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Electron Beam Divergence Due to Self Potential

Introduction

When modeling the propagation of a charged particle beam at a high current, the electric field due to the space charge of the beam significantly affects the trajectories of the charged particles. Perturbations to these trajectories, in turn, affect the space charge distribution. In order to accurately predict the properties of the beam, the particle trajectories and fields must be computed in a self-consistent manner. The Charged Particle Tracing interface can use an iterative procedure to efficiently compute the strongly coupled particle trajectories and electric field for systems operating under steady-state conditions. Such a procedure reduces the required number of model particles by several orders of magnitude, compared to methods based on explicit modeling of Coulomb interactions between the beam particles. A mesh refinement study confirms that the solution agrees with the analytical expression for the shape of a nonrelativistic, paraxial beam envelope.

Note: This application requires the Particle Tracing Module.

Model Definition

This model computes the shape of an electron beam propagating through free space. When the magnitude of the beam current is large enough that Coulomb interactions are significant, the shape of the beam may be determined by solving a set of strongly coupled equations for the beam potential and the electron trajectories,

$$\nabla \cdot \varepsilon_0 \nabla V = \sum_{i=1}^{N} e\delta(\mathbf{r} - \mathbf{q}_i)$$

$$\frac{d}{dt}(m_e v) = e\nabla V$$

The beam electrons are assumed to be nonrelativistic so that magnetic forces can be neglected. Modeling the beam electrons and the resulting electric potential using a time-dependent study would require a very large number of model particles to be released at a large number of time intervals. Instead, this model computes the shape of the electron beam by coupling a time-dependent study step for computing the particle trajectories to a stationary step for computing the electric potential. This algorithm is suitable for modeling beams which operate at steady-state conditions. It consists of the following steps:

1 Compute the particle trajectories, assuming no space charge effects are present, using a time-dependent solver. From these trajectories, compute the space charge density using the **Electric Particle Field Interaction** node.
2 Compute the electric potential due to the space charge density of the beam, using a stationary solver. The model uses an **Infinite Element Domain** region to apply appropriate boundary conditions for a beam propagating in free space.
3 Use the electric potential calculated in step 2 to compute the perturbed particle trajectories. Recalculate the space charge density using these perturbed trajectories.
4 Repeat steps 2 and 3 until a specified number of iterations has been reached.

After several iterations, the particle trajectories and the corresponding space charge density and electric field reach a stable, self-consistent solution. For a nonrelativistic, paraxial beam of electrons, the shape of the beam envelope is given by Ref. 1 as

$$z = \frac{R_0 F(\chi)}{\sqrt{2K}} \tag{1}$$

where z is the distance from the beam waist, R_0 is the waist radius, K is the generalized beam perveance,

$$K = \frac{eI_0}{2\pi\varepsilon_0 m_e v_z^3}$$

χ is the ratio of the beam radius to the beam waist radius, and

$$F(\chi) = \int_1^{\chi} \frac{dy}{\sqrt{\ln(y)}} \tag{2}$$

This analytical expression for the relationship between axial position and beam envelope radius is used to determine the accuracy of the solution. A mesh refinement study confirms that the agreement between the solutions improves as the mesh element size is reduced.

In this example, **Specify current** is selected from the **Particle release specification** list in the physics interface **Particle Properties** section. As a result, each model particle represents a continuous stream of particles, released at regular time intervals, rather than the instantaneous position of a charge. For the purpose of modeling particle-field interactions, each model particle leaves behind a trail of space charge in its wake. The contribution of each model particle to the total space charge density of the beam is found by evaluating the sum

$$\frac{d\rho}{dt} = eZ\sum_{i=1}^{N} f_{\mathrm{rel}}\delta(\mathbf{r}-\mathbf{q}_i)$$

where e is the elementary charge, Z is the charge number of the particles, δ is the Dirac delta function, and f_{rel} is the effective frequency of release of the particle. The frequency of release is the number of particles per model particle per second. To avoid the infinite potential associated with an infinitesimally small point charge, the space charge density is distributed uniformly over each mesh element before the electrostatics problem is solved.

Results and Discussion

After several iterations, the model reaches a self-consistent solution for the trajectories of the electrons and the beam potential. The electron trajectories are plotted in Figure 1. The expression `r-at(0,r)` is used to define a color expression for the trajectories. The `at` operator is used to evaluate an expression at the initial time, rather than the current time. Thus the color expression gives the radial displacement of each particle due to space charge effects.

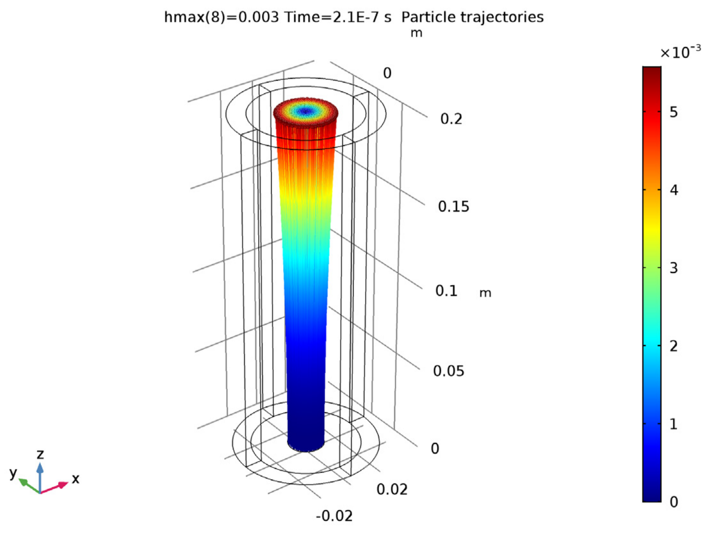

Figure 1: A beam of electrons with a waist located at z = 0 diverges due to transverse beam forces. The color represents the radial displacement of each electron from its initial position.

The electric potential distribution in the beam is shown in Figure 2. Since the beam propagates from left to right, and the beam electrons initially move in the positive

z direction, the left end of the plot corresponds to the beam waist. This is also the location where the beam radius is smallest in magnitude.

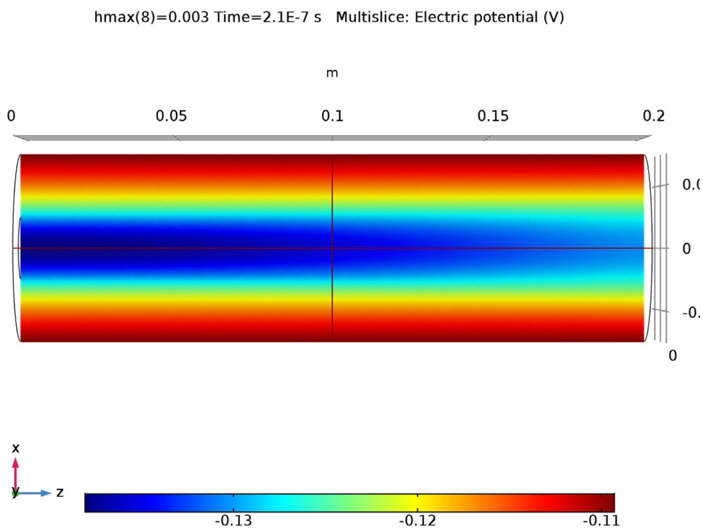

Figure 2: Plot of the electric potential of the electron beam. The potential is greatest in magnitude close to the beam waist.

A mesh refinement study confirms that the shape of the beam envelope agrees more closely with the analytical expression of Equation 1 as the maximum mesh element size is reduced. The distance from the beam waist as a function of beam radius is compared to the result of this expression, and the relative error is plotted in Figure 3. For all values of the maximum element size, the error shown is computed after three iterations of the solver loop.

These results show that a self-consistent solution for the particle trajectories and the fields due to their space charge density can be obtained using an iterative solver sequence. This requires much less time and memory than a fully coupled time-dependent study of the individual beam particles and their fields. The accuracy of the solution clearly improves as the mesh element size is reduced, enabling more accurate computation of the electron trajectories and beam potential.

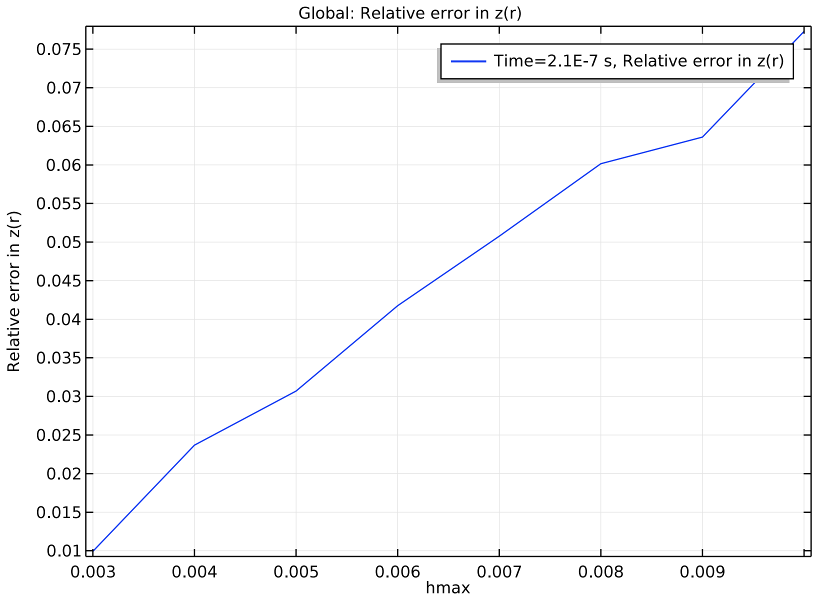

Figure 3: The results of a mesh refinement study indicate that the observed relationship between beam radius and distance from the beam waist converges to the expected value as the mesh is refined. The comparison is made at a location 0.2 meters from the waist.

Reference

1. S. Humphries, *Charged Particle Beams*, Dover Publications, New York, 2013.

Application Library path: `ACDC_Module/Particle_Tracing/electron_beam_divergence`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.
2 In the **Select Physics** tree, select **AC/DC>Particle Tracing>Particle Field Interaction, Non-Relativistic**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Bidirectionally Coupled Particle Tracing**.
6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

   To save time, the parameters can be loaded from a file.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
3 Click **Load from File**.
4 Browse to the model's Application Libraries folder and double-click the file `electron_beam_divergence_parameters.txt`.

GEOMETRY 1

Cylinder 1 (cyl1)

1 On the **Geometry** toolbar, click **Cylinder**.
2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
3 In the **Radius** text field, type `r2`.
4 In the **Height** text field, type `L`.
5 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	tlayer

6 Right-click **Cylinder 1 (cyl1)** and choose **Build Selected**.

Work Plane 1 (wp1)

1 On the **Geometry** toolbar, click **Work Plane**.
2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane type** list, choose **Face parallel**.

4 Find the **Planar face** subsection. Select the **Active** toggle button.

5 On the object **cyl1**, select Boundary 10 only.

6 Click **Show Work Plane**.

Circle 1 (c1)

1 On the **Work Plane** toolbar, click **Primitives** and choose **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `r0beam`.

4 Right-click **Circle 1 (c1)** and choose **Build Selected**.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permittivity	epsilonr	1	1	Basic

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
qr	sqrt(qx^2+qy^2)	m	Radial distance from beam axis
qrmax	cpt.cptmaxop1(qr)	m	Beam radius
z_avg	cpt.cptaveop1(qz)	m	Average z-coordinate
chi	qrmax/at(0,qrmax)		Ratio of beam radius to waist radius

To model a drifting electron beam propagating in a large, open area, surround the modeling domain with an **Infinite Element Domain**. This results in appropriate boundary conditions for the electric potential.

Infinite Element Domain 1 (ie1)

1 On the **Definitions** toolbar, click **Infinite Element Domain**.
2 In the **Settings** window for **Infinite Element Domain**, locate the **Geometry** section.
3 From the **Type** list, choose **Cylindrical**.
4 Select Domains 1, 2, 4, and 5 only.

CHARGED PARTICLE TRACING (CPT)

Inlet 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Charged Particle Tracing (cpt)** and choose **Inlet**.
2 Select Boundary 12 only.
3 In the **Settings** window for **Inlet**, locate the **Release Current Magnitude** section.
4 In the *I* text field, type `Ibeam`.
5 Locate the **Initial Position** section. From the **Initial position** list, choose **Density**.
6 In the *N* text field, type `1000`.
7 Locate the **Initial Velocity** section. Specify the $\mathbf{v}_0$ vector as

0	x
0	y
v0beam	z

Electric Force 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Electric Force 1**.
2 Select Domain 3 only.
3 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.
4 From the $\mathbf{E}$ list, choose **Electric field (es/ccn1)**.
5 Locate the **Advanced Settings** section. Select the **Use piecewise polynomial recovery on field** check box.

ELECTROSTATICS (ES)

On the **Physics** toolbar, click **Charged Particle Tracing (cpt)** and choose **Electrostatics (es)**.

Ground 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrostatics (es)** and choose **Ground**.
2. Select Boundaries 2, 3, 14, and 22 only.

MESH 1

Free Tetrahedral 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Free Tetrahedral**.
2. In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.
3. From the **Geometric entity level** list, choose **Domain**.
4. Select Domain 3 only.

Size 1

1. Right-click **Component 1 (comp1)>Mesh 1>Free Tetrahedral 1** and choose **Size**.
2. In the **Settings** window for **Size**, locate the **Element Size** section.
3. Click the **Custom** button.
4. Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.
5. In the associated text field, type `hmax`.

Distribution 1

1. In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.
2. Right-click **Swept 1** and choose **Distribution**.
3. In the **Settings** window for **Distribution**, click **Build All**.

STUDY 1

Step 1: Bidirectionally Coupled Particle Tracing

1. In the **Settings** window for **Bidirectionally Coupled Particle Tracing**, locate the **Study Settings** section.
2. Click **Range**.
3. In the **Range** dialog box, type `1e-8` in the **Step** text field.
4. In the **Stop** text field, type `21e-8`.
5. Click **Replace**.
6. In the **Settings** window for **Bidirectionally Coupled Particle Tracing**, locate the **Iterations** section.

7 From the **Termination method** list, choose **Convergence of global variable**.

8 In the **Global variable** text field, type `qrmax`.

9 In the **Relative tolerance** text field, type `1E-5`.

10 In the **Relative tolerance threshold** text field, type `0.015`.

11 In the **Maximum number of iterations** text field, type `8`.

Use a **Parametric Sweep** to confirm that a finer mesh results in closer agreement with the expected beam envelope size.

Parametric Sweep

1 On the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
hmax		

5 Click **Range**.

6 In the **Range** dialog box, type `0.01` in the **Start** text field.

7 In the **Step** text field, type `-0.001`.

8 In the **Stop** text field, type `0.003`.

9 Click **Replace**.

The smallest mesh size requires about 5 GB RAM.

10 On the **Study** toolbar, click **Compute**.

RESULTS

Plot the trajectories of the electrons, using a **Color Expression** to observe their radial displacement over time.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Results>Particle Trajectories (cpt)** node, then click **Particle Trajectories 1**.

2 In the **Settings** window for **Particle Trajectories**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Type** list, choose **Line**.

Color Expression 1

1 In the **Model Builder** window, expand the **Particle Trajectories 1** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `qr-at(0,qr)`.

4 On the **Particle Trajectories (cpt)** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar. This plot should look like Figure 1.

Data Sets

The electric potential can be visualized more clearly by excluding the selection of the **Infinite Element Domain** from the **Study 1/Parametric Solutions 1 (sol2)** data set.

Study 1/Parametric Solutions 1 (sol2)

In the **Model Builder** window, expand the **Results>Data Sets** node, then click **Study 1/Parametric Solutions 1 (sol2)**.

Selection

1 On the **Results** toolbar, click **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 3 only.

Electric Potential (es)

1 In the **Model Builder** window, under **Results** click **Electric Potential (es)**.

2 In the **Settings** window for **3D Plot Group**, click to expand the **Color legend** section.

3 Locate the **Color Legend** section. From the **Position** list, choose **Bottom**.

4 Click the **Go to ZX View** button on the **Graphics** toolbar. This plot should look like Figure 2.

For each mesh size, compare the beam envelope shape to the analytical solution for a paraxial, nonrelativistic beam.

1D Plot Group 3

1 On the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

4 From the **Time selection** list, choose **Last**.

Global 1

1. Right-click **1D Plot Group 3** and choose **Global**.
2. In the **Settings** window for **Global**, type `Relative Error in Longitudinal Beam Displacement` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`abs((r0beam/sqrt(2*K)*integrate(1/sqrt(log(s)),s,1+eps,chi)-z_avg)/z_avg)`		`Relative error in z(r)`

   This expression is Equation 1, where the first argument of the `integrate` operator is the integrand of Equation 2. The lower limit of integration is increased by the floating point relative accuracy `eps` (machine epsilon, 2^{-52} or about 2.2204×10^{-16}) to avoid division by zero during numerical integration.

4. Locate the **x-Axis Data** section. From the **Axis source data** list, choose **hmax**.
5. On the **1D Plot Group 3** toolbar, click **Plot**. This plot should look like Figure 3.