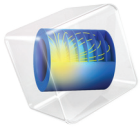

Particle Tracing Module

Application Library Manual

5.3

COMSOL

Particle Tracing Module Application Library Manual

Version: COMSOL 5.3

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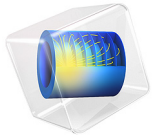


Brownian Motion

Introduction

Particle tracing offers an attractive alternative to continuum-based numerical methods, such as the finite element method, for modeling species transport in strongly convecting flows because the particle tracing method is insensitive to the magnitude of the Péclet number. In most real systems, species transport has both a convective and diffusive component. Particle tracing can be used to solve purely convective motion, purely diffusive motion and anything in-between. Thus using a particle-based approach the entire spectrum of Péclet numbers can be handled without encountering the numerical instabilities associated with the continuum approach.

In this example the agreement between the continuum and particle-based numerical methods is verified in the case of purely diffusive motion.

Model Definition

The diffusion equation is solved in two different ways. First, the species concentration is computed using the Transport of Diluted Species interface, which uses a continuum model in which the concentration is discretized using a finite element mesh in the modeling domain. The equation governing the evolution of the concentration c (SI unit: $\mathrm{mol/m^3}$) in a stagnant background fluid ($\mathbf{u}=\mathbf{0}$) is:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = 0$$

where the diffusion coefficient D (SI unit: $\mathrm{m^2/s}$) is defined as

$$D = \frac{k_\mathrm{B} T}{6\pi\mu r_p}$$

where

- $k_\mathrm{B} = 1{,}3806488 \times 10^{-23}$ J/K is Boltzmann's constant,
- T (SI unit: K) is the absolute fluid temperature,
- μ (SI unit: Pa s) is the fluid viscosity, and
- r_p (SI unit: m) is the particle radius.

The initial concentration is given by a Dirac delta function at $(0, 0)$:

$$c_0 = \delta(0, 0)$$

That is, the initial concentration is infinitely large at the origin and zero everywhere else, such that the surface integral over any region containing the origin is unity. Because an initial condition that is infinitely large at a point is impractical to model, the initial concentration is instead given a very large finite value in a small area surrounding the origin.

The model geometry consists of two concentric circles as shown in Figure 1. The initial concentration diffuses from (0, 0) radially outwards in all directions. After 100 seconds, some of the initial concentration has diffused from the inner circular domain to the outer domain. The transmission probability for diffusion from the inner domain to the outer domain is defined as:

$$\alpha = \frac{\int_O c\,dS}{\int_I c\,dS + \int_O c\,dS}$$

where I denotes the inner domain and O the outer.

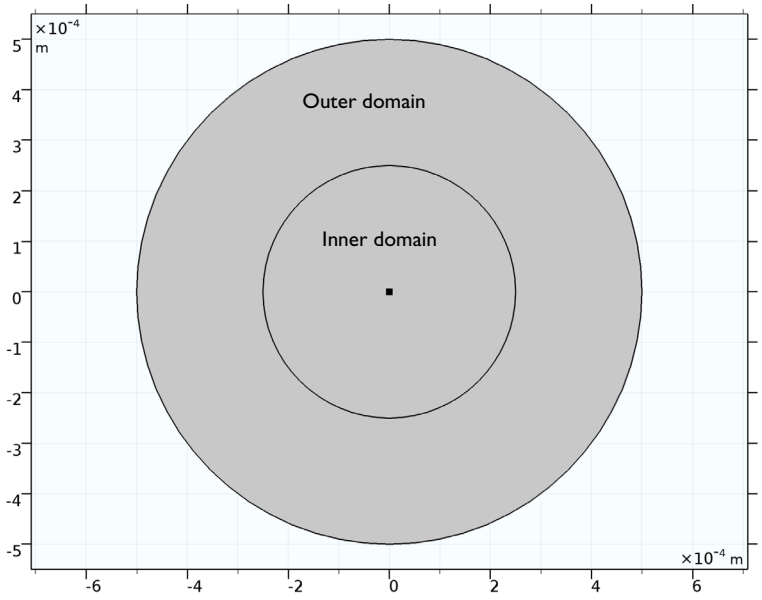


Figure 1: Model geometry. The concentration is initially a delta function at (0,0) and the particles are all released at (0,0) with an initial velocity of zero.

Diffusion can also be modeled using a particle-based approach. The combination of the **Brownian Force** and the **Drag Force** results in diffusion of particles from regions of high to low number density. The equations of motion are:

$$\frac{d}{dt}(m_p \mathbf{v}) = \mathbf{F}_D + \mathbf{F}_b$$

$$\mathbf{F}_D = \left(\frac{1}{\tau_p}\right) m_p (\mathbf{u} - \mathbf{v})$$

$$\tau_p = \frac{\rho_p d_p^2}{18\mu}$$

This is the *Stokes* drag law, which is appropriate when the relative Reynolds number of the particles in the fluid is small. Because the fluid is stagnant, the Stokes drag law is applicable in this example. The Brownian force is given by

$$\mathbf{F}_b = \boldsymbol{\zeta} \sqrt{\frac{12\pi k_B \mu T r_p}{\Delta t}}$$

- m_p (SI unit: kg) is the particle mass,
- d_p (SI unit: m) is the particle diameter,
- τ_p (SI unit: s) is the particle velocity response time,
- $\mathbf{v}$ (SI unit: m/s) is the velocity of the particle,
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity, which in this example is set to zero representing a stagnant background fluid,
- Δt (SI unit: s) is the time step taken by the solver, and
- $\boldsymbol{\zeta}$ (dimensionless) is a vector of independent, normally distributed random numbers with zero mean and unit standard deviation.

As explained in Ref. 1, independent values are chosen for all components of $\boldsymbol{\zeta}$. A different value of $\boldsymbol{\zeta}$ is created for each particle, at each time step for each component of the Brownian force. The Brownian force leads to spreading of particles from regions of high particle density to low density.

Initially, 5000 particles are released at the point (0, 0) with initial velocity components all zero. The transmission probability from the inner to the outer domain is computed by counting the number of particles in the outer domain and dividing it by the total number of particles.

Results and Discussion

The computed transmission probability for the two different methods is shown in Table 1. Since the Brownian force uses random number generators, the problem is solved 5 times. In each case the transmission probability is slightly different but all cases agree with the result from solving the diffusion equation.

TABLE 1: TABLE OF RESULTS FOR THE COMPUTED TRANSMISSION PROBABILITY

METHOD	TRANSMISSION PROBABILITY
Diffusion Equation	0.23697
Particle Tracing 1	0.2374
Particle Tracing 2	0.239
Particle Tracing 3	0.241
Particle Tracing 4	0.2422
Particle Tracing 5	0.2418

Figure 2 plots the location of the particles at the final solution time for 4 different runs.

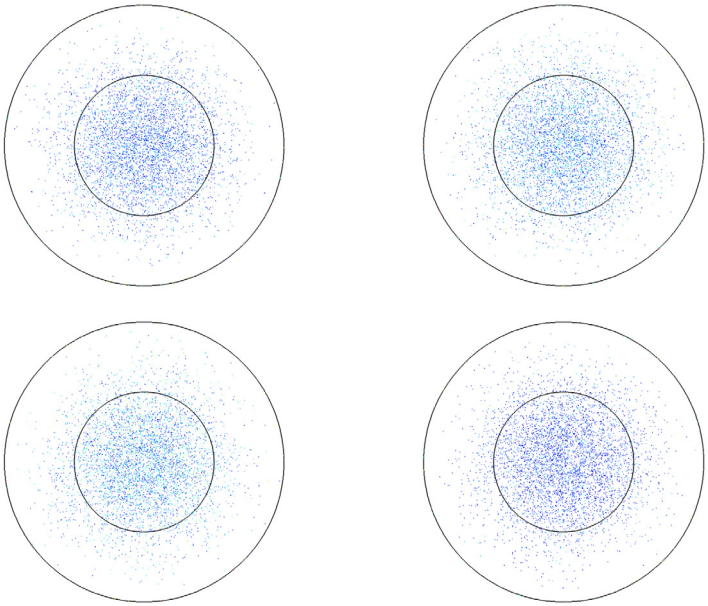


Figure 2: Plot of the particle location after 100 seconds. For each run, different random numbers were generated.

It is clear from these results that diffusive processes can be modeled using a particle-based approach. Furthermore, if a significant non-zero background fluid velocity were applied, the particle based approach would remain numerically stable.

Reference

1. M. Kim and A.L. Zydney, "Effect of Electrostatic, Hydrodynamic, and Brownian Forces on Particle Trajectories and Sieving in Normal Flow Filtration," *J. Colloid and Interface Science*, vol. 269, pp. 425–431, 2004.

Application Library path: `Particle_Tracing_Module/Tutorials/brownian_motion`

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 **2D**.

2 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species (tds)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Start by adding some definitions for the geometry and physical properties of the background fluid.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
router	0.0005	5E-4	Outer radius
rinner	0.00025	2.5E-4	Inner radius
rp	1E-7[m]	1E-7 m	Particle radius
T	300[K]	300 K	Temperature
eta	2E-5[Pa*s]	2E-5 Pa·s	Fluid viscosity
D	k_B_const*T/(6*pi*eta*rp)	1.0987E-10 m²/s	Diffusivity
ds	1	1	Input to random number generator

GEOMETRY 1

Circle 1 (c1)

1 On the **Geometry** 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 `router`.

Circle 2 (c2)

1 On the **Geometry** 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 `rinner`.

Point 1 (pt1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Point**.

2 In the **Settings** window for **Point**, click **Build All Objects**.

3 Click the **Zoom Extents** button on the **Graphics** toolbar. The geometry should look like Figure 1.

DEFINITIONS

Construct an expression for the initial concentration, which is a smoothed delta function.

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
smooth	2E-7		Smoothing distance
xd	x[1/m]		x coordinate
yd	y[1/m]		y coordinate
c0	1		Peak initial concentration
c_init	2*c0*(1-flc2hs(xd^2+yd^2-smooth^2,5e-11))		Initial concentration

Define a pair of **Integration** component couplings so that the fraction of the concentration that diffuses from the inner domain to the outer domain can be computed.

Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 Select Domain 1 only.

Integration 2 (intop2)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 Select Domain 2 only.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Clear the **Convection** check box.

Concentration 1

1 Right-click **Component 1 (comp1)>Transport of Diluted Species (tds)** and choose **Concentration**.

2 Select Boundaries 1, 2, 5, and 8 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

Transport Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 In the D_c text field, type `D`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *c* text field, type `c_init`.

Use a very fine mesh at the point (0, 0).

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

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

3 From the **Element size** list, choose **Extra fine**.

Scale 1

1 Right-click **Component 1 (comp1)>Mesh 1** and choose **Scale**.

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

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

4 Select Point 5 only.

5 Locate the **Scale** section. In the **Element size scale** text field, type `0.05`.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Times** text field, type `0 100`.

3 From the **Tolerance** list, choose **User controlled**.

4 In the **Relative tolerance** text field, type `1E-4`.

5 On the **Home** toolbar, click **Compute**.

RESULTS

Derived Values

Use the **Global Evaluation** feature to compute the fraction of the total concentration that diffused from the inner domain to the outer domain.

Global Evaluation 1

1 On the **Results** toolbar, click **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
`intop1(c)/(intop1(c)+intop2(c))`	1	

5 Click **New Table**.

COMPONENT 1 (COMP1)

Now solve the same problem using a particle-based approach.

ADD PHYSICS

1 On the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Particle Tracing>Particle Tracing for Fluid Flow (fpt)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1**.

5 Click **Add to Component** in the window toolbar.

6 On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for the **Transport of Diluted Species (tds)** interface.

4 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

5 Click **Add Study** in the window toolbar.

6 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

ROOT

In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

PARTICLE TRACING FOR FLUID FLOW (FPT)

On the **Physics** toolbar, click **Transport of Diluted Species (tds)** and choose **Particle Tracing for Fluid Flow (fpt)**.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Particle Tracing for Fluid Flow (fpt)**.

2 In the **Settings** window for **Particle Tracing for Fluid Flow**, click to expand the **Advanced settings** section.

3 Locate the **Advanced Settings** section. From the **Wall accuracy order** list, choose **1**.

4 From the **Arguments for random number generation** list, choose **User defined**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Particle Tracing for Fluid Flow (fpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Properties** section.

3 In the d_p text field, type `2*rp`.

Drag Force 1

1 In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Forces>Drag Force**.

2 In the **Settings** window for **Drag Force**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Drag Force** section. From the μ list, choose **User defined**. In the associated text field, type `eta`.

Brownian Force 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Forces>Brownian Force**.

2 In the **Settings** window for **Brownian Force**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Model Inputs** section. In the T text field, type `T`.

5 Locate the **Brownian Force** section. From the μ list, choose **User defined**. In the associated text field, type `eta`.

6 Locate the **Advanced Settings** section. In the i text field, type `ds`.

Release 5000 particles at (0, 0) with an initial velocity of zero.

Release from Grid 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Velocity** section.

3 From the **Initial velocity** list, choose **Constant speed, spherical**.

4 In the v_0 text field, type `0`.

5 In the N_{vel} text field, type `5000`.

Particle Counter 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose the domain setting **Particle Counter**.

2 Select Domain 1 only.

3 In the **Settings** window for **Particle Counter**, locate the **Particle Counter** section.

4 From the **Release feature** list, choose **Release from Grid 1**.

The Brownian force depends on the time step taken by the solver. The default tolerances are very strict for the particle tracing interfaces. When including forces with random components such as the Brownian force the tolerances need to be relaxed, otherwise the solver will take very small time steps and the model will take a long time to solve.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `0 100`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1E-3`.

Solution 2 (sol2)

1 On the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute tolerance** section.

4 Locate the **Absolute Tolerance** section. From the **Tolerance method** list, choose **Manual**.

5 In the **Absolute tolerance** text field, type `1E-3`.

6 Clear the **Update scaled absolute tolerance** check box.

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

RESULTS

Global Evaluation 2

1 On the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.

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

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Model>Component 1>Particle Tracing for Fluid Flow>Particle Counter 1> fpt.pcnt1.alpha - Transmission probability**.

6 Click **Evaluate**.

ROOT

Finally, add another study and solve the same problem 4 times, with different random numbers generated for each run. A **Parametric Sweep** over the parameter `ds` is used to create unique random numbers for each run.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for the **Transport of Diluted Species (tds)** interface.

4 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

5 Click **Add Study** in the window toolbar.

6 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `0 100`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1E-3`.

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
ds	2 3 4 5	

Solution 3 (sol3)

1 On the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, locate the **Absolute Tolerance** section.

4 From the **Tolerance method** list, choose **Manual**.

5 In the **Absolute tolerance** text field, type `1E-3`.

6 Clear the **Update scaled absolute tolerance** check box.

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

RESULTS

Global Evaluation 3

1 On the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 3/Parametric Solutions 1 (sol4)**.

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

5 From the **Table columns** list, choose **Time**.

6 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Model>Component 1>Particle Tracing for Fluid Flow>Particle Counter 1> fpt.pcnt1.alpha - Transmission probability**.

7 Click the arrow next to the **Evaluate** button and select **New table**.

Particle Trajectories (fpt) 1

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (fpt) 1**.

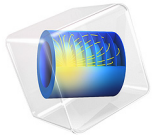
2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Parameter value (ds)** list, choose **2**.

4 On the **Particle Trajectories (fpt) 1** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

View the particle trajectories for other parameter values by selecting different options from the **Parameter value (ds)** list. Note that the distributions all look similar but that the particle positions are distinct in each plot. Four such plots are shown in Figure 2.



Child's Law Benchmark

Introduction

Space charge limited emission is a phenomenon that restricts the current of charged particles that can be released from a surface. As the electron current released by a cathode increases, so does the charge density in the immediate vicinity of the cathode. This distribution of charge density exerts an electric force on the emitted electrons, directed toward the cathode. The space charge limited current is the maximum current that can be released such that the emitted particles are not repelled back toward the cathode.

The uniform space charge limited current J in a plane-parallel vacuum diode is given by Child's Law,

$$J = \frac{4\varepsilon_0}{9}\sqrt{\frac{2e}{m_e}}\frac{V^{3/2}}{d^2}$$

Where J is the norm of the current density, ε_0 is the vacuum permittivity, e is the electron charge, m_e is the electron mass, V is the potential at the anode, and d is the distance between the cathode and the anode.

In this example, the space charge limited current in a plane-parallel vacuum diode is computed using COMSOL Multiphysics and the Particle Tracing Module. The resulting electric potential distribution and current are compared with the analytical solution given by Child's Law. The current density is computed using a study that establishes a bidirectional coupling between the particle trajectories and the electric potential.

Model Definition

Electrons are emitted from a grounded cathode located at $x = 0$ and propagate toward an extraction grid at a fixed potential V_0 located at $x = d$. Space charge limited emission occurs when any further increase in current would repel electrons back toward the cathode; this is equivalent to enforcing the boundary condition

$$\mathbf{n} \cdot \nabla V = 0$$

on the cathode surface.

The space charge limited current is computed using an iterative process in which the particle trajectories and electric potential are computed in alternating steps. The values of variables not solved for in one step are always taken from the most recent iteration of the other. In this way, successively better approximations of the current can be computed. However, if the space charge limited current is significantly overestimated during any iteration, then the particles are immediately repelled back toward the cathode and the

charge density becomes saturated in the mesh elements adjacent to the cathode. To avoid this overestimation of the space charge limited current, only a small fraction of the space charge density is used to calculate the electric potential during early iterations. This fraction of the space charge density is gradually increased until it reaches unity in the **Number of iterations** specified in the Settings window for the Electric Particle Field Interaction node.

To reduce the probability of the particles immediately being repelled back toward the cathode, it is convenient to release the particles from a surface a short distance away from the cathode, at which the potential gradient is nonzero. To do so, the Space Charge Limited Emission feature is applied to the boundary at $x = 0$. Instead of representing the cathode, the left side of the geometry represents an emission surface a short distance d_{buf} away from the cathode. The electric potential is computed in the narrow region between the cathode and the emission surface, allowing the initial particle velocity at the emission surface to be defined. The electric potential to the right of the emission surface can then be computed using the space charge density computed by the Electric Particle Field Interaction node.

The Bidirectionally Coupled Particle Tracing study step sets up a solver loop in which the particle trajectories are computed using a time-dependent solver, while the electric potential is computed using a stationary solver. The solver sequence alternates between these two solvers for a specified number of iterations, always using the previous solution for the variables not solved for. In this way, a self-consistent solution, in which the particle trajectories and the electric potential affect each other, is obtained.

Results and Discussion

For space charge limited emission (Ref. 1), the electric potential varies with position as

$$V(x) = V_0\left(\frac{x + d_{\text{buf}}}{d + d_{\text{buf}}}\right)^{4/3} \tag{1}$$

where d is the distance from the emission surface to the anode and x is the distance from the emission surface to a given point.

The comparison between the analytical solution given by Equation 1 and the computed result is shown in Figure 1. The relative error is shown in Figure 2.

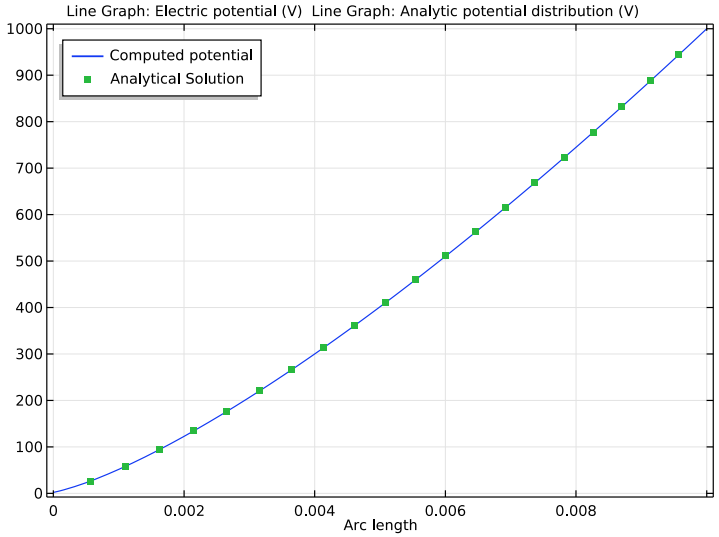


Figure 1: Comparison of the computed electric potential and the analytic solution given by Child's Law.

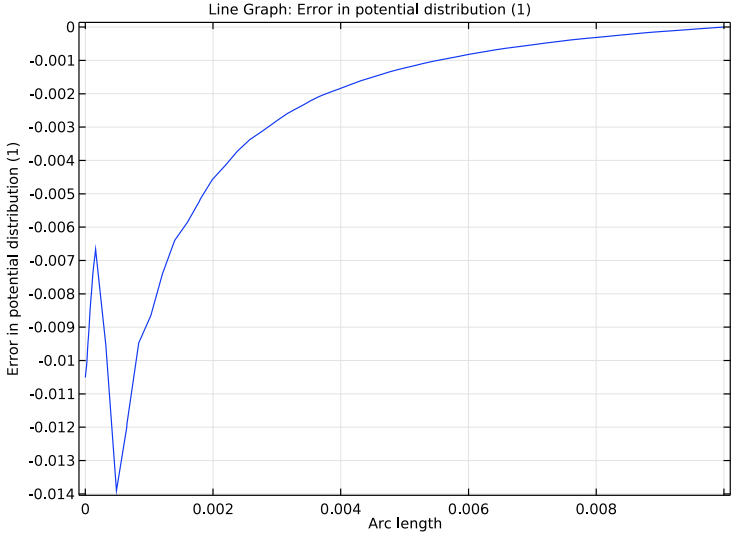


Figure 2: Relative error between the computed electric potential and the analytic solution given by Child's Law.

Reference

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

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/childs_law_benchmark`

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 **2D**.

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**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
V0	1000[V]	1000 V	Potential difference across gap
d	1[cm]	0.01 m	Length of the modeling domain

Name	Expression	Value	Description
dbuf	0.01[cm]	1E-4 m	Length of the buffer region
H	2[cm]	0.02 m	Height of the modeling domain
Depth	1[m]	1 m	Depth into the modeling domain
Jan	(4*epsilon0_const/9)*sqrt(2*V0*e_const/me_const)*V0/d^2	738.06 A/m²	Analytic current density
Ian	Jan*H*Depth	14.761 A	Analytic total current

GEOMETRY 1

Rectangle 1 (r1)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type d.
4. In the **Height** text field, type H.

DEFINITIONS

Variables 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
2. In the **Settings** window for **Variables**, locate the **Variables** section.
3. In the table, enter the following settings:

Name	Expression	Unit	Description
Van	V0*((x+dbuf)/(d+dbuf))^(4/3)	V	Analytic potential distribution
rel_err	(V-Van)/Van		Error in potential distribution

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

CHARGED PARTICLE TRACING (CPT)

Electric Force 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Electric Force 1**.

2 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

3 From the **E** list, choose **Electric field (es/ccn1)**.

ELECTROSTATICS (ES)

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

Electric Potential 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrostatics (es)** and choose **Electric Potential**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the V_0 text field, type `V0`.

Set up space charge limited emission of electrons at the left boundary.

MULTIPHYSICS

Space Charge Limited Emission 1 (scle1)

1 On the **Physics** toolbar, click **Multiphysics** and choose **Boundary> Space Charge Limited Emission**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Space Charge Limited Emission**, locate the **Extra Dimension Settings** section.

4 In the o_s text field, type `dbuf`.

The iterative scheme employed when solving can be made more stable by ramping up the computed space charge density over a number of iterations. The rate at which the space charge density is ramped up is controlled by the **Number of iterations** check box in the settings window for the Electric Particle Field Interaction node. Further stability can

be achieved by selecting the **Use cumulative space charge density** check box, which treats the charge density as the average over successive iterations. The number of iterations should typically be around 15, depending on the size of the buffer zone specified in the Space Charge Limited Emission feature. The smaller the buffer zone, the larger the number of iterations should be. In addition, the number of iterations over which to ramp up to full space charge density should be 10-15 less than the number specified in the Bidirectionally Coupled Particle Tracing study settings.

5 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Electric Particle Field Interaction 1 (epfi1)**.

6 In the **Settings** window for **Electric Particle Field Interaction**, locate the **Continuation Settings** section.

7 Select the **Use cumulative space charge density** check box.

8 In the β text field, type 15.

Use a boundary layer mesh immediately in front of the emission surface for higher accuracy.

MESH 1

Size

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Finer**.

Boundary Layers 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, click to expand the **Transition** section.

3 Clear the **Smooth transition to interior mesh** check box.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Layer Properties** section.

4 In the **Number of boundary layers** text field, type 4.

5 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. From the **Time unit** list, choose **ns**.
3. In the **Times** text field, type `range(0,0.1,3)`.
4. Locate the **Iterations** section. From the **Termination method** list, choose **Convergence of global variable**.
5. In the **Global variable** text field, type `scle1.rc`.
6. In the **Maximum number of iterations** text field, type `35`.
7. On the **Home** toolbar, click **Compute**.

RESULTS

Data Sets

Use the **Cut Line 2D** data set to visualize the relative error in the electric potential versus the prediction of Child's Law.

Cut Line 2D 1

1. On the **Results** toolbar, click **Cut Line 2D**.
2. In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
3. In row **Point 1**, set **y** to `1[cm]`.
4. In row **Point 2**, set **x** to `1[cm]` and **y** to `1[cm]`.

1D Plot Group 3

1. On the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Comparison With Child's Law` in the **Label** text field.
3. Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.
4. From the **Time selection** list, choose **Last**.
5. Click to expand the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1. Right-click **Comparison With Child's Law** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, click to expand the **Legends** section.
3. Select the **Show legends** check box.

4 From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
Computed potential

Line Graph 2

1 In the **Model Builder** window, under **Results** right-click **Comparison With Child's Law** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `Van`.

4 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

6 In the **Number** text field, type `20`.

7 Locate the **Legends** section. Select the **Show legends** check box.

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
Analytical Solution

10 On the **Comparison With Child's Law** toolbar, click **Plot**. The plot should look like Figure 1.

1D Plot Group 4

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Relative Error` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

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

Line Graph 1

1 Right-click **Relative Error** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `rel_err`.

4 On the **Relative Error** toolbar, click **Plot**. The plot should look like Figure 2.

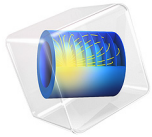
Check that the computed current matches the analytical solution.

Global Evaluation 1

1. On the **Results** toolbar, click **Global Evaluation**.
2. In the **Settings** window for **Global Evaluation**, locate the **Data** section.
3. From the **Time selection** list, choose **Last**.
4. Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Model>Global Definitions>Parameters>Ian - Analytic total current**.
5. Click **Evaluate**.

Global Evaluation 2

1. On the **Results** toolbar, click **Global Evaluation**.
2. In the **Settings** window for **Global Evaluation**, locate the **Data** section.
3. From the **Time selection** list, choose **Last**.
4. Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Model>Component 1>Currents and Charge>scle1.rc - Release current magnitude**.
5. Click the arrow next to the **Evaluate** button and click **Table 1 - Global Evaluation 1 (Ian)**.



Dielectrophoretic Separation of Platelets from Red Blood Cells

Introduction

By exploiting the fact that platelets are the smallest cells in blood, it is possible to perform size-based fractionation of blood (that is, separate platelets from red blood cells) using dielectrophoresis. This model demonstrates the continuous separation of platelets from red blood cells (RBCs) using the Dielectrophoretic Force feature available in the Particle Tracing for Fluid Flow interface.

This model also requires one of the following: CFD Module, Microfluidics Module, or Subsurface Flow Module.

Model Definition

Dielectrophoresis is the movement of particles in a non-uniform electric field due to the interaction of the particles' induced dipoles with the spatial gradient of the electric field norm.

When the electric field is computed in the frequency domain, the **Dielectrophoretic Force** feature adds the following contribution to the total force applied on the particles:

$$\mathbf{F}_{\text{ext}} = 2\pi r_p^3 \varepsilon_0 \,\text{real}(\varepsilon_f^*)\,\text{real}\left(\frac{\varepsilon_p^* - \varepsilon_f^*}{\varepsilon_p^* + 2\varepsilon_f^*}\right)\nabla|\mathbf{E}_{\text{rms}}|^2$$

where ε_f^* (dimensionless) is the complex relative permittivity of the fluid, ε_p^* (dimensionless) is the complex relative permittivity of the particle, and $\mathbf{E}_{\text{rms}}$ is the root mean square electric field. For fields that are computed in the frequency domain, the complex permittivity can be expressed as

$$\varepsilon^* = \varepsilon - \frac{i\sigma}{\omega}$$

where ε is the permittivity, σ is the electrical conductivity, and ω is the angular frequency of the electric field.

The **Shell** subnode can be added to the **Dielectrophoretic Force** node to model the dielectrophoretic force on particles with thin dielectric shells. The complex permittivity of the shell can differ from the complex permittivity of the rest of the particle. When computing the dielectrophoretic force, the complex permittivity of the particle is replaced by the equivalent complex relative permittivity $\varepsilon_{\text{eq}}^*$ of a homogeneous particle comprising both the shell and the interior of the particle:

$$\varepsilon_{eq}^{*} = \varepsilon_{s}^{*} \frac{\left(\frac{r_0}{r_i}\right)^3 + 2\left(\frac{\varepsilon_p^{*} - \varepsilon_s^{*}}{\varepsilon_p^{*} + 2\varepsilon_s^{*}}\right)}{\left(\frac{r_0}{r_i}\right)^3 - \left(\frac{\varepsilon_p^{*} - \varepsilon_s^{*}}{\varepsilon_p^{*} + 2\varepsilon_s^{*}}\right)}$$

where r_0 and r_i (SI unit: m) are the outer and inner radii of the shell, respectively; ε_p^{*} (dimensionless) is the complex relative permittivity of the particle, and ε_s^{*} (dimensionless) is the complex relative permittivity of the outer shell. For this model, the shell parameters for platelets and RBCs are respectively obtained from Ref. 2 and Ref. 3.

The present model is based on a lab-on-a-chip device described in detail in Ref. 1. It consists of two inlets, two outlets and a separation region in which a non-uniform electric field created by an arrangement of electrodes of alternating polarity alter the particle trajectories. Figure 1 shows the schematic of the modeled geometry. As seen on the figure, the inlet velocity for the lower inlet is significantly higher (853 μm/s) than the upper inlet (154 μm/s) in order to focus all the injected particles toward the upper outlet.

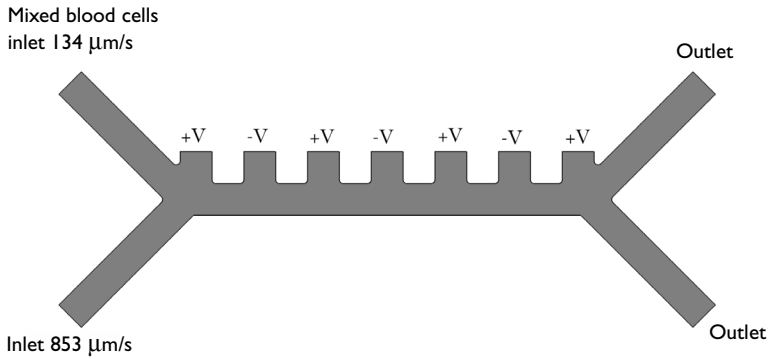


Figure 1: Two dimensional geometry of the modeled device. Details are presented in Ref. 1. *The inlet velocity for the bottom inlet is significantly higher than the upper inlet to focus all the injected particles toward the upper outlet (Flow Focusing).*

The model uses the following physics interfaces:

1. Creeping Flow (Microfluidics Module) to model the fluid flow,
2. Electric Currents to model the electric field in the microchannel, and

3 Particle Tracing for Fluid Flow (Particle Tracing Module) to compute the trajectories of RBCs and platelets under the influence of drag and dielectrophoretic forces

Three studies are also used:

1 Study 1 solves for the steady state fluid dynamics and frequency domain (AC) electric potential.

2 Study 2 uses a Time Dependent study step which utilizes the solution from Study 1 and estimates the particle trajectories without the dielectrophoretic force, as a result of which all particles (platelets and RBC) are focused to the same outlet.

3 Study 3 computes the particle trajectories while including the effect of the dielectrophoretic force.

Results and Discussion

Figure 2 shows the electric potential in the microfluidic device. When no dielectrophoretic force is applied, the red blood cells and platelets follow the same path and exit through the same outlet, as shown in Figure 3. When the dielectrophoretic force is applied, the two species are separated due to the differences in their dielectric properties, as shown in Figure 4.

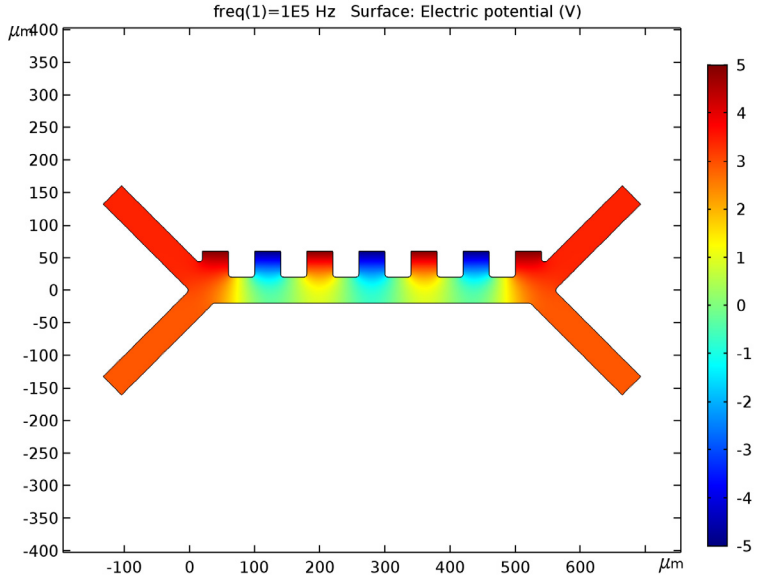


Figure 2: Spatial variation of the electric potential in the microfluidic channel.

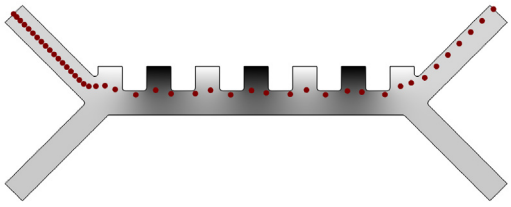


Figure 3: Particle trajectories without dielectrophoretic force applied. The RBCs are displayed in red and the platelets in blue. Since the particles are released at the same time and follow a similar path, the platelets are hidden behind the RBCs on the figure.

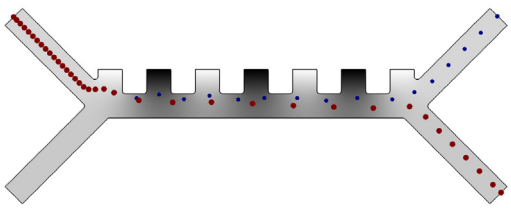


Figure 4: Particle trajectories with dielectrophoretic force applied. The RBCs are displayed in red and the platelets in blue. For sake of visualization, the relative size of the RBCs has been divided by two.

References

1. N. Piacentini, G. Mernier, R. Tornay, and P. Renaud, "Separation of platelets from other blood cells in continuous-flow by dielectrophoresis field-flow-fractionation," *Biomicrofluidics*, vol. 5, 034122, 2011.

2. M. Egger and E. Donath, "Electrorotation measurements of diamide-induced platelet activation changes," *Biophysical Journal*, vol. 68, pp. 364–372, 1995.

3. S. Park, Y. Zhang, T.H. Wang, and S. Yang, "Continuous dielectrophoretic bacterial separation and concentration from physiological media of high conductivity," Supplementary information, *Lab on a Chip*, vol. 11, pp. 2893–2900, 2011.

Application Library path: `Particle_Tracing_Module/Fluid_Flow/dielectrophoretic_separation`

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 **2D**.
2. In the **Select Physics** tree, select **AC/DC>Electric Currents (ec)**.
3. Click **Add**.
4. In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Creeping Flow (spf)**.
5. Click **Add**.
6. In the **Select Physics** tree, select **Fluid Flow>Particle Tracing> Particle Tracing for Fluid Flow (fpt)**.
7. Click **Add**.
8. Click **Done**.

GEOMETRY 1

Insert the prepared geometry sequence from file. You can read the instructions for creating the geometry in the appendix.

1 On the **Geometry** toolbar, click **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `dielectrophoretic_separation_geom_sequence.mph`.

GLOBAL DEFINITIONS

Parameters

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

Load the model parameters 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 `dielectrophoretic_separation_parameters.txt`.

ELECTRIC CURRENTS (EC)

Electric Potential 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electric Currents (ec)** and choose **Electric Potential**.

2 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

3 In the V_0 text field, type `5`.

4 Select Boundaries 8, 17, 26, and 34 only.

Electric Potential 2

1 In the **Model Builder** window, right-click **Electric Currents (ec)** and choose **Electric Potential**.

2 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

3 In the V_0 text field, type `-5`.

4 Select Boundaries 13, 21, and 30 only.

CREEPING FLOW (SPF)

Inlet 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Creeping Flow (spf)** and choose **Inlet**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Inlet**, locate the **Velocity** section.

4 In the U_0 text field, type `134[um/s]`.

Inlet 2

1 In the **Model Builder** window, right-click **Creeping Flow (spf)** and choose **Inlet**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Inlet**, locate the **Velocity** section.

4 In the U_0 text field, type `853[um/s]`.

Outlet 1

1 Right-click **Creeping Flow (spf)** and choose **Outlet**.

2 Select Boundaries 40 and 41 only.

PARTICLE TRACING FOR FLUID FLOW (FPT)

Wall 1

1 In the **Model Builder** window, expand the **Particle Tracing for Fluid Flow (fpt)** node, then click **Wall 1**.

2 In the **Settings** window for **Wall**, locate the **Wall Condition** section.

3 From the **Wall condition** list, choose **Bounce**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Particle Tracing for Fluid Flow (fpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Properties** section.

3 In the ρ_p text field, type `rho_p`.

4 In the d_p text field, type `dp1`.

Override Properties 1

1 In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Override Properties**.

2 In the **Settings** window for **Override Properties**, locate the **Particle Properties** section.

3 In the ρ_p text field, type `rho_p`.

4 In the d_p text field, type `dp2`.

Inlet 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Inlet**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Inlet**, locate the **Release Times** section.

4 In the **Release times** text field, type `range(0,0.05,3)`.

5 Locate the **Initial Position** section. From the **Initial position** list, choose **Uniform distribution**.

6 Locate the **Initial Velocity** section. From the **u** list, choose **Velocity field (spf)**.

Inlet 2

1 Right-click **Component 1 (comp1)>Particle Tracing for Fluid Flow (fpt)>Inlet 1** and choose **Duplicate**.

2 In the **Settings** window for **Inlet**, click to expand the **Inherit properties** section.

3 Locate the **Inherit Properties** section. From the **Inherit properties** list, choose **Override Properties 1**.

Outlet 1

1 In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Outlet**.

2 Select Boundaries 40 and 41 only.

Drag Force 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Forces>Drag Force**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Drag Force**, locate the **Drag Force** section.

4 From the **u** list, choose **Velocity field (spf)**.

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
Electrical conductivity	sigma	`sigma_f`	S/m	Basic
Relative permittivity	epsilonr	`epsilon_f`	1	Basic

Property	Name	Value	Unit	Property group
Density	rho	`rho_f`	kg/m³	Basic
Dynamic viscosity	mu	`mu_f`	Pa·s	Basic

Add a **Stationary** and a **Frequency Domain** study step to respectively solve the fluid flow and electric potential in the channel.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Electric Currents (ec)** and **Particle Tracing for Fluid Flow (fpt)**.

5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies>Stationary**.

6 Click **Add Study** in the window toolbar.

7 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 1

Step 2: Frequency Domain

1 On the **Study** toolbar, click **Study Steps** and choose **Frequency Domain> Frequency Domain**.

2 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `f0`.

4 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Creeping Flow (spf)** and **Particle Tracing for Fluid Flow (fpt)**.

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

RESULTS

Electric Potential (ec)

Click the **Zoom Extents** button on the **Graphics** toolbar. Compare the resulting plot to Figure 2.

Add a **Time Dependent** study to compute the trajectories of the particles without the **Dielectrophoretic Force** feature.

ADD STUDY

1 On the **Study** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Electric Currents (ec)** and **Creeping Flow (spf)**.

5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

6 Click **Add Study** in the window toolbar.

7 On the **Study** toolbar, click **Add Study** to close the **Add Study** window.

Change the relative tolerance for better accuracy.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,0.05,3)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1.0E-3`.

Check the values of variables not solve for in order to get access to the velocity field and electric potential computed in the first study.

6 Click to expand the **Values of dependent variables** section. Locate the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

7 From the **Method** list, choose **Solution**.

8 From the **Study** list, choose **Study 1, Frequency Domain**.

Get the initial solution. The purpose is to generate a plot of the particule trajectories and use it to plot the particles while solving for them.

Particle Trajectories (fpt)

On the **Study** toolbar, click **Get Initial Value**.

Modify the plot to display the particle size and electric potential.

RESULTS

Particle Trajectories (fpt)

For clearer visualization use an `if` statement to display the RBCs with a diameter two times smaller than their real size.

Particle Trajectories 1

1. In the **Model Builder** window, expand the **Results>Particle Trajectories (fpt)** node, then click **Particle Trajectories 1**.
2. In the **Settings** window for **Particle Trajectories**, locate the **Coloring and Style** section.
3. Find the **Point style** subsection. In the **Point radius expression** text field, type `if(fpt.dp==dp2,dp2/2,dp1)`.

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 `fpt.dp`.
4. Locate the **Coloring and Style** section. From the **Color table** list, choose **Wave**.

Surface 1

1. In the **Model Builder** window, under **Results** right-click **Particle Trajectories (fpt)** and choose **Surface**.
2. In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
3. From the **Color table** list, choose **GrayScale**.
4. Click the **Zoom Extents** button on the **Graphics** toolbar.

Plot the particle trajectories while solving. Note that the dielectrophoretic force isn't applied in this study, so all of the particles appear follow approximately the same trajectory.

STUDY 2

Step 1: Time Dependent

1. In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.
2. In the **Settings** window for **Time Dependent**, click to expand the **Results while solving** section.
3. Locate the **Results While Solving** section. Select the **Plot** check box.
4. From the **Plot group** list, choose **Particle Trajectories (fpt)**.

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

RESULTS

Particle Trajectories (fpt)

Click the **Zoom Extents** button on the **Graphics** toolbar. The plot should look like Figure 3.

Now add another **Time Dependent** study to compute the effect of the dielectrophoretic force on the particle trajectories.

ADD STUDY

1 On the **Study** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Electric Currents (ec)** and **Creeping Flow (spf)**.

5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

6 Click **Add Study** in the window toolbar.

7 On the **Study** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,0.05,3)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1.0E-3`.

6 Click to expand the **Values of dependent variables** section. Locate the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

7 From the **Method** list, choose **Solution**.

8 From the **Study** list, choose **Study 1, Frequency Domain**.

COMPONENT 1 (COMP1)

In the **Model Builder** window, expand the **Component 1 (comp1)** node.

PARTICLE TRACING FOR FLUID FLOW (FPT)

In the **Model Builder** window, expand the **Component 1 (comp1)>** **Particle Tracing for Fluid Flow (fpt)** node.

Dielectrophoretic Force 1

1. Right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Forces>** **Dielectrophoretic Force**.
2. Click in the **Graphics** window and then press Ctrl+A to select all domains.
3. In the **Settings** window for **Dielectrophoretic Force**, locate the **Dielectrophoretic Force** section.
4. From the **E** list, choose **Electric field (ec/cucn1)**.
5. Locate the **Particle Properties** section. In the $\varepsilon_{r,\,p}$ text field, type `epsilon_p1`.
6. In the σ_p text field, type `sigma_p1`.
7. Locate the **Advanced Settings** section. Select the **Use piecewise polynomial recovery on field** check box.
8. From the **Particles to affect** list, choose **Single species**.

Shell 1

1. Right-click **Component 1 (comp1)>Particle Tracing for Fluid Flow (fpt)>** **Dielectrophoretic Force 1** and choose **Shell**.
2. In the **Settings** window for **Shell**, locate the **Shell Properties** section.
3. In the t_s text field, type `th_s1`.
4. In the $\varepsilon_{r,\,s}$ text field, type `epsilon_s1`.
5. In the σ_s text field, type `sigma_s1`.

Dielectrophoretic Force 2

1. Right-click **Dielectrophoretic Force 1** and choose **Duplicate**.
2. In the **Settings** window for **Dielectrophoretic Force**, locate the **Particle Properties** section.
3. In the $\varepsilon_{r,\,p}$ text field, type `epsilon_p2`.
4. In the σ_p text field, type `sigma_p2`.
5. Locate the **Advanced Settings** section. From the **Affected particle properties** list, choose **Override Properties 1**.

Shell 1

1. In the **Model Builder** window, expand the **Dielectrophoretic Force 2** node, then click **Shell 1**.

2 In the **Settings** window for **Shell**, locate the **Shell Properties** section.

3 In the t_s text field, type `th_s2`.

4 In the $\varepsilon_{r,\,s}$ text field, type `epsilon_s2`.

5 In the σ_s text field, type `sigma_s2`.

Get the initial solution in order to view the particle trajectories while running the study.

STUDY 3

Particle Trajectories (fpt) 1

On the **Study** toolbar, click **Get Initial Value**.

RESULTS

Particle Trajectories 1

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

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

3 Find the **Point style** subsection. In the **Point radius expression** text field, type `if(fpt.dp==dp2,dp2/2,dp1)`.

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 `fpt.dp`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Wave**.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Particle Trajectories (fpt) 1** and choose **Surface**.

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

3 From the **Color table** list, choose **GrayScale**.

4 On the **Particle Trajectories (fpt) 1** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

Plot the particle trajectories while solving. Note that the dielectrophoretic force separates the particles.

STUDY 3

Step 1: Time Dependent

1. In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.
2. In the **Settings** window for **Time Dependent**, click to expand the **Results while solving** section.
3. Locate the **Results While Solving** section. Select the **Plot** check box.
4. From the **Plot group** list, choose **Particle Trajectories (fpt) 1**.
5. On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (fpt) 1

1. In the **Model Builder** window, click **Particle Trajectories (fpt) 1**.
2. On the **Particle Trajectories (fpt) 1** toolbar, click **Plot**.
3. Click the **Zoom Extents** button on the **Graphics** toolbar. Compare the resulting plot to Figure 4.

Appendix — Geometry Instructions

On the **Home** toolbar, click **Component** and choose **Add Component>2D**.

GEOMETRY 1

1. In the **Model Builder** window, click **Geometry 1**.
2. In the **Settings** window for **Geometry**, locate the **Units** section.
3. From the **Length unit** list, choose **µm**.

Rectangle 1 (r1)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `560/2`.
4. In the **Height** text field, type `40`.
5. Locate the **Position** section. In the **y** text field, type `-20`.

Rectangle 2 (r2)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type 40.

4 In the **Height** text field, type 200.

5 Locate the **Position** section. In the **x** text field, type 9.

6 In the **y** text field, type -9.

7 Locate the **Rotation Angle** section. In the **Rotation** text field, type 45.

Mirror 1 (mir1)

1 On the **Geometry** toolbar, click **Transforms** and choose **Mirror**.

2 Select the object **r2** only.

3 In the **Settings** window for **Mirror**, locate the **Normal Vector to Line of Reflection** section.

4 In the **x** text field, type 0.

5 In the **y** text field, type 1.

6 Locate the **Input** section. Select the **Keep input objects** check box.

Mirror 2 (mir2)

1 On the **Geometry** toolbar, click **Transforms** and choose **Mirror**.

2 Click in the **Graphics** window and then press Ctrl+A to select all objects.

3 In the **Settings** window for **Mirror**, locate the **Input** section.

4 Select the **Keep input objects** check box.

5 Locate the **Point on Line of Reflection** section. In the **x** text field, type 560/2.

Square 1 (sq1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Square**.

2 In the **Settings** window for **Square**, locate the **Size** section.

3 In the **Side length** text field, type 40.

4 Locate the **Position** section. In the **x** text field, type 20.

5 In the **y** text field, type 20.

Array 1 (arr1)

1 On the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 Select the object **sq1** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 In the **x size** text field, type 7.

5 Locate the **Displacement** section. In the **x** text field, type 80.

Union 1 (uni1)

1 On the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

Use the select box icon to select all the geometry objects.

2 Click the **Select Box** button on the **Graphics** toolbar.

3 Click in the **Graphics** window and then press Ctrl+A to select all objects.

4 In the **Settings** window for **Union**, locate the **Union** section.

5 Clear the **Keep interior boundaries** check box.

Fillet 1 (fil1)

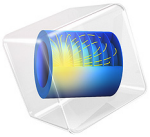
1 On the **Geometry** toolbar, click **Fillet**.

2 On the object **uni1**, select Points 5, 6, 8, 9, 11, 13, 15, 17, 19, 22, 24, 26, 28, 30, 32, 34, 35, and 37 only.

3 In the **Settings** window for **Fillet**, locate the **Radius** section.

4 In the **Radius** text field, type `5`.

5 Click **Build All Objects**.



Ideal Cloak[1]

1. This model is courtesy of Yaroslav Urzhumov, Center for Metamaterials and Integrated Plasmonics, Duke University Durham, NC.

Introduction

Electromagnetic or optical invisibility can be achieved by coating an object with a transparent gradient-index structure that bends the rays of light around the concealed object (Ref. 1). The structure has to be able to do so with radiation incident from any direction, which can be achieved by making it rotationally invariant. Inside this transparent shell, situated is a nontransparent object whose scattering properties in free space are inessential as long as the cloak operates perfectly by preventing any light rays from hitting the object. The concept of invisibility based on omnidirectional cloaking was introduced by Sir John Pendry (Imperial College, UK) and his collaborators in 2006 (Ref. 1).

The cloak of invisibility modeled here is a concentric spherical shell, whose interior surface represents the concealed cavity. Omnidirectional cloaks require anisotropic material properties, which can be calculated using the transformation optics theory (Ref. 1). Although ray and beam bending can be achieved with a gradient of isotropic refractive index, index gradient alone is not sufficient for omnidirectional invisibility. This can be shown by means of the uniqueness theorem that applies to scattering problems involving bodies composed of isotropic materials (Ref. 2).

The refractive index in the azimuthal directions (normal to the radial direction) experiences a gradual change from unity on the exterior surface of the cloak, where it matches free space, down to zero on the interior surface. With a proper choice of index distribution, you can ensure that any ray hitting the cloak never reaches the interior surface, and thus never probes the object. The refractive index in the radial direction is not continuous in this particular cloak design. The resulting index discontinuity at the exterior surface does not lead to reflections because only the index in the tangential direction affects reflectivity.

This model demonstrates the use of optical tracing for studying optically large gradient-index structures with anisotropic optical properties. Additionally, the model introduces a smoothing technique for handling discontinuities of refractive index on curved surfaces, which are typical in conventional optical devices such as lenses.

Model Definition

There is no explicit support for modeling geometrical optics in the Particle Tracing Module, but an analogy between the Hamilton equations and the equations for rays in the zero wavelength limit allows us to solve the problem. The analogy is as follows:

- The wave vector, $\mathbf{k}$ (SI unit: 1/m) plays the same role in geometrical optics as the momentum, $\mathbf{p}$, of particles in classical mechanics.

- The angular frequency, ω (SI unit: $1/\mathrm{s}$) plays the role of the Hamiltonian, H.

  For a classical particle, Hamilton's equations are:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}, \frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}$$

  and using the analogy above:

$$\frac{d\mathbf{k}}{dt} = -\frac{\partial \omega}{\partial \mathbf{q}}, \frac{d\mathbf{q}}{dt} = \frac{\partial \omega}{\partial \mathbf{k}}$$

- The particle mass should be set to 1.

For geometric optics, the angular frequency is given by

$$\omega = \frac{c|\mathbf{k}|}{n}$$

where n is the refractive index of the material. For vacuum, the refractive index is simply 1. Inside the cloak, the refractive index is anisotropic, so it is more convenient to express the wave vector using spherical coordinates:

$$\begin{bmatrix} k_r \\ k_\vartheta \\ k_\phi \end{bmatrix} = \begin{bmatrix} \sin\vartheta\cos\phi & \sin\vartheta\sin\phi & \cos\vartheta \\ \cos\vartheta\cos\phi & \cos\vartheta\sin\phi & -\sin\vartheta \\ -\sin\phi & \cos\phi & 0 \end{bmatrix} \begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix}$$

The angular frequency is hence given by:

$$\omega = c\left(\frac{k_r^2}{n_r^2} + \frac{k_\vartheta^2}{n_\vartheta^2} + \frac{k_\phi^2}{n_\phi^2}\right)^{\frac{1}{2}}$$

Results and Discussion

The trajectory of the rays is plotted in Figure 1. The rays reach the cloak and bend around the inner sphere, which would appear invisible to an observer.

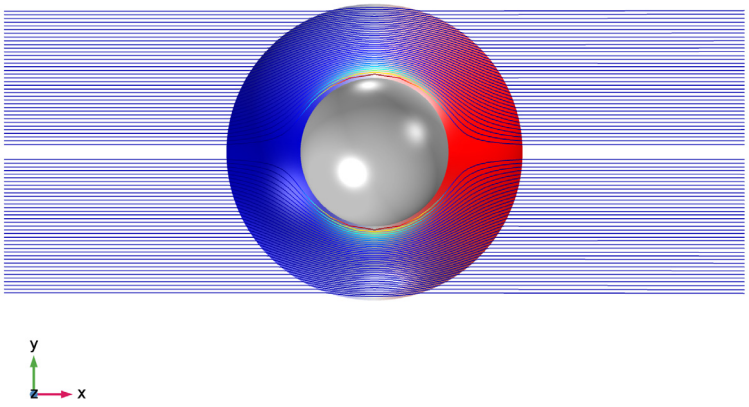


Figure 1: Plot of the light rays traveling through the cloak.

A better way of determining whether the incoming rays are returned to their original trajectory is by using Poincaré maps or phase portraits. Figure 2 shows a Poincaré map in the yz-plane at the initial time step (red dots) and at the final time step (blue dots). The map shows the y-location of the particle on the x-axis, and the z-location of the particles on the y-axis. This is because the Poincaré section is defined in the yz-plane. The particle position after traveling through the cloak is almost exactly the same as it was initially. There are deviations close to $x = 0$ due to some small numerical error.

Figure 3 shows the change in the particles' position in the yz-plane after traveling through the cloaking device. The particles at the maximum and minimum y-coordinates have greater absolute error in their final positions despite being deflected at lower angles compared to the particles passing through the middle of the cloak. The higher absolute error may be due to these particles entering the anisotropic domain at a very oblique angle of incidence.

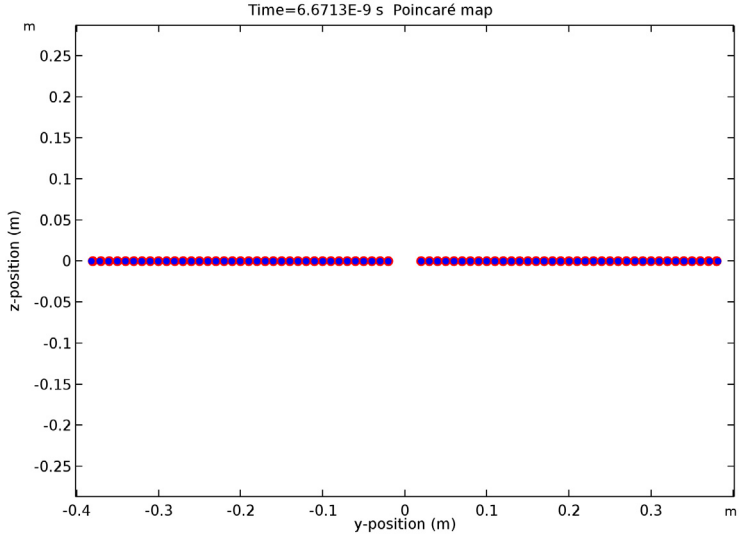


Figure 2: Poincaré map in the yz-plane at for Poincaré sections at $x = -1$ *(red) and* $x = 1$ *(blue).*

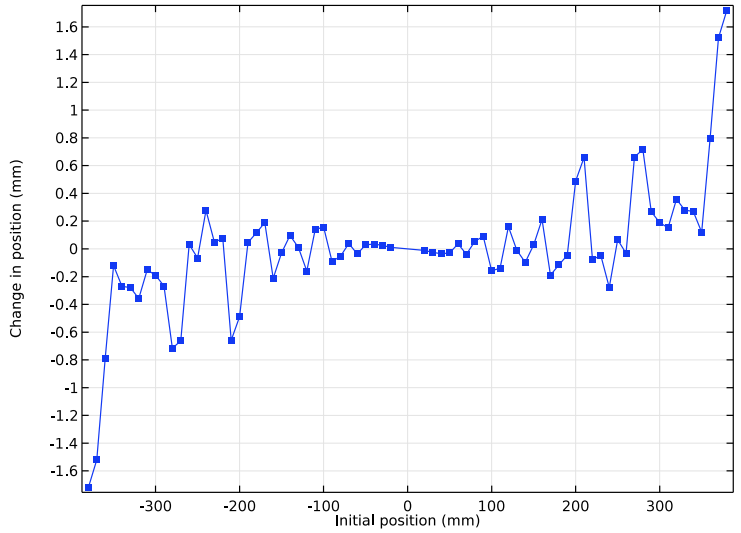


Figure 3: Change in the y-component of the particle position after traveling through the cloaking device.

References

1. J. Pendry, D. Schurig, and D.R. Smith, "Controlling Electromagnetic Fields," *Science*, vol. 312, no. 5781, pp. 1780–1782, 2006.

2. A.I. Nachman, "Reconstruction from Boundary Measurements," *Ann. Math.*, vol. 128, pp. 531–576, 1988.

Application Library path: `Particle_Tracing_Module/Tutorials/ideal_cloak`

Modeling Instructions

This model comes courtesy of Yaroslav Urzhumov, Center for Metamaterials and Integrated Plasmonics, Duke University.

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 **Mathematics>Mathematical Particle Tracing (pt)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GLOBAL DEFINITIONS

Specify the dimensions of the air domain and the cloak.

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
L	1[m]	1 m	Box length
a	0.2[m]	0.2 m	Inner radius
b	0.4[m]	0.4 m	Outer radius
n_air	1	1	Refractive index of air
hmax	L*0.2	0.2 m	Maximum element size in volume
hmax_cloak	b*0.05	0.02 m	Maximum element size in cloak

GEOMETRY 1

Block 1 (blk1)

1 On the **Geometry** toolbar, click **Block**.

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

3 In the **Width** text field, type `2*L`.

4 In the **Depth** text field, type `2*L`.

5 In the **Height** text field, type `2*L`.

6 Locate the **Position** section. From the **Base** list, choose **Center**.

Sphere 1 (sph1)

1 On the **Geometry** toolbar, click **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

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

Sphere 2 (sph2)

1 On the **Geometry** toolbar, click **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

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

4 Click **Build All Objects**.

5 Click **Go to Default View**.

DEFINITIONS

Now add the expressions which transform the refractive index of the cloak from Cartesian to spherical coordinates. The wave vector must also be transformed.

Variables 1

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

Load the variable definitions from a file.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `ideal_cloak_variables.txt`.

Using the analogy presented in the introduction section above, enter an expression for the angular frequency, which is called `H_photon` in this case.

MATHEMATICAL PARTICLE TRACING (PT)

1 In the **Model Builder** window, expand the **Definitions** node, then click **Component 1 (comp1)>Mathematical Particle Tracing (pt)**.

2 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Hamiltonian**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Hamiltonian** section.

3 In the H text field, type `H_photon`.

4 Locate the **Particle Mass** section. In the m_p text field, type `1`.

Next, release the particles in the y direction for a fixed x and z coordinate.

Release from Grid 1

1 On the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{x,\,0}$ text field, type `-1`.

4 In the $q_{y,\,0}$ text field, type `range(-0.38,0.01,-0.02) range(0.02,0.01,0.38)`.

5 In the $q_{z,\,0}$ text field, type `0`.

6 Locate the **Initial Velocity** section. Specify the $\mathbf{v}_0$ vector as

1	x
0	y
0	z

Because the Hamiltonian formulation is being used to model rays, the settings entered for the **Initial velocity** determine the initial wave vector direction, not the velocity of the model particles.

The mesh needs to be fine in the cloak region so that the particle trajectories can be computed to a high degree of accuracy.

MESH 1

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Free Tetrahedral**.

2 Right-click **Free Tetrahedral 1** and choose **Size**.

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

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

5 Select Domain 2 only.

6 Click to expand the **Element size parameters** section. Locate the **Element Size** section. Click the **Custom** button.

7 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

8 In the associated text field, type `hmax_cloak`.

9 Select the **Minimum element size** check box.

10 In the associated text field, type `hmax_cloak/2`.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **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. In the **Maximum element size** text field, type `hmax`.

5 In the **Minimum element size** text field, type `hmax/2`.

6 In the **Model Builder** window, click **Mesh 1**.

7 In the **Settings** window for **Mesh**, click **Build All**.

To accurately compute the particle trajectories in an anisotropic medium, the default solver tolerances need to be made more strict. Do this by first showing the default solver, and then reducing the relative and absolute tolerances.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 Click **Range**.

4 In the **Range** dialog box, type `2[m]/c_const` in the **Stop** text field.

5 From the **Entry method** list, choose **Number of values**.

6 In the **Number of values** text field, type `301`.

7 Click **Replace**.

8 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

9 From the **Tolerance** list, choose **User controlled**.

10 In the **Relative tolerance** text field, type `1e-6`.

Solution 1 (sol1)

1 On the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)** click **Time-Dependent Solver 1**.

4 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time stepping** section.

5 Locate the **Time Stepping** section. From the **Method** list, choose **Runge-Kutta**.

6 From the **Runge-Kutta method** list, choose **Dormand-Prince 5**.

7 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)> Time-Dependent Solver 1** click **Fully Coupled 1**.

8 In the **Settings** window for **Fully Coupled**, click to expand the **Method and termination** section.

9 Locate the **Method and Termination** section. From the **Jacobian update** list, choose **Minimal**.

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

RESULTS

Particle Trajectories (pt)

The path of the rays is best visualized by adding selections for the cloak inner and outer surfaces.

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot data set edges** check box.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 In the **Model Builder** window, expand the **Particle Trajectories (pt)** node.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Results>Particle Trajectories (pt)> Particle Trajectories 1** 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**.

4 Find the **Point style** subsection. From the **Type** list, choose **None**.

Color Expression 1

1 In the **Model Builder** window, under **Results>Particle Trajectories (pt)> Particle Trajectories 1** click **Color Expression 1**.

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

3 Clear the **Color legend** check box.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Particle Trajectories (pt)** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Solution 1 (sol1)**.

4 Locate the **Expression** section. In the **Expression** text field, type `cos_phi`.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **WaveLight**.

6 Clear the **Color legend** check box.

Selection 1

1 Right-click **Results>Particle Trajectories (pt)>Surface 1** and choose **Selection**.

2 Select Boundaries 6, 8, 14, and 18 only.

Surface 2

1 In the **Model Builder** window, under **Results** right-click **Particle Trajectories (pt)** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Solution 1 (sol1)**.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Gray**.

Selection 1

1 Right-click **Results>Particle Trajectories (pt)>Surface 2** and choose **Selection**.

2 Select Boundaries 10–13, 16, 17, 19, and 20 only.

DEFINITIONS

View 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **View 1**.

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

3 Clear the **Show grid** check box.

RESULTS

Particle Trajectories 1

1 In the **Model Builder** window, under **Results>Particle Trajectories (pt)** click **Particle Trajectories 1**.

2 On the **Particle Trajectories (pt)** toolbar, click **Plot**.

3 Click the **Go to XY View** button on the **Graphics** toolbar. The plot should look like Figure 1.

To see how well the cloak performs, look at the rays in phase space before and after they pass through the cloak. You can do this in two different ways.

The first method is to define a pair of **Cut Plane** data sets on the incoming and outgoing sides of the cloak, then plot a **Poincaré Map** of the ray positions as they intersect each plane.

Cut Plane 1

1 On the **Results** toolbar, click **Cut Plane**.

2 In the **Settings** window for **Cut Plane**, locate the **Data** section.

3 From the **Data set** list, choose **Particle 1**.

4 Locate the **Plane Data** section. In the **x-coordinate** text field, type `-0.99`.

Cut Plane 2

1 Right-click **Cut Plane 1** and choose **Duplicate**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 In the **x-coordinate** text field, type `0.99`.

2D Plot Group 2

1 On the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Ray Position Relative to Initial Position` in the **Label** text field.

3 Locate the **Plot Settings** section. Select the **x-axis label** check box.

4 In the associated text field, type `y-position (m)`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `z-position (m)`.

Poincaré Map 1

1 On the **Ray Position Relative to Initial Position** toolbar, click **More Plots** and choose **Poincaré Map**.

2 In the **Settings** window for **Poincaré Map**, locate the **Data** section.

3 From the **Cut plane** list, choose **Cut Plane 1**.

4 On the **Ray Position Relative to Initial Position** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

Poincaré Map 2

1 Right-click **Poincaré Map 1** and choose **Duplicate**.

2 In the **Settings** window for **Poincaré Map**, locate the **Data** section.

3 From the **Cut plane** list, choose **Cut Plane 2**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

5 Select the **Radius scale factor** check box.

6 In the associated text field, type `0.004`.

7 Click to expand the **Title** section. From the **Title type** list, choose **None**.

8 On the **Ray Position Relative to Initial Position** toolbar, click **Plot**.

9 Click the **Zoom Extents** button on the **Graphics** toolbar. The plot should look like Figure 2.

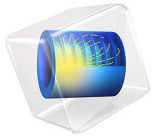
The second method is to construct a **Phase Portrait** of the rays and verify that their positions and velocities are the same before and after passing through the cloak.

1D Plot Group 3

1. On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Change in Lateral Position` in the **Label** text field.
3. Locate the **Data** section. From the **Data set** list, choose **Particle 1**.
4. From the **Time selection** list, choose **Last**.
5. Locate the **Plot Settings** section. Select the **x-axis label** check box.
6. In the associated text field, type `Initial position (mm)`.
7. Select the **y-axis label** check box.
8. In the associated text field, type `Change in position (mm)`.

Particle 1

1. On the **Change in Lateral Position** toolbar, click **More Plots** and choose **Particle**.
2. In the **Settings** window for **Particle**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `qy-at(0,qy)`.
4. From the **Unit** list, choose **mm**.
5. Click to expand the **Title** section. From the **Title type** list, choose **None**.
6. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
7. In the **Expression** text field, type `at(0,qy)`.
8. From the **Unit** list, choose **mm**.
9. Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
10. From the **Positioning** list, choose **In data points**.
11. On the **Change in Lateral Position** toolbar, click **Plot**. The plot should look like Figure 3. You can see that the rays do indeed return to their original position after passing through the cloak.



Ion Cyclotron Motion

Introduction

If a charged particle is placed in a uniform magnetic field, it moves in a helical pattern about a fixed gyro radius. The gyro radius, which is also known as the Larmor or cyclotron radius, is given by the simple equation:

$$r_L = \frac{mv_\perp}{ZeB}$$

- r_L (SI unit: m) is the Larmor radius,
- $v_\perp$ (SI unit: m/s) is the velocity component orthogonal to the magnetic field,
- Z (dimensionless) is the particle charge number,
- $e = 1{,}60217656 \times 10^{-19}\ C$ is the elementary charge,
- m (SI unit: kg) is the particle mass, and
- B (SI unit: T) is the magnitude of the magnetic flux density.

This model computes the trajectory of an ion in a uniform magnetic field using the Newtonian, Lagrangian, and Hamiltonian formulations available in the Mathematical Particle Tracing interface.

Model Definition

The equations of motion for a charge in a magnetic field can be determined from the Lagrange equations:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{\partial L}{\partial \mathbf{q}} \tag{1}$$

where $\mathbf{v}$ is the particle velocity, $\mathbf{q}$ is the particle position, and L (SI unit: J) is the Lagrangian, which is defined as:

$$L = \frac{m(\mathbf{v}\cdot\mathbf{v})}{2} + q(\mathbf{v}\cdot\mathbf{A})$$

This form of the Lagrangian is valid for nonrelativistic particles; that is, the particle velocity is much less than the speed of light. The contribution due to the electric potential is neglected. The Hamiltonian is related to the Lagrangian via:

$$H = \mathbf{v}\cdot\frac{\partial L}{\partial \mathbf{v}} - L$$

Introducing the generalized momentum of the particle, $\mathbf{P}$ (SI unit: kg·m/s), the Hamiltonian becomes:

$$H = \frac{(\mathbf{P} - q\mathbf{A})^2}{2m}$$

In order to derive the equations of motion for the Newtonian formulation, start with the right-hand side of Equation 1:

$$\frac{\partial L}{\partial \mathbf{q}} = \nabla L = q\nabla(\mathbf{A}\cdot\mathbf{v}) = q(\mathbf{v}\cdot\nabla)\mathbf{A} + q(\mathbf{v}\times\nabla\times\mathbf{A}) \tag{2}$$

The left-hand side of Equation 1 becomes

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{d}{dt}(\mathbf{p} + q\mathbf{A}) = \frac{d\mathbf{p}}{dt} + q(\mathbf{v}\cdot\nabla)\mathbf{A} + q\frac{\partial \mathbf{A}}{\partial t}. \tag{3}$$

Equating Equation 2 and Equation 3 and canceling like terms yields

$$\frac{d\mathbf{p}}{dt} = q(\mathbf{v}\times\mathbf{B}) \tag{4}$$

for a stationary magnetic field. Here, the magnetic flux density has been introduced as

$$\mathbf{B} = \nabla\times\mathbf{A} \tag{5}$$

When the particle velocity is small compared to the speed of light Equation 4 yields the classical equation of motion for a charged particle in a stationary, uniform magnetic field

$$\frac{d}{dt}(m\mathbf{v}) = q(\mathbf{v}\times\mathbf{B})$$

Results and Discussion

The model is solved in COMSOL using the Lagrangian, Hamiltonian, and Newtonian formulations. The Larmor radius is compared to the analytic solution and given in Table 1. All three formulations agree with the analytic expression to within 0.05 %. The Hamiltonian formulation gives slightly different results because it solves two first-order differential equations as opposed to a single second-order equation.

TABLE 1: TABLE COMPARING THE LARMOR RADIUS FOR THE DIFFERENT FORMULATIONS

	ANALYTIC	LAGRANGIAN	HAMILTONIAN	NEWTONIAN
Larmor radius (um)	414.57	414.42	414.53	414.42

The particle trajectories for the three different formulations are plotted below.

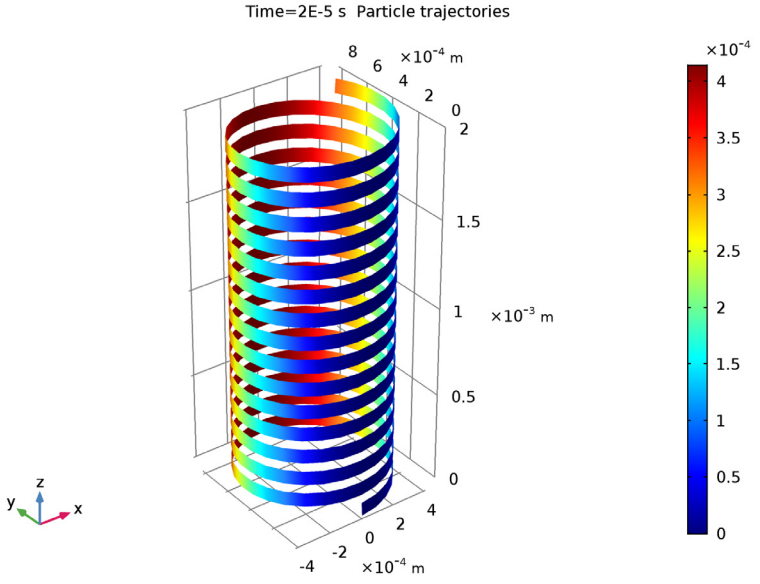


Figure 1: Plot of the ion trajectory for the Lagrangian formulation.

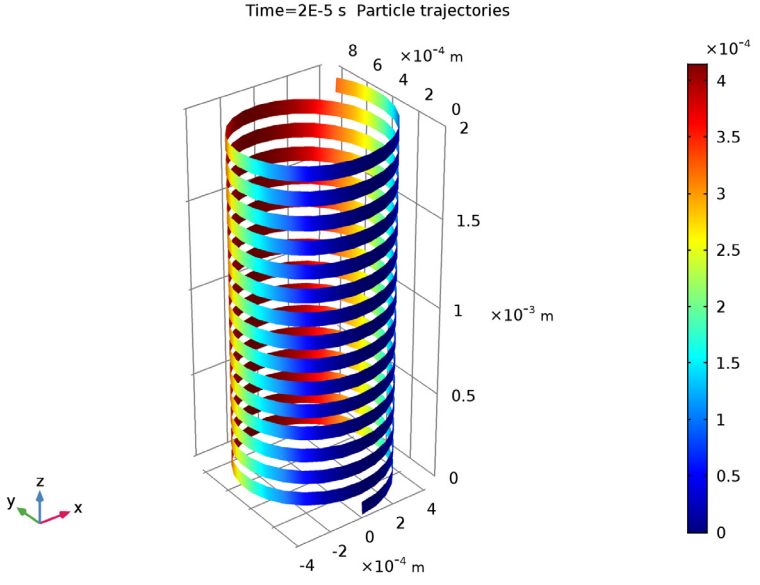


Figure 2: Plot of the ion trajectory for the Hamiltonian formulation.

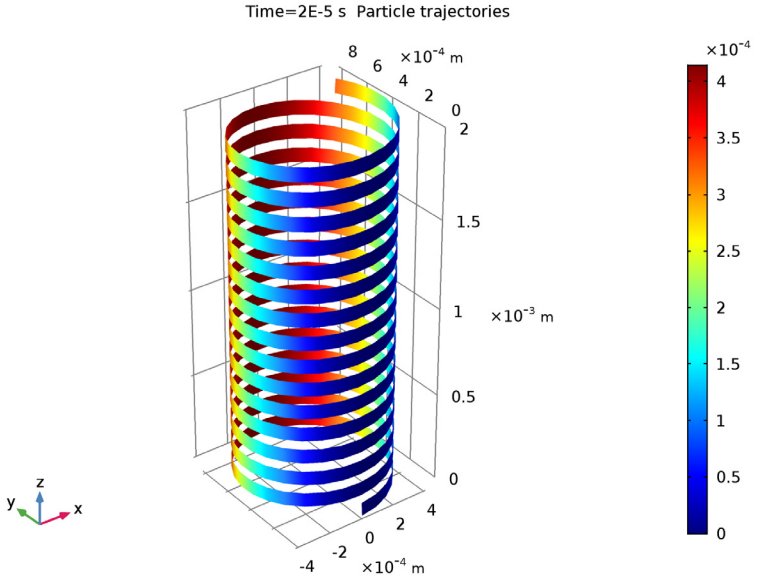


Figure 3: Plot of the particle trajectory for the Newtonian formulation.

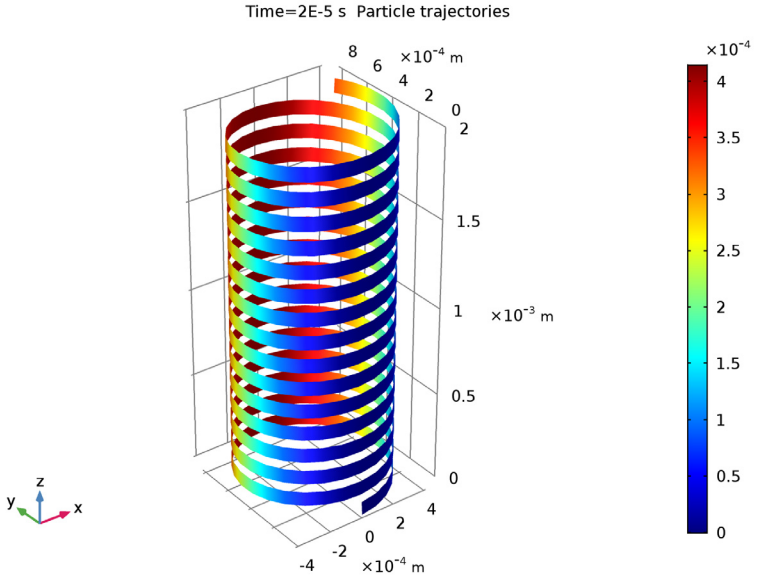


Figure 4: Plot of the particle trajectory for the first-order Newtonian formulation.

Reference

1. L.D. Landau and E.M. Lifshitz, *The Classical Theory of Fields*, 4th ed., Elsevier, 2005.

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/ion_cyclotron_motion`

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 **Mathematics>Mathematical Particle Tracing (pt)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

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 `2e-3`.

4 In the **Height** text field, type `2e-3`.

5 On the **Geometry** toolbar, click **Build All**.

GLOBAL DEFINITIONS

Define parameters for the particle mass, magnetic flux density, initial particle velocity, and Larmor radius. The Larmor radius is only used during results processing.

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
mp	0.04[kg/mol]/ N_A_const	6.6422E-26 kg	Ion mass
B	2[T]	2 T	Magnetic flux density
v0	2E3[m/s]	2000 m/s	Particle velocity, perpendicular to the magnetic field
rL	mp*v0/(e_const*B)	4.1457E-4 m	Larmor radius

Now define an analytic expression for the magnetic vector potential, which results in a uniform magnetic field in the z-direction.

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
Ax	1[Wb/m]*y[1/m]	Wb/m	Magnetic vector potential, x-component
Ay	-1[Wb/m]*x[1/m]	Wb/m	Magnetic vector potential, y-component
Az	0[Wb/m]	Wb/m	Magnetic vector potential, z-component
Bx	d(Az,y)-d(Ay,z)	T	Magnetic flux density, x-component
By	d(Ax,z)-d(Az,x)	T	Magnetic flux density, y-component
Bz	d(Ay,x)-d(Ax,y)	T	Magnetic flux density, z-component

Release a single particle at the origin with an initial velocity in the x-direction so that the Lorentz force is non-zero. Also add a small initial velocity in the z-direction so that you can clearly see the particle trajectory after solving.

MATHEMATICAL PARTICLE TRACING (PT)

In the **Model Builder** window, expand the **Component 1 (comp1)> Mathematical Particle Tracing (pt)** node.

Release from Grid 1

1. Right-click **Mathematical Particle Tracing (pt)** and choose **Release from Grid**.
2. In the **Settings** window for **Release from Grid**, locate the **Initial Velocity** section.
3. Specify the $\mathbf{v}_0$ vector as

v0	x
0	y
1e2	z

The first formulation you will use is **Lagrangian**. The Lagrangian for a particle in a magnetic field is the sum of the particle kinetic energy, which is here defined as `pt.Ep`, and the dot product of the particle velocity and the magnetic potential, multiplied by the particle charge.

4. In the **Model Builder** window, click **Mathematical Particle Tracing (pt)**.
5. In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.
6. From the **Formulation** list, choose **Lagrangian**.

Particle Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** click **Particle Properties 1**.
2. In the **Settings** window for **Particle Properties**, locate the **Particle Mass** section.
3. In the m_p text field, type `mp`.
4. Locate the **Lagrangian** section. In the L text field, type `pt.Ep+e_const*(pt.vx*Ax+pt.vy*Ay+pt.vz*Az)`.

Use a coarse mesh. The field is entered using an analytic expression, so the accuracy of the solution is independent of the mesh element size.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

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

3 From the **Element size** list, choose **Extra coarse**.

4 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,5.0e-8,2.0e-5)`.

4 In the **Model Builder** window, click **Study 1**.

5 In the **Settings** window for **Study**, type `Lagrangian Study` in the **Label** text field.

6 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (pt)

In order to be able to see the radius of the particle orbit, plot the *y*-component of the particle location as a color expression.

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, type `Lagrangian Results` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Particle Trajectories 1

Render the particle trajectory as a ribbon. The default ribbon orientation is in the direction of the unit binormal, or the direction out of the plane tangent to the curved trajectory.

1 In the **Model Builder** window, expand the **Results>Lagrangian Results** 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 **Ribbon**.

4 Select the **Width scale factor** check box.

5 In the associated text field, type `4E-5`.

6 Find the **Point style** subsection. From the **Type** list, choose **None**.

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 `qy/2`.

4 On the **Lagrangian Results** toolbar, click **Plot**.

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

Particle Evaluation 1

1 On the **Results** toolbar, click **More Derived Values** and choose **Other>Particle Evaluation**.

2 In the **Settings** window for **Particle Evaluation**, locate the **Data** section.

3 In the **Time** list, select **0**.

4 Locate the **Expression** section. In the **Expression** text field, type `rL`.

5 Click the arrow next to the **Evaluate** button and click **New Table**.

Particle Evaluation 2

1 On the **Results** toolbar, click **More Derived Values** and choose **Other>Particle Evaluation**.

2 In the **Settings** window for **Particle Evaluation**, locate the **Data** section.

3 In the **Time** list, select **0**.

4 Locate the **Expression** section. In the **Expression** text field, type `timemax(0,2E-5,qy)/2`.

5 Click the arrow next to the **Evaluate** button and select **Table 1 - Particle Evaluation 1 (rL)**.

Now switch formulation from **Lagrangian** to **Hamiltonian**. When you do this, the particle momentum components are added as additional degrees of freedom. The momentum has three components: p_x, p_y, and p_z. This results in a doubling of the number of degrees of freedom in the model.

MATHEMATICAL PARTICLE TRACING (PT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mathematical Particle Tracing (pt)**.

2 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Hamiltonian**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Hamiltonian** section.

3 In the H text field, type `((px-e_const*Ax)^2+(py-e_const*Ay)^2+(pz-e_const*Az)^2)/(2*pt.mp)`.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,5.0e-8,2.0e-5)`.

4 In the **Model Builder** window, click **Study 2**.

5 In the **Settings** window for **Study**, type `Hamiltonian Study` in the **Label** text field.

6 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (pt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, type `Hamiltonian Results` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Results>Hamiltonian Results** 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 **Ribbon**.

4 Select the **Width scale factor** check box.

5 In the associated text field, type `4E-5`.

6 Find the **Point style** subsection. From the **Type** list, choose **None**.

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 `qy/2`.

4 On the **Hamiltonian Results** toolbar, click **Plot**.

5 Click **Go to Default View**. The plot should look like Figure 2.

Particle Evaluation 3

1 On the **Results** toolbar, click **More Derived Values** and choose **Other>Particle Evaluation**.

2 In the **Settings** window for **Particle Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Particle 2**.

4 In the **Time** list, select **0**.

5 Locate the **Expression** section. In the **Expression** text field, type `timemax(0,2E-5,qy)/2`.

6 Click the arrow next to the **Evaluate** button and select **Table 1 - Particle Evaluation 1 (rL)**.

Switch to the **Newtonian** formulation and add the Lorentz force manually.

MATHEMATICAL PARTICLE TRACING (PT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mathematical Particle Tracing (pt)**.

2 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Newtonian**.

Force 1

1 Right-click **Component 1 (comp1)>Mathematical Particle Tracing (pt)** and choose **Force**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Force**, locate the **Force** section.

4 Specify the **F** vector as

`e_const*(Bz*pt.vy-By*pt.vz)`	x
`e_const*(-Bz*pt.vx+Bx*pt.vz)`	y
`e_const*(By*pt.vx-Bx*pt.vy)`	z

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,5.0e-8,2.0e-5)`.

4 In the **Model Builder** window, click **Study 3**.

5 In the **Settings** window for **Study**, type `Newtonian Study` in the **Label** text field.

6 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (pt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, type `Newtonian Results` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Results>Newtonian Results** 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 **Ribbon**.

4 Select the **Width scale factor** check box.

5 In the associated text field, type `4E-5`.

6 Find the **Point style** subsection. From the **Type** list, choose **None**.

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 `qy/2`.

4 On the **Newtonian Results** toolbar, click **Plot**.

5 Click **Go to Default View**. The plot should look like Figure 3.

Particle Evaluation 4

1 On the **Results** toolbar, click **More Derived Values** and choose **Other>Particle Evaluation**.

2 In the **Settings** window for **Particle Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Particle 3**.

4 In the **Time** list, select **0**.

5 Locate the **Expression** section. In the **Expression** text field, type `timemax(0,2E-5,qy)/2`.

6 Click the arrow next to the **Evaluate** button and select **Table 1 - Particle Evaluation 1 (rL)**.

Finally, switch to the **Newtonian, first order** formulation.

MATHEMATICAL PARTICLE TRACING (PT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mathematical Particle Tracing (pt)**.

2 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Newtonian, first order**.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 4

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 4** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,5.0e-8,2.0e-5)`.

4 In the **Model Builder** window, click **Study 4**.

5 In the **Settings** window for **Study**, type `Newtonian, First Order Study` in the **Label** text field.

6 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (pt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, type `Newtonian, First Order Results` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Results>Newtonian, First Order Results** 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 **Ribbon**.

4 Select the **Width scale factor** check box.

5 In the associated text field, type `4E-5`.

6 Find the **Point style** subsection. From the **Type** list, choose **None**.

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 `qy/2`.

4 On the **Newtonian, First Order Results** toolbar, click **Plot**.

5 Click **Go to Default View**. The plot should look like Figure 4.

Particle Evaluation 5

1 On the **Results** toolbar, click **More Derived Values** and choose **Other>Particle Evaluation**.

2 In the **Settings** window for **Particle Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Particle 4**.

4 In the **Time** list, select **0**.

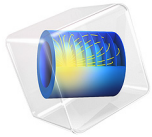
5 Locate the **Expression** section. In the **Expression** text field, type `timemax(0,2E-5,qy)/2`.

6 Click the arrow next to the **Evaluate** button and select **Table 1 - Particle Evaluation 1 (rL)**.

TABLE

1 Go to the **Table** window.

The Larmor radius shows good agreement with the analytic expression for all four formulations.



Ion Drift Velocity Benchmark

Introduction

When ions are subjected to a static electric field in a rarefied buffer gas, the combined effect of the electric force and collisions between nearby neutral particles causes the average ion velocity to approach an equilibrium value known as the ion drift velocity. The ability to accurately predict the drift velocity is important for the operation of devices such as ion mobility spectrometers, which are capable of accurately analyzing gas mixtures containing many different ion species by sorting the different species based on small variations in their drift velocity.

In this example, the average drift velocity of a group of argon ions is computed and compared to experimental data. The ions are modeled using the Charged Particle Tracing interface. Collisions with a neutral background gas are applied using the **Collisions** node, which supports various stochastic collision models including **Elastic** collisions and **Resonant Charge Exchange** reactions. The resulting average ion drift velocity and ion temperature agree closely with values from the literature.

Model Definition

The model consists of a group of Ar+ ions which are released in a neutral background gas of Ar atoms at a given temperature and number density. The background gas is assumed to follow a Maxwellian velocity distribution:

$$f(v_i) = \sqrt{\frac{m_p}{2\pi k_B T_0}} \exp\left(-\frac{m_p(v_i^2)}{2k_B T_0}\right)$$

At each time step taken by the solver, for each model particle a background gas particle is sampled at random from the Maxwellian distribution. The frequency of elastic collisions is then computed from the collision cross-section, background gas number density, and the relative velocity of the model particle with respect to the randomly sampled background gas particle:

$$\nu = N_d \sigma |\mathbf{v}_p - \mathbf{v}_g| \tag{1}$$

where the collision cross section is generally a function of the particle kinetic energy. The collision probability is then computed as a function of the collision frequency and the time step size:

$$P = 1 - \exp(-\nu \Delta t)$$

The particles can be subjected to many different collision types in the same model. In this example, the Ar+ ions are subjected to **Elastic** collisions, in which only momentum is exchanged between the model particle and the neutral background Argon atom; and **Resonant Charge Exchange** reactions, in which both charge and momentum are exchanged between the model particle and the background gas. It is possible to specify different collision cross sections for each type of reaction; the collision frequency in Equation 1 is then computed based on the sum of all of the specified cross sections. When a collision is detected, one of the available collision types is applied at random, with probabilities proportional to their respective collision cross sections. Only one type of collision can be applied to a single particle in a single time step taken by the solver.

In addition to the elastic and charge exchange collisions, the ions are also subjected to a uniform static electric field polarized in the z-direction. When the sample size of the model particles is sufficiently large, the average z-component of the particle velocity then approaches an equilibrium value, the ion drift velocity.

To obtain an accurate solution with a stochastic collision model, strict or manual time stepping is recommended. The maximum time step taken by the solver should be small compared to the average time between elastic collisions, so that the particles can be correctly accelerated by the electric force in the time between successive collisions. However, the number of collisions also must be sufficiently large to achieve statistical convergence.

One viable approach to ensure that a sufficient number of collisions have occurred, without wasting additional computational resources and time, is to modify the solver sequence to include a **Stop Condition** based on the total number of collisions. To keep track of the total number of elastic collisions or charge exchange reactions that each particle undergoes, select the **Count collisions** check box for each reaction type. You can also select the **Count all collisions** check box in the settings window for the parent **Collisions** node to monitor the total number of collisions of any type that occur for each model particle. The sum of the number of collisions over all model particles can be evaluated using the built-in component coupling `comp1.cpt.cptop1(expr)`, which computes the sum of the expression `expr` over all model particles.

Results and Discussion

The relationship between the reduced electric field magnitude and the average ion drift velocity is shown in Figure 1. The average ion temperature is shown in Figure 2.

In both plots, the computed solution shows good agreement with experimental data from Ref. 1.

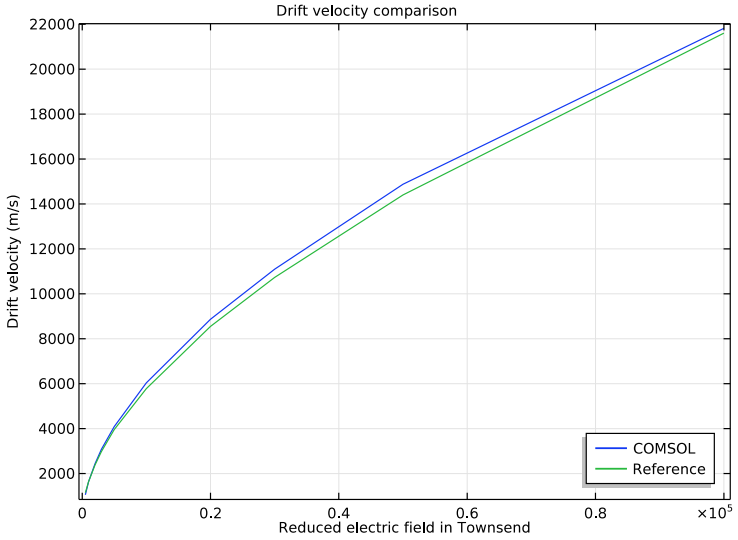


Figure 1: Plot of the drift velocity of Ar+ ions in a background gas of neutral argon. The average drift velocity is compared to experimental data.

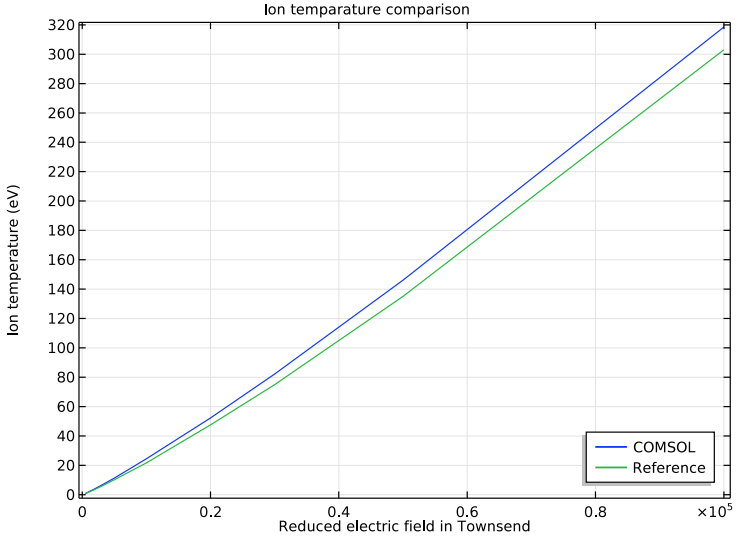


Figure 2: Plot of the ion temperature of Ar+ ions in a background gas of neutral argon. The average ion temperature is compared to experimental data.

Reference

1. A.V. Phelps, "Cross Sections and Swarm Coefficients for Nitrogen Ions and Neutrals in N2 and Argon Ions and Neutrals in Ar for Energies from 0.1eV to 10keV," *J. Phys. Chem. Ref. Data*, vol. 20, no. 3, pp. 557–573, 1991.

2. A. V. Phelps, "The application of scattering cross sections to ion flux models in discharge sheaths," *J. Appl. Phys.* vol. 76, pp. 747-753, 1994.

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/ion_drift_velocity_benchmark`

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>Charged Particle Tracing (cpt)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
mAr	0.04[kg/mol]/ N_A_const	6.6422E-26 kg	Ar+ ion mass
ND	3.2956e22[1/m^3]	3.2956E22 1/m³	Background gas number density
EoverN	500	500	Reduced electric field in Townsend
Ez	1e-21[V*m^2]* EoverN*ND	16478 V/m	Electric field magnitude
T0	300[K]	300 K	Gas temperature
maxCol	1e5	1E5	Maximum number of collisions for termination

DEFINITIONS

Enter raw data from Ref. 1 for the ion drift velocity as a function of the reduced electric field for elastic collisions between Ar+ ions and neutral Ar atoms.

Interpolation 1 (int1)

1 On the **Home** toolbar, click **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `ion_drift_velocity_benchmark_velocity.txt`.

6 Click **Import**.

7 Locate the **Units** section. Clear the **Arguments** text field.

8 In the **Function** text field, type `m/s`.

9 Locate the **Definition** section. In the **Function name** text field, type `Vdrift`.

Enter raw data from Ref. 1 for the ion temperature (eV) as a function of the reduced electric field.

Interpolation 2 (int2)

1 On the **Home** toolbar, click **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `ion_drift_velocity_benchmark_temperature.txt`.

6 Click **Import**.

7 Locate the **Units** section. Clear the **Arguments** text field.

8 In the **Function** text field, type `eV`.

9 Locate the **Definition** section. In the **Function name** text field, type `ionTemp`.

Enter the analytic approximation for momentum cross section for elastic scattering between Ar+ ions and neutral Ar atoms from Ref. 2, which depends on the kinetic energy of the particles.

Analytic 1 (an1)

1 On the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type `Qm` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `1.15e-18*x^(-0.1)*(1+0.015/x)^0.6`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

Enter the analytic approximation for isotropic elastic collision between Ar+ ions and neutral Ar atoms from Ref. 2, which depends on the kinetic energy of the particles.

Analytic 2 (an2)

1 On the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type `Qi` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `2e-19/(x^(0.5)*(1+x))+3e-19*x/(1+x/3)^(2.3)`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

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 `2`.

4 In the **Height** text field, type 3.

5 Click **Build All Objects**.

CHARGED PARTICLE TRACING (CPT)

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Mass** section.

3 In the m_p text field, type `mAr`.

4 Locate the **Charge Number** section. In the Z text field, type 1.

Wall 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Wall 1**.

2 In the **Settings** window for **Wall**, locate the **Wall Condition** section.

3 From the **Wall condition** list, choose **Bounce**.

Release from Grid 1

1 In the **Model Builder** window, right-click **Charged Particle Tracing (cpt)** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{z,\,0}$ text field, type 1.

4 Locate the **Initial Velocity** section. From the **Initial velocity** list, choose **Maxwellian**.

5 In the $N_{\mathbf{v}}$ text field, type 30.

6 In the T_0 text field, type T0.

Electric Force 1

1 Right-click **Charged Particle Tracing (cpt)** and choose **Electric Force**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

4 Specify the $\mathbf{E}$ vector as

0	x
0	y
Ez	z

Collisions 1

1 Right-click **Charged Particle Tracing (cpt)** and choose **Collisions**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Collisions**, locate the **Fluid Properties** section.

4 In the N_d text field, type `ND`.

5 In the T text field, type `T0`.

6 Locate the **Collision Statistics** section. Select the **Count all collisions** check box.

Elastic 1

1 Right-click **Component 1 (comp1)>Charged Particle Tracing (cpt)>Collisions 1** and choose **Elastic**.

2 In the **Settings** window for **Elastic**, locate the **Collision Frequency** section.

3 In the σ text field, type `Qi(cpt.Ep)`.

4 Locate the **Collision Statistics** section. Select the **Count collisions** check box.

Resonant Charge Exchange 1

1 Right-click **Collisions 1** and choose **Resonant Charge Exchange**.

2 In the **Settings** window for **Resonant Charge Exchange**, locate the **Collision Frequency** section.

3 In the σ text field, type `(Qm(cpt.Ep)-Qi(cpt.Ep))/2`.

4 Locate the **Collision Statistics** section. Select the **Count collisions** check box.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, click **Build All**.

STUDY 1

Parametric Sweep

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

Sweep the reduced electric field from 500 Td to 1e5 Td.

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
EoverN	`5e2, 1e3, 2e3, 3e3, 5e3, 1e4, 2e4, 3e4, 5e4, 1e5`	

To produce an accurate solution, the number of time steps taken by the solver should be at least an order of magnitude larger than the average number of collisions. To ensure that a proper amount of collisions occur within each time step for any values of the reduce electric field, set a fixed time step in the solver settings proportional to `sqrt(maxCol/EoverN)`. This choice of time step size and the use of a **Stop Condition** on the maximum number of collisions allows the computation time to be considerably reduced without compromising accuracy. In order to keep the file size relatively small, store output at only two time steps in the study settings.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `0,5.0e-8*sqrt(maxCol/EoverN)`.

Solution 1 (sol1)

1 On the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time stepping** section.

4 Locate the **Time Stepping** section. From the **Steps taken by solver** list, choose **Manual**.

5 In the **Time step** text field, type `5e-11*sqrt(maxCol/EoverN)`.

6 In the **Amplification for high frequency** text field, type `1`.

7 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

Set the stop condition to stop the time-dependent solver when the maximum number of collisions is reached. Make sure to store the solution at the time steps before and after the stop condition is fulfilled.

8 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

9 Click **Add**.

10 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.cpt.cptop1(comp1.cpt .col1.cex1.Nc)>maxCol`	true	√	`Stop expression 1`

11 Locate the **Output at Stop** section. From the **Add solution** list, choose **Steps before and after stop**.

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

RESULTS

1D Plot Group 2

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Compare the drift velocity to the tabulated data. Make this comparison at the last time step, after the drift velocity has reached an equilibrium value.

2 In the **Settings** window for **1D Plot Group**, type `Drift Velocity` in the **Label** text field.

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

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

5 Click to expand the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Drift Velocity** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`cpt.cptaveop1(cpt.vz)`	`m/s`	
`Vdrift(EoverN)`	`m/s`	

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `EoverN`.

7 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
COMSOL
Reference

Drift Velocity

1 In the **Model Builder** window, under **Results** click **Drift Velocity**.

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

3 Select the **y-axis label** check box.

4 In the associated text field, type `Drift velocity (m/s)`.

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Drift velocity comparison`.

7 On the **Drift Velocity** toolbar, click **Plot**. The resulting image should look like Figure 1.

Now compare the ion energy to tabulated data. From Ref. 1, the average ion energy corresponds to a one dimensional energy distribution, i.e. $E_p = k_B T/(2e)$.

Drift Velocity 1

1 In the **Model Builder** window, right-click **Drift Velocity** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Ion Temperature` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Results>Ion Temperature** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`cpt.cptaveop1(2*cpt.Ep)`	eV	
`ionTemp(EoverN)`	eV	

Ion Temperature

1 In the **Model Builder** window, under **Results** click **Ion Temperature**.

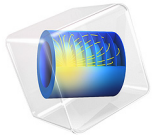
2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 In the **y-axis label** text field, type `Ion temperature (eV)`.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Ion temparature comparison`.

6 On the **Ion Temperature** toolbar, click **Plot**. The resulting image should look like Figure 2.



Particle Trajectories in a Laminar Static Mixer

Introduction

In static mixers, also called motionless or in-line mixers, a fluid is pumped through a pipe containing stationary blades. This mixing technique is particularly well suited for laminar flow mixing because it generates only small pressure losses in this flow regime. This example studies the flow in a twisted-blade static mixer. It evaluates the mixing performance by calculating the trajectory of suspended particles through the mixer.

Model Definition

This model studies the mixing of one species dissolved in water at room temperature. The geometry consists of a tube with three twisted blades of alternating rotations (Figure 1).

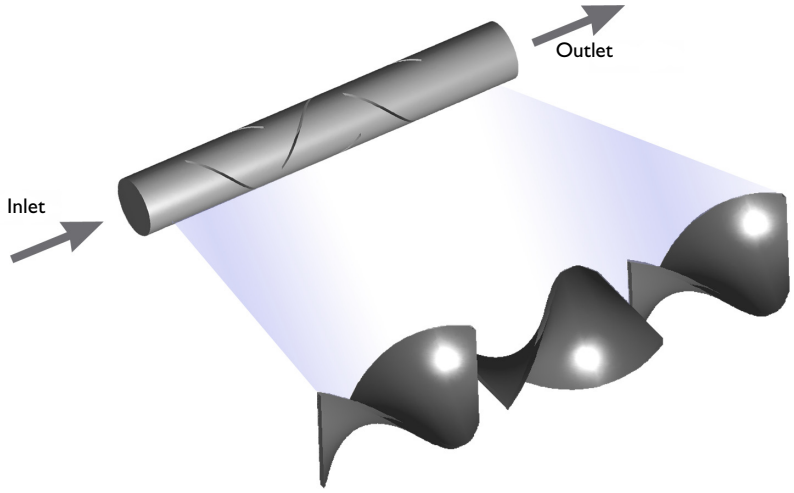


Figure 1: Depiction of a laminar static mixer containing three blades with alternating rotations.

The tube's radius, r_a, is 3 mm, the length is $14r_a$, and the length of each blade is $3r_a$. The inlet flow is laminar and fully developed with an average velocity of 1 cm/s. At the outlet, the model specifies a constant reference pressure of 0 Pa. The Laminar Flow interface is used in 3D, and the solved equations are:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]$$
$$\nabla\cdot\mathbf{u} = 0$$

Here μ denotes the dynamic viscosity (SI unit: kg/(m·s)), $\mathbf{u}$ is the velocity (SI unit: m/s), ρ is the fluid density (SI unit: kg/m^3), and p if the pressure (SI unit: Pa).

The particle trajectories are computed using a Newtonian formulation with the Stokes drag law,

$$\frac{d}{dt}(m_p\mathbf{v}) = \frac{1}{\tau_p}m_p(\mathbf{u}-\mathbf{v})$$

where $\mathbf{v}$ is the particle velocity and τ_p is the particle velocity response time:

$$\tau_p = \frac{\rho_p d_p^2}{18\mu}$$

where ρ_p is the density of the particles and d_p is the particle diameter. There are 3000 particles released. The density of the particles released is normalized according to the magnitude of the fluid velocity at the inlet. This means that there are more particles released where the inlet velocity magnitude is highest and fewer particles released where the velocity magnitude is low.

Results and Discussion

The particle trajectories are plotted in Figure 1. Because the particles have mass, they do not necessarily all reach the outlet; some of the particles get stuck to the mixer walls. The transmission probability is defined as the ratio of the number of particles that reach the outlet to the total number of particles released. For this specific configuration the transmission probability is about 0.80. This means that about 20% of the particles remain trapped in the mixer.

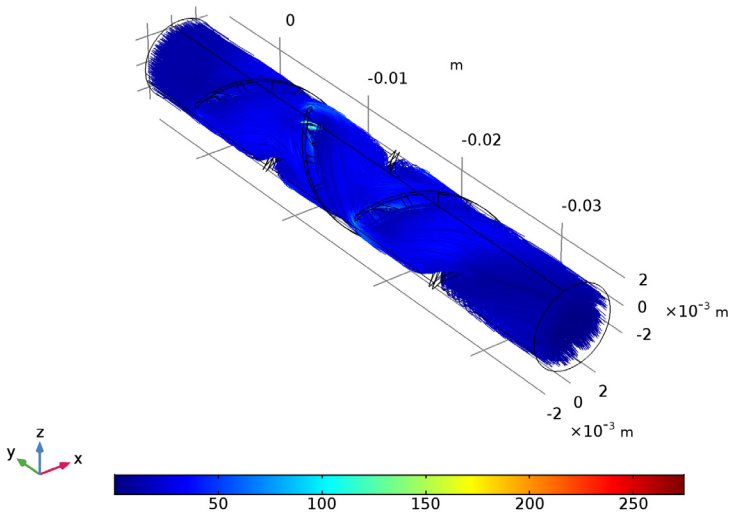


Figure 2: Plot of the particle trajectories inside the laminar mixer. The color is the shear rate.

One useful way of visualizing how to particles mix is to use a Poincaré plot. The Poincaré plot places a colored dot for each particles at the location at which the particle passes through a cut plane (known as a Poincaré section). In Figure 3, the location of the particles at 6 Poincaré sections are shown. The color represents the location of the particle at its initial position. So, particles marked as red had an initial position of $x < 0$ and particles marked as blue had an initial position of $x > 0$. The `at` operator is used to mark the particles with the color of their initial position. The first Poincaré section (the one furthest to the left in Figure 3) clearly indicates which particles start with coordinates of $x < 0$. As the particles begin to follow the flow field, they begin to mix together. By the end of the mixer, the particles have not mixed completely—there are still significant pockets of only red and only blue particles.

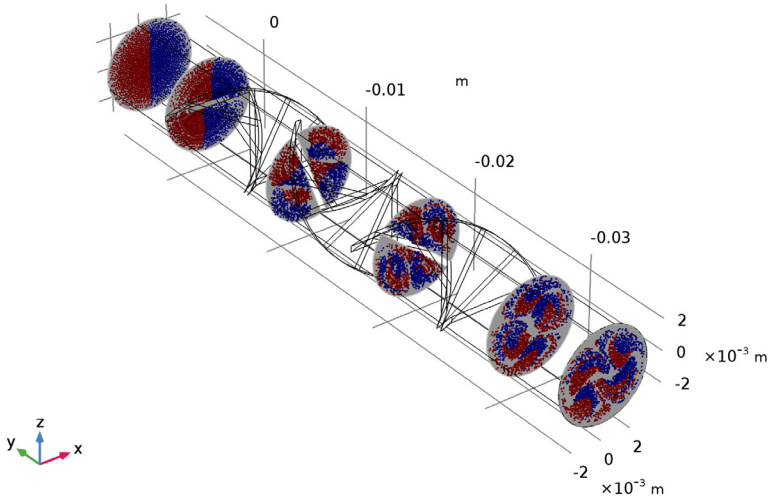


Figure 3: Poincaré maps of the particle trajectories at different Poincaré sections. The color is a logical expression indicating which particles had an initial position at $x < 0$.

A phase portrait can also be used to visualize the effect of particle mixing, but it is not as useful as the Poincaré map because it applies to all particles at a given snapshot in time rather than a plane in space. A standard phase portrait plots the particle position versus velocity (or momentum), but in COMSOL the default expressions can be overridden. In Figure 4 the x-axis represents the y-location of the particles, and the y-axis represents the z-location of the particles at different snapshots in time. At $t = 5$ s there are still pockets where only blue and only red particles exist, indicating that if 2 distinct streams were introduced at the inlet, they would not be completely mixed.

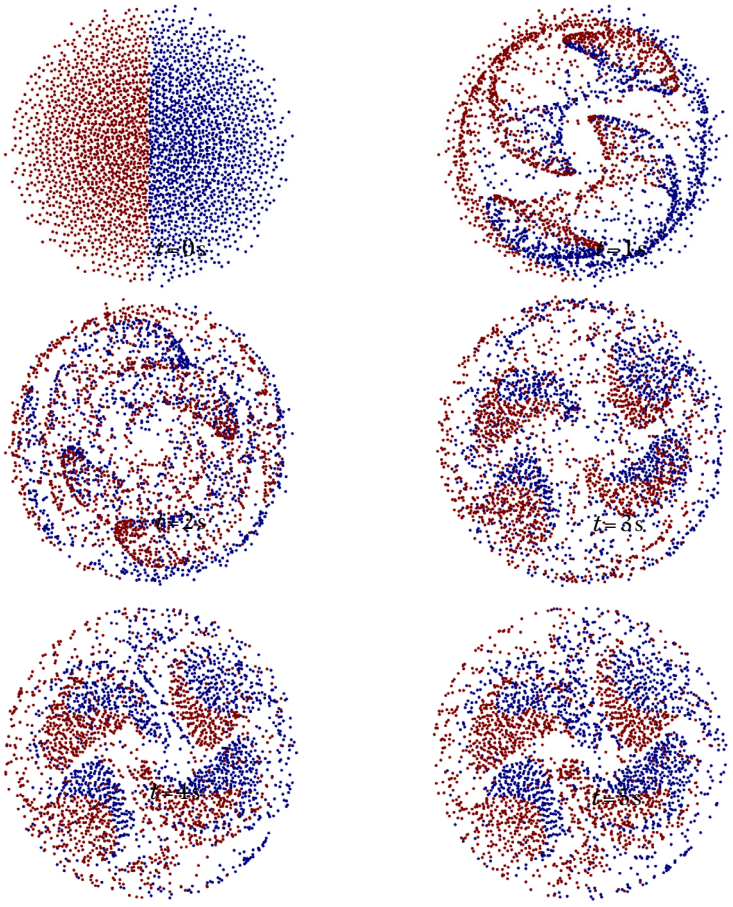


Figure 4: Plot of the particle position in the xz-plane at different points in time. The red colored particles had an initial position of $x < 0$ and the blue colored particles had an initial position of $x > 0$.

Notes About the COMSOL Implementation

The model is solved in two stages: first the fluid velocity and pressure are computed, then, using a separate study, the particle trajectories are computed.

Reference

1. R. Perry and D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

Application Library path: `Particle_Tracing_Module/Fluid_Flow/laminar_mixer_particle`

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 **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Stationary**.

6 Click **Done**.

GEOMETRY 1

The mixer geometry is quite complicated so start by importing it from a file.

Import 1 (imp1)

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

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

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `laminar_mixer_particle.mphbin`.

5 Click **Import**.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Ra	3[mm]	0.003 m	Tube radius
u_av	1[cm/s]	0.01 m/s	Mean velocity

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
Density	rho	1000	kg/m³	Basic
Dynamic viscosity	mu	1e-3	Pa·s	Basic

LAMINAR FLOW (SPF)

Now add an expression for the inflow velocity which is parabolic.

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Laminar Flow (spf)** node.

Inlet 1

1 Right-click **Laminar Flow (spf)** and choose **Inlet**.

2 Select Boundary 23 only.

3 In the **Settings** window for **Inlet**, locate the **Velocity** section.

4 In the U_0 text field, type `2*(1-(x^2+z^2)/Ra^2)*u_av`.

The boundary condition which was just added was rather complicated but necessary to get a fully developed flow profile. The CFD, Microfluidics, and Plasma modules all have

a special **Laminar inflow** boundary condition which ensures a fully developed flow profile at the inlet. It is not necessary to enter a complicated expression for the velocity profile, just the average velocity or flowrate.

Outlet 1

1 Right-click **Laminar Flow (spf)** and choose **Outlet**.

2 Select Boundary 20 only.

MESH 1

The mesh needs to be quite fine to ensure that the particle motion is accurate through the modeling domain. In this case, take care to ensure that the mesh is fine on the mixing blades.

1 On the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

Free Triangular 1

1 Click the **Wireframe Rendering** button on the **Graphics** toolbar.

2 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Free Triangular 1**.

3 Select Boundaries 5, 16–18, and 53–55 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Extremely fine**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

4 Click the **Custom** button.

5 Locate the **Element Size Parameters** section. In the **Curvature factor** text field, type `0.15`.

6 On the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

Free Triangular 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Free Triangular 2**.

2 Select Boundary 23 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Free Triangular 2** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Extra fine**.

5 On the **Mesh** toolbar, click **Free Tetrahedral**.

Free Tetrahedral 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Free Tetrahedral 1**.

2 In the **Settings** window for **Free Tetrahedral**, click **Build All**.

STUDY 1

On the **Home** toolbar, click **Compute**.

RESULTS

Velocity (spf)

Now that the flow field has been computed, add the interface to compute the particle trajectories.

ADD PHYSICS

1 On the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Particle Tracing>Particle Tracing for Fluid Flow (fpt)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1**.

5 Click **Add to Component** in the window toolbar.

6 On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for the **Laminar Flow (spf)** interface.

5 Click **Add Study** in the window toolbar.

6 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

PARTICLE TRACING FOR FLUID FLOW (FPT)

On the **Physics** toolbar, click **Laminar Flow (spf)** and choose **Particle Tracing for Fluid Flow (fpt)**.

The drag force feature should get the fluid velocity field and viscosity from the **Laminar flow** interface.

1 In the **Model Builder** window, expand the **Particle Tracing for Fluid Flow (fpt)** node.

Drag Force 1

1 Right-click **Component 1 (comp1)>Particle Tracing for Fluid Flow (fpt)** and choose **Forces>Drag Force**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Drag Force**, locate the **Drag Force** section.

4 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

5 From the μ list, choose **Dynamic viscosity (spf/fp1)**.

The goal is to release particles with a number density proportional to the magnitude of the fluid velocity.

Inlet 1

1 In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow (fpt)** and choose **Inlet**.

2 Select Boundary 23 only.

3 In the **Settings** window for **Inlet**, locate the **Initial Position** section.

4 From the **Initial position** list, choose **Density**.

5 In the N text field, type `3000`.

6 In the ρ text field, type `spf.U`.

7 Locate the **Initial Velocity** section. From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

Particle Counter 1

1 Right-click **Particle Tracing for Fluid Flow (fpt)** and choose the boundary condition **Particle Counter**.

2 Select Boundary 20 only.

3 In the **Settings** window for **Particle Counter**, locate the **Particle Counter** section.

4 From the **Release feature** list, choose **Inlet 1**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Particle Tracing for Fluid Flow (fpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Properties** section.

3 In the d_p text field, type `5E-7[m]`.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, click to expand the **Values of dependent variables** section.

3 Locate the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1, Stationary**.

6 Locate the **Study Settings** section. Click **Range**.

7 In the **Range** dialog box, type `0.2` in the **Step** text field.

8 In the **Stop** text field, type `5`.

9 Click **Replace**.

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

RESULTS

Particle Trajectories (fpt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (fpt)**.

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 to expand the **Title** section. From the **Title type** list, choose **None**.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Particle Trajectories (fpt)** 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**.

4 Find the **Point style** subsection. From the **Type** list, choose **None**.

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**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Laminar Flow>Velocity and pressure>spf.sr - Shear rate**.

3 On the **Particle Trajectories (fpt)** toolbar, click **Plot**.

4 Click **Go to Default View**. The resulting plot should look like Figure 2.

Global Evaluation 1

1 On the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.

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

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Model>Component 1>Particle Tracing for Fluid Flow>Particle Counter 1> fpt.pcnt1.alpha - Transmission probability**.

6 Click **Evaluate**.

Cut Plane 1

1 On the **Results** toolbar, click **Cut Plane**.

2 In the **Settings** window for **Cut Plane**, locate the **Data** section.

3 From the **Data set** list, choose **Particle 1**.

4 Locate the **Plane Data** section. From the **Plane** list, choose **xz-planes**.

5 In the **y-coordinate** text field, type `0.006`.

6 Select the **Additional parallel planes** check box.

7 In the **Distances** text field, type `0.006 0.016 0.026 0.036 0.042`.

8 Click **Plot**.

3D Plot Group 4

1 On the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Poincaré Maps` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

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

5 Locate the **Title** section. From the **Title type** list, choose **None**.

Poincaré Map 1

1 On the **Poincaré Maps** toolbar, click **More Plots** and choose **Poincaré Map**.

2 In the **Settings** window for **Poincaré Map**, locate the **Data** section.

3 From the **Cut plane** list, choose **Cut Plane 1**.

4 Locate the **Coloring and Style** section. Select the **Radius scale factor** check box.

5 In the associated text field, type `6E-5`.

6 On the **Poincaré Maps** toolbar, click **Plot**.

Color Expression 1

1 Right-click **Poincaré Map 1** and choose **Color Expression**.

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

3 In the **Expression** text field, type `at(0,qx<0)`.

4 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Poincaré Maps** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Data** section.

3 From the **Data set** list, choose **Cut Plane 1**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

6 From the **Color** list, choose **Gray**.

7 On the **Poincaré Maps** toolbar, click **Plot**.

8 Click **Go to Default View**. The resulting plot should look like Figure 3.

2D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Phase Portrait` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

4 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

Phase Portrait 1

1 On the **Phase Portrait** toolbar, click **More Plots** and choose **Phase Portrait**.

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

3 From the **x-axis** list, choose **Manual**.

4 In the **Expression** text field, type `comp1.qx`.

5 From the **y-axis** list, choose **Manual**.

6 In the **Expression** text field, type `comp1.qz`.

7 Locate the **Coloring and Style** section. Select the **Radius scale factor** check box.

8 In the associated text field, type `3E-5`.

Color Expression 1

1 Right-click **Phase Portrait 1** and choose **Color Expression**.

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

3 Clear the **Color legend** check box.

4 Locate the **Expression** section. In the **Expression** text field, type `at(0,qx<0)`.

5 On the **Phase Portrait** toolbar, click **Plot**.

Phase Portrait

1 In the **Model Builder** window, under **Results** click **Phase Portrait**.

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

3 From the **View** list, choose **View 2D 2**.

4 Click **Go to Source**.

By default the **Phase Portrait** plot scales the coordinate axes so that the plot fits in the Graphics window. This is to ensure that the phase portrait is shown clearly even if the two axes correspond to quantities with vastly different orders of magnitude, like position and momentum. In the present case, both axes represent position components, so by selecting **View 2D 2** a reasonable-looking 1:1 aspect ratio is enforced.

Axis

1 In the **Model Builder** window, expand the **View 2D 2** node, then click **Axis**.

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

3 From the **View scale** list, choose **None**.

Phase Portrait

1 In the **Model Builder** window, under **Results** click **Phase Portrait**.

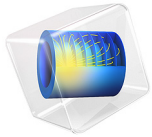
2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **0**.

4 On the **Phase Portrait** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

Plot the phase portrait at different solution times by selecting values from the **Time (s)** list. The phase portraits at 1-second intervals are shown in Figure 4.



Rössler Attractor

Introduction

A Rössler attractor is a system of three nonlinear ordinary differential equations. The Rössler attractor is similar in nature to the Lorenz attractor. The coupled nonlinear equations can be solved using the Massless formulation available in the Mathematical Particle Tracing interface.

Model Definition

The governing differential equations for a Rössler attractor are

$$\frac{dx}{dt} = -y - z$$

$$\frac{dy}{dt} = x + ay$$

$$\frac{dz}{dt} = b + z(x - c)$$

where a, b, and c are constants. This model uses the original parameters used by Rössler: $a = 0.2$, $b = 0.2$ and $c = 5.7$. The particles are released from an initial grid in the y direction at $x = 0$ and $z = 0$. In total, 31 particles are released uniformly between $y = 3$ and $y = 8$.

Results and Discussion

After the initial release of the particles, they travel anticlockwise in the xy-plane at $z = 0$. Once they cross to the positive side of the yz-plane the particles rise very sharply in the z direction. The particles with the largest radial coordinate in the xy-plane acquire the highest velocity and thus reach the highest point the z direction; see Figure 1. The region where the particles reach high elevations in a short period of time is called the upswing region. The particles with the outermost radial coordinate entering the upswing region end up at the innermost radial coordinate after the downswing region.

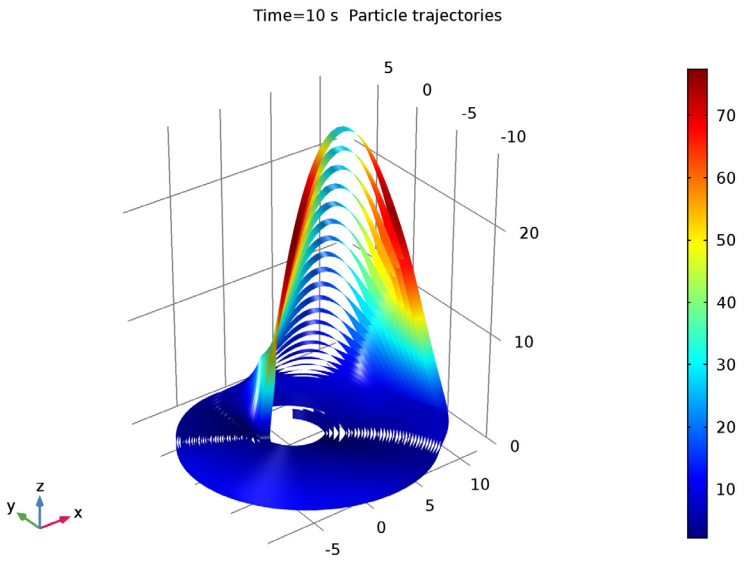


Figure 1: Plot of the Rössler attractor after 10 seconds.

The average particle velocity is plotted in Figure 2. There is a double-peak in maximum velocity, corresponding to the upswing and downswing regions. A Poincaré map of the particle trajectories at 10 seconds is shown in Figure 3. In the region $x < 0$ the particles clearly only ever exist at $z = 0$ in the xz-plane. In the region $x > 0$ the particles can acquire a significant elevation in the xz-plane.

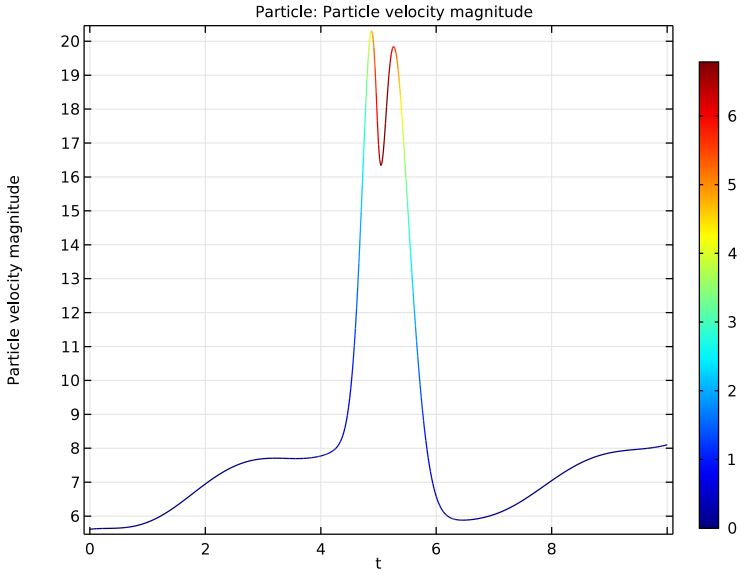


Figure 2: Plot of the average particle velocity versus time.

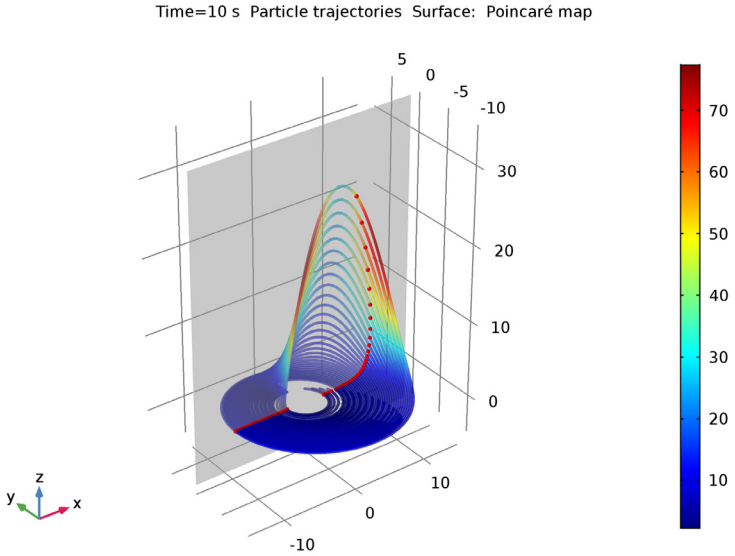


Figure 3: Particle trajectories with a Poincaré map superimposed (red dots) and Poincaré section shown (gray cut plane).

Reference

1. Wikipedia, http://en.wikipedia.org/wiki/R%C3%B6ssler_attractor

Application Library path: `Particle_Tracing_Module/Tutorials/rossler_attractor`

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 **Mathematics>Mathematical Particle Tracing (pt)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.

GEOMETRY 1

The geometry is designated to be large enough so that the particle trajectories do not make contact with the walls.

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 `15`.
4. In the **Height** text field, type `40`.
5. Locate the **Position** section. In the **z** text field, type `-5`.
6. On the **Geometry** toolbar, click **Build All**.

COMPONENT 1 (COMP1)

1 In the **Model Builder** window, click **Component 1 (comp1)**.

2 In the **Settings** window for **Component**, locate the **General** section.

3 From the **Unit system** list, choose **None**.

GLOBAL DEFINITIONS

Define the constants a, b and c as parameters. This means they could, in principle, be varied as part of a **Parametric Sweep** when solving.

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
a	0.2	0.2	Model parameter
b	0.2	0.2	Model parameter
c	5.7	5.7	Model parameter

MATHEMATICAL PARTICLE TRACING (PT)

The **Massless** formulation allows a system of first order ordinary differential equations to be solved.

1 In the **Model Builder** window, expand the **Component 1 (comp1)> Mathematical Particle Tracing (pt)** node, then click **Mathematical Particle Tracing (pt)**.

2 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Massless**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Velocity** section.

3 Specify the **v** vector as

-y-z	x
x+a*y	y
b+z*(x-c)	z

Release from Grid 1

1 In the **Model Builder** window, right-click **Mathematical Particle Tracing (pt)** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{y,\,0}$ text field, type `range(3,5/30,8)`.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,0.02,10)`.

4 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories 1

Render the particle trajectories as ribbons. The default ribbon orientation is in the direction of the unit binormal, or the direction out of the plane tangent to the curved trajectory.

1 In the **Model Builder** window, expand the **Particle Trajectories (pt)** 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 **Ribbon**.

4 Select the **Width scale factor** check box.

5 In the associated text field, type `0.5`.

6 Find the **Point style** subsection. From the **Type** list, choose **None**.

Particle Trajectories (pt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot data set edges** check box.

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

5 Click **Go to Default View**. The plot should look like Figure 1.

Now plot the average particle velocity using the **1D Plot Group** and a **Particle** plot type.

1D Plot Group 2

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Average Particle Velocity Magnitude` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

Particle 1

1 On the **Average Particle Velocity Magnitude** toolbar, click **More Plots** and choose **Particle**.

2 In the **Settings** window for **Particle**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Mathematical Particle Tracing>Velocity and energy>pt.V - Particle velocity magnitude**.

3 Locate the **Data Series Operation** section. From the **Operation** list, choose **Average**.

Color Expression 1

1 Right-click **Particle 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Mathematical Particle Tracing>Particle position>qz - Particle position, z component**.

3 On the **Average Particle Velocity Magnitude** toolbar, click **Plot**. The plot should look like Figure 2.

A **Cut Plane** data set can be used to visualize how the particles cross a specific area of interest in the modeling domain. A **Poincaré map** is created using the intersection points of the trajectories with the plane.

Cut Plane 1

1 On the **Results** toolbar, click **Cut Plane**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 From the **Plane** list, choose **ZX-planes**.

4 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

Particle Trajectories (pt) 1

1 In the **Model Builder** window, under **Results** right-click **Particle Trajectories (pt)** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Particle Trajectories and Poincaré Map` in the **Label** text field.

Particle Trajectories 1

1. In the **Model Builder** window, expand the **Results>Particle Trajectories and Poincaré Map** 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 **Tube**.
4. In the **Tube radius expression** text field, type `10`.

Surface 1

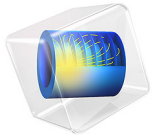
1. In the **Model Builder** window, under **Results** right-click **Particle Trajectories and Poincaré Map** and choose **Surface**.
2. In the **Settings** window for **Surface**, locate the **Data** section.
3. From the **Data set** list, choose **Cut Plane 1**.
4. Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
5. From the **Color** list, choose **Gray**.
6. Click the **Transparency** button on the **Graphics** toolbar.

Particle Trajectories and Poincaré Map

In the **Model Builder** window, under **Results** click **Particle Trajectories and Poincaré Map**.

Poincaré Map 1

1. On the **Particle Trajectories and Poincaré Map** toolbar, click **More Plots** and choose **Poincaré Map**.
2. In the **Settings** window for **Poincaré Map**, locate the **Data** section.
3. From the **Cut plane** list, choose **Cut Plane 1**.
4. On the **Particle Trajectories and Poincaré Map** toolbar, click **Plot**.
5. Locate the **Coloring and Style** section. Select the **Radius scale factor** check box.
6. In the associated text field, type `0.25`.
7. On the **Particle Trajectories and Poincaré Map** toolbar, click **Plot**.
8. Click the **Zoom Extents** button on the **Graphics** toolbar. The plot should look like Figure 3.



Rotating Galaxy

Introduction

It is possible to define arbitrary interaction forces between particles using the **Particle-Particle Interaction** feature. This tutorial model shows how to add a custom particle-particle interaction force, the force due to gravitational attraction.

Model Definition

For each star in a galaxy the following ordinary differential equation is solved:

$$\frac{d}{dt}(m_i \mathbf{v}_i) = \mathbf{F}_i$$

where the force on the i^{th} particle is given by:

$$\mathbf{F}_i = -Gm_i^2 \sum_{j=1}^{N} \frac{(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

where G is the gravitational constant, and m_i is the mass of the i^{th} planet, and the case $i = j$ is excluded from the sum. The mass of all stars is the same in this model. The variable $\mathbf{r}_i$ is the position vector of particle i and $\mathbf{r}_j$ is the position vector of particle j.

The stars all start out as a rigid body with initial position vector:

$$q_{x,i} = \frac{1}{2} + R\cos\theta$$

$$q_{y,i} = \frac{1}{2} + \alpha R\sin\theta$$

where R is a uniformly distributed random number between 0 and 0.25, and θ is a uniformly distributed random number between 0 and 2π. The constant α is 0.25. This results in a higher initial density of stars near to the center of rotation. The initial velocity is an anti-clockwise rigid body rotation:

$$u_{x,i} = -VD\sin\theta$$

$$u_{y,i} = VD\cos\theta$$

where V is 50 and D is defined as:

$$D = \sqrt{x^2 + y^2}$$

Results and Discussion

As shown in Figure 1 the stars all start off with an elliptical shape and the density of stars is higher towards the center of rotation. After 25 time intervals the galaxy has some of its stars far away from the high-density region which is close to the galaxy center. By the last time step the galaxy has evolved to the familiar spiral shape seen in basic astrophysics text books.

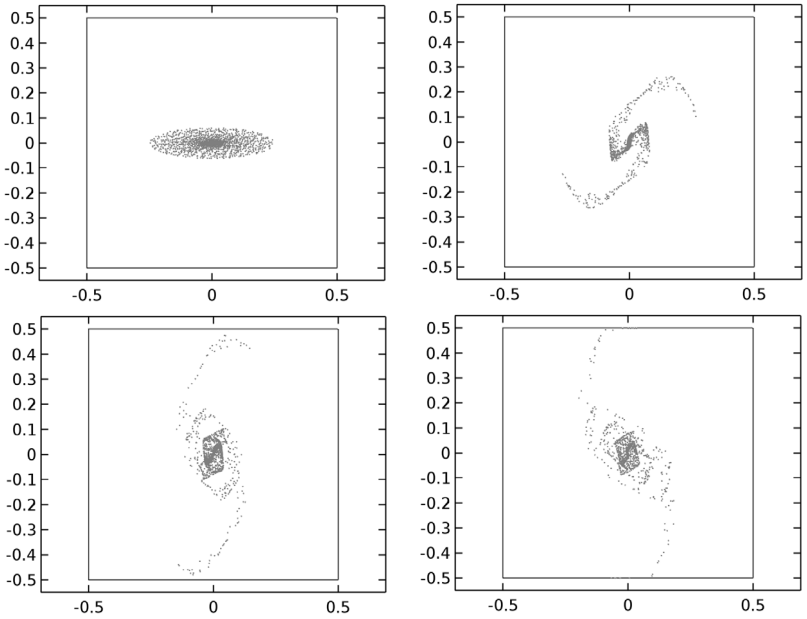


Figure 1: Plot of the position of the stars at different points in time. Top left is the initial position, top right is after 25 time intervals, bottom right after 40 and lower right after 50.

Notes About the COMSOL Implementation

There is specific syntax which must be used to specify user-defined interaction forces. The particle degrees of freedom are given the variable names `qx` and `qy`, but to access the position vector of neighboring particles use the expression `dest(qx)` and `dest(qy)`. For the gravitational force in this example, the force on particle i depends on its position vector and mass of all other particles:

$$\mathbf{F}_i = -Gm^2 \sum_{j=1}^{N} \frac{(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

where $\mathbf{r}_i$ is the position vector of the i^{th} particle, G is the gravitational constant, and m is the mass. To enter this as a user-defined force, enter:

```
G*m^2*(qx-dest(qx))/sqrt((qx-dest(qx))^2+(qy-dest(qy))^2+tol)^3
G*m^2*(qy-dest(qy))/sqrt((qx-dest(qx))^2+(qy-dest(qy))^2+tol)^3
```

where `tol` is a user-defined parameter, in this case 0.01, to prevent division by zero for the i^{th} particle. In practice it is quite difficult to chose the value of `tol`. It should in general be a small fraction of the smallest distance you want to allow between particles.

Application Library path: `Particle_Tracing_Module/Tutorials/rotating_galaxy`

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 **2D**.
2. In the **Select Physics** tree, select **Mathematics>Mathematical Particle Tracing (pt)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.

ROOT

1. In the **Model Builder** window, click the root node.
2. In the root nodes'**Settings** window, locate the **Unit System** section.
3. From the **Unit system** list, choose **None**.

GEOMETRY 1

Draw a rectangle and an ellipse. The ellipse is used to make it easier to specify the initial position and velocity of the stars in the galaxy.

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Position** section.

3 From the **Base** list, choose **Center**.

4 Click **Build All Objects**.

Ellipse 1 (e1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Ellipse**.

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

3 In the **a-semiaxis** text field, type `1/4`.

4 In the **b-semiaxis** text field, type `1/16`.

5 Click **Build All Objects**.

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
G	0.05		Gravitational constant
m	1		Normalized solar mass
V0	50		Initial velocity
R	sqrt(x^2+y^2)		Distance from the origin
r	sqrt((qx-dest(qx))^2+(qy-dest(qy))^2+0.01)		Sum of the distance between particles

MATHEMATICAL PARTICLE TRACING (PT)

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Mass** section.

3 In the m_p text field, type 1.

The gravitational force means that every particle interacts with every other particle. To model this effect, add a **Particle-Particle Interaction** feature. There is no predefined interaction force available for gravitational attraction, so use the **User defined** option.

Particle-Particle Interaction 1

1 In the **Model Builder** window, right-click **Mathematical Particle Tracing (pt)** and choose **Particle-Particle Interaction**.

2 Click in the **Graphics** window and then press Ctrl+A to select both domains.

3 In the **Settings** window for **Particle-Particle Interaction**, locate the **Force** section.

4 From the **Interaction force** list, choose **User defined**.

5 Specify the $\mathbf{F}_u$ vector as

-G*m^2*(dest(qx)-qx)/r^3	x
-G*m^2*(dest(qy)-qy)/r^3	y

Because every particle interacts with every other particle, a full Jacobian matrix is generated at every time step. This makes the problem impractical to solve because assembling and factorizing a full 2400-by-2400 matrix at every time step is computationally very expensive. The sparsity of the Jacobian matrix can be preserved by selecting **Exclude Jacobian contribution for particle-particle interactions**. This is also the default setting. The drawback of this option is that the solver may end up taking much smaller time steps when solving.

Release 1200 particles from the ellipse domain in such a way that there are more particles released close to the origin. Set the initial velocity to correspond to rigid body motion.

Release 1

1 Right-click **Mathematical Particle Tracing (pt)** and choose **Release**.

2 Select Domain 2 only.

3 In the **Settings** window for **Release**, locate the **Initial Position** section.

4 From the **Initial position** list, choose **Density**.

5 In the N text field, type 1200.

6 In the ρ text field, type 1/sqrt(x^2+16*y^2+1E-4).

7 Locate the **Initial Velocity** section. Specify the $\mathbf{v}_0$ vector as

`-V0*R*sin(atan2(y,x))`	x
`V0*R*cos(atan2(y,x))`	y

MESH 1

The accuracy of the particle motion is not affected by the mesh size in this case because the particle trajectories are not coupled to any fields. However, the initial release of the particles is somewhat mesh-dependent. Therefore, use a very fine mesh on the inner ellipse.

Free Triangular 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Domain Selection** section.

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

4 Select Domain 2 only.

5 Click to expand the **Tessellation** section. From the **Method** list, choose **Delaunay**.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

4 Click to expand the **Element size parameters** section. Locate the **Element Size** section. Click the **Custom** button.

5 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

6 In the associated text field, type `0.005`.

Free Triangular 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Tessellation** section.

3 From the **Method** list, choose **Delaunay**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Finer**.

4 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Times** text field, type `range(0,0.1/50,0.1)`.

Solution 1 (sol1)

1 On the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1>Solver Configurations> Solution 1 (sol1)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, click to expand the **Method and termination** section.

5 Locate the **Method and Termination** section. From the **Jacobian update** list, choose **Minimal**.

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

DEFINITIONS

Hide for Physics 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** right-click **View 1** and choose **Hide for Physics**.

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

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

4 Select Boundaries 5–8 only.

RESULTS

Particle Trajectories (pt)

In the **Model Builder** window, expand the **Particle Trajectories (pt)** node.

Color Expression 1

1 In the **Model Builder** window, expand the **Results>Particle Trajectories (pt)> 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 `1`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **GrayScale**.

5 Clear the **Color legend** check box.

Particle Trajectories (pt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (pt)**.

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

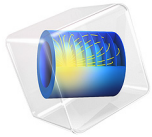
3 From the **Title type** list, choose **None**.

4 Locate the **Data** section. From the **Time (s)** list, choose **0**.

5 On the **Particle Trajectories (pt)** toolbar, click **Plot**.

6 Click the **Zoom Extents** button on the **Graphics** toolbar.

Plot the particle positions at later times by selecting different values from the **Time (s)** list. The plot in Figure 1 shows the initial positions of the stars and the positions after 25 time intervals, 40 intervals, and 50 intervals.



Motion of Trapped Protons in Earth's Magnetic Field

Introduction

The Earth has a substantial magnetic field that extends outward for many thousands of kilometers. It is thought that this magnetic field is generated by circulating currents within a spinning metal liquid core—the dynamo effect. This magnetic field closely resembles a dipole field; however, there is a tilt between the spin axis of the Earth and that of the magnetic dipole. There are also other asymmetries in the Earth's magnetic field that require the use of software models to describe fully. These models are constructed using data obtained from orbiting spacecraft.

Having an accurate model of the Earth's magnetic field is very important in studies of the Earth's deep interior, its crust, and its ionosphere and magnetosphere. Therefore, a standard model is maintained by the International Association of Geomagnetism and Aeronomy (IAGA). This model is referred to as the International Geomagnetic Reference Field (IGRF). The IGRF model is updated every few years and is currently on its 11th generation (Ref. 1).

The influence of the solar wind means that the full extended shape of the Earth's magnetosphere is very different from a dipole. However, within a few Earth radii, simpler models of the Earth's magnetic field are sufficient.

Charged particles in the Earth's magnetic field travel in helical paths around the field lines. The angle between the direction of the magnetic field and a particle's trajectory is referred to as the pitch angle. As particles move along the magnetic field lines, they approach a pole in the magnetic field. Near the poles, the particles get closer to earth, causing the magnetic field to increase in magnitude and thus causing the pitch angle to increase. If the pitch angle reaches 90 degrees while the particle is still outside of the atmosphere (>100 km), the particle motion reverses direction back along the field line. The point at which this occurs is referred to as a mirror, or bounce, point. The particle similarly bounces off the other mirror point in the other hemisphere.

Particles are considered trapped if they are not lost to the Earth's atmosphere during this motion. Particles can also be liberated due to scattering by electromagnetic waves.

The latitude of a mirror point (λ_m) is related to the particle's pitch angle at the equatorial plane, or its equatorial pitch angle (α_{eq}). As the equatorial pitch angle increases, the mirror point latitude decreases. Any particles that have equatorial pitch angles that give mirror points outside the atmosphere are said to be outside the atmospheric loss cone and are trapped.

Particles that bounce from mirror point to mirror point also exhibit a drift motion around the Earth, switching from field line to field line. This is due to the fact that the magnetic

field magnitude is increasing as the particle moves towards the Earth, so that its gyration is not circular, but has in fact a smaller radius on the side closer to the Earth.

As electrons and protons drift in opposite directions around the Earth, an electric current (ring current) is set up. The magnitude of the ring current increases during solar storms, and its effect can be measured on the ground as a weakening of the measured magnetic field. The disturbance storm time index, Dst, is one such measure of this ring current and is used to assess the severity of magnetic storms from the Sun.

These motions of trapped charge particles lead to "belts" of energetic charged particles in the near Earth environment and are referred to as the Van Allen radiation belts. They extend from about 1000 to 60,000 km (~0.15 to ~10 Earth radii) above the Earth's surface and therefore pose a real threat to space-based microelectronics.

Model Definition

Mathematically, the IGRF model consists of the Gauss coefficients, which define a spherical harmonic expansion of the magnetic scalar potential:

$$V(r, \Phi, \theta) = a \sum_{l=1}^{L} \sum_{m=-l}^{l} \left(\frac{R_e}{r}\right)^{l+1} (g_l^m \cos m\Phi + h_l^m \sin m\Phi) P_l^m(\cos\theta)$$

where r is the radial distance from the Earth's center, L is the maximum degree of the expansion, Φ is East longitude, θ is colatitude (polar angle), R_e is the Earth's radius, g_l^m and h_l^m are Gauss coefficients, and $P_l^m \cos\theta$ are the Schmidt normalized associated Legendre functions of degree l and order m.

The model uses a simple sphere of radius R_e to represent the Earth within a larger spherical simulation domain of radius $5R_e$ where this particle trajectories are computed. The geometry is shown in Figure 1.

The Magnetic Force feature in the Charged Particle Tracing interface and the Particle Tracing for Fluid Flow interface includes a built-in option to compute magnetic fields using the data from the IGRF model. To access this data, in a 3D model select **Earth's magnetic field** from the **Magnetic flux density** list in the settings window for the Magnetic Force feature.

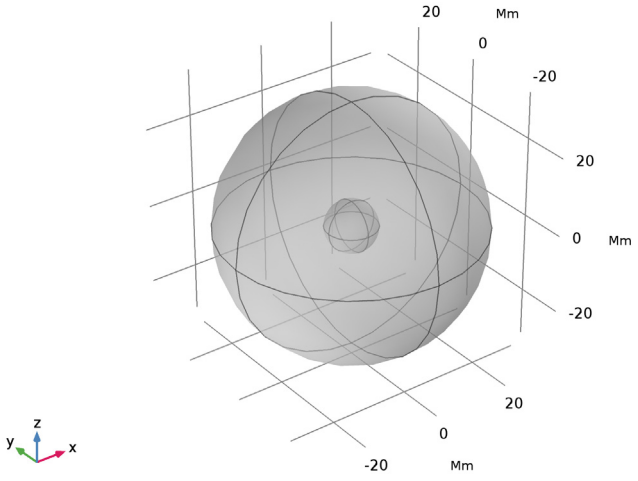


Figure 1: Geometry of the simulation domain, which extends from radius Re to 5Re.

Figure 2 shows the IGRF magnetic field lines. The difference from a simple dipole is not really evident in this figure, but asymmetries exist in both latitude and longitude.

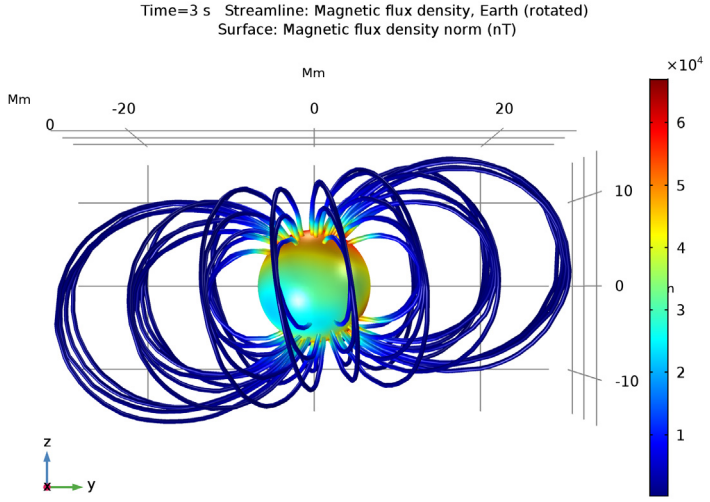


Figure 2: IGRF magnetic field lines.

The model uses the Charged Particle Tracing interface only, together with a Time Dependent study.

Results and Discussion

A single 10 MeV proton is released from the equatorial plane at a distance of $2R_e$ from the center of the Earth. It is released with an equatorial pitch angle of 30 degrees. The three components of its motion (gyration, bounce and drift) are clearly visible in Figure 3. The timescales for the drift motion are much longer than that of the bounce motion, which in turn is much longer than the gyration period.

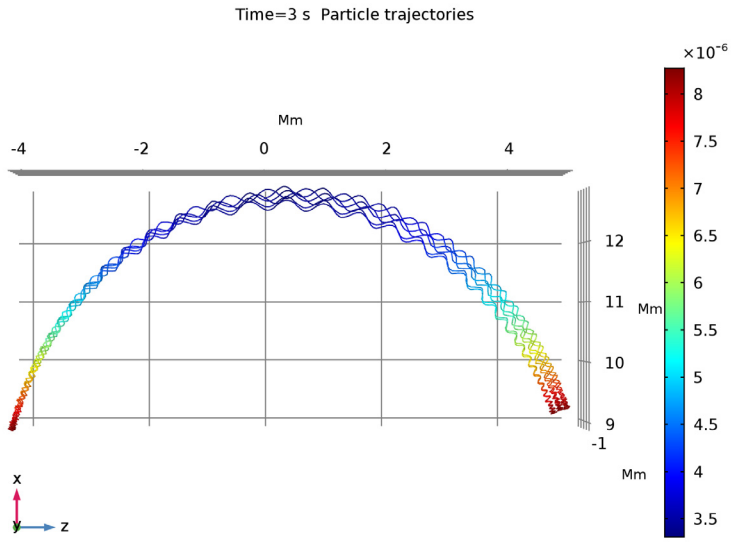


Figure 3: Particle trajectory of a single 10 MeV proton in Earth's magnetic field. Particle gyration, bounce and drift motion are clearly visible.

Due to the large changes in the magnitude of the magnetic field in different parts of the simulation domain, care has to be taken to ensure an appropriate time step is used for the particles. An good indication of how well the time steps are resolving the gyration of the particles is to plot the particle energy as a function of time and observe little or no change. Figure 4 plots the relative change in the particle kinetic energy as a function of time. This relative error is of the order 10^{-3} and so we can be certain we are resolving most of the particle motion.

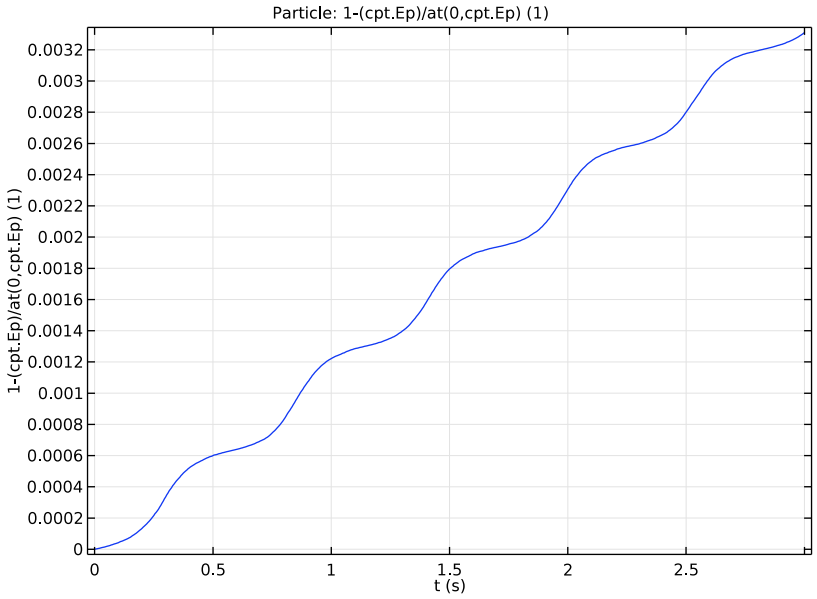


Figure 4: Relative error in particle kinetic energy.

There are many aspects of the particle motion that can be investigated using this model, but the scope of this tutorial is limited to investigating how the mirror point latitude is affected by the equatorial pitch angle of the released protons.

As mentioned above, as the equatorial pitch angle of a particle decreases, the mirror point latitude is expected to increase. At the limits, a particle with an equatorial pitch angle of 90 degrees would remain in the equatorial plane whereas one with a pitch angle of zero degrees would travel directly along the field line without bouncing.

Figure 6 shows the mirror point latitude vs. equatorial pitch angle for 15 particles with equatorial pitch angles ranging from 5 degrees to 80 degrees.

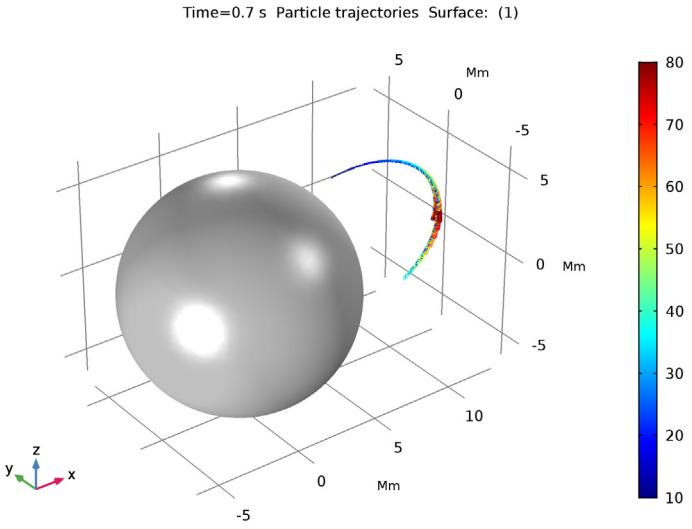


Figure 5: Trajectories of several trapped protons. The color expression corresponds to the equatorial pitch angle of each proton.

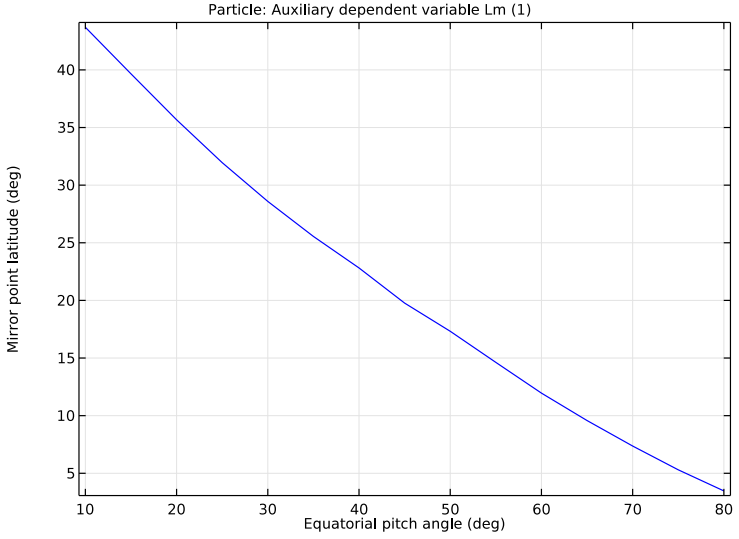


Figure 6: Mirror point latitude (λ_m) against particle equatorial pitch angle (Ea).

References

1. International Geomagnetic Reference Field website, http://www.ngdc.noaa.gov/IAGA/vmod/igrf.html.

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/trapped_protons`

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>Charged Particle Tracing (cpt)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Re	6371.2[km]	6.3712E6 m	Radius of the Earth
E0	10[MeV]	1.6022E-12 J	Initial particle energy
alpha	30[deg]	0.5236 rad	Equatorial pitch angle

Add a sphere with radius `Re` within a larger simulation domain of radius `5*Re`.

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **Mm**.

Sphere 1 (sph1)

1 On the **Geometry** toolbar, click **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

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

Sphere 2 (sph2)

1 On the **Geometry** toolbar, click **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

3 In the **Radius** text field, type `5*Re`.

Difference 1 (dif1)

1 On the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **sph2** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Find the **Objects to subtract** subsection. Select the **Active** toggle button.

5 Click the **Transparency** button on the **Graphics** toolbar.

6 Select the object **sph1** only.

7 Click **Build All Objects**.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

9 Click the **Transparency** button on the **Graphics** toolbar.

Hide the outermost boundary to facilitate setup of the Charged Particle Tracing interface.

DEFINITIONS

View 1

1 In the **Model Builder** window, expand the **Definitions** node.

2 Right-click **View 1** and choose **Hide for Geometry**.

3 In the **Settings** window for **Hide for Geometry**, locate the **Selection** section.

4 From the **Geometric entity level** list, choose **Boundary**.

5 On the object **dif1**, select Boundaries 1–4, 9, 10, 13, and 16 only.

Add a **Ball** selection containing all boundaries on the Earth's surface.

Ball 1

1 On the **Definitions** toolbar, click **Ball/Disk**.

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

3 From the **Level** list, choose **Boundary**.

4 Locate the **Ball Radius** section. In the **Radius** text field, type `Re`.

CHARGED PARTICLE TRACING (CPT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Charged Particle Tracing (cpt)**.

2 In the **Settings** window for **Charged Particle Tracing**, locate the **Particle Release and Propagation** section.

3 From the **Formulation** list, choose **Newtonian, first order**.

In this example, the particles are relativistic protons.

4 Select the **Relativistic correction** check box.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Charge Number** section.

3 In the Z text field, type `1`.

4 Locate the **Particle Rest Mass** section. In the m_r text field, type `mp_const`.

Exert a magnetic force on the particles using the Earth's magnetic field.

Magnetic Force 1

1 On the **Physics** toolbar, click **Domains** and choose **Magnetic Force**.

2 In the **Settings** window for **Magnetic Force**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Magnetic Force** section. From the $\mathbf{B}$ list, choose **Earth's magnetic field**.

Set up the **Release from Grid** feature to release a single 10 MeV proton at a distance of 2 Earth radii along the x-axis. Set its velocity x-component to zero, and its y- and z-components using the equatorial pitch angle.

Release from Grid 1

1 On the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{x,\,0}$ text field, type `2*Re`.

4 Locate the **Initial Velocity** section. From the **Initial velocity** list, choose **Kinetic energy and direction**.

5 In the E_0 text field, type `E0`.

6 Specify the $\mathbf{L}_0$ vector as

`0`	`x`
`sin(alpha)`	`y`
`cos(alpha)`	`z`

Define two auxiliary dependent variables for the mirror point latitude and equatorial pitch angle. These auxiliary dependent variables will be disabled in Study 1 but will be needed in Study 2.

Auxiliary Dependent Variable 1

1 On the **Physics** toolbar, click **Global** and choose **Auxiliary Dependent Variable**.

2 In the **Settings** window for **Auxiliary Dependent Variable**, locate the **Auxiliary Dependent Variable** section.

3 In the **Field variable name** text field, type `Lm`.

Auxiliary Dependent Variable 2

1 On the **Physics** toolbar, click **Global** and choose **Auxiliary Dependent Variable**.

2 In the **Settings** window for **Auxiliary Dependent Variable**, locate the **Auxiliary Dependent Variable** section.

3 In the **Field variable name** text field, type `Ea`.

The **Velocity Reinitialization** feature can be used to detect when a particle bounces, and set the auxiliary dependent variable `Lm` to the instantaneous value of the latitude at that point.

Velocity Reinitialization 1

1 On the **Physics** toolbar, click **Domains** and choose **Velocity Reinitialization**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 In the **Settings** window for **Velocity Reinitialization**, locate the **Velocity Reinitialization** section.

4 In the *e* text field, type `(cpt.vx*cpt.mf1.Berx+cpt.vy*cpt.mf1.Bery+cpt.vz*cpt.mf1.Berz)<0 && Lm==0`.

This expression is true for the first time step at which the angle between the particle velocity and the Earth's magnetic field is greater than 90 degrees.

5 From the **Effect on primary particle** list, choose **None**.

6 Click to expand the **New value of auxiliary dependent variables** section. Locate the **New Value of Auxiliary Dependent Variables** section. Select the **Assign new value to auxiliary variable : Lm** check box.

7 In the $\mathrm{Lm}_{\mathrm{new}}$ text field, type `(-acos(qz/sqrt(qx^2+qy^2+qz^2))+pi/2)*(180/pi)`.

Release from Grid 1

Duplicate the release feature to create a separate release feature for the second study.

Release from Grid 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** right-click **Release from Grid 1** and choose **Duplicate**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Velocity** section.

3 Specify the $\mathbf{L}_0$ vector as

0	x
sin(Ea)	y
cos(Ea)	z

The second **Release from Grid** feature stores the initial equatorial pitch angle of each particle.

4 Locate the **Initial Value of Auxiliary Dependent Variables** section. From the **Distribution function** list, choose **List of values**.

5 Click **Range**.

6 In the **Range** dialog box, type `10[deg]` in the **Start** text field.

7 In the **Step** text field, type `5[deg]`.

8 In the **Stop** text field, type `80[deg]`.

9 Click **Replace**.

Since the initial direction will be defined in terms of the equatorial pitch angle, specify that this auxiliary variable must be initialized before the particle momentum.

10 In the Settings window for Release from Grid, locate the **Initial Value of Auxiliary Dependent Variables** section.

11 Select the second **Initialize before particle momentum** check box, which corresoponds to the variable for equatorial pitch angle `Ea`.

STUDY 1

Step 1: Time Dependent

Disable the features that are not needed for the first study.

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify physics tree and variables for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Charged Particle Tracing (cpt)>Auxiliary Dependent Variable 1**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Charged Particle Tracing (cpt)>Auxiliary Dependent Variable 2**.

7 Click **Disable**.

8 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Charged Particle Tracing (cpt)>Velocity Reinitialization 1**.

9 Click **Disable**.

10 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Charged Particle Tracing (cpt)>Release from Grid 2**.

11 Click **Disable**.

12 In the **Model Builder** window, click **Step 1: Time Dependent**.

13 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

14 Click **Range**.

15 In the **Range** dialog box, type `0.005` in the **Step** text field.

16 In the **Stop** text field, type `3`.

17 Click **Replace**.

18 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (cpt)

1. In the **Model Builder** window, under **Results** click **Particle Trajectories (cpt)**.
2. In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
3. Clear the **Plot data set edges** check box.

Particle Trajectories 1

1. In the **Model Builder** window, expand the **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 **Tube**.
4. Select the **Radius scale factor** check box.
5. In the associated text field, type `0.01`.
6. From the **Interpolation** list, choose **Uniform**.
7. In the **Number of interpolated times** text field, type `2000`.
8. Find the **Point style** subsection. From the **Type** list, choose **None**.

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**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Charged Particle Tracing>Fields>cpt.mf1.normB - Magnetic flux density norm**.
3. On the **Particle Trajectories (cpt)** toolbar, click **Plot**.
4. Click the **Go to ZX View** button on the **Graphics** toolbar. Compare the resulting plot with Figure 3.

Data Sets

Create some additional data sets to visualize the magnetic field using a **Streamline** plot.

Cut Plane 1

1. On the **Results** toolbar, click **Cut Plane**.
2. In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.
3. From the **Plane** list, choose **XY-planes**.

Selection

1 In the **Model Builder** window, under **Results>Data Sets** right-click **Study 1/ Solution 1 (sol1)** and choose **Duplicate**.

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

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

4 From the **Geometric entity level** list, choose **Boundary**.

5 From the **Selection** list, choose **Ball 1**.

3D Plot Group 2

1 On the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Magnetic Flux Density` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Streamline 1

1 Right-click **Magnetic Flux Density** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Charged Particle Tracing>Fields>cpt.mf1.Berx,...,cpt.mf1.Berz - Magnetic flux density, Earth (rotated)**.

3 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Start point controlled**.

4 In the **Points** text field, type `50`.

5 From the **Along curve or surface** list, choose **Cut Plane 1**.

6 Locate the **Coloring and Style** section. From the **Line type** list, choose **Tube**.

Color Expression 1

1 Right-click **Results>Magnetic Flux Density>Streamline 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Charged Particle Tracing>Fields>cpt.mf1.normB - Magnetic flux density norm**.

3 Locate the **Expression** section. From the **Unit** list, choose **nT**.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Magnetic Flux Density** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Solution 1 (2) (sol1)**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Charged Particle Tracing>Fields>cpt.mf1.normB - Magnetic flux density norm**.

5 Locate the **Expression** section. From the **Unit** list, choose **nT**.

6 Click to expand the **Inherit style** section. Locate the **Inherit Style** section. From the **Plot** list, choose **Streamline 1**.

7 On the **Magnetic Flux Density** toolbar, click **Plot**.

8 Click the **Go to YZ View** button on the **Graphics** toolbar. Compare the resulting plot with Figure 2.

1D Plot Group 3

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Energy Loss` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

Particle 1

1 On the **Energy Loss** toolbar, click **More Plots** and choose **Particle**.

Verify that energy is conserved throughout the study.

2 In the **Settings** window for **Particle**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `1-(cpt.Ep)/at(0,cpt.Ep)`.

4 On the **Energy Loss** toolbar, click **Plot**. Compare the resulting plot with Figure 4.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

STUDY 2

Step 1: Time Dependent

1 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

2 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

3 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

4 Select the **Modify physics tree and variables for study step** check box.

5 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Charged Particle Tracing (cpt)>Release from Grid 1**.

6 Click **Disable**.

7 Locate the **Study Settings** section. Click **Range**.

8 In the **Range** dialog box, type `0.001` in the **Step** text field.

9 In the **Stop** text field, type `0.7`.

10 Click **Replace**.

11 On the **Home** toolbar, click **Compute**.

RESULTS

Particle Trajectories (cpt) 1

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (cpt) 1**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot data set edges** check box.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Particle Trajectories (cpt) 1** 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**.

4 Find the **Point style** subsection. From the **Type** list, choose **None**.

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 `Ea*180/pi`.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Particle Trajectories (cpt) 1** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Solution 1 (2) (sol1)**.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Gray**.

6 On the **Particle Trajectories (cpt) 1** toolbar, click **Plot**.

7 Click **Go to Default View**. Compare the resulting plot with Figure 5.

1D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Mirror Point Latitude` in the **Label** text field.

Plot the particle mirror point latitude against equatorial pitch angle.

3 Locate the **Data** section. From the **Data set** list, choose **Particle 2**.

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

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Equatorial pitch angle (deg)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Mirror point latitude (deg)`.

Particle 1

1 On the **Mirror Point Latitude** toolbar, click **More Plots** and choose **Particle**.

2 In the **Settings** window for **Particle**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `Lm`.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `Ea*180/pi`.

6 On the **Mirror Point Latitude** toolbar, click **Plot**.

7 Click the **Zoom Extents** button on the **Graphics** toolbarCompare the resulting plot with Figure 6.