Spectral Calculations of Isotropic Turbulence: Efficient Removal of Aliasing Interactions
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This is plotted in Fig. 2. Evidently, in the region beyond \( \xi \approx 1.3 \), the vertical gradient is stable. This would tend to compress an eddy of uniform temperature (corresponding to an entrained blob) vertically, resulting in a lateral expansion. We can estimate this effect quantitatively. The maximum vertical gradient is approximately

\[
\frac{\partial}{\partial z} \left( \bar{T} - \bar{T}_0 \right) \big|_{\text{max}} = 0.32 \frac{\theta}{z}, \tag{2}
\]

if we make the approximation that \( J \sim \exp \left( -\frac{1}{2} \xi \right) \).

A force gradient per unit mass will be given by \( g/\theta T_0 \) times this, and an effective strain rate will be given by multiplying by a time that an eddy is subjected to the temperature field. The maximum radial velocity is in this region (a very flat maximum near \( \xi \approx 2.5 \)) with a value of roughly \( -\frac{1}{2} U_s / R_T \). At this velocity an eddy would traverse its own width \( l \) in a time \( 2z / U_s \). This time is evidently the time spent by the eddy in the temperature field; in addition, it is of the same order as the time for appreciable development of the flow defined by

\[
(\nu U_s / l)^{-1} \approx z / U_s \tag{3}
\]

and as the time during which the eddies are accelerated.

That is, the accelerating force per unit mass is \( g\theta / T_0 \); applied over a certain time, this results in a velocity \( U_s \). The time is evidently

\[
\frac{U_s}{g\theta / T_0} \approx \frac{z}{U_s}, \tag{4}
\]

using \( g\theta / T_0 = U_s / R_T \), and \( R_T l = z \). Using \( 2z / U_s \) for the time, the effective strain rate is

\[
(0.32 \theta / z) (g / T_0) (2z / U_s) \approx 0.64 U_s / z. \tag{5}
\]

We must compare this with the strain rate tending to compress the eddies horizontally, or expand them vertically:

\[
\frac{\partial U}{\partial z} = -\left( \frac{1}{2} + \xi \right) U_s / z; \quad \frac{\partial U}{\partial z} \bigg|_{\text{max}} = 0.62 U_s / z,
\]

using \( f = \exp \left( -\frac{1}{2} \xi \right) \).

These effects are thus seen to be of the same order of magnitude, and of opposite sign. It appears likely, therefore, that they counteract each other, resulting in a dynamical situation more like the wake, and a lower value of \( R_T \).

The excellent numerical agreement between (5) and (6) must be regarded as fortuitous; somewhat different definitions than those we have adopted could result in a factor of 2 in either direction.

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3. Reference 1, p. 189.
5. In Fig. 1 and in the equation we are making the approximation, sufficiently accurate for this discussion, that the length scales of the temperature and velocity distributions are equal. In fact (Ref. 2) the length scale of the temperature distribution is about 16% greater than that of the velocity distribution.
6. A blob of entrained fluid ("eddy") gradually mixes with its surroundings, slowly losing its buoyancy; there is, of course, no sharply defined "time that an eddy is subjected to the temperature field." We are trying to estimate a time characteristic of this process, say a mean half-life of the buoyancy of an entrained blob.
7. Reference 1, p. 96.

Spectral Calculations of Isotropic Turbulence: Efficient Removal of Aliasing Interactions

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An algorithm is given for the rapid calculation of the convolution sums appearing in the Fourier-transformed Navier–Stokes equations. In three space dimensions, the new algorithm is a factor of 4 more efficient than previously suggested algorithms.

Numerical simulation of isotropic incompressible turbulence usually involves solving the Navier–Stokes equations in a cubical box with periodic boundary conditions. In this case, it seems that the best procedure is to expand the velocity field in a Fourier series and perform the calculation in wave-vector space.13 The convolution sums that appear in the Fourier-trans-
formed Navier–Stokes equations are most efficiently evaluated using a discrete form of the convolution theorem and the very efficient fast Fourier transform algorithm. However, straightforward application of the fast Fourier transform introduces “aliasing” errors. The fast Fourier transform, being a discrete Fourier transform, is unable to distinguish between wave-vector components modulo $2K$, where $K$ is the maximum wave-vector component considered in the calculation. Standard methods to remove aliasing do so at the cost of requiring a factor $2^n$ additional Fourier transforms, and hence a factor $2^n$ in computing time. Here, $n$ is the number of space dimensions. In this note, we derive an algorithm that requires only a factor $2$ additional transforms (a speedup of a factor $2^{n-1}$ over the old algorithm) at the additional cost of truncating those Fourier modes that lie outside a sphere of radius $\alpha K$, $\alpha \geq 2\sqrt{2}/3 \approx 0.94$. Since the truncated modes have little physical significance when the calculation is done with a wave-vector component cutoff of $K$, the cost of the new algorithm is minimal.

The three-dimensional velocity field $\mathbf{v}(\mathbf{x})$ is defined only on points of the discrete $N \times N \times N$ grid $\mathbf{x} = 2\pi n/N$ with $0 \leq n < N$ (i.e., $0 \leq n_a < N$ for $\alpha = 1, 2, 3$) and $n_a$ integral. Similarly, the Fourier coefficients $\mathbf{u}(\mathbf{k})$ are defined on the grid $\mathbf{k} \in C_K$, where $\mathbf{k} \in C_K$ is defined to mean $-K \leq n_a < K$ for $\alpha = 1, 2, 3$ and $N = 2K$. Then, $\mathbf{v}(\mathbf{x})$ and $\mathbf{u}(\mathbf{k})$ form a discrete Fourier transform pair:

$$\mathbf{v}(\mathbf{x}) = \sum_{\mathbf{k} \in C_K} \mathbf{u}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x});$$

$$\mathbf{u}(\mathbf{k}) = (1/N^3) \sum_{0 \leq n < N} \mathbf{v}(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}).$$

The nonlinear terms in the Fourier-transformed Navier–Stokes equations appear as convolution sums of the form

$$U_{\theta_\gamma}(\mathbf{k}) = \left[1/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q}) \quad (\mathbf{k} \in C_K).$$

Instead of computing these sums directly, we compute them using the convolution theorem by transforming $\mathbf{u}_p$ and $\mathbf{u}_q$ to real space, forming $\mathbf{v}_p(\mathbf{x}) \mathbf{v}_q(\mathbf{x})$, and transforming back to wave-vector space. Three fast Fourier transforms require order $3N^3 \log_2 N^3$ operations instead of order $(N^3)^2$ operations required for direct evaluation of the convolution sum. However, because of aliasing (which arises from the discreteness of the grid used in the transforms (1)), the result obtained as the inverse transform of $\mathbf{v}_p(\mathbf{x}) \mathbf{v}_q(\mathbf{x})$ is not $U_{\theta_\gamma}(\mathbf{k})$ but rather the aliased sum

$$A_{\theta_\gamma}(\mathbf{k}) = \left[1/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q}) \quad (\mathbf{k} \in C_K),$$

where $a_n(\mathbf{q}) = q_n - 2K$ if $q_n \geq K$, $a_n(\mathbf{q}) = q_n + 2K$ if $q_n < -K$, and $a_n(\mathbf{q}) = q_n$ otherwise.

Expanding the aliased convolution sum, it follows that

$$A_{\theta_\gamma}(\mathbf{k}) = U_{\theta_\gamma}(\mathbf{k}) + \sum_{a_n(\mathbf{q}) = -2K} \left[1/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q}).$$

The term involving $\mathbf{e}$ represents the spurious aliasing interactions. If instead of using just the single discrete grid $\mathbf{x}$ defined above, we introduce new discrete grids shifted from the $\mathbf{x}$ grid by constant vectors $\pi \hat{\mathbf{e}}/N$ with $\hat{e}_\alpha = 0, 1$, so that the new grid points are $\mathbf{x} + \pi \hat{\mathbf{e}}/N$ and the new velocity field is $\mathbf{v}(\mathbf{x} + \pi \hat{\mathbf{e}}/N)$, it is straightforward to deduce from (1) and (2) that

$$\exp(-i\pi \mathbf{k} \cdot \hat{\mathbf{e}}/N) \sum_{0 \leq n < N} \mathbf{v}_n(\mathbf{x} + \pi \hat{\mathbf{e}}/N) \mathbf{v}_n(\mathbf{x} + \pi \hat{\mathbf{e}}/N)$$

$$\times \exp(-i\mathbf{k} \cdot \mathbf{x}) = \left[1/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q})$$

$$+ \sum_{a_n(\mathbf{q}) = -2K} \exp(i\pi \mathbf{e} \cdot \hat{\mathbf{e}})$$

$$\times \left[1/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q}).$$

Noting that $\exp(i\pi \mathbf{e} \cdot \hat{\mathbf{e}}) = \pm 1$, it follows that by summing (3) over all eight possible vectors $\hat{\mathbf{e}}$ the aliasing interactions are completely eliminated. The price, however, is 8 times as many transforms over the 8 shifted grids in real space.

Instead, if we set $\hat{\mathbf{e}} = (1, 1, 1)$ and sum (2) and (3), we find

$$T_{\text{FFT}}[\mathbf{v}_\theta(\mathbf{x}) \mathbf{v}_\gamma(\mathbf{x})]$$

$$+ \exp(-i\pi \mathbf{k} \cdot \hat{\mathbf{e}}/N) T_{\text{FFT}}[\mathbf{v}_\theta(\mathbf{x} + \pi \hat{\mathbf{e}}/N) \mathbf{v}_\gamma(\mathbf{x} + \pi \hat{\mathbf{e}}/N)]$$

$$= \left[2/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q})$$

$$+ \sum_{a_n(\mathbf{q}) = -2K} \left[2/(2K)^3\right] \sum_{p+q=k} \mathbf{u}_p(\mathbf{p}) \mathbf{u}_q(\mathbf{q}),$$

where the operator $T_{\text{FFT}}$ denotes the fast Fourier transform, and the primed summation is over only those vectors $\mathbf{e}$ with precisely two nonzero components. The second term on the right-hand side of (4) involves only “doubly aliased” interactions, in which precisely two of the components of $\mathbf{k}$ are aliased. The singly and triply aliased interactions vanish since $\exp(i\pi \mathbf{e} \cdot \hat{\mathbf{e}}) = -1$ if $\hat{\mathbf{e}} = (1, 1, 1)$ and the number of nonzero components of $\mathbf{e}$ is odd. According to (4), the number of aliasing interactions may be greatly reduced, although not totally eliminated, at the cost of doubling the numbers of fast Fourier transforms.

If the set of allowable modes $C_K$ is reduced by considering only those modes within a sphere of radius $\alpha K$ and if $\alpha$ is chosen small enough, then no modes exist to contribute to the doubly aliased term on the right-hand side of (4). That is, if $S_K$ is the set of modes with
because for $\alpha$ small enough one cannot find any modes $k, p, q$ satisfying $k = p + q + 2Ke$ lying within the sphere $S_K$. We will show below that $\alpha$ need not be less than $2\sqrt{2}/3 \approx 0.94$ and $S_K$ contains about half as many modes as $C_K$. Moreover, nearly all the discarded modes lie in the corners of $C_K$ and an accurate simulation requires that all these modes be weakly excited relative to those within the sphere $S_K$. Thus, Eq. (4) may be used to compute alias-free convolution sums with $C_K$ replaced by $S_K$.

The largest value of $\alpha$ for which (5) is generally true is precisely given by

$$ \alpha^* = 2M^2 $$

if $2K = 3M$,

$$ = M^2 + (M+1)^2 \quad \text{if } 2K = 3M + 1, $$

$$ = 2(M+1)^2 \quad \text{if } 2K = 3M + 2, $$

where $K, M$ are integral. Note that, if $2K = 3M$, $\alpha^* = \frac{8}{2}$, and that in all cases $\alpha^* \leq \frac{8}{2}$ as $K \to \infty$.

The proof of (6) is based on the observation that the largest $\alpha$ for which (5) is generally true is given by the smallest value of $\alpha$ for which these exist a solution $k, p, q$ to the relations

$$ k_1^2 + k_2^2 + k_3^2 \leq \alpha^2 K^2; $$

$$ p_1^2 + p_2^2 + p_3^2 \leq \alpha^2 K^2; $$

$$ q_1^2 + q_2^2 + q_3^2 \leq \alpha^2 K^2; $$

$$ k_1 - p_1 - q_1 = 2K; $$

$$ k_2 - p_2 - q_2 = 2K; $$

$$ k_3 - p_3 - q_3 = 0, $$

where we have chosen $e = (1, 1, 0)$ without any loss of generality. Clearly, a minimum for $\alpha$ will occur with $k_1 = p_2 = q_3 = 0$ and $p_1, p_3, q_1, q_2$ negative. These properties of the minimum solution may be demonstrated analytically at some increase in complexity of the following analysis. Set $x_1 = k_1, x_2 = k_2, x_3 = -p_1, x_4 = -p_2, x_5 = -q_1, x_6 = -q_2$, so that the $x_i$ are all positive. Define the additional nonnegative variables $s_3$ as the defects in the inequalities in (7). With these definitions, (7) becomes

$$ x_1^2 + x_2^2 + x_3^2 = \alpha^2 K^2; $$

$$ x_3^2 + x_4^2 + s_3^2 = \alpha^2 K^2; $$

$$ x_5^2 + x_6^2 + s_3^2 = \alpha^2 K^2; $$

$$ x_1 + x_2 + x_3 = 2K; $$

$$ x_4 + x_5 + x_6 = 2K. $$

To solve (8) for minimum $\alpha$, it is more convenient to sum the first three equations of (8), retain the two linear constraints, and minimize $3\alpha^2 K^2 - (s_1^2 + s_2^2 + s_3^2)$. From the set of optimal points of this latter system, it is easy to deduce the optimal point for the system (8).

We must find the minimum $L$ such that

$$ \sum_{i=1}^{4} x_i^2 = L; \quad x_1 + x_2 + x_3 = 2K; \quad x_4 + x_5 + x_6 = 2K. $$

Using conventional techniques (such as the method of Lagrange multipliers), a minimum is obtained when

$$ x_i = \frac{2K}{3} (i = 1, \cdots, 6), \quad \alpha^2 = \frac{8}{2}. $$

This gives an integer solution, however, only when $2K$ is divisible by 3. To force an integer solution when $2K$ is not divisible by 3, additional constraints must be devised. If $2K = 3M + 1$, set

$$ x_1 \geq M + 1, \quad x_4 \geq M + 1, $$

without loss of generality. If $2K = 3M + 2$, set

$$ x_1 \leq M, \quad x_4 \leq M, $$

without loss of generality, since an integral solution is sought. These additional constraints are deducible from the last two equations of (9) for integer $\alpha$. The choice of $x_1, x_4$ is arbitrary except for noting that choosing $x_1, x_4$ will give a solution optimal for (9) but not for (8). Optimal points for the last two cases can be found by applying the method of Lagrange multipliers after removing the inequalities by the artifice of defining additional nonnegative variables $s_1, s_2$ as the defects in the inequalities for $x_1, x_4$. Thus, for $2K = 3M + 1, x_1 - x_2 = M + 1, x_4 - x_5 = M + 1$. The results can be summarized as follows:

<table>
<thead>
<tr>
<th>$K$</th>
<th>$\alpha^2 K^2$</th>
<th>$\alpha K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>61</td>
<td>7.8</td>
</tr>
<tr>
<td>16</td>
<td>242</td>
<td>15.6</td>
</tr>
<tr>
<td>32</td>
<td>925</td>
<td>30.4</td>
</tr>
</tbody>
</table>

and for each case, $\alpha^2 K^2 = \max(k_1^2 + k_2^2, p_1^2 + p_2^2, q_1^2 + q_2^2)$. For some typical values of $K$, the results for $\alpha$ are

$$ x_1^2 + x_2^2 + x_3^2 = \alpha^2 K^2; $$

$$ x_3^2 + x_4^2 + s_3^2 = \alpha^2 K^2; $$

$$ x_5^2 + x_6^2 + s_3^2 = \alpha^2 K^2; $$

$$ x_1 + x_2 + x_3 = 2K; $$

$$ x_4 + x_5 + x_6 = 2K. $$

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Convergence of the Long-Wavelength Expansions in a Classical Fluid

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The convergence of Irving and Kirkwood's long-wavelength expansion for the stress tensor is examined. The convergence is shown to be only asymptotic for realistic intermolecular potentials.

Although exact expressions for the stress tensor and heat flux of a single component system of spherical molecules have been derived from the principles of classical statistical mechanics, for most applications interest has centered on the behavior of these quantities for systems near local thermodynamic equilibrium. For such systems macroscopic variables change little over distances on the order of a molecular correlation length and are characteristically referred to as long-wavelength phenomena.

Two decades ago expansions for the stress tensor and heat flux were derived by Irving and Kirkwood to describe hydrodynamic, or long-wavelength phenomena. Since that time these expansions have become a cornerstone of the statistical theory of transport. One unfortunate feature of the expansions is that they quickly diverge for realistic intermolecular potentials. In fact, they diverge for any potential which goes as \((1/r)^n\) for large \(r\), where \(n\) is a positive integer and \(r\) is the internuclear separation. The purpose of this communication is to demonstrate that the Irving and Kirkwood expansions converge asymptotically for realistic potentials. We shall restrict ourselves to an examination of the stress tensor. The arguments and conclusions for the case of the heat flux are easily seen to be identical.

The exact expression for the stress tensor may be written as follows:

\[
\tau = -m^{-1} \int d^3P (\mathbf{P} - \mathbf{\bar{P}}) (\mathbf{P} - \mathbf{\bar{P}}) f(\mathbf{x}, \mathbf{P})
+ \frac{1}{2} \int d^3r \mathbf{r} r (r^{-1} \frac{d\phi}{dr}) \gamma(r, \mathbf{x}).
\]  

(1)

In Eq. (1) \(\tau\) is the stress tensor evaluated at the position \(\mathbf{x}\) and time \(t\), \(m\) is the mass of a molecule, \(\phi\) is the intermolecular potential, \(f(\mathbf{x}, \mathbf{P})\) is the singlet distribution function in position and momentum space, and \(\mathbf{\bar{P}}\) is the average momentum of a molecule located at \(\mathbf{x}\) at the time \(t\). The distribution function \(\gamma\) may be expressed in terms of the instantaneous pair distribution function \(g(\mathbf{x}_1, \mathbf{x}_2)\) as follows. Let

\[
\gamma(r, \mathbf{x}) = g(\mathbf{x} - \frac{1}{2} \mathbf{r}, \mathbf{x} + \frac{1}{2} \mathbf{r}),
\]

so that \(\gamma\) is the pair distribution function expressed in terms of relative coordinates \(\mathbf{r}\) and center-of-mass coordinates \(\mathbf{x}\)

\[
\mathbf{r} = \mathbf{x} - \mathbf{x}_i, \quad \mathbf{x} = \frac{1}{2} (\mathbf{x}_1 + \mathbf{x}_2).
\]

The distribution function \(\gamma\) then has the convenient representation

\[
\hat{\gamma}(r, \mathbf{x}) = \int_{-1/2}^{1/2} d\eta \gamma(r, \mathbf{x} + \eta \mathbf{r}).
\]  

(2)

Hence, \(\hat{\gamma}\) is the average of \(\gamma\) taken by fixing \(\mathbf{r}\) and integrating over the center-of-mass dependence on a line connecting \(\mathbf{x} - \frac{1}{2} \mathbf{r}\) and \(\mathbf{x} + \frac{1}{2} \mathbf{r}\).

Although Irving and Kirkwood were unable to obtain an expression for \(\tau\) in closed form, to reproduce their result we merely perform a Taylor series expansion of the integrand of Eq. (2) in powers of \(\eta\). Integrating by term and inserting the result into the expression for the intermolecular contribution of \(\tau\) yields

\[
\tau_{int} = \frac{1}{2} \int d^3r \mathbf{r} r \left( r^{-1} \frac{d\phi}{dr} \right) \hat{\gamma}(r, \mathbf{x})
= \sum_0^\infty \left( (2n+1)! \right)^{-1} \int d^3r \mathbf{r} r \left( r^{-1} \frac{d\phi}{dr} \right) \times \left( r \frac{\partial}{\partial r} \right)^{2n} \gamma(r, \mathbf{x}).
\]  

(3)

The motivation for the expansion is that, for long-wavelength phenomena, \(\gamma\) varies little in its dependence on \(\mathbf{x}\) over distances comparable to the "range" of the intermolecular potential.

Let \(G\) be the Fourier transform of \(\gamma\) in \(\mathbf{x}\):

\[
G(\mathbf{K}, \mathbf{r}) = \int d\mathbf{x} \gamma(\mathbf{x}) \exp(-i\mathbf{K} \cdot \mathbf{x}).
\]

In terms of \(G\), we find

\[
\hat{\gamma} = \int dK G(\mathbf{K}, \mathbf{r}) \exp(i\mathbf{K} \cdot \mathbf{r})
\]

In the Fourier representation which is suitable for examining the convergence properties of the series, the Irving and Kirkwood expansion is obtained by...