

# A highly accurate high-order method to solve the Neumann boundary condition problem for the 3D Laplace equation

M.L.Shashikant<sup>†</sup>, Martin Berz<sup>‡</sup>

Department of Physics and Astronomy, MSU

Email: <sup>†</sup>manikond@msu.edu

The 3D Laplace equation is one of the important PDEs of Physics and describes the phenomenology of electrostatics and magnetostatics. Frequently very precise solution of this PDE is required; but with conventional finite element or finite difference codes this is difficult to achieve because of the need for an exceedingly fine mesh which leads to often prohibitive CPU time.

We present an alternate approach based on high-order quadrature and a high-order finite element method. Both of the ingredients become possible via the use of high-order automatic differentiation. Various examples of the method and the precision that can be achieved will be given. For example, using only about 100 finite elements of order 7, accuracies in the range of  $10^{-7}$  can be obtained in the 3D case.

## 1 Introduction

The Neumann problem for the  $n$  dimensional Laplace equation is the solution of the PDE

$$\Delta\psi(\vec{r}) = 0 \text{ in the volume } \Omega(\mathbb{R}^n) \\ \text{where } \nabla\psi(\vec{r}) = \vec{f}(\vec{r}) \text{ on surface } \partial\Omega(\mathbb{R}^n)$$

The three dimensional (3D) case is of particular interest because it describes static problems in electromagnetism, heat conduction, and a variety of other problems. The existence and uniqueness of the solution for the 3D case can easily be shown through the application of Green's formulae.

It is well known that the analytic closed form solution for the 3D case can be found for problems with certain regular geometries where a separation of variables can be performed. However, in most practical cases, numerical methods are the only way to proceed. Usually the finite difference or finite element approach are used to find the numerical solution as data set in the region of interest. But because of their relatively low approximation order, for the problem of precise solution of PDEs, the methods have very limited success because of the prohibitively large number of mesh points required.

In the following we develop a method that determines local finite elements of in principle unlimited order, and show results of computations up to order 9. We begin by representing the solution of the PDE via Helmholtz' theorem, which states that for any vector field  $\vec{v}$  satisfying

$$[\nabla \cdot \vec{v}]_{\infty} = 0, \quad [\nabla \times \vec{v}]_{\infty} = 0,$$

the solution may be written as the sum of an irrotational part and a solenoidal part as  $\vec{v}(\vec{r}) = \vec{\nabla} \times \vec{A}_t(\vec{r}) + \vec{\nabla} \phi_n(\vec{r})$

where

$$\begin{aligned}\phi_n(\vec{r}) &= \frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{r}_s) \cdot \vec{f}(\vec{r}_s)}{|\vec{r} - \vec{r}_s|} d^2\vec{r}_s \\ \vec{A}_t(\vec{r}) &= -\frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{r}_s) \times \vec{f}(\vec{r}_s)}{|\vec{r} - \vec{r}_s|} d^2\vec{r}_s.\end{aligned}$$

Here  $\vec{r}_s$  denotes points on the surface  $\partial\Omega$  and  $\vec{r}$  denote points within  $\Omega$ .  $\vec{n}$  is a unit vector perpendicular to  $\partial\Omega$  that points away from  $\Omega$ .

The  $\phi_n(\vec{r})$  and  $\vec{A}_t(\vec{r})$  are completely determined from the normal and the tangential components of  $\vec{v}$  on surface  $\partial\Omega$ .

## 2 Surface integration and finite elements via AD

Since these expressions are analytic, they are expandable. The idea is now to expand them to higher orders in BOTH the surface variables  $r_s$  and the volume variables  $\vec{r}$ . The dependence on the surface variables will be integrated over surface sub-cells, which results in a highly accurate integration formula. The dependence on the volume variables will be retained, which leads to a high order finite element method. By using sufficiently high order, high accuracy can be achieved with a small number of surface elements, and, more importantly, a small number of volume elements.

Within this abstract, we forego all algebraic details, and illuminate the behavior of the method with an example.

### 2.1 An Analytical Example: the Bar Magnet

As a reference problem we consider the magnetic field of rectangular iron bars with inner surfaces ( $y = \pm y_0$ ) parallel to the mid-plane ( $y = 0$ ) as shown below. The geometry of these uniformly magnetized bars, which are assumed to be infinitely extended in the  $\pm y$ -directions, is defined by:

$$x_1 \leq x \leq x_2, \quad |y| \geq y_0, \quad z_1 \leq z \leq z_2$$

From this bar magnet one can obtain analytic solution for the magnetic field  $\vec{B}(x, y, z)$  of the form

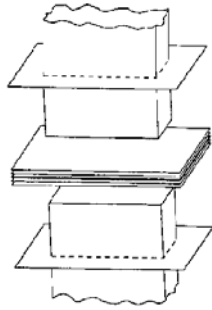
$$\begin{aligned}B_y(x, y, z) &= \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[ \arctan\left(\frac{X_i \cdot Z_j}{Y_+ \cdot R_{ij}^+}\right) + \arctan\left(\frac{X_i \cdot Z_j}{Y_- \cdot R_{ij}^-}\right) \right] \\ B_x(x, y, z) &= \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[ \ln\left(\frac{Z_j + R_{ij}^-}{Z_j + R_{ij}^+}\right) \right] \\ B_z(x, y, z) &= \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[ \ln\left(\frac{X_j + R_{ij}^-}{X_j + R_{ij}^+}\right) \right]\end{aligned}$$

where  $i, j = 1, 2$ ,

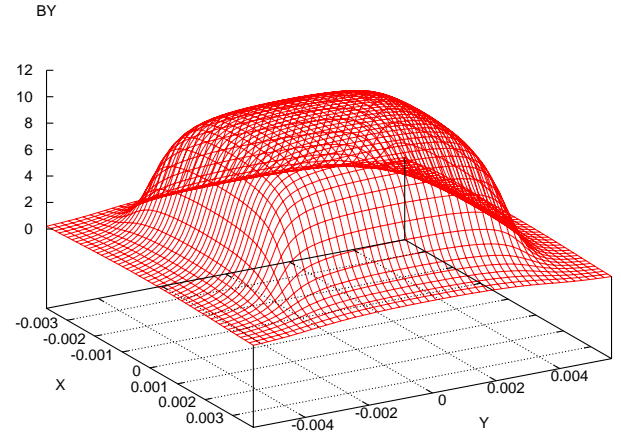
$$X_i = x - x_i, \quad Y_{\pm} = y_0 \pm y, \quad Z_i = z - z_i$$

$$\text{and } R_{\pm} = (X_i^2 + Y_j^2 + Z_{\pm}^2)^{\frac{1}{2}}$$

The mid plane field of such magnet is shown below



Bar Magnet



$B_y$  on Mid plane of Barbmagnet

## 2.2 Results and Analysis

As a first step, we study the performance of the surface integration method. To this end, the six surfaces are each subdivided into a  $44 \times 44$  mesh. On each of the mesh cells, the contribution from the Helmholtz integral is Taylor expanded, and the resulting polynomial is integrated. The following figure shows the accuracy of the predicted field, compared with the exact solution, as a function of the order of expansion within the surface mesh cells. Results are shown for the points  $(0, 0, 0)$  and  $(.1, .1, .1)$ . It can be seen that at order six, an accuracy of approximately  $10^{-13}$  is reached, which is very high compared to conventional numerical field solvers.

For the next example, we split the volume inside the bar magnet into  $5 \times 5 \times 5$  finite elements of width  $\pm 0.2$ . Within each of the elements, a Taylor expansion is carried out, resulting in a polynomial representation of the field within the cell. The polynomial representation is used to evaluate the field at 1000 randomly chosen points within the cell, and comparing the result with the analytical answer. We show the resulting RMS error for finite elements centered around  $(0, 0, 0)$  and  $(.1, .1, .1)$ . It can be seen that at order 7, an accuracy of approximately  $10^{-7}$  is reached.

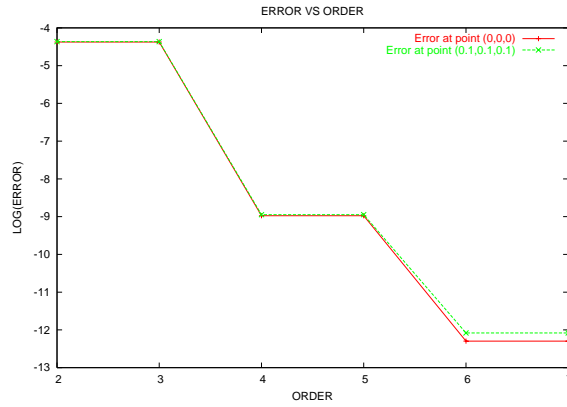


Figure 1: Error for the field calculated for the bar magnet example for individual points  $(0, 0, 0)$  and  $(.1, ., 1, .1)$

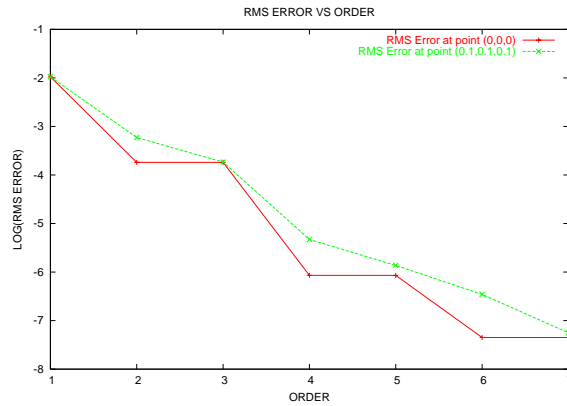


Figure 2: Average error for the field calculated for the bar magnet example for finite elements of width 0.4 around points  $(0, 0, 0)$  and  $(.1, ., 1, .1)$

We see that the method of simultaneous surface and volume expansion leads to accuracies that are significantly less than those of conventional finite element tools, even when unusually large finite elements are used.

The final paper will contain detailed comparisons to conventional finite element methods with regard to accuracy and speed.