

A Highly Accurate High-Order Verified Method to Solve the 3D Poisson Equation

S.L. Manikonda, M. Berz, K. Makino

Argonne National Laboratory
Michigan State University

Definition (Taylor Model)

Let $f : D \subset \mathbb{R}^v \longrightarrow \mathbb{R}$ be a function that is $(n + 1)$ times continuously partially differentiable on an open set containing the domain D . Let x_0 be a point in D and P the n -th order Taylor polynomial of f around x_0 . Let I be an interval such that

$$f(x) \in P(x - x_0) + I \text{ for all } x \in D.$$

Then the pair (P, I) is called an n -th order Taylor model of f around x_0 on D .

Definition

For an n -th order Taylor model $T = (P, I)$ and $k = 1, \dots, v$, let

$$Q_k = \int_0^{x_k} P_{(n-1)}(x_1, \dots, x_{k-1}, \xi_k, x_{k+1}, \dots, x_v) d\xi_k.$$

The antiderivative ∂_k^{-1} of T is defined by

$$\partial_k^{-1}(P, I) = \left(Q_k, \left(B \left(P_{(n)} - P_{(n-1)} \right) + I \right) \cdot 2 \right).$$

- D is $[-1, 1]^v \subset \mathbb{R}^v$.

The Taylor Model integration

Finite integration of a Taylor model,

$$J^{(v-1)} = \int_{-1}^1 T^v(x_1, \dots, x_{k-1}, \xi_k, x_{k+1}, \dots, x_v) d\xi_k,$$

Steps to compute the Taylor model $J^{(v-1)}$ using the antiderivative $\partial_{\xi_1}^{-1}$ operator.

- 1 Split the Taylor Model $T^v = (P, I)$ into a polynomial P of order n and interval I .
- 2 Construct a new Taylor model $G^v = (P, I_\epsilon)$, where $I_\epsilon = [0, 0]$.
- 3 Apply the antiderivative operator $\partial_{\xi_1}^{-1}$ to the Taylor model G^v .
- 4 Evaluate the Taylor models $\partial_{\xi_1}^{-1} G^v$ (at $\xi_1 = 1$) and $\partial_{\xi_1}^{-1} G^v$ (at $\xi_1 = -1$) and subtract them to obtain a new Taylor model R^{v-1} .
- 5 Add the interval $2 \cdot I$ to the Taylor model R^{v-1} to give the Taylor model after integration with respect to the ξ_1 variable.

The steps 1 through 5 can be repeated for the integration in more than one variable.

The Poisson Problem

Goal: Determine an accurate solution of the Poisson equation when derivatives of the solution are specified on the boundary

$$\begin{aligned}\nabla^2 \phi'(\vec{r}) &= \rho(\vec{r}) \text{ in the bounded volume } \Omega \subset \mathbb{E}^3 \\ \nabla \phi'(\vec{r}) &= \vec{g}(\vec{r}) \text{ on the surface } \partial\Omega\end{aligned}$$

- Motivation: Modelling space charge effects in Accelerators, Extraction of transfer maps

Splitting the problem

$$\phi'(\vec{r}) = \phi(\vec{r}) + \psi(\vec{r})$$

- The potential $\psi(\vec{r})$ satisfies the Poisson equation

$$\nabla^2 \psi(\vec{r}) = \rho(\vec{r}) \text{ in the bounded volume } \Omega \subset \mathbb{E}^3$$

- The potential $\phi(\vec{r})$ is the solution to the Laplace equation

$$\begin{aligned}\nabla^2 \phi(\vec{r}) &= 0 \text{ in the bounded volume } \Omega \subset \mathbb{E}^3 \\ \nabla \phi(\vec{r}) &= \vec{g}(\vec{r}) - \nabla \psi(\vec{r}) \text{ on the surface } \partial\Omega\end{aligned}$$

- The solution for ψ can be found using

$$\psi(\vec{r}) = \int_V \frac{1}{4\pi\epsilon_0} \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\Omega',$$

- Hence the Poisson BVP translates to solving the Laplace BVP
- The above splitting is good for electrostatic problems. However, similar treatment can be done for magnetostatic problems (the potential satisfies Ampere's equation). The method developed hold for both the electrostatic and magnetostatic case.

The Laplace BVP

$$\begin{aligned}\nabla^2 \phi(\vec{r}) &= 0 \text{ in the bounded volume } \Omega \subset \mathbb{E}^3 \\ \nabla \phi(\vec{r}) &= \vec{g}(\vec{r}) \text{ on the surface } \partial\Omega\end{aligned}$$

Goal:

- Provide solution as local expansion of the field ($\phi(\vec{r})$ and $\partial_{x_i}^n \phi(\vec{r})$)
- Highly accurate and work for case with large variation of field in the region of interest
- Computationally inexpensive
- Provide information about the field quality of measured data

Analytic closed form solution can only be found for few problems with certain regular geometries (separation of variables method, power series, finite Fourier transform)

- Finite Difference, Finite element methods
 - Numerical solution as data set in the region of interest
 - Relatively low approximation order
 - Often large number of mesh points and careful meshing required
 - Usually multipole expansion of the field can not be computed
- Methods using surface data
 - Boundary integral methods and source-based field models
 - Require knowledge of Green's function for the problem
 - 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.
 - Methods using the **Helmholtz theorem**

The Helmholtz Theorem

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

$$\vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}_t(\vec{x}) + \vec{\nabla} \phi_n(\vec{x}) \text{ where}$$

$$\phi_n(\vec{x}) = \frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s) \cdot \vec{B}(\vec{x}_s)}{|\vec{x} - \vec{x}_s|} ds - \frac{1}{4\pi} \int_{\Omega} \frac{\vec{\nabla} \cdot \vec{B}(\vec{x}_v)}{|\vec{x} - \vec{x}_v|} dV$$

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

$\partial\Omega$ is a surface which bounds the volume Ω

\vec{x}_s and \vec{x}_v denote points on $\partial\Omega$ and within Ω

$\vec{\nabla}$ denotes the gradient with respect to \vec{x}_v

\vec{n} is a unit normal vector pointing away from $\partial\Omega$

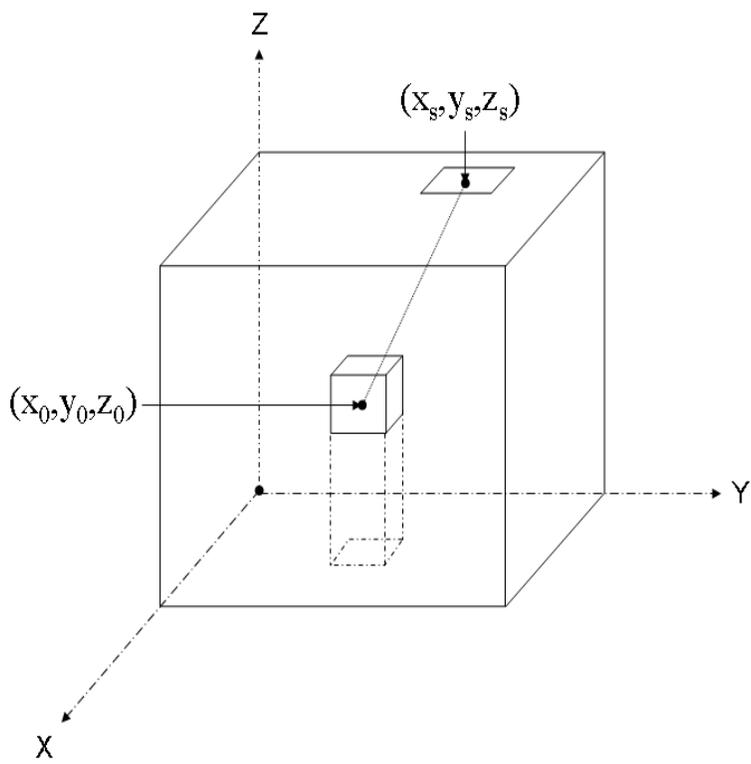
- If \vec{B} is the magnetic/electric field in the source free region, we have $\vec{\nabla} \times \vec{B}(\vec{x}_v) = 0$ and $\vec{\nabla} \cdot \vec{B}(\vec{x}_v) = 0$, and the volume integral terms vanish
- $\phi_n(\vec{x})$ and $\vec{A}_t(\vec{x})$ are completely determined from the normal and the tangential field data on surface $\partial\Omega$ via

$$\phi_n(\vec{x}) = \frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s) \cdot \vec{B}(\vec{x}_s)}{|\vec{x} - \vec{x}_s|} ds$$

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

$$\vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}_t(\vec{x}) + \vec{\nabla} \phi_n(\vec{x})$$

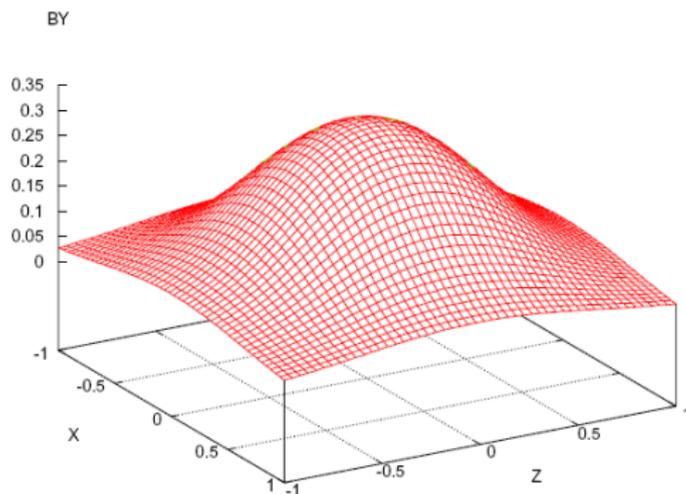
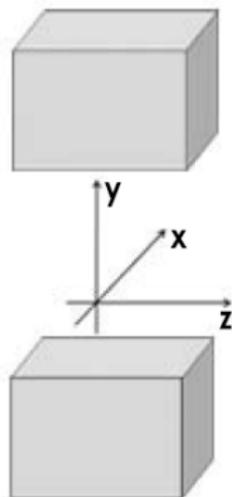
- The Helmholtz theorem can be used to find field directly from the surface field data
- Integral kernels that provides interior fields in terms of the boundary fields or source are smoothing
- Since the expressions are analytic, they can be expanded at least locally



Implementation

- 1 Discretize the surface $\partial\Omega$ into individual surface cells S_i with centers s_i and the volume Ω into volume cells V_j with centers v_j .
- 2 Pick a volume cell V_j .
- 3 For each surface cell S_i , evaluate the kernels for ϕ_n and A_t using Taylor model arithmetic to obtain a Taylor model representations in BOTH the surface variables of S_i AND the volume variables of V_j , i.e. in a total of five variables.
- 4 Use the Taylor model anti-derivation operation twice to perform integration over the surface variables of each cell S_i .
 - The dependence on the surface variables (x_s, y_s) are integrated over surface sub-cells Γ_i , which results in a highly accurate integration formula
 - The dependence on the volume variables (x, y, z) 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
- 5 Add up all results to obtain a three dimensional Taylor model enclosing the field \vec{B} over the volume cell V_j .

Analytic example: Bar magnet



- Interior of the magnet: $-0.5 \leq x \leq 0.5$, $|y| \leq 0.5$, and $-0.5 \leq z \leq 0.5$
- Analytic solution for the magnetic field are know

Analytic solution

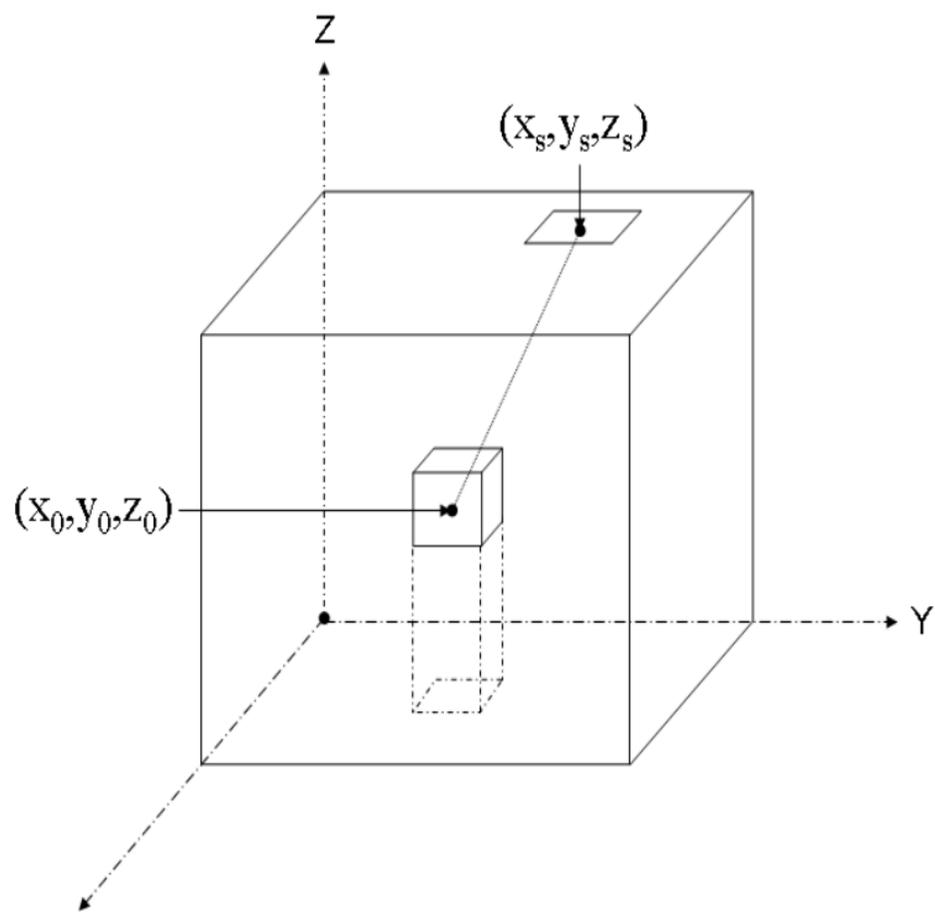
$$B_y(x, y, z) = \frac{B_0}{4\pi} \sum_{i,j=1}^2 (-1)^{i+j} \left[\arctan \left(\frac{X_i \cdot Z_j}{Y_+ \cdot R_{ij}^+} \right) + \arctan \left(\frac{X_i \cdot Z_j}{Y_- \cdot R_{ij}^-} \right) \right]$$

$$B_x(x, y, z) = \frac{B_0}{4\pi} \sum_{i,j=1}^2 (-1)^{i+j} \left[\ln \left(\frac{Z_j + R_{ij}^-}{Z_j + R_{ij}^+} \right) \right]$$

$$B_z(x, y, z) = \frac{B_0}{4\pi} \sum_{i,j=1}^2 (-1)^{i+j} \left[\ln \left(\frac{X_j + R_{ij}^-}{X_j + R_{ij}^+} \right) \right]$$

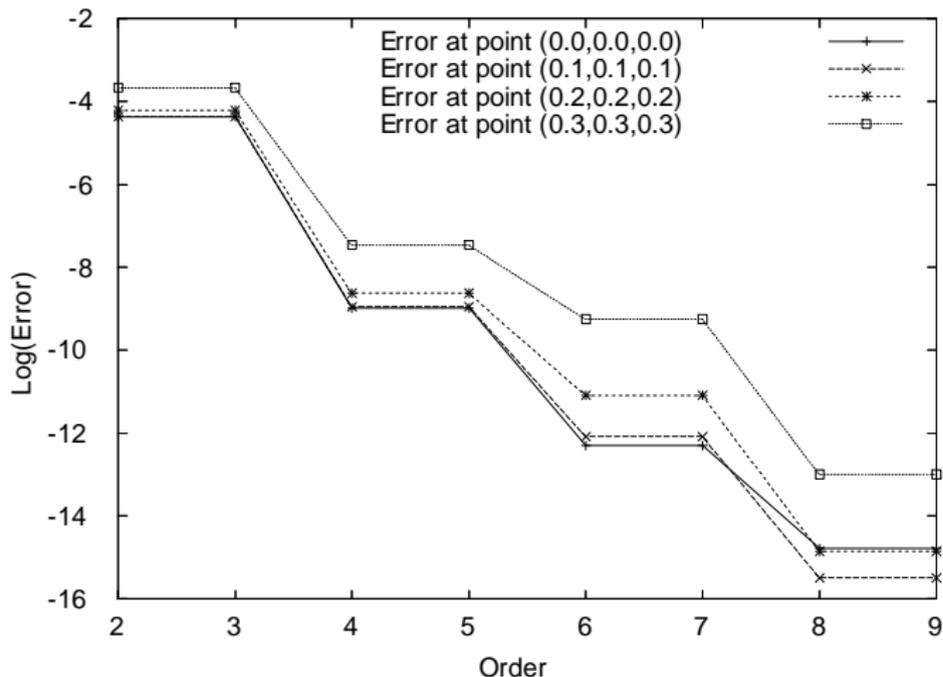
where $X_i = x - x_i$, $Y_{\pm} = y_0 \pm y$, $Z_i = z - z_i$, and $R_{ij}^{\pm} = \left(X_i^2 + Y_{\pm}^2 + Z_{\pm}^2 \right)^{\frac{1}{2}}$

- Using the analytic formulas we specify magnetic field on the surface enclosing the volume of interest
- We use the Helmholtz method to compute the field inside
- We compare the results with the analytic formulas (three plots)

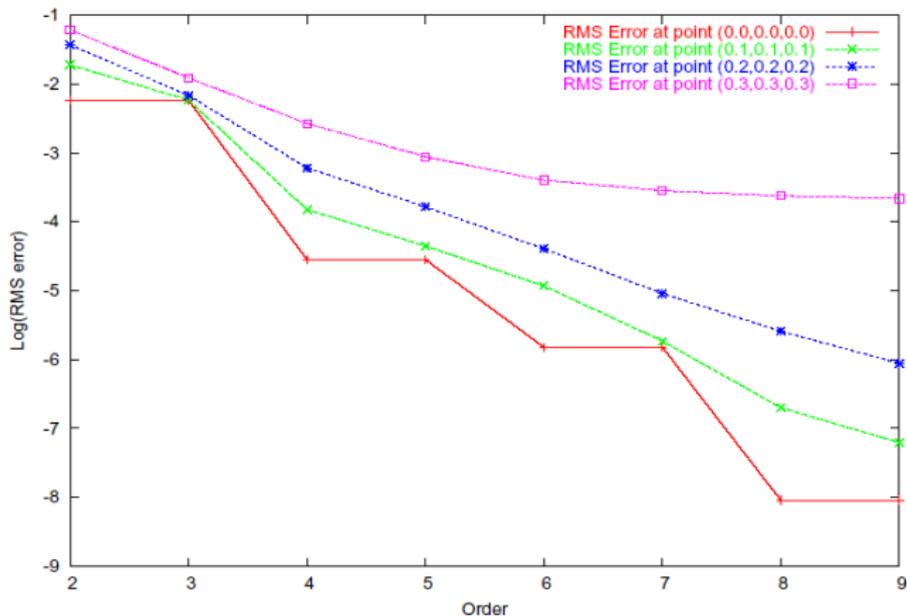


Performance of surface integration method

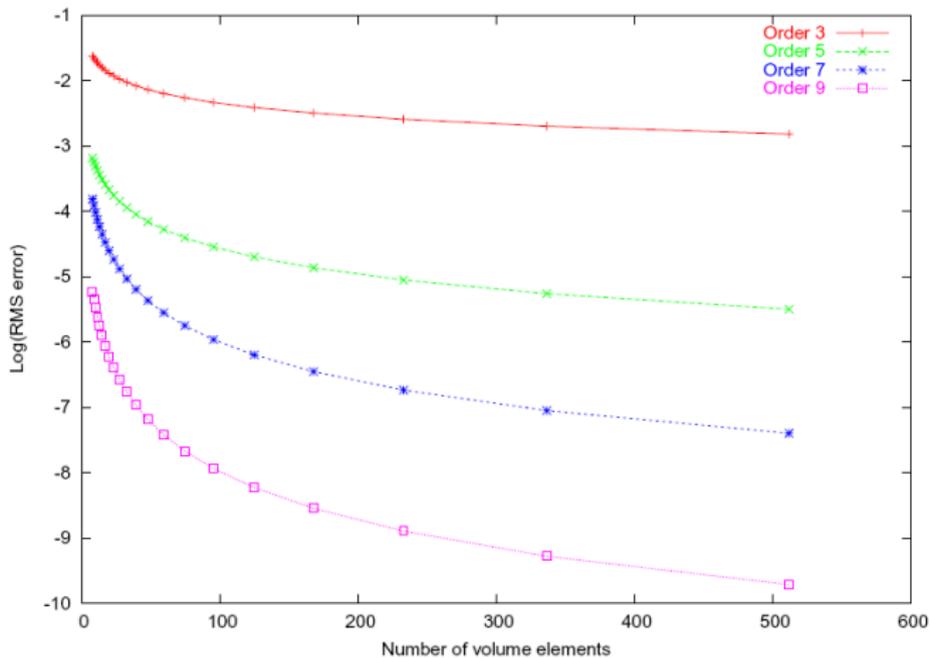
- Choose a cube of edge length 0.8 centered at origin
- each face is covered by 44×44 mesh (surface elements)
- Field data is specified on the surface mesh using analytic formulas



- Split the cube into $4 \times 4 \times 4$ volume elements of width 0.2
- Express magnetic field in each volume element by a local expansion about the center of the element
- The RMS average error for 1000 points



Dependency of the average error on the number of volume element.



Parallel implementation

- Contribution due to each surface element is independent of the other surface elements
- The large summation over all the surface elements can be parallelized
- NERSC (National Energy Research Scientific Computing Center) IBM RS6000 Seaborg Cluster consisting of 6080 processors
 - 380 computing nodes with each node having 16 processors (shared memory pool of 16 to 64 GBytes)
 - Communication between the processors within a node is much faster
- Implementation
 - $(NPR \text{ processors}) = (N2 \text{ groups}) \times (N1 \text{ processors})$
 - $N1 = INT \left(2 \cdot \sqrt{NPR} \right)$
 - Two parallel loop are used to make the summation efficient and also minimizes cross-communication

```

{Loop over N2 groups}
PLOOP JJ 1 N2;

    {Loop over N1 processors}
    PLOOP II 1 N1;

        {Evaluate the processor number PP}
        PP:=II+(JJ-1)*N1;

        [Code to identify the surface elements JBEG through JEND
        for which the processor PP will evaluate the partial sum]

        {Loop to compute the partial sum of the scalar and vector potential
        contributions over surface elements JBEG through JEND}
        LOOP IL JBEG JEND;
            :
            [Code to compute the scalar and the vector potential
            contribution of a surface element IL.]
            :
        ENDLOOP;

        {End the parallel loop over the group of N1 processors and
        send the results to sub-master processor using communication mode 4}
        ENDPLOOP 4 PN1 _SCLPOT PN1 _VECPOT;

        {Loop to evaluate group partial sum of N1 processors}
        LOOP II 1 N1;
            :
            [Summation to get group partial sum GN2_SCLPOT and GN2_VECPOT]
            :
        ENDLOOP;

        {End the parallel loop over the N2 groups and send the results to master processor}
        ENDPLOOP 4 GN2 _SCLPOT GN2 _VECPOT;

        {Loop to evaluate sum over N2 groups}
        LOOP JJ 1 N2;
            :
            [Summation to get sum SCLPOT and VECPOT]
            :
        ENDLOOP;

        [Code to evaluate the divergence of SCLPOT and the curl of VECPOT and sum them
        to get the magnetic field]

```

Table 3.3.1. The code for the parallel algorithm.

- 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 Order for different surface element length for x component of Magnetic field
- 2 Study the dependency of the Interval part of the B field on the volume element length
 - The surface element length is locked at 1/128
 - Plot of interval width VS volume element length for y component of Magnetic field

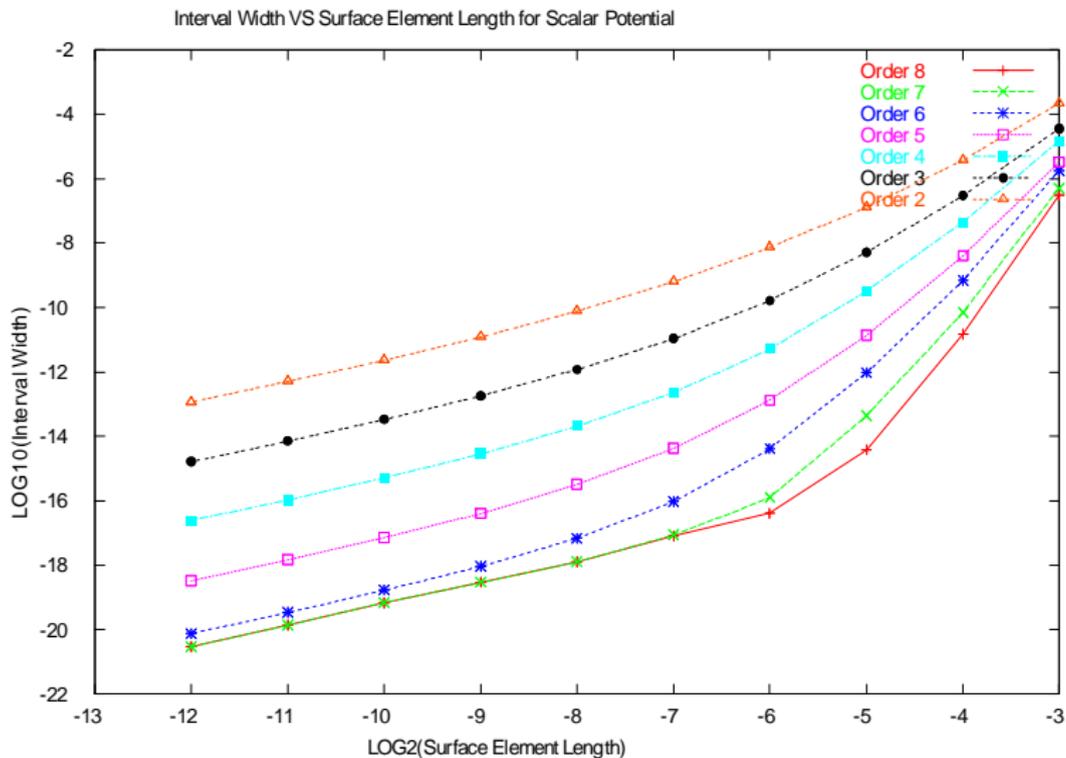


Figure: Integration over single surface element (for ϕ)

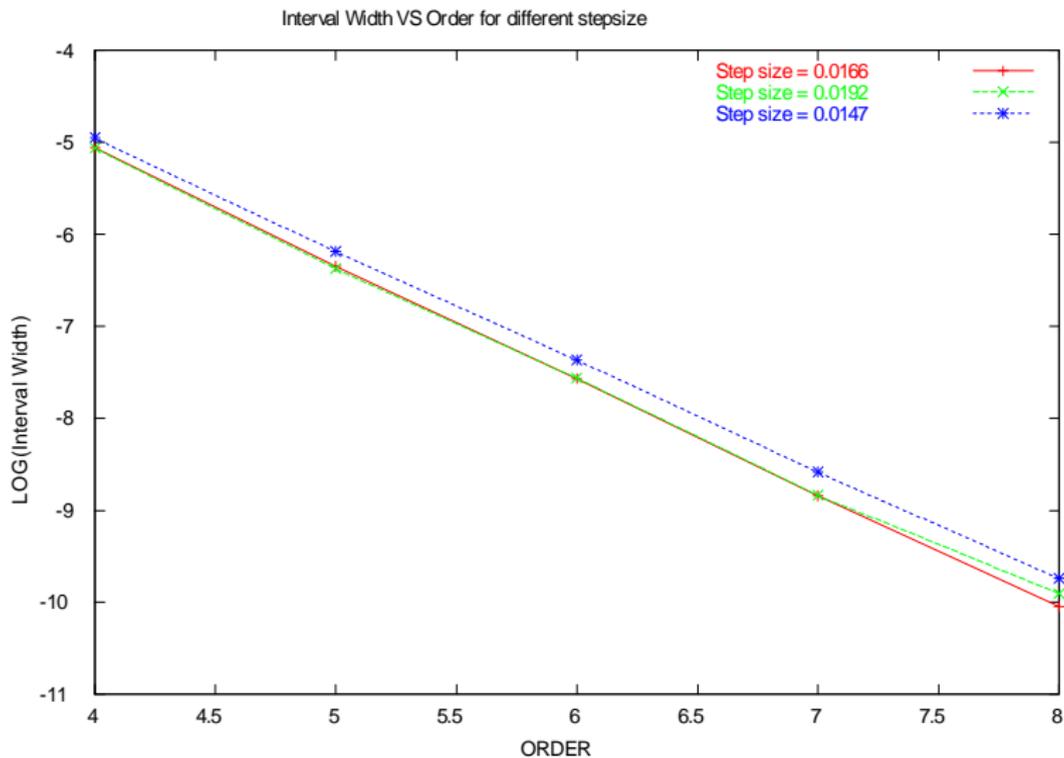


Figure: Interval width VS Order (for different step size)

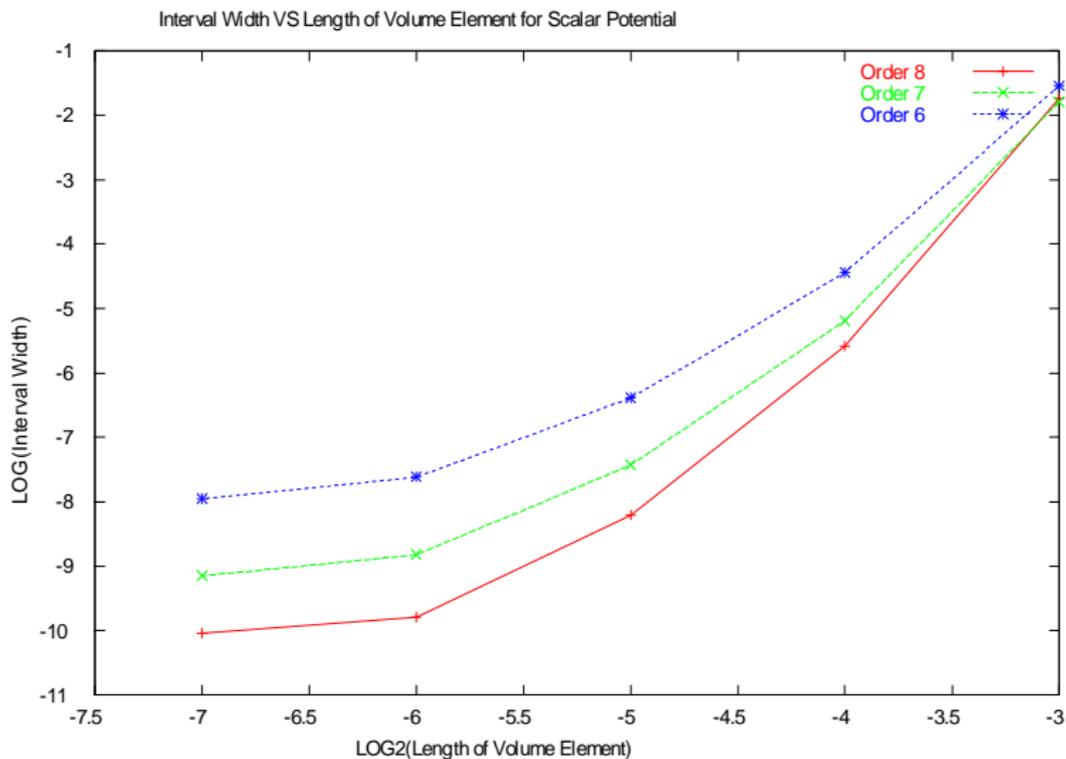


Figure: Interval width VS Volume element length (for ϕ)

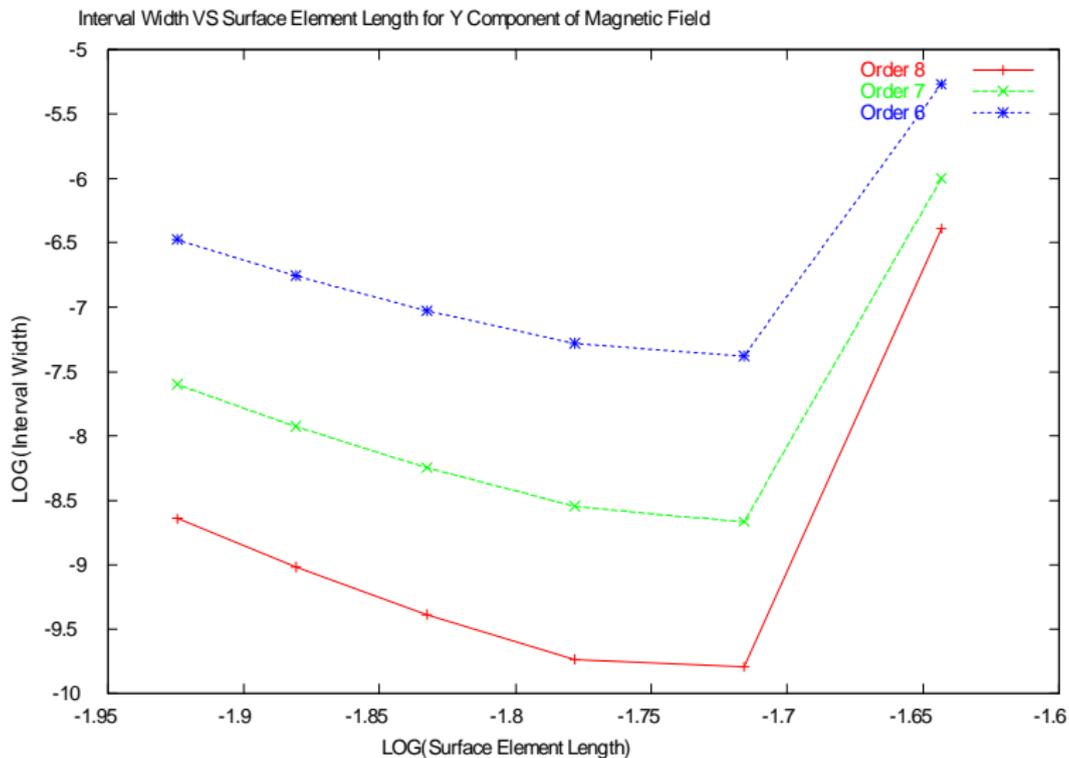


Figure: Interval width VS Volume element length for B_y

$$\psi(\vec{r}) = \int_V \frac{1}{4\pi\epsilon_0} \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\Omega',$$

2D Example: Elliptic beam with constant charge density:

$$E(x) = \frac{4\lambda}{a^2 - b^2} \left[\bar{z} - \left(\bar{z}^2 - a^2 + b^2 \right)^{1/2} \right] \quad \text{outside}$$

$$= \frac{4\lambda}{a^2 - b^2} \left(\frac{bx}{a} + i \frac{ay}{b} \right) \quad \text{inside}$$

For point (2, -1) where the field is $E_x=0.804087298$,

I	COEFFICIENT	ORDER	EXPONENTS
1	0.8040872977134209	0	0 0 0 0 0 0
2	-.2016096082544022	1	1 0 0 0 0 0
3	-.3947986319240676	1	0 1 0 0 0 0
4	-.3639403897170208E-01	2	2 0 0 0 0 0
5	0.4323711148810844	2	1 1 0 0 0 0
6	0.3639403897170199E-01	2	0 2 0 0 0 0
7	0.8519948776613888E-01	3	3 0 0 0 0 0
8	-.2193724610529883	3	2 1 0 0 0 0
9	-.2555984632984171	3	1 2 0 0 0 0
10	0.7312415368432942E-01	3	0 3 0 0 0 0
11	-.5968849793167204E-01	4	4 0 0 0 0 0
12	-.7794142886791706E-02	4	3 1 0 0 0 0
13	0.3581309875900321	4	2 2 0 0 0 0
14	0.7794142886791850E-02	4	1 3 0 0 0 0