Appendix-B

Total kinetic energy, E_K, can be obtained from kinetic energy spectrum, $E_K(k)$ as

$$E_K = \int_0^{\infty} E_K(k)dk \tag{i}$$

Also, using the fact that $E_K = \iiint_V \frac{u_i(\underline{x})u_i(\underline{x})}{2} dV$, $u_{rms} = \sqrt{\frac{1}{V}\iiint_V \frac{u_i(\underline{x})u_i(\underline{x})}{3} dV}$ and $V = (2\pi l)^3$ in our periodic box of side l, we get

$$E_K = {}^3\!/_2\, u_{rms}^2 (2\pi l)^3 \tag{ii}$$

Inputting the initial spectrum, E(k), in eq. (i), and comparing with eq. (ii),

$$\int_0^{k_{max}} \left(Ak^4 e^{-2k^2/k_p^2}\right)dk = {}^3\!/_2\, u_{rms}^2 (2\pi l)^3 \tag{iii}$$

Integrating by parts (assuming $k_{max} >> k_p$),

$$\int_0^{k_{max}} \left(k^4 e^{-2k^2/k_p^2}\right)dk = \underbrace{-k^3 \frac{k_p^2}{4} e^{-2k^2/k_p^2}\Big|_0^{k_{max}}}_{\approx 0} + \int_0^{k_{max}} \left(3k^2 \frac{k_p^2}{4} e^{-2k^2/k_p^2}\right)dk$$

$$= \underbrace{-3k \frac{k_p^4}{16} e^{-2k^2/k_p^2}\Big|_0^{k_{max}}}_{\approx 0} + \int_0^{k_{max}} \left(3 \frac{k_p^4}{16} e^{-2k^2/k_p^2}\right)dk$$

This last integral can be estimated for large k_{max} using the following:

$$\int_0^{k_{max}} e^{-2k^2/k_p^2} dk \approx {}^{k_p}\!/_{\sqrt{2}} \times \int_0^{\infty} e^{-x^2} dx = {}^{k_p}\!/_2 \sqrt{{}^{\pi}\!/_2} \tag{iv}$$

Substituting in eq. (iii) and simplifying, we get

$$A = \frac{16 u_{rms}^2 (2\pi l)^3}{k_p^5 \sqrt{{}^{\pi}\!/_2}} \tag{v}$$

Consider that for isotropic flows, $E_K(k) = 2\pi k^2 \phi_{i,i}(\underline{k})$. Thus,

$$\hat{u}_i(\underline{k})\hat{u}_i^*(\underline{k}) = \frac{E_K(k)}{\pi k^2} = \frac{Ak^2}{\pi} e^{-2k^2/k_p^2} \tag{vi}$$

Let, for a given vector $\underline{k} = k_1\hat{\imath} + k_2\hat{\jmath} + k_3\hat{k}$, $\hat{u}_i(\underline{k}) = a_i e^{i\phi_i}\ \forall\ i \in \{1,2,3\}$. Here, ϕ_i's are the randomly chosen phases in [0,2π], while a_i's are the unknown magnitudes of spectral velocity in each direction. Since the initial velocity field is solenoidal, $\underline{k} \cdot \underline{\hat{u}}(\underline{k}) = 0$. Then, we get

$$\sum_{j=1}^{3} a_j k_j \cos\phi_j + i \sum_{m=1}^{3} a_m k_m \sin\phi_m = 0 \tag{vii}$$

Subtracting cos(ϕ_1)*Im(eq. (vii)) from sin(ϕ_1)*Re(eq. (vii)), we get

$$a_2 k_2 \sin(\phi_1 - \phi_2) + a_3 k_3 \sin(\phi_1 - \phi_3) = 0$$

$$\therefore \frac{a_2 k_2}{\sin(\phi_3 - \phi_1)} = \frac{a_3 k_3}{\sin(\phi_1 - \phi_2)}$$

Generating similar equation between a_1 and a_3, we can get the following:

$$\frac{a_1}{\frac{\sin(\phi_2 - \phi_3)}{k_1}} = \frac{a_2}{\frac{\sin(\phi_3 - \phi_1)}{k_2}} = \frac{a_3}{\frac{\sin(\phi_1 - \phi_2)}{k_3}} = \lambda \tag{viii}$$

Each a_i can be written in terms of a single variable λ. It may be noted that for the case of some k_i=0, a_i=0 to keep mean velocity zero. The variable λ can now be easily found using eq.(vi), which can be written as ${a_1}^2 + {a_2}^2 + {a_3}^2 = {Ak^2}/{\pi}\, e^{-2k^2/k_p^2}$.

Appendix-C

We consider the dissipation free dimensionless momentum equation

$$\frac{\partial(\rho u_i)}{\partial t}+\nabla\left(\rho u_i \underline{u}\right)+\frac{1}{M_c^2}\frac{\partial p}{\partial x_i}=0. \qquad \text{(i)}$$

The term ρu_i can be written as $\sqrt{\rho}w_i$ where $w_i=\sqrt{\rho}u_i$. Expanding eq. (i), we get

$$\sqrt{\rho}\frac{\partial w_i}{\partial t}+\frac{w_i}{2\sqrt{\rho}}\frac{\partial \rho}{\partial t}+\sqrt{\rho}\nabla\left(w_i\underline{u}\right)+w_i\underline{u}\frac{\nabla\rho}{2\sqrt{\rho}}+\frac{1}{M_c^2}\frac{\partial p}{\partial x_i}=0.$$

Or,
$$\frac{\partial w_i}{\partial t}+\frac{u_i}{2\sqrt{\rho}}\left(\frac{\partial \rho}{\partial t}+\underline{u}\nabla\rho\right)+\nabla\left(w_i\underline{u}\right)+\frac{1}{M_c^2\sqrt{\rho}}\frac{\partial p}{\partial x_i}=0.$$

Using continuity equation, we get the evolution equation of w_i as

$$\frac{\partial w_i}{\partial t}+\underline{u}\nabla w_i+\frac{w_i\nabla\underline{u}}{2}+\frac{1}{M_c^2\sqrt{\rho}}\frac{\partial p}{\partial x_i}=0. \qquad \text{(ii)}$$

Taking Fourier transformation, and simplifying, we get

$$\begin{aligned}\frac{d\widehat{w_i}(\underline{K})}{dt}=&-\left\langle\left(\sum_{\underline{K'}}\hat{\underline{u}}(\underline{K'})e^{i\underline{K'}.\underline{x}}\right).\left(\sum_{\underline{K"}}i\underline{K"}\widehat{w_i}(\underline{K"})e^{i\underline{K"}.\underline{x}}\right)e^{-i\underline{K}.\underline{x}}\right\rangle_L\\&-{}^1\!/_2\left\langle\left(\sum_{\underline{K'}}\widehat{w_i}(\underline{K'})e^{i\underline{K'}.\underline{x}}\right).\left(\sum_{\underline{K"}}i\underline{K"}\hat{\underline{u}}(\underline{K"})e^{i\underline{K"}.\underline{x}}\right)e^{-i\underline{K}.\underline{x}}\right\rangle_L\\&-\frac{1}{M_c^2}\left\langle\left(\sum_{\underline{K'}}\hat{a}(\underline{K'})e^{i\underline{K'}.\underline{x}}\right)\left(\sum_{\underline{K"}}i\underline{K"}\hat{p}(\underline{K"})e^{i\underline{K"}.\underline{x}}\right)e^{-i\underline{K}.\underline{x}}\right\rangle_L.\end{aligned}$$

$$\begin{aligned}\frac{d\widehat{w_i}(\underline{K})}{dt}=&-i\sum_{\underline{K'}}\hat{\underline{u}}(\underline{K'}).\left(\underline{K}-{}^{\underline{K'}}\!/_2\right)\widehat{w_i}(\underline{K}-\underline{K'})\\&-{}^i\!/_{M_c^2}\sum_{\underline{K'}}\hat{a}(\underline{K'})(K_i-K'_i)\hat{p}(\underline{K}-\underline{K'}).\end{aligned} \qquad \text{(iii)}$$

Here $\hat{a}$ is the Fourier transform of square root of density, $1/\sqrt{\rho}$. We now multiply equation (iii) with $w_i{}^*$, add the complex conjugate of this and divide by 2. The LHS will then be the time derivative of spectral kinetic energy.

$$\frac{dE_K(\underline{K})}{dt} = Im\left\{\sum_{\underline{K'}} \underline{\hat{u}}(\underline{K'}).\left(\underline{K} - {}^{\underline{K'}}\!/_2\right)\widehat{w_i}(\underline{K} - \underline{K'})\widehat{w_i}(-\underline{K}) + {}^1\!/_{M_c^2}\sum_{\underline{K'}} \hat{a}(\underline{K'})(K_i - K'_i)\hat{p}(\underline{K} - \underline{K'})\widehat{w_i}(-\underline{K})\right\}. \quad \text{(iv)}$$

$E(\underline{K}) = \widehat{w_i}(\underline{K})\widehat{w_i}^*(\underline{K}) = \widehat{w_i}(\underline{K})\widehat{w_i}(-\underline{K})$ is being called the spectral kinetic energy as it will sum up to the kinetic energy over all wavenumbers following the Parseval's theorem.

Now, we consider a triad of wavenumbers $\underline{k}(= -\underline{K})$, $\underline{q}(= \underline{K'})$ and $\underline{p}(= \underline{K} - \underline{K'})$ such that $\underline{k} + \underline{p} + \underline{q} = 0$. From equation (iv), the rate of change of $E(\underline{k})(= E(-\underline{k}))$ due to this triad alone can be found to be

$$\frac{dE_K(\underline{k})}{dt} = \underbrace{Im\left\{\left(\frac{\underline{p} - \underline{k}}{2}\right).\underline{\hat{u}}\left(\underline{q}\right)\underline{\widehat{w}}\left(\underline{p}\right).\underline{\widehat{w}}(\underline{k})\right\}}_{S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right)} + \underbrace{Im\left\{\left(\frac{\underline{q} - \underline{k}}{2}\right).\underline{\hat{u}}\left(\underline{p}\right)\underline{\widehat{w}}\left(\underline{q}\right).\underline{\widehat{w}}(\underline{k})\right\}}_{S^{ww}\left(\underline{k}|\underline{q}|\underline{p}\right)} + \underbrace{{}^1\!/_{M_c^2}\, Im\left\{\underline{p}.\underline{\widehat{w}}(\underline{k})\hat{a}\left(\underline{q}\right)\hat{p}\left(\underline{p}\right)\right\}}_{S^{wp}\left(\underline{k}|\underline{q}|\underline{p}\right)} + \underbrace{{}^1\!/_{M_c^2}\, Im\left\{\underline{q}.\underline{\widehat{w}}(\underline{k})\hat{a}\left(\underline{p}\right)\hat{p}\left(\underline{q}\right)\right\}}_{S^{wp}\left(\underline{k}|\underline{p}|\underline{q}\right)}. \quad \text{(v)}$$

The quantity $S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right)$ denotes the inertial component of the mode-to-mode kinetic energy transfer rate to receiver wavenumber $\underline{k}$ from donor wavenumber $\underline{p}$ due to the mediator wavenumber $\underline{q}$. This definition is justified because

$$S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right) + S^{ww}\left(\underline{p}|\underline{k}|\underline{q}\right) = Im\left\{\left(\frac{\underline{p} - \underline{k}}{2}\right).\underline{\hat{u}}\left(\underline{q}\right)\underline{\widehat{w}}\left(\underline{p}\right).\underline{\widehat{w}}(\underline{k}) + \left(\frac{\underline{k} - \underline{p}}{2}\right).\underline{\hat{u}}\left(\underline{q}\right)\underline{\widehat{w}}(\underline{k}).\underline{\widehat{w}}\left(\underline{p}\right)\right\} = 0. \quad \text{(vi)}$$

The above definition draws parallel from the mode-to-mode energy transfer definition provided by Verma (2019).

The quantity $S^{wp}\left(\underline{k}|\underline{p}|\underline{q}\right)$ denotes the pressure component of the mode-to-mode kinetic energy transfer rate to receiver wavenumber $\underline{k}$. However, the donor wavenumber here is not $\underline{p}$ alone, as $S^{wp}\left(\underline{k}|\underline{p}|\underline{q}\right) + S^{wp}\left(\underline{p}|\underline{k}|\underline{q}\right) \neq 0$. Further, this quantity is responsible for transferring kinetic energy to/from internal energy, and hence, cannot be expected to be conserved.

To find the mode-to-mode kinetic energy transfer rates due to triadic interaction between given modes k, p, and q, we can take average over all possible combinations of wavenumbers $\underline{k}$, $\underline{p}$ and $\underline{q}$.

$$S^{ww}(k|p|q) = \frac{\sum_{|\underline{k}|=k-\Delta k}^{k+\Delta k} \sum_{|\underline{p}|=p-\Delta p}^{p+\Delta p} \sum_{|\underline{q}|=q-\Delta q}^{q+\Delta q} S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right)}{N}. \tag{vi}$$

Here, Δk, Δp and Δq are the shell thicknesses in the wavenumber space, while N is the number of valid triads. The total number of such terms will be of the order of k_{max}^6, which will require extensive computation & memory. To ease computation, a limit may be set on the number of pairs used for each (k,p,q) triplet, which will reduce the no. of quantities to be computed to order of k_{max}^3.

Another computation consideration is that in simulation, only positive z-component of all Fourier space vectors (including wavenumber vectors) are stored. This means that only about 1/8th of the $(\underline{k}, \underline{p}, \underline{q})$ triplets are available. To include the missing numbers, we consider wavenumbers $\underline{k_2}$ and $\underline{p_2}$ having negative z-component (thus not available for computation), and corresponding available wavenumbers $\underline{k_1} = -\underline{k_2}$ and $\underline{p_1} = -\underline{p_2}$.

Following is the list of possible $\underline{q}$ for different combinations of these wavenumbers, found in terms of available wavenumbers.

$$\underline{q} = \begin{cases} \underline{q_1} = -\left(\underline{k_1} + \underline{p_1}\right) \\ \underline{q_2} = -\left(\underline{k_1} + \underline{p_2}\right) = -\underline{k_1} + \underline{p_1} \\ \underline{q_3} = -\left(\underline{k_2} + \underline{p_1}\right) = \underline{k_1} - \underline{p_1} \\ \underline{q_4} = -\left(\underline{k_2} + \underline{p_2}\right) = \underline{k_1} + \underline{p_1} \end{cases}.$$

$\underline{q_1}$ is bound to have a negative z-component, and hence, $-\underline{q_1}$ needs to be used for computation. Complex conjugate of any Fourier space variable found at this representative $\underline{q}$ will have to be taken for maintaining consistency in computation. Similarly, $\underline{q_2}$ will have negative z-component for $k_{1z} > p_{1z}$, and $\underline{q_3}$ for $k_{1z} < p_{1z}$. Triadic interaction will be

$$S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right) = \begin{cases} Im\left\{\left(\frac{\underline{\underline{p_1}} - \underline{\underline{k_1}}}{2}\right).\underline{\hat{u}}^*\left(\underline{q_1}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}\left(\underline{k_1}\right)\right\};\ \underline{q_1} = \left(\underline{k_1} + \underline{p_1}\right) \\ Im\left\{-\left(\frac{\underline{\underline{p_1}} + \underline{\underline{k_1}}}{2}\right).\underline{\hat{u}}\left(\underline{q_2}\right)\underline{\hat{w}}^*\left(\underline{p_1}\right).\underline{\hat{w}}\left(\underline{k_1}\right)\right\};\ \underline{q_2} = \underline{p_1} - \underline{k_1}; k_{1z} < p_{1z} \\ Im\left\{-\left(\frac{\underline{\underline{p_1}} + \underline{\underline{k_1}}}{2}\right).\underline{\hat{u}}^*\left(\underline{q_2}\right)\underline{\hat{w}}^*\left(\underline{p_1}\right).\underline{\hat{w}}\left(\underline{k_1}\right)\right\};\ \underline{q_2} = \underline{k_1} - \underline{p_1}; k_{1z} \geq p_{1z} \\ Im\left\{\left(\frac{\underline{\underline{p_1}} + \underline{\underline{k_1}}}{2}\right).\underline{\hat{u}}^*\left(\underline{q_3}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}^*\left(\underline{k_1}\right)\right\};\ \underline{q_3} = \underline{p_1} - \underline{k_1}; k_{1z} < p_{1z} \\ Im\left\{\left(\frac{\underline{\underline{p_1}} + \underline{\underline{k_1}}}{2}\right).\underline{\hat{u}}\left(\underline{q_3}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}^*\left(\underline{k_1}\right)\right\};\ \underline{q_3} = \underline{k_1} - \underline{p_1}; k_{1z} \geq p_{1z} \\ Im\left\{\left(\frac{\underline{\underline{k_1}} - \underline{\underline{p_1}}}{2}\right).\underline{\hat{u}}\left(\underline{q_4}\right)\underline{\hat{w}}^*\left(\underline{p_1}\right).\underline{\hat{w}}^*\left(\underline{k_1}\right)\right\}\underline{q_4} = \left(\underline{k_1} + \underline{p_1}\right) \end{cases}.$$

Thus, a given $\underline{k}, \underline{p}$ pair in the computational domain gives more than one triadic interaction. We can sum the first and last formula and combine the other four formulae to get a complete formula that includes all possible triadic interactions.

$$S^{ww}\left(\underline{k}|\underline{p}|\underline{q}\right) = \begin{cases} Im\left\{\left(\underline{p_1} - \underline{k_1}\right).\underline{\hat{u}}^*\left(\underline{q}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}\left(\underline{k_1}\right)\right\};\ \underline{q} = \left(\underline{k_1} + \underline{p_1}\right) \\ Im\left\{\left(\underline{p_1} + \underline{k_1}\right).\underline{\hat{u}}^*\left(\underline{q}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}^*\left(\underline{k_1}\right)\right\};\ \underline{q} = \underline{p_1} - \underline{k_1}; k_{1z} < p_{1z}. \\ Im\left\{\left(\underline{p_1} + \underline{k_1}\right).\underline{\hat{u}}\left(\underline{q}\right)\underline{\hat{w}}\left(\underline{p_1}\right).\underline{\hat{w}}^*\left(\underline{k_1}\right)\right\};\ \underline{q} = \underline{k_1} - \underline{p_1}; k_{1z} \geq p_{1z} \end{cases} \quad \text{(vii)}$$