The potential of a homogeneous voxel

Below, we generalize the formula derived in (Hummer, 1996) to the case of anisotropic voxels and simplify the expressions. Let the voxel be given by the rectangular volume $[-a, a] \times [-b, b] \times [-c, c]$ for certain constants $a, b, c > 0$ and suppose that $\rho = 1$ on the rectangle. The electric potential is then is given by

$$V(u,v,w) = \frac{1}{4\pi}\int_{-a}^{a}\int_{-b}^{b}\int_{-c}^{c}\frac{dxdydz}{\sqrt{\sigma_y\sigma_z(x-u)^2+\sigma_z\sigma_x(y-v)^2+\sigma_x\sigma_y(z-w)^2}} \tag{1}$$

Integrating by parts yields

$$\begin{aligned} 2V(u,v,w) &= \frac{1}{4\pi}\int_{-a-u}^{a-u}\int_{-b-v}^{b-v}\frac{zdxdy}{\sqrt{\sigma_u^2x^2+\sigma_v^2y^2+\sigma_w^2z^2}}\Big|_{z_0}^{z_1} \\ &+ \frac{1}{4\pi}\int_{-a-u}^{a-u}\int_{-c-w}^{c-w}\frac{ydxdz}{\sqrt{\sigma_u^2x^2+\sigma_v^2y^2+\sigma_w^2z^2}}\Big|_{y_0}^{y_1} \\ &+ \frac{1}{4\pi}\int_{-b-v}^{b-v}\int_{-c-w}^{c-w}\frac{xdydz}{\sqrt{\sigma_u^2x^2+\sigma_v^2y^2+\sigma_w^2z^2}}\Big|_{x_0}^{x_1}, \end{aligned}$$

where we have defined $\sigma_u = \sqrt{\sigma_y\sigma_z}$, $\sigma_v = \sqrt{\sigma_z\sigma_x}$ and $\sigma_w = \sqrt{\sigma_x\sigma_y}$. By using the identities

$$\int_{y_0}^{y_1}\frac{dy}{\sqrt{x^2+y^2+z^2}} = \log\frac{\sqrt{x^2+y_1^2+z^2}+y_1}{\sqrt{x^2+y_0^2+z^2}+y_0},$$

and

$$\begin{aligned} \int_{x_0}^{x_1}\log\left(\sqrt{x^2+y^2+z^2}+y\right)dx &= y\log\left(\sqrt{x^2+y^2+z^2}+x\right) \\ &+ x\log\left(\sqrt{x^2+y^2+z^2}+y\right) \\ &- z\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right) \\ &- x + z\arctan\left(\frac{x}{z}\right), \end{aligned}$$

we organize the solution to by defining functions f, g and h as follows:

$$\begin{aligned} f(x,y,z) &= yz\log\left(\sqrt{x^2+y^2+z^2}+x\right) + xz\log\left(\sqrt{x^2+y^2+z^2}+y\right) - \\ & z^2\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right), \end{aligned}$$

which is well-defined for all x, y, z, including at the origin where the argument of the arctan function above assumes the limiting value $1/\sqrt{3}$,

$$\begin{aligned} g(x_1,x_0,y_1,y_0,z_1,z_0) &= [\{f(x_1,y_1,z_1) - f(x_0,y_1,z_1)\} - \{f(x_1,y_0,z_1) - f(x_0,y_0,z_1)\}] - \\ & [\{f(x_1,y_1,z_0) - f(x_0,y_1,z_0)\} - \{f(x_1,y_0,z_0) - f(x_0,y_0,z_0)\}], \end{aligned}$$

and

$$\begin{aligned} h(a,b,c,u,v,w) &= g(a-u,-a-u,b-v,-b-v,c-w,-c-w) + \\ & g(b-v,-b-v,c-w,-c-w,a-u,-a-u) + \\ & g(c-w,-c-w,a-u,-a-u,b-v,-b-v). \end{aligned}$$

In terms of these functions, and in the case of $\sigma_x = \sigma_y = \sigma_z = 1$, the potential is given by

$$V(u, v, w) = \frac{1}{4\pi} \frac{h(a, b, c, u, v, w)}{2}$$

The general solution to follows by a shift in the arguments of h: $a \to \sigma_u a$, $b \to \sigma_v b$, $c \to \sigma_w c$, $u \to \sigma_u u$, $v \to \sigma_v v$, $w \to \sigma_w w$ and a multiplicative factor:

$$V(u, v, w) = \frac{1}{4\pi} \frac{h(\sigma_u a,\ \sigma_v b,\ \sigma_w c,\ \sigma_u u,\ \sigma_v v,\ \sigma_w w)}{2\sigma_u \sigma_v \sigma_w}. \tag{2}$$