Appendix B
Ordering of Fourier Coefficients

Due to algorithmic details of the fast Fourier transform the Fourier coefficients are ordered in a somewhat "strange" manner, at least for a newby. This causes problems especially when calculating derivatives of functions in Fourier space, as calculating the derivative corresponds to a multiplication with a real wave number (or vector in more than one spatial dimension). Hence the wave vectors have to be stored in a real array with exactly the same ordering as the Fourier coefficients. A complex field f sampled by N grid points is transformed to a complex array $\tilde{f}$ of Fourier coefficients being ordered according to

$$\tilde{f}_0, \tilde{f}_1, \ldots, \tilde{f}_{\frac{N}{2}}, \tilde{f}_{-\frac{N}{2}+1}, \tilde{f}_{-\frac{N}{2}+2}, \ldots, \tilde{f}_{-1} \tag{B.1}$$

If we consider a real field f the Fourier coefficients exhibit a symmetry $\tilde{f}_{-j} = \tilde{f}_j^*$. This is exploited by most Fourier transform by only storing roughly half of the array, reducing the memory needed for holding the coefficients and giving a speed increase of roughly a factor of two. The Fourier coefficients in Fourier space are then ordered according to

$$\tilde{f}_0, \tilde{f}_1, \ldots, \tilde{f}_{\frac{N}{2}} \tag{B.2}$$

Let L denote the physical length of the simulation domain. The real array of wave numbers then takes the form

$$k(i) = \begin{cases} \frac{2\pi}{L} i & \text{if} \quad i = 0, \ldots, \frac{N}{2} \\ \frac{2\pi}{L}(-N+i) & \text{if} \quad i = \frac{N}{2}+1, \ldots, N-1 \end{cases} \tag{B.3}$$

In case of a real field, the above-mentioned symmetry may be exploited. Then the array holding the wave vectors has also roughly half the size resulting in the index i running only $i = 0, \ldots, \frac{N}{2}$. These considerations are generalized to a two-dimensional field $f(x,t)$ in a straight-forward manner. In this case we have a two-dimensional array for the Fourier coefficients. In case f represents a complex field, the wave vectors are arranged according to

$$k_x(i,j) = \begin{cases} \frac{2\pi}{L} i & \text{if} \quad i = 0, \ldots, \frac{N}{2} \\ \frac{2\pi}{L}(-N+i) & \text{if} \quad i = \frac{N}{2}+1, \ldots, N-1 \end{cases} \tag{B.4}$$

$$k_y(i,j) = \begin{cases} \frac{2\pi}{L} j & \text{if} \quad j = 0, \ldots, \frac{N}{2} \\ \frac{2\pi}{L}(-N+j) & \text{if} \quad j = \frac{N}{2}+1, \ldots, N-1 \end{cases}$$

In case of a real field, half of the Fourier coefficients suffice and the index i for the wave vectors reduces to $i = 0, \ldots, \frac{N}{2}$. One should note that different implementations of the fast Fourier algorithms exhibit a different ordering of Fourier coefficients. The ordering presented here is for example used by the `FFTW` library.