

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. To validate the model, the change in beam radius from the waist position is compared to an analytic expression for the shape a nonrelativistic, paraxial beam envelope.

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,

$$\nabla \cdot \varepsilon_0 \nabla V(\mathbf{r}) = \sum_{i=1}^N e \delta(\mathbf{r} - \mathbf{q}_i)$$
$$\frac{\mathrm{d}}{\mathrm{d}t} \left(m_\mathrm{e} \frac{\mathrm{d}\mathbf{q}_i}{\mathrm{d}t} \right) = e \nabla V$$

where

- $m_{\rm e} = 9.10938356 \times 10^{-31}$ kg is the electron mass,
- $e = 1.602176634 \times 10^{-19}$ C is the elementary charge,
- $\varepsilon_0 = 8.854187817 \times 10^{-12}$ F/m is the permittivity of vacuum,
- V (SI unit: V) is the electric potential,
- N (dimensionless) is the total number of particles,
- **r** (SI unit: m) is the position vector,
- \mathbf{q}_i (SI unit: m) is the position of the *i*th particle, and
- δ (SI unit: 1/m³) is the Dirac delta function.

The beam electrons are assumed 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** analysis of the particle trajectories to a **Stationary** analysis of the electric potential. The two different types of solver are combined using the dedicated **Bidirectionally Coupled Particle Tracing** study step. This algorithm is suitable for modeling beams which operate at steady-state conditions. It consists of the following steps:

- I Compute the particle trajectories in the time domain, ignoring Coulomb forces. Compute the space charge density using the **Electric Particle Field Interaction** node.
- **2** Compute the stationary electric potential due to the space charge density of the beam.
- **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, or until some other user-specified convergence criterion has been met.

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 should follow the equation

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

where z (SI unit: m) is the distance from the beam waist, R_0 (SI unit: m) is the waist radius, K (dimensionless) is the generalized beam perveance,

$$K = \frac{eI_0}{2\pi\varepsilon_0 m_{\rm e} v_z^3}$$

 χ (dimensionless) is the ratio of the beam radius to the beam waist radius, and

$$F(\chi) = \int_{1}^{\chi} \frac{dy}{\sqrt{\ln(y)}}$$
(2)

In this example, each model particle actually represents a continuous stream of electrons, released at regular time intervals, rather than the instantaneous position of a single 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 particle to the total space charge density of the beam is found by evaluating the sum

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

where f_{rel} (SI unit: 1/s) is a proportionality factor that indicates the number of real electrons that each model particle represents. 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 electron trajectories and the beam potential. The trajectories are shown 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 from its position at the waist.



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 **Global Evaluation** is then used to compare the shape of the beam envelope to the analytic solution given by Equation 1. The results differ only by a few percentage points, which can be attributed to discretization error since the contribution of each particle to the space charge density is discretized using constant shape functions over each mesh element.

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.

Reference

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

Application Library path: Particle_Tracing_Module/ Charged_Particle_Tracing/electron_beam_divergence

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click 🔗 Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 间 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> Charged Particle Tracing>Bidirectionally Coupled Particle Tracing.
- 6 Click M Done.

GLOBAL DEFINITIONS

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

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 I

Cylinder I (cyl1)

- I In the Geometry toolbar, click 问 Cylinder.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r0.
- **4** In the **Height** text field, type L.
- 5 Click 틤 Build Selected.

Work Plane I (wp1)

I In 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 On the object cyll, select Boundary 3 only.

It might be easier to select the correct boundary by using the **Selection List** window. To open this window, in the **Home** toolbar click **Windows** and choose **Selection List**. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)

5 Click 📥 Show Work Plane.

Work Plane I (wp1)>Circle I (c1)

- I In the Work Plane toolbar, click 📀 Circle.
- 2 In the Settings window for Circle, locate the Size and Shape section.
- 3 In the Radius text field, type r0beam.
- 4 Click 틤 Build Selected.

ADD MATERIAL

- I In the Home toolbar, click 🙀 Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Perfect vacuum.
- 4 Click Add to Component in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Material to close the Add Material window.

DEFINITIONS

Variables I

- I In the Home toolbar, click a= 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.max(qr)	m	Beam radius
z_avg	cpt.ave(qz)	m	Average z-coordinate
chi	qrmax/at(0,qrmax)		Ratio of beam radius to waist radius

CHARGED PARTICLE TRACING (CPT)

Particle Properties 1

- I In the Model Builder window, under Component I (compl)>Charged Particle Tracing (cpt) click Particle Properties I.
- 2 In the Settings window for Particle Properties, locate the Particle Species section.
- 3 From the Particle species list, choose Electron.

Inlet I

- I In the Physics toolbar, click 🔚 Boundaries and choose Inlet.
- **2** Select Boundary 5 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	у
vObeam	z

Electric Force 1

- I In the Model Builder window, click Electric Force I.
- **2** Select Domain 1 only.
- 3 In the Settings window for Electric Force, locate the Electric Force section.
- 4 From the **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)

In the Model Builder window, under Component I (compl) click Electrostatics (es).

Ground I

I In the Physics toolbar, click 📄 Boundaries and choose Ground.

2 Select Boundaries 1, 2, 6, and 7 only.



MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Sequence Type section.
- 3 From the list, choose User-controlled mesh.

Size

- I In the Model Builder window, under Component I (compl)>Mesh I click Size.
- 2 In the Settings window for Size, click to expand the Element Size Parameters section.
- 3 In the Maximum element size text field, type hmax.
- 4 Click 📗 Build All.

STUDY I

- Step 1: Bidirectionally Coupled Particle Tracing
- In the Model Builder window, under Study I click
 Step I: Bidirectionally Coupled Particle Tracing.
- 2 In the Settings window for Bidirectionally Coupled Particle Tracing, locate the Study Settings section.
- 3 Click Range.
- 4 In the Range dialog box, type 1e-8 in the Step text field.

- 5 In the Stop text field, type 21e-8.
- 6 Click Replace.
- 7 In the Settings window for Bidirectionally Coupled Particle Tracing, locate the Iterations section.
- 8 From the Termination method list, choose Convergence of global variable.
- 9 In the Global variable text field, type qrmax.
- **IO** In the **Relative tolerance** text field, type **1E-5**.
- II In the Relative tolerance threshold text field, type 0.015.
- 12 In the Maximum number of iterations text field, type 8.
- **I3** In the **Home** toolbar, click **= Compute**.

RESULTS

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

Particle Trajectories 1

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

- I In the Model Builder window, expand the Particle Trajectories I node, then click Color Expression I.
- 2 In the Settings window for Color Expression, locate the Expression section.
- 3 In the Expression text field, type qr-at(0,qr).
- 4 Locate the Coloring and Style section. Click Change Color Table.
- 5 In the Color Table dialog box, select Linear>Viridis in the tree.
- 6 Click OK.
- 7 In the Particle Trajectories (cpt) toolbar, click 🗿 Plot.
- 8 Click the Figure 1. **Zoom Extents** button in the **Graphics** toolbar. This plot should look like

Electric Potential (es)

- I In the Model Builder window, under Results click Electric Potential (es).
- 2 In the Settings window for 3D Plot Group, locate the Color Legend section.

- **3** From the **Position** list, choose **Bottom**.
- 4 In the Graphics window toolbar, click ▼ next to ↓ Go to Default View, then choose Go to ZX View. This plot should look like Figure 2.

Global Evaluation 1

- I In the Results toolbar, click (8.5) Global Evaluation.
- 2 In the Settings window for Global Evaluation, locate the Data section.
- **3** From the **Time selection** list, choose **Last**.
- **4** Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
<pre>r0beam/sqrt(2*K)*integrate(1/ sqrt(log(s)),s,1+eps,chi)</pre>	m	Expected z-coordinate for beam radius
z_avg	m	Average z-coordinate

5 Click **= Evaluate**.

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