Green's Function for Potential Field Extrapolation

1. Some Preliminaries on the Potential Magnetic Field

By definition, a potential magnetic field is one for which the electric current density vanishes. That is,

$$\begin{aligned} \boldsymbol{J} &= \frac{c}{4\pi}\boldsymbol{\nabla}\times\boldsymbol{B} \\ &= 0. \end{aligned} \tag{1}$$

In addition, the magnetic field must also satisfy Maxwell's equations, in particular Gauss's law:

$$\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0. \tag{2}$$

Any function which satisfies these two constraints is a valid potential field.

It is often convenient to write the magnetic field in terms of a scalar potential, Φ, in the following way:

$$\boldsymbol{B} = -\boldsymbol{\nabla}\Phi. \tag{3}$$

This automatically satisfies the condition that the current density vanishes, since *any* scalar has the property that the curl of the gradient vanishes. Thus one only has to take into account the condition on the divergence, which can be written

$$\begin{aligned} \boldsymbol{\nabla}\cdot\boldsymbol{B} &= 0 \\ \boldsymbol{\nabla}^2\Phi &= 0. \end{aligned} \tag{4}$$

This is Laplace's equation for the scalar potential, which has been solved (in terms of various special functions) in something like 11 coordinate systems. For this exercise, we will be using only standard Cartesian coordinates. To define a unique solution in a volume, the normal component of the magnetic field may be specified on the closed surface bounding the volume. In some cases, this volume will be taken as semi-infinite, for example, the half-space above a plane. In this case, the condition that the normal component of the field be specified "at infinity" is satisfying by requiring that the magnitude of the field fall off rapidly enough with distance above the plane.

2. The Green's Function

For a potential field, the Green's function has a reasonably simple form:

$$G_x = \frac{x - x'}{r^3}, \tag{5}$$

$$G_y = \frac{y - y'}{r^3}, \tag{6}$$

$$G_z = \frac{z}{r^3}, \tag{7}$$

where $r^2 = (x - x')^2 + (y - y')^2 + z^2$, and the boundary is assumed to be at $z' = 0$. The field at any point is then constructed from

$$B_i(\boldsymbol{x}) = \frac{1}{2\pi} \int dx'\, dy'\, G_i(\boldsymbol{x}, \boldsymbol{x}') B_z(x', y', 0). \tag{8}$$

3. Application to Discrete Data

Now comes the fun part: applying this to $\boldsymbol{B}$ measured at discrete points. It's not as simple as one might think, because one does *not* want the field due to a series of point sources at each place there is a measurement. Instead, require that the vertical field be constant across each pixel. That is, let

$$\begin{aligned} B_z(x, y, 0) = & \sum_{i,j} \left[\Theta\left(x - x_i - \frac{\Delta x}{2}\right) - \Theta\left(x - x_i + \frac{\Delta x}{2}\right)\right] \\ & \times \left[\Theta\left(y - y_j - \frac{\Delta y}{2}\right) - \Theta\left(y - y_j + \frac{\Delta y}{2}\right)\right] B_{ij} \end{aligned} \tag{9}$$

Use this expression for the field in the integral with the Green's function.

$$\begin{aligned} B_l(x, y, z) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' B_z(x', y', 0) G_l(x, y, z, x', y') \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' \sum_{i,j} \left[\Theta\left(x - x_i - \frac{\Delta x}{2}\right) - \Theta\left(x - x_i + \frac{\Delta x}{2}\right)\right] \\ &\quad \times \left[\Theta\left(y - y_j - \frac{\Delta y}{2}\right) - \Theta\left(y - y_j + \frac{\Delta y}{2}\right)\right] B_{ij} G_l(x, y, z, x', y') \\ &= \frac{1}{2\pi} \sum_{i,j} B_{ij} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} dx' \int_{y_j - \Delta y/2}^{y_j + \Delta y/2} dy'\, G_l(x, y, z, x', y') \\ &= \frac{1}{2\pi} \sum_{i,j} B_{ij} \int_{x - x_i + \Delta x/2}^{x - x_i - \Delta x/2} d(-\tilde{x}) \int_{y - y_j + \Delta y/2}^{y - y_j - \Delta y/2} d(-\tilde{y})\, G_l(x, y, z, x', y') \end{aligned}$$

$$= \frac{1}{2\pi}\sum_{i,j} B_{ij}\int_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} d\tilde{x}\int_{y-y_j-\Delta y/2}^{y-y_j+\Delta y/2} d\tilde{y}\, G_l(x,y,z,x',y') \qquad (10)$$

with $r^2 = (x-x')^2 + (y-y')^2 + z^2$, $\tan\theta = (y-y')/(x-x')$, and $\tilde{x} = x - x'$, $\tilde{y} = y - y'$. Start with the z-component, and try to do the integrals explicitly.

$$\begin{aligned}
B_z(x,y,z) &= \frac{1}{2\pi}\sum_{i,j} B_{ij}\int_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} d\tilde{x}\int_{y-y_j-\Delta y/2}^{y-y_j+\Delta y/2} d\tilde{y}\frac{z}{(\tilde{x}^2+\tilde{y}^2+z^2)^{3/2}} \\
&= \frac{z}{2\pi}\sum_{i,j} B_{ij}\int_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} d\tilde{x}\frac{\tilde{y}}{(\tilde{x}^2+z^2)(\tilde{x}^2+\tilde{y}^2+z^2)^{1/2}}\Big|_{y-y_j-\Delta y/2}^{y-y_j+\Delta y/2} \\
&= \frac{z}{2\pi}\sum_{i,j} B_{ij}\int_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} d\tilde{x}\Big[\frac{\tilde{y}_j+\Delta y/2}{(\tilde{x}^2+z^2)[\tilde{x}^2+(\tilde{y}_j+\Delta y/2)^2+z^2]^{1/2}} \\
&\qquad -\frac{\tilde{y}_j-\Delta y/2}{(\tilde{x}^2+z^2)[\tilde{x}^2+(\tilde{y}_j-\Delta y/2)^2+z^2]^{1/2}}\Big] \\
&= \frac{z}{2\pi}\sum_{i,j} B_{ij}\Big\{\frac{\tilde{y}_j+\Delta y/2}{z(\tilde{y}_j+\Delta y/2)}\tan^{-1}\Big[\frac{\tilde{x}(\tilde{y}_j+\Delta y/2)}{z\sqrt{\tilde{x}^2+(\tilde{y}_j+\Delta y/2)^2+z^2}}\Big]\Big|_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} \\
&\qquad -\frac{\tilde{y}_j-\Delta y/2}{z(\tilde{y}_j-\Delta y/2)}\tan^{-1}\Big[\frac{\tilde{x}(\tilde{y}_j-\Delta y/2)}{z[\tilde{x}^2+(\tilde{y}_j-\Delta y/2)^2+z^2]^{1/2}}\Big]\Big|_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2}\Big\} \\
&= \sum_{i,j}\frac{B_{ij}}{2\pi}\Big\{\tan^{-1}\Big[\frac{(\tilde{x}_i+\Delta x/2)(\tilde{y}_j+\Delta y/2)}{z\sqrt{(\tilde{x}_i+\Delta x/2)^2+(\tilde{y}_j+\Delta y/2)^2+z^2}}\Big] \\
&\qquad -\tan^{-1}\Big[\frac{(\tilde{x}_i-\Delta x/2)(\tilde{y}_j+\Delta y/2)}{z\sqrt{(\tilde{x}_i-\Delta x/2)^2+(\tilde{y}_j+\Delta y/2)^2+z^2}}\Big] \\
&\qquad +\tan^{-1}\Big[\frac{(\tilde{x}_i-\Delta x/2)(\tilde{y}_j-\Delta y/2)}{z\sqrt{(\tilde{x}_i-\Delta x/2)^2+(\tilde{y}_j-\Delta y/2)^2+z^2}}\Big] \\
&\qquad -\tan^{-1}\Big[\frac{(\tilde{x}_i+\Delta x/2)(\tilde{y}_j-\Delta y/2)}{z\sqrt{(\tilde{x}_i+\Delta x/2)^2+(\tilde{y}_j-\Delta y/2)^2+z^2}}\Big]\Big\} \qquad (11)
\end{aligned}$$

where $\tilde{x}_i = x - x_i$, $\tilde{y}_j = y - y_j$. This is rather unwieldy, but at least it's an analytic expression that does not involve integrals. Next, try the x-component.

$$\begin{aligned}
B_x(x,y,z) &= \frac{1}{2\pi}\sum_{i,j} B_{ij}\int_{x-x_i-\Delta x/2}^{x-x_i+\Delta x/2} d\tilde{x}\int_{y-y_j-\Delta y/2}^{y-y_j+\Delta y/2} d\tilde{y}\frac{\tilde{x}}{(\tilde{x}^2+\tilde{y}^2+z^2)^{3/2}} \\
&= -\frac{1}{2\pi}\sum_{i,j} B_{ij}\int_{y-y_i-\Delta y/2}^{y-y_i+\Delta y/2} d\tilde{y}\frac{1}{(\tilde{y}^2+\tilde{x}^2+z^2)^{1/2}}\Big|_{x-x_j-\Delta x/2}^{x-x_j+\Delta x/2} \\
&= \frac{1}{2\pi}\sum_{i,j} B_{ij}\int_{y-y_i-\Delta y/2}^{y-y_i+\Delta y/2} d\tilde{y}\Big[\frac{1}{(\tilde{y}^2+(\tilde{x}_i-\Delta x/2)^2+z^2)^{1/2}}
\end{aligned}$$

$$
\begin{aligned}
& \qquad - \frac{1}{(\tilde{y}^2 + (\tilde{x}_i + \Delta x/2)^2 + z^2)^{1/2}} \Bigg] \\
= & \ \frac{1}{2\pi} \sum_{i,j} B_{ij} \Bigg\{ \ln \left[\tilde{y} + (\tilde{y}^2 + (\tilde{x}_i - \Delta x/2)^2 + z^2)^{1/2} \right] \Bigg|_{y-y_i-\Delta y/2}^{y-y_i+\Delta y/2} \\
& \qquad - \ln \left[\tilde{y} + (\tilde{y}^2 + (\tilde{x}_i + \Delta x/2)^2 + z^2)^{1/2} \right] \Bigg|_{y-y_i-\Delta y/2}^{y-y_i+\Delta y/2} \Bigg\} \\
= & \ \sum_{i,j} \frac{B_{ij}}{2\pi} \ln \left[\frac{\tilde{y} + (\tilde{y}^2 + (\tilde{x}_i - \Delta x/2)^2 + z^2)^{1/2}}{\tilde{y} + (\tilde{y}^2 + (\tilde{x}_i + \Delta x/2)^2 + z^2)^{1/2}} \right] \Bigg|_{y-y_i-\Delta y/2}^{y-y_i+\Delta y/2} \\
= & \ \sum_{i,j} \frac{B_{ij}}{2\pi} \Bigg\{ \ln \left[\frac{(\tilde{y}_j + \Delta y/2) + [(\tilde{y}_j + \Delta y/2)^2 + (\tilde{x}_i - \Delta x/2)^2 + z^2]^{1/2}}{(\tilde{y}_j + \Delta y/2) + [(\tilde{y}_j + \Delta y/2)^2 + (\tilde{x}_i + \Delta x/2)^2 + z^2]^{1/2}} \right] \\
& \qquad - \ln \left[\frac{(\tilde{y}_j - \Delta y/2) + [(\tilde{y}_j - \Delta y/2)^2 + (\tilde{x}_i - \Delta x/2)^2 + z^2]^{1/2}}{(\tilde{y}_j - \Delta y/2) + [(\tilde{y}_j - \Delta y/2)^2 + (\tilde{x}_i + \Delta x/2)^2 + z^2]^{1/2}} \right] \Bigg\} \qquad (12)
\end{aligned}
$$

and this expression will also hold for the y-component by appropriately interchanging x and y.

4. Solution for a Box

Consider now the case in which one wishes to determine the field in the volume $0 < x < a$, $0 < y < b$, $0 < z < c$, given the normal component of the field on all six of the faces of the box. Following the discussion in Jackson (1975), construct six separate scalar potentials, each of which has a non-vanishing normal derivative on only one of the walls. Then the scalar potential for the solution will be simply the sum of the six. Try to construct this in such a way that FFTs can be used, by taking the exponential solutions to be in the direction normal to the face on which the derivative of the potential does not vanish. So, let

$$
\Phi_0(\boldsymbol{x}) = \sum_{m,n} A^0_{mn} \cos(m\pi x/a) \cos(n\pi y/b) \cosh \left[\pi \sqrt{\frac{m^2}{a^2} + \frac{n^2}{b^2}} (z - c) \right] \qquad (13)
$$

which by construction satisfies $\nabla^2 \Phi_0 = 0$, and hence $\boldsymbol{\nabla} \cdot \boldsymbol{B} = \boldsymbol{\nabla} \cdot (-\boldsymbol{\nabla} \Phi) = 0$. With this definition,

$$
\begin{aligned}
\frac{\partial \Phi_0}{\partial x}\bigg|_{0,a} &= -\sum_{m,n} \frac{m\pi}{a} A^0_{mn} \sin(m\pi x/a) \cos(n\pi y/b) \cosh \left[\pi \sqrt{\frac{m^2}{a^2} + \frac{n^2}{b^2}} (z - c) \right] \bigg|_{0,a} \\
&= 0 \qquad (14) \\
\frac{\partial \Phi_0}{\partial y}\bigg|_{0,b} &= -\sum_{m,n} \frac{n\pi}{b} A^0_{mn} \cos(m\pi x/a) \sin(n\pi y/b) \cosh \left[\pi \sqrt{\frac{m^2}{a^2} + \frac{n^2}{b^2}} (z - c) \right] \bigg|_{0,b}
\end{aligned}
$$

$$
\begin{aligned}
&= 0 &(15)\\
\left.\frac{\partial\Phi_0}{\partial z}\right|_c &= \sum_{m,n}\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}A^0_{mn}\cos(m\pi x/a)\cos(n\pi y/b)\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\Big|_c\\
&= 0 &(16)\\
\left.\frac{\partial\Phi_0}{\partial z}\right|_0 &= \sum_{m,n}\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}A^0_{mn}\cos(m\pi x/a)\cos(n\pi y/b)\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\Big|_0\\
B_z(x,y,0) &= \sum_{m,n}\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}A^0_{mn}\cos(m\pi x/a)\cos(n\pi y/b)\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}c\right] &(17)
\end{aligned}
$$

Try to simplify at least the notation somewhat by starting with

$$
\begin{aligned}
\Phi_3(\boldsymbol{x}) &= \frac{1}{\pi}\sum_{m,n}\left[\frac{m^2}{a^2}+\frac{n^2}{b^2}\right]^{-1/2}\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\\
&\quad\times\left\{C^+_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}z\right]+C^-_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\right\} &(18)
\end{aligned}
$$

thus

$$
\begin{aligned}
\left.\frac{\partial\Phi_3}{\partial x}\right|_{0,a} &= -\sum_{m,n}\frac{m}{a}\left[\frac{m^2}{a^2}+\frac{n^2}{b^2}\right]^{-1/2}\sin\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\Big|_{x=0,a}\\
&\quad\times\left\{C^+_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}z\right]+C^-_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\right\}\\
&= 0 &(19)\\
\left.\frac{\partial\Phi_3}{\partial y}\right|_{0,b} &= -\sum_{m,n}\frac{n}{b}\left[\frac{m^2}{a^2}+\frac{n^2}{b^2}\right]^{-1/2}\cos\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi y}{b}\right)\Big|_{y=0,b}\\
&\quad\times\left\{C^+_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}z\right]+C^-_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\right\}\\
&= 0 &(20)\\
\left.\frac{\partial\Phi_3}{\partial z}\right|_{0,c} &= \sum_{m,n}\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)\\
&\quad\times\left\{C^+_{mn}\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}z\right]+C^-_{mn}\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}(z-c)\right]\right\}\\
B_z(x,y,0) &= \sum_{m,n}\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right)C^-_{mn}\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}c\right]\\
C^-_{mn} &= \frac{4}{ab\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}c\right]}\int_0^a dx\int_0^b dy\,B_z(x,y,0)\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right) &(21)
\end{aligned}
$$

$$
\begin{aligned}
B_z(x,y,c) &= -\sum_{m,n} \cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right) C^{+}_{mn}\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}c\right] \\
C^{+}_{mn} &= -\frac{4}{ab\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{b^2}}c\right]}\int_0^a dx\int_0^b dy\, B_z(x,y,c)\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi y}{b}\right) \qquad (22)
\end{aligned}
$$

Similarly, let

$$
\begin{aligned}
\Phi_1(\boldsymbol{x}) &= \frac{1}{\pi}\sum_{m,n}\left[\frac{m^2}{b^2}+\frac{n^2}{c^2}\right]^{-1/2}\cos\left(\frac{m\pi y}{b}\right)\cos\left(\frac{n\pi z}{c}\right) \\
&\quad \times\left\{A^{+}_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{b^2}+\frac{n^2}{c^2}}x\right]+A^{-}_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{b^2}+\frac{n^2}{c^2}}(x-a)\right]\right\} \qquad (23)
\end{aligned}
$$

where

$$
\begin{aligned}
A^{-}_{mn} &= \frac{4}{bc\sinh\left[\pi\sqrt{\frac{m^2}{b^2}+\frac{n^2}{c^2}}a\right]}\int_0^b dy\int_0^c dz\, B_x(0,y,z)\cos\left(\frac{m\pi y}{b}\right)\cos\left(\frac{n\pi z}{c}\right) \qquad (24) \\
A^{+}_{mn} &= -\frac{4}{bc\sinh\left[\pi\sqrt{\frac{m^2}{b^2}+\frac{n^2}{c^2}}a\right]}\int_0^b dy\int_0^c dz\, B_x(a,y,z)\cos\left(\frac{m\pi y}{b}\right)\cos\left(\frac{n\pi z}{c}\right) \qquad (25)
\end{aligned}
$$

and

$$
\begin{aligned}
\Phi_2(\boldsymbol{x}) &= \frac{1}{\pi}\sum_{m,n}\left[\frac{m^2}{a^2}+\frac{n^2}{c^2}\right]^{-1/2}\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi z}{c}\right) \\
&\quad \times\left\{B^{+}_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{c^2}}y\right]+B^{-}_{mn}\cosh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{c^2}}(y-b)\right]\right\} \qquad (26)
\end{aligned}
$$

where

$$
\begin{aligned}
B^{-}_{mn} &= \frac{4}{ac\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{c^2}}b\right]}\int_0^a dx\int_0^c dz\, B_y(x,0,z)\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi z}{c}\right) \qquad (27) \\
B^{+}_{mn} &= -\frac{4}{ac\sinh\left[\pi\sqrt{\frac{m^2}{a^2}+\frac{n^2}{c^2}}b\right]}\int_0^a dx\int_0^c dz\, B_y(x,b,z)\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{n\pi z}{c}\right) \qquad (28)
\end{aligned}
$$

and the vector potential for the complete solution is simply $\Phi = \Phi_1 + \Phi_2 + \Phi_3$.

4.1. Application to Discrete Data

The above formulation provides a general solution, given the normal component of the field on all six faces of a box. Now consider the case in which the normal field is given at discrete (regularly spaced) points on each of the faces, with the goal of converting as much as possible of this into Fourier Transforms. There are two ways we can proceed: turn the sine and cosine expansions into discrete Fourier transforms by redefining the boundary over a larger area, with the appropriate symmetry, or take the real part of each Fourier transform as it is performed. Start with the latter, since it will use transforms of smaller array sizes, which will be faster. Note that for the discrete case, the integrals will be represented as sums, in the following form

$$\int_0^{L_j} dx^j\, f(\boldsymbol{x}) \quad \rightarrow \quad \frac{L_j}{N_j-1}\Big[\frac{f(x^j=0)+f(x^j=L_j)}{2} + \sum_{m=1}^{N_j-2} f(x^j=x^j_m)\Big] \tag{29}$$

where $x^j_m = mL_j/(N_j-1)$. Note that this implies a particular choice for the walls of the box, namely that the wall falls on the outermost grid point in each dimension. This assumption is different from the "standard" periodic boundary conditions used in `fff.pro`, for example, and also different from the walls in Yuhong's simulation, in which the wall is midway between the last grid point and a "ghost" grid point outside the wall. So, the factor of a half in the first and last grid points represents the fact that only half the pixel is contained within the walls.

To begin with, change notation once again, this time using $(1,2,3)$ in place of (x,y,z). With this notation, assume that the volume of interest is $0 \le x^j \le L_j$, with $j=1,2,3$, and let

$$\begin{aligned}\Phi^l(\boldsymbol{x}) \quad = \quad & \frac{1}{\pi}\sum_{m=0}^{N_j-1}\sum_{n=0}^{N_k-1}\left[\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}\right]^{-1/2}\cos\Big(\frac{m\pi x^j}{L_j}\Big)\cos\Big(\frac{n\pi x^k}{L_k}\Big) \\ & \times\Big\{A^{l+}_{mn}\cosh\Big[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}x^l\Big] + A^{l-}_{mn}\cosh\Big[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}(x^l-L_l)\Big]\Big\}\end{aligned} \tag{30}$$

hence

$$\begin{aligned}B^{l\pm} \quad = \quad & -\sum_{m=0}^{N_j-1}\sum_{n=0}^{N_k-1}\cos\Big(\frac{m\pi x^j}{L_j}\Big)\cos\Big(\frac{n\pi x^k}{L_k}\Big) \\ & \times\Big\{A^{l+}_{mn}\sinh\Big[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}x^l\Big] + A^{l-}_{mn}\sinh\Big[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}(x^l-L_l)\Big]\Big\}\Big|_{x^l=0,L_l} \\ = \quad & \mp\sum_{m=0}^{N_j-1}\sum_{n=0}^{N_k-1}A^{l\pm}_{mn}\sinh\Big[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\Big]\cos\Big(\frac{m\pi x^j}{L_j}\Big)\cos\Big(\frac{n\pi x^k}{L_k}\Big) \\ & \mp\int_0^{L_j} dx^j\, B^{l\pm}\cos\Big(\frac{r\pi x^j}{L_j}\Big)\end{aligned}$$

$$
\begin{aligned}
&= \sum_{m=0}^{N_j-1}\sum_{n=0}^{N_k-1} A^{l\pm}_{mn}\sinh\left[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\right]\cos\left(\frac{n\pi x^k}{L_k}\right)\int_0^{L_j} dx^j\,\cos\left(\frac{m\pi x^j}{L_j}\right)\cos\left(\frac{r\pi x^j}{L_j}\right)\\
&\quad\mp\int_0^{L_j} dx^j\int_0^{L_k} dx^k\, B^{l\pm}\cos\left(\frac{r\pi x^j}{L_j}\right)\cos\left(\frac{s\pi x^k}{L_k}\right)\\
&= \frac{L_j}{2}(1+\delta_{r0})\sum_{n=0}^{N_k-1} A^{l\pm}_{rn}\sinh\left[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\right]\int_0^{L_k} dx^k\,\cos\left(\frac{n\pi x^k}{L_k}\right)\cos\left(\frac{s\pi x^k}{L_k}\right)\\
&\quad\mp\int_0^{L_j} dx^j\int_0^{L_k} dx^k\, B^{l\pm}\cos\left(\frac{r\pi x^j}{L_j}\right)\cos\left(\frac{s\pi x^k}{L_k}\right)\\
&= \frac{L_jL_k}{4}(1+\delta_{r0})(1+\delta_{s0})A^{l\pm}_{rs}\sinh\left[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\right]
\end{aligned}
$$

$$
A^{l\pm}_{mn} = \mp\frac{(2-\delta_{m0})(2-\delta_{n0})}{L_jL_k\sinh\left[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\right]}\int_0^{L_j} dx^j\int_0^{L_k} dx^k\, B^{l\pm}\cos\left(\frac{m\pi x^j}{L_j}\right)\cos\left(\frac{n\pi x^k}{L_k}\right) \quad (31)
$$

Note that this expression is not really well defined for $m = n = 0$ (as is the expression for Φ), but since this is the Φ = constant term, and so does not contribute to the magnetic field, I'm not going to treat it properly. It may need to be handled differently when coded, however. Also, I am assuming flux balance, so there is no term of the form $\Phi = \boldsymbol{B}_0\cdot\boldsymbol{x}$.

4.1.1. Using Real Parts

This is not as straightforward as I thought, because one ends up with a "missing" factor of 2 in the cosine terms. Numerical Recipes has a way (actually, several ways) to deal with this, by constructing fast cosine transforms, but for now, proceed with the "slow" method of doubling the dimensions. Thus, this section is not complete.

4.1.2. Expanding the Boundary

In order to make use of the standard FFT, and in fact, with the further goal of performing this with repeated calls to `fff.pro`, which assumes only the lower boundary is given, and that the boundary conditions are periodic with period L, define a symmetrized version of B^l in the volume $0 \le x_1 < 2L_1$, $0 \le x_2 < 2L_2$, $0 \le x_3 < 2L_3$, and assume that B^l vanishes outside of this region. Do this by letting

$$
B^3(2L_1 - x^1, x^2, 0) = B^3(x^1, x^2, 0), \quad (32)
$$

$$\begin{aligned} B^3(2L_1 - x^1, x^2, L_3) &= B^3(x^1, x^2, L_3), & (33)\\ B^3(x^1, 2L_2 - x^2, 0) &= B^3(x^1, x^2, 0), & (34)\\ B^3(x^1, 2L_2 - x^2, L_3) &= B^3(x^1, x^2, L_3), & (35)\end{aligned}$$

and similarly for B^1, B^2. *Note that this definition is a little different from the "standard" periodic boundary conditions.* With this definition, and making use of the vanishing of B^3 outside the area of interest, evaluate

$$\begin{aligned}
& \int_0^{2L_1} dx^1 B^3(x^1,x^2,0) \exp\Big(-\frac{2\pi i m x^1}{2L_1}\Big) \\
&= \int_0^{L_1} dx^1 B^3(x^1,x^2,0)\Big[\cos\Big(\frac{2\pi m x^1}{2L_1}\Big) - i\sin\Big(\frac{2\pi m x^1}{2L_1}\Big)\Big] \\
&\quad + \int_{L_1}^{2L_1} dx^1 B^3(x^1,x^2,0)\Big[\cos\Big(\frac{2\pi m x^1}{2L_1}\Big) - i\sin\Big(\frac{2\pi m x^1}{2L_1}\Big)\Big] \\
& 2L_1 \int_{-\infty}^{\infty} d\Big(\frac{x^1}{2L_1}\Big) B^3(x^1,x^2,0) \exp\Big(-\frac{2\pi i m x^1}{2L_1}\Big) \\
&= \int_0^{L_1} dx^1 B^3(x^1,x^2,0)\Big[\cos\Big(\frac{2\pi m x^1}{2L_1}\Big) - i\sin\Big(\frac{2\pi m x^1}{2L_1}\Big)\Big] \\
&\quad + \int_0^{L_1} d\tilde{x}^1 B^3(2L_1-\tilde{x}^1,x^2,0)\Big[\cos\Big(2\pi m - \frac{2\pi m \tilde{x}^1}{2L_1}\Big) - i\sin\Big(2\pi m - \frac{2\pi m \tilde{x}^1}{2L_1}\Big)\Big] \\
2L_1\mathtt{FFT}_1(B^3) &= \int_0^{L_1} dx^1 B^3(x^1,x^2,0)\Big[\cos\Big(\frac{2\pi m x^1}{2L_1}\Big) - i\sin\Big(\frac{2\pi m x^1}{2L_1}\Big)\Big] \\
&\quad + \int_0^{L_1} dx^1 B^3(x^1,x^2,0)\Big[\cos\Big(\frac{2\pi m x^1}{2L_1}\Big) + i\sin\Big(\frac{2\pi m x^1}{2L_1}\Big)\Big] \\
\mathtt{FFT}_1(B^3) &= \frac{1}{L_1}\int_0^{L_1} dx^1 B^3(x^1,x^2,0)\cos\Big(\frac{\pi m x^1}{L_1}\Big) \qquad (36)
\end{aligned}$$

which has been calculated without making the change to discrete data, but presumably must also hold, provided the FFT is defined properly.

Now go back to the expressions for the coefficients in the cosine expansion,

$$\begin{aligned}
A^{l\pm}_{mn} &= \frac{\mp(2-\delta_{m0})(2-\delta_{n0})}{L_j L_k \sinh\Big[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\Big]} \int_0^{L_j} dx^j \int_0^{L_k} dx^k\, B^l(x^l=0,L_l)\cos\Big(\frac{m\pi x^j}{L_j}\Big)\cos\Big(\frac{n\pi x^k}{L_k}\Big) \\
&= \frac{\mp(2-\delta_{m0})(2-\delta_{n0})}{\sinh\Big[\pi L_l\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}\Big]} \mathtt{FFT}_{jk}(B^l(x^l=0,L_l)) \qquad (37)
\end{aligned}$$

where the FFT is taken in the forward direction to correspond to IDL's normalization.

In the discrete version, if B^3_{mn} is given for $m = 0, N_1 - 1$, $n = 0, N_2 - 1$, then the expanded version of the field is given explicitly by

$$B^3_{2(N_1-1)-m,n} = B^3_{mn}, \tag{38}$$
$$B^3_{m,2(N_1-1)-n} = B^3_{mn}, \tag{39}$$

Because of the expanded dimensions for B^l, the coefficients are only meaningful for $m < N_j$, $n < N_k$. That is, the $A^{l\pm}_{mn}$ are not all independent. In particular, $A^{l\pm}_{mn} = A^{l\pm}_{2(N_j-1)-m,n} = A^{l\pm}_{m,2(N_k-1)-n}$.

Having determined the coefficients in terms of FFTs, next tackle the series for the scalar potential itself. To do this, it will be convenient to define a new set of coefficients, given by

$$\alpha^l_{mn} = \left[\frac{m^2}{L_j^2} + \frac{n^2}{L_k^2}\right]^{-1/2} \left\{ A^{l+}_{mn} \cosh\left[\pi\sqrt{\frac{m^2}{L_j^2} + \frac{n^2}{L_k^2}} x^l\right] + A^{l-}_{mn} \cosh\left[\pi\sqrt{\frac{m^2}{L_j^2} + \frac{n^2}{L_k^2}} (x^l - L_l)\right]\right\} \tag{40}$$

for $m < N_j, n < N_k$, and let

$$\alpha^l_{2(N_1-1)-m,n} = \alpha^l_{mn}, \tag{41}$$
$$\alpha^l_{m,2(N_1-1)-n} = \alpha^l_{mn}. \tag{42}$$

Now evaluate

$$\begin{aligned}
\mathtt{FFT}^{-1}_{jk}(\alpha^l) &= \frac{1}{4(N_j-1)(N_k-1)} \sum_{m=0}^{2N_j-1} \sum_{n=0}^{2N_k-1} \alpha^l_{mn} \exp\left[\frac{2\pi imp}{2(N_j-1)}\right] \exp\left[\frac{2\pi inq}{2(N_k-1)}\right] \\
&= \frac{1}{4(N_j-1)(N_k-1)} \sum_{m=0}^{2N_j-3} \exp\left[\frac{i\pi mp}{N_j-1}\right] \sum_{n=0}^{2N_k-3} \alpha^l_{mn} \left[\cos\left(\frac{\pi nq}{N_k-1}\right) + i\sin\left(\frac{\pi nq}{N_k-1}\right)\right] \\
&= \frac{1}{4(N_j-1)(N_k-1)} \sum_{m=0}^{2N_j-3} \exp\left[\frac{i\pi mp}{N_j-1}\right] \left\{ \sum_{n=1}^{N_k-2} \alpha^l_{mn} \left[\cos\left(\frac{\pi nq}{N_k-1}\right) + i\sin\left(\frac{\pi nq}{N_k-1}\right)\right] \right. \\
&\quad \left. + \alpha^l_{m0} + \alpha^l_{m,N_k-1}\cos(\pi q) + \sum_{n=N_k}^{2N_k-3} \alpha^l_{mn} \left[\cos\left(\frac{\pi nq}{N_k-1}\right) + i\sin\left(\frac{\pi nq}{N_k-1}\right)\right]\right\} \\
&= \frac{1}{4(N_j-1)(N_k-1)} \sum_{m=0}^{2N_j-3} \exp\left[\frac{i\pi mp}{N_j-1}\right] \left\{ \sum_{n=1}^{N_k-2} \alpha^l_{mn} \left[\cos\left(\frac{\pi nq}{N_k-1}\right) + i\sin\left(\frac{\pi nq}{N_k-1}\right)\right] \right. \\
&\quad + \sum_{\tilde{n}=1}^{N_k-2} \alpha^l_{m,2(N_k-1)-\tilde{n}} \left[\cos\left(2\pi q - \frac{\pi \tilde{n} q}{N_k-1}\right) + i\sin\left(2\pi q - \frac{\pi\tilde{n}q}{N_k-1}\right)\right] \\
&\quad \left. + \alpha^l_{m0} + \alpha^l_{m,N_k-1}\cos(\pi q)\right\}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{m=0}^{2N_j-3}\exp\left[\frac{i\pi mp}{N_j-1}\right]\Big\{\sum_{n=1}^{N_k-2}2\alpha^l_{mn}\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad +\alpha^l_{m0}+\alpha^l_{m,N_k-1}\cos(\pi q)\Big\} \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{m=0}^{2N_j-3}\exp\left[\frac{i\pi mp}{N_j-1}\right]\sum_{n=0}^{N_k-1}(2-\delta_{n0}-\delta_{nN_k})\alpha^l_{mn}\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{n=0}^{N_k-1}(2-\delta_{n0}-\delta_{nN_k})\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad \times\Big\{\sum_{m=0}^{2N_j-3}\alpha^l_{mn}\cos\left(\frac{\pi mp}{N_j-1}\right)+i\sin\left(\frac{\pi mp}{N_j-1}\right)\Big\} \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{n=0}^{N_k-1}(2-\delta_{n0}-\delta_{nN_k})\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad \times\Big\{\sum_{m=1}^{N_j-2}\alpha^l_{mn}\cos\left(\frac{\pi mp}{N_j-1}\right)+i\sin\left(\frac{\pi mp}{N_j-1}\right)+\alpha^l_{0,n}+\alpha^l_{N_j-1,n}\cos(\pi p) \\
&\quad +\sum_{m=N_j}^{2N_j-3}\alpha^l_{mn}\cos\left(\frac{\pi mp}{N_j-1}\right)+i\sin\left(\frac{\pi mp}{N_j-1}\right)\Big\} \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{n=0}^{N_k-1}(2-\delta_{n0}-\delta_{nN_k})\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad \times\Big\{\sum_{m=1}^{N_j-2}\alpha^l_{mn}\cos\left(\frac{\pi mp}{N_j-1}\right)+i\sin\left(\frac{\pi mp}{N_j-1}\right)+\alpha^l_{0,n}+\alpha^l_{N_j-1,n}\cos(\pi p) \\
&\quad +\sum_{\tilde{m}=1}^{N_j-2}\alpha^l_{2(N_j-1)-\tilde{m},n}\cos\left(2\pi p-\frac{\pi\tilde{m}p}{N_j-1}\right)+i\sin\left(2\pi p-\frac{\pi\tilde{m}p}{N_j-1}\right)\Big\} \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{n=0}^{N_k-1}(2-\delta_{n0}-\delta_{nN_k})\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad \times\Big\{\sum_{m=1}^{N_j-2}2\alpha^l_{mn}\cos\left(\frac{\pi mp}{N_j-1}\right)+\alpha^l_{0,n}+\alpha^l_{N_j-1,n}\cos(\pi p)\Big\} \\
&= \frac{1}{4(N_j-1)(N_k-1)}\sum_{m=0}^{N_j-1}\sum_{n=0}^{N_k-1}\cos\left(\frac{\pi mp}{N_j-1}\right)\cos\left(\frac{\pi nq}{N_k-1}\right) \\
&\quad \times\alpha^l_{mn}(2-\delta_{n0}-\delta_{nN_k})(2-\delta_{m0}-\delta_{mN_j})
\end{aligned}
\tag{43}
$$

which (basically) gives the expression for the scalar potential. Slightly redefine α in order to get the various components of $\boldsymbol{B}$. So, for example, to get the component of the field normal to the wall, let

$$\begin{aligned}\alpha_{mn}^{ll} &= \left\{A_{mn}^{l+}\sinh\left[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}x^l\right]+A_{mn}^{l-}\sinh\left[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}(x^l-L_l)\right]\right\} \\ &\quad\times(1+\delta_{m0}+\delta_{mN_j})(1+\delta_{n0}+\delta_{nN_k}) \qquad (44)\end{aligned}$$

for $m<N_j, n<N_k$, in which case

$$B^l = \mathtt{FFT}_{jk}^{-1}(\alpha^{ll}). \qquad (45)$$

Note that this is only the contribution to one component from one wall, so still have to sum over the other five walls, as well as calculate the other components. For a component perpendicular to the wall under consideration, let

$$\begin{aligned}\alpha_{mn}^{lj} &= \frac{m}{L_j}\left[\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}\right]^{-1/2}\left\{A_{mn}^{l+}\cosh\left[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}x^l\right]+A_{mn}^{l-}\cosh\left[\pi\sqrt{\frac{m^2}{L_j^2}+\frac{n^2}{L_k^2}}(x^l-L_l)\right]\right\} \\ &\quad\times(1+\delta_{m0}+\delta_{mN_j})(1+\delta_{n0}+\delta_{nN_k}) \qquad (46)\end{aligned}$$

for $m<N_j, n<N_k$, and let

$$\alpha_{2(N_1-1)-m,n}^{l} = -\alpha_{mn}^{l}, \qquad (47)$$

$$\alpha_{m,2(N_1-1)-n}^{l} = \alpha_{mn}^{l}. \qquad (48)$$

in order to get a sin instead of a cos term. Note that now the expression for the field will be

$$B^j = -i\mathtt{FFT}_{jk}^{-1}(\alpha^{jl}). \qquad (49)$$

4.2. Flux Balance

The previous analysis requires that at least the flux through any pair of parallel walls vanish. Consider adding the following scalar potential, suggested by Dana Longcope, to the solution, to allow flux to exit through any combination of walls.

$$\Phi = A_1(x^2-y^2)+A_2(x^2-z^2)+A_3(y^2-z^2) \qquad (50)$$

with corresponding field components

$$\begin{aligned}B_x &= -2(A_1+A_2)x \\ B_y &= 2(A_1-A_3)y \\ B_z &= 2(A_2+A_3)z \qquad (51)\end{aligned}$$

Check that the diverence of this vanishes:

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{B} &= -2(A_1+A_2)+2(A_1-A_3)+2(A_2+A_3) \\ &= 0. \end{aligned} \tag{52}$$

The flux through the walls is given by

$$\begin{aligned}\Phi_x &= \int_0^{L_y} dy \int_0^{L_z} dz\, B_x|_{x=0,L_x} \\ &= -2(A_1+A_2)\int_0^{L_y} dy \int_0^{L_z} dz\, x|_{x=0,L_x} \\ &= -2(A_1+A_2)L_y L_z x|_{x=0,L_x} \end{aligned} \tag{53}$$

$$\begin{aligned}\Phi_y &= \int_0^{L_x} dx \int_0^{L_z} dz\, B_y|_{y=0,L_y} \\ &= 2(A_1-A_3)\int_0^{L_x} dx \int_0^{L_z} dz\, y|_{y=0,L_y} \\ &= 2(A_1-A_3)L_x L_z y|_{y=0,L_y} \end{aligned} \tag{54}$$

$$\begin{aligned}\Phi_z &= \int_0^{L_x} dx \int_0^{L_y} dy\, B_z|_{z=0,L_z} \\ &= 2(A_2+A_3)\int_0^{L_x} dx \int_0^{L_y} dy\, z|_{z=0,L_z} \\ &= 2(A_2+A_3)L_x L_y z|_{z=0,L_z} \end{aligned} \tag{55}$$

In order to balance the flux, don't need all of these terms, so deal with the flux in both the $x-$ and $y-$ directions by adding/subtracting a corresponding amount to the flux through the top boundary. Thus, keep only the terms involving A_2 and A_3, thus

$$\begin{aligned}\Phi_x &= -2A_2 L_x L_y L_z \\ \Phi_y &= -2A_3 L_x L_y L_z \end{aligned} \tag{56}$$

REFERENCES

Jackson, J. D. 1975, Classical Electrodynamics, 2nd edn. (New York: John Wiley & Sons)
