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Using differential algebra techniques for electromagnetic field simulations

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Overview

- Background
- Transfer Maps
 - Maps for known fields
 - Maps from measured fields
- New map extraction techniques
 - Laplace solver
 - Field from current sources
- Applications
- Conclusion and future outlook

Description of a Beam

- An ensemble of particles with similar phase space coordinates is called a beam
- The position and momenta are usually sufficient to describe the motion (spin and charge)
- We can choose a reference particle for which the motion is known (reference curve or design orbit)
- We can uniquely define a coordinate system attached to the reference particle
- Motion of a particle = *Motion of the reference particle* + *Motion in relative coordinates*
- The arc length S along the reference orbit is used as the independent variable

Motion of Reference Particle

$$\chi_{m0} = \frac{p_0}{ze} \quad \text{Magnetic rigidity}$$

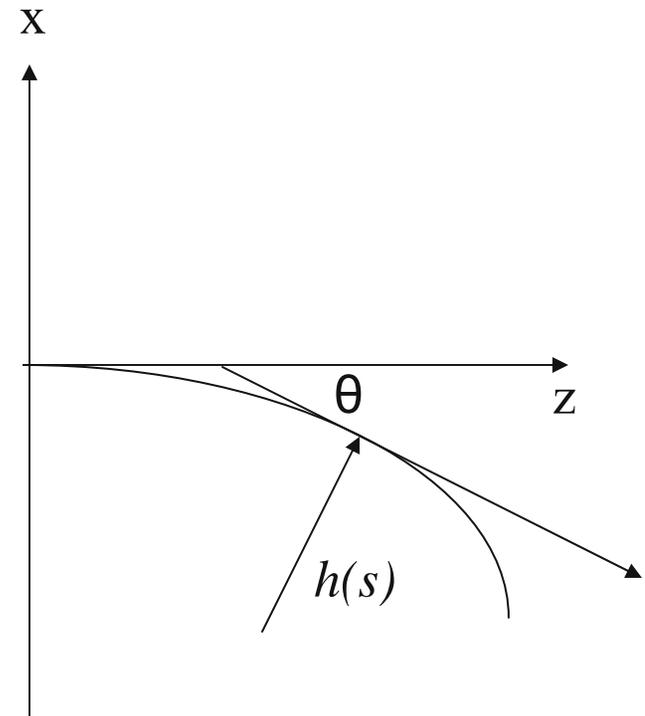
$$\chi_{e0} = \frac{p_0 v_0}{ze} \quad \text{Electric rigidity}$$

ODE's for reference particle

$$\frac{dX}{ds} = -\sin(\theta)$$

$$\frac{dZ}{ds} = \cos(\theta)$$

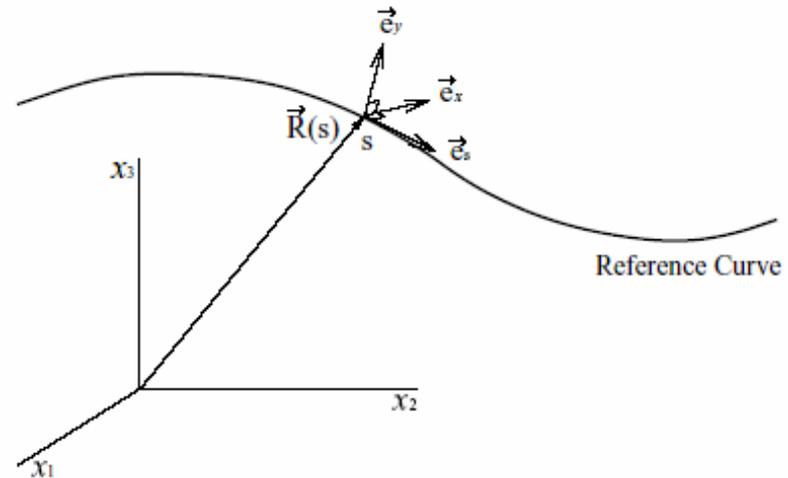
$$\frac{d\theta}{ds} = h(s) = \frac{B_Y}{\chi_{m0}} - \frac{(E_X \sin(\theta) + E_Z \cos(\theta))}{\chi_{e0}}$$



- Motion of the reference particle is restricted to a plane
- \mathbf{p}_0 is a fixed momentum and \mathbf{v}_0 and z are the velocity and the charge of the reference particle

Relative coordinates

$$\vec{Z}(s) = \begin{pmatrix} x \\ a = \frac{p_x}{p_0} \\ y \\ b = \frac{p_y}{p_0} \\ l = k(t - t_0) \\ \delta = \frac{(E - E_0)}{E_0} \end{pmatrix}$$



- \mathbf{x} and \mathbf{y} are the position of particle in relative coordinates
- \mathbf{a} and \mathbf{b} are the momentum slopes, \mathbf{E} is the total energy, \mathbf{l} a length like coordinate
- \mathbf{p}_0 is a fixed momentum and \mathbf{E}_0 and \mathbf{t}_0 are the energy and the time of flight of the reference particle

ODE's of motion

$$E = E_0 (1 + \delta)$$

$$\eta = \frac{E - eV(x)}{mc^2},$$

$$\frac{p_0}{p_s} = \left(\frac{\eta(2 + \eta)}{\eta_0(2 + \eta_0)} \cdot \frac{m^2}{m_0^2} - a^2 - b^2 \right)^{-\frac{1}{2}}$$

$$x' = a(1 + hx) \frac{p_0}{p_s},$$

$$y' = b(1 + hx) \frac{p_0}{p_s},$$

$$l' = \left\{ (1 + hx) \frac{1 + \eta \frac{p_0}{p_s}}{1 + \eta_0 \frac{p_0}{p_s}} - 1 \right\} \frac{k}{v_0},$$

$$a' = \left[\frac{1 + \eta \frac{p_0}{p_s}}{1 + \eta_0 \frac{p_0}{p_s}} \frac{E_x}{\chi_{e0}} + b \frac{B_z}{\chi_{m0}} \frac{p_0}{p_s} - \frac{B_y}{\chi_{m0}} \right] \cdot (1 + hx) + h \frac{p_s}{p_0},$$

$$b' = \left[\frac{1 + \eta \frac{p_0}{p_s}}{1 + \eta_0 \frac{p_0}{p_s}} \frac{E_y}{\chi_{e0}} + \frac{B_x}{\chi_{m0}} - a \frac{B_z}{\chi_{m0}} \frac{p_0}{p_s} \right] \cdot (1 + hx),$$

$$\delta' = 0 \quad \text{No time dependence of the field}$$

What is a Transfer Map?

The transfer map \mathcal{M} relates $\vec{Z}(s_0)$ to $\vec{Z}(s)$

$$\vec{Z}(s) = \mathcal{M}(s_0, s) \left(\vec{Z}(s_0) \right)$$

- For a deterministic system the transfer map is the flow of ODEs

$$\frac{d\vec{z}}{ds} = \vec{f}(\vec{z}, s)$$

- Transfer maps are origin preserving $\mathcal{M}(\vec{0}) = \vec{0}$
- $\mathcal{M}(s_1, s_2) \circ \mathcal{M}(s_0, s_1) = \mathcal{M}(s_0, s_2)$
- Transfer map of any Hamiltonian system satisfies symplectic condition
- For weakly non-linear systems, like an accelerator system, the map can be expanded as a Taylor series (**Taylor Map**)
- Due to practical limitations we have to truncate the map at certain order

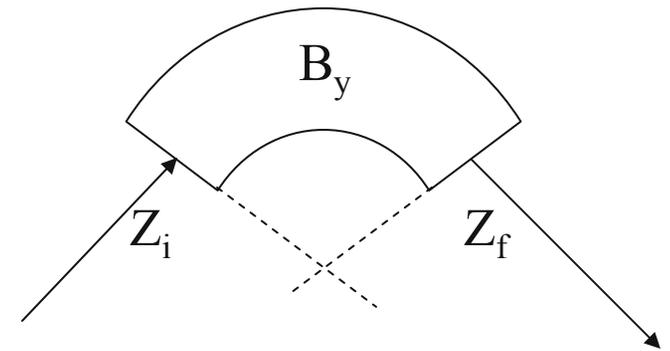
Second order Taylor map for a dipole (2D)

$$x_f = \cos(hL)x_i + \frac{1}{h}\sin(hL)a_i - \frac{h\sin(hL)^2}{2}x_i^2 + \frac{\sin(2hL)}{2}x_ia_i + \frac{\cos(hL)\cdot(1-\cos(hL))}{2h}a_i^2 - \frac{(1-\cos(hL))}{2h}b_i^2$$

$$a_f = -h\sin(hL)x_i + \cos(hL)a_i - \frac{\sin(hL)}{2}a_i^2 - \frac{\sin(hL)}{2}b_i^2$$

$$y_f = y_i + Lb_i + \sin(hL)x_ib_i + \frac{(1-\cos(hL))}{h}a_ib_i$$

$$b_f = b_i$$



$$Z = (x, a, y, b)$$

- For the case of $h=1.666$ and $hL=59$ degrees and

$$x_f = 0.5150381x_i + 0.5143004a_i - 0.6122798x_i^2 + 0.4414738x_ia_i + 0.0749321a_i^2 - 0.1454886b_i^2$$

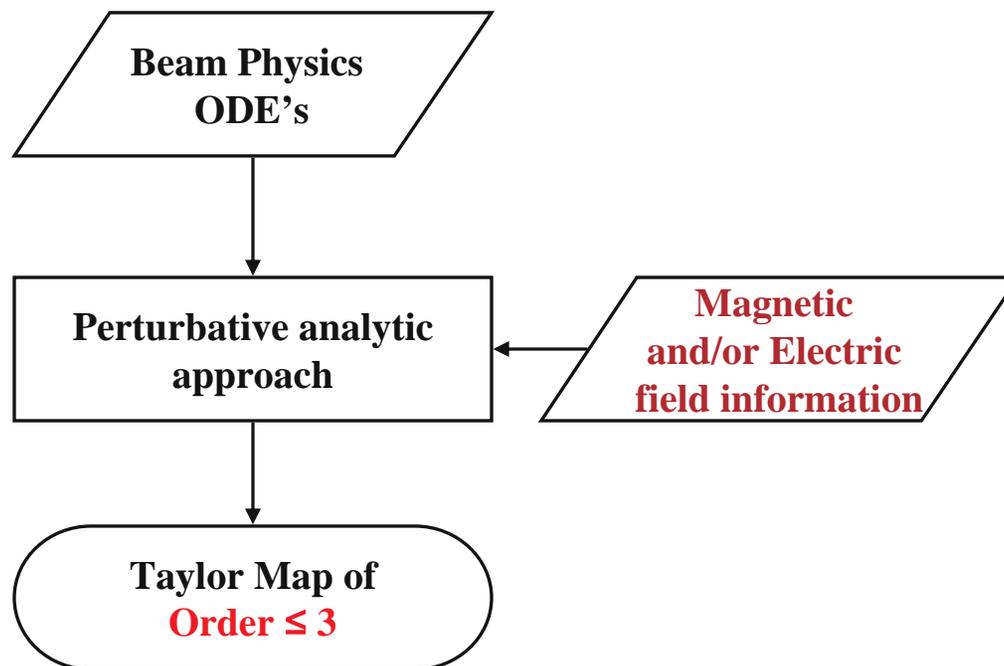
$$a_f = -1.428612x_i + 0.5150381a_i - 0.4285837a_i^2 - 0.4285837b_i^2$$

$$y_f = y_i + 0.6178466b_i + 0.8571673x_ib_i + 0.2909772a_ib_i$$

$$b_f = b_i$$

x_f	a_f	y_f	b_f	$x_ia_fy_fb_f$
0.5150381	-1.428612	0.000000	0.000000	1000
0.5143004	0.5150381	0.000000	0.000000	0100
0.000000	0.000000	1.000000	0.000000	0010
0.000000	0.000000	0.6178466	1.000000	0001
-0.6122798	0.000000	0.000000	0.000000	2000
0.4414738	0.000000	0.000000	0.000000	1100
0.7493216E-01	-0.4285837	0.000000	0.000000	0200
0.000000	0.000000	0.8571673	0.000000	1001
0.000000	0.000000	0.2909772	0.000000	0101
-0.1454886	-0.4285837	0.000000	0.000000	0002

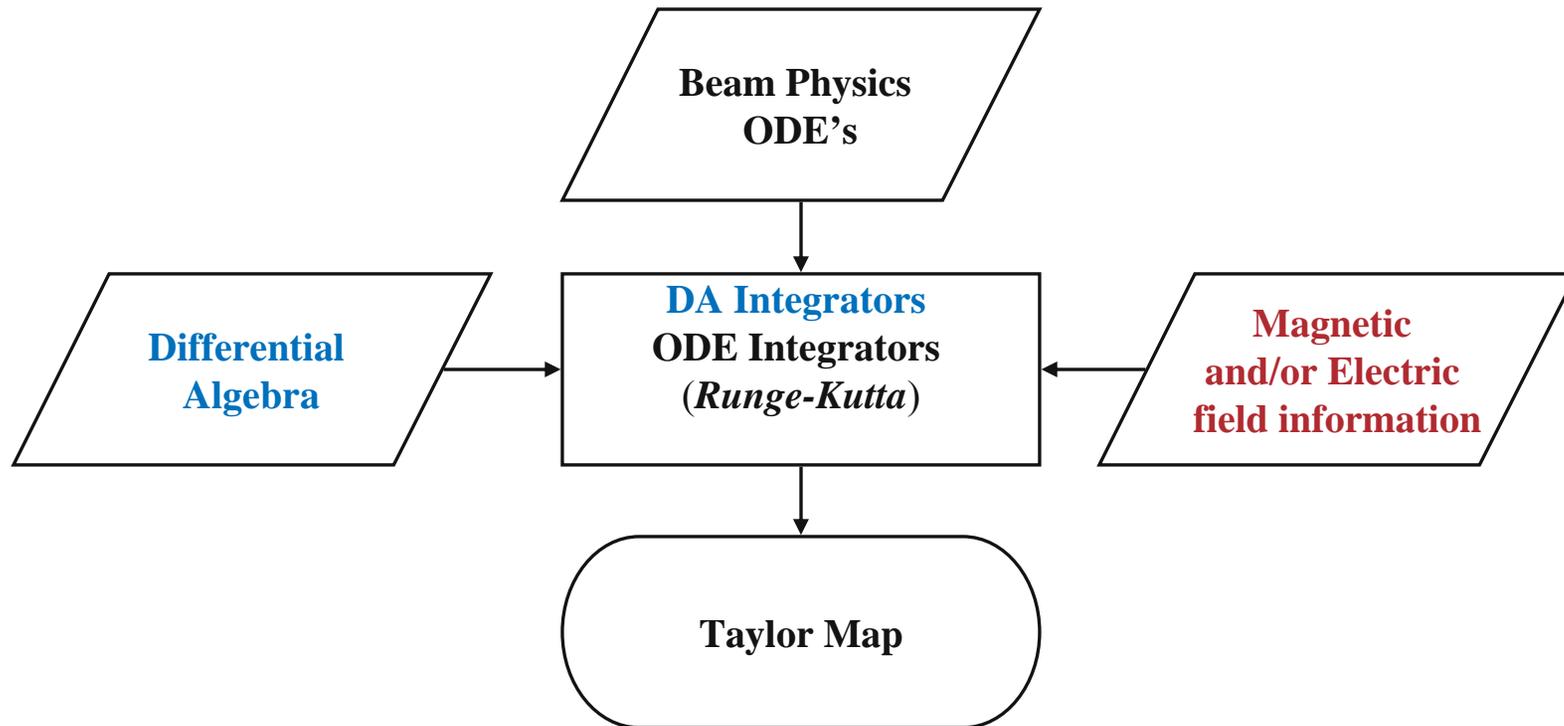
Maps for known fields



- Method can be used to compute transfer map of order ≤ 3
- Analytic or local Taylor expansion (multipole decomposition) of the magnetic field should be specified
- Present/future accelerators require much higher order description

Obtaining Maps using DA

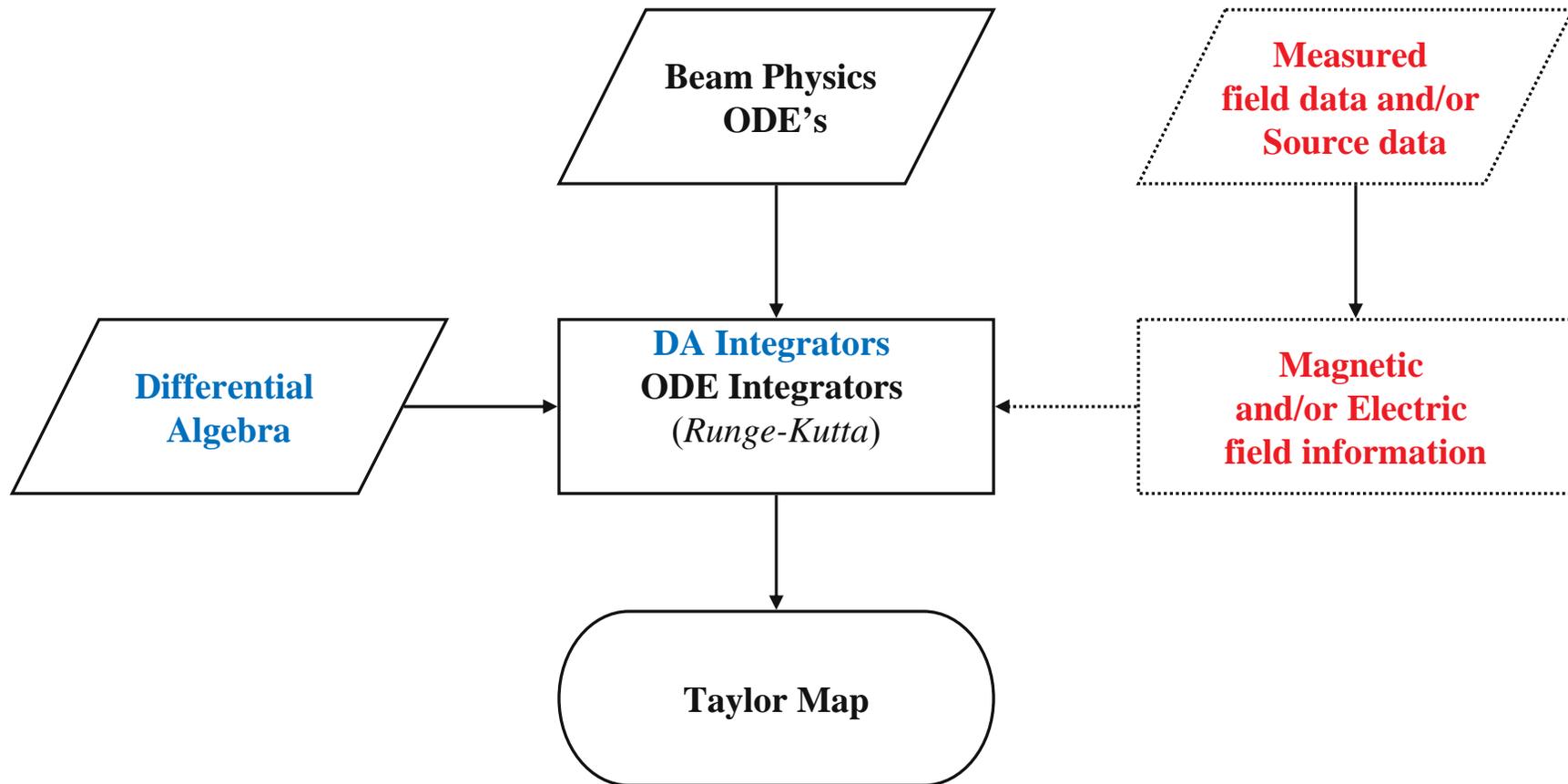
- DA methods were introduced to compute maps to in principle arbitrary order
- Analytic formula or local expansion of the field should be specified



Maps from measured field data or source distribution

- Usual practice: Magnetic field is approximated by an analytic model. Fringe fields are treated separately
- High resolution spectrographs, LHC (and future HEP accelerators) require magnets to be modelling to high accuracy
- However, high accuracy require the use of realistic fields obtained from
 - experimental measurements
 - 3D FEM magnet modelling codes like TOSCA
 - the knowledge of current coil configuration and shielding
- Methods in use:
 - Using field data on the mid-plane or on the central axis (unstable, large error)
 - Methods using image charge (inversion of large matrix, lot of guess work)
- **Current methods can not obtain high accuracy maps directly from the measured data or the source distribution.**

Goal



- Local expansion of the field from measured data (**Laplace BVP**)
- Local expansion of the field from current distribution (**Biot-Savart Law**)

(1) The Laplace BVP

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

What are we looking for ?

- 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)

Numerical Methods

- 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**

2D Laplace equation

$$\nabla^2 \phi(\vec{r}) = 0 \text{ in the bounded volume } \Omega \subset \mathbb{E}^2$$

Using Cauchy's formula

$$\phi(\alpha) = \frac{1}{2\pi i} \oint_{\partial\Omega} \frac{\phi(z)}{z - \alpha} dz$$

- α is a point within Ω
- Cauchy's formula is an integral representation of f which permits us to compute f anywhere in the interior of $\partial\Omega$, knowing only the value of f on Ω
- Kernel is smoothing
- Simple extension does not exist for 3D

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

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

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

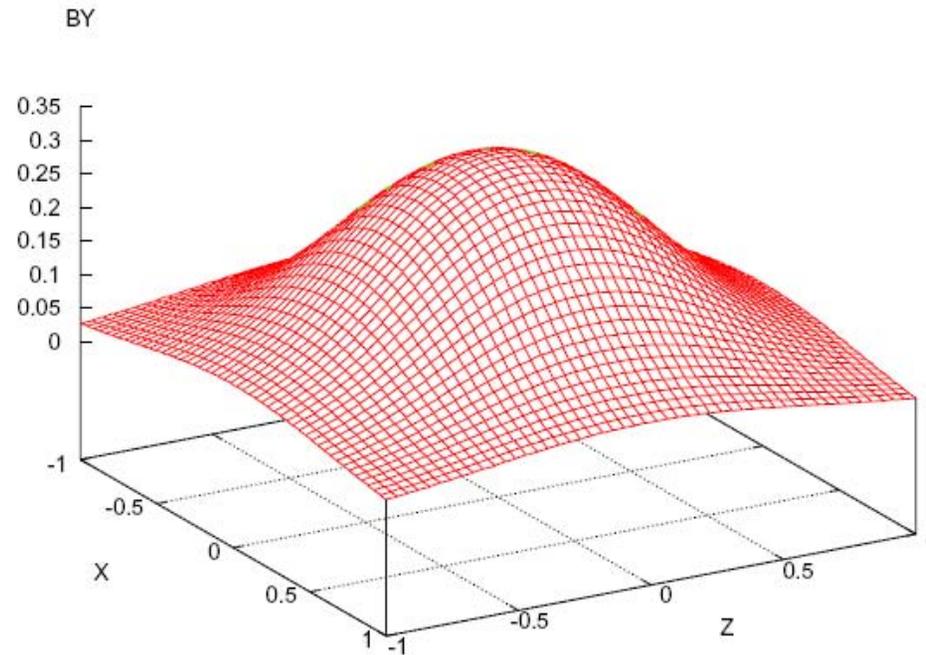
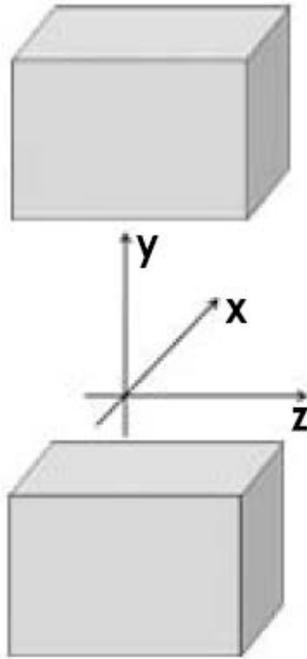
$$\vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}_t(\vec{x}) + \vec{\nabla} \phi_n(\vec{x})$$

- 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

- Split domain of integration $\partial\Omega$ in to smaller regions Γ_i , $i = 1 \dots N$
- Describe the surface element Γ_i in two variables $\vec{r}_s(x_s, y_s)$
- Expand the kernel to higher orders in two surface variables (x_s, y_s) and the three volume variables (x, y, z)
- 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
- Implemented using the high-order multivariate differential algebraic tools available in the arbitrary order code COSY INFINITY
 - local expansion, surface integration, curl and divergence
 - Field representation to any order without any manual computations

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

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

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

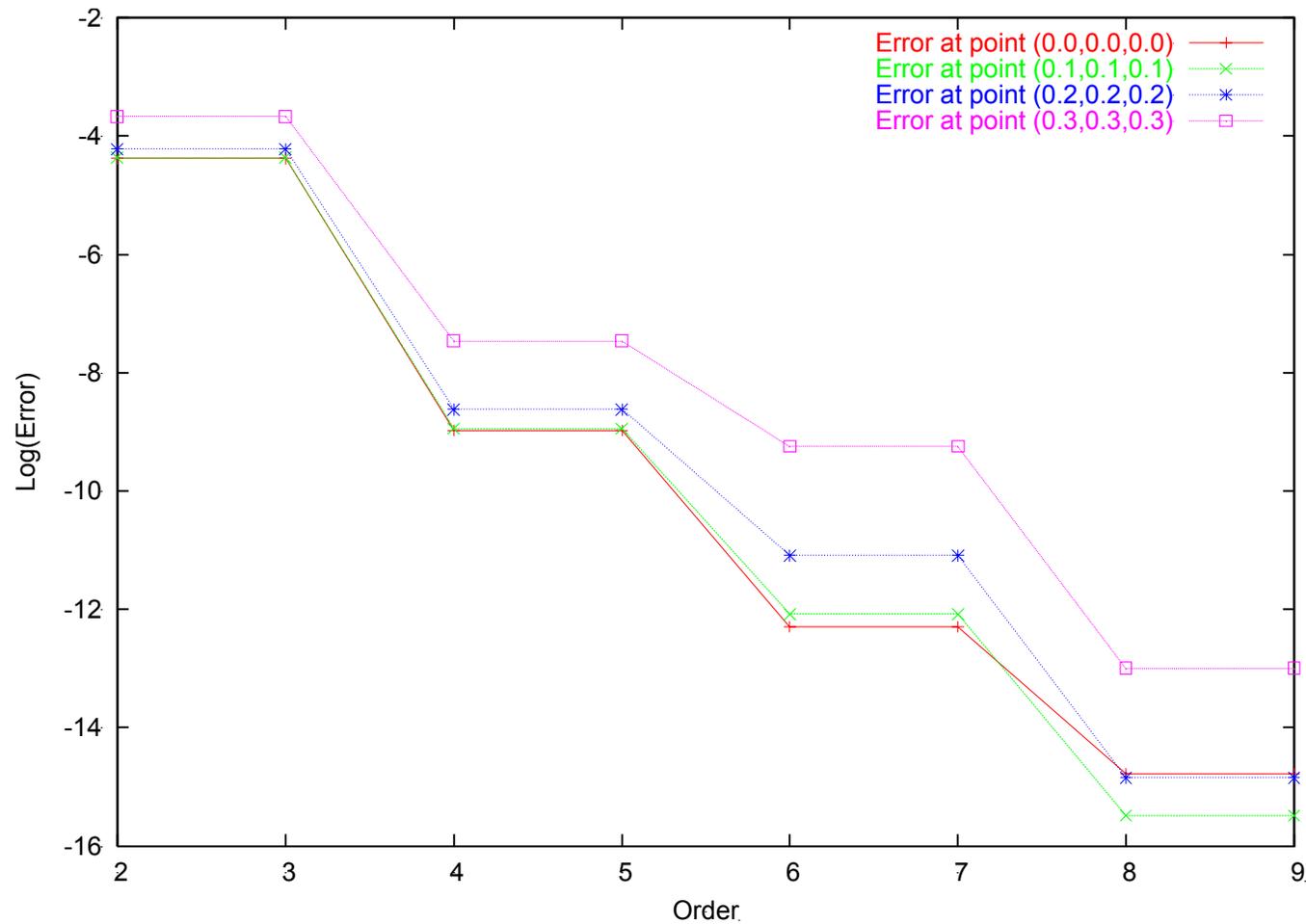
$$B_z(x, y, z) = \frac{B_0}{4\pi} \sum_{i,j=1}^2 (-1)^{i+j} \left[\ln \left(\frac{X_j + R_{ij}^-}{X_j + R_{ij}^+} \right) \right]$$

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

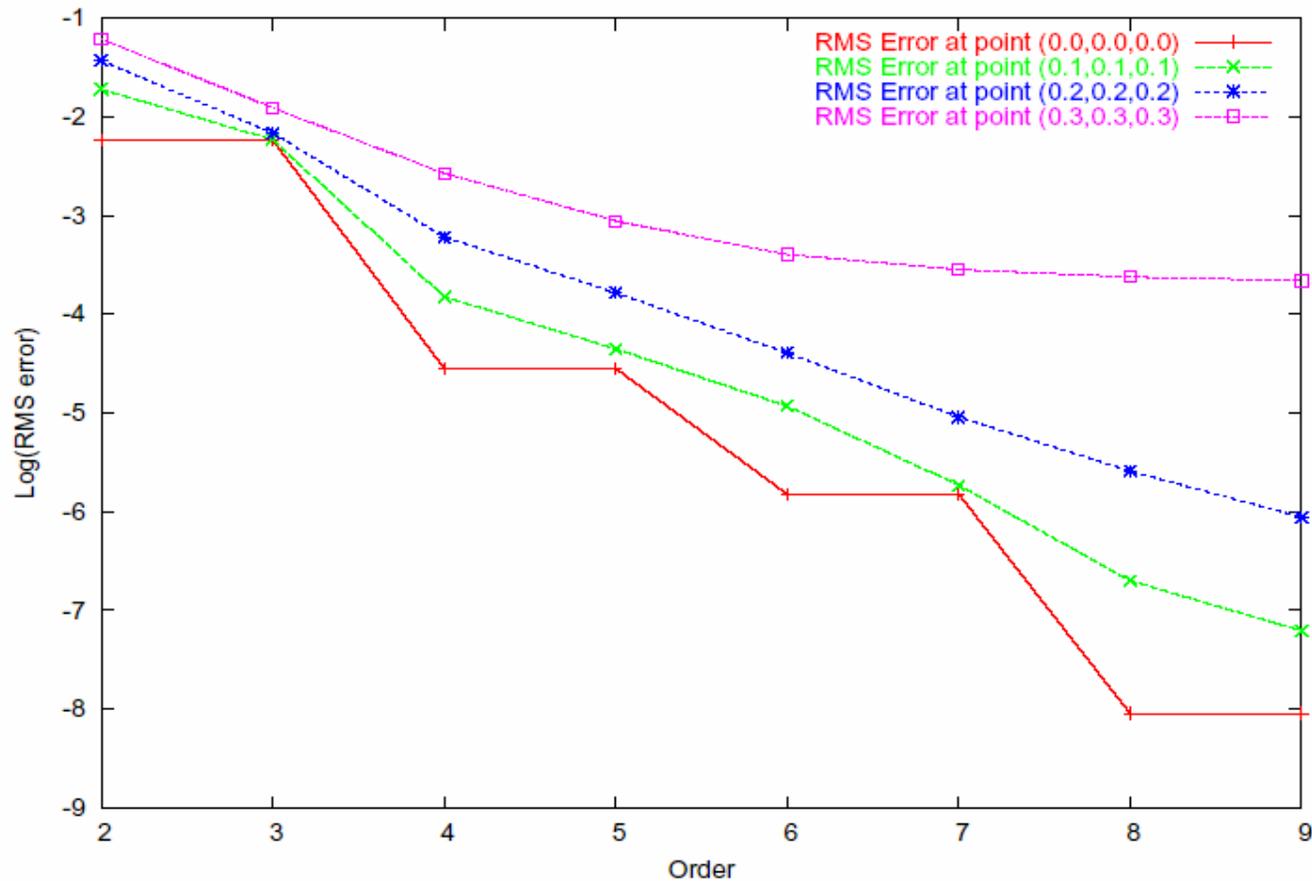
- Using the analytic formulas we specify magnetic field on the surface enclosing the volume of interest
- We use the Helmholtz method to compute the field inside
- We compare the results with the analytic formulas (three plots)

Performance of surface integration method

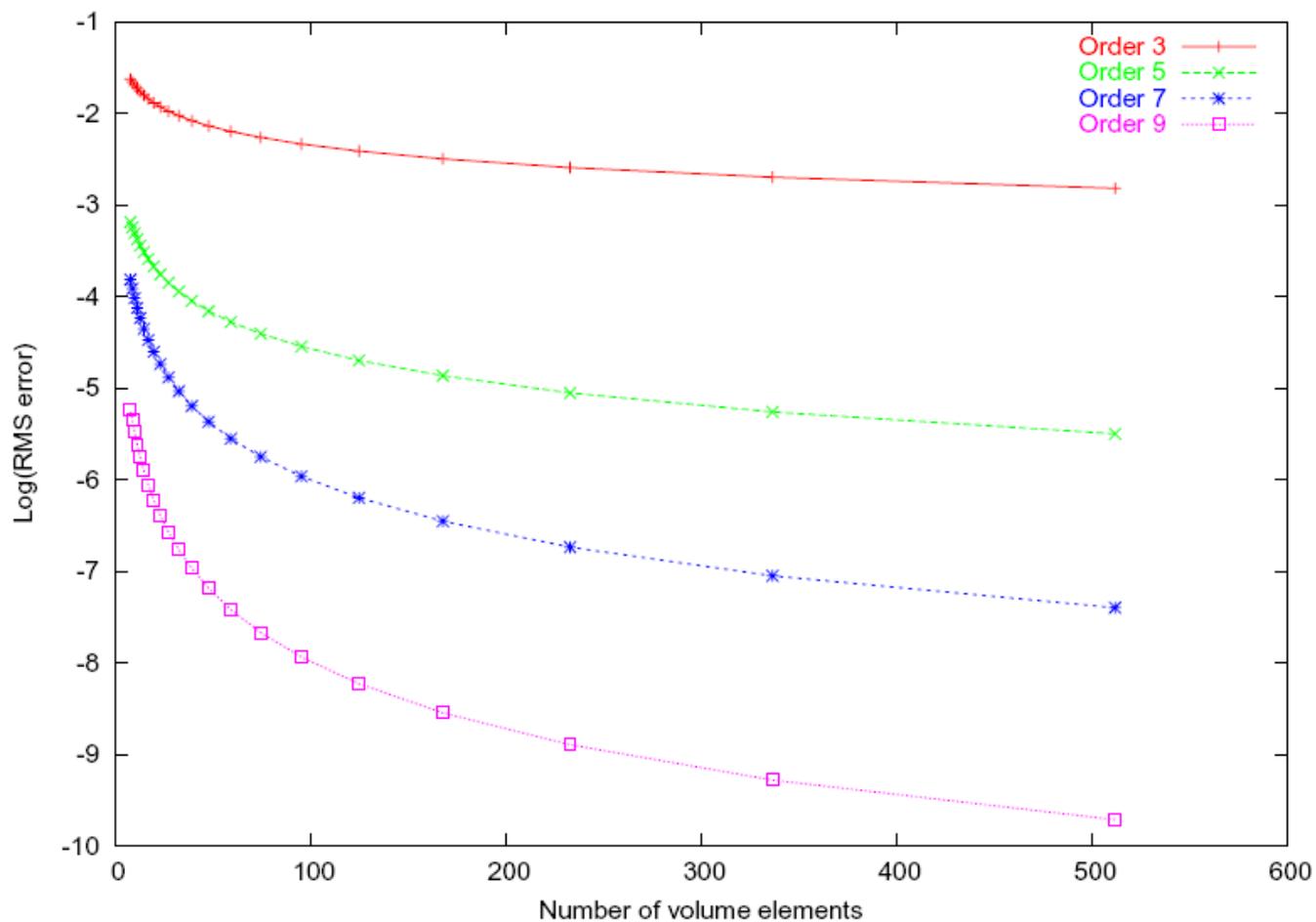
- Choose a cube of edge length 0.8m centered at origin
- Each face is covered by 44x44 mesh (surface elements)



- Split the cube into 4x4x4 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

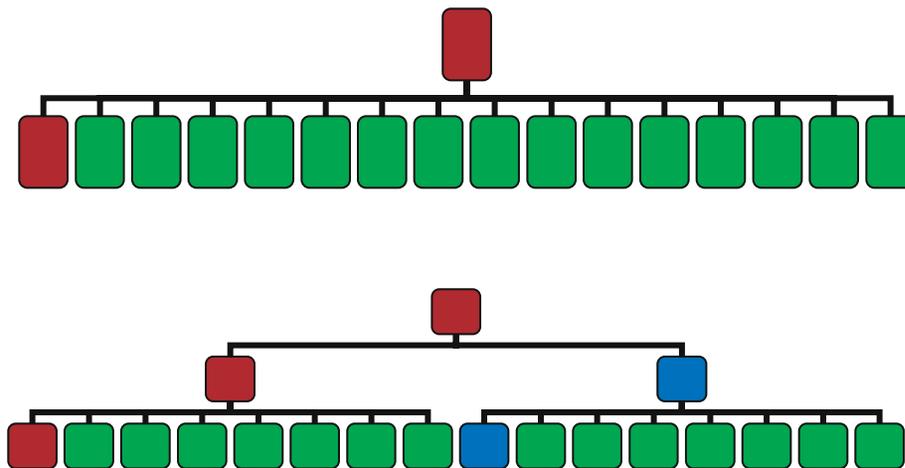


■ Dependency of the average error on the number of volume element.



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
 - $(NPR \text{ processors}) = (N2 \text{ groups}) \times (N1 \text{ processors})$
 - $N1 = \text{INT}(2\sqrt{NPR})$
 - Two parallel loop are used to make the summation efficient and also minimizes cross-communication



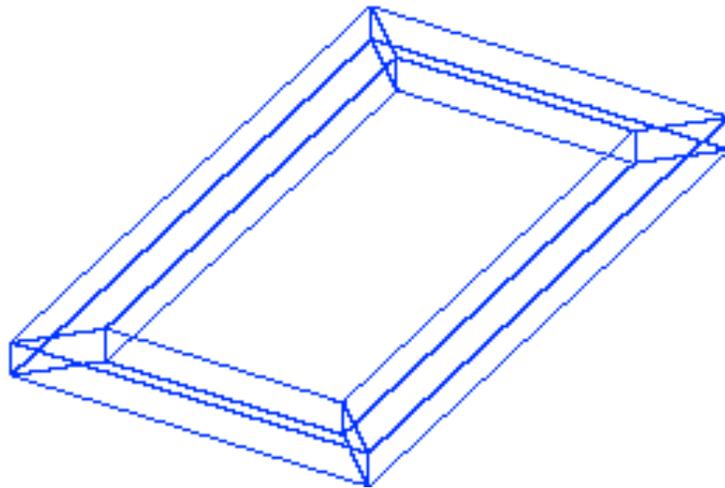
(2) Magnetic field due to arbitrary current distribution

- Magnetic field due to arbitrary current distribution is computed using the Biot-Savart law or Ampere's law
- Implementation is similar to the Laplace solver case
 - Discretize the domain into current elements
 - DA framework is developed to describe a current element for the line, surface and volume case
 - Expand the kernel for the Biot-Savart law or Ampere's law
 - Integrate with respect to the variables describing the current elements
 - Sum over all the current elements
- The curl and the divergences for the field computed is always zero in the current free region.

Tools

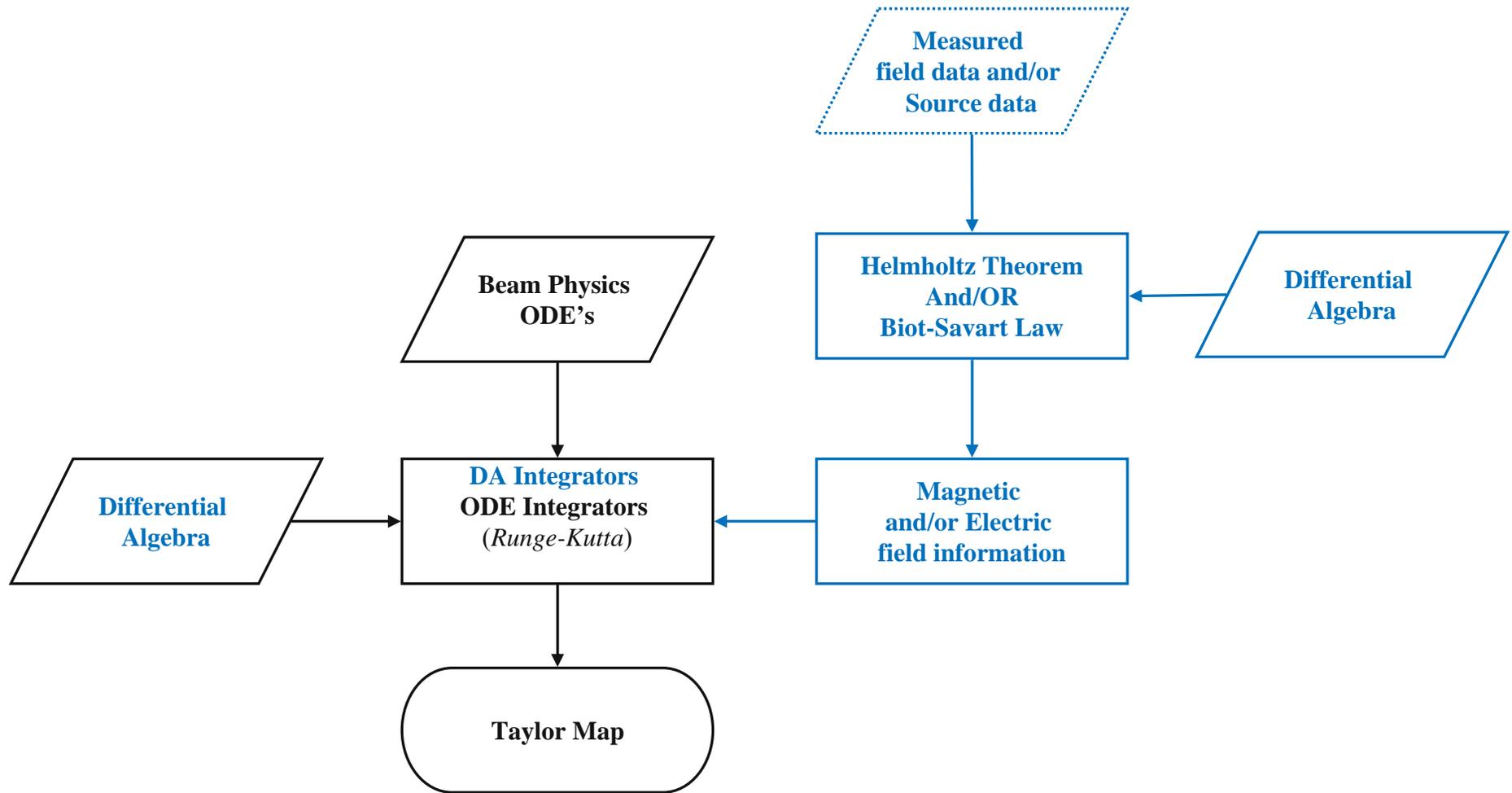
Due to their frequent use in the accelerator magnet applications, a dedicated set of tools has been written in the code COSY INFINITY for

- Infinitely long rectangular cross section current wire(2D design)
- Finite length rectangular cross section current wire
 - *Current coil of rectangular cross section (3D design)*



In addition to extracting the transfer maps these tools can be used to design magnets

Complete Picture: Map Extraction



In the case of measured data we will be constrained by the quality (accuracy, divergence, curl free etc) of the data

Check: Transfer map for analytic quadrupole magnet case

Quadrupole example: $\vec{B}(x, y, s) = (k_q y, k_q x, 0)$

- Transfer map from quadrupole field is known
- From the analytic formulas we create surface data and extract transfer map
- Difference between the map computed using the analytic formulas and surface data

```
-.7127632E-13 -.7115593E-12 .0000000E+00 .0000000E+00 .0000000E+00 100000
-.4718448E-14 -.7105427E-13 .0000000E+00 .0000000E+00 .0000000E+00 010000
.0000000E+00 .0000000E+00 .7149836E-13 .7143869E-12 .0000000E+00 001000
.0000000E+00 .0000000E+00 .4718448E-14 .7127632E-13 .0000000E+00 000100
.0000000E+00 .0000000E+00 .0000000E+00 .0000000E+00 -.7057580E-15 200000
.0000000E+00 .0000000E+00 .0000000E+00 .0000000E+00 .3560542E-13 110000
.0000000E+00 .0000000E+00 .0000000E+00 .0000000E+00 .2366163E-14 020000
.0000000E+00 .0000000E+00 .0000000E+00 .0000000E+00 -.7064949E-15 002000
.0000000E+00 .0000000E+00 .0000000E+00 .0000000E+00 -.3588926E-13 001100
.3567199E-13 -.7027697E-15 .0000000E+00 .0000000E+00 .0000000E+00 100001
.4732326E-14 .3557007E-13 .0000000E+00 .0000000E+00 .0000000E+00 010001
.0000000E+00 .0000000E+00 -.3581380E-13 -.7045552E-15 .0000000E+00 001001
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Applications



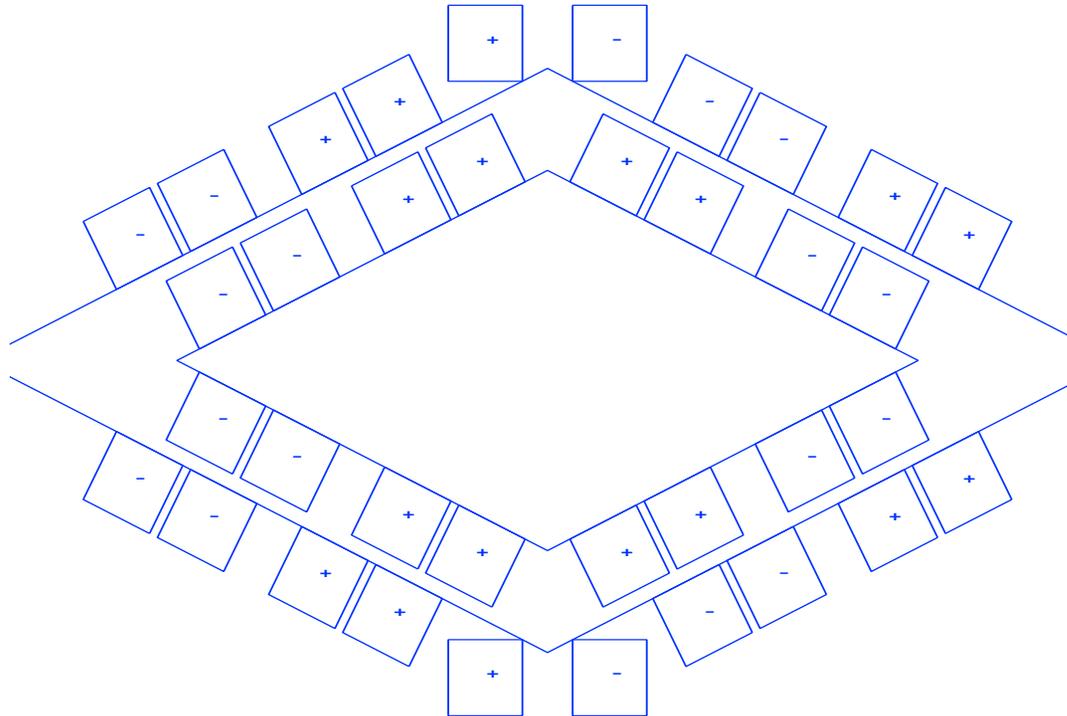
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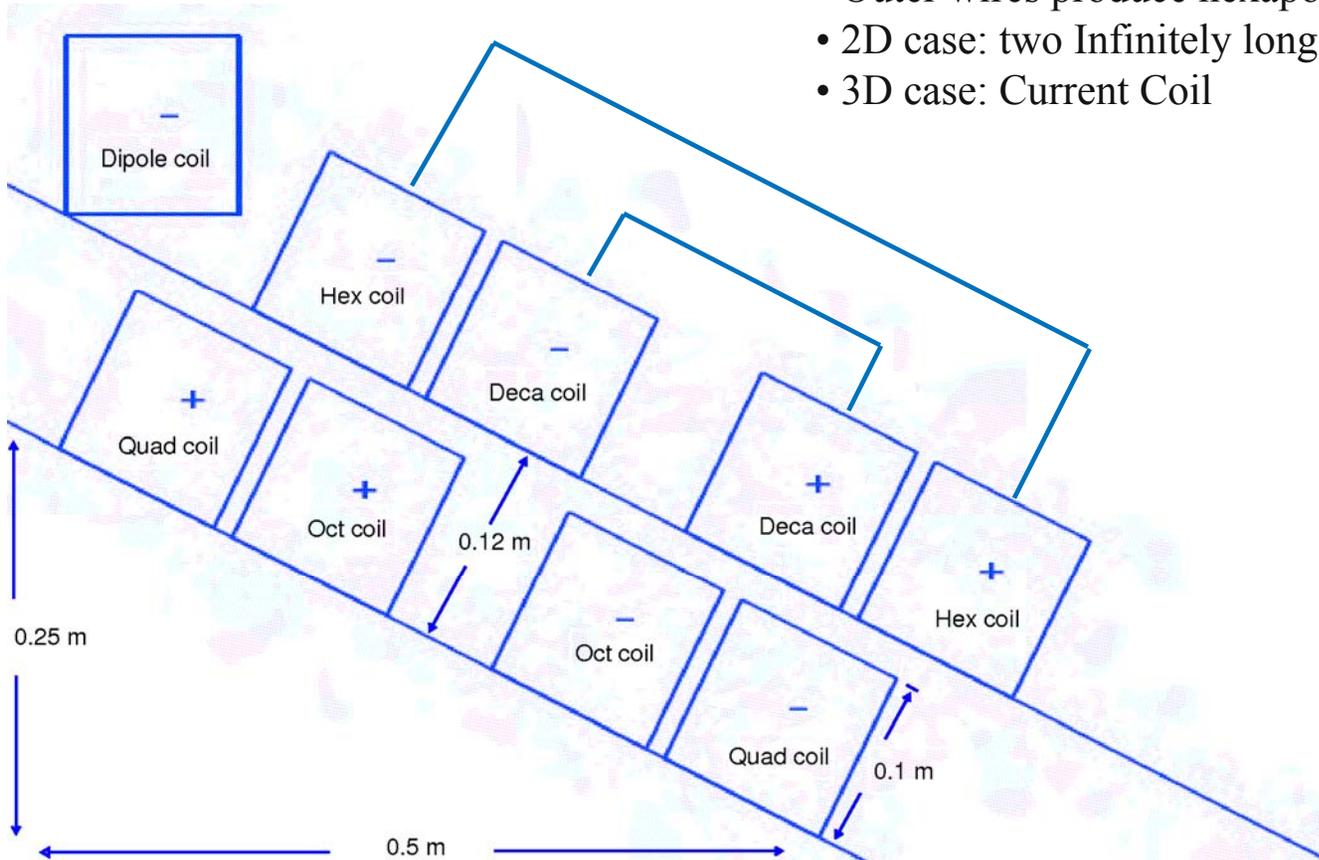
(1) Design of quadrupole magnet with an elliptic cross section

For beam wider in the dispersive plane than the transverse plane it is cost efficient to utilize magnets with elliptic cross sections



- 18 superconducting racetrack coils ($\pm 10^8 \text{A/m}^2$)
- Rhombic prism support structure (elliptic aperture 1:2)

- "+" produces a positive multipole term
- Inner wires produce quadrupole and octupole fields
- Outer wires produce hexapole and decapole fields
- 2D case: two Infinitely long current wires
- 3D case: Current Coil



Using DA we can make the currents as parameters and find the functional dependence Of the multipole components on the coil currents.

The relationship between the currents and the principle multipole components can be given by a simple matrix

$$\begin{bmatrix} B_0^y \\ B_{(x)}^y \\ B_{(xx)}^y \\ B_{(xxx)}^y \\ B_{(xxxx)}^y \end{bmatrix} = \begin{bmatrix} 0 & 0 & -0.25 & -0.04 & +0.37 \\ +5.76 & +2.40 & 0 & 0 & 0 \\ 0 & 0 & -3.89 & -2.08 & -1.45 \\ -0.40 & +15.44 & 0 & 0 & 0 \\ 0 & 0 & +1.66 & -2.32 & +2.99 \end{bmatrix} \cdot \begin{bmatrix} QI \\ OI \\ HI \\ DI \\ I \end{bmatrix}$$

$$B_{(yy)}^y = -B_{(xx)}^y$$

$$B_{(xyy)}^y = -3B_{(xxx)}^y$$

$$-\frac{B_{(xxyy)}^y}{6} = B_{(yyyy)}^y = B_{(xxxx)}^y$$

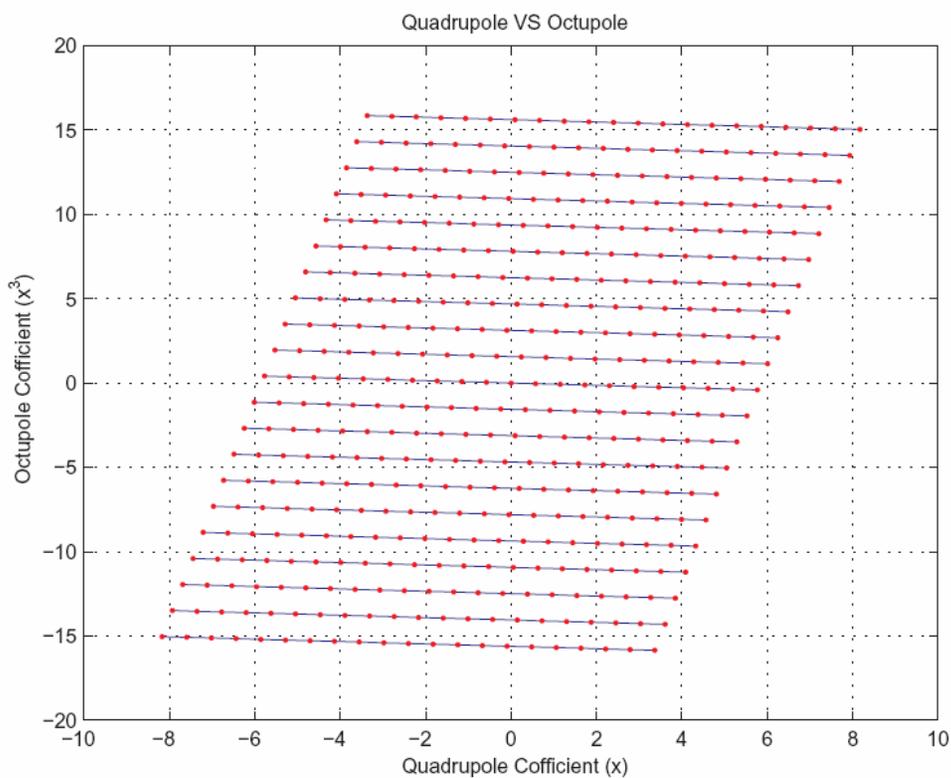
$$B_{(y)}^x = B_{(x)}^y$$

$$B_{(xy)}^x = 2B_{(xx)}^y$$

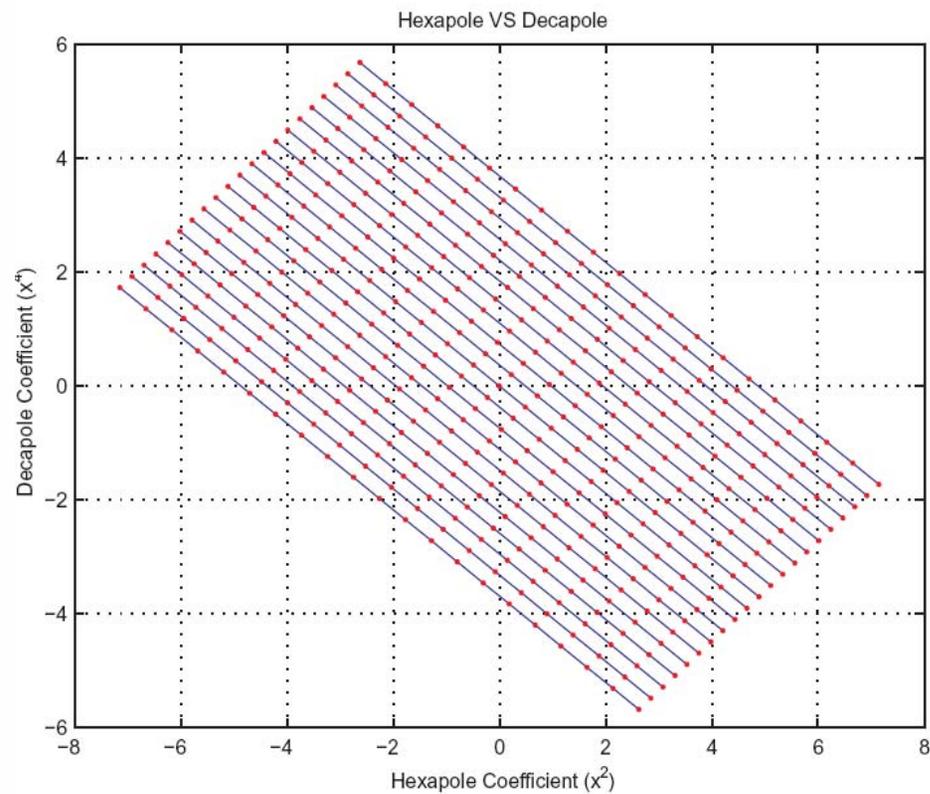
$$\frac{B_{(xxy)}^x}{3} = -B_{(yyy)}^x = B_{(xxx)}^y$$

$$B_{(xxxy)}^x = -B_{(xyyy)}^x = 4B_{(xxxx)}^y$$

Operational Plot



Quadrupole and the octupole terms

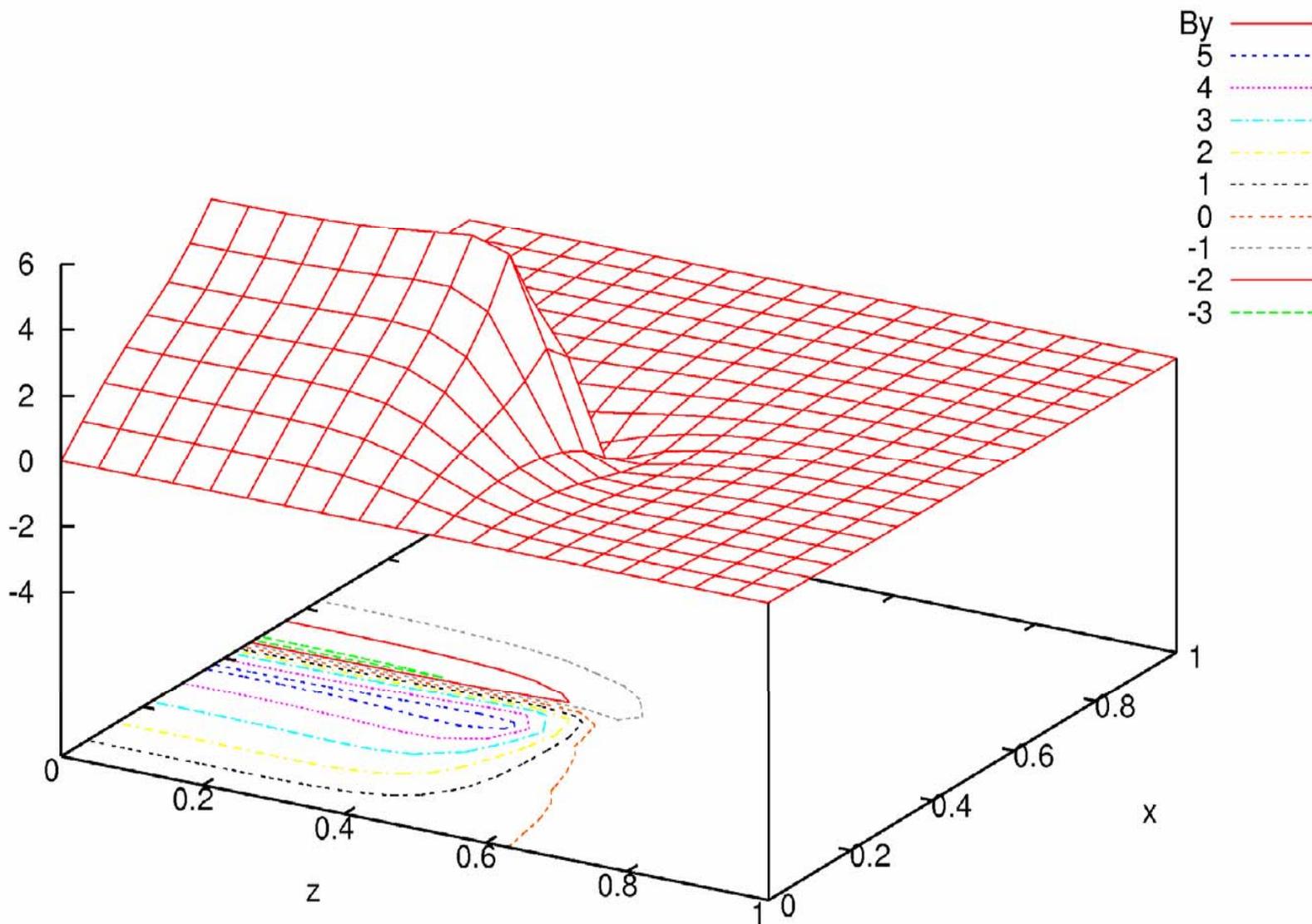


Hexapole and the Decapole terms

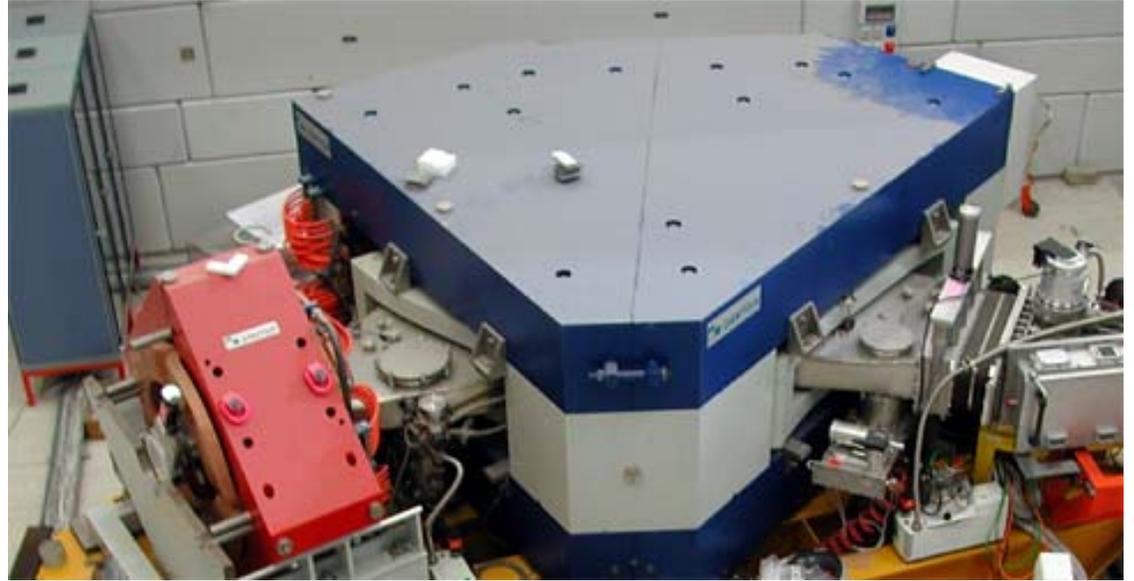
- The coefficients are computed at the horizontal half aperture
- The current density was varied between $\pm 10^8 \text{ A/m}^2$

3D Design: Fringe field

The plot of the magnetic field on the midplane, $y = 0$ m. Only the magnetic field in the first quadrant is shown.

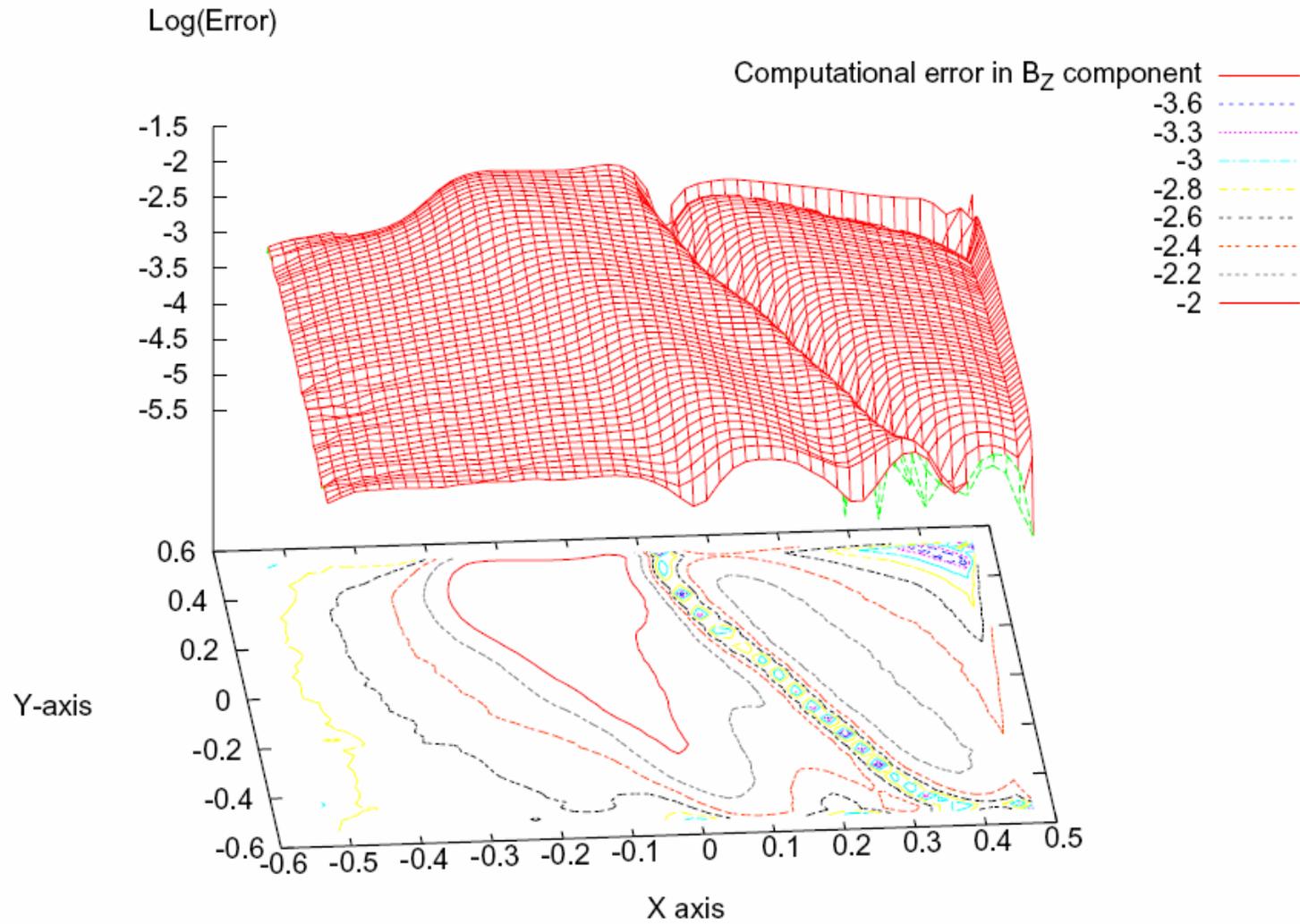


(2) MAGNEX spectrometer dipole magnet

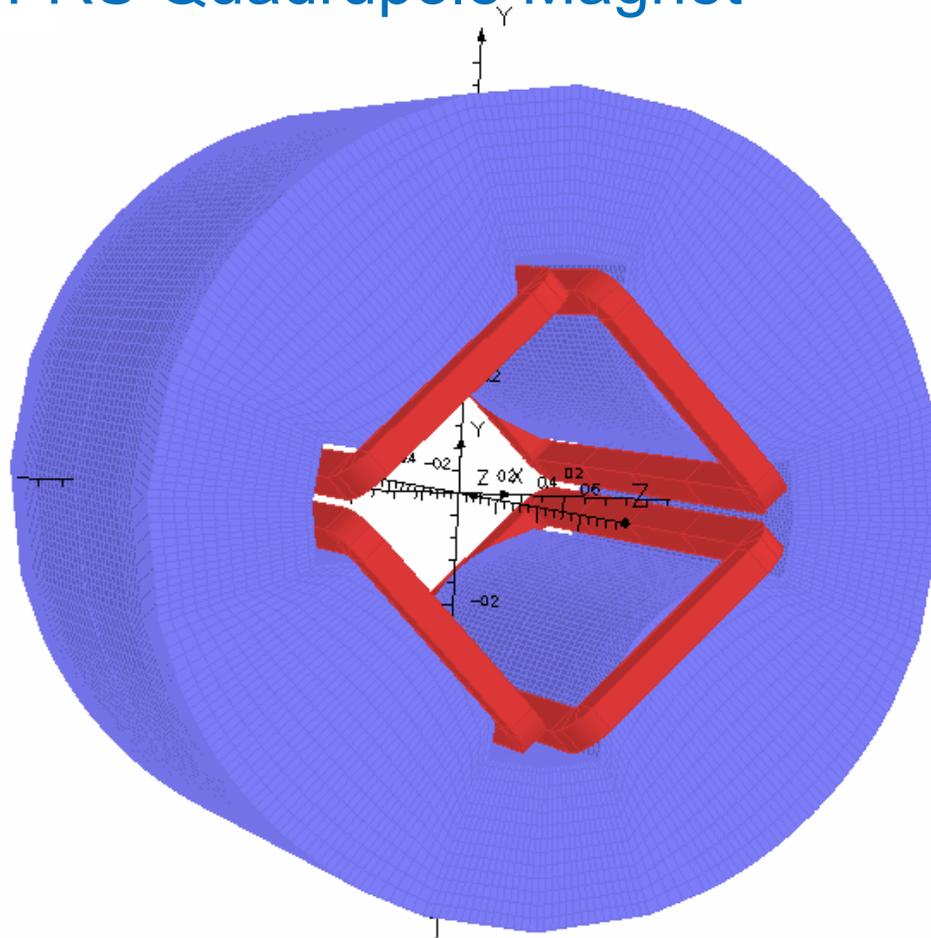


Magnetic field data is measured on the grids for 7 different planes
 $\langle \Delta B_i / B_i \rangle = 5 \times 10^{-4}$

Contour plot of magnetic field errors for the mid-plane (region 1)



(3) Super-FRS Quadrupole Magnet



V VECTOR FIELDS

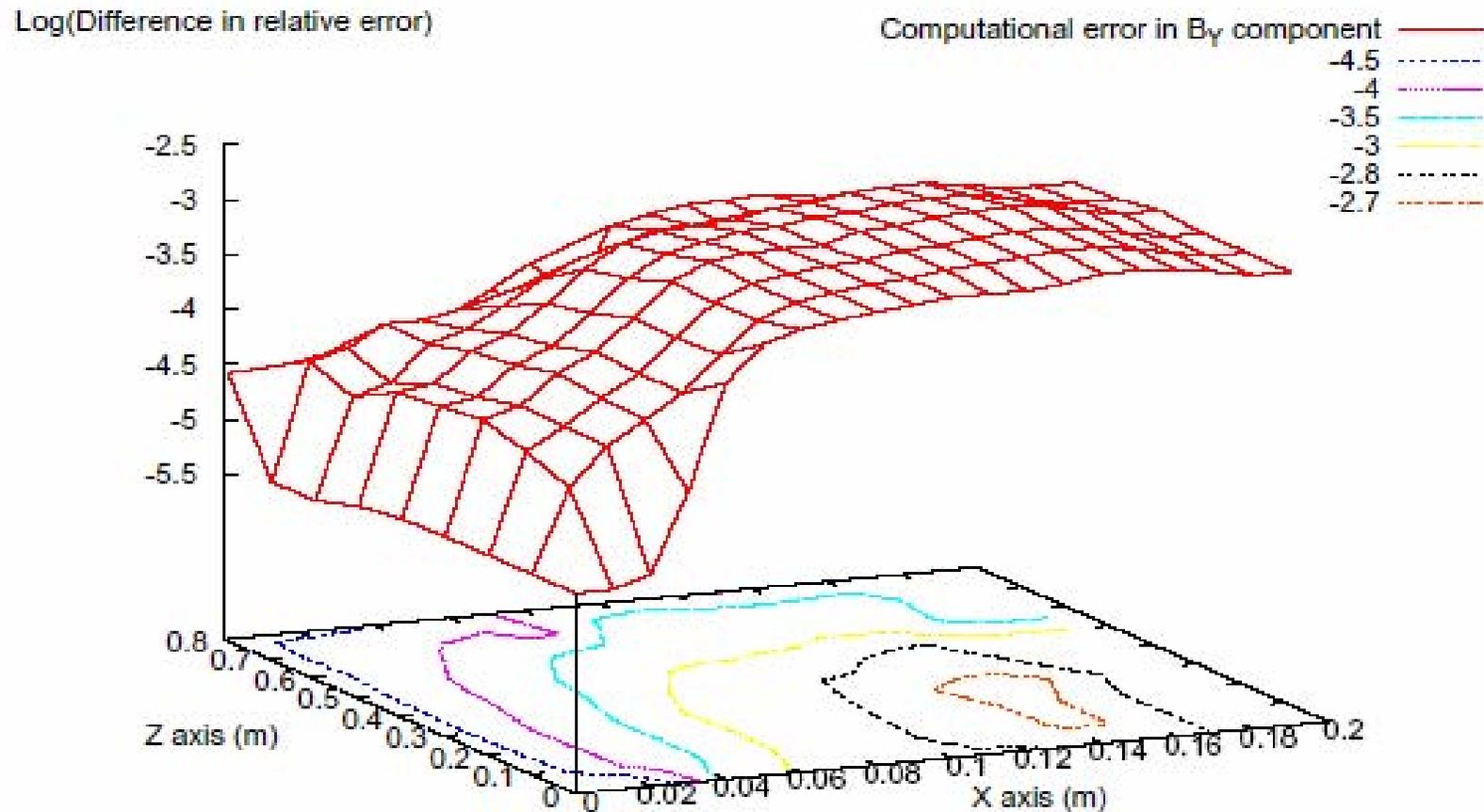
UNITS	
Length	m
Magn Flux Density	T
Magn Field	A/m
Magn Scalar Pot	A
Magn Vector Pot	Wb/m
Elec Flux Density	C/m ²
Elec Field	V/m
Conductivity	S/m
Current Density	A/m ²
Power	W
Force	N
Energy	J

PROBLEM DATA	
cr_sf_2.op3	
TOSCA Magnetostatic	
Non-linear materials	
Simulation No 1 of 1	
87740 elements	
367338 nodes	
1 conductor	
Nodally interpolated fields	

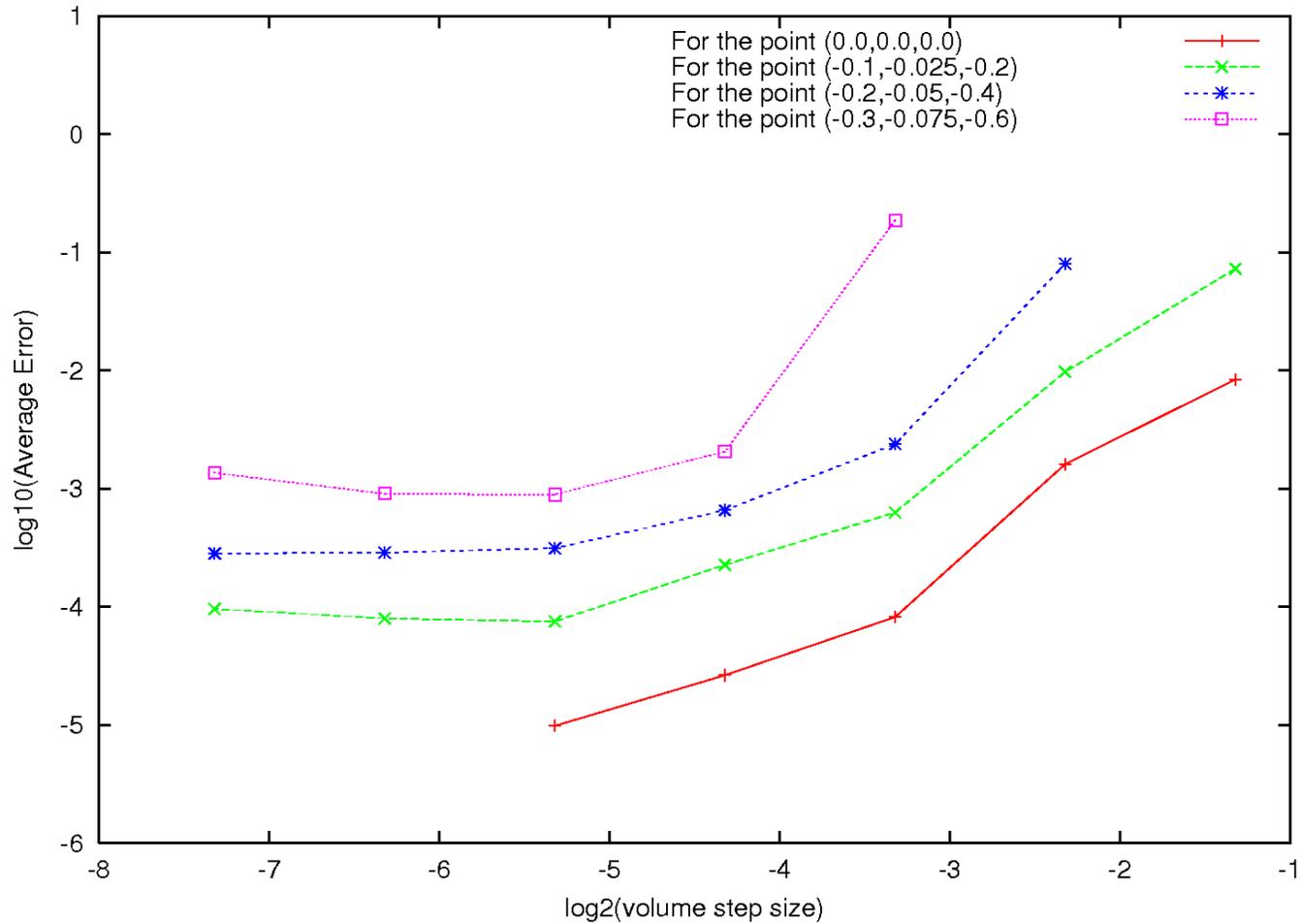
Local Coordinates	
Origin: 0.0, 0.0, 0.0	
Local XYZ = Global XYZ	

- The TOSCA model for the quadrupole magnet $\Delta B/B = 70 \times 10^{-4}$
- Length of 0.8 m with the usable horizontal aperture of ± 0.2 m and the vertical aperture of 0.1 m
- The surface was discretized with a step size of 5 mm, leading to a discretization of 80x40x320 surface elements.

The difference between the relative error of the y component of the magnetic field on the mid plane for first quadrant



- The RMS average difference between the TOSCA simulation result and the new Laplace solver technique versus the volume element length

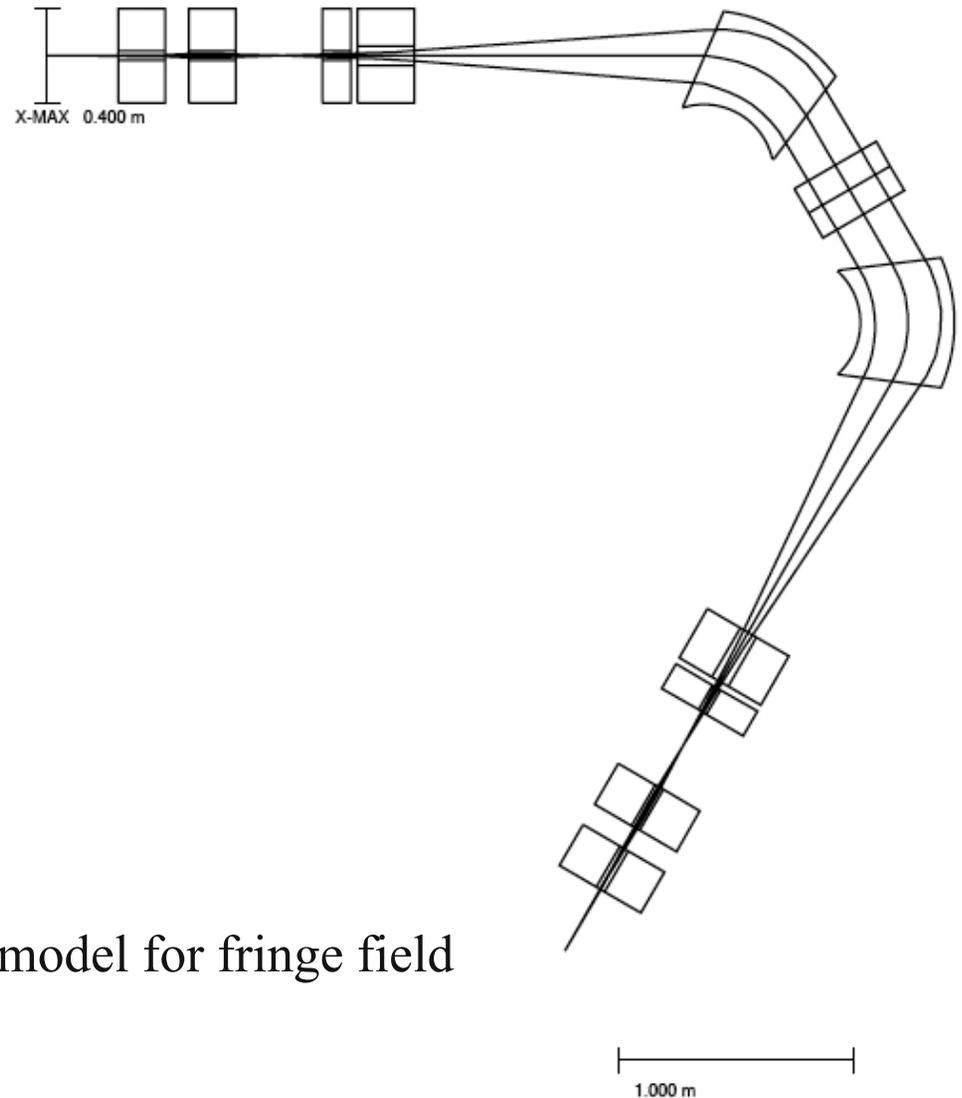
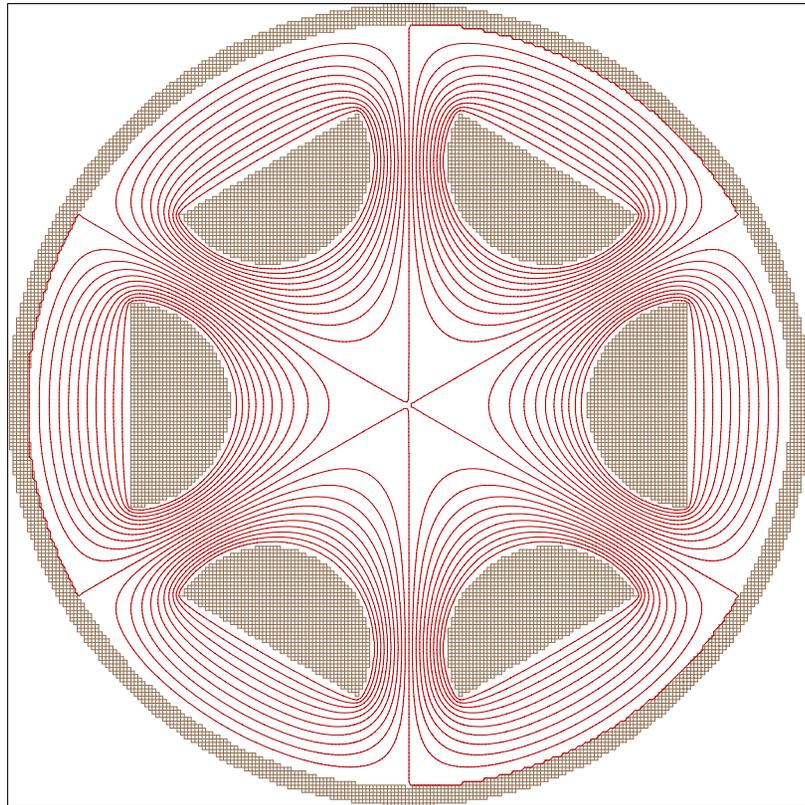


Extracted Transfer map to second order

-0.4705674	-1.394826	0.000000	0.000000	0.000000	100000
0.5581815	-0.4705674	0.000000	0.000000	0.000000	010000
0.000000	0.000000	3.837901	4.272580	0.000000	001000
0.000000	0.000000	3.213394	3.837901	0.000000	000100
0.000000	0.000000	0.000000	0.000000	1.000000	000010
0.000000	0.000000	0.000000	0.000000	0.3989286	000001
0.1284348E-14	0.1535115E-14	0.000000	0.000000	-0.4476261	200000
0.1159401E-14	0.9402369E-15	0.000000	0.000000	0.4865291E-01	110000
-0.1197808E-14	-0.3977569E-14	0.000000	0.000000	-0.1627172	020000
0.1930759E-13	0.5931886E-13	0.000000	0.000000	-2.059670	002000
0.3353931E-13	0.9565057E-13	0.000000	0.000000	-3.933253	001100
0.4768188	-0.4891389	0.000000	0.000000	0.000000	100001
0.1259816	0.4768188	0.000000	0.000000	0.000000	010001
0.000000	0.000000	-1.858375	-0.9955222	0.000000	001001
0.1398535E-13	0.3825810E-13	0.000000	0.000000	-1.984025	000200
0.000000	0.000000	-2.589889	-1.858375	0.000000	000101
0.000000	0.000000	0.000000	0.000000	-0.2995974	000002

(4) CARABU electric sextapole magnets (work in progress)

- The CALifornium Rare Isotope Breeder Upgrade
- Sextapole magnet are dominated by fringe fields



Good agreement to third order with the Enge model for fringe field

Conclusion

- Using of DA methods multipole expansion solution of the field to high order can be obtained. Which also leads to small number of volume elements
- Using the surface data and Helmholtz theorem leads to technique that are naturally smoothing
- Design of accelerator magnets is possible with the tools developed
- The DA frame work developed can be used for other PDEs for which the solution can be expressed as an integral equation

