nu\boldsymbol{\nabla}\mathbf{U}\cdot\boldsymbol{\nabla}\ln(h+Z)+\frac{\mathbf{t}}{\rho(h+Z)}+\mathbf{S}'_U,$$

with

$$\mathbf{S}'_U=-\langle(\delta\mathbf{u}\cdot\boldsymbol{\nabla})\,\delta\mathbf{u}\rangle_{\mathbf{X}}+\nu\frac{\langle\boldsymbol{\nabla}\,\delta\zeta\cdot\boldsymbol{\nabla}\,\delta\mathbf{u}\rangle_{\mathbf{X}}}{h+Z}+\nu\langle\delta\zeta\boldsymbol{\nabla}\,\delta\mathbf{u}\rangle_{\mathbf{X}}\cdot\boldsymbol{\nabla}\left(\frac{1}{h+Z}\right).$$

The corresponding model is

$$\left\langle \delta u_k \frac{\partial \delta \mathbf{u}}{\partial x_k} \right\rangle_{\mathbf{X}} = \frac{\Delta^2}{24} \frac{\partial U_k}{\partial X_l} \frac{\partial^2 \mathbf{U}}{\partial X_l \partial X_k} + O(\Delta^3),$$

$$\left\langle \frac{\partial \delta \zeta}{\partial x_k} \frac{\partial \delta \mathbf{u}}{\partial x_k} \right\rangle_{\mathbf{X}} = \frac{\Delta^2}{24} \frac{\partial^2 Z}{\partial X_l \partial X_k} \frac{\partial^2 \mathbf{U}}{\partial X_l \partial X_k} + O(\Delta^3),$$

$$\left\langle \delta \zeta \frac{\partial \delta \mathbf{u}}{\partial x_k} \right\rangle_{\mathbf{X}} = \frac{\Delta^2}{24} \frac{\partial Z}{\partial X_l} \frac{\partial^2 \mathbf{U}}{\partial X_l \partial X_k} + O(\Delta^3).$$

IV. CONCLUSIONS

In conclusion, we have presented a formalism for obtaining closed large-scale fluid equations easily applicable to complex systems. In the case of the incompressible NS equations the formalism reproduces the differential approximation (to the order Δ^3) of the similarity model, which has the highest correlation found in *a priori* tests. Moreover, the analytically obtained model constant compares very well with the empirically determined one. As is the case for most models (for an exception see Ref. [6], in which explicit subgrid forcing is incorporated into the SGSS), the presented formalism is expected to be applicable when the forcing of the flow, given either by explicit body forces or by boundary conditions, acts at resolved scales only, in such a way that the subgrid scales are excited by nonlinear interactions among resolved scales. In this case the amplitude of the unresolved scale component of a field does usually remain sufficiently small to produce a smooth large-scale flow.

It is important to note that the particular definitions of fluctuations and corresponding averaging procedure that lead to relations (5) (which are fundamental, in the applications to complex system, to avoid the proliferation of SGSS) do not preclude the use of statistical theories to help model the SGSS so defined, allowing to complement the formalism presented. However, single-point closures cannot be used but rather two-point closures, as done in [7].

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APPENDIX

In this Appendix we analyze in some detail the different approximations made in the main text, and show that the resulting errors in the final expressions are of order Δ^3 only. For notational purposes, if the error in some expression is of order Δ^p we refer to that expression as $o(\Delta^p)$ accurate. To begin, consider the simplest average

$$A(\mathbf{X},\lambda) = \langle a(\mathbf{x}) \rangle_{\mathbf{X}}^{(\lambda)},$$

where the scale dependence has been indicated, and the right hand side is explicitly given by (in d-dimensional space)

$$\langle a(\mathbf{x}) \rangle_{\mathbf{X}}^{(\lambda)} \equiv \frac{1}{(\lambda \Delta_0)^d} \int_{X_1 - \lambda\Delta_0/2}^{X_1 + \lambda\Delta_0/2} dx_1 \cdots \int_{X_d - \lambda\Delta_0/2}^{X_d + \lambda\Delta_0/2} dx_d a(\mathbf{x}). \tag{A1}$$

By expressing $a(\mathbf{x})$ in terms of its Fourier transform

$$a(\mathbf{x}) = \frac{1}{(2\pi)^d} \int e^{i\mathbf{K}\cdot\mathbf{x}} \tilde{a}(\mathbf{K}) d^d K = \frac{1}{(\pi\Delta_0)^d} \int e^{i2\mathbf{k}\cdot\mathbf{x}/\Delta_0} \tilde{a}(\mathbf{k}) d^d k, \tag{A2}$$

conveniently written in terms of the dimensionless wave vector $\mathbf{k} = \Delta_0 \mathbf{K}/2$, after performing the spatial integral in Eq. (A1) one immediately obtains the Fourier transform of the average as

$$\tilde{A}(\mathbf{k},\lambda) = \tilde{a}(\mathbf{k}) S(\mathbf{k},\lambda), \tag{A3}$$

where

$$S(\mathbf{k},\lambda) = \frac{\sin(\lambda k_1)}{\lambda k_1} \cdots \frac{\sin(\lambda k_d)}{\lambda k_d}. \tag{A4}$$

We now analyze the approximation (18) applied to $A(\mathbf{X},\lambda)$:

$$A(\mathbf{X},2\lambda) \simeq A(\mathbf{X},\lambda) + \lambda \frac{\partial A(\mathbf{X},\lambda)}{\partial \lambda} + \frac{\lambda^2}{2} \frac{\partial^2 A(\mathbf{X},\lambda)}{\partial \lambda^2} = \frac{1}{(\pi\Delta_0)^d} \int e^{i2\mathbf{k}\cdot\mathbf{X}/\Delta_0} \tilde{a}(\mathbf{k}) S_{\mathrm{app}}(\mathbf{k},2\lambda) d^d k,$$

where, from Eq. (A3),

$$S_{\mathrm{app}}(\mathbf{k},2\lambda) = S(\mathbf{k},\lambda) + \lambda \frac{\partial S(\mathbf{k},\lambda)}{\partial \lambda} + \frac{\lambda^2}{2} \frac{\partial^2 S(\mathbf{k},\lambda)}{\partial \lambda^2}. \tag{A5}$$

It is now convenient to consider the derivative, easily obtained from Eq. (A4),

$$\frac{\partial S(\mathbf{k},\lambda)}{\partial \lambda} = \frac{S(\mathbf{k},\lambda)}{\lambda} \sum_{i=1}^{d} [\lambda k_i \cot(\lambda k_i) - 1].$$

Taylor expanding the summand we can write

$$\frac{\partial \ln S(\mathbf{k},\lambda)}{\partial \ln \lambda} = -\frac{\lambda^2}{3} \sum_{i=1}^{d} k_i^2 - \frac{\lambda^4}{45} \sum_{i=1}^{d} k_i^4 + O(\lambda^6 k^6).$$

For the scales of $A(\mathbf{X},\lambda)$, $\lambda k \lesssim \pi/2$, the order k^4 and higher terms can be neglected, which allows a simple integration to yield

$$S(\mathbf{k},\lambda) = \exp(-\lambda^2 k^2/6), \tag{A6}$$

from which

$$S(\mathbf{k},2\lambda) = \exp(-2\lambda^2 k^2/3) = \exp(-\lambda^2 k^2/6) \times \left(1 - \frac{\lambda^2 k^2}{2} + \frac{\lambda^4 k^4}{8} + O(\lambda^6 k^6)\right), \tag{A7}$$

while, from Eq. (A5),

$$S_{\mathrm{app}}(\mathbf{k},2\lambda)=\exp(-\lambda^2k^2/6)\times\left(1-\frac{\lambda^2k^2}{2}+\frac{\lambda^4k^4}{18}+O(\lambda^6k^6)\right). \quad \text{(A8)}$$

Equations (A7) and (A8) then differ in terms of order $(\lambda k)^4$ [consistent with the approximation leading to Eq. (A6)], which means that approximation (18) for simple averages (A1) is $o(\Delta^4)$ accurate.

Similarly, approximation (22) applied to the single average (A1) can be analyzed directly from Eq. (A6) from which we can write

$$S(\mathbf{k},\lambda')=S(\mathbf{k},\lambda)\left(1+\frac{(\lambda^2-\lambda'^2)k^2}{6}+O(k^4)\right). \quad \text{(A9)}$$

For $\lambda'\leqslant\lambda$ the second term between brackets is always smaller than $\lambda^2k^2/6$, which, for a source q corresponding to a simple average (A1), translates to

$$q(\mathbf{X},\lambda')=q(\mathbf{X},\lambda)+O(\Delta^2). \quad \text{(A10)}$$

Since Eq. (21) is of order Δ^2, approximation (22) leads in this case to $o(\Delta^4)$ accurate results in Eq. (24).

In general, however, both Eqs. (18) and (22) are applied to averages more complex than Eq. (A1) [see Eqs. (15) and (16)]. These averages can always be expressed in terms of simple averages of the form (A1) or products thereof, for instance,

$$\langle \delta a(\mathbf{X},\mathbf{x})\,\delta b(\mathbf{X},\mathbf{x})\rangle_{\mathbf{X}}=\langle a(\mathbf{x})b(\mathbf{x})\rangle_{\mathbf{X}}-A(\mathbf{X})B(\mathbf{X}), \quad \text{(A11)}$$

and

$$\langle \delta a(\mathbf{X},\mathbf{x})\,\delta b(\mathbf{X},\mathbf{x})\,\delta c(\mathbf{X},\mathbf{x})\rangle_{\mathbf{X}}=\langle a(\mathbf{x})b(\mathbf{x})c(\mathbf{x})\rangle_{\mathbf{X}}-A(\mathbf{X})\langle b(\mathbf{x})c(\mathbf{x})\rangle_{\mathbf{X}}-B(\mathbf{X})\times\langle a(\mathbf{x})c(\mathbf{x})\rangle_{\mathbf{X}}-C(\mathbf{X})\langle a(\mathbf{x})b(\mathbf{x})\rangle_{\mathbf{X}}+2A(\mathbf{X})B(\mathbf{X})C(\mathbf{X}). \quad \text{(A12)}$$

Approximation (18) can now be analyzed term by term in Eqs. (A11) and (A12). The first term in the right-hand side of both expressions is an average of the form (A1) so that Eq. (18) applied to it produces $o(\Delta^4)$ accurate results. The rest of the terms are the product of either two or three simple averages. Let us consider as an example the term $A(\mathbf{X},\lambda)B(\mathbf{X},\lambda)$, where the scale dependence has been explicitly indicated. Approximation (18) applied to it is expressed as

$$A(\mathbf{X},2\lambda)B(\mathbf{X},2\lambda)=A(\mathbf{X},\lambda)B(\mathbf{X},\lambda)+\lambda\frac{\partial}{\partial\lambda}[A(\mathbf{X},\lambda)B(\mathbf{X},\lambda)]+\frac{\lambda^2}{2}\frac{\partial^2}{\partial\lambda^2}[A(\mathbf{X},\lambda)B(\mathbf{X},\lambda)]. \quad \text{(A13)}$$

Since approximation (18) for simple averages gives $o(\Delta^4)$ accurate results, it can be applied to each term in the left-hand side of Eq. (A13) to evaluate the product at this level of accuracy. If this is done, and the derivatives in the right-hand side performed, it is easy to verify that both sides of Eq. (A13) so evaluated differ in terms of order Δ^3, that is, approximation (18) applied to the product of two simple averages gives $o(\Delta^3)$ accurate results. The same conclusion is similarly verified for the product of three simple averages, leading then to $o(\Delta^3)$ accurate results for both fluctuation averages (A11) and (A12).

Analogously, using Eq. (A10) for each simple average, it is immediately verified that Eq. (A10) is also valid for the product of two or more simple averages, leading to $o(\Delta^4)$ accurate results when approximation (22) is used in Eq. (24).

The accuracy in the final expressions is then limited to the $o(\Delta^3)$ accuracy of approximation (18).

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