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Accuracy Analysis of Charged Particle Trajectory CAE Software

Content

Executive Summary

Though there exists extensive literature on the subject of charged particle beam analysis, most often only the simplest of geometries can be treated analytically. Advances in numerical solutions of both ordinary and partial differential equations have led to the development of **Computer Aided Engineering** (**CAE**) software packages that permit the simulation of more complex systems that include “real world” deviations that inevitably occur.

Since accuracy of simulation results is fundamental for the selection of beam analysis software, this paper will use that criterion to examine the most popular numerical methods and illustrate techniques for evaluating their suitability. We will limit the scope of our studies to accuracy assessments, while acknowledging that additional features (such as capabilities to model emission regimes, secondary emissions, space charge effects, etc.) are required in a fully functional beam analysis package.

Overview of Charged Particle Beam Analysis

Charged particle beam analysis requires the solution of both **initial value** and **boundary value** problems. The analysis may be further complicated by physical effects such as beam dispersion due to Coulomb forces. Often an iterative approach is required to modify the boundary value solution until convergence is obtained.

Analytic solutions for initial value problems can be easily obtained if the field solution can be assumed as constant. This situation is common for beam deflection systems and for certain types of particle traps. However, analytic techniques fail for regions with non-uniform fields. Fortunately, several advanced numerical methods are available for the solution of Ordinary Differential Equations (**ODE**s). Numerical methods utilize calculated field values at each solution step, and any specified level of accuracy can usually be obtained by simply using a small enough step size (assuming, of course, that the field calculations are accurate enough).

Although analytic field solutions of boundary value problems can be obtained for certain specialized geometries, they cannot be applied in general and usually cannot account for fringe fields or end effects. In these cases, numerical solutions for Partial Differential Equations (**PDE**s) are usually obtained through **Finite Element Method** (**FEM**) or **Boundary Element Method** (**BEM**) simulations. Both methods discretize models of physical systems by creating meshes of geometric elements (typically 2D triangles and/or 3D tetrahedra) and, as a general rule, accuracy improves as more elements are used (similar to reducing the time step in the case of **ODE** solvers).

CAE software suitable for beam analysis must provide a high level of accuracy for both the ODE and PDE solutions. Obtaining accurate solutions requires both the selection of appropriate solver methods, and sufficiently fine discretization (time step for the ODE solver, element mesh for the PDE solver). Depending on the nature of the problem, some solver methods may be more "efficient" in the sense that they can obtain high accuracy without the need for excessively fine levels of discretization. Generally the more efficient algorithms will produce faster solutions.

The remainder of this paper will demonstrate examples of different solution methods applied to field distributions commonly encountered in charge particle beam systems.

Types of Field Distributions

In order to evaluate the accuracy of numerical solutions, we will use field distributions which produce fairly simple trajectories that can be solved by analytic methods. We will consider two cases:

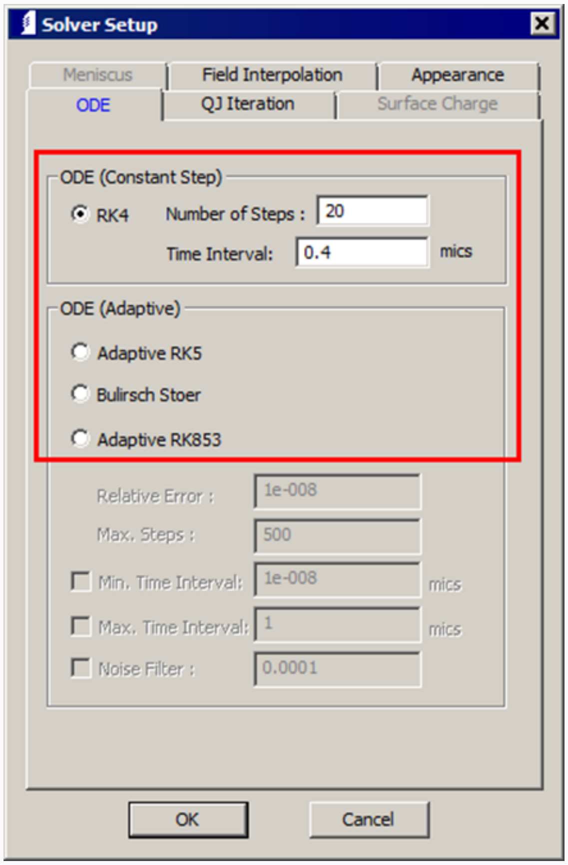
- Constant Electric Fields: Used in electrostatic deflectors. Charged particles will follow parabolic trajectories.
- Constant Magnetic Fields: Used in cyclotrons, steering magnets and particle traps. Particles will describe circular arcs including complete circular paths.

In practice, it is often difficult to create devices that produce exactly the ideal fields described above. However, the ideal approximation is often acceptably accurate for design purposes, especially over small regions.

Simulating Trajectories using the LORENTZ CAE Software Suite

The particle trajectory simulations in this paper will be produced using programs from the **LORENTZ** suite of CAE software products developed by **Integrated Engineering Software**. The **LORENTZ** programs incorporate both ODE and PDE solvers in the same package.

The picture at right shows the ODE solver types that can be selected for trajectory simulations.



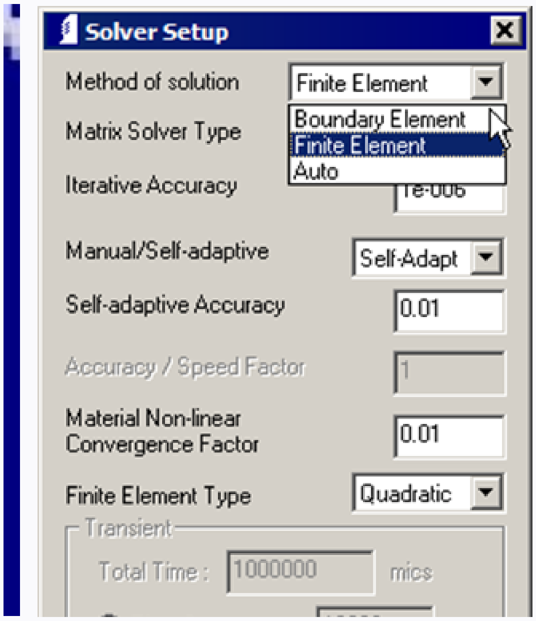
The simplest ODE solver type is the constant time step **fourth order Runge-Kutta** method which is abbreviated as **RK4**.

In addition, there are **adaptive** step methods such as the **Bulirsch Stoer**, **RK5** and **RK853** Runge-Kutta methods. These can often produce at least equivalent (and often better) accuracy with fewer simulation steps than the constant step **RK4** method.

We will compare results from all four solver methods in the course of this paper.

The ODE solvers generally employ field values calculated from PDE solution, but it is also possible to import external field data as we will describe in a later section.

LORENTZ programs contain both **Boundary Element Method** (**BEM**) and **Finite Element Method** (**FEM**) field solvers as shown at right. We will solve several field models using both methods for comparison.

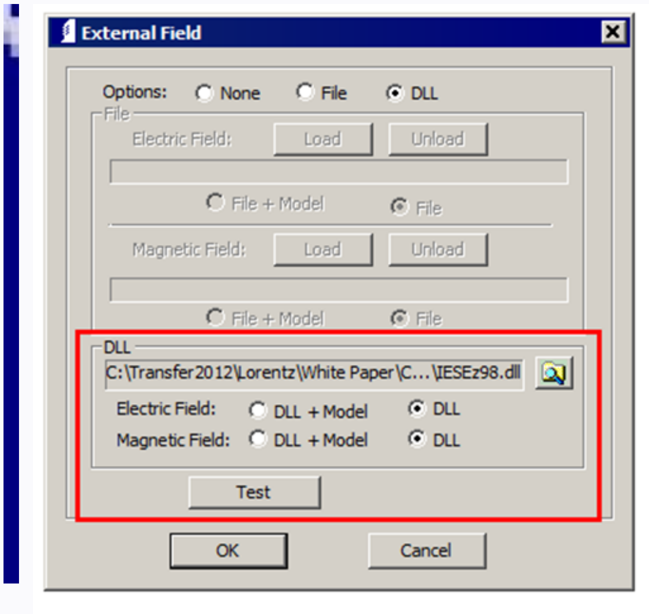


It is obvious that the trajectory simulations calculated by the ODE solvers are fundamentally dependent on the accuracy of the field simulations calculated by the PDE solvers. If actual trajectory simulations differ from expected analytic results, it can be difficult to determine whether the errors are due to bad ODE solutions or simply to errors in field values supplied from the PDE solution. In the next section we will explain how imported field values can be used to validate the ODE solver methods independently of the PDE solvers.

Isolating ODE Solution Errors

In order to compare the accuracy of the different ODE solvers, it is necessary to eliminate the possibility of errors due to the PDE solvers. Fortunately, the **LORENTZ** programs permit the use of field values which can be exactly defined by mathematical formulas using the **External Field** option.

The picture at right shows the **External Field** dialog box used to import field solutions. Fields can be imported using discrete data points from text files, or calculated from formulas coded into **Dynamic Link Library** (**DLL**) modules. The imported fields can either supplement or entirely replace fields obtained from the **PDE** solution.



The fields we will import will be DLL files created from **C++** code.

Constant E Field Simulations

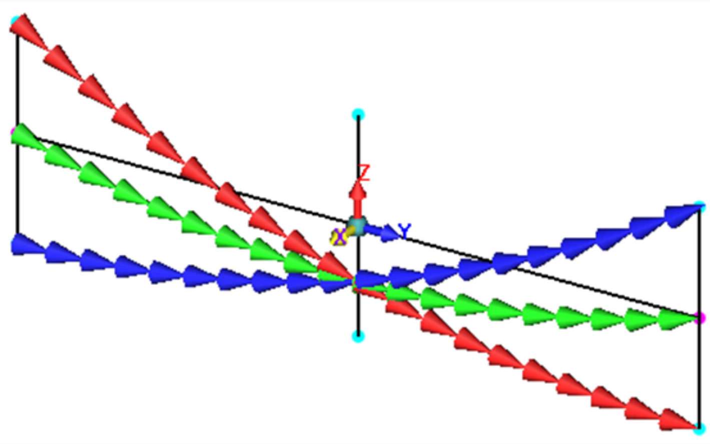
Overview

Charged particles launched in the region of a constant electric field will experience a constant force and acceleration in the direction of the field.

At right we show three trajectories of positive particles under the influence of a **Z** directed **E** field.

The blue trajectory was launched with an initial velocity in the **Y** direction, while the red and green trajectories had initial velocities that also contained negative **Z** components.

All three trajectories follow parabolic arcs, which can be calculated by simple analytic formulas.



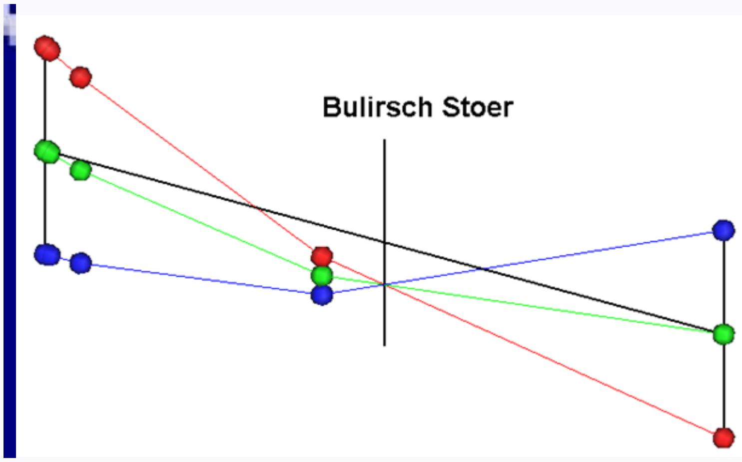
ODE Solutions for Mathematically Defined External Field

The trajectories shown above were computed by the **RK4** method, using field values defined mathematically in a **DLL** module. Only about 20 points were used so there are small discrepancies between the calculated points and the analytic formulas. However, the results can be made essentially the same as analytic calculations by simply reducing the time step.

The adaptive step ODE solvers also produce excellent results, though at first sight they may appear crude.

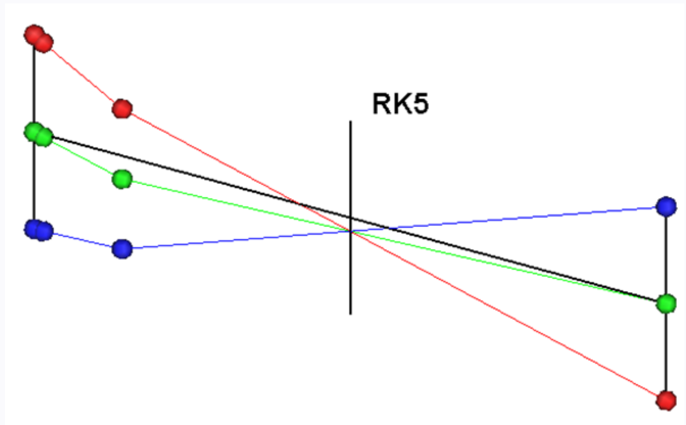
At right we show the results obtained from the **Bulirsch Stoer** method. Each trajectory consists of only 8 points, but the first 5 points are clustered closely together because the initial time steps are very small (this is a default setting that can be changed by the user).

As the algorithm adapts to the field variations, larger time steps are used for the last 3 points.



The simulated trajectory points do in fact follow the analytically calculated parabolas. This is easy to see for the start and end points, and can be verified for the intermediate points. The numerical efficiency of the adaptive step algorithms does have the drawback of producing poorer visualizations of the particle trajectories.

The **RK853** solver produces essentially the same results as the **Bulirsch Stoer**, but the **RK5** computes one less step as shown at right. Again the results are in excellent agreement with theoretical expectations.



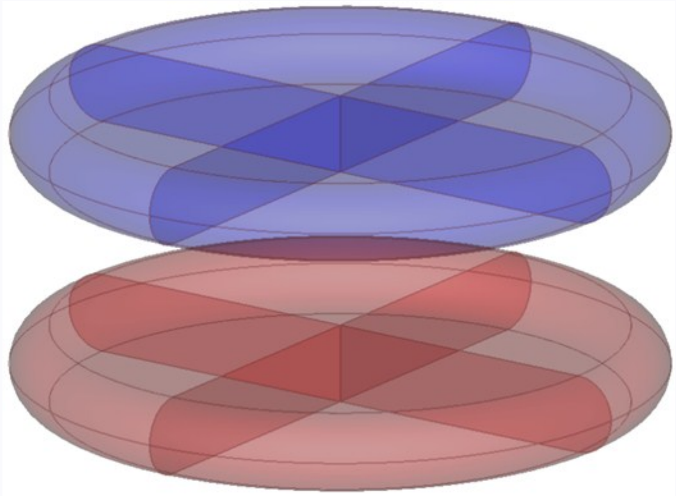
Approximate Physical Model

The electric field in the gap between parallel electrodes at different potentials will be approximately uniform. We will use this as a basis for creating a physical model which we will then solve using **BEM** and **FEM** algorithms.

At right we show the model we will use to approximate a constant field.

The system consists of a lower disk at a positive potential and an upper disk at a negative potential.

We will assign voltages such that the **E** field will be approximately **100 V/m** in the region between the disks.



Field Solver Methods

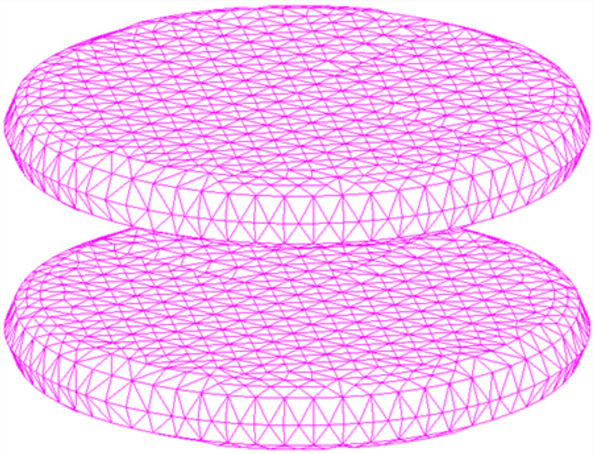
The most common field solvers used for electromagnetic applications are based on either the **Finite Element Method (FEM)** or the **Boundary Element Method (BEM)**. Both methods essentially convert the problem of solving the partial differential field equations into the numerical analysis problem of solving large systems of linear equations. However, the two methods have fundamental differences in the types of unknowns that are solved for, and in the type of meshing required.

FEM is the older of the two methods and was originally developed to solve structural analysis problems. As applied to electromagnetics, **FEM** formulates a system of linear equations that solves for a potential function, and the field solution is then obtained through a process of numerical differentiation.

BEM uses the approach of solving for equivalent sources (such as charges or currents) and obtains the field solution through a process of numerical integration.

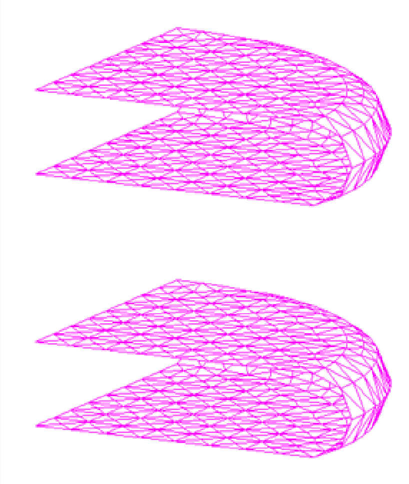
At right we show the type of mesh required for **BEM** analysis. The surfaces of the disks have been subdivided by a mesh of 2D triangles.

Note that there is no mesh required in the empty space region between or around the disks.



In the case of our disk system, the size of the model can be reduced by using symmetry or periodicity.

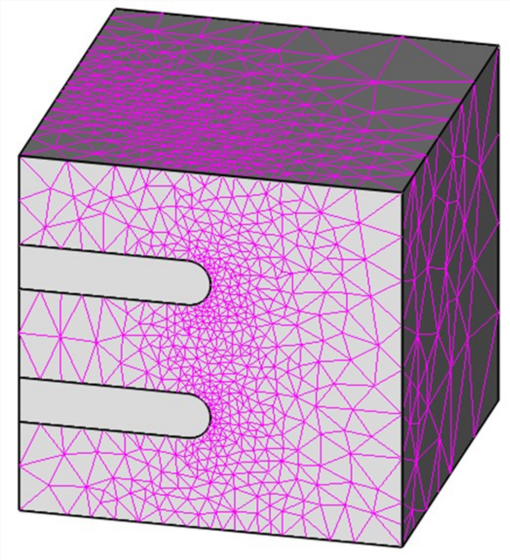
At right we have used two planes of symmetry to reduce the size of the model by a factor of four. The mesh on the reduced model clearly shows that only the outer surfaces require elements.



The same symmetric model will require a very different mesh for **FEM** simulation, as shown in the picture at right.

First note that a **FEM** solution requires the construction of an artificial boundary box to truncate the model space. The outer surfaces of the box (except symmetry surfaces) are assigned zero potential which terminates the field.

Also, a mesh of 3D tetrahedral elements must be constructed throughout the solution space around and in between the disks (no tetrahedra are required in the disk volumes however, since there outer surfaces are assigned constant potentials).



For the sake of clarity, the boundary box we have shown here was deliberately constructed to be roughly ***twice*** the disk dimensions. In practice, this would be too small to give an accurate solution. The normal rule of thumb is to use a factor of ***five times*** model dimensions, and we will use this convention for the models in this paper.

Comparison of Field Solutions

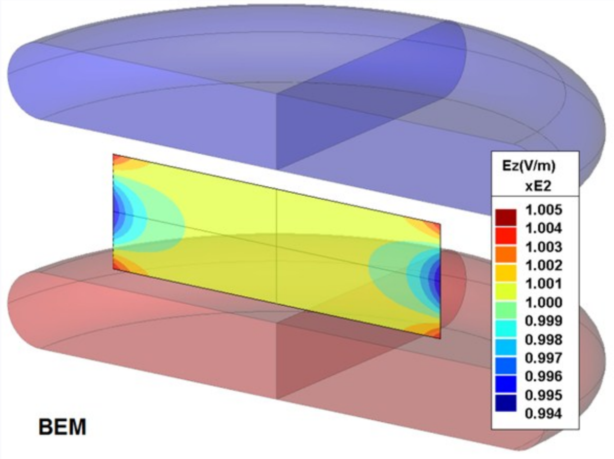
We will compare field plots for models solved using **BEM**, and **FEM**. Also we will show **FEM** results for both **linear** and **quadratic** basis function elements (using the same mesh in both cases).

We will begin with the **BEM** results.

At right we show a contour plot of the **axial (Z)** component of the **E** field on a plane in the center of the gap between the disks.

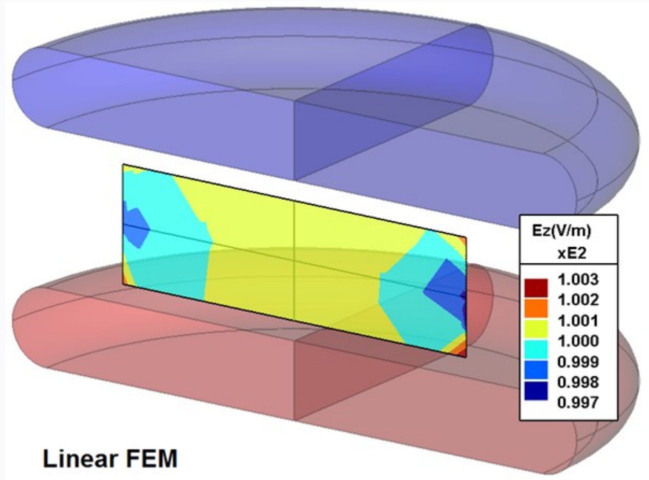
The field is extremely uniform in the center of the plots, but varies at the outer edges. In addition, the **radial** component of the field is extremely small in the center, but will become significant near the edges.

Note that the results are symmetric and show smooth variations between contour bands.



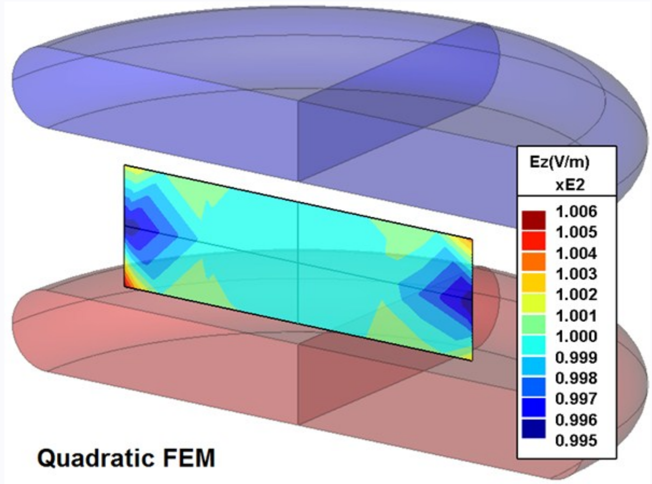
Next we show the result from **FEM** using **linear** basis elements.

The field magnitude is very close to the **BEM** results but the plot is no longer symmetric, and the edges of contour bands are straight line paths instead of continuous curves. These artifacts are unavoidable consequences caused by discrete nature of the mesh elements, and the differentiation of the potential solution used to calculate field values.



Using **Quadratic** basis function elements produces some improvement, but the asymmetry and sharp transitions are still present as shown at right.

Better results can be obtained with **FEM** by forcing a denser mesh, though this will of course increase the time needed to compute the field solution. This may or may not be needed depending on the accuracy criteria required.



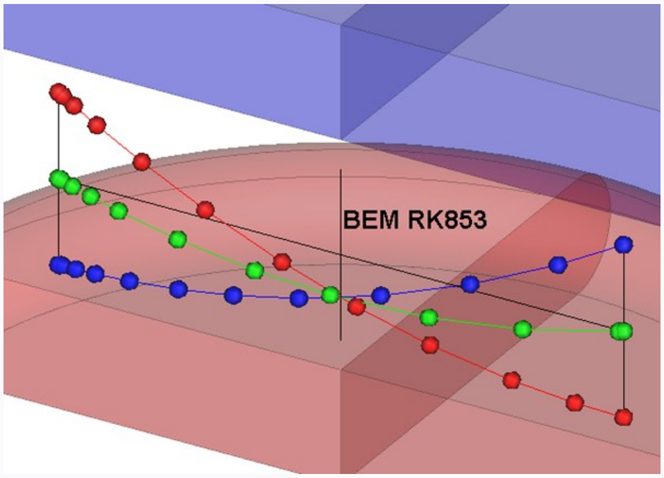
The fields defined by the **DLL** were mathematically ideal, consisting of only a constant **Z** component. The disk model produces a fairly uniform axial field, but it is not exactly constant and will contain radial components. The uniformity could be improved, and the radial components could be reduced by increasing the diameter of the disks and limiting trajectories to small regions near the disk center. The numerical solutions could also be improved by using finer levels of meshing. However, all numerical field solutions will inevitably contain some deviations from theoretically ideal fields.

Comparison of Trajectories Results from Field Solutions

The field results from all methods were good enough that the **RK4** simulations show no noticeable differences from the **DLL** model. The main differences occur when the adaptive step ODE solvers are used.

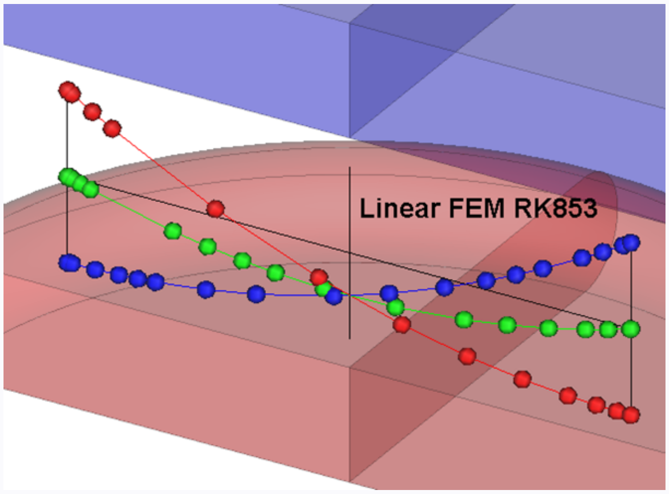
The non-ideal nature of the field created by our physical model combined with inevitable imperfections in the numerical field solutions cause the adaptive ODE solvers to use more trajectory steps.

At right we show the trajectory points calculated by the **RK853** algorithm using the **BEM** field solution. Note the initial dense clustering followed by essentially constant spacing.



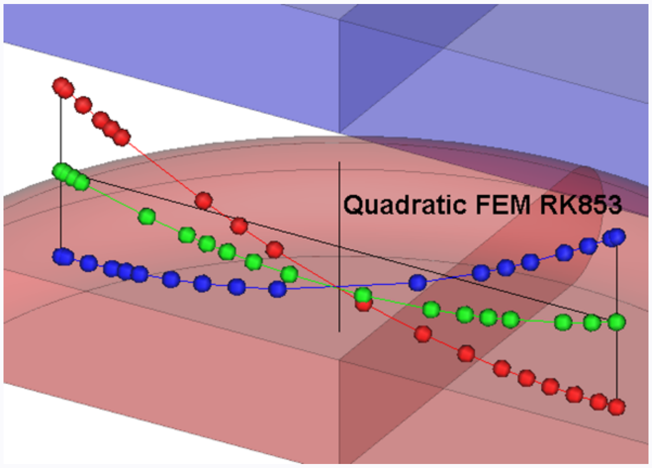
The **Linear FEM** results show additional clustering of points for sections where the calculated field changes abruptly.

However, the field uniformity is sufficient for the trajectories to be essentially parabolic arcs.



Similarly the **Quadratic FEM** results display additional clustering due to sharp field transitions.

In all three cases the results are extremely close to those of the ideal **DLL** model. Though we have referred to “abrupt” field changes the absolute value of field variations is on the order of one percent.



Constant B Field Simulations

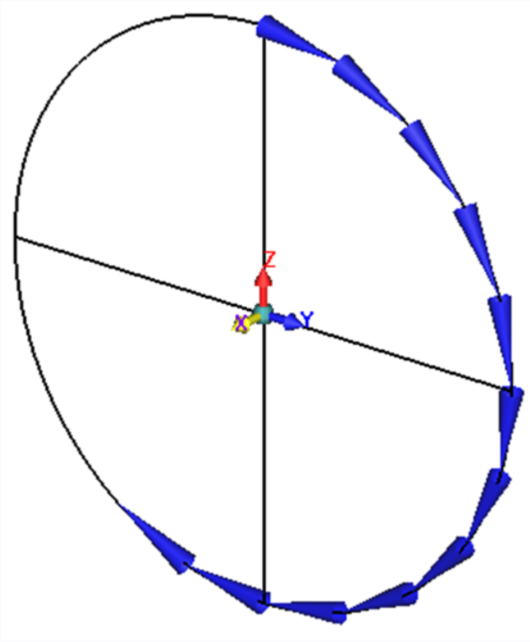
Overview

According to the **Lorentz Force** equation, charged particles traveling in a region with a magnetic field will experience a force determined by the cross product of the particle’s velocity vector and the **B** field vector.

If the **B** field is constant and the initial velocity vector is perpendicular to the field, the particle will describe a circular path with an axis parallel to the **B** field.

This situation is shown at right where the **B** field consists only of a positive **X** component, and the particle is launched in the positive **Y** direction.

Once again we will use a **DLL** to supply a constant field value in order to validate the ODE solvers. For the example shown, the **RK4** solver was used with step size set so that **20** points are calculated per cycle.

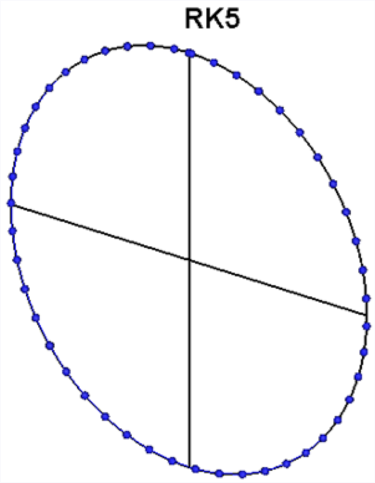


ODE Solutions for Mathematically Defined External Field

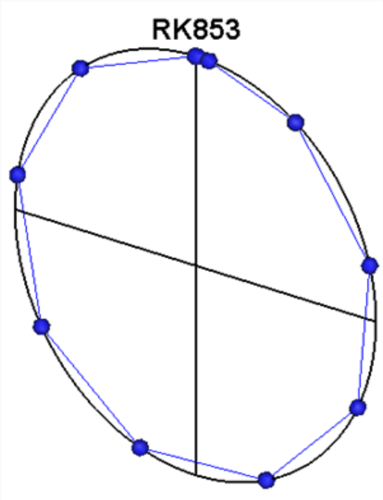
For an exact mathematically defined field and perpendicular launch, the particle should describe a circular path indefinitely.

Though the **RK4** method appears to produces a circular path for as few as **10** steps per cycle, the particle energy and path radius decreases with each cycle indicating too coarse of a step size. Using **20** steps per cycle largely corrects this.

The adaptive step **RK5** solver algorithm starts with the default minimum step size but quickly stabilizes at about **50** steps per cycle.

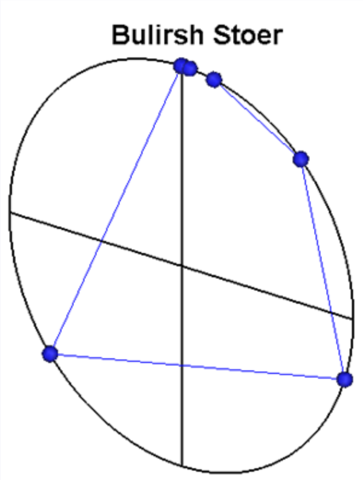


The **RK853** solver stabilizes at a fairly large interval and can produce excellent results with only **10** steps per cycle.



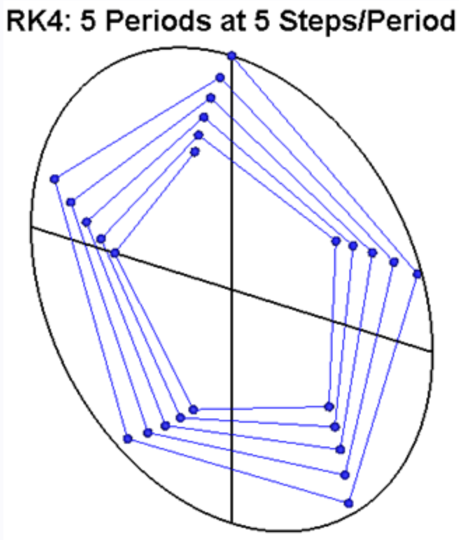
The **Bulirsch Stoer** algorithm is particularly efficient requiring less than **three** steps per cycle.

Note that though only a few points are calculated, they lie on the circle predicted by theoretical analysis.

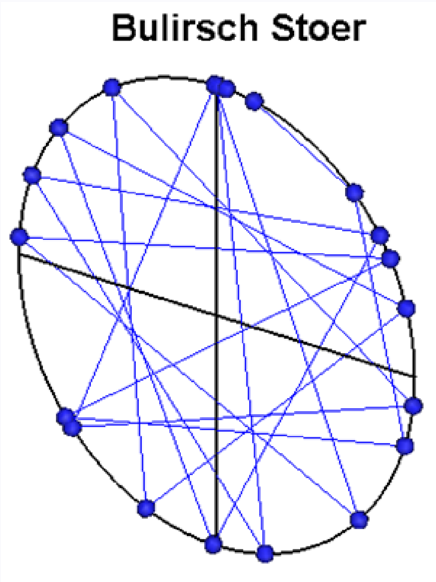


Stability over Several Cycles

In applications such as ion traps and cyclotrons, particle paths may describe several cycles, so it is of interest to know if the ODE solvers produce stable solutions.



As an example of an unstable solution, we used the **RK4** solver with the step size increased to one fifth the period for a complete cycle. The picture at right shows a simulation over five cycles. The results show a continuous loss of energy causing the particle to trace out ever smaller paths with each cycle. This clearly is not consistent with the physics of the system, and shows the ODE step size is too large for accurate results.



As a test the simulation time was increased to allow **ten** complete cycles. The adaptive step solvers produce outstanding results showing almost no energy loss, while the **RK4** with 20 steps/cycle shows a final loss of less than **0.3%**.

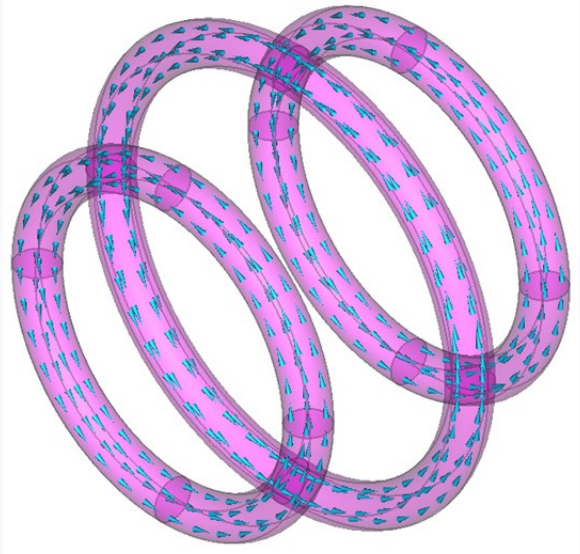
At right we show the **Bulirsch Stoer** solution which required only **24** steps for **ten** cycles. Final energy is about **0.24 parts per million** greater than the initial launch energy.

Approximate Physical Model

To generate an extremely uniform magnetic field we will use a **Maxwell Coil** model as shown at right.

Maxwell Coil systems are an improvement over the more common **Helmholtz Coil** systems. Though three coils are required, the resulting field has a greater degree of uniformity.

Our system will produce an axial field with an **X** component in the center of the coil region.



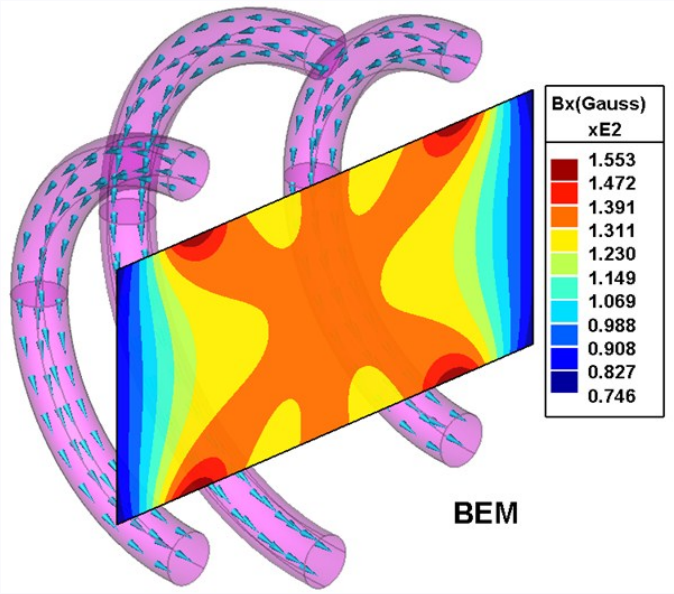
Comparison of Field Solutions

We will begin again with the **BEM** results.

At right we show a contour plot of the **axial (X)** component of the **B** field on a plane in the center of the coils.

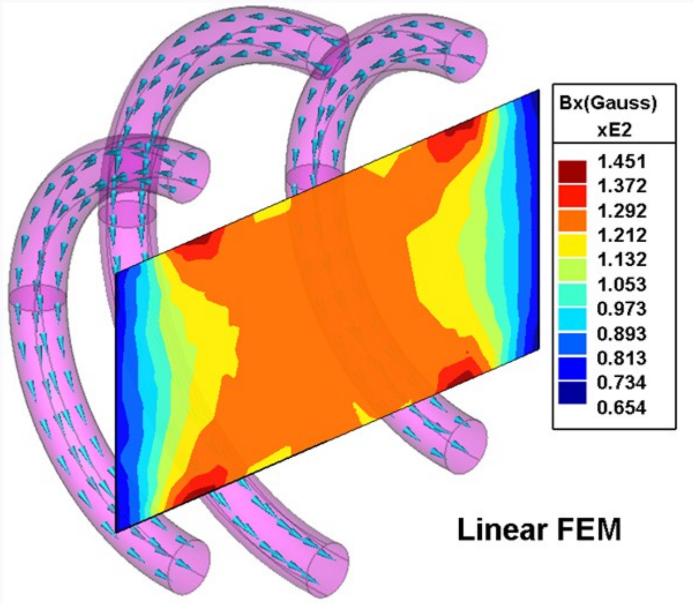
Unlike the **E** field results for the disk model, the **B** field contours have complex patterns. However there is a large central region where the field is uniform.

As in the electric field model, **BEM** results are again symmetric and show smooth variations between contour bands. Also the magnitude of the field at the coil center agrees very well with theoretical calculations.



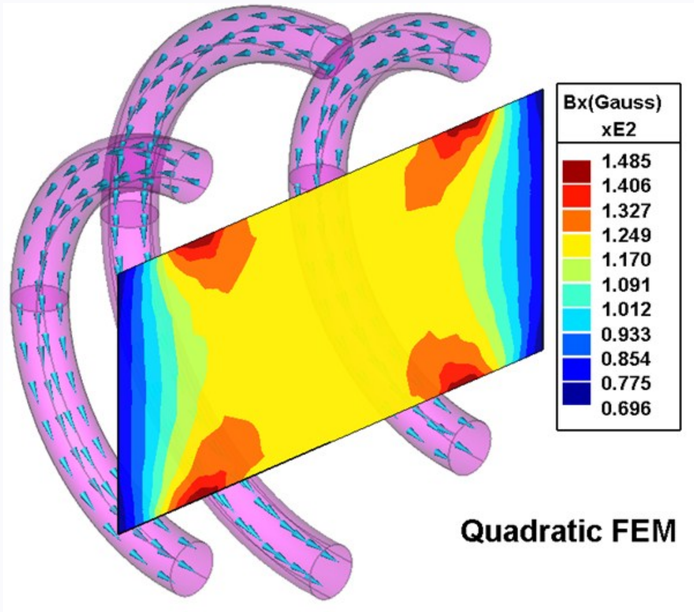
Next we show the result from **FEM** using **linear** basis elements.

The field magnitude at the center is about **92%** of the **BEM** results. The sharp field transitions are again apparent.



Using **Quadratic** basis function elements produces a field which is about **96%** of the **BEM** results, and slightly better contour transitions.

The slightly smaller **FEM** field values could be improved by using a larger boundary box. However, we will simply scale the currents to produce more or less equivalent **B** values (in order to use the same launch energies to produce approximately similar trajectories).

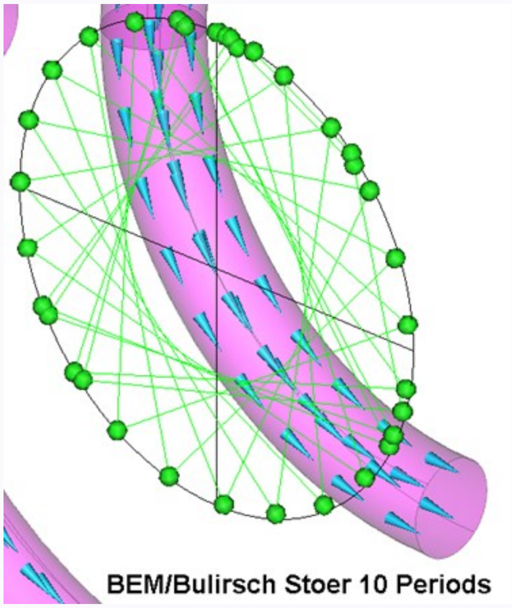


Comparison of Trajectories Results from Field Solutions

In attempting to compare results, it was found that the **FEM** solutions would not produce stable circular paths for the fields generated by the **Maxwell Coil** system. We will explain why this occurs.

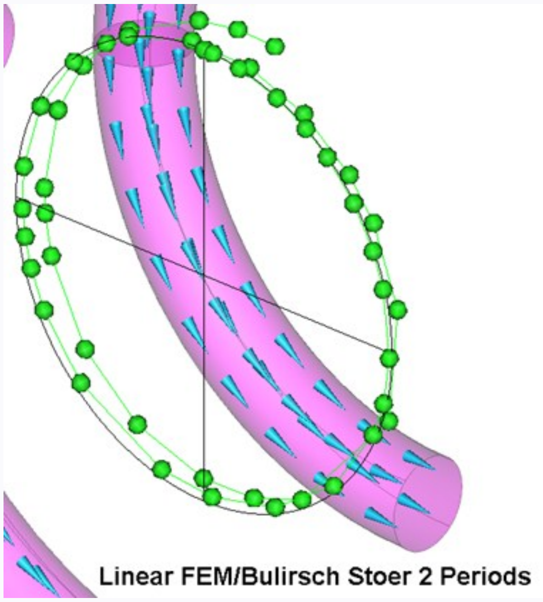
First note that if the **BEM** field solver is used, stable trajectories will be produced ***provided*** that the particles are launched exactly in the **X=0 (YZ)** plane.

At right we show the results for **10** periods using a combination of the **BEM** PDE and **Bulirsch Stoer** ODE solvers.

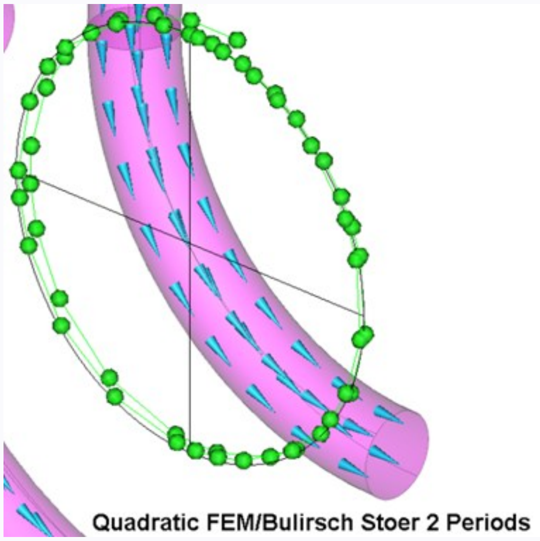


Problems arise with both **Linear** and **Quadratic FEM** field solvers for even a single period, but they become more apparent as simulation times increase so we will show results for two periods.

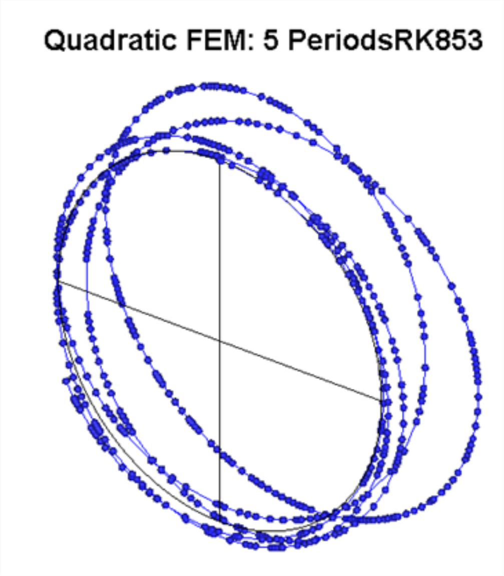
The **Linear FEM** results show a spiral path with a drift in the negative **X** direction.



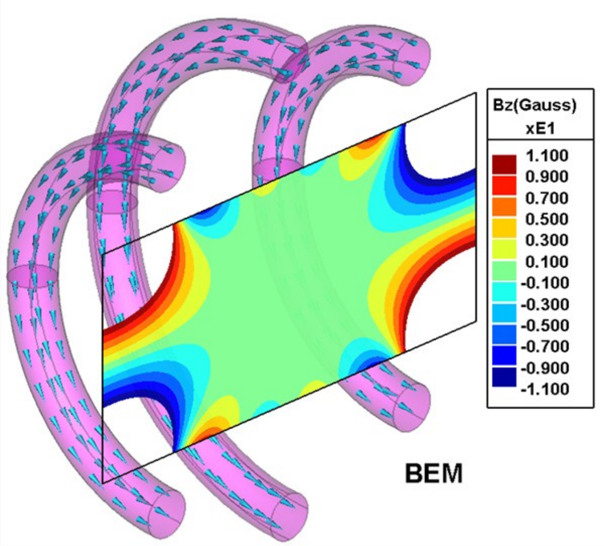
Similarly the **Quadratic FEM** results also display a drift in the **X** direction, though it is not as extreme.



As the simulation time is increased, the **FEM** trajectories show a "mirror" effect, oscillating back and forth in the **X** direction while spiraling around the **X** axis.



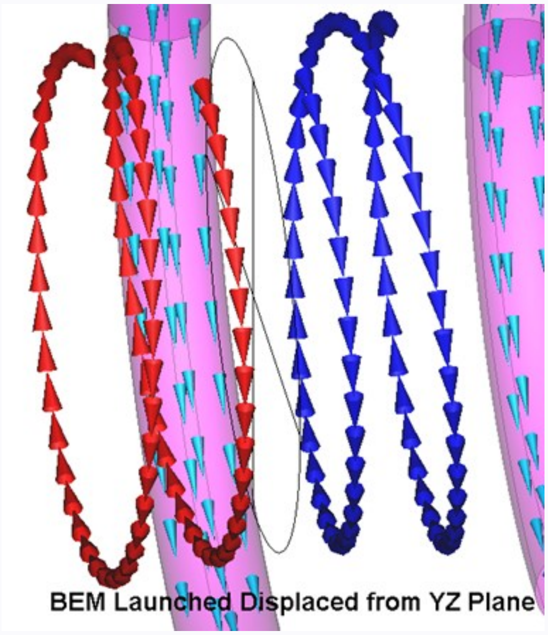
The explanation for this is that though the coils produce a predominantly **axial** field, the **radial** field components are not identically zero, except for certain regions such as the coil axis, and the perpendicular plane of the central coil.



This is shown by the contour plot of the **Z** component of the field in the **Y=0 (XZ)** plane.

Any radial components will produce drifting in the axial direction. The **BEM** solution is accurate enough that the radial components in the launch plane are negligible. However, the **FEM** solver errors result in significant radial components.

A similar effect can be produced with the **BEM** field solution if we deliberately launch at some displacement from the **YZ** plane as shown at right.



Though the inaccuracies of **FEM** solutions had little effect for the constant **E** field simulations, they can produce significant errors for constant **B** field simulations.

Summary

Charged particle beam analysis requires a high degree of accuracy for both PDE and ODE solutions. Obtaining an accurate solution of the electromagnetic fields is a critical prerequisite for accurate trajectory simulations.

Based on the models studied in this paper, we can draw the following conclusions.

- Adaptive step ODE solvers have a distinct advantage both in terms of calculation efficiency, and (perhaps more important) in terms of stability of solutions.

- The **Boundary Element Method (BEM)** field solvers appear to have an inherent advantage over **Finite Element Method (FEM)** solvers both in accuracy, and in ease of obtaining solutions.

Because of the wide range of particle beam applications, it is certainly desirable to have a variety of options for both the PDE and ODE solutions, since no one analysis method is best for all possible situations.

As a final comment, we will note that while accurate ODE and PDE solvers are essential for any CAE beam simulation software, a fully functional package must also be capable of modeling complex physical phenomena such as space charge effects and emission regimes; as well as providing sophisticated analysis options such as Emittance plots and Spot Size calculations. Whenever possible, it is highly desirable to test software on a trial evaluation period to confirm its suitability before making a purchase decision.

About INTEGRATED Engineering Software

Since its inception in 1984, INTEGRATED Engineering Software has created simulation tools that reflect the inspiration of our customers: thousands of engineers and scientists who, everyday, push the boundaries to envision what is possible. They take their ideas from a realm that is almost science fiction and bring them to reality.

As the name of our company suggests, all our programs are seamlessly integrated, starting from a concept, through entry of the geometry and physics of the problem, to the selection of type of solver and the problem's solution. Once the problem has been solved, a vast number of parameters can be calculated or the field quantities displayed.

INTEGRATED Engineering Software is a leading developer of hybrid simulation tools for electromagnetic and particle trajectory analysis. We provide a complete line of fully integrated 2 and 3 dimensional simulation software.

Since the creation of our company, our focus has always been here and our experience has grown hand-by-hand with a great recognition in our market.

INTEGRATED is staffed with leading R&D engineers in areas such as electrical engineering, magnetics, and high frequency applications. Our tools are used in a wide variety of industries, including manufacturing, automotive, medical, telecommunications, power, health care and aerospace markets, as well as universities and research laboratories.

INTEGRATED products allow engineers and scientists to reduce design cycles, save time and money and deliver more efficient products to the market faster than ever before.

INTEGRATED empowers engineers and scientists with many options to choose from:
The best solvers for each specific application: Boundary Element Method (BEM), Finite Element Method (FEM) or Finite Difference Time Domain (FDTD) solvers. The best optimization tool for each particular design: parametric analysis, scripting or application programming interface (API)

INTEGRATED’s commitment is to provide designers with the most sophisticated analysis tools to assist them in the creation of the future.

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