Highly Accurate 3D Field Gradient Computation Using Local Post-solving

Koen Delaere, Uwe Pahner, Ronnie Belmans and Kay Hameyer
Dept. EE (ESAT), Div. ELEN, Kardinaal Mercierlaan 94, Katholieke Universiteit Leuven, B3000 Leuven, Belgium

Abstract—To enhance the accuracy of finite element based computations of field quantities and their derivatives, a post-solving technique with superconvergent properties is presented. This technique uses an analytical expression for the magnetic field potential inside a closed region. The coefficients of the analytical expression are evaluated using a FE solution as boundary condition. All second derivatives of the analytical expression are calculated, leading to values for the flux density $B$ and its derivatives. These values are highly accurate, even when based upon a FE solution. As an example, the (edge) write gradient in a notch write head is evaluated.

*Index Terms*—Convergence of Numerical Methods, Finite Element Methods, Magnetic Fields, Magnetic Recording.

I. INTRODUCTION

To enhance the accuracy of finite element (FE) based computations of field and force quantities, post-solving techniques with superconvergent properties are commonly used [1]–[2]. These techniques use an analytical expression for the magnetic field potential inside a closed region without sources and consisting of one material only. The coefficients in the analytical expression are evaluated using a FE solution as boundary condition. Several applications of this method have been investigated, usually in order to improve FE based force calculations, which are very sensitive to the accuracy of the underlying field quantities [3]. In [4] it is shown that the energy error decreases as $O(h^2)$ for decreasing uniform mesh size $h$.

The first and second order derivatives of the analytical expression can be calculated without numerical differentiation, giving flux density $B$ and its derivatives with the same accuracy as the original FE solution. The calculation of the derivatives of the flux density $B$ is presented, using a double differentiation of the analytical expression for the magnetic potential. This results in a more reliable value for the field gradient than usually can be obtained using a FE solution. Field gradients are important in evaluating recording head performance, e.g. the edge write gradient in a notch write head [5]. The results of this method will be compared to the results obtained using two numerical differentiation steps.

II. FLUX DENSITY

Inside a closed spherical region without sources, the magnetic scalar potential $u(r,\theta,\phi)$ satisfies Laplace’s equation $\nabla^2 u = 0$. The general solution in spherical co-ordinates $(r,\theta,\phi)$ can be formulated as

$$u = \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} \left[ p_{mn} \cdot c_{mn}(\theta,\phi) + q_{mn} \cdot s_{mn}(\theta,\phi) \right] \cdot r^n, \quad (1)$$

where $p_{mn}$ and $q_{mn}$ are coefficients depending on the boundary condition, and $c_{mn}(\theta,\phi)$ and $s_{mn}(\theta,\phi)$ are the surface harmonic functions

$$c_{mn}(\theta,\phi) = P_m^n(\cos \theta) \cdot \cos m\phi,$$

$$s_{mn}(\theta,\phi) = P_m^n(\cos \theta) \cdot \sin m\phi,$$

using the associated Legendre polynomials of the first kind $P_m^n$. The coefficients $p_{mn}$ and $q_{mn}$ are evaluated using a FE solution as a boundary condition for (1) on a finite number of points distributed over a sphere with radius $R$. Details about this procedure and the resulting explicit form of $p_{mn}$ and $q_{mn}$ are given in [4].

The flux density $B(r,\theta,\phi)$ anywhere within the spherical region ($r < R$) can be expressed in terms of the coefficients $p_{mn}$ and $q_{mn}$. The flux density in the centre of the sphere ($r = 0$) acquires the simple expression

$$\left( B_x, B_y, B_z \right)_{r=0} = -\mu_0 \left( \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z} \right)_{r=0} \quad (3)$$

$$= -\mu_0 \cdot \left( p_{11}, q_{11}, p_{01} \right). \quad (4)$$

III. DERIVATIVES OF FLUX DENSITY

Not only the flux density $B$ but also its spatial derivatives are related to the magnetic potential $u$ and can be expressed in terms of $p_{mn}$ and $q_{mn}$. They acquire simple expression for values at the centre of the sphere.

A. $\partial B_x/\partial x$, $\partial B_y/\partial y$, $\partial B_z/\partial z$.

First, the derivative is transformed into the spherical co-ordinate formulation, e.g. for the x-direction:

$$\frac{\partial B_x}{\partial x} \bigg|_{y=0, z=0} = -\mu_0 \frac{\partial^2 u}{\partial x^2} \bigg|_{y=0, z=0} = -\mu_0 \frac{\partial^2 u}{\partial r^2} \bigg|_{r=\pi/2, \theta=0}. \quad (5)$$

where the spherical co-ordinates are defined as

$$x = r \sin \theta \cos \phi,$$

$$y = r \sin \theta \sin \phi, \quad (6)$$

$$z = r \cos \theta.$$
From (1) it is seen that the potential \( u \) can be interpreted as a polynomial in \( r \):
\[
  u(r, \theta, \phi) = \alpha(\theta, \phi) + \beta(\theta, \phi) \cdot r + \gamma(\theta, \phi) \cdot r^2 + \ldots,
\]
so the second derivative w.r.t. \( r \) in (6) is given by
\[
  -\mu_0 \frac{\partial^2 u}{\partial r^2} \bigg|_{\theta=\pi/2, \phi=0} = -\mu_0 \cdot 2\gamma \left( \frac{\pi}{2}, 0 \right). \tag{8}
\]

The function \( \gamma(\theta, \phi) \) can be retrieved recognising that it is the coefficient in \( r^2 \) in (1). Only the integer combinations \((m,n)\)=(0,2), (1,2) and (2,2) result in a term in \( r^2 \):
\[
  \gamma(\theta, \phi) = p_{02} P_2^0 (\cos \theta) + (p_{12} \cos \phi + q_{12} \sin \phi) P_2^1 (\cos \theta) + (p_{22} \cos 2\phi + q_{22} \sin 2\phi) P_2^2 (\cos \theta). \tag{9}
\]

The associated Legendre polynomials \( P_n^m \) are based upon the ordinary Legendre polynomials \( P_n \) as follows:
\[
  P_n^m(x) = (-1)^m (1-x^2)^{m/2} \cdot \frac{d^m}{dx^m} P_n(x). \tag{10}
\]

The three Legendre terms in (9) are
\[
  P_2^0 (\cos \theta) = \frac{1}{2} (3 \cos^2 \theta - 1), \]
\[
  P_2^1 (\cos \theta) = -3 \cos \theta \cdot \sin \theta, \]
\[
  P_2^2 (\cos \theta) = 3 \sin^2 \theta. \tag{11}
\]

Now \( \gamma(\theta, \phi) \) can be evaluated using \( \theta=\pi/2 \) and \( \phi=0 \) to give the derivative \( \partial B_x/\partial \theta \) at the origin. By using the appropriate values for \( \theta \) and \( \phi \), the derivatives \( \partial B_x/\partial \phi \) and \( \partial B_z/\partial \theta \) at the origin are found immediately:
\[
  \frac{\partial B_x}{\partial x} = -2\mu_0 \gamma \left( \frac{\pi}{2}, 0 \right) = 2\mu_0 (p_{02} \cdot P_2^0 - p_{22}) \]
\[
  \frac{\partial B_y}{\partial y} = -2\mu_0 \gamma \left( \frac{\pi}{2}, 0 \right) = 2\mu_0 (p_{02} \cdot P_2^1 - q_{22}) \]
\[
  \frac{\partial B_z}{\partial z} = -2\mu_0 \gamma (0, \phi) = -2\mu_0 p_{02} \cdot P_2^1. \tag{12}
\]

B. \( \partial B_x/\partial \theta \) and \( \partial B_y/\partial \phi \)

Since the values at the centre of the sphere are the target, and since these derivatives only involve the co-ordinates \( x \) and \( y \), the analysis can be performed in the plane \( z=0 \). The potential \( u \) restricted to the plane \( z=0 \) (\( \theta=\pi/2 \)) is
\[
  u \bigg|_{z=0} = \sum_{m=0, n|m} \left[ P_{mn} c_{mn} \left( \frac{\pi}{2}, \phi \right) + q_{mn} s_{mn} \left( \frac{\pi}{2}, \phi \right) \right] r^n, \tag{13}
\]
with \( r^2=x^2+y^2 \) and \( \phi=\arctan(x/y) \). The derivative of (13) w.r.t. \( x \) is given by
\[
  \frac{\partial u}{\partial x} \bigg|_{z=0} = \sum_{m=0, n|m} \left[ P_{mn} c_{mn} \left( \frac{\pi}{2}, \phi \right) + q_{mn} s_{mn} \left( \frac{\pi}{2}, \phi \right) \right] n x r^{n-2} + \sum_{m=1, n \neq m} \left[ m P_{mn} c_{mn} \left( \frac{\pi}{2}, \phi \right) - m q_{mn} s_{mn} \left( \frac{\pi}{2}, \phi \right) \right] \cdot y r^{n-2}. \tag{14}
\]

The derivative (14) has to be derived further w.r.t. \( y \). Before doing this, (14) can be confined to the \( y \)-axis without losing its validity, i.e. \( x=0 \). Care must be taken to perform the derivations \( \partial/\partial x \) and \( \partial/\partial y \) and simplifications \((z=0 \text{ and } x=0)\) in the correct order. For \( x=0 \) (\( \phi=\pi/2 \), \( r=y \) and (14) becomes
\[
  \frac{\partial u}{\partial y} \bigg|_{x=0} = \sum_{m=0, n=m} \sum_{m=0, n=m} m P_{mn} c_{mn} (0) \cdot y^{n-1} \tag{15}
\]
and the derivative w.r.t. \( y \) is
\[
  \frac{\partial^2 u}{\partial y^2} \bigg|_{x=0} = \sum_{m=0, n=m} \sum_{m=0, n=m} m P_{mn} c_{mn} (0) \cdot (n-1) y^{n-2}. \tag{16}
\]

For the value of this derivative at the centre of the sphere, \( y=0 \) still needs to be filled in. The only terms in the double sum of (16) that do not disappear for \( y=0 \) are the combinations \((m,n)\) with \( n=0 \), i.e. (1,2) and (2,2):}
\[
  \frac{\partial^2 u}{\partial y^2} \bigg|_{x=0} = 1 \cdot p_{12} P_2^1 (0) + 2 \cdot p_{22} P_2^2 (0). \tag{17}
\]

Evaluating the Legendre terms gives \( P_2^1 (0) = 0 \) and \( P_2^2 (0) = 3 \), which yields the field gradient
\[
  \frac{\partial B_x}{\partial y} \bigg|_{x=0} = \frac{\partial B_y}{\partial y} \bigg|_{x=0} = -6\mu_0 P_{22}. \tag{18}
\]

C. \( \partial B_z/\partial \phi \), \( \partial B_x/\partial \phi \), \( \partial B_y/\partial \phi \), \( \partial B_z/\partial \phi \)

The procedure is illustrated for the first pair. Since these derivatives only involve co-ordinates \( y \) and \( z \), the analysis can be performed in the plane \( x=0 \). The potential \( u \) is first restricted to the plane \( x=0 \) (\( \phi=\pi/2 \)) and subsequently derived w.r.t. \( z \) and evaluated at \( z=0 \), giving
\[
  \frac{\partial u}{\partial z} \bigg|_{z=0} = \sum_{m=0, n=m} \sum_{m=0, n=m} m q_{mn} y^{n-1} \frac{d}{dt} \left[ P_{mn} (t) \right] \bigg|_{t=0}, \tag{19}
\]
where the term in brackets is a constant. Next, (19) is derived w.r.t. \( y \) and subsequently evaluated at \( y=0 \):
The only terms in the double sum (20) that do not disappear for  \( y = 0 \) are the combinations \((m,n)\) with \( n - 2 = 0 \), i.e. \((0,2)\), \((1,2)\) and \((2,2)\). The final result is obtained as

\[
\frac{\partial B_x}{\partial y} \bigg|_{y=0} = \frac{\partial B_y}{\partial z} \bigg|_{z=0} = -3 \mu_0 q_{12} \quad (21)
\]

and in a similar fashion it is found that

\[
\frac{\partial B_x}{\partial x} \bigg|_{x=0} = \frac{\partial B_x}{\partial z} \bigg|_{z=0} = -3 \mu_0 p_{12} \quad (22)
\]

IV. EXAMPLE: WRITE GRADIENT

Fig.1 shows a coarse FE mesh of a notch write head with write gap \( g = 0.5 \mu \)m (first order elements). The field gradient \( \frac{\partial B_y}{\partial y} \) is calculated along the indicated plane in front of the recording head. The field gradient in this plane is calculated using (12) (Fig.2a) and compared to the value obtained using two numerical differentiations of the FE solution (Fig.2b). The superconvergent formulae clearly show a more realistic and reliable pattern for the gradient, although the FE mesh is very coarse and first order.

Fig.3 shows a front view of the recording head and a contour plot of \( \frac{\partial B_y}{\partial y} \) in this plane. This information is used to indicate the region in front of the recording head where the (edge) write gradient reaches the media coercitivity \( H_C \). It is well known that this limit contour reaches further along the recording head edges than is the case in the middle of the track (on-track position) [5]. The contour plot is slightly asymmetric due to the error in the FE solution because of the coarse meshing.

The total CPU time consists of calculation and tetrahedron searching. The calculation time is proportional to the number of points where the field solution is sampled. For double numerical differentiation, this is the number of points \( N_P \) that is sampled in the plane. For local post-solving, the number of samples is \( N_D \), where \( D \) is the number of points sampled on one sphere. For good results, \( D \geq 400 \) is recommended [4]. Fast searching algorithms for localising the tetrahedron that contains a given point will decrease the CPU time considerably since most time is spent searching for the next tetrahedron. In total, the local post-solving technique typically requires 20 times the CPU time of double differentiation.

VI. CONCLUSION

Calculating the second derivatives of an analytical expression for the magnetic scalar potential satisfying Laplace's equation, leads to highly accurate formulae for all field gradients. The values obtained are considerably more reliable than the values obtained using double numerical derivation. These formulae can bring important improvement to FE based results of recording head characteristics, e.g. edge write gradients.

REFERENCES