Outline

• What’s new in V5.0
• Overview of Particle Tracing Module physics interfaces
• Boundary conditions
• Release features
• Secondary particle emission
• Monte Carlo modeling
• Accumulators
• Results and visualization
• Model Library examples
Particle Tracing Module

• Add-on to COMSOL Multiphysics.

• Combines with any COMSOL Multiphysics Module.

• Includes three physics interfaces for computing particle trajectories.
Particle Tracing

- Particle tracing can be used as an alternative to the finite element method for solving real world physics problems.
- Advantages:
  - No numerical instabilities which occur in the finite element method due to high Peclet numbers.
  - Much simpler mathematics involved in formulating the problem.
  - Solves a different class of problems than continuum methods.

Ion motion in a quadrupole mass spectrometer. Ion motion is influenced by both AC and DC fields.
Key Applications

- **AC/DC**
  - Mass spectrometry
  - Beam physics and ion optics
  - Multipaction
- **Fluid Flow**
  - Fluid flow visualization
  - Sprays
  - Separation, filtration, and erosion
  - Brownian motion and particle diffusion
  - Rarefied gas dynamics
- **RF**
  - Ray tracing for smoothly graded materials (limited ray tracing)
- **Plasma**
  - Ion angular energy distribution function
  - Etching
- **Acoustics**
  - Acoustophoretic forces
- **Mathematics**
  - Classical mechanics

Ion cyclotron motion due to uniform external magnetic field computed using the Lagrangian formulation

Histogram of the ion angular energy distribution function in an inductively coupled plasma. The x-axis is the angle of incidence of the ions striking the wafer (deg), the y-axis is the energy (eV). The height is the relative count.
New in V5.0

• Accumulators
  – Communicate information from particles to the underlying mesh.
  – Enhances multiphysics capability.
New in V5.0

• Improvements to secondary particle emission
  – Domain-based release.
  – Multiple species.
New in V5.0

• New options for built-in forces
  – High Knudsen number corrections.
  – New drag laws.
Physics Interfaces

• Mathematical Particle Tracing
  – Specify the equations of motion using Massless, Newtonian, Lagrangian or Hamiltonian formulations.
  – Complete freedom over the equations solved allows, for example, ray tracing to be modeled.

• Charged Particle Tracing
  – Model ion and electron trajectories in electric and magnetic fields.
  – Easy to define electric, magnetic and collisional forces.
  – Allows one-way or two-way coupling to electric fields.

• Particle Tracing for Fluid Flow
  – Model microscopic and macroscopic particles in a fluid.
  – Includes drag, gravitational, dielectrophoretic, acoustophoretic and many other forces.
  – Can model fluid-particle interactions.
Charged Particle Tracing

• Use this to model ion and electron trajectories in electric and magnetic fields.
• Predefined forces.
• Monte Carlo modeling of interaction with background gases
• Typically the fields are pre-computed from one of the AC/DC interfaces.
• Coulomb force for particle-particle interactions.

Multipaction due to secondary electron emission in an RF device operating at a very specific frequency
Particle Tracing for Fluid Flow

- Use this to model motion of microscopic particles in a fluid.
- Predefined forces.
- Sticking probabilities and secondary particle emission.
- Typically the velocity field is pre-computed using one of the interfaces in the CFD or Microfluidics modules.
- Particle-particle interactions.

Particle trajectories in a laminar static mixer visualized using a comet tail plot.
Mathematical Particle Tracing

- Complete freedom over the equations solved for each particle.
- Analogous to the PDE modes offered in COMSOL Multiphysics.
- Many different ways of solving the same problem, for example:

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Equation of motion</th>
<th>Charged Particle in a Magnetic Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lagrangian</td>
<td>( \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} )</td>
<td>( L = \frac{m(v \cdot v)}{2} + q(v \cdot A) )</td>
</tr>
<tr>
<td>Hamiltonian</td>
<td>( \frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} ), ( \frac{d\mathbf{p}}{dt} = \frac{\partial H}{\partial \mathbf{x}} )</td>
<td>( H = \frac{(\mathbf{P} - q\mathbf{A})^2}{2m} )</td>
</tr>
<tr>
<td>Newtonian</td>
<td>( \frac{d}{dt} (m\mathbf{v}) = \mathbf{F} )</td>
<td>( \frac{d}{dt} (m\mathbf{v}) = q(\mathbf{v} \times \mathbf{B}) )</td>
</tr>
<tr>
<td>Massless</td>
<td>( \frac{dq}{dt} = \mathbf{v} )</td>
<td>N/A</td>
</tr>
</tbody>
</table>
Boundary Conditions

• Freeze, Stick, Disappear – Stops a particle at the boundary.
  — Freeze: Retains information about the velocity.
  — Stick: Sets the velocity to zero.
  — Disappear: Completely removes the particle.

• Pass through – Ignores the boundary.

• General reflection – Particles are reflected in a user-defined direction.
Boundary Conditions, Continued

- Bounce – Specular reflection at surfaces.

- Diffuse scattering – Reflect particles in a random direction based on Knudsen’s cosine law.

- Mixed diffuse and specular reflection – Assign a probability of specular reflection.
Conditional Particle-Wall Interactions

- Sticking probabilities and expressions:
  - Particles making contact with the wall are subjected to one of two wall conditions according to an arbitrary expression, or a probability (between 0 and 1).
- It is also possible to change the value of an auxiliary dependent variable when the particle crosses or touches a boundary.

Animation: Particles freeze on all walls with a probability of 0.5, otherwise they bounce.
Releasing Particles from Domains

- Release node: release particles using the mesh. Particle positions can be weighted using a density function.

Mesh-based, refinement factor = 1.

Mesh-based, refinement factor = 2.

Density proportional to $1/r$
Releasing Particles from a Grid

- Release from Grid node: Specify initial coordinates. The particles are then released at a grid of points.
Releasing Particles from Boundaries

- Inlet node: release particles from a boundary. The release can be mesh-based, weighted by a density function, or at a uniform grid of points.
Initializing particle velocity

- **Expression** – User-defined expressions for the initial velocity components.
  - At inlets, the initial velocity can be specified using tangential and normal components.
- **Constant speed**: spherical, hemispherical, or cone – Releases a group of particles uniformly throughout a sphere, hemisphere, or cone in velocity space.
- **Maxwellian** – Particle velocity components are sampled from a Maxwellian distribution at a user-defined temperature.
- **Using kinetic energy and direction.**

The Constant speed, cone setting can be used to model sprays in devices such as CVD chambers.
Particle Velocity Reinitialization

- Velocity Reinitialization: Resets the velocity to some expression when a condition is met.
- Elastic Collision Force, Monte Carlo: Particles are randomly scattered by a background gas.
- Auxiliary dependent variables can be reset.

Electrodynamic ion funnel: particles are accelerated by AC and DC fields and collide with a buffer gas, causing them to be focused into a small area.
Additional Particle Properties

- Using the Override Properties node, it is possible to release multiple species of particle in a single model.
- When releasing particles, you can decide what species the released particles should be.

Dielectrophoretic separation: red blood cells are separated from platelets using dielectrophoresis.
Secondary Particle Emission

- Secondary particles can be created when a particle hits a boundary or when a certain condition is met.
- Secondary emission is available as a subnode to many features.

Multipaction due to secondary electron emission in an RF device operating at a very specific frequency.
Secondary Emission at Boundaries

- Secondary Emission subnodes can be added to Wall and Outlet features.
- Secondary particles are released when particles hit the boundaries.
- Multiple species of secondary particle can be released at once.
- Secondary emission can be based on a probability or a logical expression.

Exponential electron growth due to secondary emission in a photomultiplier
Secondary Emission from Domains

- Velocity Reinitialization: Can release secondary particles whenever the velocity is reinitialized.
- Secondary particles can be offset from the primary particle location.
- Multiple species can be released.
Accumulators

• Accumulators can be used to communicate information from the particle position to dependent variables defined on the underlying mesh.
  – Domain-level Accumulators
  – Boundary-level Accumulators
  – Nonlocal Accumulators
Accumulator (Domain)

- Change the values of domain variables using each particle’s current position or the time history of particle positions.
- Specialized features: Particle-Field Interaction and Fluid-Particle Interaction.

S-bend benchmark: a comparison of the number density in the s-bend using the Free Molecular Flow interface (bottom) and a domain-level Accumulator (top), assuming molecules reflect diffusely at the walls.

Body load created by a spray of particles in a cross-flow.
Accumulator (Boundary)

- Subnode to Wall and Outlet nodes.
- Changes the value of a dependent variable when particles hit walls.
- Specialized accumulator features
  - Etch (Charged Particle Tracing)
  - Erosion (Particle Tracing for Fluid Flow)
Nonlocal Accumulator

- Communicates information about a particle’s current position to the location from which it was released.
- Can be used to model radiative heat transfer between diffusely and specularly reflecting surfaces.

Parallel plates: Rays are released from each surface and query the temperature of whatever surface they hit. The incident heat flux at each plate is computed using Nonlocal Accumulators.
Advanced Modeling Tools

- Weak contributions on particles.
- Self-consistent particle-field and fluid-particle interactions.
- Auxiliary dependent variables.
  - Solve additional equations for each particle.
- Compatible with Deformed Geometry and Moving Mesh.
- User-defined forces.

Charge exchange cell: An auxiliary dependent variable is used to change the charge number of a particle when a collision with a background gas occurs. As a result, some particles are deflected by a charged plate while others are not.
Particle Trajectory Plots

• Visualize particle trajectories using:
  – Lines
  – Tubes
  – Points
  – Comet Tails
• Color particles with arbitrary expressions.

Elastic particles suspended in a fluid due to the acoustophoretic force. The color represents the radiation potential.

Particle motion in a stirred micromixer. The particle streams are colored differently for the 3 different inlets.
Particle Plot

- Plot a particle variable versus time for all particles, or plot two particle variables against each other at selected time steps.
- When plotting over time, use data series operations to compute the following quantities over all particles:
  - Average
  - Sum
  - RMS
  - Maximum
  - Minimum
  - Standard deviation
  - Variance

Rossler attractor (left). The average particle speed is plotted over time (right) using a Particle plot.
Other Plot Types

Poincaré map (red dots) in a baffled mixer

Phase portrait of particle speed vs. position in a mixer

Histogram of the ion angular energy distribution function in an inductively coupled plasma. The x-axis is the angle of incidence of the ions striking the wafer (deg), the y-axis is the energy (eV). The height is the relative count.
Other Visualization Tools

- Filters
- Particle evaluation
- Animate Particle Trajectories plots

All particles rendered (left) and only 10% of particles rendered (right)
Model Library Examples

• Benchmark Models
  – Ion drift velocity benchmark

• Fluid Flow
  – Dielectrophoretic separation
  – Laminar mixer particle

• Tutorial Models
  – Brownian motion
  – Ion cyclotron motion
  – Rossler attractor
  – Rotating galaxy
  – Trapped protons

Rotating galaxy: A custom particle-particle interaction force is used to model gravitational attraction between stars.
Model Library Examples

- Ray Tracing
  - Ideal cloak
  - Luneburg lens
- ACDC Module
  - Electron beam divergence
  - Ion funnel
  - Magnetic lens
  - Quadrupole mass filter
  - Quadrupole mass spectrometer
- Acoustics Module
  - Acoustic levitator
Model Library Examples

- **CFD Module**
  - Micromixer particle tracing
  - Thermophoresis
- **Heat Transfer Module**
  - Parallel plates diffuse specular
- **Molecular Flow Module**
  - Charge exchange cell
  - RF coupler
  - S-bend benchmark
- **Plasma Module**
  - Ion energy distribution function
Brownian Motion

- Particle tracing methods can be used to avoid instabilities due to high Peclet numbers.
- The Particle Tracing for Fluid Flow interface includes a Brownian Force for Monte Carlo simulations of diffusion of particles.

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

• Imports data about the Earth’s magnetic field using an external library.
• Computes the mirror point latitude of protons in the magnetic field as a function of equatorial pitch angle.

Magnetic field lines. Data is imported using an external library.

Proton trajectory in the Earth’s magnetic field. The proton changes direction at certain latitudes known as mirror points.
Electron Beam Divergence

- Sets up a bidirectional coupling between particle trajectories and the electric potential.
- Uses a time-dependent solver and stationary solver in an iterative loop.
- The self-consistent solution agrees with the analytical expression for the shape of a nonrelativistic beam envelope.
Summary

• Flexible modeling tool with a wide variety of built-in forces.
• Can be used in one-way or two-way coupling to other physics, or used on its own for powerful Monte Carlo simulations.
• Dedicated postprocessing tools.