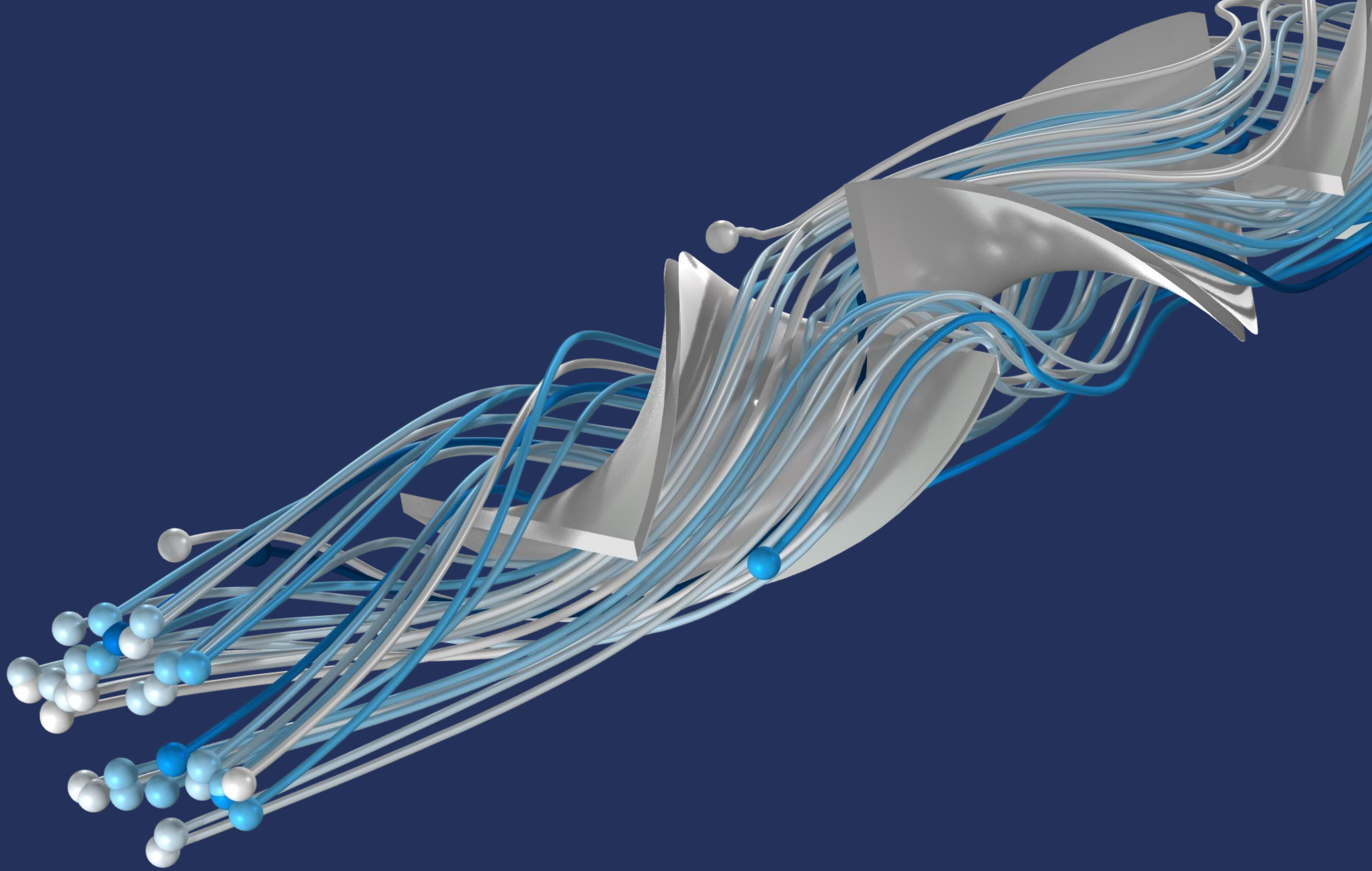
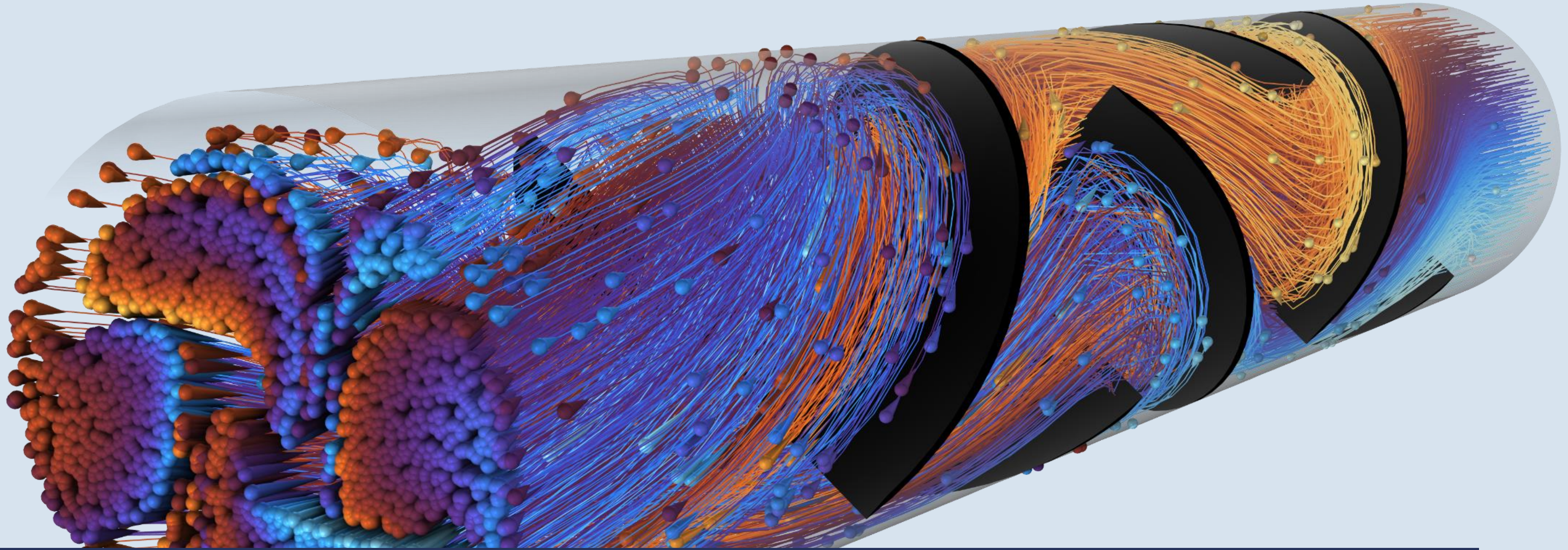


Particle Tracing Module

Tomáš Vrbata
HUMUSOFT s.r.o.



Particle Tracing Module

Particle Tracing

- Positions and velocities of particles over time
- Wide variety of particle releases, boundary conditions, forces, …
- Alternative to field-based methods

Physics Interfaces

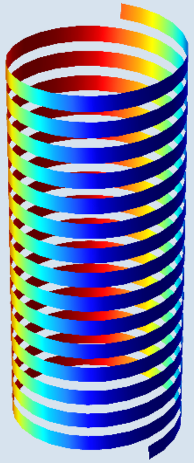
- Mathematical Particle Tracing
- Charged Particle Tracing
- Particle Tracing for Fluid Flow

Application Areas

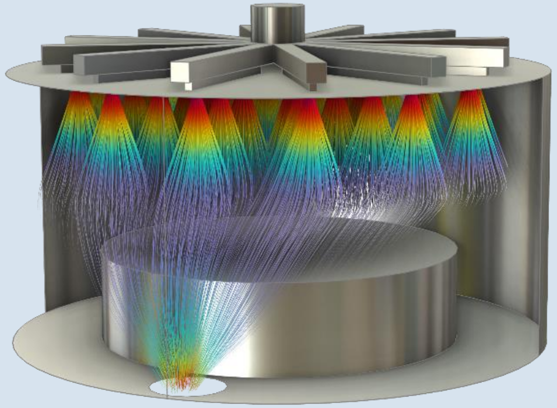
- Mass spectrometry
- Separation and filtration
- Droplets and sprays
- Erosion
- Plasmas

MODELING CAPABILITIES

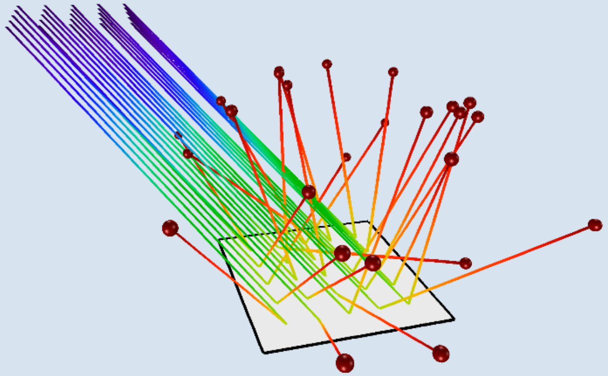
Particle Tracing Functionalities



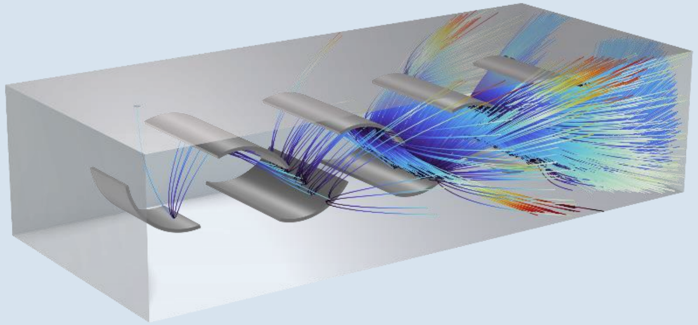
Multiple formulations to solve same problems.



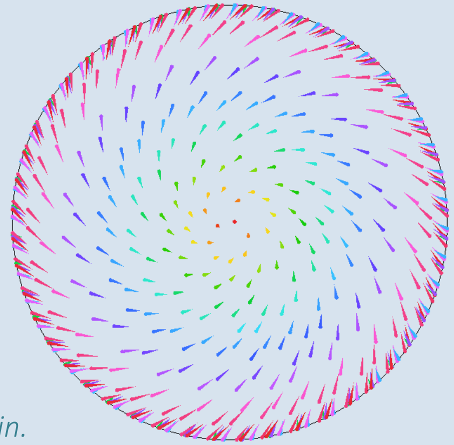
Particle position and velocity initialization.



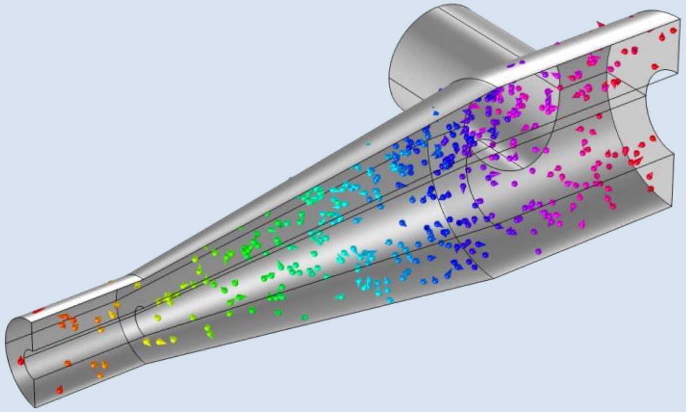
Multiple boundary conditions.



Secondary particle emissions.



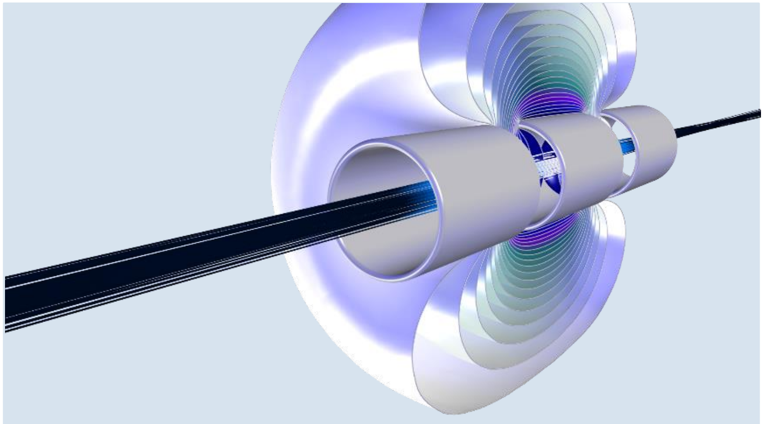
Rotating domain.



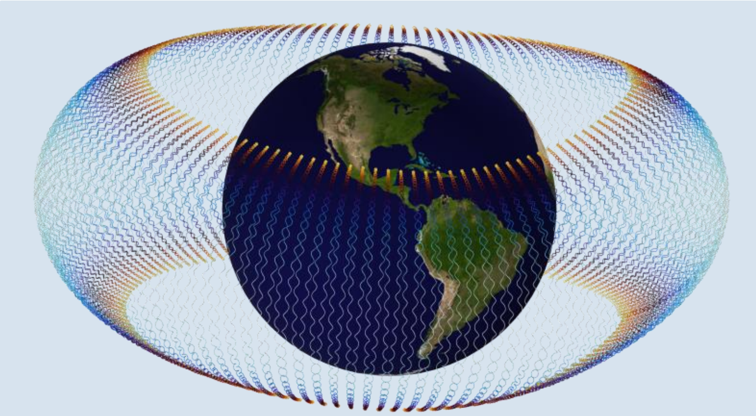
Coupling with varieties of physics.

MODELING CAPABILITIES

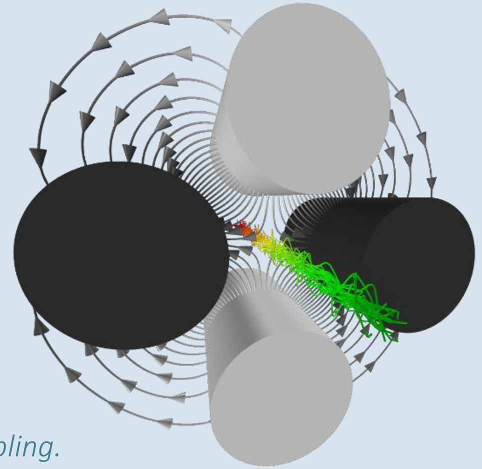
Charged Particle Tracing



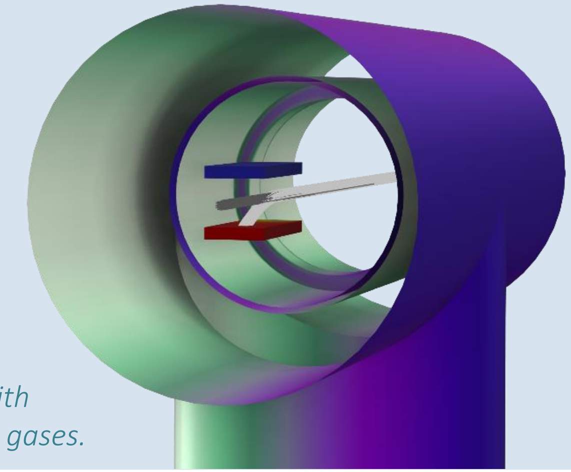
Particle tracing in electric field.



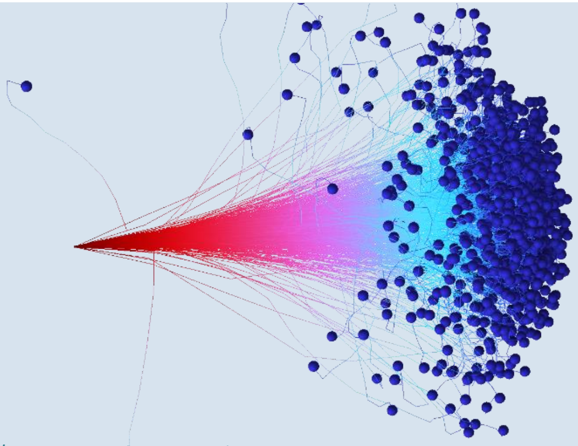
Particle tracing in magnetic field.



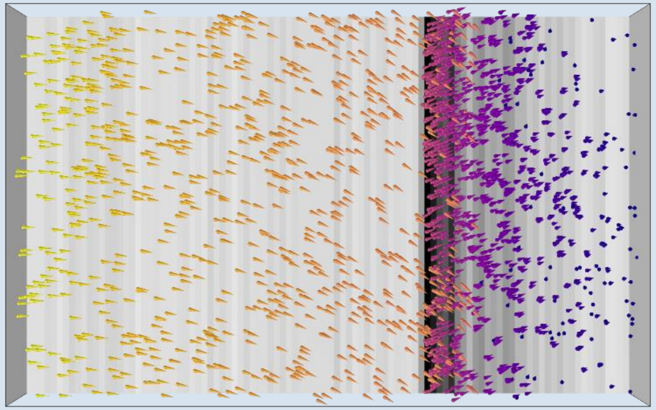
Various built-in
forces and coupling.



Collisions with
background gases.



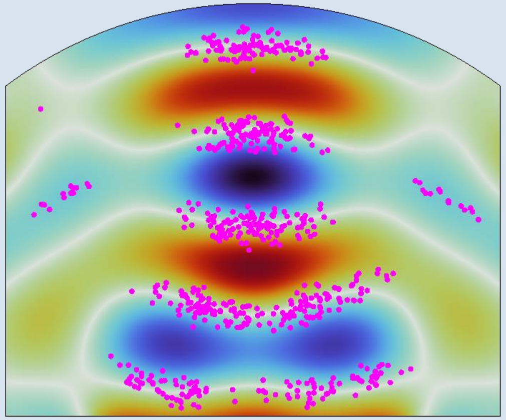
Particle matter interaction.

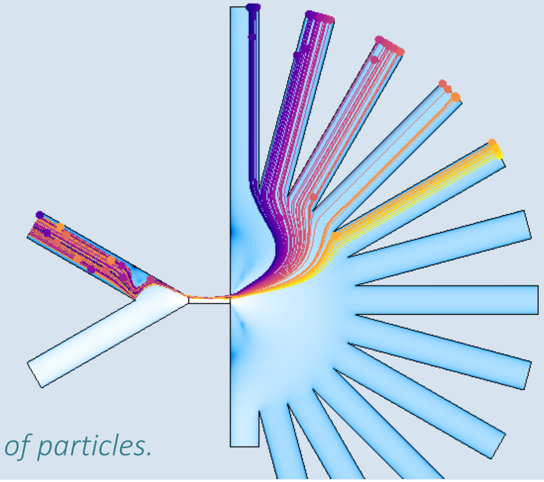


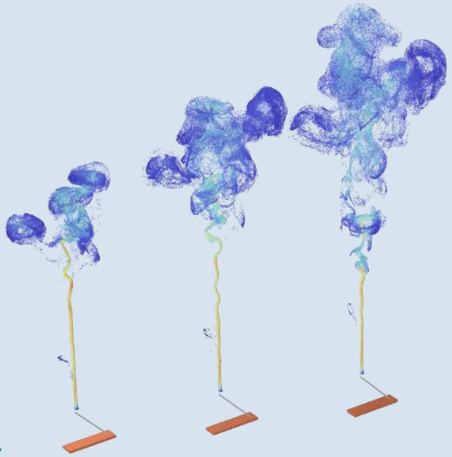
Particle field interaction.

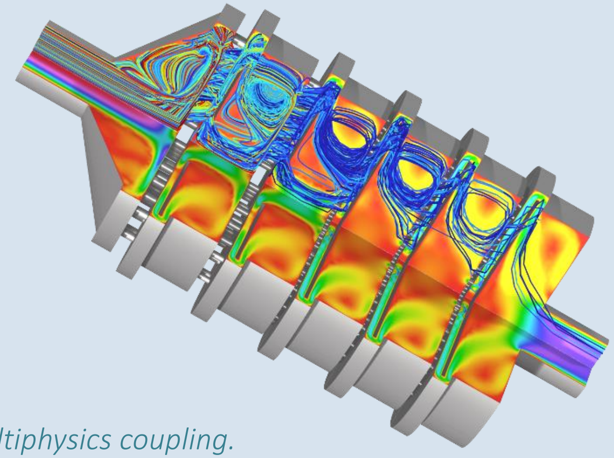
MODELING CAPABILITIES

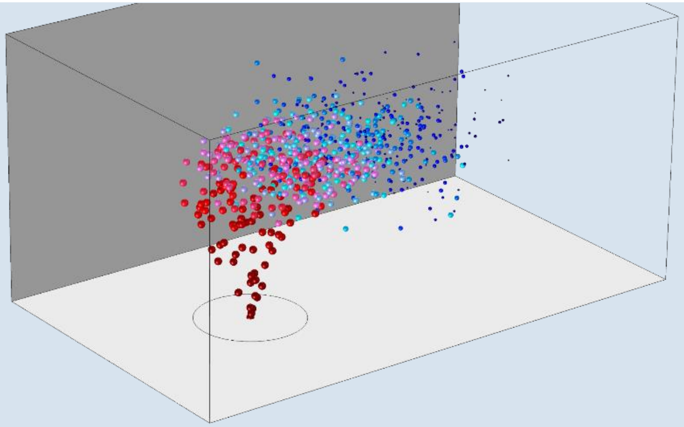
Particle Tracing for Fluid Flow

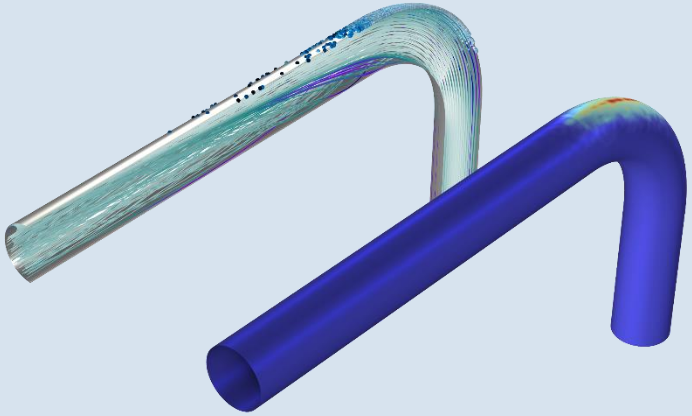

Multiple built-in forces.


Multi species of particles.


Particle tracing in turbulent fluid flow.

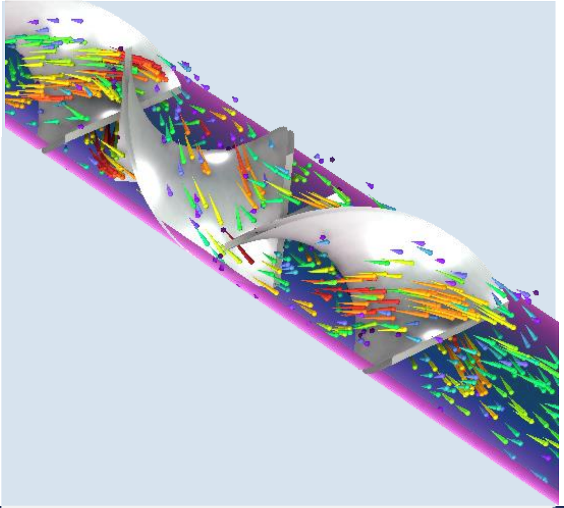

Multiphysics coupling.


Droplet spraying and evaporation.


Erosion modeling.

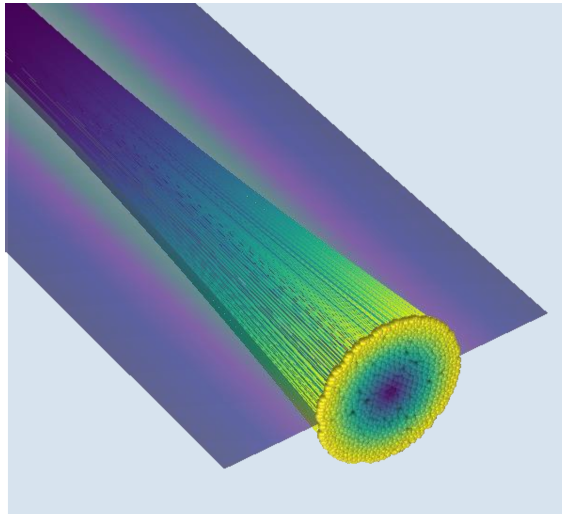
MODELING CAPABILITIES

Multiphysics Couplings with Particle Tracing



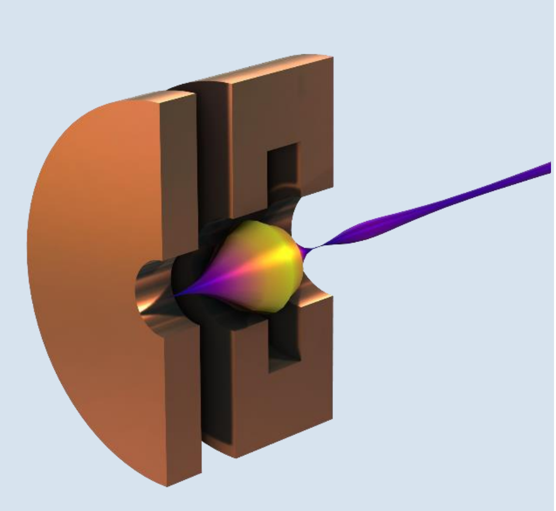
Fluid-Particle Interaction

This capability computes drag force exerted on particles in each mesh element in selected domains.



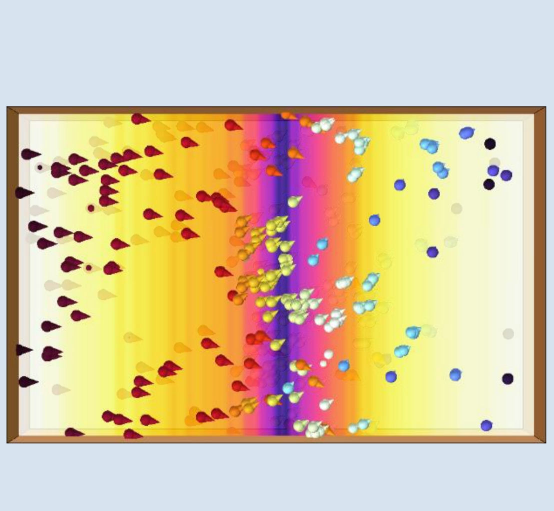
Electric Particle Field Interaction

You can compute space charge density due to particles and also apply it as a source when computing the electric potential



Magnetic Particle Field Interaction

You can compute accumulated current density due to motion of charged particles and use it as a source for the computation of the magnetic vector potential.



Space Charge limited Emission

This Multiphysics coupling models the space charge limited emission of electrons from a surface.

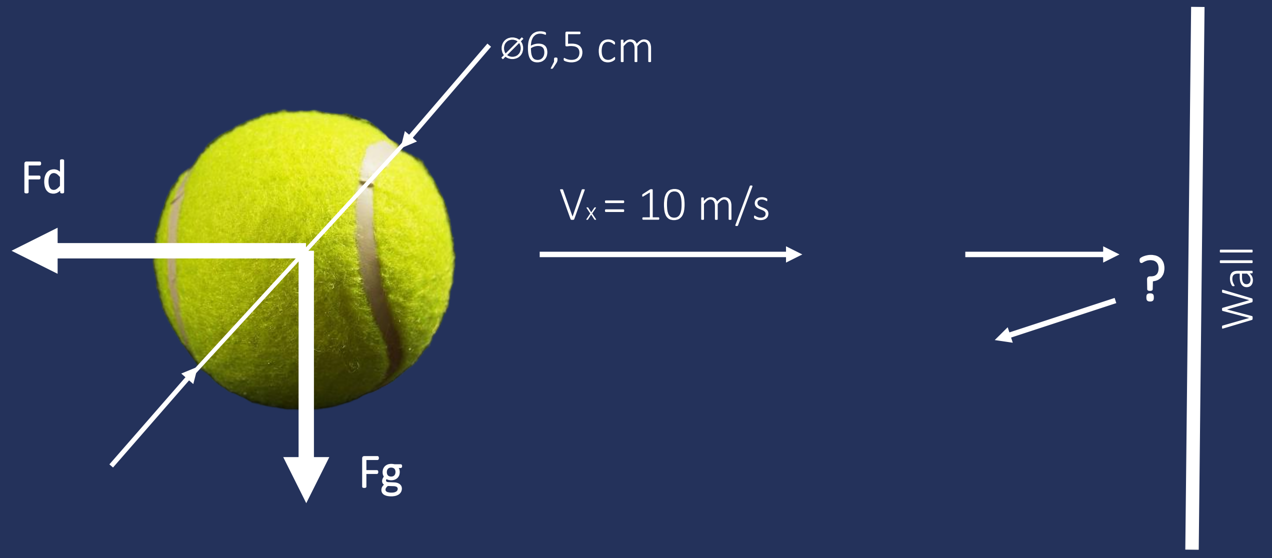
*Requires the CFD Module and Acoustics Module.

A) What?

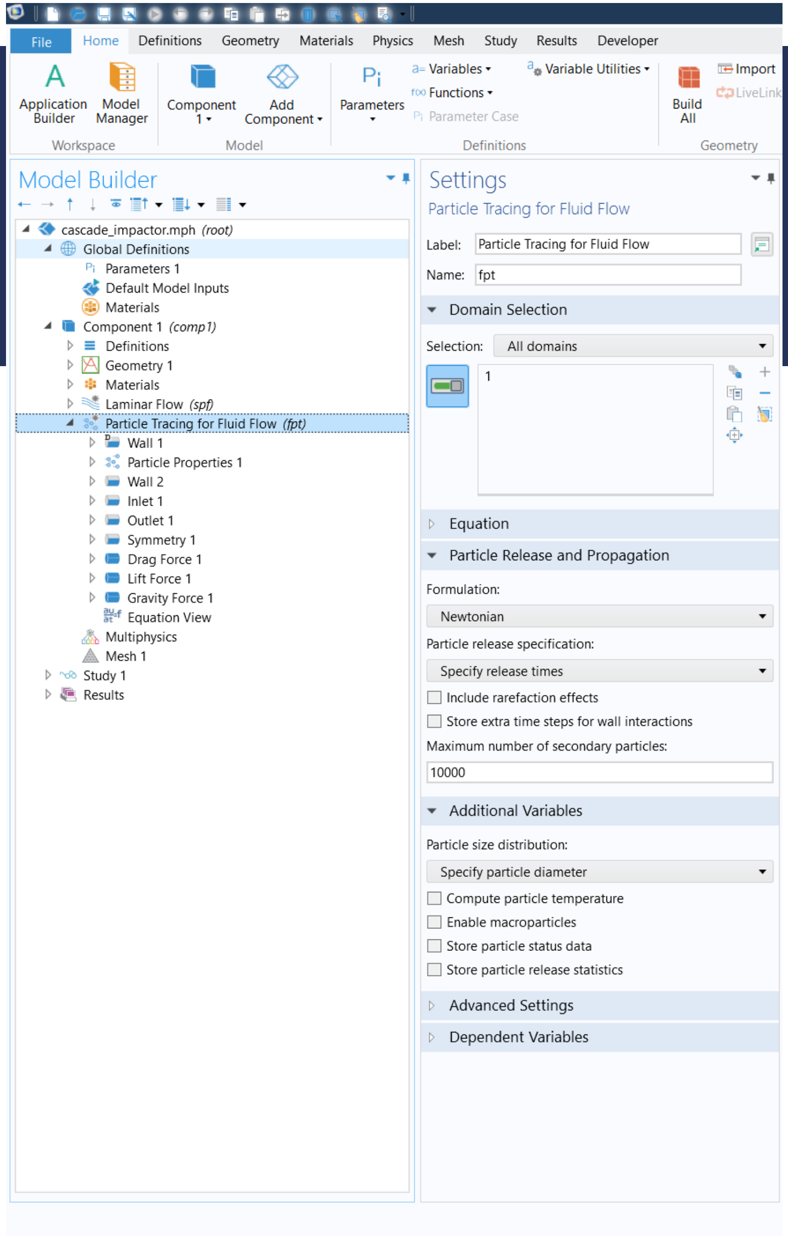
B) From?

C) What happens on walls?

D) Which forces?

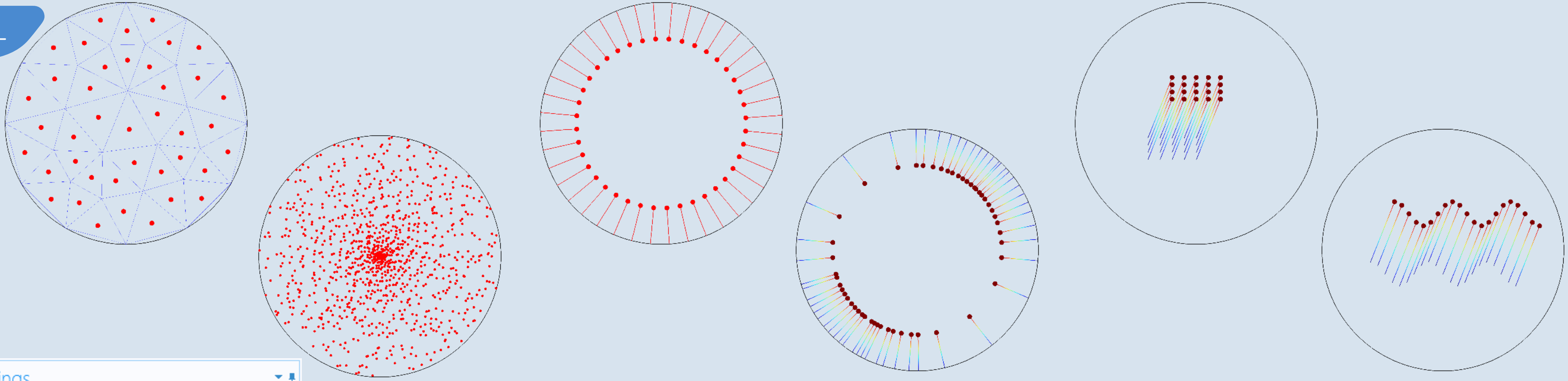


Essential Features in a PT Modul

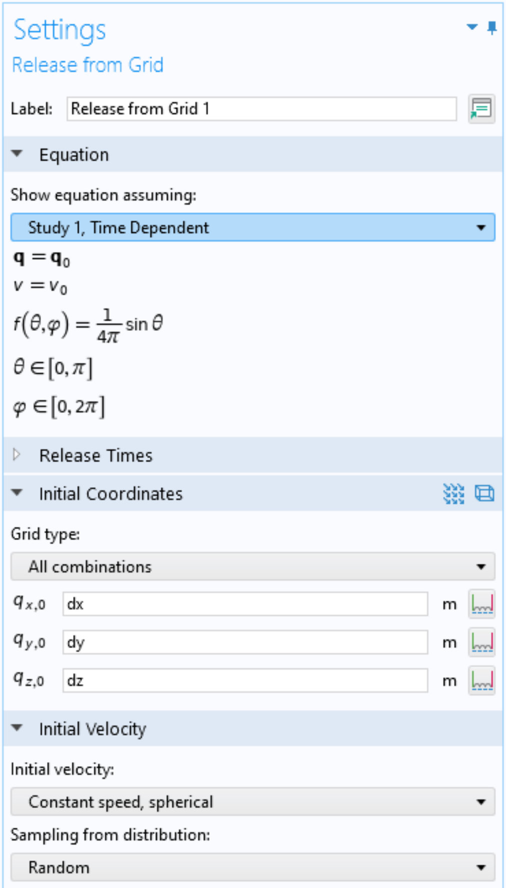


Essential Features in a PT Model

- At least one Particle Properties node (particle size, etc.)
- At least one release feature (Release, Inlet, etc.)
- At least one boundary condition (a default Wall node)
- Applied Forces
- (Optional) – Domain interactions
  - – Secondary particle emissions



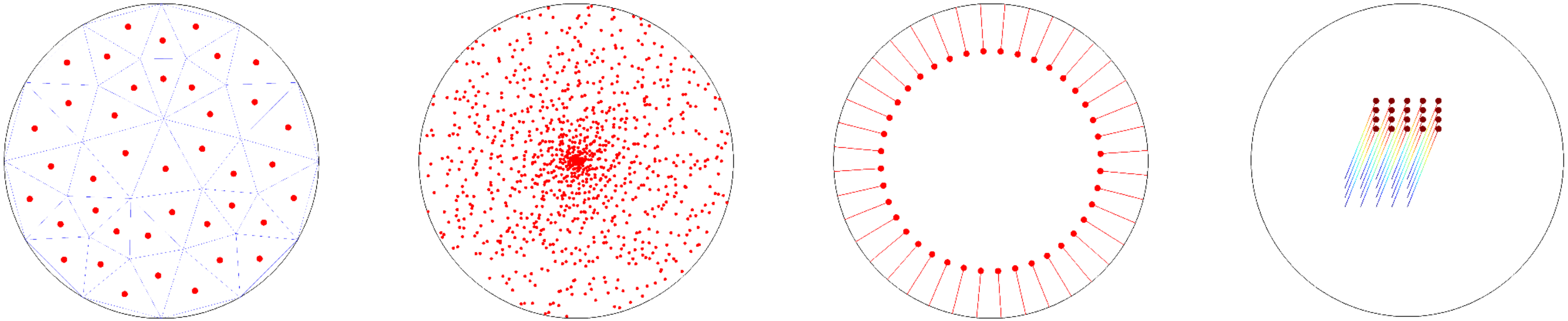
Releasing Particles



- Release from grid or data file
- Release from data file
- Release from domain, boundary, edges, and points based on user-defined density functions, uniform, or random

Guess the Method of Release

- A) Rectangular grid
- B) Density proportional to an expression
- C) Mesh-based
- D) Arbitrary grid
- E) Uniform release from boundary



Guess the Method of Release

- A) Rectangular grid
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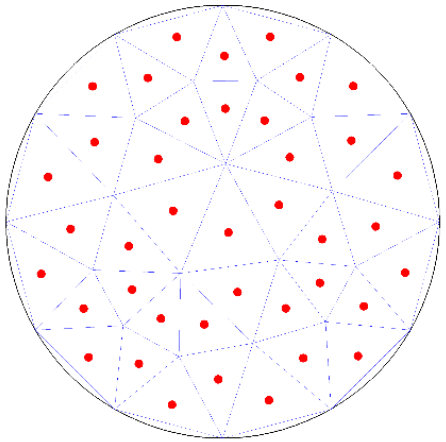
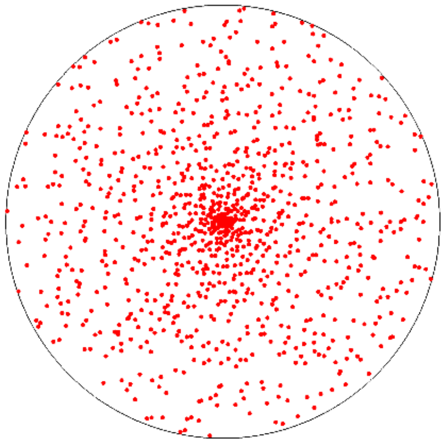
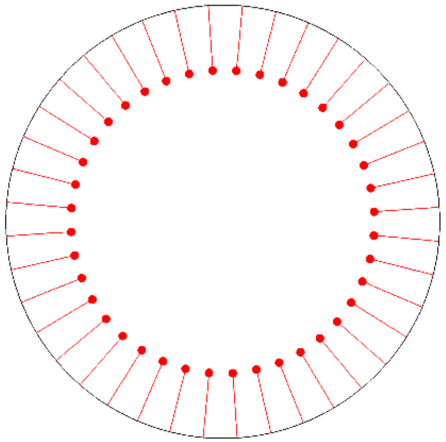


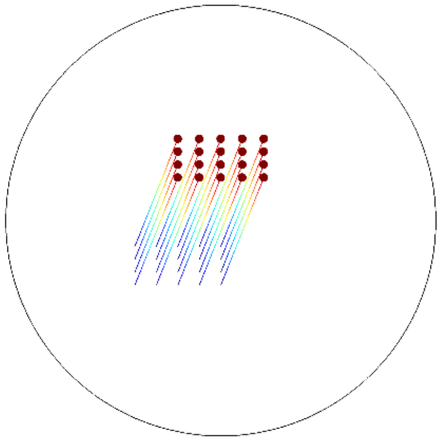
Mesh-based



Density proportional



Uniform release from boundary

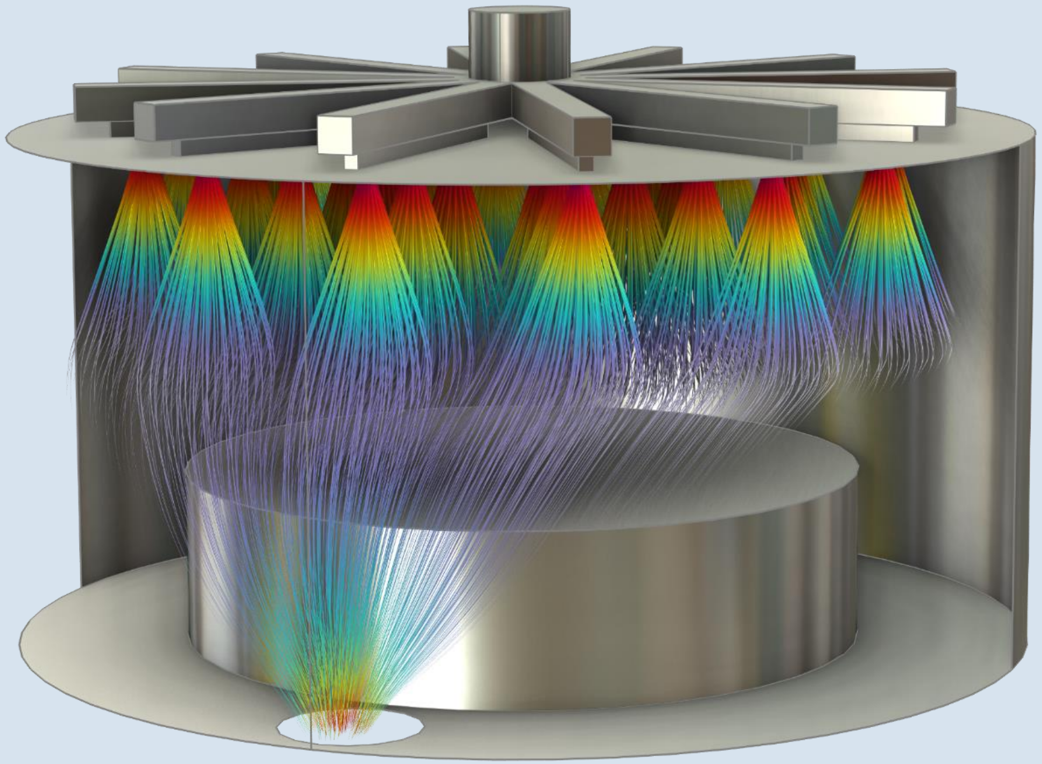


Rectangular grid

Initializing Particle Velocity

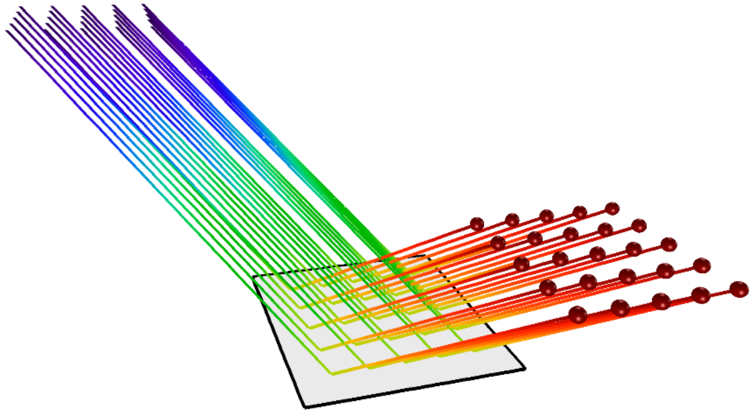
Initialize velocity by:

- Specifying components directly
- Using kinetic energy and direction
- Uniform distributions:
  - Sphere
  - Hemisphere
  - Cone
  - Lambertian

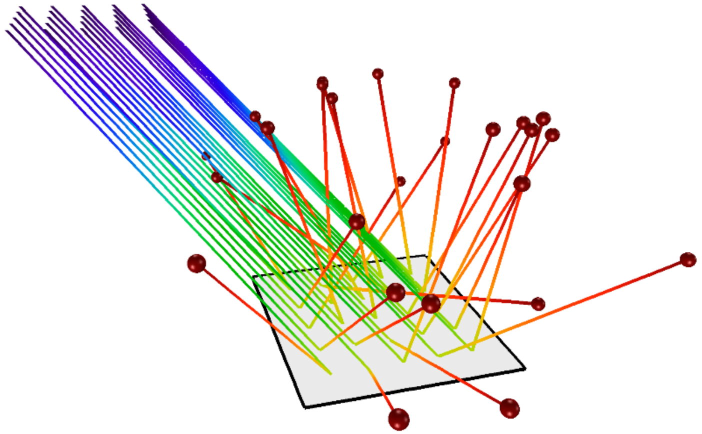


Cone-based release of particles can be used to model sprays in devices such as CVD chambers.

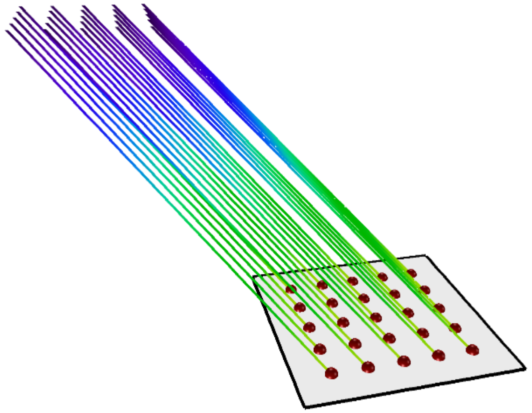
WIDE VARIETY OF BOUNDARY CONDITIONS



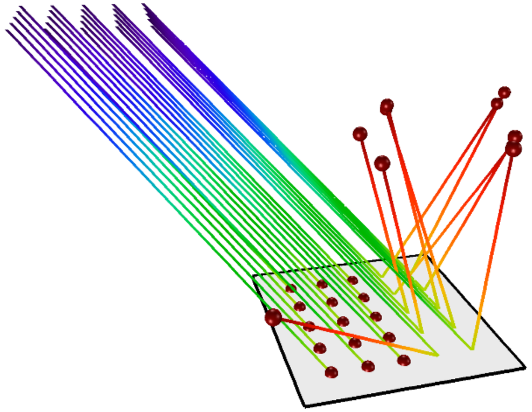
Specular reflection.



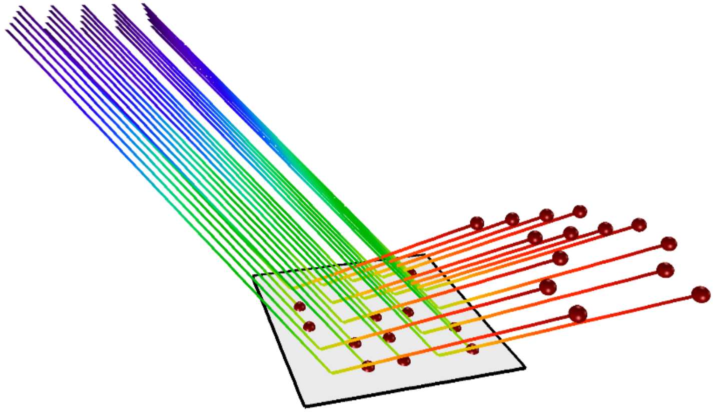
Diffuse or isotropic scattering.



Absorption: stop or remove particles.



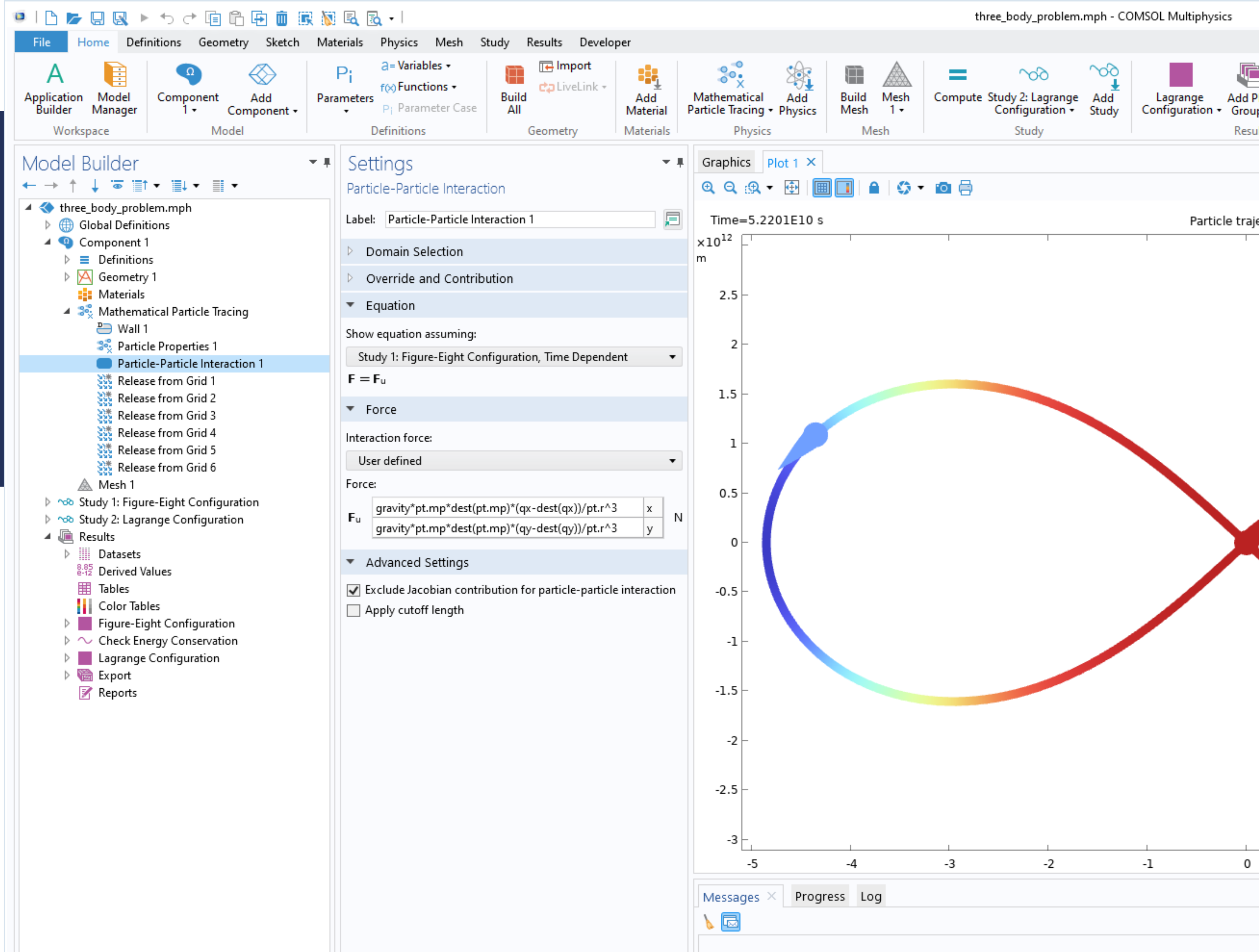
Conditional interactions, based on a custom expression.



Conditional interactions, based on probability.

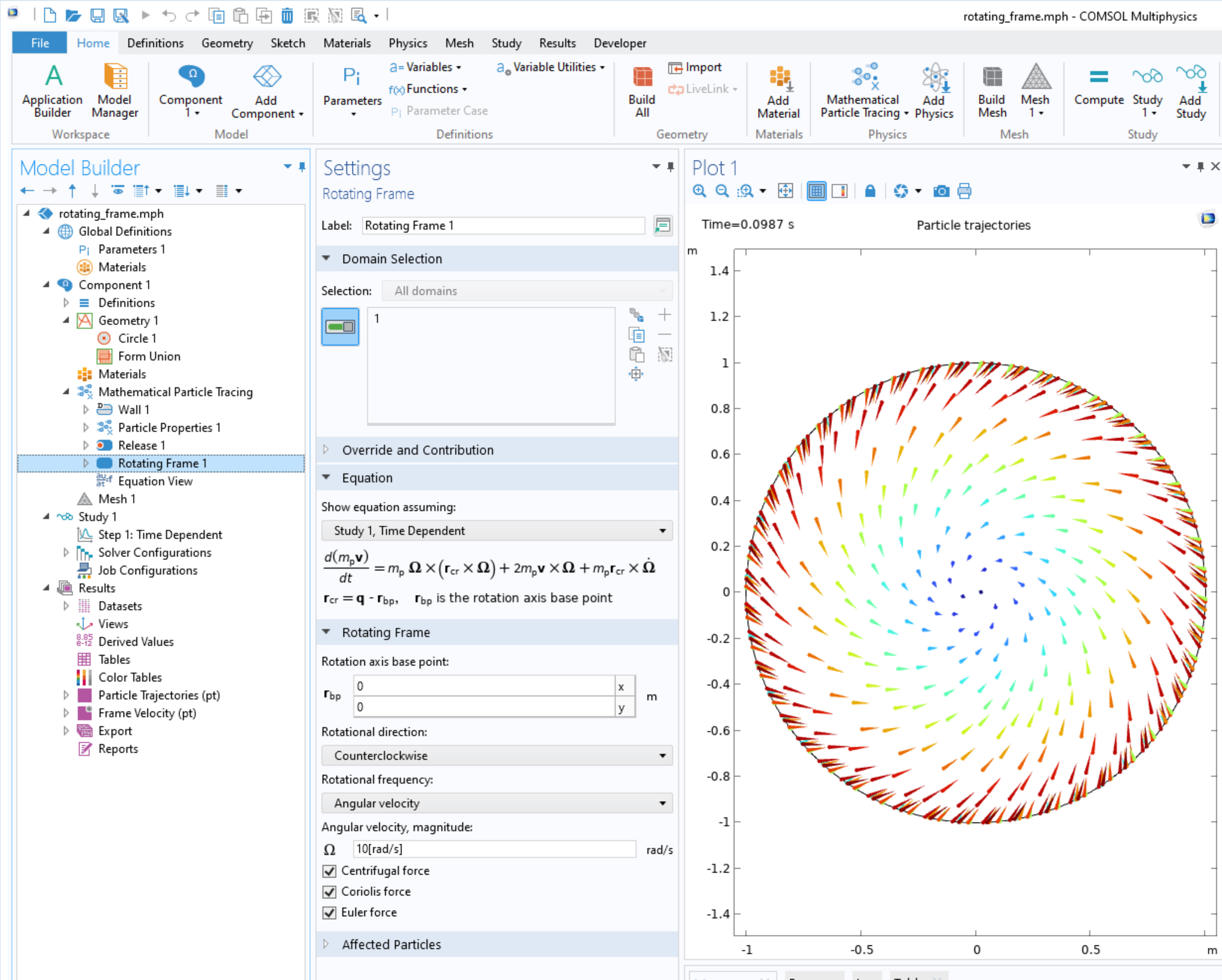
Forces

- User-defined expressions
- Can query any field variable defined in the modeling domain
- Particle-particle interactions
- Many forces can be combined in a single model
- Forces can apply to all particles or just to a certain species



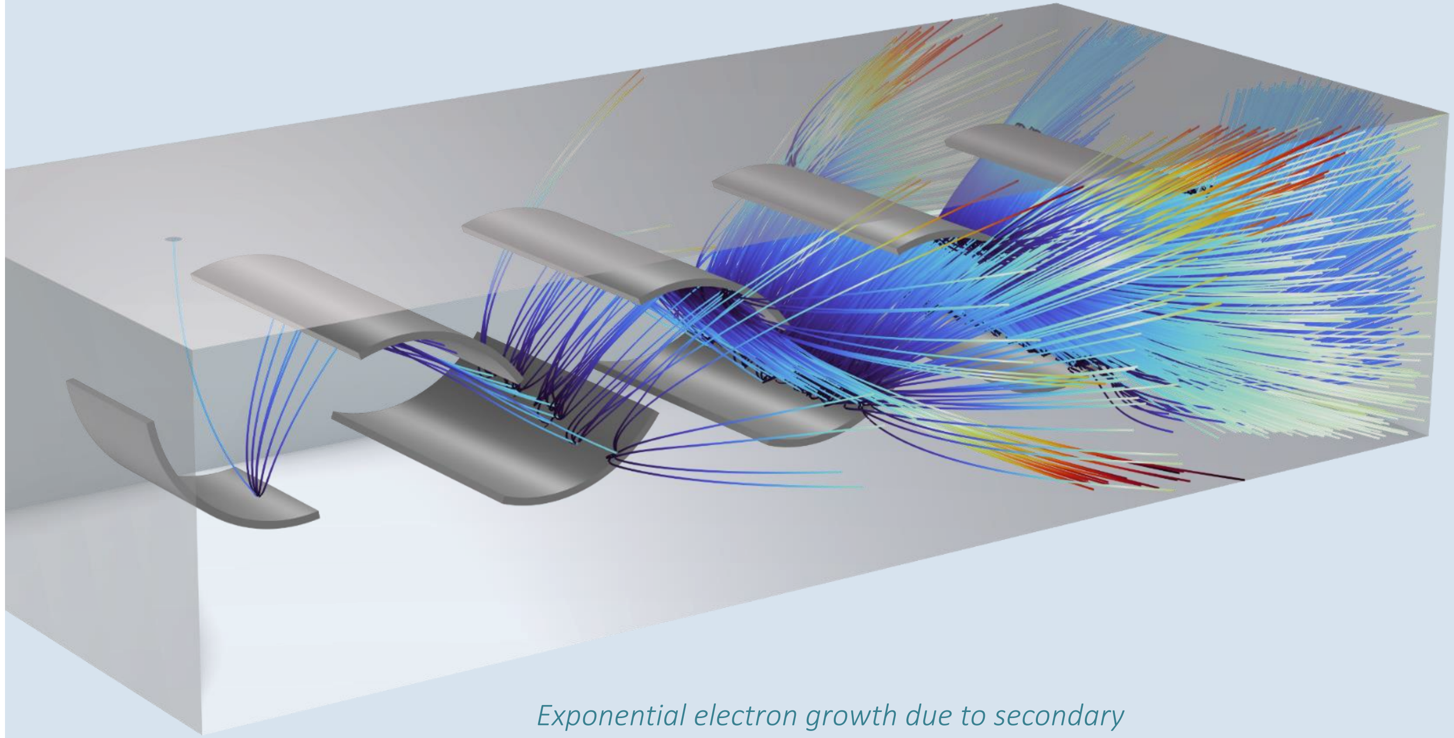
Fictitious Forces in Rotating Frames

- Centrifugal force
- Coriolis force
- Euler force



Secondary Particle Emission

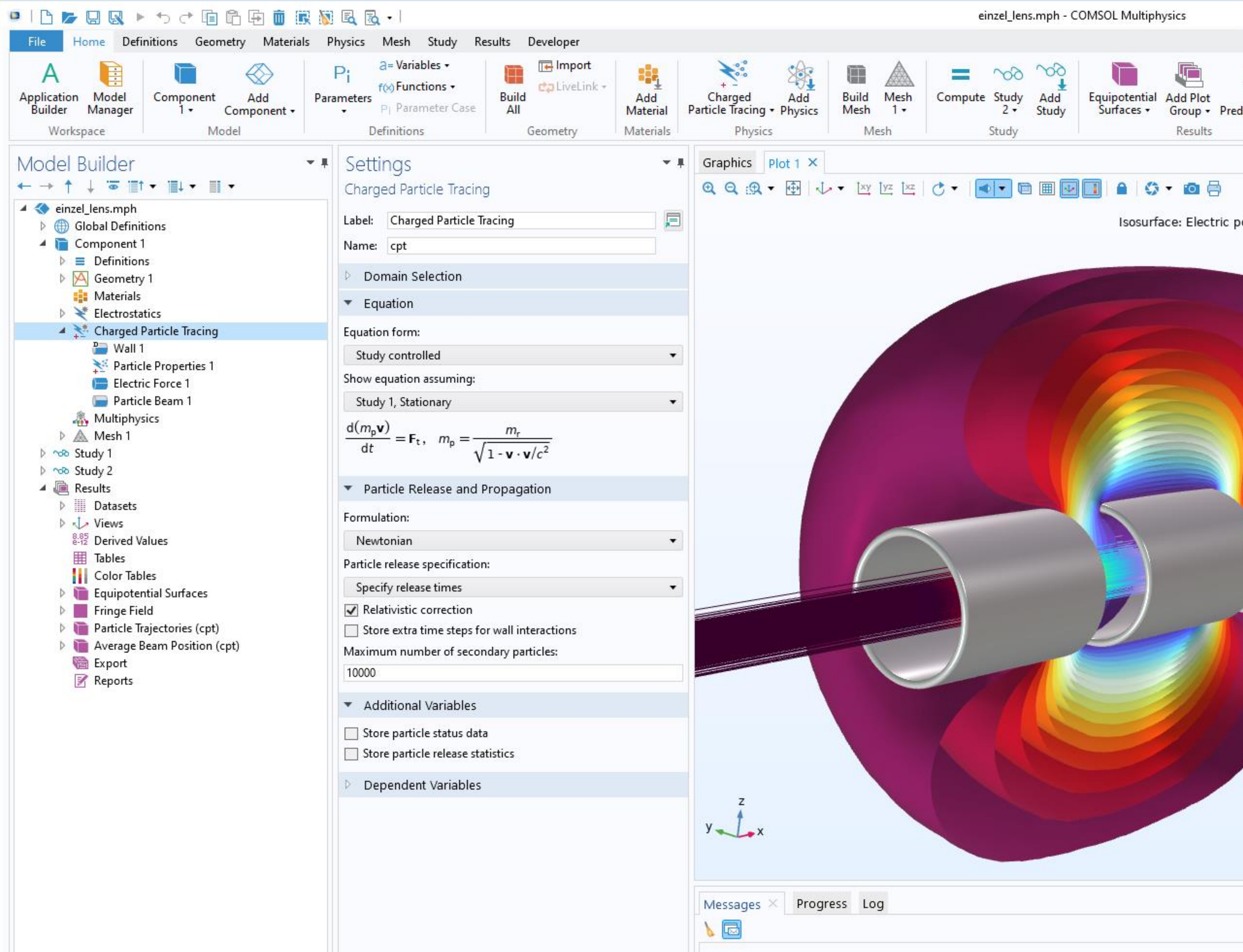
- Particles in a model can release secondary particles in domains or while hitting boundaries
- Secondary emission can be based on a probability or a logical expression



Exponential electron growth due to secondary emission in a photomultiplier.

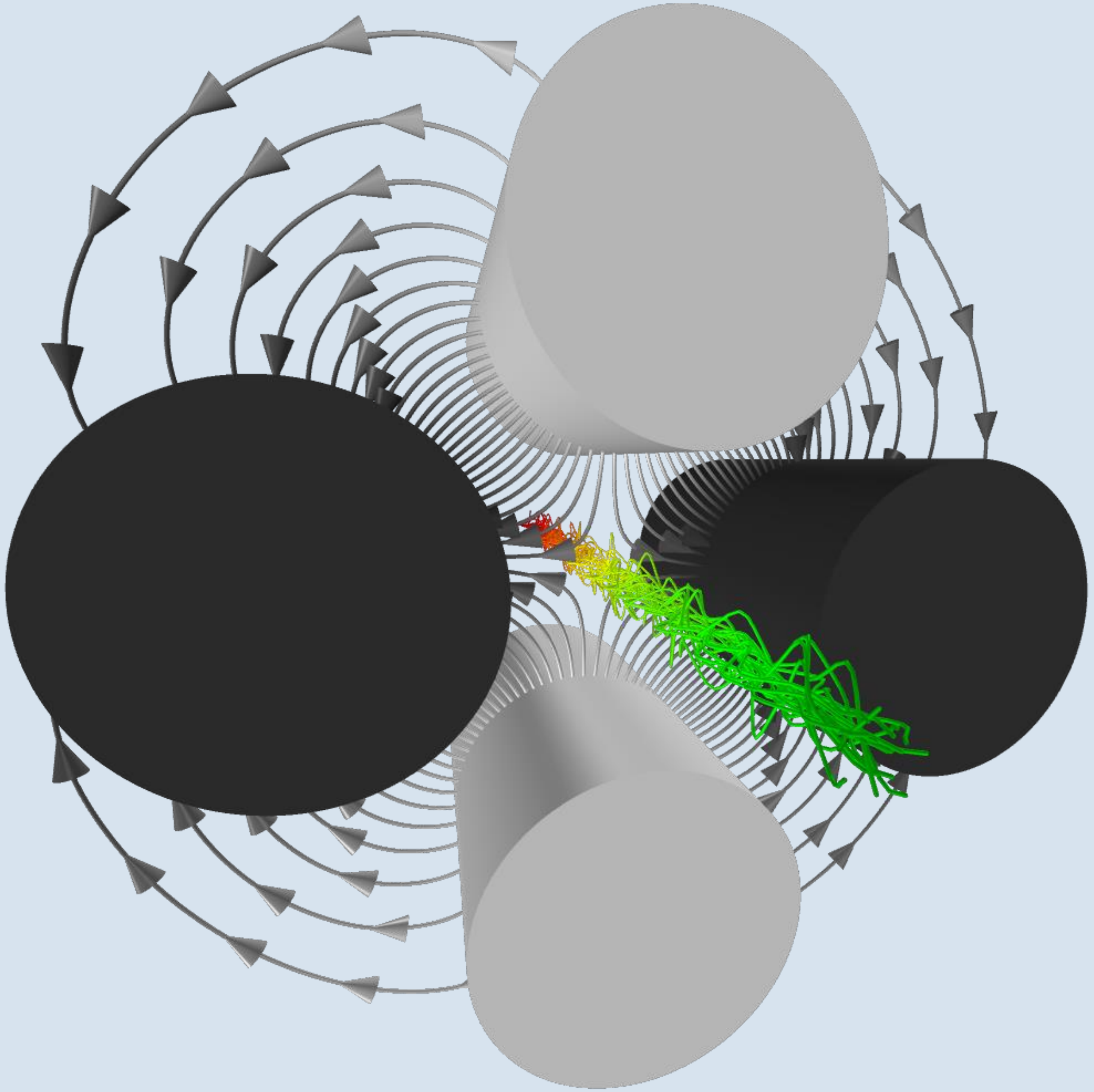
Charged Particle Tracing Interface

- For computing ion and electron trajectories
- Built-in electric and magnetic forces
- Easy coupling to electric or magnetic fields solved for by one of the AC/DC interfaces
- Monte Carlo collision model for rarefied gases

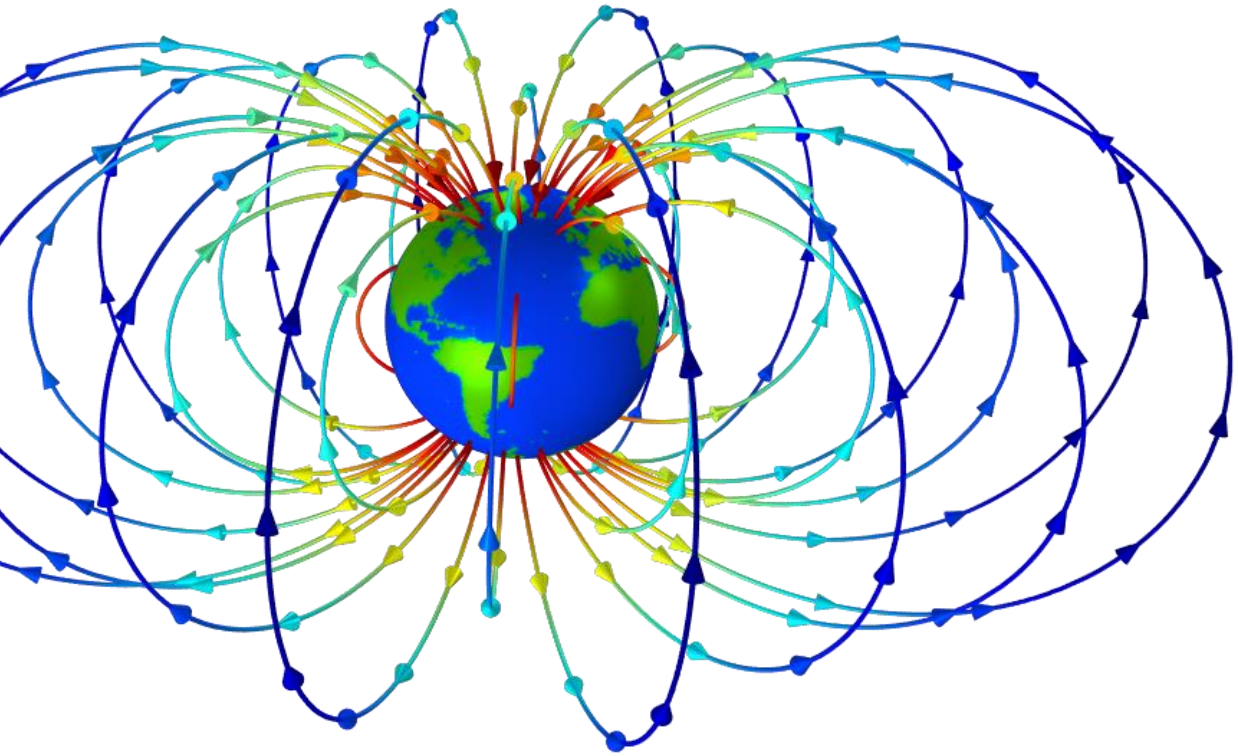


Electric and Magnetic Forces

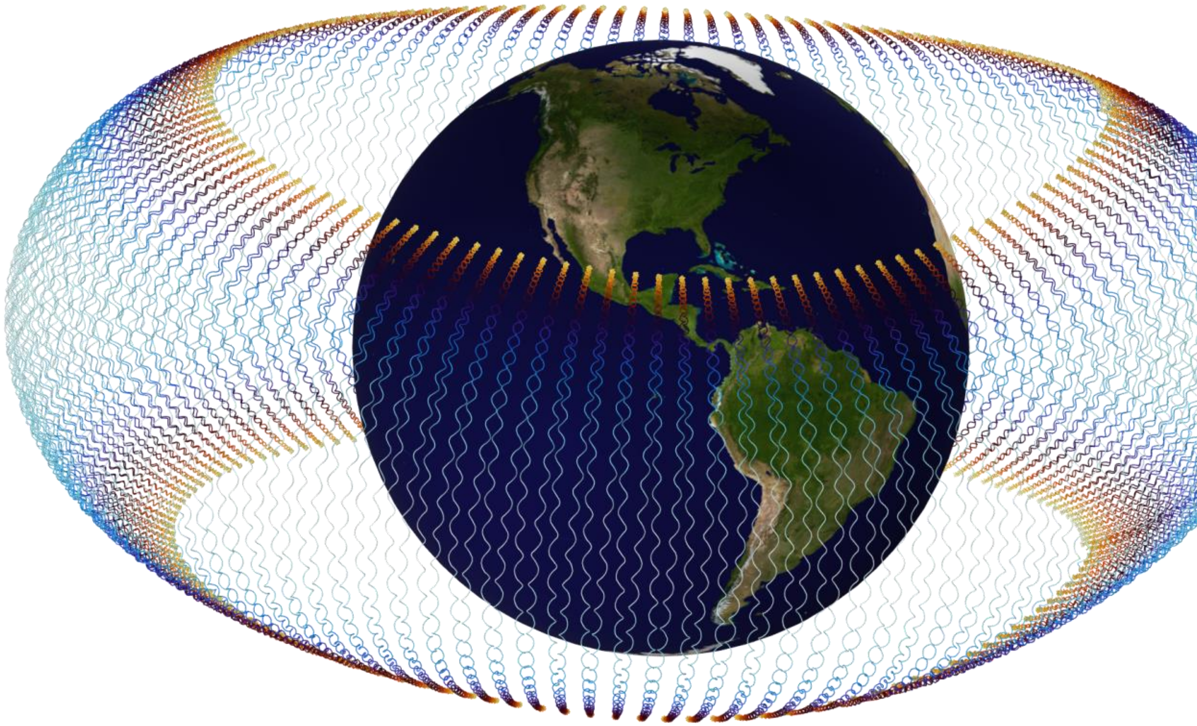
- Automatically couple electric and magnetic forces to previously computed potentials or fields
- Combinations of stationary, transient, time-harmonic, and other time-periodic fields



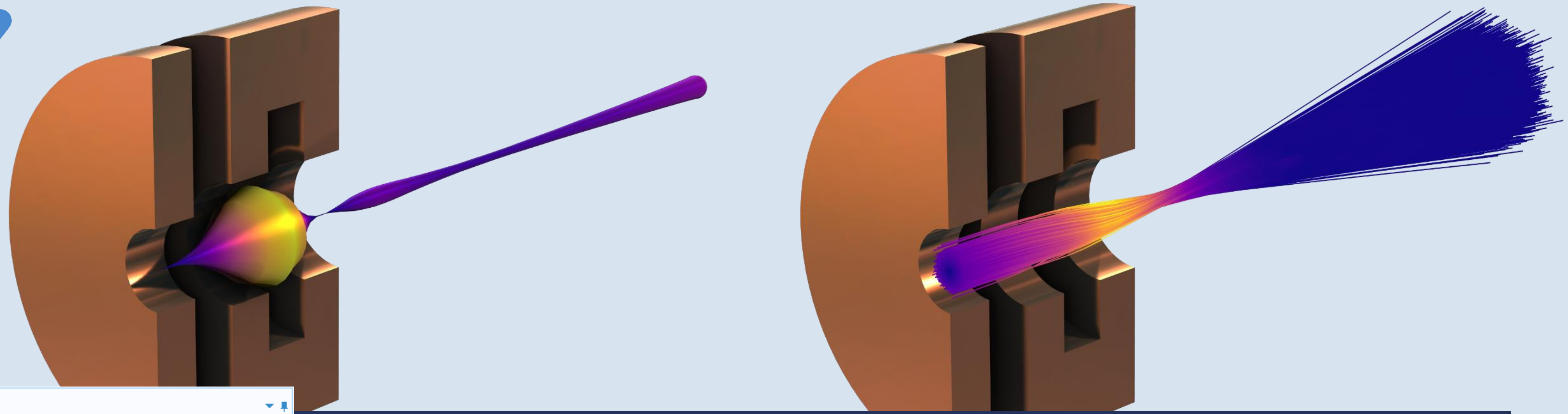
Quadrupole mass spectrometer: ions are trapped by the combined AC and DC fields of two oppositely biased pairs of electrodes.



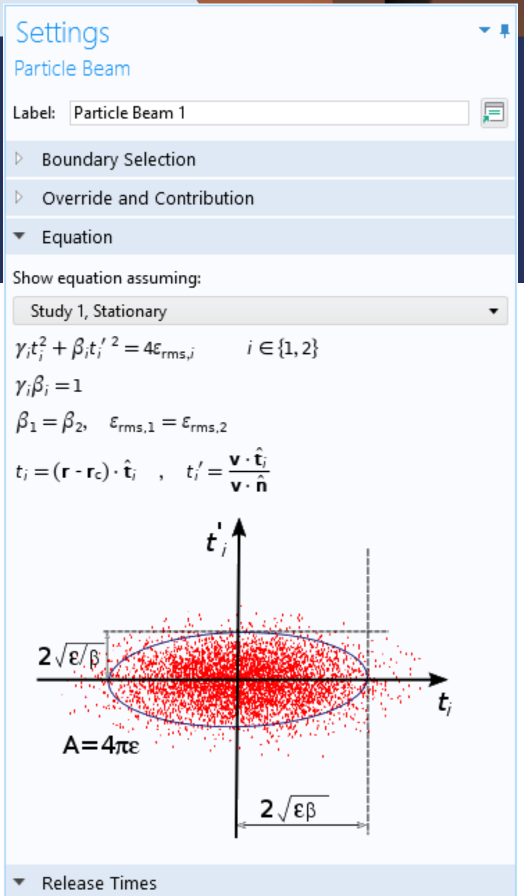
Field lines of Earth's magnetic field, from the International Geomagnetic Reference Field (IGRF).



Proton trajectory.



Beam Simulations

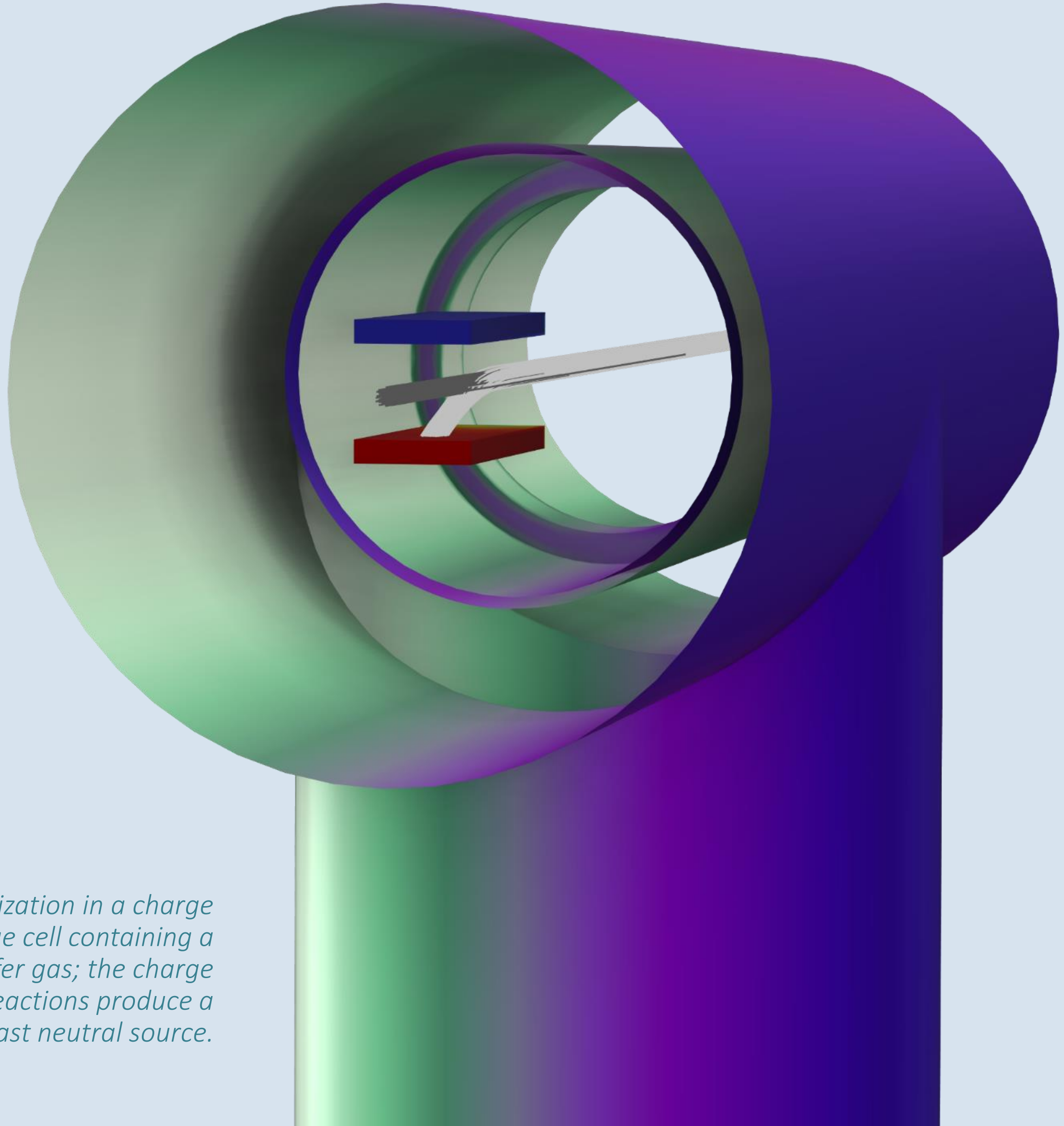


- Release nonlaminar beams of charged particles with ellipses or Gaussian distributions in transverse phase space
- Symmetric or asymmetric beams in 3D
- Specify either beam dimensions or initial Twiss parameters
- Built-in variables for computing Twiss parameters and beam emittance

Monte Carlo Collision Modeling

Built-in options are available for modeling collisions between particles and a background gas:

- Elastic
- Inelastic
- Attachment
- Ionization
- Resonant and nonresonant charge exchange
- User-defined expressions

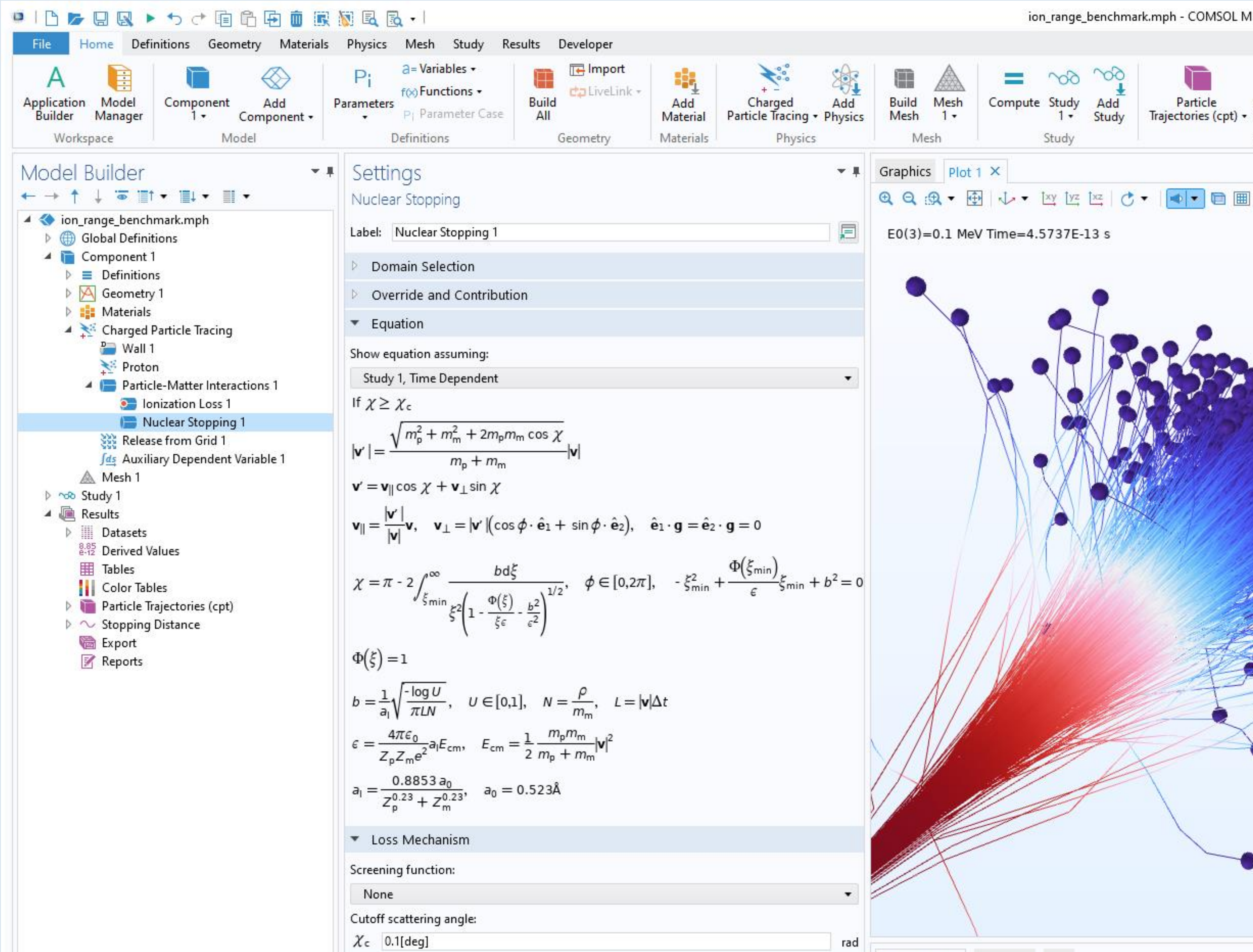


Beam neutralization in a charge exchange cell containing a rarefied buffer gas; the charge exchange reactions produce a fast neutral source.

Ion Interactions with Solid Matter

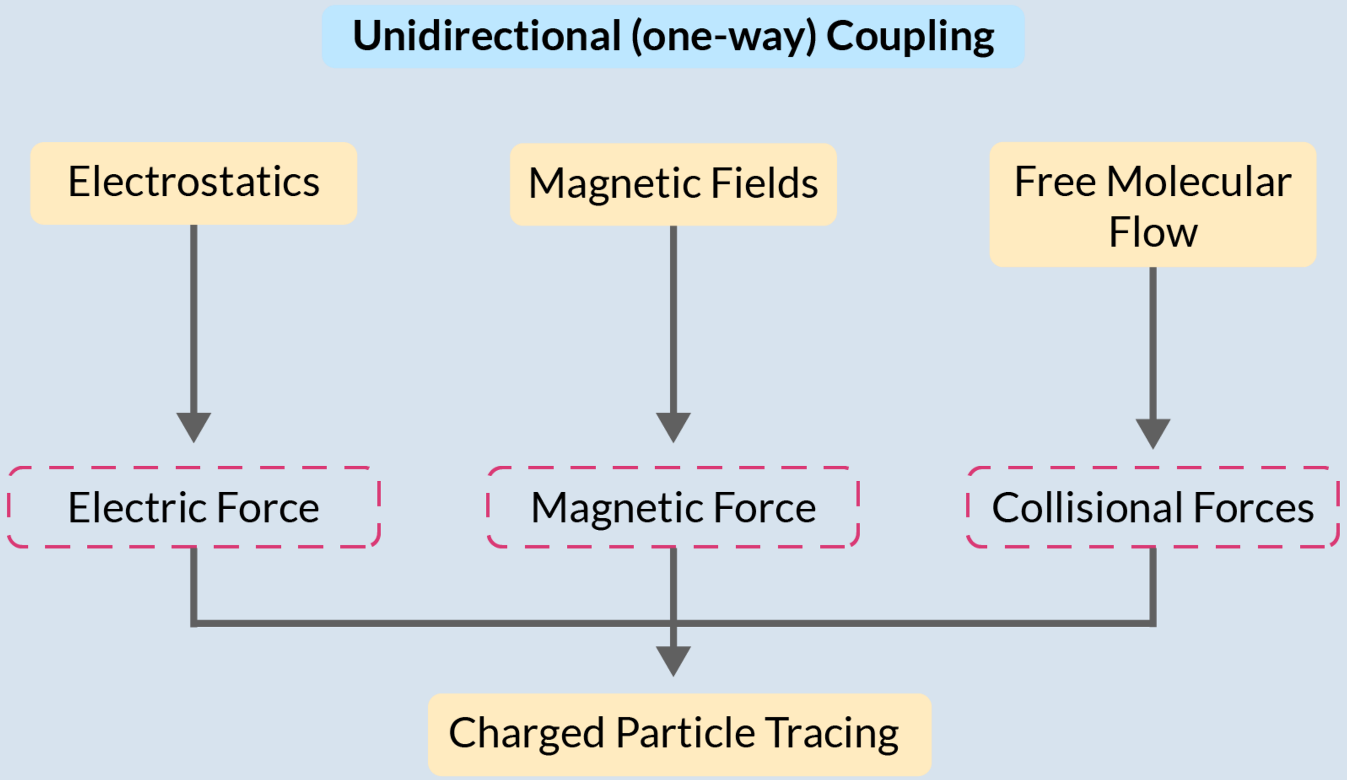
Built-in features for modeling interaction of energetic ions with solids:

- Ionization Loss: continuous deceleration from interaction with target electrons
- Nuclear Stopping: discrete scattering by target nuclei



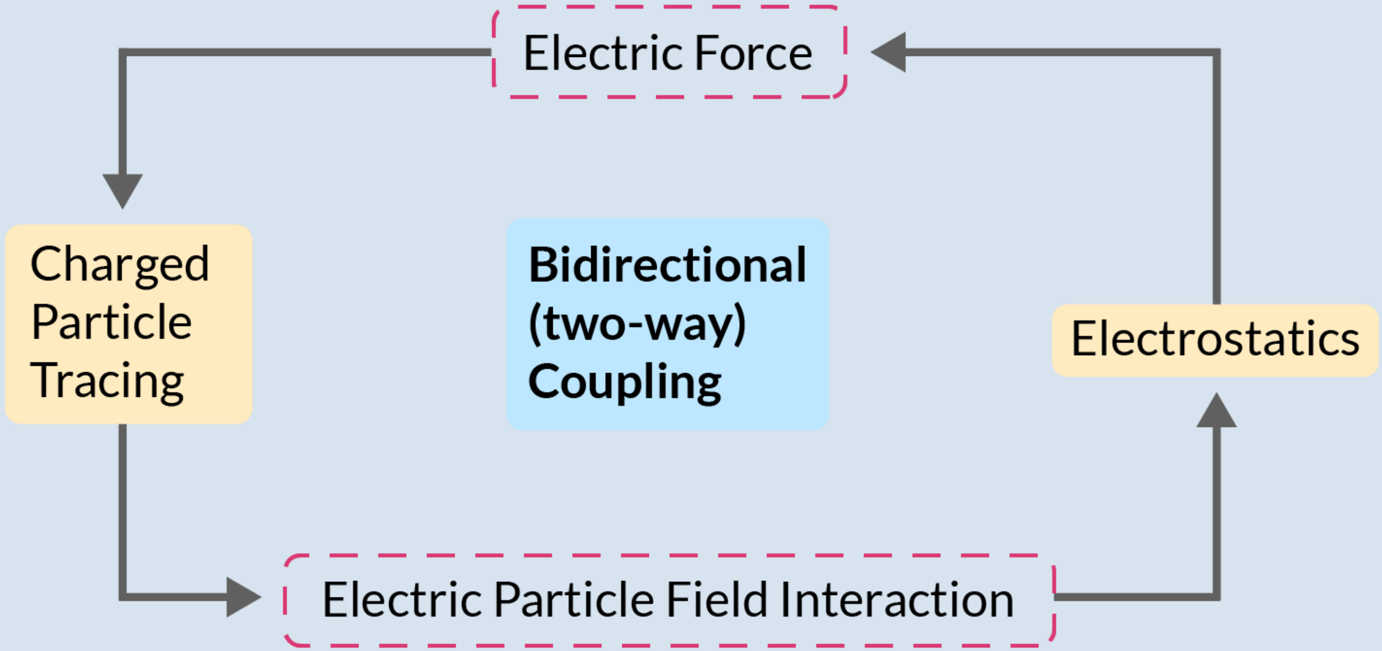
Coupling Particles and Fields

- Unidirectional couplings – simplest and fastest to solve
- Fields are solved for first
- Fields exert forces on particles
- Particle trajectories are computed last
- Particles don't have a large effect on the fields



Two-way Particle Field Interactions

- Solve for electric potential and particle trajectories together
- Particles are affected by electric forces
- Fields are affected by the space charge density of particles
- More complicated and computationally demanding than the unidirectional coupling



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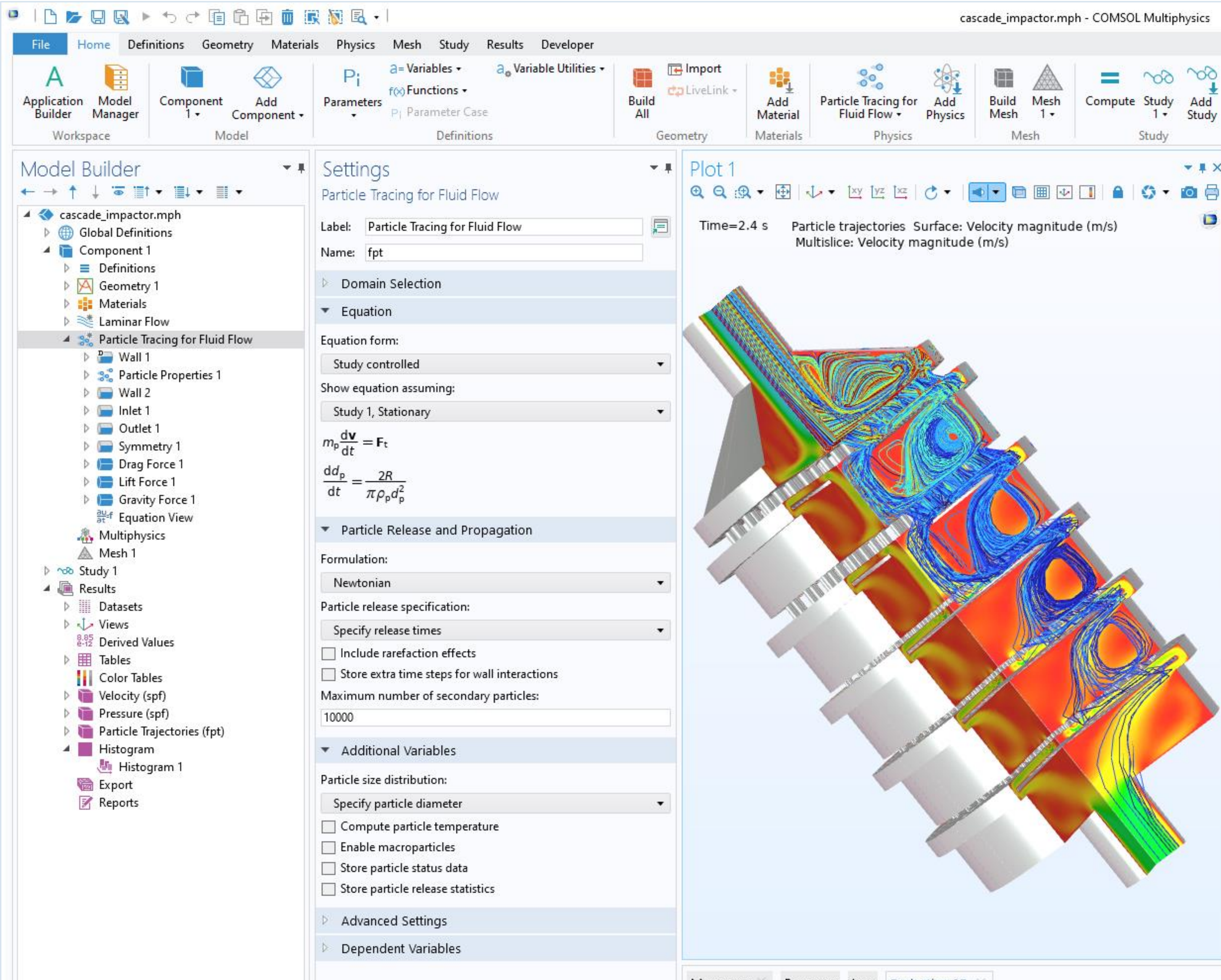
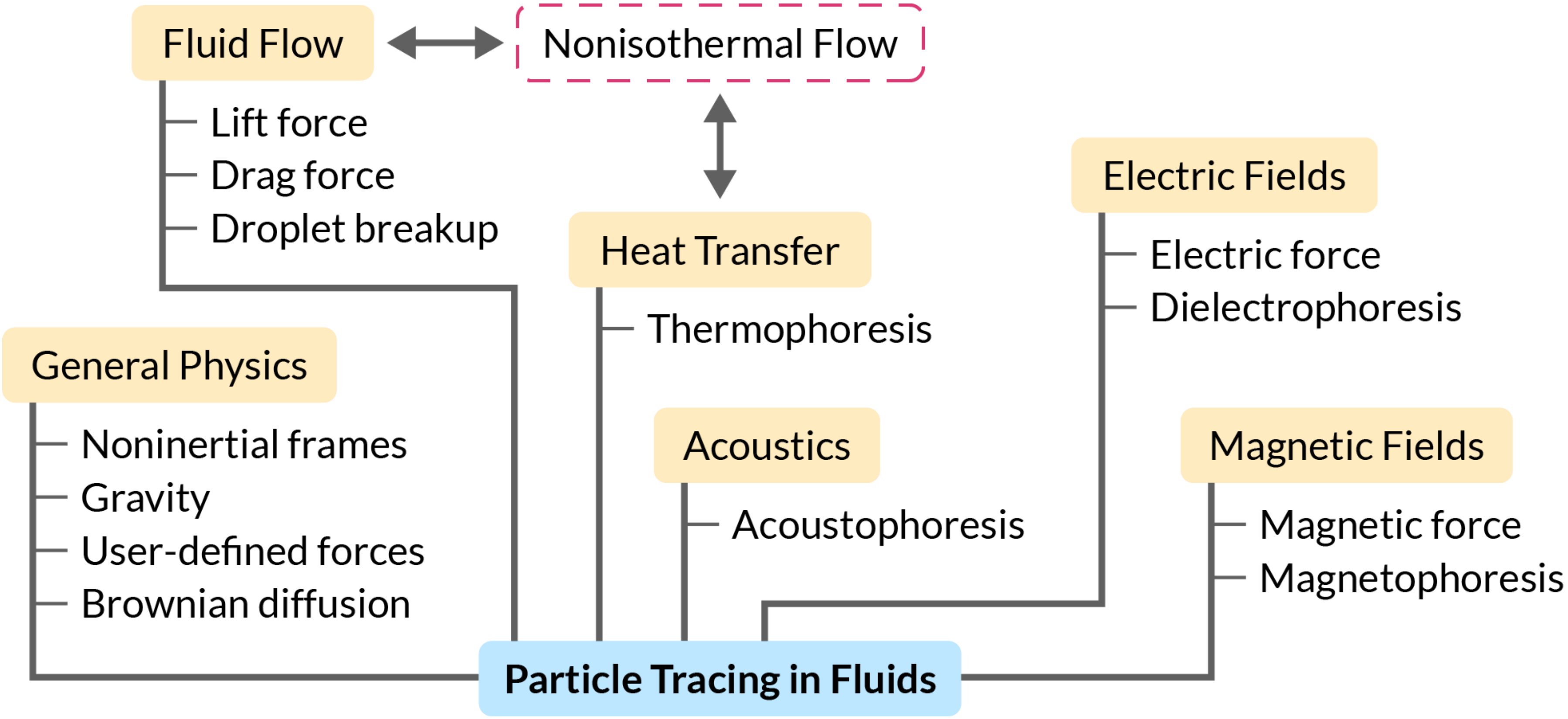
Particle Tracing for Fluid Flow Interface

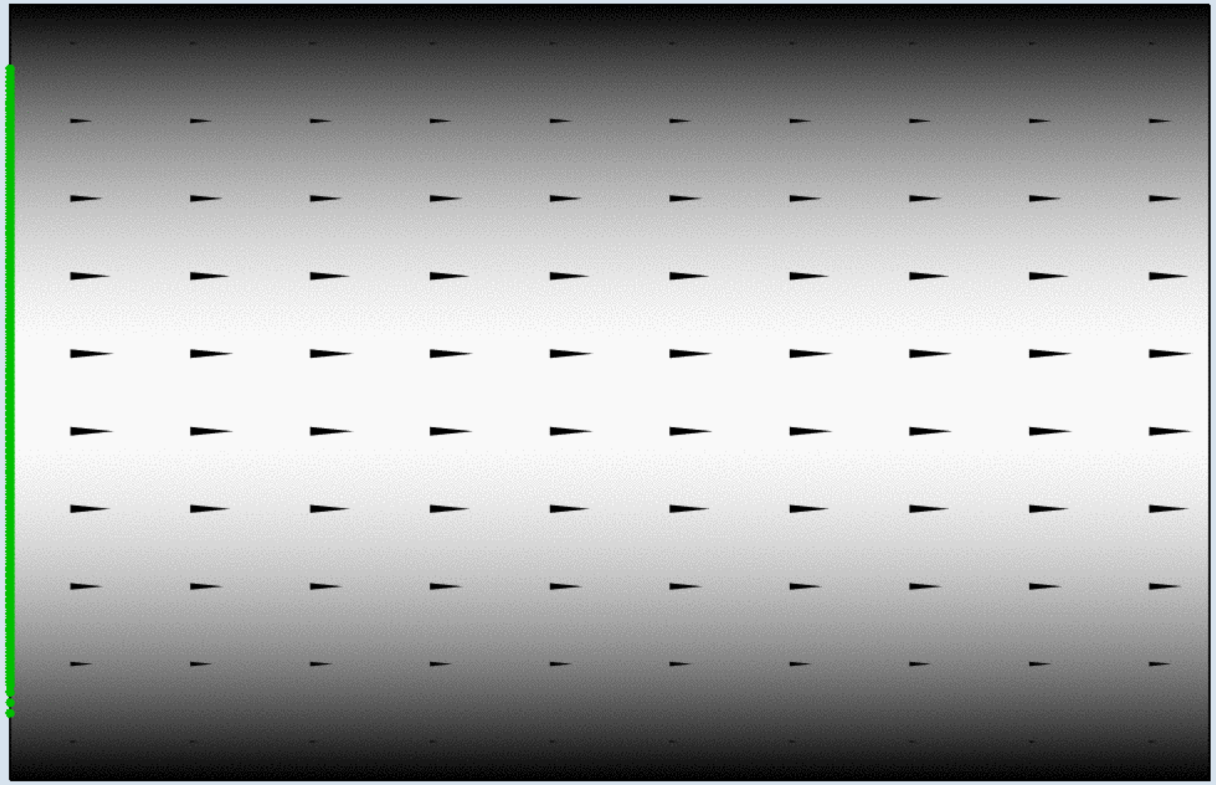
- Compute trajectories of particles in a fluid
- Separate formulations for inertial particle tracing (for larger particles) and for smaller particles with negligible inertia
- Wide variety of predefined forces




Fluid Flow
Nonisothermal Flow
Lift force
Drag force
Droplet breakup
Heat Transfer
Thermophoresis
Electric Fields
Electric force
Dielectrophoresis
General Physics
Noninertial frames
Gravity
User-defined forces
Brownian diffusion
Acoustics
Acoustophoresis
Magnetic Fields
Magnetic force
Magnetophoresis
Particle Tracing in Fluids

Lift and Drag Forces

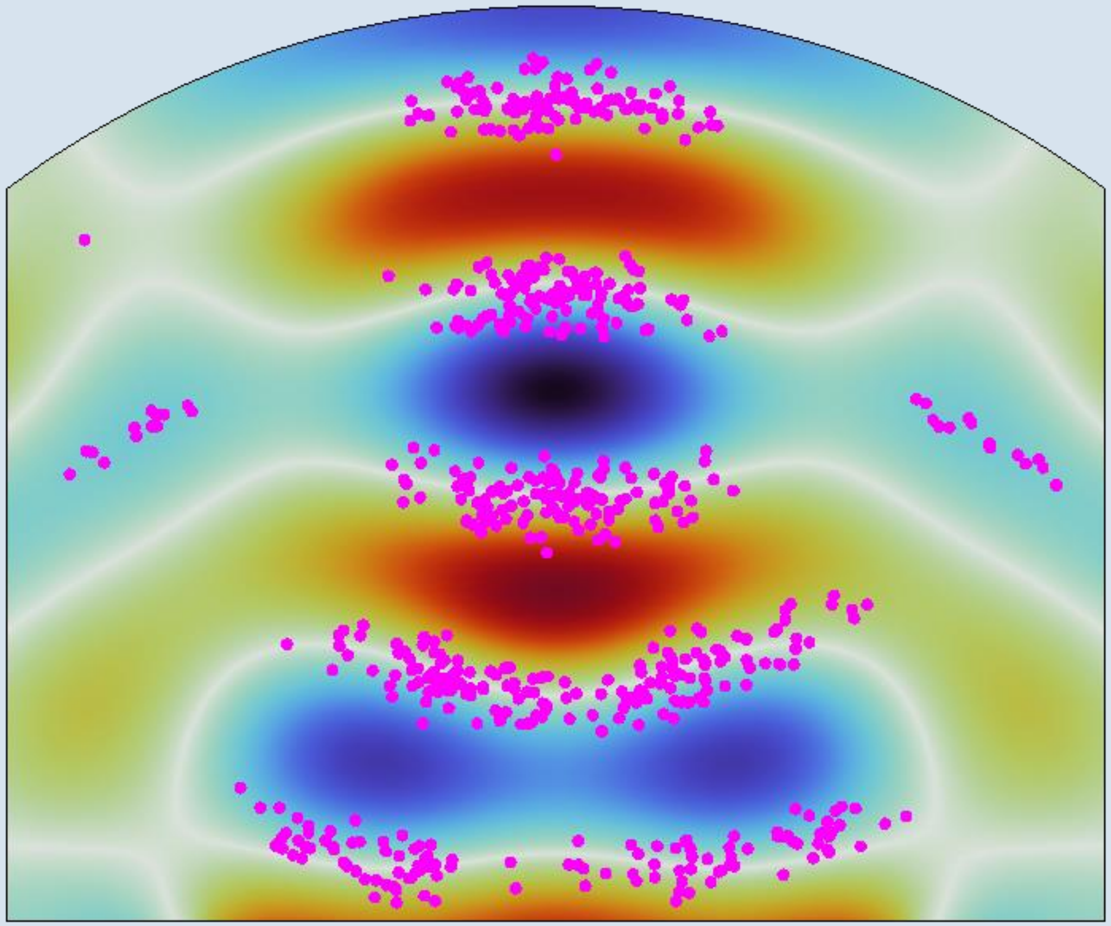
- Drag forces:
  - Different drag models for high and low relative Reynolds numbers
- Lift forces



Inertial focusing: Neutrally buoyant particles in a channel with a parabolic velocity profile approach equilibrium positions relative to the channel walls due to lift and drag forces.

Other Built-in Forces

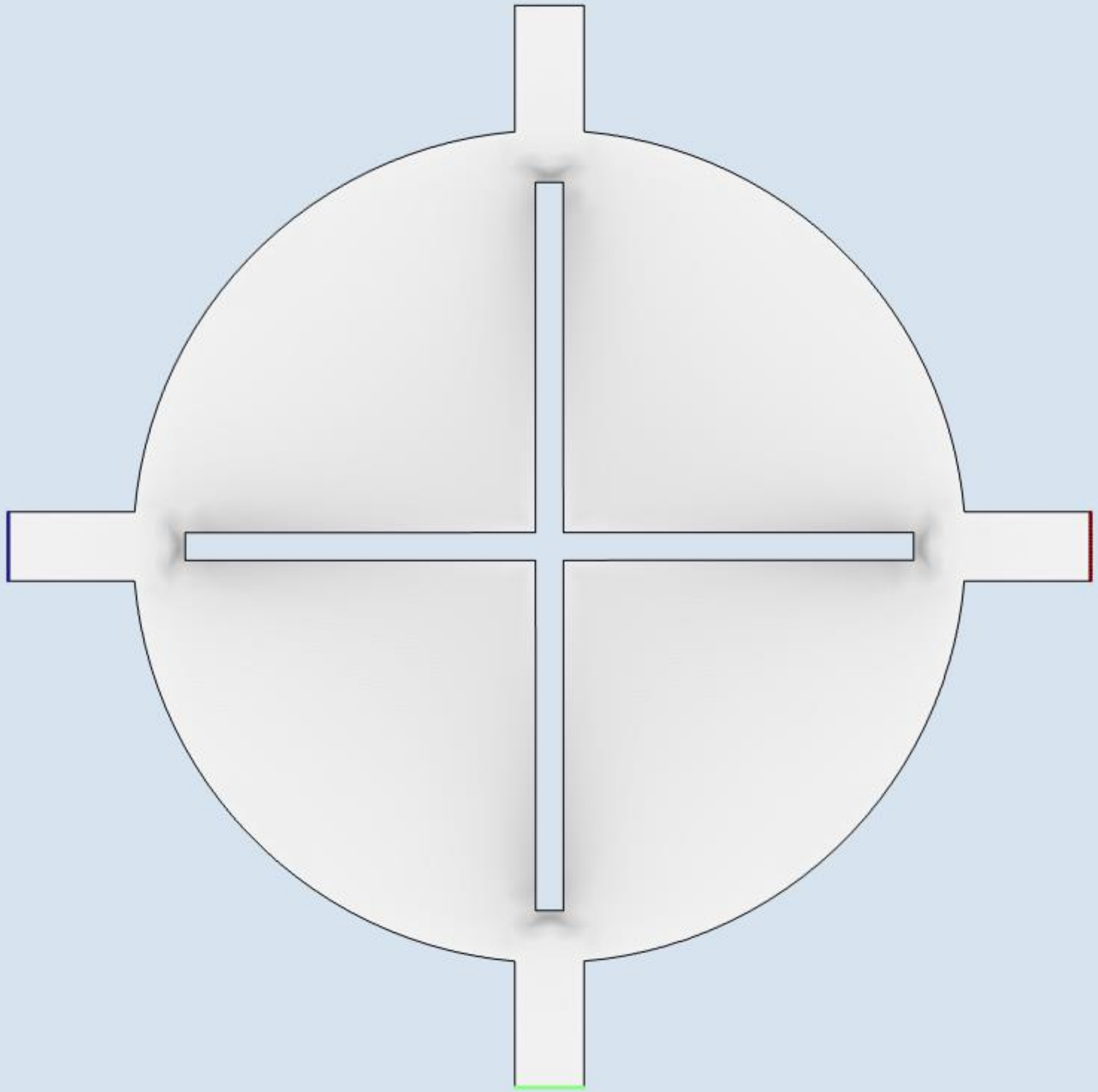
- Electric, magnetic, dielectrophoretic, and magnetophoretic:
  - Coupling to electric and magnetic fields
- Thermophoretic:
  - Coupling to temperature field
- Acoustophoretic radiation force:
  - Coupling to sound pressure field
- Gravity



Acoustic levitator: particles are suspended by the balance of gravitational and acoustophoretic radiation forces. The grayscale background shows the sound pressure level in dB.

Mixer Modeling

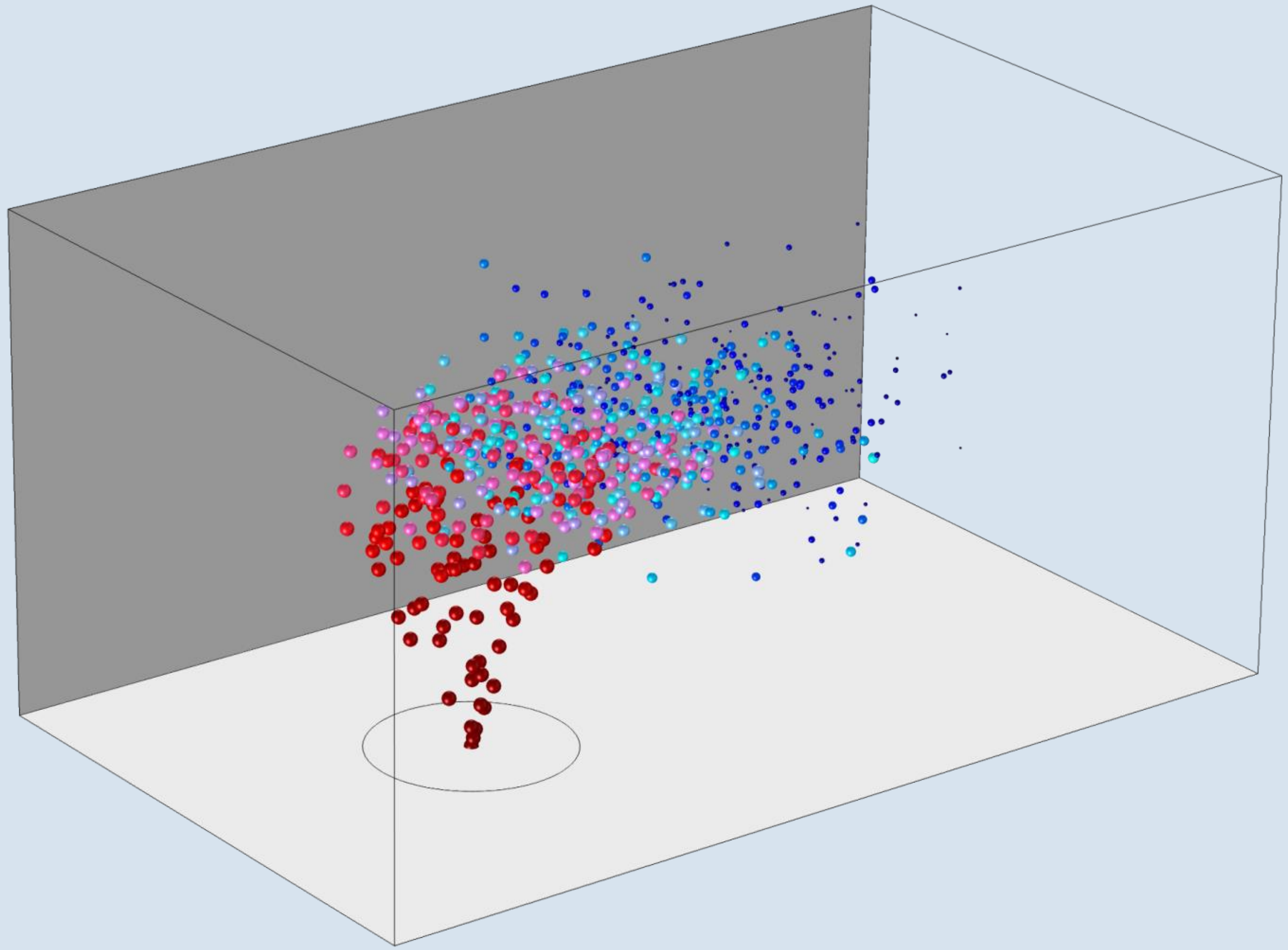
- Fully compatible with Deformed Geometry / Moving Mesh (ALE)
- Combines with fluid flow physics in rotating domains
- Moving boundaries can strike or capture particles
- Particles can stick to, and then follow, a moving boundary



Three species of particles mixed by micromixer.

Spray Modeling

- Model solid particles, liquid droplets, or gas bubbles
- Built-in features for modeling breakup of liquid droplets
- Built-in feature to model the release of a spray from a nozzle
- Built-in droplet evaporation models
  - Maxwell
  - Stefan-Fuchs
  - User defined

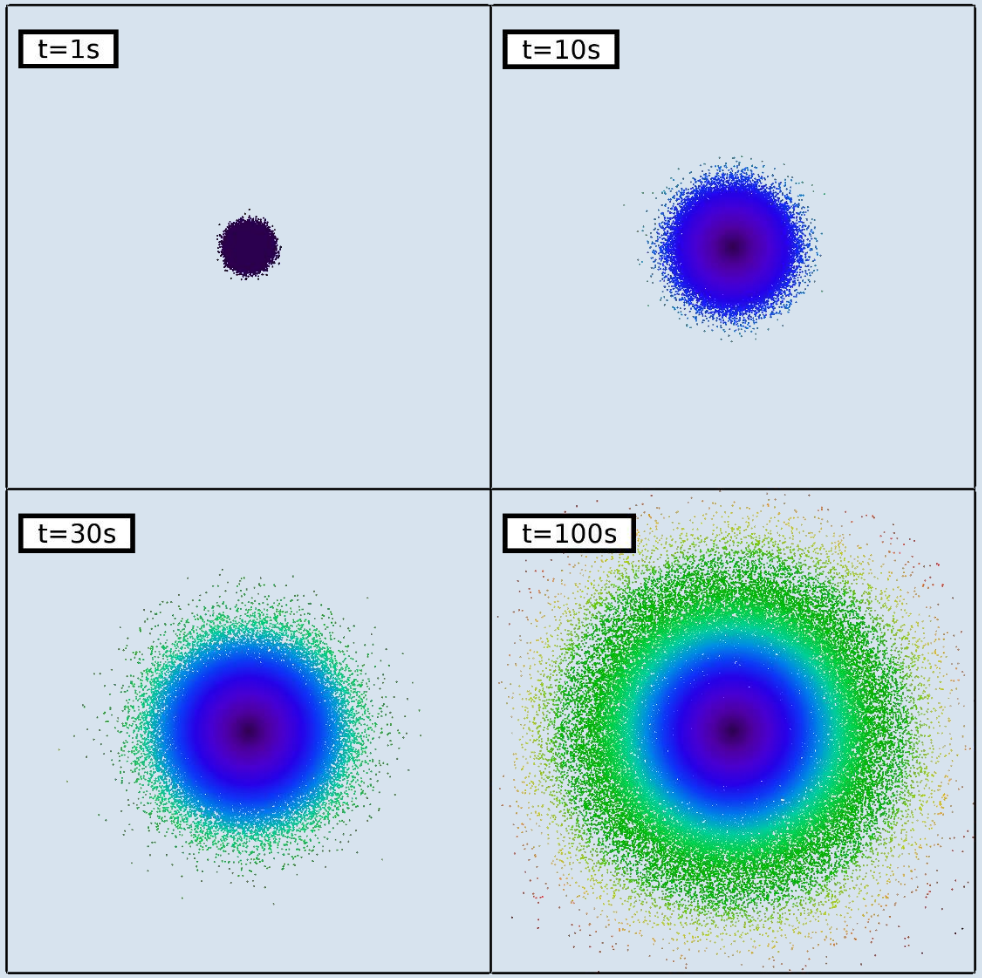


Liquid droplets are sprayed into a channel. As they accelerate due to the drag force, they also break up into a smaller droplets. The child droplets spread out due to turbulent dispersion in the channel.

COMSOL

Brownian Motion

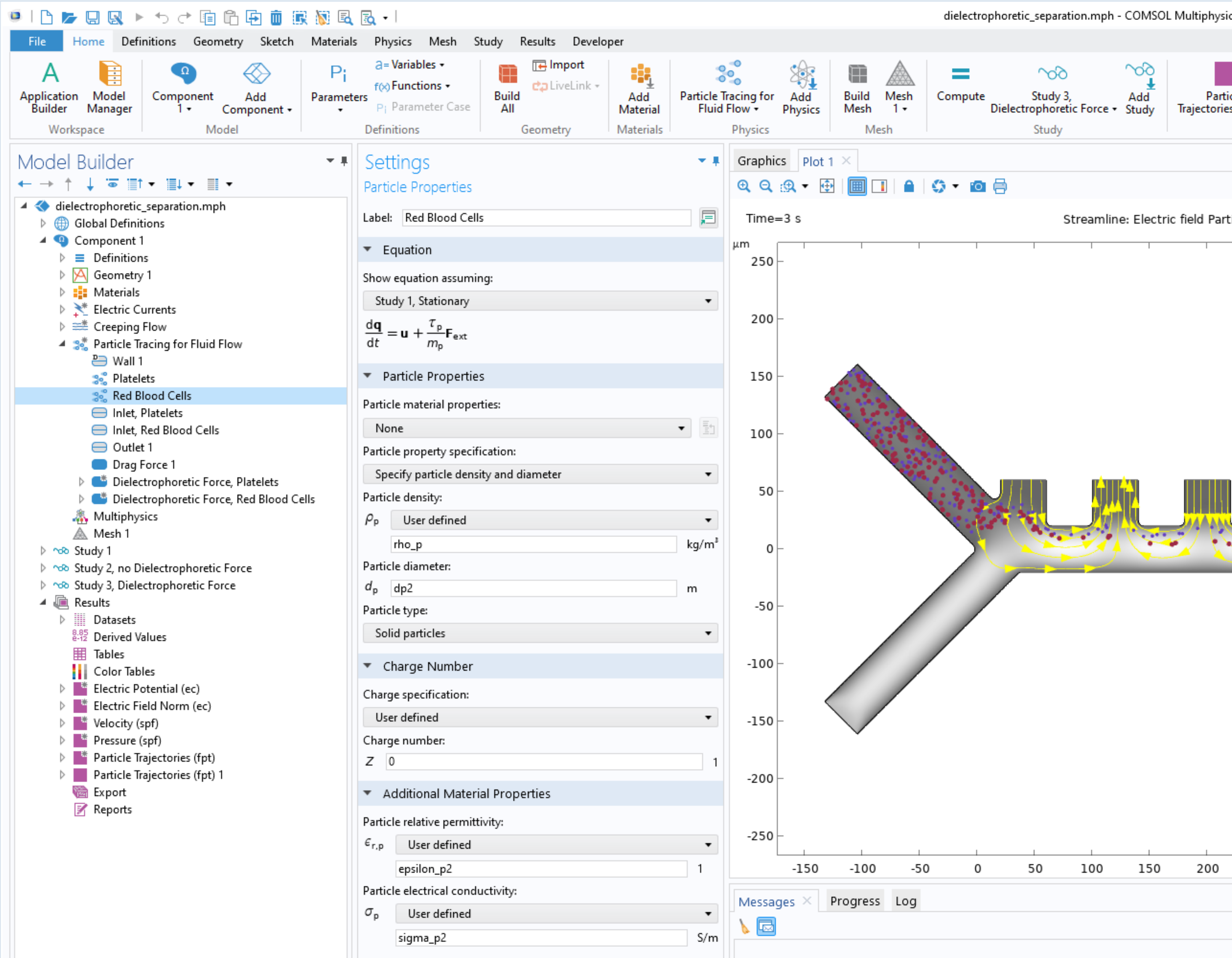
- Built-in Brownian force for Monte Carlo diffusion models
- Random contributions to particle motion at each time step taken by the solver
- The computed transmission probability agrees with the value computed by solving the diffusion equation



Diffusion of particles in a background fluid due to the Brownian force.

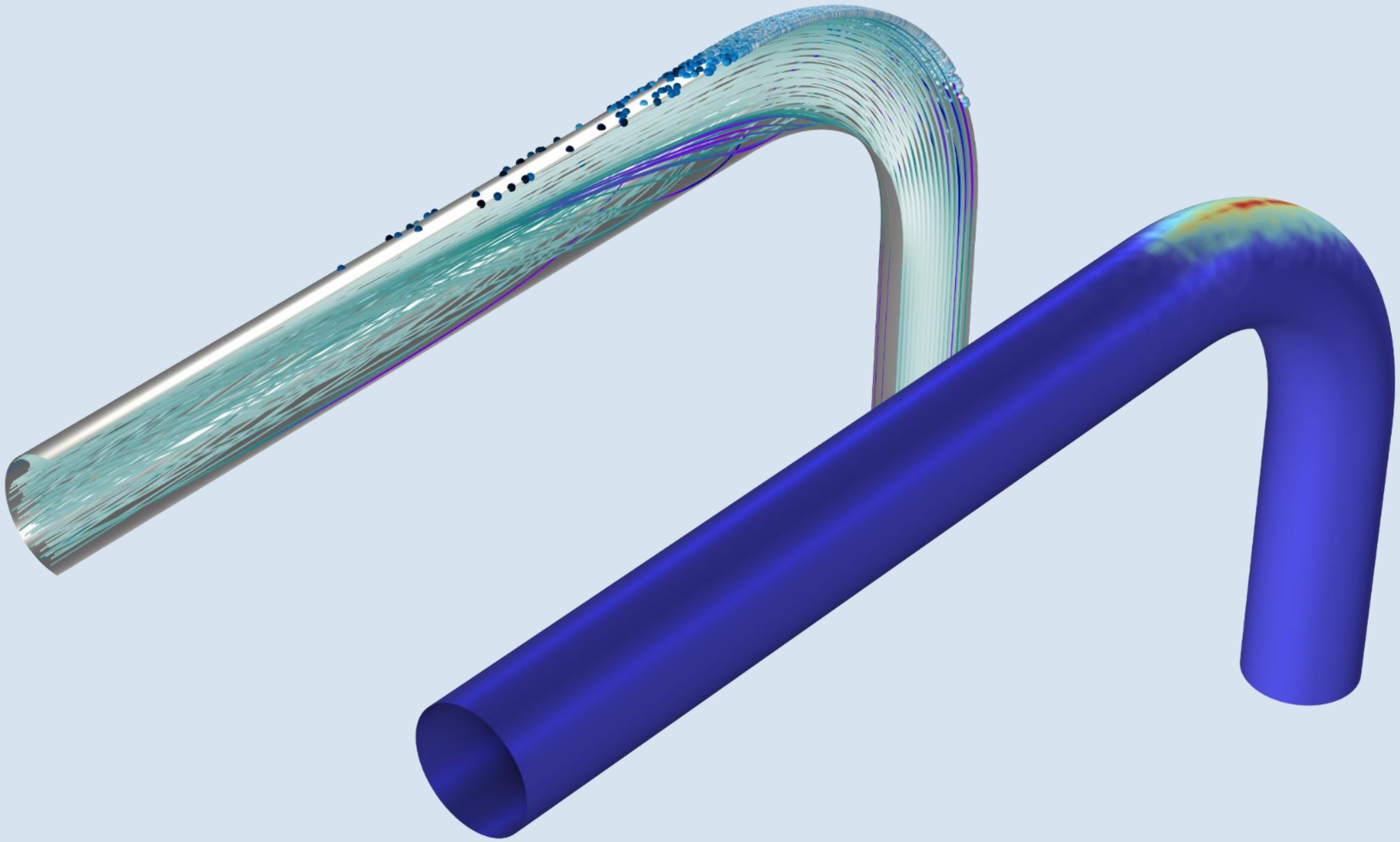
Simulate with Multiple Species

- Define several sets of particle properties
- Choose which species to release
- Apply forces to specific particle types



Erosion Modeling

- Built-in variables for rate of erosive wear at boundaries
- Variety of built-in erosion models

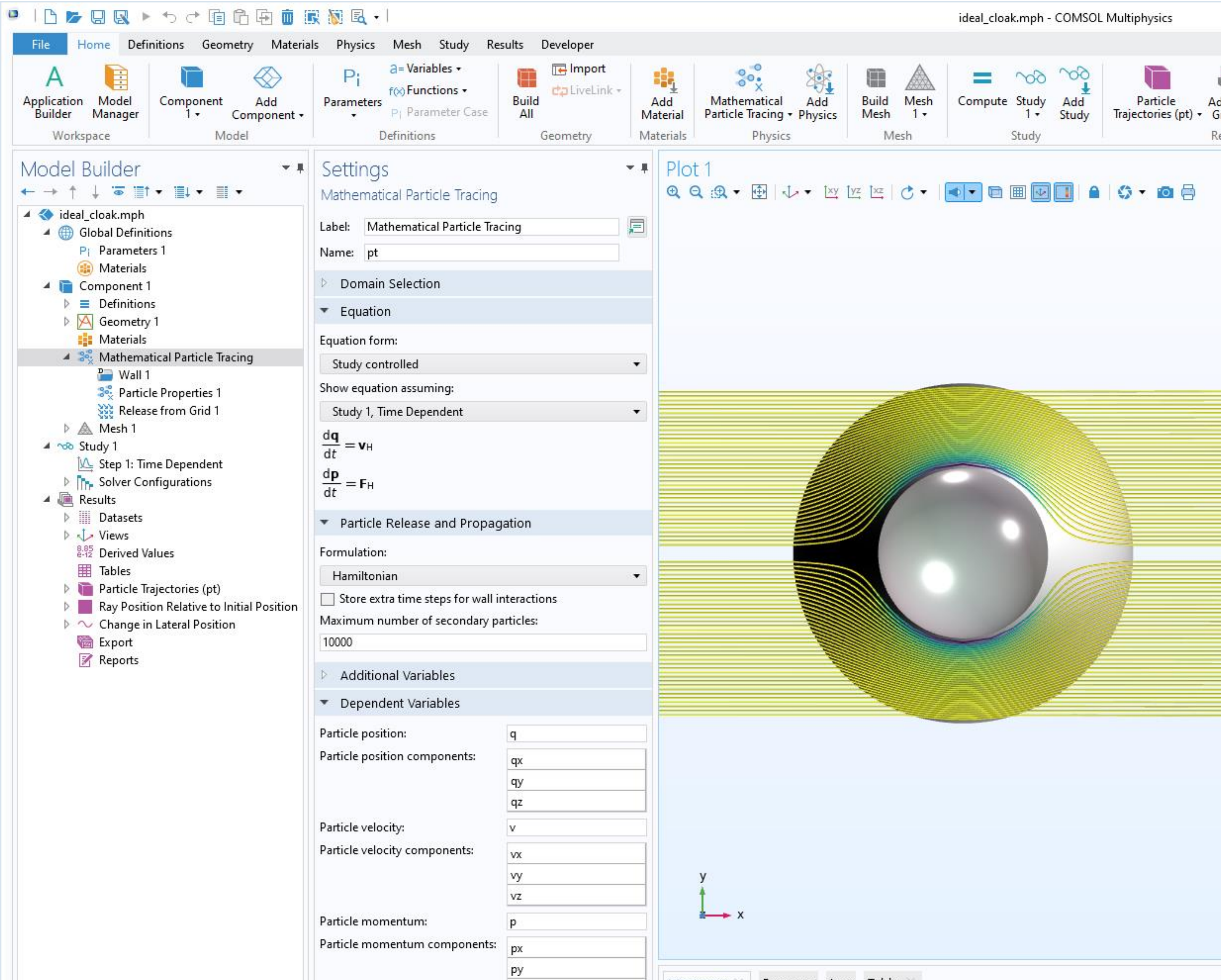


Particle trajectories in a pipe elbow (left) and rate of erosive wear on the surface (right).

COMSOL

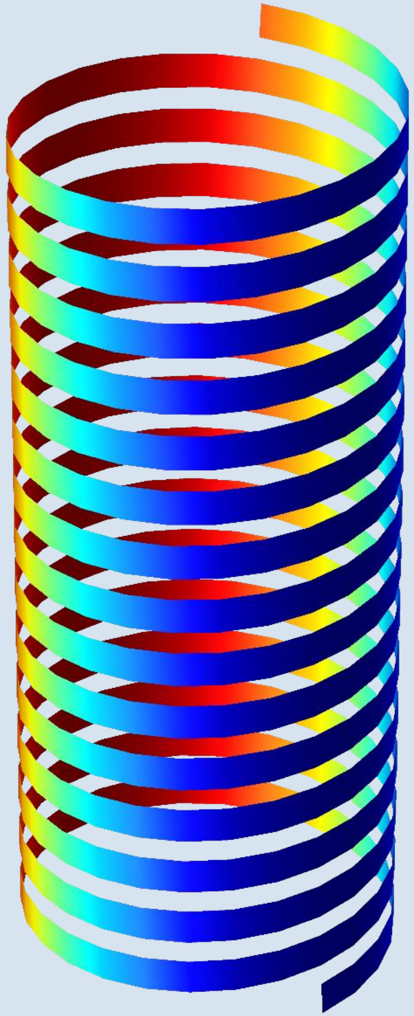
Mathematical Particle Tracing Interface

- Complete freedom over the equations solved for each particle
- Different formulations to solve the same problem
  - Lagrangian
  - Hamiltonian
  - Newtonian
  - Massless



Mathematical Particle Tracing

Formulation	Equation of motion	Charged Particle in a Magnetic field
Lagrangian	$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \mathbf{v}} = \frac{\partial L}{\partial \mathbf{q}}$	$L = \frac{m_\mathrm{p}(\mathbf{v}\cdot\mathbf{v})}{2} + eZ(\mathbf{v}\cdot\mathbf{A})$
Hamiltonian	$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}, \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}}$	$H = \frac{(\mathbf{p}-eZ\mathbf{A})^2}{2m_\mathrm{p}}$
Newtonian	$\frac{\mathrm{d}}{\mathrm{d}t}(m_\mathrm{p}\mathbf{v}) = \mathbf{F}$	$\frac{\mathrm{d}}{\mathrm{d}t}(m_\mathrm{p}\mathbf{v}) = eZ(\mathbf{v}\times\mathbf{B})$
Massless	$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{v}$	N/A



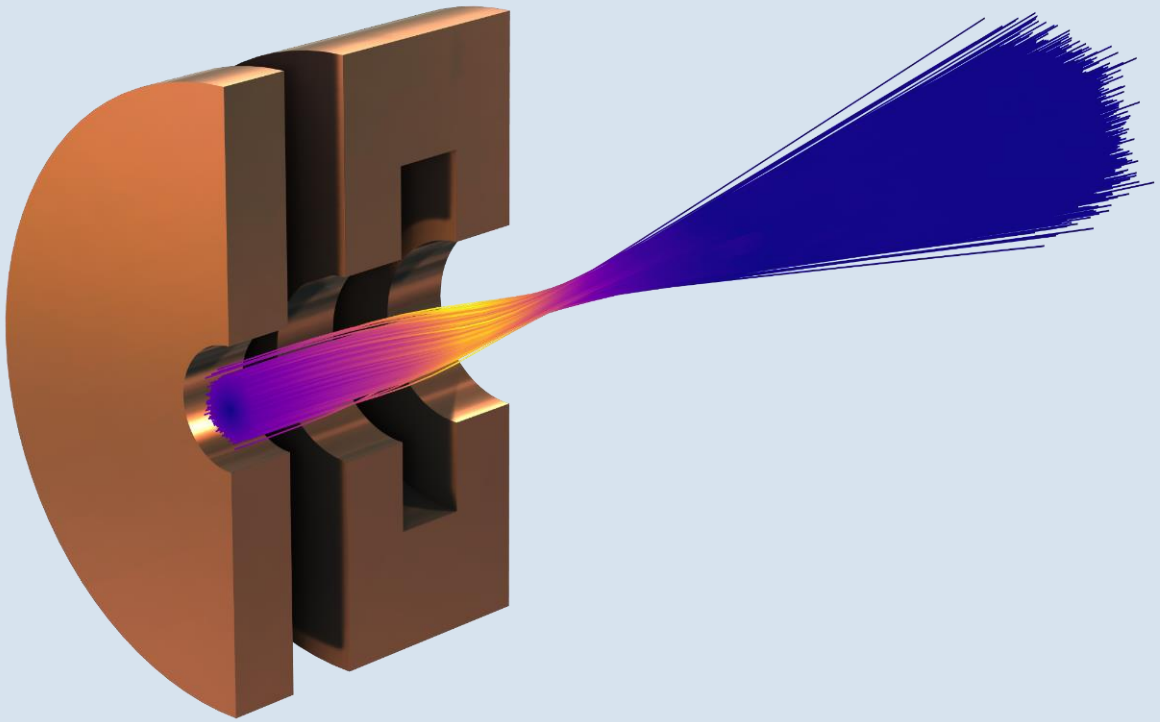
Motion of a charged particle in a uniform magnetic field.

Demonstration of the Module on User Cases

USER CASE

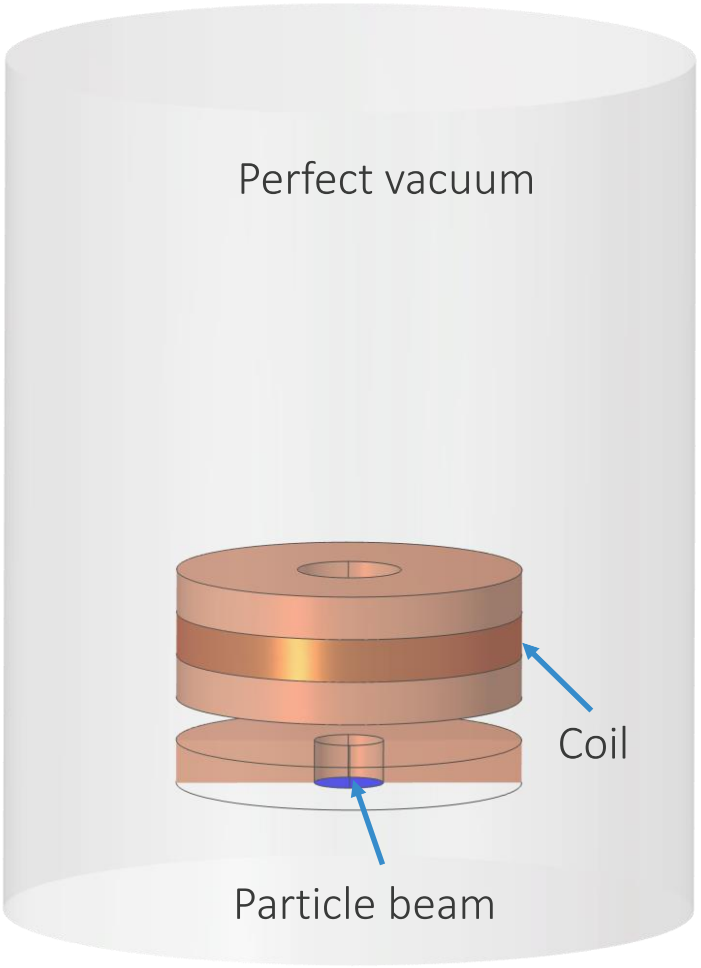
Charged Particle Tracing

Magnetic Lens



Model Setup

- Magnetic Field
- Coil
- Perfect vacuum
- Electrons
- Particle beam



Untitled.mph - COMSOL Multiphysics

File Home Definitions Geometry Materials Physics Mesh Study Results Developer

New

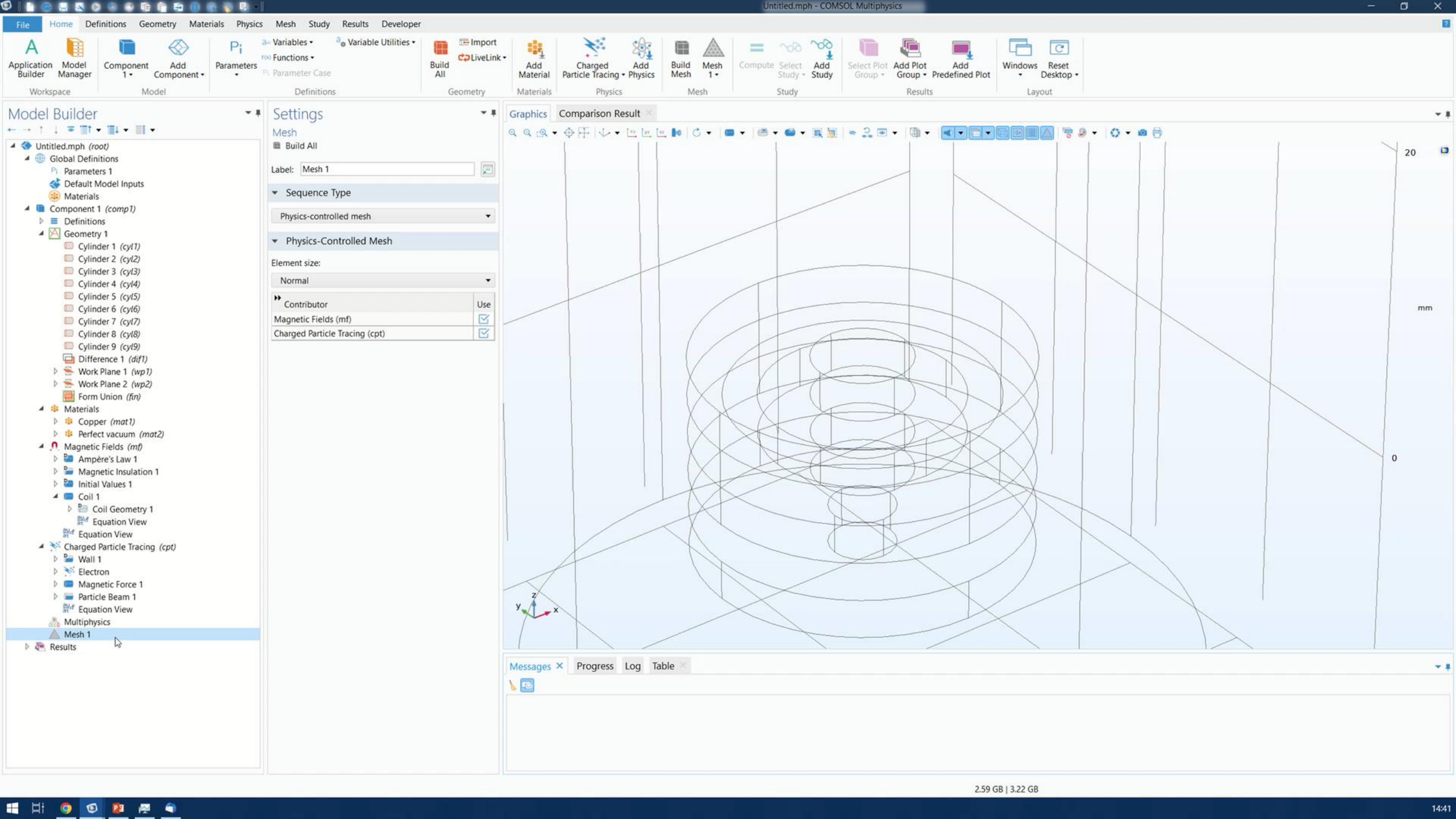
Model Wizard

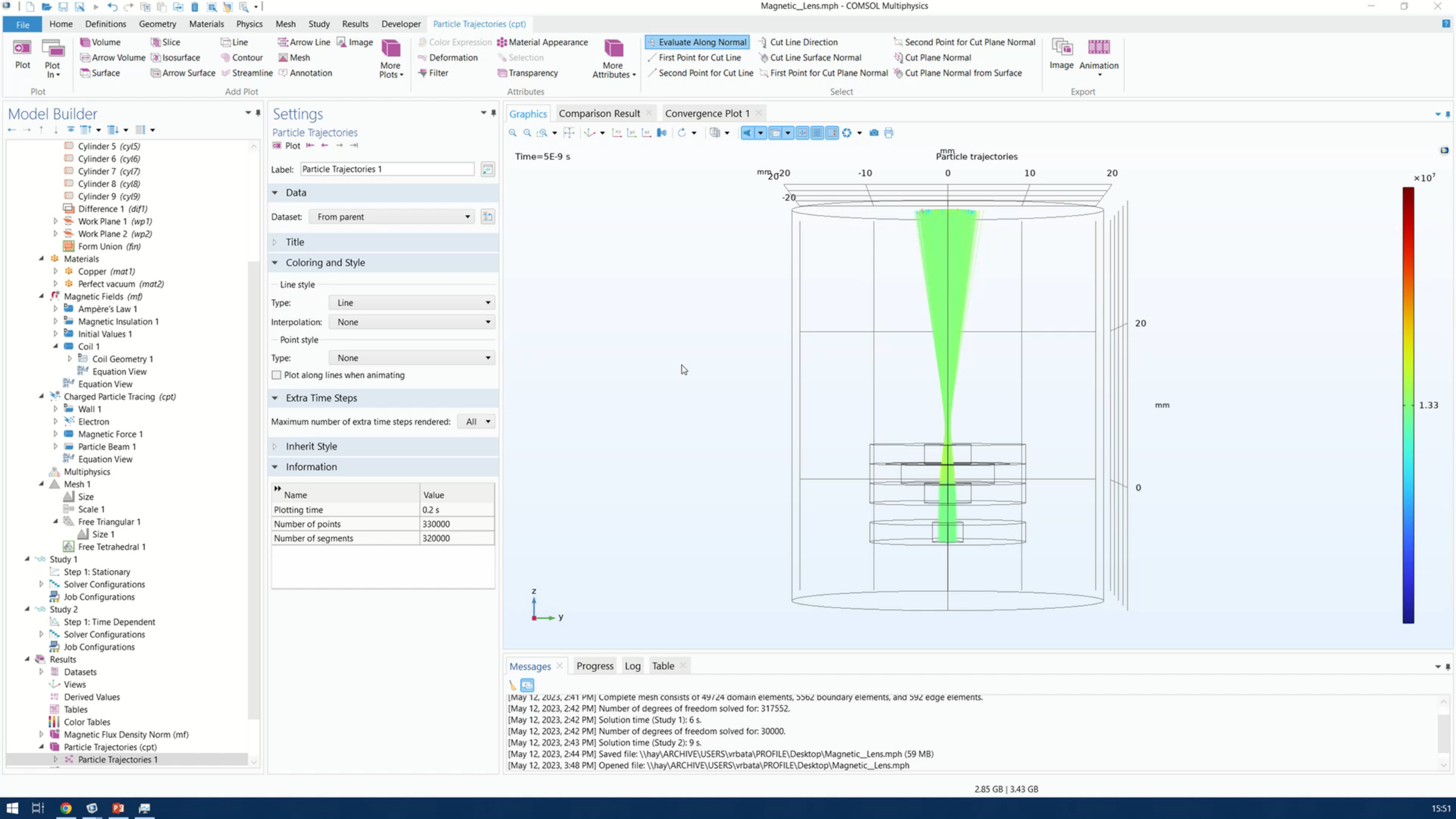
Blank Model

Help Cancel Show on startup

2.22 GB | 2.89 GB

14:03

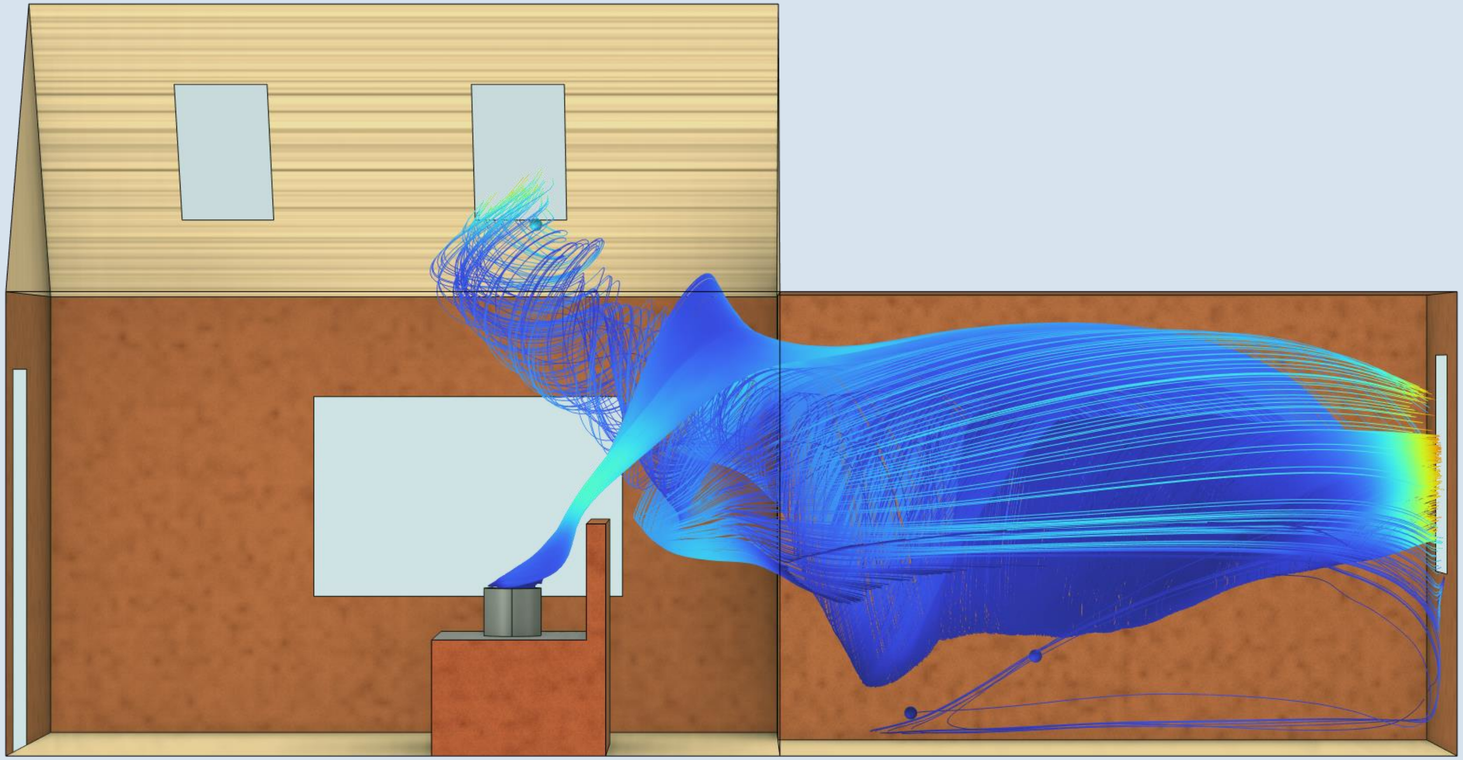

Untitled.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Model Manager
Workspace
Component 1
Add Component
Model
Parameters
Variables
Functions
Parameter Case
Variable Utilities
Definitions
Build All
Import
LiveLink
Geometry
Add Material
Materials
Charged Particle Tracing
Add Physics
Physics
Build Mesh
Mesh 1
Mesh
Compute
Select Study
Add Study
Study
Select Plot Group
Add Plot Group
Add Predefined Plot
Results
Windows
Reset Desktop
Layout
Model Builder
Untitled.mph (root)
Global Definitions
Parameters 1
Default Model Inputs
Materials
Component 1 (comp1)
Definitions
Geometry 1
Cylinder 1 (cyl1)
Cylinder 2 (cyl2)
Cylinder 3 (cyl3)
Cylinder 4 (cyl4)
Cylinder 5 (cyl5)
Cylinder 6 (cyl6)
Cylinder 7 (cyl7)
Cylinder 8 (cyl8)
Cylinder 9 (cyl9)
Difference 1 (dif1)
Work Plane 1 (wp1)
Work Plane 2 (wp2)
Form Union (fin)
Materials
Copper (mat1)
Perfect vacuum (mat2)
Magnetic Fields (mf)
Ampère's Law 1
Magnetic Insulation 1
Initial Values 1
Coil 1
Coil Geometry 1
Equation View
Equation View
Charged Particle Tracing (cpt)
Wall 1
Electron
Magnetic Force 1
Particle Beam 1
Equation View
Multiphysics
Mesh 1
Results
Settings
Mesh
Build All
Label: Mesh 1
Sequence Type
Physics-controlled mesh
Physics-Controlled Mesh
Element size:
Normal
Contributor
Use
Magnetic Fields (mf)
Charged Particle Tracing (cpt)
Graphics
Comparison Result
20
mm
0
z
y
x
Messages
Progress
Log
Table
2.59 GB | 3.22 GB
14:41


Magnetic__Lens.mph - COMSOL Multiphysics
File Home Definitions Geometry Materials Physics Mesh Study Results Developer Particle Trajectories (cpt)
Plot
Plot In
Volume
Arrow Volume
Surface
Slice
Isosurface
Arrow Surface
Line
Contour
Streamline
Arrow Line
Mesh
Annotation
Image
More Plots
Add Plot
Color Expression
Deformation
Filter
Material Appearance
Selection
Transparency
More Attributes
Attributes
Evaluate Along Normal
First Point for Cut Line
Second Point for Cut Line
Cut Line Direction
Cut Line Surface Normal
First Point for Cut Plane Normal
Second Point for Cut Plane Normal
Cut Plane Normal
Cut Plane Normal from Surface
Select
Image
Animation
Export
Model Builder
Cylinder 5 (cyl5)
Cylinder 6 (cyl6)
Cylinder 7 (cyl7)
Cylinder 8 (cyl8)
Cylinder 9 (cyl9)
Difference 1 (dif1)
Work Plane 1 (wp1)
Work Plane 2 (wp2)
Form Union (fin)
Materials
Copper (mat1)
Perfect vacuum (mat2)
Magnetic Fields (mf)
Ampère's Law 1
Magnetic Insulation 1
Initial Values 1
Coil 1
Coil Geometry 1
Equation View
Equation View
Charged Particle Tracing (cpt)
Wall 1
Electron
Magnetic Force 1
Particle Beam 1
Equation View
Multiphysics
Mesh 1
Size
Scale 1
Free Triangular 1
Size 1
Free Tetrahedral 1
Study 1
Step 1: Stationary
Solver Configurations
Job Configurations
Study 2
Step 1: Time Dependent
Solver Configurations
Job Configurations
Results
Datasets
Views
Derived Values
Tables
Color Tables
Magnetic Flux Density Norm (mf)
Particle Trajectories (cpt)
Particle Trajectories 1
Settings
Particle Trajectories
Plot
Label: Particle Trajectories 1
Data
Dataset: From parent
Title
Coloring and Style
Line style
Type: Line
Interpolation: None
Point style
Type: None
Plot along lines when animating
Extra Time Steps
Maximum number of extra time steps rendered: All
Inherit Style
Information
Name | Value
Plotting time | 0.2 s
Number of points | 330000
Number of segments | 320000
Graphics
Comparison Result
Convergence Plot 1
Time=5E-9 s
Particle trajectories
mm
-20 -10 0 10 20
20
0
mm
×10^7
1.33
z
y
Messages
Progress
Log
Table
[May 12, 2023, 2:41 PM] Complete mesh consists of 49724 domain elements, 5562 boundary elements, and 592 edge elements.
[May 12, 2023, 2:42 PM] Number of degrees of freedom solved for: 317552.
[May 12, 2023, 2:42 PM] Solution time (Study 1): 6 s.
[May 12, 2023, 2:42 PM] Number of degrees of freedom solved for: 30000.
[May 12, 2023, 2:43 PM] Solution time (Study 2): 9 s.
[May 12, 2023, 2:44 PM] Saved file: \\hay\ARCHIVE\USERS\vrbata\PROFILE\Desktop\Magnetic__Lens.mph (59 MB)
[May 12, 2023, 3:48 PM] Opened file: \\hay\ARCHIVE\USERS\vrbata\PROFILE\Desktop\Magnetic__Lens.mph
2.85 GB | 3.43 GB
15:51

USER CASE

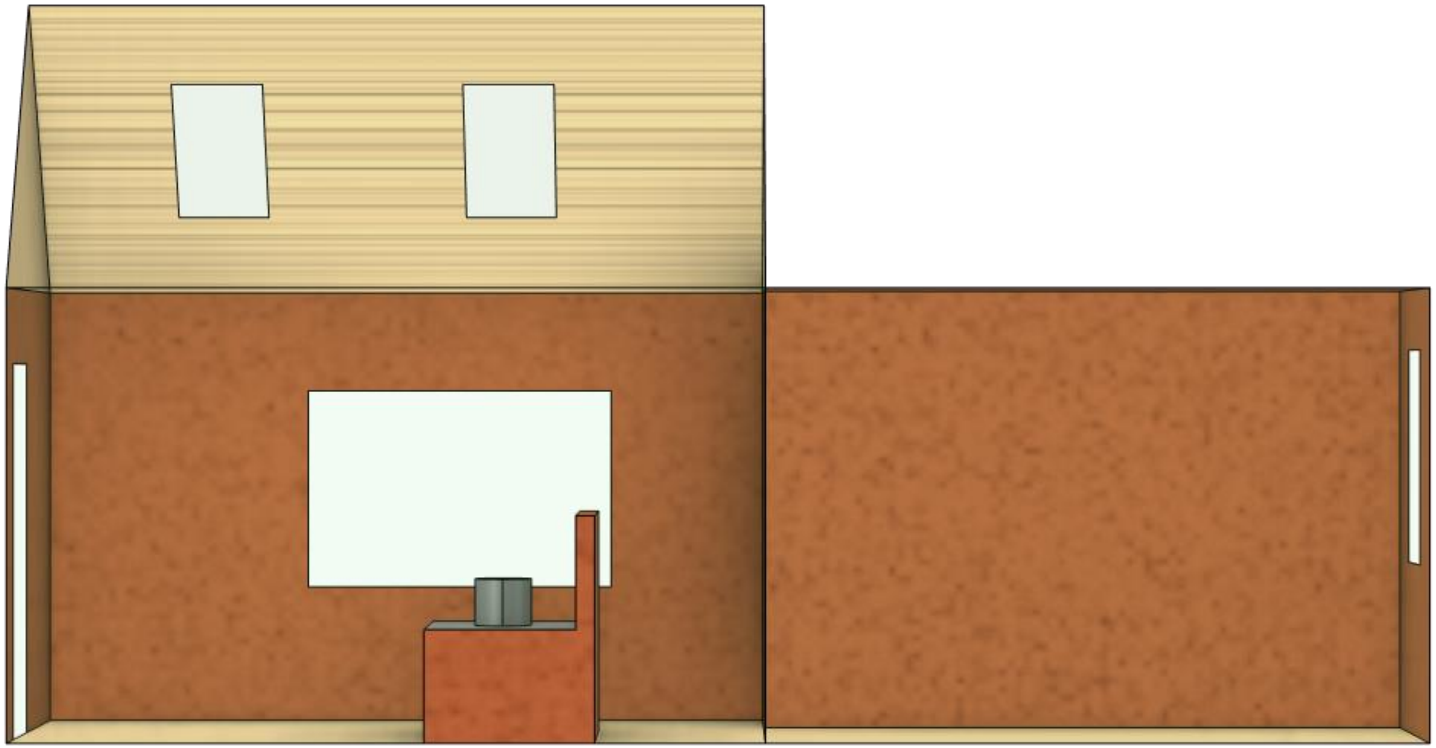
Particle Tracing For Fluid Flow

Ventilation Of The House



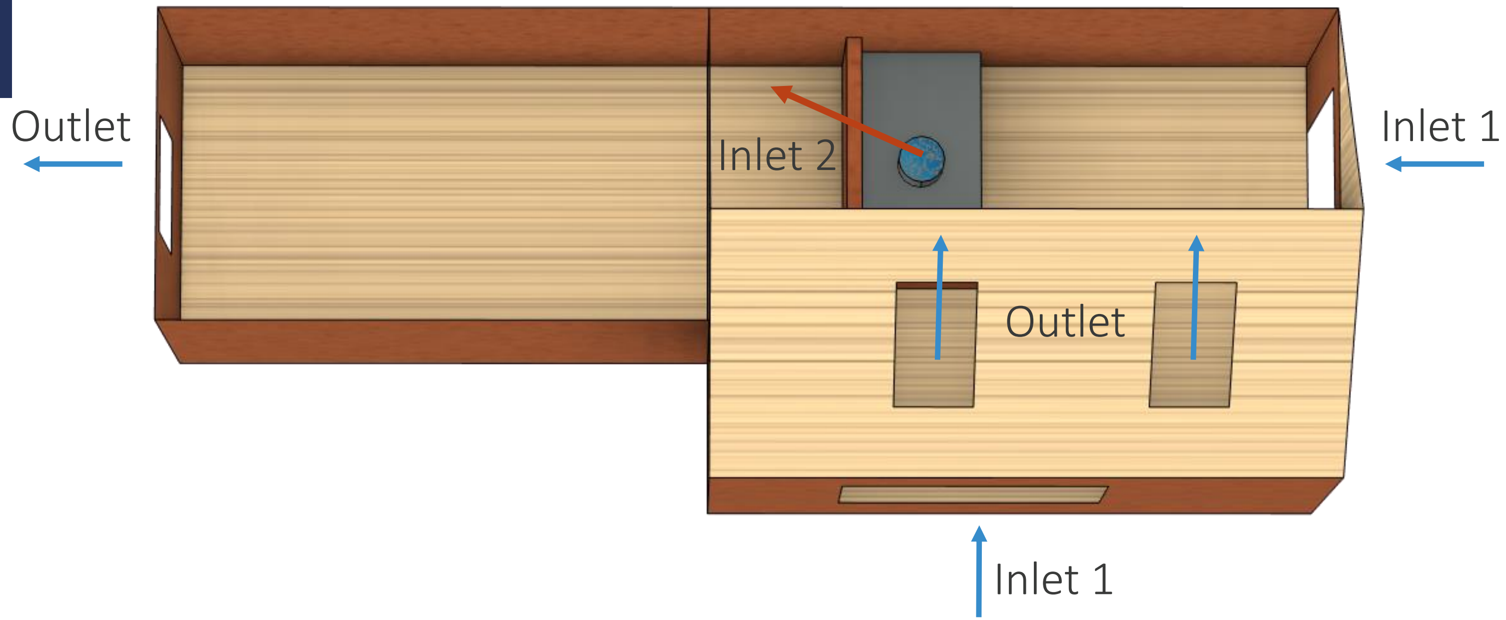
Model Description

- Family house
- Stinking pot
- Open windows and doors
- Air



Model Setup

- Turbulent flow
- Inlet 1 (fresh air): 0.1 m/s
- Inlet 2 (pot): 0.01 m/s
- Pressure outlet
- Massless particles



Untitled.mph - COMSOL Multiphysics

File Home Definitions Geometry Materials Physics Mesh Study Results Developer

New

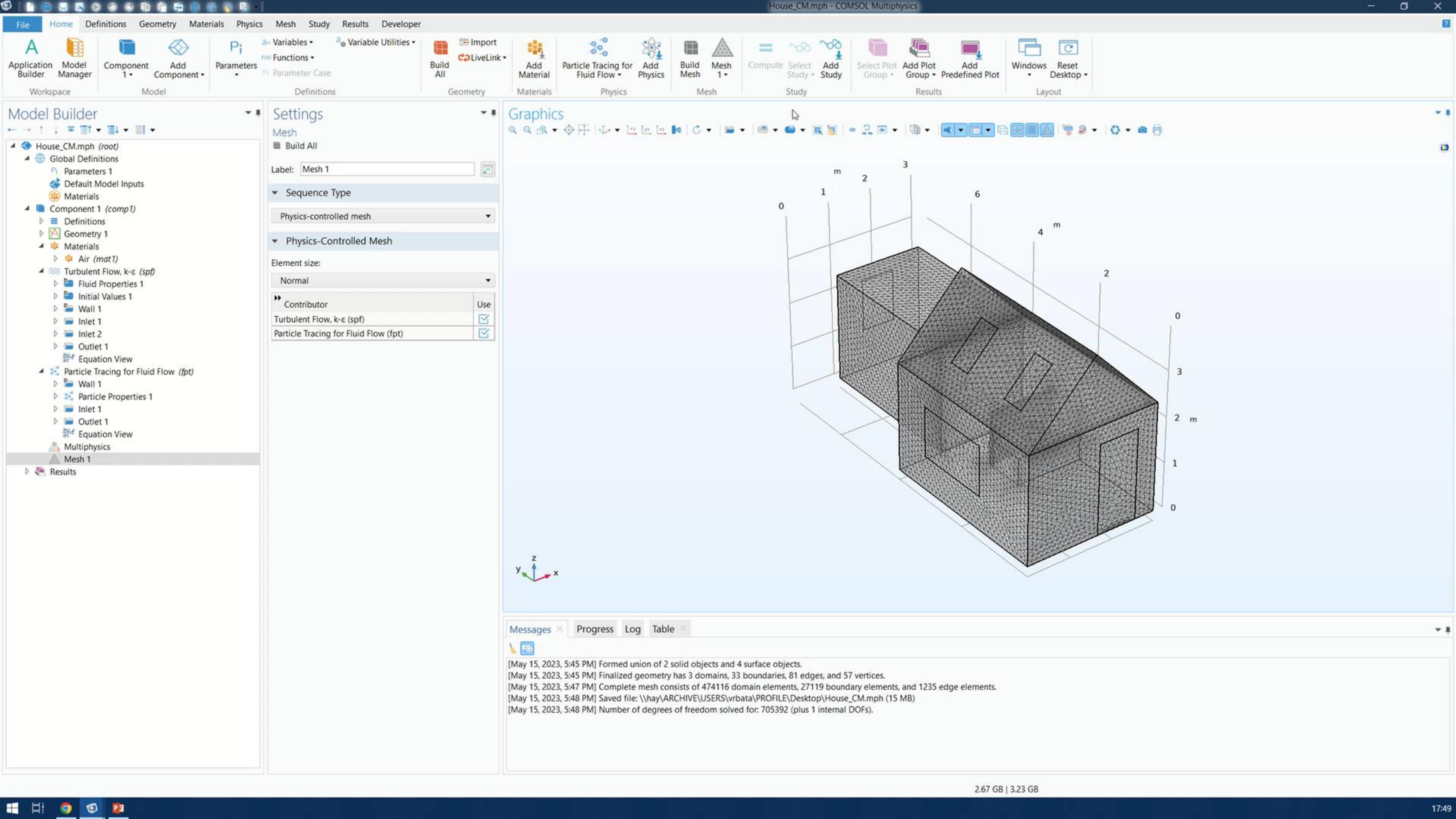
Model Wizard

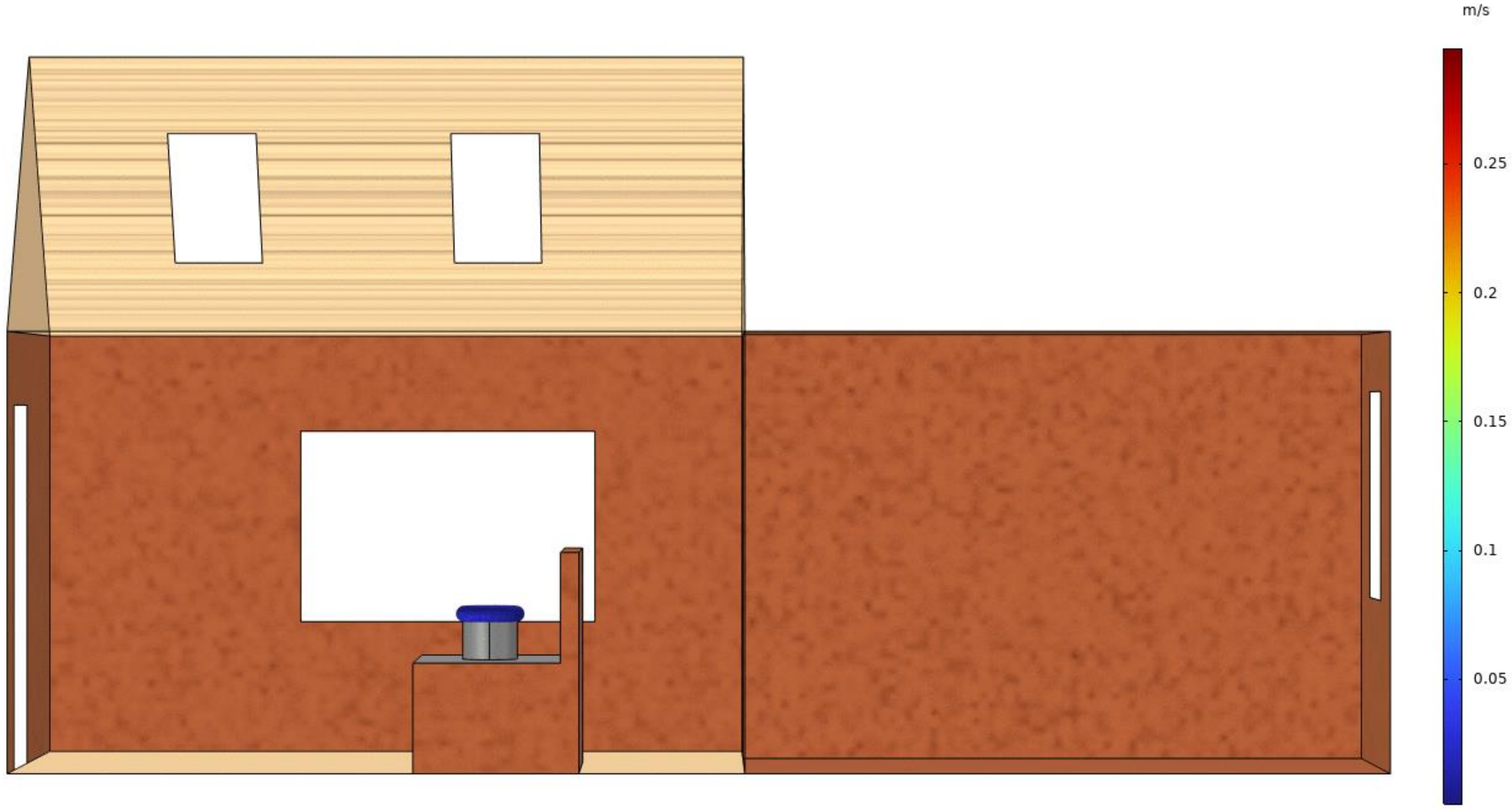
Blank Model

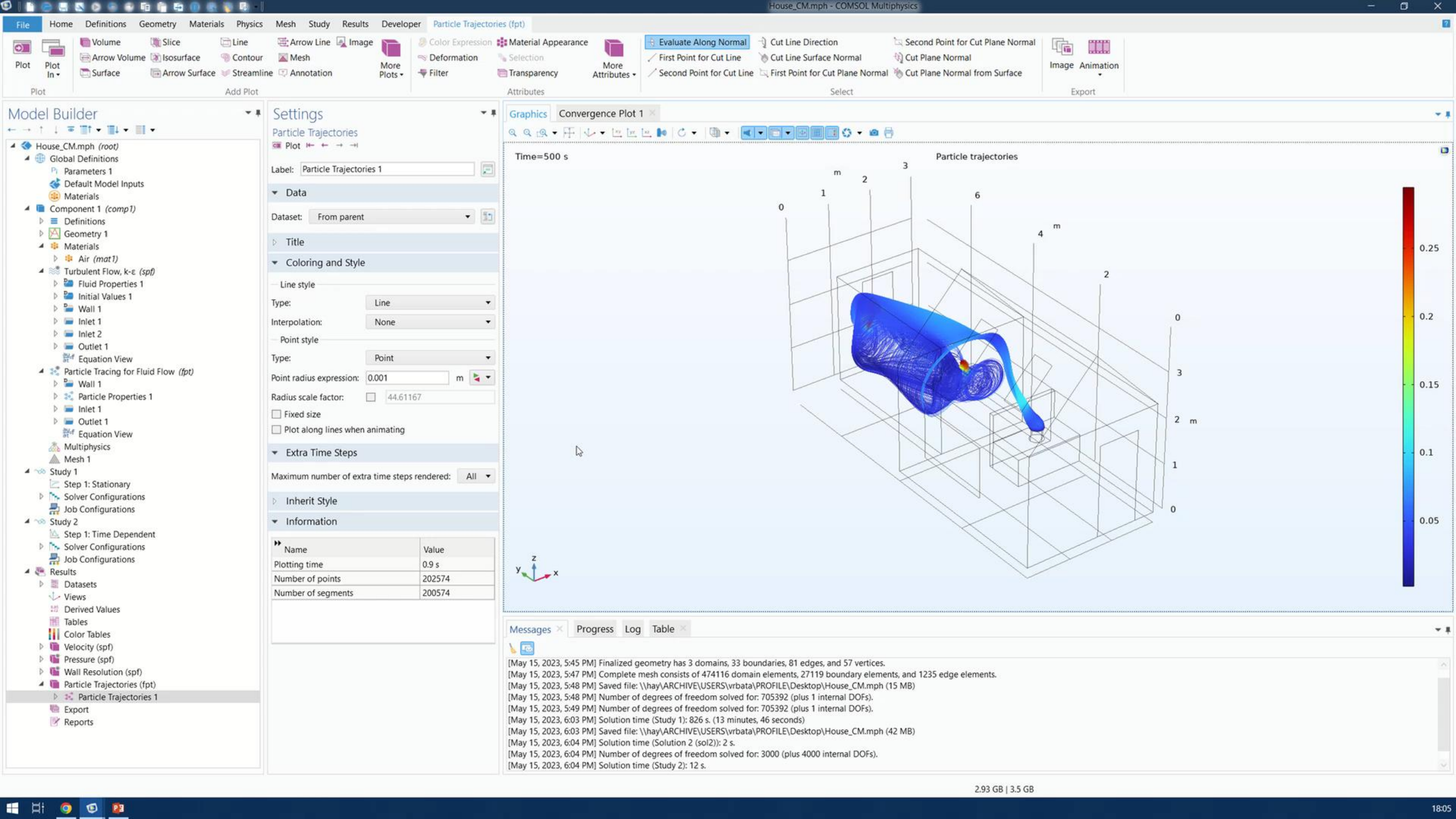
Help Cancel Show on startup

2.58 GB | 3.18 GB

17:44


House_CM.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Model Manager
Workspace
Component 1
Add Component
Model
Parameters
Variables
Functions
Parameter Case
Variable Utilities
Definitions
Build All
Import
LiveLink
Geometry
Add Material
Materials
Particle Tracing for Fluid Flow
Add Physics
Physics
Build Mesh
Mesh 1
Mesh
Compute
Select Study
Add Study
Study
Select Plot Group
Add Plot Group
Add Predefined Plot
Results
Windows
Reset Desktop
Layout
Model Builder
House_CM.mph (root)
Global Definitions
Parameters 1
Default Model Inputs
Materials
Component 1 (comp1)
Definitions
Geometry 1
Materials
Air (mat1)
Turbulent Flow, k-ε (spf)
Fluid Properties 1
Initial Values 1
Wall 1
Inlet 1
Inlet 2
Outlet 1
Equation View
Particle Tracing for Fluid Flow (fpt)
Wall 1
Particle Properties 1
Inlet 1
Outlet 1
Equation View
Multiphysics
Mesh 1
Results
Settings
Mesh
Build All
Label: Mesh 1
Sequence Type
Physics-controlled mesh
Physics-Controlled Mesh
Element size:
Normal
Contributor
Use
Turbulent Flow, k-ε (spf)
Particle Tracing for Fluid Flow (fpt)
Graphics
Messages
Progress
Log
Table
[May 15, 2023, 5:45 PM] Formed union of 2 solid objects and 4 surface objects.
[May 15, 2023, 5:45 PM] Finalized geometry has 3 domains, 33 boundaries, 81 edges, and 57 vertices.
[May 15, 2023, 5:47 PM] Complete mesh consists of 474116 domain elements, 27119 boundary elements, and 1235 edge elements.
[May 15, 2023, 5:48 PM] Saved file: \\hay\ARCHIVE\USERS\vrbata\PROFILE\Desktop\House_CM.mph (15 MB)
[May 15, 2023, 5:48 PM] Number of degrees of freedom solved for: 705392 (plus 1 internal DOFs).
2.67 GB | 3.23 GB
17:49

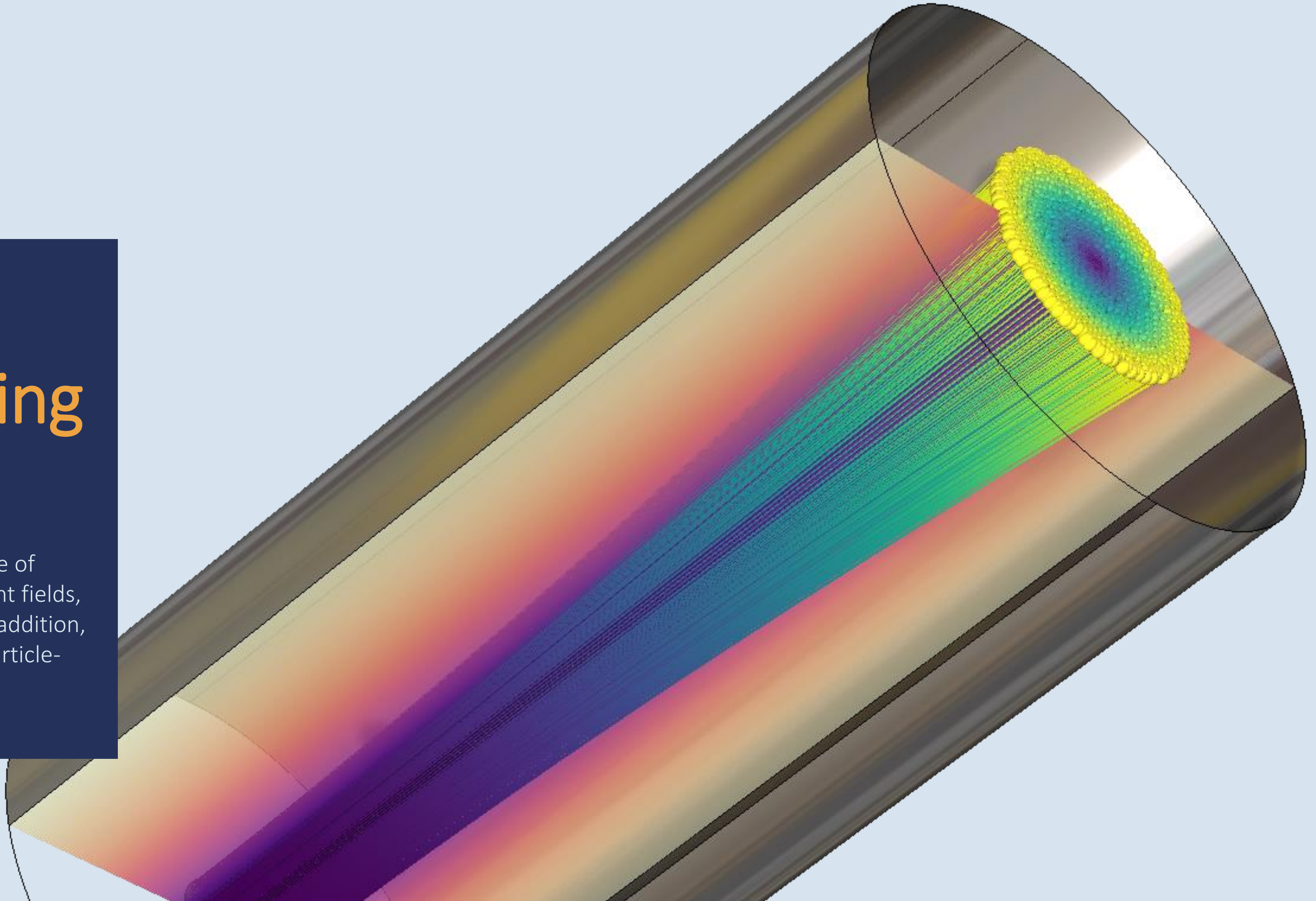

m/s
0.25
0.2
0.15
0.1
0.05


House_CM.mph - COMSOL Multiphysics
File Home Definitions Geometry Materials Physics Mesh Study Results Developer Particle Trajectories (fpt)
Plot
Plot In
Volume
Arrow Volume
Surface
Slice
Isosurface
Arrow Surface
Line
Contour
Streamline
Arrow Line
Mesh
Annotation
Image
More Plots
Add Plot
Color Expression
Deformation
Filter
Material Appearance
Selection
Transparency
More Attributes
Attributes
Evaluate Along Normal
First Point for Cut Line
Second Point for Cut Line
Cut Line Direction
Cut Line Surface Normal
First Point for Cut Plane Normal
Second Point for Cut Plane Normal
Cut Plane Normal
Cut Plane Normal from Surface
Select
Image
Animation
Export
Model Builder
House_CM.mph (root)
Global Definitions
Parameters 1
Default Model Inputs
Materials
Component 1 (comp1)
Definitions
Geometry 1
Materials
Air (mat1)
Turbulent Flow, k-ε (spf)
Fluid Properties 1
Initial Values 1
Wall 1
Inlet 1
Inlet 2
Outlet 1
Equation View
Particle Tracing for Fluid Flow (fpt)
Wall 1
Particle Properties 1
Inlet 1
Outlet 1
Equation View
Multiphysics
Mesh 1
Study 1
Step 1: Stationary
Solver Configurations
Job Configurations
Study 2
Step 1: Time Dependent
Solver Configurations
Job Configurations
Results
Datasets
Views
Derived Values
Tables
Color Tables
Velocity (spf)
Pressure (spf)
Wall Resolution (spf)
Particle Trajectories (fpt)
Particle Trajectories 1
Export
Reports
Settings
Particle Trajectories
Plot
Label: Particle Trajectories 1
Data
Dataset: From parent
Title
Coloring and Style
Line style
Type: Line
Interpolation: None
Point style
Type: Point
Point radius expression: 0.001 m
Radius scale factor: 44.61167
Fixed size
Plot along lines when animating
Extra Time Steps
Maximum number of extra time steps rendered: All
Inherit Style
Information
Name | Value
Plotting time | 0.9 s
Number of points | 202574
Number of segments | 200574
Graphics
Convergence Plot 1
Time=500 s
Particle trajectories
0.25
0.2
0.15
0.1
0.05
Messages Progress Log Table
[May 15, 2023, 5:45 PM] Finalized geometry has 3 domains, 33 boundaries, 81 edges, and 57 vertices.
[May 15, 2023, 5:47 PM] Complete mesh consists of 474116 domain elements, 27119 boundary elements, and 1235 edge elements.
[May 15, 2023, 5:48 PM] Saved file: \\hay\ARCHIVE\USERS\vrbata\PROFILE\Desktop\House_CM.mph (15 MB)
[May 15, 2023, 5:48 PM] Number of degrees of freedom solved for: 705392 (plus 1 internal DOFs).
[May 15, 2023, 5:49 PM] Number of degrees of freedom solved for: 705392 (plus 1 internal DOFs).
[May 15, 2023, 6:03 PM] Solution time (Study 1): 826 s. (13 minutes, 46 seconds)
[May 15, 2023, 6:03 PM] Saved file: \\hay\ARCHIVE\USERS\vrbata\PROFILE\Desktop\House_CM.mph (42 MB)
[May 15, 2023, 6:04 PM] Solution time (Solution 2 (sol2)): 2 s.
[May 15, 2023, 6:04 PM] Number of degrees of freedom solved for: 3000 (plus 4000 internal DOFs).
[May 15, 2023, 6:04 PM] Solution time (Study 2): 12 s.
2.93 GB | 3.5 GB
18:05

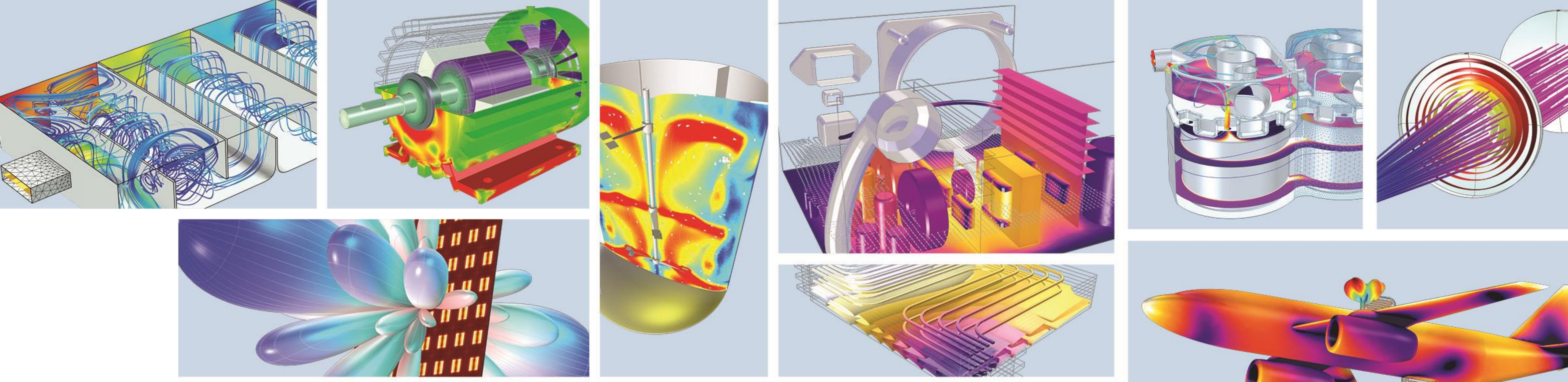
CONCLUDING REMARKS

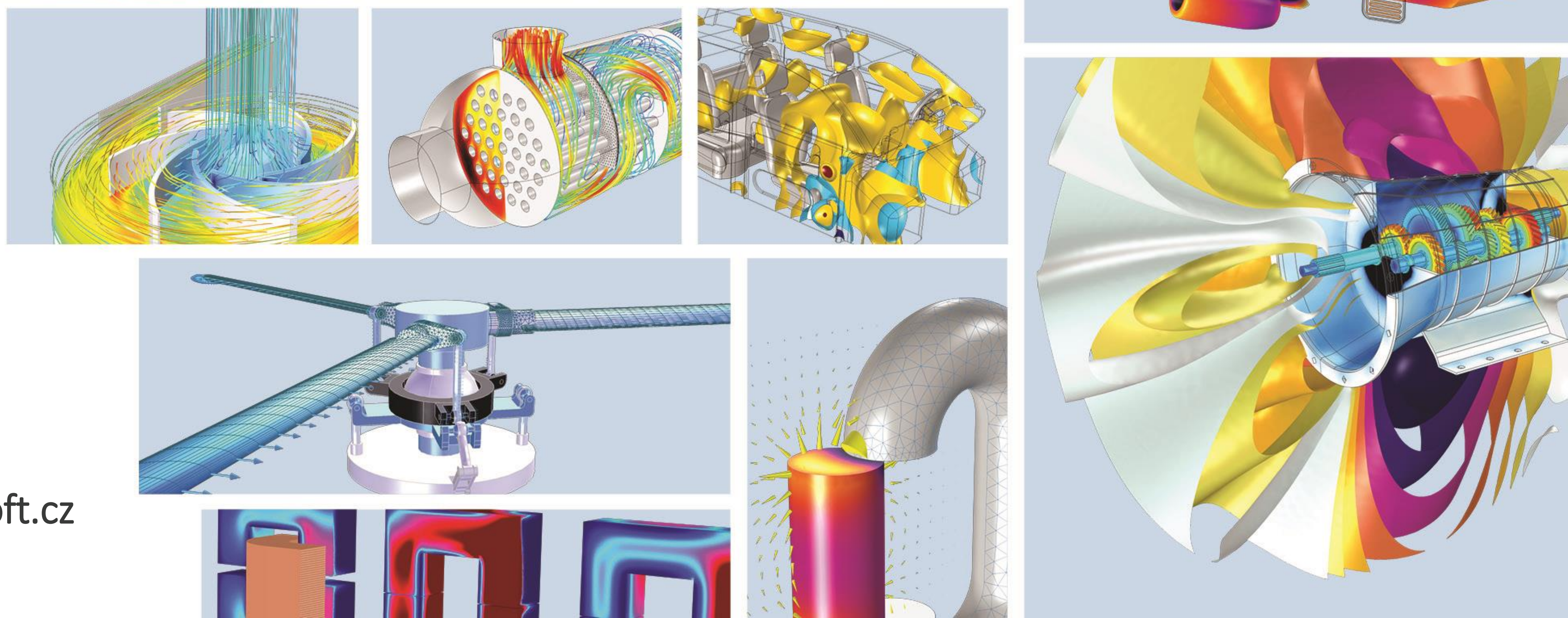
The Particle Tracing Module

The Particle Tracing Module features a wide range of functionality for computing the impact of different fields, such as electric fields, on particle trajectories. In addition, it has the unique ability to model bidirectional particle-field interactions.



Thank you for your attention





Contact Us

support@humusoft.cz