Discrete Fourier Lagrangian

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The discrete Lagrangian is using the second difference

$$\Delta_h U_j{}^n = \sum_{i=1}^{d} \frac{U^n{}_{j+e_i} - 2U^n{}_j + U^n{}_{j-e_i}}{h_i^2} \tag{1}$$

we believe following [1] that it will be easier to solve this equation in Fourier space, we use the discrete Fourier transform, for simplicity we will work in two dimensions in an $m_1 \times m_2$ grid . The discrete Fourier transform is then, see [2]

$$\widehat{U^n}[k] = \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right]$$

We need the Fourier transform of the discrete Lagrangian (1). Using the linearity of the Fourier transform we have

$$\begin{aligned}
\Delta_h \widehat{U_{j_1,j_2}}{}^n &= \sum_{i=1}^{d} \frac{\widehat{U^n{}_{j+e_i}} - 2\widehat{U^n{}_j} + \widehat{U^n{}_{j-e_i}}}{h_i^2} \\
&= \frac{\sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1+e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] - 2\sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right]}{h_1^2} \\
&+ \frac{\sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1-e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right]}{h_1^2} + \frac{\sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2+e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right]}{h_2^2} \\
&+ \frac{-2\sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] + \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2-e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right]}{h_2^2} \\
&= \frac{1}{h_1^2} \exp\left[2\pi i \frac{k_1}{m_1}\right] \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1+e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 (j_1+e_1)}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] \\
&+ \frac{1}{h_2^2} \exp\left[2\pi i \frac{k_2}{m_2}\right] \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2+e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 (j_2+e_2)}{m_2}\right)\right] \\
&- \left(\frac{2}{h_1^2} + \frac{2}{h_2^2}\right) \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] \\
&+ \frac{1}{h_1^2} \exp\left[-2\pi i \frac{k_1}{m_1}\right] \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1-e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 (j_1-e_1)}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] \\
&+ \frac{1}{h_2^2} \exp\left[-2\pi i \frac{k_2}{m_2}\right] \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2-e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 (j_2-e_2)}{m_2}\right)\right]
\end{aligned}$$

Using the changes of variables $j_i = j_i \pm e_i$ for $i = 1, 2$ we have

$$\begin{aligned}
\widehat{U^n}[k] &= \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1+e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 (j_1 + e_1)}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] \\
&= \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2+e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 (j_2 + e_2)}{m_2}\right)\right] \\
&= \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1-e_1,j_2} \exp\left[-2\pi i \left(\frac{k_1 (j_1 - e_1)}{m_1} + \frac{k_2 j_2}{m_2}\right)\right] \\
&= \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n{}_{j_1,j_2-e_2} \exp\left[-2\pi i \left(\frac{k_1 j_1}{m_1} + \frac{k_2 (j_2 - e_2)}{m_2}\right)\right]
\end{aligned}$$

our discrete Lagrangian becomes

$$\begin{aligned}
\widehat{\Delta_h U_j^n} &= \sum_{i=1}^{d} \frac{1}{h_i^2} \left(\exp\left[\frac{2\pi i k_i}{m_i}\right] - 2 + \exp\left[-\frac{2\pi i k_i}{m_i}\right]\right) \widehat{U^n}[k] \\
&= \sum_{i=1}^{d} \frac{2}{h_i^2} \left(\cos\left[\frac{2\pi k_i}{m_i}\right] - 1\right) \widehat{U^n}[k]
\end{aligned}$$

where in the second line we have used the formulation of $\cos$ in terms of exponentials. Obviously this can be extended to any domain of the form $\Omega = m_1 \times m_2 \cdots \times m_d$. Writing We use the discrete Fourier transform, for simplicity we will work in two dimensions in an $m_1 \times m_2$ grid . Writing

$$F[k] = \sum_{i=1}^{d} \frac{2}{h_i^2} \left(\cos\left[\frac{2\pi k_i}{m_i}\right] - 1\right)$$

we have

$$\widehat{\Delta_h U_j^n} = F[k] \widehat{U^n}[k] \tag{2}$$

and we see that in k-space operation of Δ_h becomes multiplication by $F[k]$.

References

[1] M. Elsey, B. Wirth A simple and efficient scheme for phase field crystal simulation, pre-print, (2012).

[2] E.S. Karlsen, supervisor: P.E. Mæland Multidimensional Multirate Sampling and Seismic Migration, Master's Thesis: University of Bergen, (2010).