Vertex corrections and ‘optimal’ subgrid models for homogeneous isotropic turbulence

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Abstract. If the Fourier modes in a DNS of homogeneous isotropic turbulence are separated into ‘resolved’ ($k < k_c$) and ‘unresolved’ ($k > k_c$) modes by introducing a partition wavevector $k_c$, projection of the part of the nonlinear interaction containing unresolved modes onto the resolved velocity gives a numerical eddy viscosity that models the effect of the unresolved interactions on the resolved velocity field. Evaluation of this eddy viscosity by DIA gives a result in fair overall agreement with numerical data. We consider the extension of this formalism to projection of the unresolved nonlinearity onto quadratic products of the resolved velocity. We evaluate this projection by perturbation theory, and attempt to relate the result to the vertex corrections predicted by Martin-Siggia-Rose theory. Non-Gaussian properties of turbulence prove to have a crucial role. We discuss the constraints imposed by Galilean invariance on this type of computation.

1. Introduction

The Navier-Stokes equations in Fourier variables are

$$\dot{u}_i(k) = -\frac{i}{2} P_{imn}(k) \int dp \, dq \, \delta(k - p - q) u_m(p) u_n(q) - \nu k^2 u_i(k)$$

where, in one form of the standard notation, $P_{imn}(k) = k_m P_{in}(k) + k_n P_{im}(k)$ and $P_{in}(k) = \delta_{in} - k_i k_n k^{-2}$ is the transverse projection operator that projects any vector into the plane perpendicular to $k$: physically, $\delta_{in}$ gives the advective part of the nonlinearity, and $k_i k_n k^{-2}$ comes from solving the pressure Poisson equation; we note that this part of the nonlinearity depends only on strains. The physical space form of the pressure Poisson equation

$$\nabla^2 p = -\frac{\partial u_m}{\partial x_n} \frac{\partial u_n}{\partial x_m}$$

makes this evident.

The factor $\delta(k - p - q)$ expressing the ‘triad condition,’ that vectors $k, p,$ and $q$ form a triangle, comes from writing the quadratic nonlinearity in physical space as a convolution in wavevector space. We review this standard material for later reference when we attempt to generalize the Navier-Stokes equations somewhat.
It will be convenient to rewrite the Navier-Stokes nonlinearity, or ‘vertex,’ first in terms of a quantity with three vector arguments as

\[ P_{imn}(k, p, q) = -\frac{i}{2} P_{imn}(k) \delta(k - p - q) \]  

that acts on the velocity field by

\[ \int d(pdq) P_{imn}(k, p, q) u_m(p) u_n(q) \]  

and then further as a quantity with three time arguments as

\[ P_{imn}(k, p, q; t, t', t'') = P_{imn}(k, p, q) \delta(t - t') \delta(t - t'') \]  

acting on velocity products as

\[ \int_0^t dt' \int_0^{t''} dt'' \int dpdq P_{imn}(k, p, q; t, t', t'') u_m(p, t') u_n(q, t'') \]  

2. Theoretical evaluation of vertex corrections

Recall the renormalized perturbation theory of Martin, Siggia & Rose (1973) (MSR). This theory groups the infinity of terms generated by treating the nonlinearity as small into classes with the same ‘structure;’ we will not attempt a summary, but refer to the original paper for details.

One type of term is an effective nonlinearity, \( \gamma_{imn}(k, p, q; t, t', t'') \delta(k - p - q) \) that acts on the velocity field by

\[ \int_0^t dt' \int_0^{t''} dt'' \int dpdq \delta(k - p - q) \gamma_{imn}(k, p, q; t, t', t'') u_m(p, t') u_n(q, t'') \]

just like the ordinary nonlinearity rewritten as Eq. (6).

We will evaluate one such term, that of lowest order, as a ‘correction’ to the Direct Interaction Approximation (DIA) of Kraichnan (1959); here, quotes are advisable since the actual inclusion of such terms in DIA need not be an improvement (Kraichnan, 1958). Yet the theoretical interest of such corrections would seem to justify an attempt to show where they come from, and at least to outline the derivation, even if the complexity of the rather elementary details precludes a complete account.

We can begin with the ‘bare’ vertex, that is, the nonlinearity of the Navier-Stokes equation itself, in the form of Eq. (3):

\[ P_{imn}(k, p, q) u_m(p, t) u_n(q, t) \]

and substitute

\[ u_m(p, t) = \int_0^t dt' G(p; t, t') P_{mrs}(p, p', p'') u_r(p', t') u_s(p'', t') \]

and make the same substitution for \( u_s(q, t) \); because we are evaluating this quantity as a correction to DIA, \( G \) is simply the DIA response function. The result is

\[ P_{mn}(k, p, q) G(p; t, t') P_{mrs}(p, p', p'') u_r(p', t') u_s(p'', t') \times \\
G(q; t, t') P_{npq}(q, q', q'') u_p(q', t') u_q(q'', t') \]
where integration over repeated wavevectors and appropriate time integrations are understood. The $P$ operators imply triad conditions

$$\mathbf{p} = \mathbf{p}' + \mathbf{p}'' \quad \mathbf{q} = \mathbf{q}' + \mathbf{q}''$$

We can contract two wavevectors in four equivalent ways, one of which is

$$\mathbf{p}' + \mathbf{q}' = 0$$

Then the remaining free wavevectors $\mathbf{p}'', \mathbf{q}''$ satisfy

$$\mathbf{k} = \mathbf{p} + \mathbf{q} = \mathbf{p}' + \mathbf{p}'' + \mathbf{q}' + \mathbf{q}'' = \mathbf{p}'' + \mathbf{q}''$$

and we obtain the first vertex correction term

$$\gamma_{1sq}^1(\mathbf{k}, \mathbf{p}'', \mathbf{q}'', t, t'; t'', t''') = \int d\mathbf{p}' G(p; t, t')G(q; t, t'')U(p'; t', t'') \times P_{imm}(\mathbf{k}, \mathbf{p}, \mathbf{q})P_{mrs}(\mathbf{p}, \mathbf{p}'', \mathbf{p}''')P_{npr}(\mathbf{q} - \mathbf{p}', \mathbf{q}'')P_{pr}(\mathbf{p}')$$

in which the wavevector arguments can be rearranged as

$$\gamma_{1sq}^1(\mathbf{k}, \mathbf{p}, \mathbf{q}; t', t'') = \int d\mathbf{q}' G(p'; t, t')G(q'; t, t'')U(|\mathbf{p}' - \mathbf{p}|; t', t'') \times P_{imm}(\mathbf{k})P_{mrs}(\mathbf{p}')P_{npr}(\mathbf{q}')P_{pr}(\mathbf{p}' - \mathbf{p})$$

A second structure is obtained by substituting Eq. (9) in Eq. (3) as before, but then substituting

$$u_r(\mathbf{p}', t') = \int_0^t dt'' G(p'; t'')P_{npr}(\mathbf{p}, \mathbf{q}'', \mathbf{q}'')u_p(\mathbf{q}', t'')u_q(\mathbf{q}'', t'')$$

The result is a second vertex correction term

$$\gamma_{1sq}^2(\mathbf{k}, \mathbf{p}'', \mathbf{q}'', t, t'; t'', t''') = \int d\mathbf{q}' G(p'; t, t')G(q'; t', t'')U(q; t, t'') \times P_{imm}(\mathbf{k}, \mathbf{p}, \mathbf{q})P_{mrs}(\mathbf{p}, \mathbf{p}'', \mathbf{p}''')P_{npr}(\mathbf{q}'', \mathbf{q}'')P_{nq}(\mathbf{q})$$

which acts (slightly differently in time from $\gamma^1$) by

$$\int_0^t dt' \int_0^{t'} dt'' \int d\mathbf{p}''d\mathbf{q}'' \delta(\mathbf{k} - \mathbf{p}'' - \mathbf{q}'') \times \gamma_{1sq}^2(\mathbf{k}, \mathbf{p}'', \mathbf{q}'', t, t'; t'', t''')u_s(\mathbf{p}'', t')u_q(\mathbf{q}'', t'')$$

Again, the wavevector arguments can be rearranged to give

$$\gamma_{1sq}^2(\mathbf{k}, \mathbf{p}, \mathbf{q}; t', t'') = \int d\mathbf{q}' G(|\mathbf{q}' + \mathbf{k}|; t'')G(|\mathbf{q}' + \mathbf{q}|; t'')U(\mathbf{q}' + \mathbf{q}; t', t'') \times P_{imm}(\mathbf{k})P_{mrs}(\mathbf{q}' + \mathbf{k})P_{npr}(\mathbf{q}' + \mathbf{q})P_{nq}(\mathbf{q}')$$

A third term is obtained by elementary symmetry operations applied to $\gamma^2$; call it $\gamma^3$ and define the total vertex correction as

$$\gamma = \gamma^1 + \gamma^2 + \gamma^3$$
3. Properties of vertex corrections

We would like to call attention to some simple properties of these quantities. First, we note that in Eqs. (15) and (19) the triad interaction between \( \mathbf{k}, \mathbf{p}, \mathbf{q} \) is now modulated by interactions with the additional wavevector \( \mathbf{q}' \): recall that this possibility was explicitly excluded in the formulation of DIA (Kraichnan, 1959); such interactions are, in Kraichnan’s terminology, indirect.

A second elementary property is a spatial nonlocality implied by the presence of \( \mathbf{p}, \mathbf{q} \) in the quantity \( \gamma \): in comparison, the bare nonlinearity contains only \( \mathbf{k} \). The consequence appears more clearly in physical space. The bare vertex in physical space is written by Carnevale & Martin (1982) as a three-argument operator as

\[
\gamma_{ijk}(x,y,z) = \frac{1}{2} \frac{\partial}{\partial x_j} \int dy dz \left[ \delta_{ik} \delta(x-y) - \frac{\partial^2}{\partial x_i \partial x_k} g(x-y) \right] \delta(y-z) + (jk)
\]

where \((jk)\) abbreviates index symmetry. We will find that, not surprisingly, vertex corrections induce a ‘smoothing’ of the term \( \delta(y-z) \). It is straightforward to repeat the previous calculation in these variables. If we isolate only the terms containing \( \delta_{jk} \), we will find a contribution to the vertex correction

\[
\int_0^t dt' \int_0^t dt'' \frac{\partial}{\partial x_j} G_{jn}(xy';tt')G_{jn}(zx';tt'') \times \frac{\partial}{\partial y_m} \frac{\partial}{\partial z_r} U_{mr}(y'z';t',t'')u_n(y',t')u_s(z',t'')
\]

The vertex correction therefore depends nontrivially on all three points \( x, y', z' \), and in particular is not proportional to \( \delta(y' - z') \). This is the ‘smoothing’ effect noted earlier.

It should be noted that the vertex correction is transverse: this is a trivial consequence of the factor \( P_{imn}(\mathbf{k}) \). It should also be verified that the vertex corrections remain energy conserving. A rather more subtle property to verify is that the integrals defining the corrections converge on a Kolmogorov spectrum; in other words, that the vertex correction is local in Fourier space. This is crucial to the vertex corrections not upsetting Kolmogorov scaling (compare Nakano (1974)). On the one hand, it seems plausible that Galilean invariance must insure convergence and locality. On the other hand, it should be noted (Yukio Kaneda, private communication) that MSR is an Eulerian theory, and therefore such consistency with Kolmogorov scaling is problematic.

Two even less obvious properties are Galilean invariance and vanishing in equipartition, which we briefly consider separately.

3.1. Galilean invariance

Perhaps the most important constraint on vertex corrections is Galilean invariance. While much has been written about this subject (for example, (Nakano, 1974; McComb, 2005)), we will only state a simple sufficient condition: since Galilean invariance does not constrain any expression that depends only on strain rates, we will insist simply that vertex corrections depend only on strain rates. One way to satisfy this condition is to require

\[
\lim_{\mathbf{p} \to -\mathbf{k}} \gamma_{imn}(\mathbf{k}, \mathbf{p}, \mathbf{q}; t, t', t'') = 0
\]
and the corresponding limit for $q$, because then, the complete vertex term $P + \gamma$ reduces in this limit to $P_{mn}(k)u_m(k)U_n = k_n u_i(k)U_n$, the Fourier transform of the spatial part of the convective derivative $U_n \partial u_i / \partial x_n$, where $U_n = u_n(q)|_{q=0}$ is understood as a mean velocity.

An example of a vertex correction that would satisfy this condition is

$$\gamma_{imn}(k, p, q) = (p \cdot q)P_{imn}(k, p, q)$$

but we emphasize that this example is intended only to illustrate the theoretical possibility of Galilean invariant vertex corrections, and is not offered as an actual model. A direct demonstration of this limit from the expressions above has not yet been accomplished.

### 3.2. Thermal equilibrium properties

Forster, Nelson & Stephen (1977) state that vertex corrections vanish in a Gaussian thermal equilibrium steady state (their 'Model A') in the limit $k \to 0$. This statement is justified by a general argument; it is not a special consequence of their renormalization group formalism. We will therefore consider this to be an additional constraint on vertex corrections. Again, a direct demonstration that the result of perturbation theory is consistent with this constraint has not yet been accomplished.

### 4. Numerical evaluation of vertex corrections

Both subgrid model formulations for LES and renormalization group formalisms introduce a cutoff wavenumber $k_c$ and rewrite the Navier-Stokes equations as

$$\dot{u}_i(k) + N_i^<(k) = -N_i^>(k) - \nu k^2 u_i(k)$$

where

$$N_i^<(k, t) = -i P_{imn}(k) \int_{\Delta^<} dp dq \, \delta(k - p - q) u_m(p, t) u_n(q, t)$$

with

$$\Delta^< = \{ p, q | p \leq k_c \text{ and } q \leq k_c \}$$

is the resolved nonlinearity, and

$$N_i^>(k, t) = P_{imn}(k) \int_{\Delta^>} dp dq \, \delta(k - p - q) u_m(p, t) u_n(q, t)$$

with

$$\Delta^> = \{ p, q | p \geq k_c \text{ or } q \geq k_c \}$$

is the unresolved nonlinearity.

Both formalisms attempt to capture the effect of modes with $k > k_c$ on the remaining modes by some modification of the equations for the modes with $k < k_c$. Langford & Moser (1999) developed the idea that the 'optimal' subgrid model is

$$\dot{u}_i(k) + N_i^<(k) = -\langle N_i^>(k) | u_i(k) \rangle - \nu k^2 u_i(k)$$

They suggested that an expansion of $\langle N^>| u^< \rangle$ in powers of $u^<$ could therefore provide a hierarchy of increasingly accurate models. It should be stressed that the significance of this approach is perhaps more theoretical than practical, since any evaluation of the terms in this series requires knowledge of the unresolved field.
The simplest construction of this type is obtained by the linear regression of $N^>$ on $u^<$, so that 
\[ \dot{u}^i(k) + N^<_i(k) = \nu(k)k^2u^i(k) \]
where (Kraichnan, 1976) \[ \nu(k)k^2 = \langle N^>_i(k)u^i(-k) \rangle / \langle u^i(k)u^i(-k) \rangle \].
This computation of an eddy viscosity from numerical data can also be considered as a kind of ‘numerical renormalization group.’ Any number of investigations (for example (Domaradzki et al., 1987)) have demonstrated that the resulting measured spectral eddy viscosity \( \nu(k) \) is well predicted by closure theories, including the main qualitative features: a ‘plateau’ for \( k \ll k_c \) and ‘cusp’ (Kraichnan, 1976) when \( k \approx k_c \).

Langford & Moser (1999) also investigated the natural next step, which adds the projection of the unresolved nonlinearity onto the resolved nonlinearity. This connects the projection formalism with vertex corrections, since the result of this computation will be a correction to the Navier-Stokes nonlinearity induced by nonlinear interactions, in this case, with the unresolved motion. The result is a model of the form
\[ \dot{u}^i(k) + N^<_i(k) = C_1(k)u^i(k) + C_2(k)N^>_i(k) \] (32)
Then the linear eddy damping \( C_1 \) and quadratic contribution \( C_2 \) satisfy the system of algebraic equations (Langford & Moser, 1999)
\[ C_1(k)\langle u^i(-k)u^i(k) \rangle + C_2(k)\langle u^i(-k)N^>_i(k) \rangle = \langle u^i(-k)N^<_i(k) \rangle \] (33)
\[ C_1(k)\langle N^<_i(-k)u^i(k) \rangle + C_2(k)\langle N^<_i(-k)N^>_i(k) \rangle = \langle N^<_i(-k)N^>_i(k) \rangle \] (34)
A notable feature of this computation appears in the inhomogeneous term in the second equation:
\[ \langle N^<_i(-k)N^>_i(k) \rangle = P_{imm}(k)P_{irs}(-k) \times \]
\[ \int_{\Delta^>} dp' dp \int_{\Delta^<} dq \delta(k - p - q)\delta(-k - p' + q') \times \]
\[ \langle u_m(p)u_r(q)u_r(p')u_s(q') \rangle \] (35)
The fourth-order correlation in this integral is part of the mean-square nonlinearity (Chen et al., 1989); we therefore have a connection between the fluctuations of the nonlinear term, a natural ‘higher order’ statistic in turbulence, and vertex corrections. The Gaussian part of this correlation vanishes, since the disjoint integration regions \( \Delta^< \) and \( \Delta^> \) do not allow the wavevectors to be grouped into pairs with opposite signs. Thus, this correlation is a cumulant, but it was shown in (Chen et al., 1989) that this cumulant can be evaluated by DIA and that the result is nonzero. This will permit a comparison between a theoretical result and the result of numerical computations, such as those of Langford & Moser (1999), and our own now in progress.

Although there is no apparent obstacle to completing this calculation, the previous discussion suggests that adding \( C_2(k)P_{imm}(k) \) to the nonlinearity modifies the advective term, and is therefore consistent with Galilean invariance only if \( C_2 \equiv 0 \) (note that the limit condition in Eq. (24) is not satisfied by the assumed vertex correction). Nevertheless, we present in Figures 1 and 2 some preliminary results in which \( C_1 \) and \( C_2 \) in Eq. (32) are evaluated using decaying turbulence DNS data at different evolution times described in the captions. Figure 1 shows the coefficient \( C_1(k) \): note that with the sign convention in Eq. (32), damping corresponds to \( C_1 \leq 0 \). Except for possible numerical artifacts near the cutoff, we find the familiar ‘plateau-cusp’ structure. Figure 2 shows the results for \( C_2 \); as in the results of Langford & Moser (1999), it is rather small, but is nevertheless clearly nonzero, and also exhibits a somewhat weaker ‘plateau-cusp’ structure than \( C_1 \). But as we have noted, such results can only be interpreted with caution, until the issues concerning Galilean invariance in this type of projection formalism are conclusively settled.
One approach to imposing Galilean invariance is to decompose the nonlinearity into its advective and pressure parts, so that

\[ N_i^c = N_i^{c<} + N_i^{p<} \]  

(36)

where

\[
N_i^{c<}(k, t) = -\frac{i}{2}(k_m \delta_{im} + k_n \delta_{in}) \int_{\Delta^c} dp dq \, \delta(k - p - q)u_m(p, t)u_n(q, t)
\]

\[
N_i^{p<}(k, t) = -ik_i k_m k_n k^{-2} \int_{\Delta^c} dp dq \, \delta(k - p - q)u_m(p, t)u_n(q, t)
\]  

(37)

with the obvious analogs for \( N^> \). Now replace Eq. (32) by

\[
\dot{u}_i(k) + N_i^{c<}(k) = C_1 u_i(k) + C_2^e(k) N_i^{c<}(k) + C_2^b(k) N_i^{p<}(k)
\]  

(38)

The problem remains that once we insist on \( C_2^e = 0 \) to maintain Galilean invariance, every term in Eq. (38) is transverse except the last, which is longitudinal; it follows then that \( C_2^b = 0 \) as well.

We should note that the calculations of this section differ rather fundamentally from the theoretical analysis based on MSR, because they consider only single-time correlations; however, it is very easy to verify that the consideration of more complex projections onto velocities evaluated at unequal times will not alter the conclusions about Galilean invariance.

For this reason, it seemed natural to generalize the formalism of (Langford & Moser, 1999) somewhat, by considering the projections onto each triad individually, leading to the model

\[
\dot{u}_i(k) + P_{imn}(k)u_m(p)u_n(q) = C_1 u_i(k) + Q_{imn}(k, p, q)u_m(p)u_n(q) - \nu k^2 u_i(k)
\]  

(39)

where it is understood that both \( p, q \leq k_c \). This type of model seems closer to the theoretical formulation of vertex corrections by MSR. It also permits the limit of Eq. (24) to be satisfied, and thus can be consistent with Galilean invariance at least in principle.

This modeling will require evaluation of correlations such as \( \langle N_i^{r<}(-k)u_m(p)u_n(q) \rangle \) where \( p, q \leq k_c \). Since

\[
\langle N_i^{r<}(-k)u_m(p)u_n(q) \rangle = -P_{irs}(k) \int_{\Delta^r} dp' dq' \, \delta(k - p' - q')\langle u_r(p')u_s(q')u_m(p)u_n(q) \rangle
\]  

(40)

it is evident that, as before, the Gaussian contribution to this fourth-order correlation vanishes because \( p', q' \geq k_c \) and \( p, q \leq k_c \). Cumulant corrections can be evaluated following (Chen et al., 1989). A representative contribution to the cumulant gives a vertex correction term

\[
P_{irs}(k)P_{bd}(k)P_{med}(p)P_{ca}(q) \int_0^t dt' \int_0^t dt'' G(p; tt''; U(q; tt''; U(k; t' t'' \times \int_{\Delta^>} dp' dq' \, \delta(k - p' - q')P_{rabs}(p')P_{cas}(q')G(p; tt'')U(q; tt')
\]  

(41)

Evidently, this result is much more complex than the MSR vertex corrections. But one property of vertex corrections is trivially true, namely the (Forster, Nelson & Stephen, 1977) condition, since the correlation in Eq. (40) vanishes if the velocity field is Gaussian. Nevertheless, it remains an open question whether this more general form actually is consistent with Galilean invariance.

We should also note the difficulty of any numerical evaluation of such triad-dependent quantities.
5. Conclusions

We have reviewed the Martin, Siggia & Rose (1973) theory of vertex corrections, and have attempted to connect this theory to the possibility of evaluating numerical vertex corrections through a projection formalism which naturally generalizes the now familiar construction of numerical eddy viscosity from numerical data. It is not clear why projection might violate Galilean invariance, or conversely, why nonzero results for this projection can be obtained at all if a nonzero projection violates Galilean invariance. Further research will be required to clarify this issue.

![Figure 1. Coefficient $C_1(k,t)$ at $u_0k_0t_n = 0.6n, n = 1,\cdots, 5$ for decaying turbulence. $k_c = 32, R_\lambda(0) = 162$](#)

![Figure 2. Coefficient $C_2(k,t)$ at $u_0k_0t_n = 0.6n, n = 1,\cdots, 5$ for decaying turbulence. $k_c = 32, R_\lambda(0) = 162$.](#)

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