Calculation of Divergence in Fourier space

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1 Idea

A field of 3x3 tensors in the form

$$\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = \boldsymbol{P}(\vec{x}) \tag{1}$$

depending on a discrete 3D vector $\vec{x}$ (spatial coordinates in real space)

$$\vec{x} \text{ with } x_1 = 1, 2, ..., N_1, \; x_2 = 1, 2, ..., N_2, \text{ and } x_3 = 1, 2, ..., N_3 \tag{2}$$

is transformed into Fourier space using the FFT (Subroutines provided by FFTW, 9 transforms of rank 3). The result is a 3x3 tensor field depending on the frequencies $\vec{\xi}$:

$$\hat{\boldsymbol{P}}(\vec{\xi}) = \mathcal{F}\left(\boldsymbol{P}(\vec{x})\right) \tag{3}$$

the divergence of a tensor is defined as:

$$\operatorname{div}(\boldsymbol{P}) = \begin{pmatrix} \frac{\partial P_{11}}{\partial x_1} + \frac{\partial P_{12}}{\partial x_2} + \frac{\partial P_{13}}{\partial x_3} \\ \frac{\partial P_{21}}{\partial x_1} + \frac{\partial P_{22}}{\partial x_2} + \frac{\partial P_{23}}{\partial x_3} \\ \frac{\partial P_{z1}}{\partial x_1} + \frac{\partial P_{z2}}{\partial x_2} + \frac{\partial P_{33}}{\partial x_3} \end{pmatrix} \tag{4}$$

It is a 3D vector. With

$$\mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right) = (2\pi i \xi)^n \hat{f}(\xi) \tag{5}$$

follows:

$$\mathcal{F}\left(\operatorname{div}(\boldsymbol{P})\right) = 2\pi i \vec{\xi} \times \hat{\boldsymbol{P}}(\vec{\xi}) \tag{6}$$

Due to the order in which FFTW stores the array, the components of the 3D frequencies can be calculated by dividing a linear list $0, 1, 2, ... N/2 - 1, \pm N/2, -(N/2 - 1), ..., -2, -1$ by the sampling length in each dimension.

2 Questions

The inverse transform of $\mathcal{F}\left(\operatorname{div}\left(\boldsymbol{P}\right)\right)$ (FFTW, 3 transforms of rank 3) should give the divergence field in real space.

My problem is, that the calculated divergence has imaginary parts after the inverse transform. That seems strange to me, as the divergence can also be computed in real space, e.g. using FDM. If a complex-to-complex transform is done, $\hat{\boldsymbol{P}}(\vec{\xi})$ possesses conjugate complex symmetry. $\operatorname{div}(\hat{\boldsymbol{P}})(\vec{x}i)$ should also have conjugate complex symmetry as it would lead to a real-only divergence after the inverse transform. Surprisingly, even for the simple derivative as given in formula eq.(**??**), the complex conjugate symmetry is also not preserved. The multiplication changes the sign of the whole term and not only of the imaginary part.

As the tensor $\boldsymbol{P}$ is a real-only tensor, it should be possible to use a real-to-complex transform for the tensor field and a complex-to-real transform for the back transform of the divergence field. Than one of the dimensions should run from 0 to $N/2+1$ only. But that implies, that the divergence in Fourier space has conjugate compley symmetry.