A highly accurate high-order validated method to solve 3D Laplace equation

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Approach

We present an approach based on high-order quadrature and a high-order finite element method to find a validated solution of the Laplace equation when derivatives of the solution are specified on the boundary

$$\Delta\psi\left(\overrightarrow{r}\right) = 0 \text{ in volume } \Omega\left(\mathrm{R}^3\right)$$
$$\nabla\psi\left(\overrightarrow{r}\right) = \overrightarrow{f}\left(\overrightarrow{r}\right) \text{ on surface } \partial\Omega\left(\mathrm{R}^3\right)$$

Where do we want to use this approach?

In accelerator/spectrometer magnets where the magnet manufacturer provides only discrete field data in the volume of interest

MAGNEX: A large acceptance MAGNetic spectrometer for EXcyt beams, at the Laboratori Nazionali del Sud - Catania (Italy).

(Fringe fields, high aspect ratio, discrete data)


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What do we expect from this method/tool ?

- Provide validated local expansion of the field ($\psi\left(\overrightarrow{r}\right)$ and $\partial^n_{x_i}\psi\left(\overrightarrow{r}\right)$)
- Highly accurate (work for case with high aspect ratio)
- Computationally inexpensive
- Provide information about the field quality and if possible reduce noise in experimentally obtained field data

Note about Laplace Equation

- Existence and uniqueness of the solution for 3D case can be shown using Green's formula

- Integral kernels that provides interior fields in terms of the boundary fields or source are smoothing

  Interior fields will be analytic even if the field/source on the surface data fails to be differentiable

- Analytic closed form solution can be found for few problems with certain regular geometries where separation of variables method can be applied

Numerical methods to solve Laplace equation

- Finite Difference, Method of weighted residuals and Finite element methods
  - Numerical solution as data set in the region of interest
  - Relatively low approximation order
  - Prohibitively large number of mesh points and careful meshing required
- Boundary integral methods or Source based field models

- Field inside of a source free volume due to a real sources outside of it can be exactly replicated by a distribution of fictitious sources on its surface. Error due to discretization of the source falls off rapidly as the field point moves away from the source.
  * Image charge method
    · Choose planes/grids to place point charges (or Gaussian dist)
    · Solve a large least square fit problem to find the charges
    · Lot of guess work and computation time involved in getting the solution
  * *Methods using Helmholtz' theorem*
    · Helmholtz' theorem is used to find electric or magnetic field directly from the surface field data

- In our approach we make use of the Taylor model frame work to implement this

Helmholtz' theorem

Any vector field $\overrightarrow{B}$ that vanishes at infinity can be written as the sum of two terms, one of which is irrotational and the other, solenoidal

$$
\begin{aligned}
\overrightarrow{B}(\vec{x}) &= \vec{\nabla} \times \vec{A}_t(\vec{x}) + \vec{\nabla}\phi_n(\vec{x}) \\
\phi_n(\vec{x}) &= \frac{1}{4\pi}\int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s)\cdot\overrightarrow{B}(\vec{x}_s)}{|\vec{x}-\vec{x}_s|}ds - \frac{1}{4\pi}\int_{\Omega}\frac{\vec{\nabla}\cdot\overrightarrow{B}(\vec{x}_v)}{|\vec{x}-\vec{x}_v|}dV \\
\vec{A}_t(\vec{x}) &= -\frac{1}{4\pi}\int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s)\times\overrightarrow{B}(\vec{x}_s)}{|\vec{x}-\vec{x}_s|}ds + \frac{1}{4\pi}\int_{\Omega}\frac{\vec{\nabla}\times\overrightarrow{B}(\vec{x}_v)}{|\vec{x}-\vec{x}_v|}dV
\end{aligned}
$$

For a source free volume we have, $\vec{\nabla} \times \overrightarrow{B}\left(\vec{x}_v\right) = 0$ and $\vec{\nabla} \cdot \overrightarrow{B}\left(\vec{x}_v\right) = 0$

Volume integral terms vanish, $\phi_n\left(\vec{x}\right)$ and $\vec{A}_t\left(\vec{x}\right)$ are completely determined from the normal and the tangential magnetic field data on surface $\partial\Omega$

$$\phi_n\left(\vec{x}\right) = \frac{1}{4\pi}\int_{\partial\Omega}\frac{\vec{n}(\vec{x}_s)\cdot\overrightarrow{B}(\vec{x}_s)}{|\vec{x}-\vec{x}_s|}ds \quad \vec{A}_t\left(\vec{x}\right) = -\frac{1}{4\pi}\int_{\partial\Omega}\frac{\vec{n}(\vec{x}_s)\times\overrightarrow{B}(\vec{x}_s)}{|\vec{x}-\vec{x}_s|}ds$$

$\vec{B}$ is Electric or Magnetic field
$\partial\Omega$ is a surface which bounds volume Ω
$\vec{x}_s$ and $\vec{x}_v$ denote points on $\partial\Omega$ and within Ω
$\vec{\nabla}$ denote the gradient with respect to $\vec{x}_v$
$\vec{n}$ is a unit normal vector pointing away from $\partial\Omega$

Implementation using Taylor Models

- Split domain of integration $\partial\Omega$ in to smaller regions Γ_i

- Expand them to higher orders in surface variables $\vec{r}_s$ and the volume variables $\vec{r}$
  - Expanded in $\vec{r}_s$ about the center of each surface element
  - Expanded in $\vec{r}$ about the center of each volume element
  - Field is chosen to be constant over each surface element

$$\int_{x_0}^{x_{N_x}} \int_{y_0}^{y_{N_y}} g(x,y)\, dx dy = \sum_{i_x=0, i_y=0, k_x=0, k_y=0}^{i_x=N_x-1, i_y=N_y-1, k_x=\infty, k_y=\infty} \frac{h_x^{2k_x+1}}{(2k_x+1)! \cdot 2^{2k_x}} \frac{h_y^{2k_y+1}}{(2k_y+1)! \cdot 2^{2k_y}} g^{2k_x, 2k_y} \left(\frac{x_{i_x+1} + x_{i_x}}{2}, \frac{y_{i_y+1} + y_{i_y}}{2} \right)$$

We can obtain:

Scalar potential $\phi_n(\vec{r})$ if we choose $g(x,y) = \vec{n}_s \cdot \frac{\vec{f}(\vec{r}_s)}{|\vec{r}-\vec{r}_s|}$

Vector potential $\vec{A}_t(\vec{r})$ if we choose $g(x,y) = \vec{n}_s \times \frac{\vec{f}(\vec{r}_s)}{|\vec{r}-\vec{r}_s|}$

- – Benefits

    * The dependence on the surface variables are integrated over surface sub-cells Γ_i, which results in a highly accurate integration formula

    * The dependence on the volume variables are 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

- Depending on the accuracy of the computation needed, we choose step sizes, order of expansion in $r\left(x,y,z\right)$ and order of expansion in $r_S\left(x_S,y_S,z_S\right)$

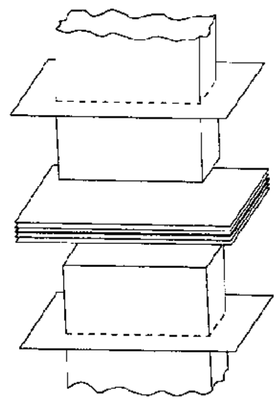
Validated Integration in COSY

$$\int_{x_{il}}^{x_{iu}} f(\vec{x})\, dx_i \in \left(P_{n,\partial^{-1}f}\left(\vec{x}|_{x_i = x_{iu} - x_{i0}} \right) - P_{n,\partial^{-1}f}\left(\vec{x}|_{x_i = x_{il} - x_{i0}} \right), I_{n,\partial^{-1}f} \right)$$

This method has following advantages:

* No need to derive quadrature formulas with weights, support points x_i, and an explicit error formula
* High order can be employed directly by just increasing the order of the Taylor model limited only by the computational resources
* Rather large dimensions are amenable by just increasing the dimensionality of the Taylor models, limited only by computational resources

An Analytical Example: the Bar Magnet



$$x_1 \le x \le x_2, \qquad |y| \ge y_0, \qquad z_1 \le z \le z_2$$

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 ($y = 0$)

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

$$B_y(x,y,z) = \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[\text{arctan}\left(\frac{X_i \cdot Z_j}{Y_+ \cdot R_{ij}^+} \right) + \text{arctan}\left(\frac{X_i \cdot Z_j}{Y_- \cdot R_{ij}^-} \right) \right]$$

$$B_x(x,y,z) = \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[\text{ln}\left(\frac{Z_j + R_{ij}^-}{Z_j + R_{ij}^+} \right) \right]$$

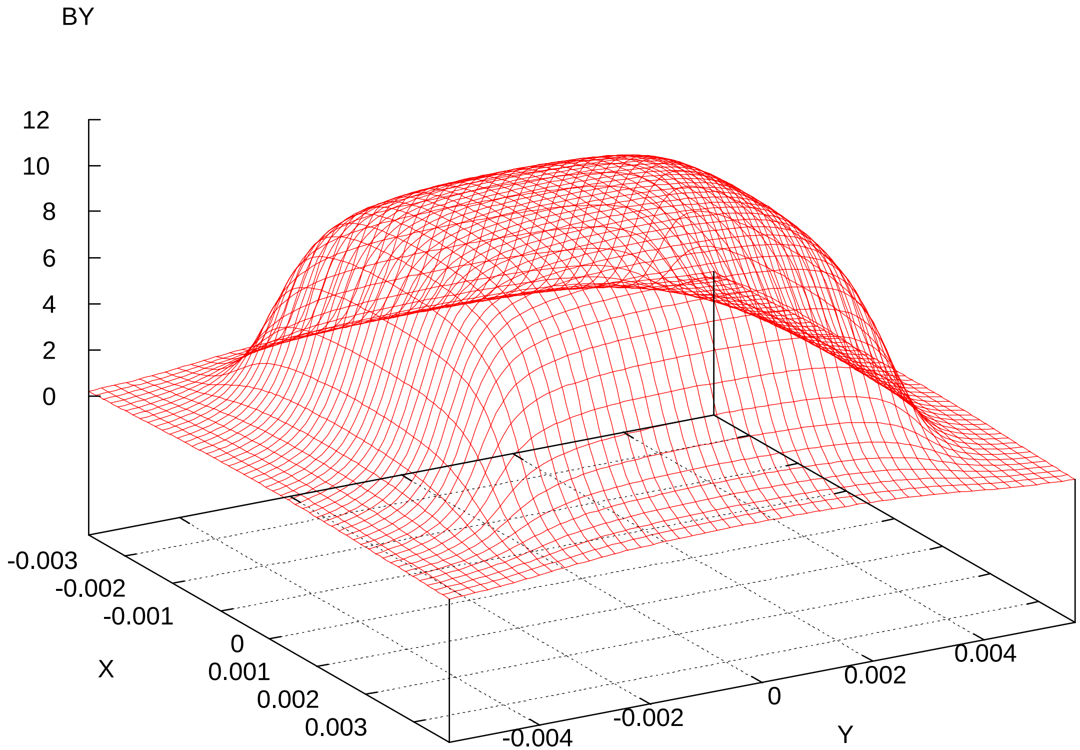
$$B_z(x,y,z) = \frac{B_0}{4\pi} \sum_{i,j} (-1)^{i+j} \left[\text{ln}\left(\frac{X_j + R_{ij}^-}{X_j + R_{ij}^+} \right) \right]$$

where $i, j = 1, 2$,

$$X_i = x - x_i, \qquad Y_\pm = y_0 \pm y, \qquad Z_i = z - z_i$$

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

We note that only even order terms exist in the Taylor expansion of this field about the origin.



B_y component of the field on the mid-plane.

Results

1. To study the dependency of the Interval part of the potentials and $\vec{B}$ field on the surface element length

   - All of the volume is considered as just one volume element

   - Examine contributions of each surface element towards the total integral

     - Expansion is done at $\vec{r} = (.1, .1, .1)$ and

     - Plot of interval width VS surface element length for scalar potential

     - Plot of interval width VS surface element length for vector potential (x component)

- Plot of interval width VS Order for different surface element length for x component of Magnetic field

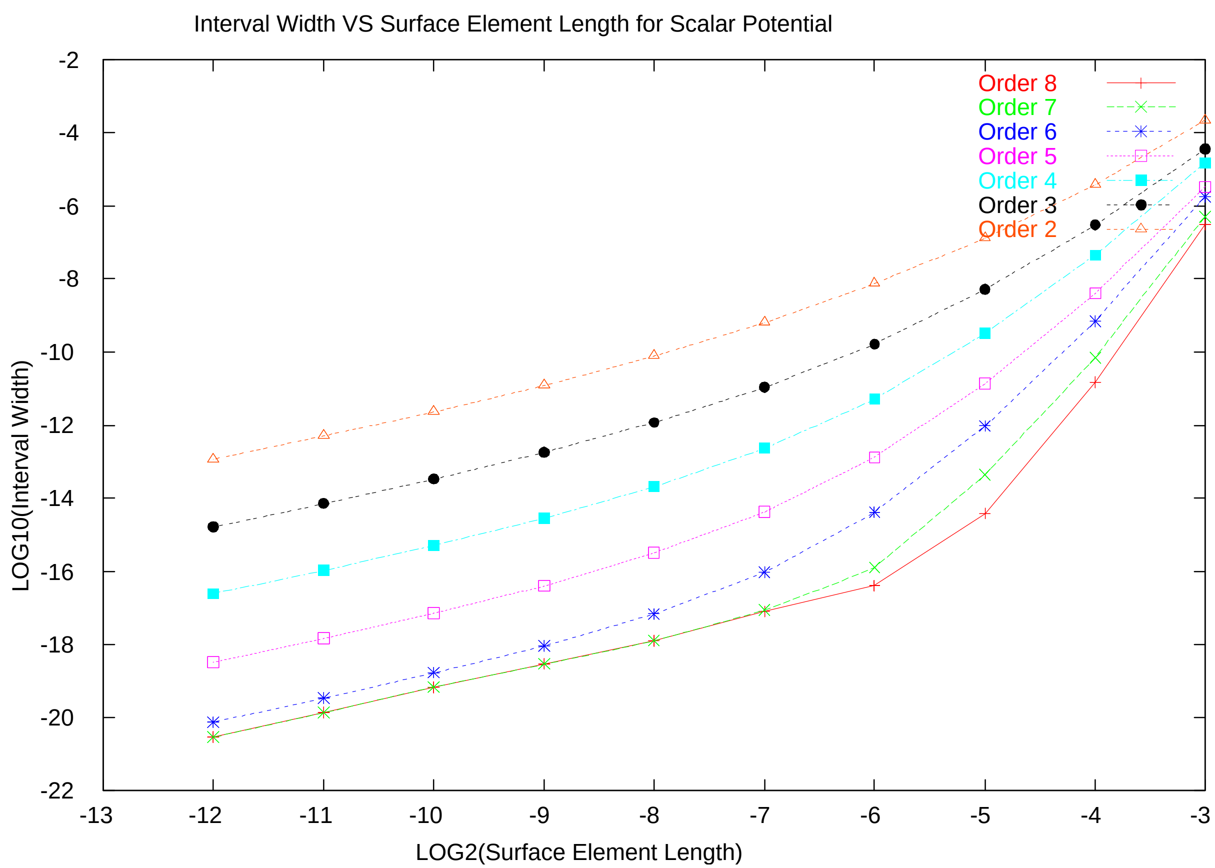


Figure 1: Integration over single surface element (for ϕ)

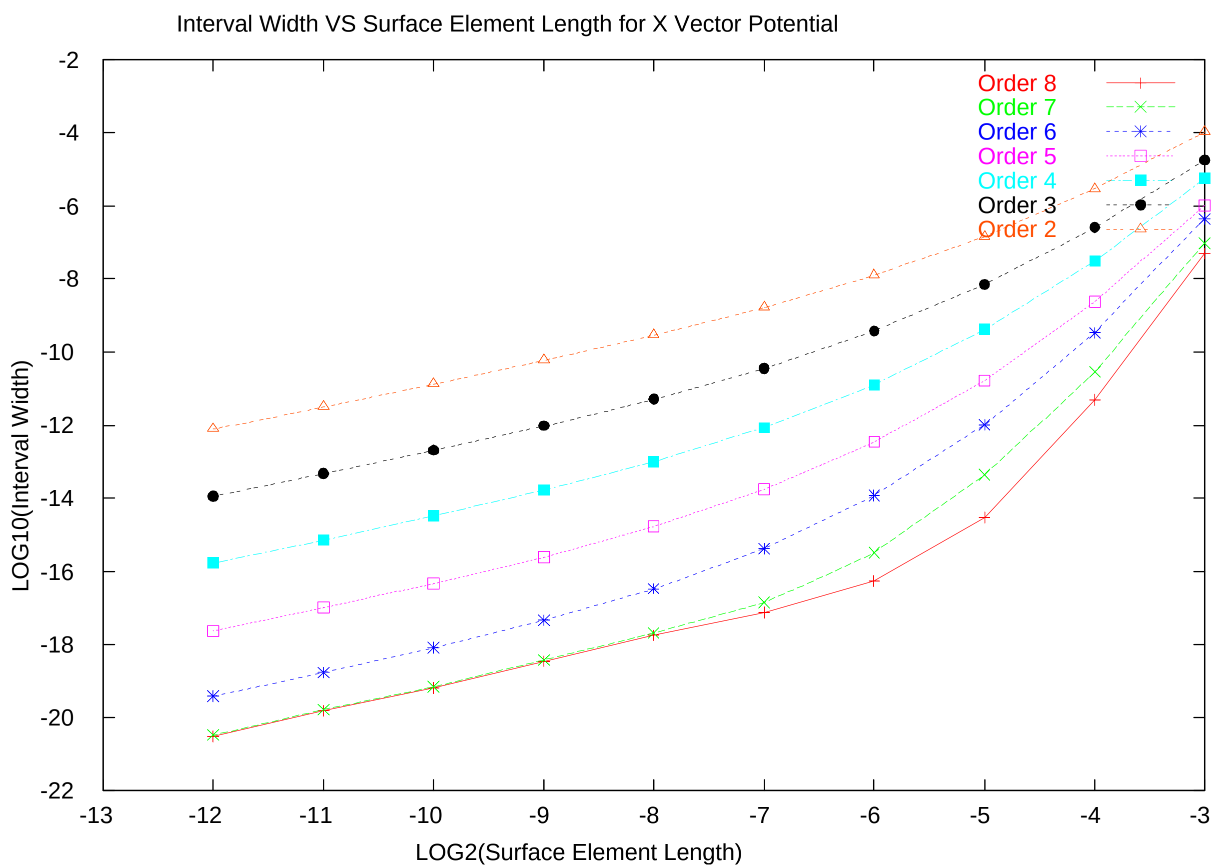


Figure 2: Integration over single surface element (for A_x)

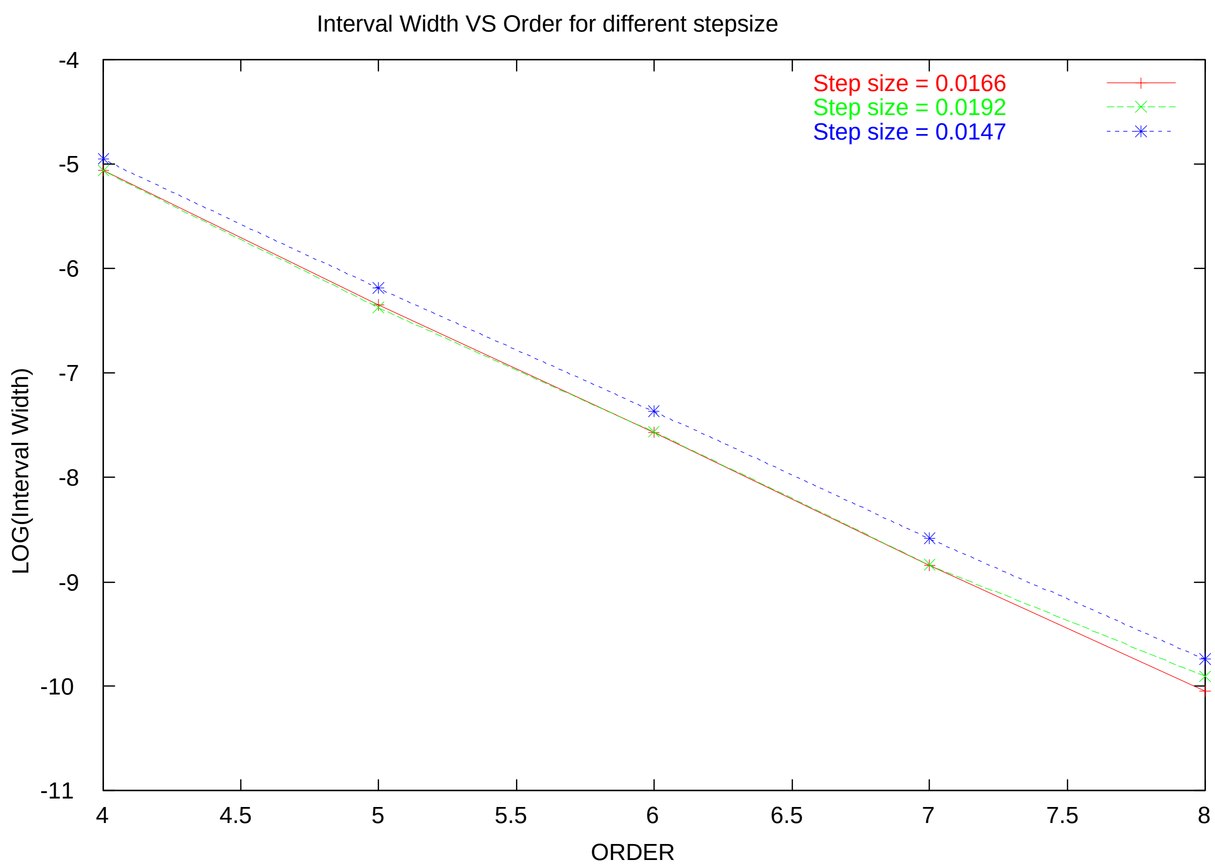


Figure 3: Interval width VS Order (for different step size)

2 Study the dependency of the Polynomial part and Interval part of the B field on the volume element length

- The surface element length is locked at $1/128$

- Plot of the error calculated for the polynomial part VS the volume element length

- Plot of interval width VS volume element length for y component of Magnetic field

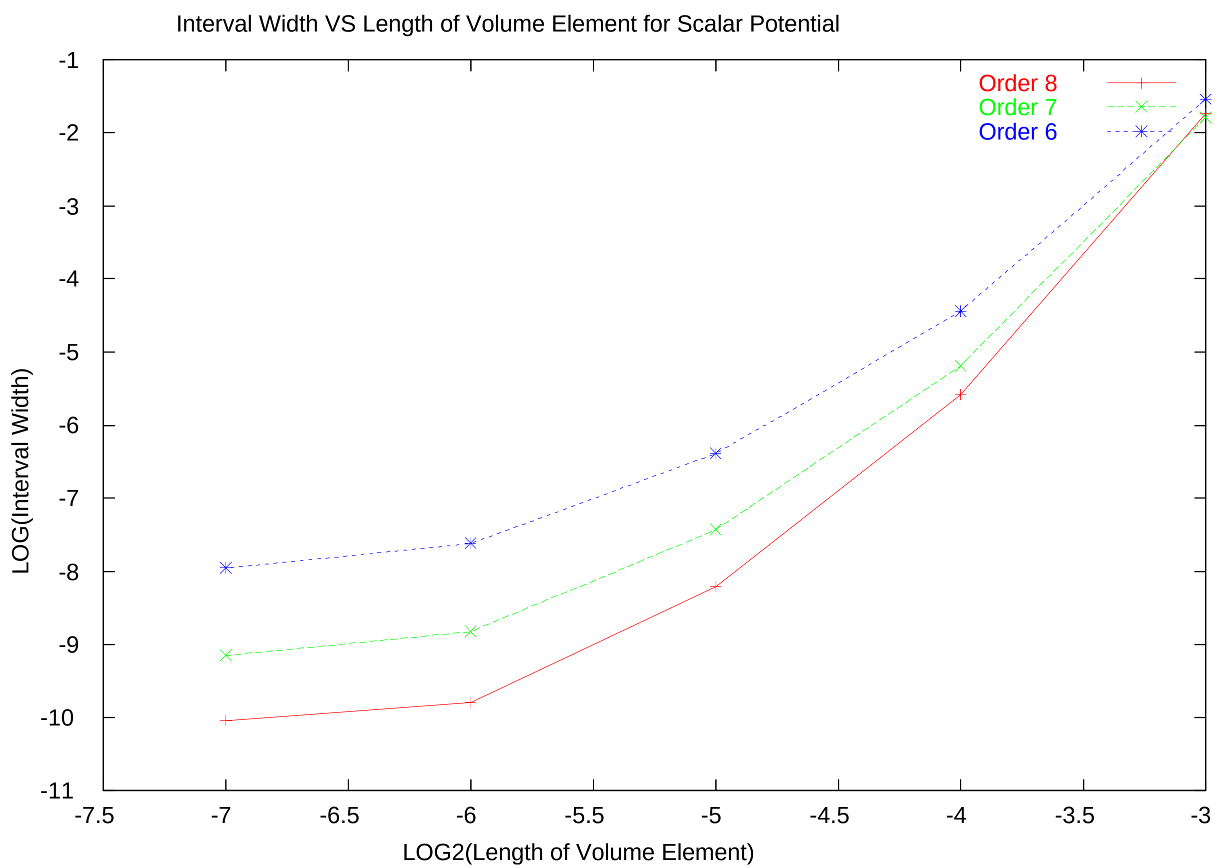


Figure 4: Interval width VS Volume element length (for ϕ)

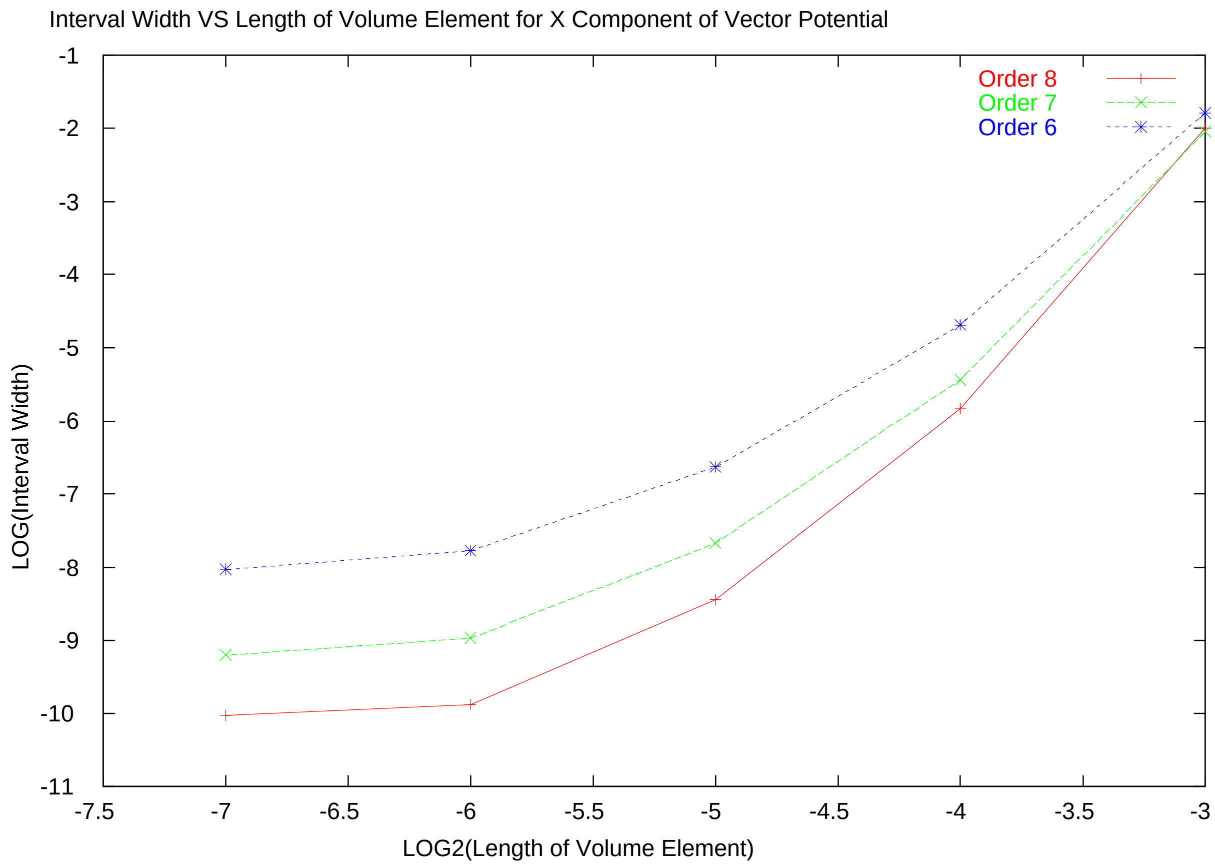


Figure 5: Interval width VS Volume element length (for A_x)

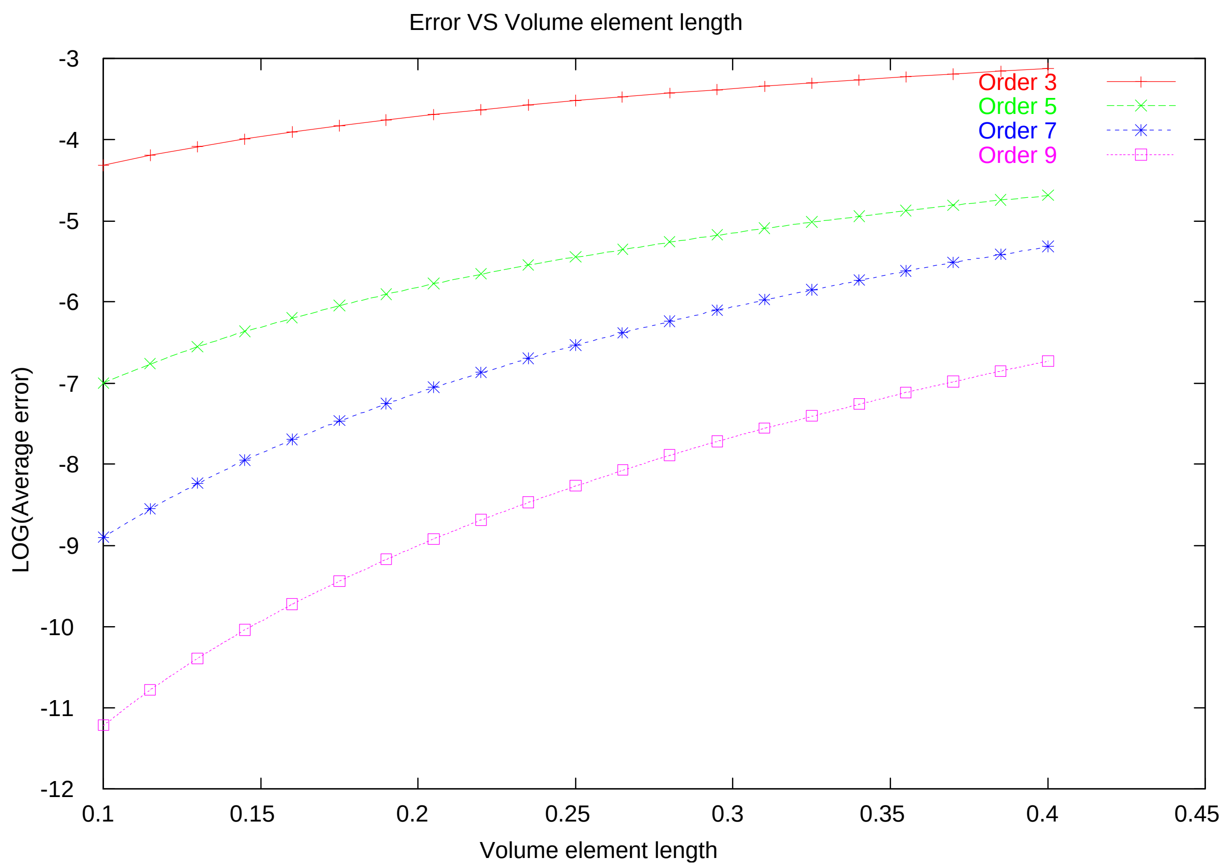


Figure 6: Error VS Volume element length for polynomial part (for B_y)

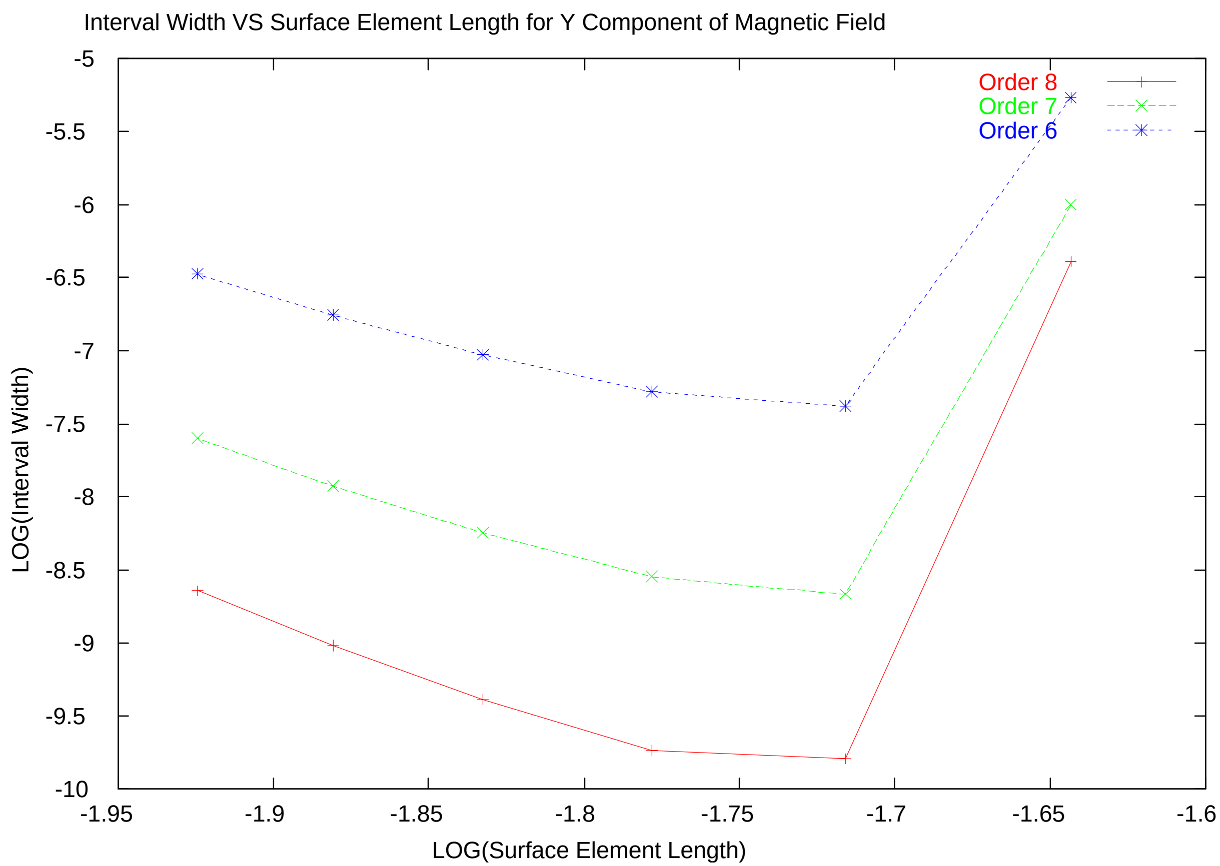


Figure 7: Interval width VS Volume element length for B_y

Summary

- Helmholtz' theorem implemented using the Taylor Model tools provide a promising approach to find local expansion of the field in the volume of interest

- Accuracy achieved is very high compared to conventional numerical field solvers

- Provides a good way to check the field quality

- This method can be extended for PDE's