Least squares computation of Dommaschk potential coefficients

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Suppose that we have a numerical representation of the vacuum magnetic field $\vec{B}$, obtained from some code, e.g. EXTENDER. We want to find some scalar χ such that

$$\nabla\chi = \vec{B}_{\mathrm{E}}. \tag{1}$$

Note that χ is a solution of the Laplace equation on a torus since $\nabla \cdot \vec{B} = 0$. Thus, χ can be written as a superposition of harmonics $\chi_{m,l}$:

$$\chi = F_0\varphi + \sum_{m,l} \chi_{m,l}, \tag{2}$$

where $\Delta\chi_{m,l} = 0$ and φ is the toroidal angle. Dommaschk gives a more explicit representation for $\widetilde{\chi}$ [1]:

$$\widetilde{\chi} = \varphi + \sum_{m,l}\left[(a_{m,l}\cos m\varphi + b_{m,l}\sin m\varphi)D_{m,l}(\widetilde{R},\widetilde{z}) + (c_{m,l}\cos m\varphi + d_{m,l}\sin m\varphi)N_{m,l-1}(\widetilde{R},\widetilde{z})\right], \tag{3}$$

where a tilde denotes normalization: $\chi = F_0\widetilde{\chi}$, $R = R_0\widetilde{R}$ and $z = R_0\widetilde{z}$.

The particular magnetic configuration is determined by the coefficients $\{a_{m,l}, b_{m,l}, c_{m,l}, d_{m,l}\}$. In order to calulate these coefficients from $\vec{B}_E$, a method involving integration over the $R = R_0$ surface was used before [2], however this method doesn't work well for some advanced stellarators where the $R = R_0$, $z = 0$ circle exits the plasma at some points. In that case, the boundary has to be extended, which is complicated and produces more numerical error that affects the end result. An alternate approach based on the minimization of the squared error will be described here.

The magnetic scalar potential can be written as follows:

$$\begin{aligned}
\chi &= \sum_i \alpha_i f_i(\widetilde{R},\widetilde{z},\phi),\\
\{\alpha_i\} &= \{F_0\} \cup \{F_0 a_{0,l}\}_{l=1}^{L} \cup \{F_0 a_{m,l}\}_{m=1,l=0}^{m=M,l=L} \cup \{F_0 b_{m,l}\}_{m=1,l=0}^{m=M,l=L}\\
&\quad \cup \{F_0 c_{m,l}\}_{m=0,l=1}^{m=M,l=L} \cup \{F_0 d_{m,l}\}_{m=1,l=1}^{m=M,l=L},\\
\{f_i\} &= \{\phi\} \cup \{D_{0,l}\}_{l=1}^{L} \cup \{D_{m,l}\cos(m\phi)\}_{m=1,l=0}^{m=M,l=L} \cup \{D_{m,l}\sin(m\phi)\}_{m=1,l=0}^{m=M,l=L}\\
&\quad \cup \{N_{m,l}\cos(m\phi)\}_{m=0,l=0}^{m=M,l=L-1} \cup \{N_{m,l}\sin(m\phi)\}_{m=1,l=0}^{m=M,l=L-1}.
\end{aligned} \tag{4}$$

Note that the cardinality of the set of coefficients is $|\{\alpha_i\}| = 1 + 2M(L+1) + 2L(M+1)$. Using the notation above, the volume-averaged squared error can be written as:

$$\begin{aligned}
S &= \langle|\nabla\chi - \vec{B}_{\mathrm{E}}|^2\rangle = \frac{1}{V}\int_{\mathcal{V}} (\nabla\chi - \vec{B}_{\mathrm{E}})^2 dV\\
&= \frac{1}{V}\int_{\mathcal{V}} \left[\left(\sum_j \alpha_j \frac{\partial f_j}{\partial R} - B_{\mathrm{E},R}\right)^2 + \left(\sum_j \alpha_j \frac{\partial f_j}{\partial z} - B_{\mathrm{E},z}\right)^2 + \left(\sum_j \frac{\alpha_j}{R}\frac{\partial f_j}{\partial \phi} - B_{\mathrm{E},\phi}\right)^2\right] dV,
\end{aligned} \tag{5}$$

where the integral is taken over a toroidal volume $\mathcal{V}$, and $V = \int_{\mathcal{V}} dV$ is the value of that volume. The derivative of the error with respect to a coefficient α_i can then be written as:

$$\frac{\partial S}{\partial \alpha_i} = \frac{2}{V} \int\limits_{\mathcal{V}} \left[\left(\sum_j \alpha_j \frac{\partial f_j}{\partial R} - B_{\mathrm{E},R} \right) \frac{\partial f_i}{\partial R} + \left(\sum_j \alpha_j \frac{\partial f_j}{\partial z} - B_{\mathrm{E},z} \right) \frac{\partial f_i}{\partial z} + \left(\sum_j \frac{\alpha_j}{R} \frac{\partial f_j}{\partial \phi} - B_{\mathrm{E},\phi} \right) \frac{1}{R} \frac{\partial f_i}{\partial \phi} \right] dV. \tag{6}$$

In order to minimize the squared error, one must set all of the derivatives to zero, which results in $1 + 2M(L+1) + 2L(M+1)$ linear equations:

$$\sum_j \alpha_j \int\limits_{\mathcal{V}} \left(\frac{\partial f_i}{\partial R} \frac{\partial f_j}{\partial R} + \frac{\partial f_i}{\partial z} \frac{\partial f_j}{\partial z} + \frac{1}{R^2} \frac{\partial f_i}{\partial \phi} \frac{\partial f_j}{\partial \phi} \right) dV = \int\limits_{\mathcal{V}} \left(B_{\mathrm{E},R} \frac{\partial f_i}{\partial R} + B_{\mathrm{E},z} \frac{\partial f_i}{\partial z} + \frac{B_{\mathrm{E},\phi}}{R} \frac{\partial f_i}{\partial \phi} \right) dV, \quad i = 1, ..., 1 + 2M(L+1) + 2L(M+1). \tag{7}$$

These equations can then be solved for the coefficients $\{\alpha_i\}$.

As compared to the previous method, the new method described here allows one to use a much lower resolution in the z direction. However, in spite of the simpler derivation, the new method requires much more time to calculate the coefficients, as it must evaluate the functions f_i at all points on the grid when integrating, which can be slow when implemented in Python.

References

[1] W. Dommaschk, *Computer Physics Communications* 40, 203-218 (1986).

[2] N. Nikulsin, R. Ramasamy, M. Hoelzl, F. Hindenlang, E. Strumberger, K. Lackner, S. Günter and the JOREK Team. *Physics of Plasmas* 29, 063901 (2022).