Finite Element Method (FEM) & COMSOL
A (very) brief introduction

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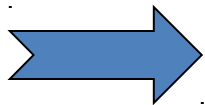HTW

Computer Simulation

- Best way to simulate complex models.

- High-end processing (processing power increasing every day)

- Is it reliable?
  - Does it accurately represent real-life conditions such as physical laws and material properties?

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Computer Simulation

- Computer simulation has become an essential part of science and engineering.

- Today a broad spectrum of options for simulation is available

  Basic programming → High level methods

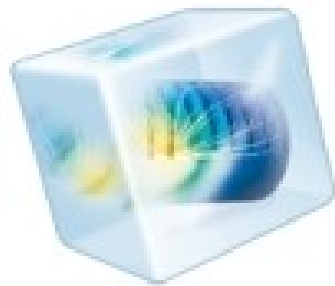- Each technique has its own unique attributes

- All share a common concern

Can you rely on the results?

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What makes software reliable???

- Intention

  → you want a model that accurately depicts what happens in the real world.

- A computer simulation environment is simply a translation of real-world physical laws in their virtual form.

- It would be ideal, then, to have a simulation environment that included the possibility to add any physical effect to your model.
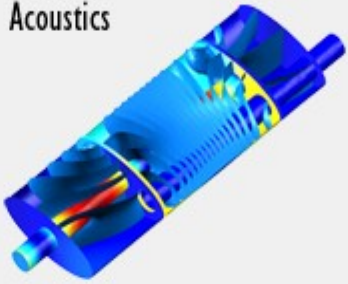
That is what Comsol is all about

COMSOL MULTIPHYSICS®

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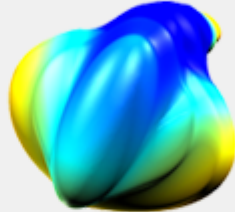Neurocenter, Saarland University Hospital
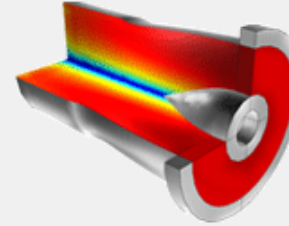
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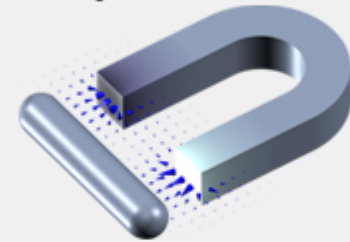
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Application fields

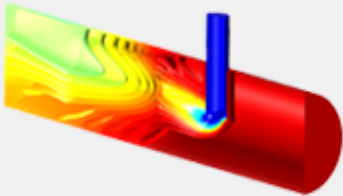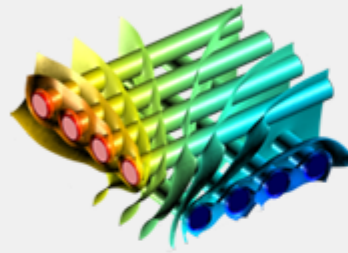Acoustics

Convection and Diffusion

Acoustics Module

Electromagnetics

Chemical Engineering Module

Heat Transfer

Fluid Dynamics
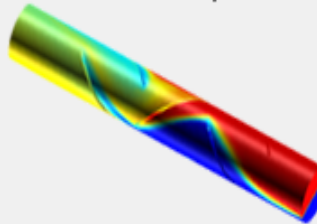
Earth Science Module
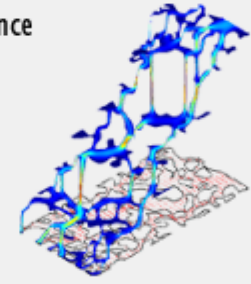
Structural Mechanics Module

RF Module

MEMS Module

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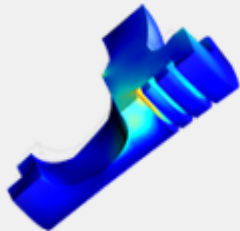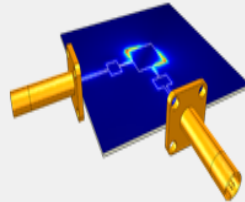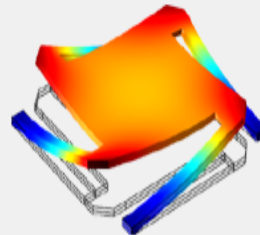
Comsol Multiphysics

Main Menu **Main Toolbar** **Settings Window**   **Graphics Window**
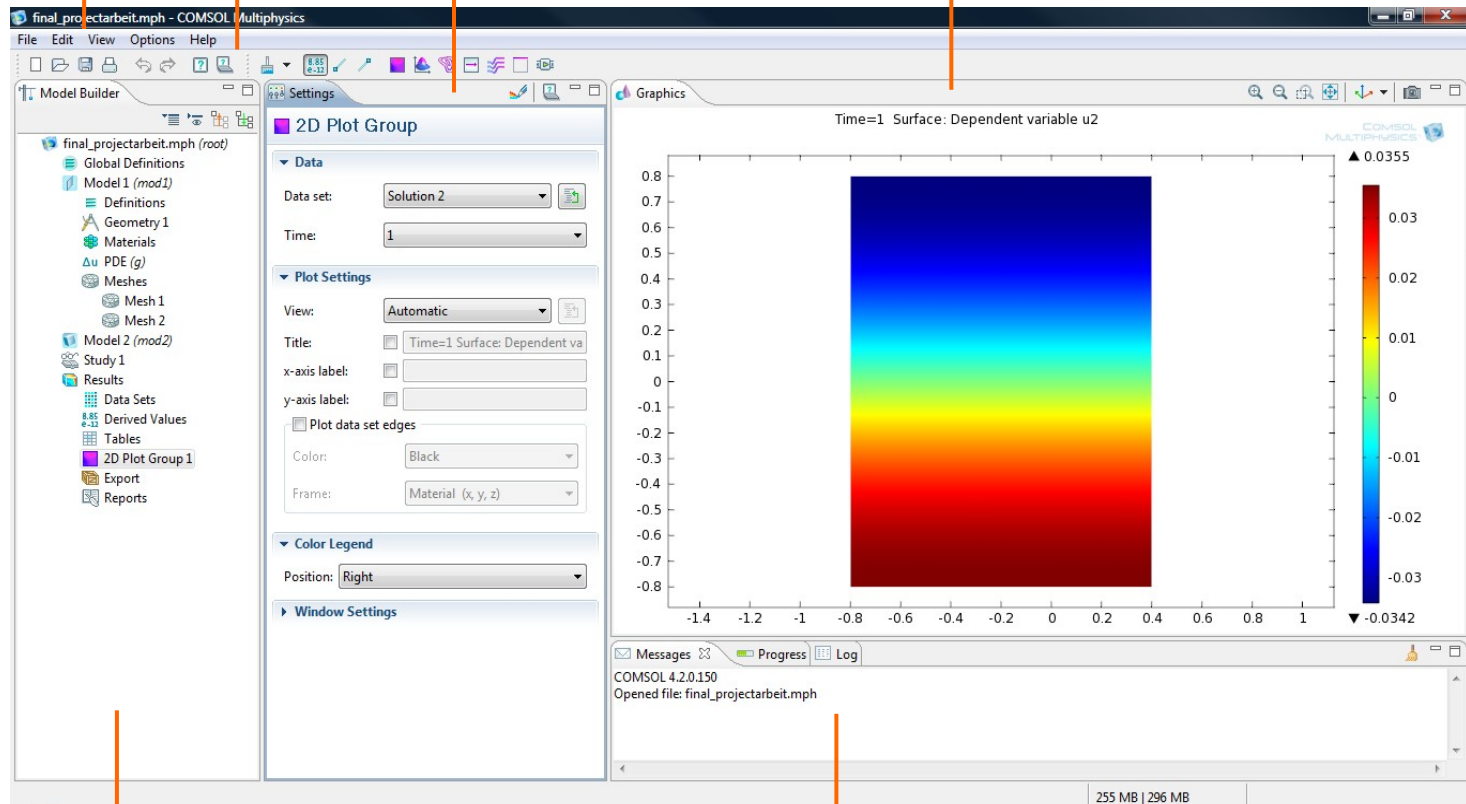
Model Builder with Model Tree   **Messages, Progress and Numerical results**

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- Most physical phenomena are described at a fundamental level by interactions between particles
  - Quarks, nucleons, mesons in Nuclear physics
  - Atoms, molecules, electrons in Classical physics
- If we were to model a physical system, we would have to consider lots of particles such as 6*10^23 per gram mole (per gram for Hydrogen)
  - Unfortunately, It would not be efficient or even realistic (numerically speaking) to represent each particle by one equation
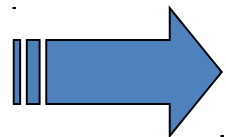
Partial Differential Equations PDEs

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1. *Laplace's equation*

$$\Delta u = \sum_{i=1}^{n} u_{x_i x_i} = 0.$$

2. *Helmholtz's (or eigenvalue) equation*

$$-\Delta u = \lambda u.$$

3. *Linear transport equation*

$$u_t + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

4. *Liouville's equation*

$$u_t - \sum_{i=1}^{n} (b^i u)_{x_i} = 0.$$

5. *Heat (or diffusion) equation*

$$u_t - \Delta u = 0.$$

6. *Schrödinger's equation*

$$iu_t + \Delta u = 0.$$

7. *Kolmogorov's equation*

$$u_t - \sum_{i,j=1}^{n} a^{ij} u_{x_i x_j} + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

8. *Fokker–Planck equation*

$$u_t - \sum_{i,j=1}^{n} (a^{ij} u)_{x_i x_j} - \sum_{i=1}^{n} (b^i u)_{x_i} = 0.$$

9. *Wave equation*

$$u_{tt} - \Delta u = 0.$$

10. *Telegraph equation*

$$u_{tt} + du_t - u_{xx} = 0.$$

11. *General wave equation*

$$u_{tt} - \sum_{i,j=1}^{n} a^{ij} u_{x_i x_j} + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

12. *Airy's equation*

$$u_t + u_{xxx} = 0.$$

13. *Beam equation*

$$u_t + u_{xxxx} = 0.$$

<u>Linear equations</u>

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1. *Eikonal equation*
$$|Du| = 1.$$

2. *Nonlinear Poisson equation*
$$-\Delta u = f(u).$$

3. *p-Laplacian equation*
$$\mathrm{div}(|Du|^{p-2}Du) = 0.$$

4. *Minimal surface equation*
$$\mathrm{div}\left(\frac{Du}{(1+|Du|^2)^{1/2}}\right) = 0.$$

5. *Monge–Ampère equation*
$$\det(D^2 u) = f.$$

6. *Hamilton–Jacobi equation*
$$u_t + H(Du, x) = 0.$$

7. *Scalar conservation law*
$$u_t + \mathrm{div}\,\mathbf{F}(u) = 0.$$

8. *Inviscid Burgers' equation*
$$u_t + u u_x = 0.$$

9. *Scalar reaction-diffusion equation*
$$u_t - \Delta u = f(u).$$

10. *Porous medium equation*
$$u_t - \Delta(u^\gamma) = 0.$$

11. *Nonlinear wave equations*
$$u_{tt} - \Delta u = f(u),$$
$$u_{tt} - \mathrm{div}\,\mathbf{a}(Du) = 0.$$

12. *Korteweg-de Vries (KdV) equation*
$$u_t + u u_x + u_{xxx} = 0.$$

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PDEs Systems

Linear Systems

1. Equilibrium equations of linear elasticity

$$\mu \Delta \mathbf{u} + (\lambda + \mu) D(\mathrm{div}\, \mathbf{u}) = \mathbf{0}.$$

2. Evolution equations of linear elasticity

$$\mathbf{u}_{tt} - \mu \Delta \mathbf{u} - (\lambda + \mu) D(\mathrm{div}\, \mathbf{u}) = \mathbf{0}.$$

3. Maxwell's equations

$$\begin{cases} \mathbf{E}_t = \mathrm{curl}\, \mathbf{B} \\ \mathbf{B}_t = -\,\mathrm{curl}\, \mathbf{E} \\ \mathrm{div}\, \mathbf{B} = \mathrm{div}\, \mathbf{E} = 0. \end{cases}$$

Non-Linear Systems

1. System of conservation laws

$$\mathbf{u}_t + \mathrm{div}\, \mathbf{F}(\mathbf{u}) = \mathbf{0}.$$

2. Reaction-diffusion system

$$\mathbf{u}_t - \Delta \mathbf{u} = \mathbf{f}(\mathbf{u}).$$

3. Euler's equations for incompressible, inviscid flow

$$\begin{cases} \mathbf{u}_t + \mathbf{u} \cdot D\mathbf{u} = -Dp \\ \mathrm{div}\, \mathbf{u} = 0. \end{cases}$$

4. Navier–Stokes equations for incompressible, viscous flow

$$\begin{cases} \mathbf{u}_t + \mathbf{u} \cdot D\mathbf{u} - \Delta \mathbf{u} = -Dp \\ \mathrm{div}\, \mathbf{u} = 0. \end{cases}$$

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PDEs

We can solve a PDE by

- **Analytical Methods**
  - Separation of variables
  - Green Functions
  - Method of characteristics
  - Transformations: Laplace and Fourier transforms

- **Numerical Methods**
  - Finite Element Method (FEM) (1D, 2D)
  - Finite Difference Method (FDM)
  - Finite Boundary Element

⟹ Comsol

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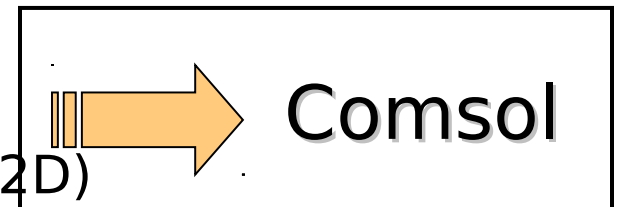
Finite Element Method

Interpretations

Physical Interpretation
– The continous physical model is divided into finite pieces called elements and laws of nature are applied on the generic element. The results are then recombined to represent the continuum.

Mathematical Interpretation
– The differential equation representing the system is converted into a variational form, which is approximated by the linear combination of a finite set of trial functions.

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Solving a PDE through FEM

- Specify the type of solver (stationary (linear/non-linear), time dependent, eigenvalue, parametric (linear/non-linear).

- Specify the domain of the equation.

- Specify the boundary conditions.

- Create a mesh (divide the domain into finite elements).

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Finite Elements

- Defined by:
  - Dimension
  - Nodes
  - Geometry
  - Degrees of Freedom (vertices)
  - Nodal forces

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Finite Elements

More info: http://www.colorado.edu/engineering/cas/courses.d/IFEM.d/

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Solving a PDE through FEM

- Once we have defined a domain (for example, an Ω domain) , we apply the boundary conditions:
  - Newman, how should the function behave when it is orthogonal to the boundary.
  - Dirichlet, it only specifies certain values for the function at the boundaries.
- When we have a 2-D PDE space with defined boundary conditions (can have both, Dirichlet and Newman), we have to find the function that satisfies both.
- Such function has to be contained in a defined space, such as the Sobolev space {like a Hilbert space, but they are all the functions in L_2 (finite energy space) for which the derivatives are also in L_2, in other words, they also have finite energy} .
- Example of Sobolev space = functions that are 0 in the Dirichlet boundary.
- So which functions??? …

Functions for FEM

- Lagrange FE function:
  - Their domain is decomposed into k triangles, and it is globally continuous. The triangle gives three degrees of freedom, for each vertex (named a_0, a_1 and a_2).
  - We describe each 2D linear function through a_0, a_1 and a_2: Each element in the domain can be represented as $a_0 + a_1 x_1 + a_2 x_2$ $a_0, a_1, a_2 \in R$.
  - All triangles together form the new domain: Each linear function is represented by one triangle. And a continuous function is represented through 2D-lineal functions (triangles). The more triangles, the most precise the representation will be.

Create a mesh

Subdivision of the mathematical model into non-overlapping components (elements)
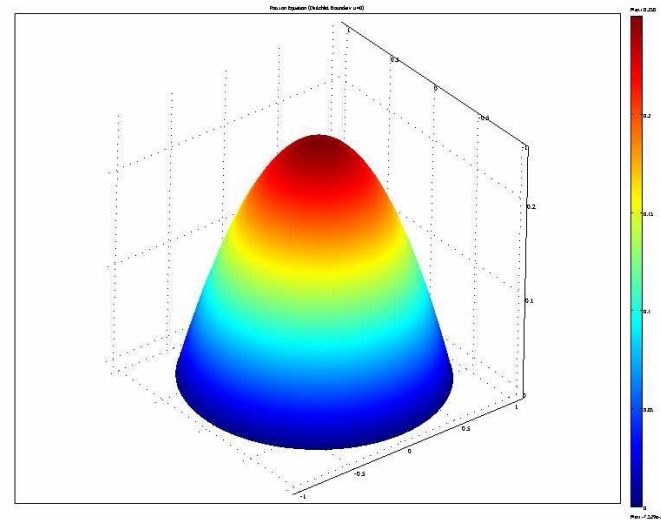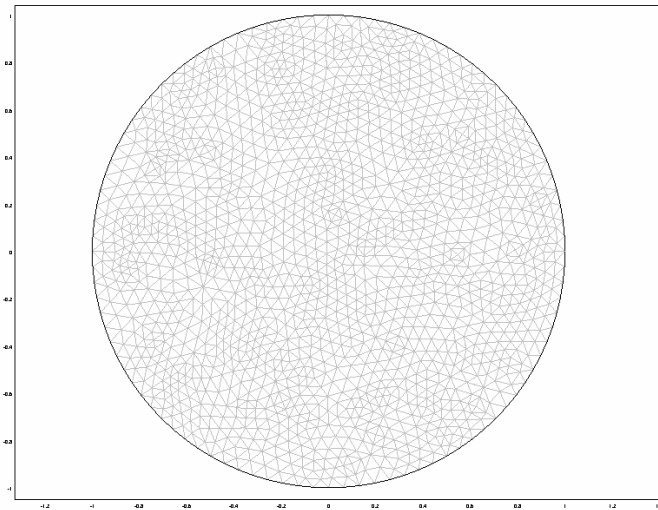
Effect of Meshes in the Solution

- More elements considered => More accuracy & More computational time (Solvers Need to be Optimized)
- Refinement in special places of the geometry improves accuracy of the solution

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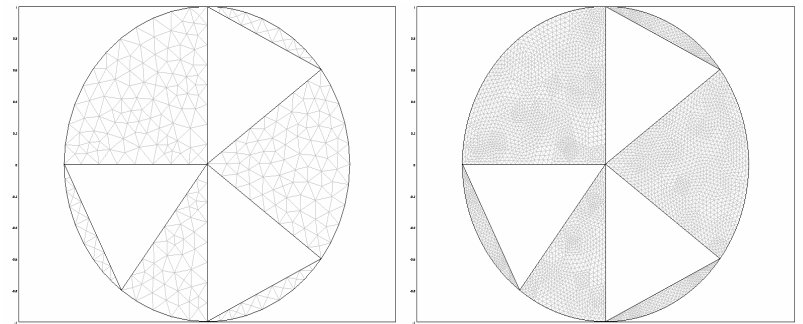
PDEs

- The iterative methods to solve the matrix equations for a system under such PDE systems are called stationary methods, since the solving equation is the same for each iteration.

- To solve such systems, we use modeling. Examples:
  - Airflow over an airplane wing
  - Magnetic drug targeting
  - Non-linear diffusion in image processing
  - Propagation of an action potential through the axon (cable equation).

- How to solve the model?

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Modeling Example

Magnetic drug targeting

(Magnetic Nanoparticles for In Vivo Applications: A Numerical Modeling Study: Trenado and Strauss, 2007)

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Magnetic Drug Targeting

1) Background of the problem

Current research on methods to target chemotherapy drugs in the human body includes the investigation of biocompatible magnetic nanocarrier systems, for example magnetic liquids such as ferrofluids. This model investigates an external magnetic field and its interaction with blood flow containing a magnetic carrier substance.

2) Graphic idealization of the model

Permanent Magnet

Human Tissue

Blood flow through vessel ⟶

Human Tissue

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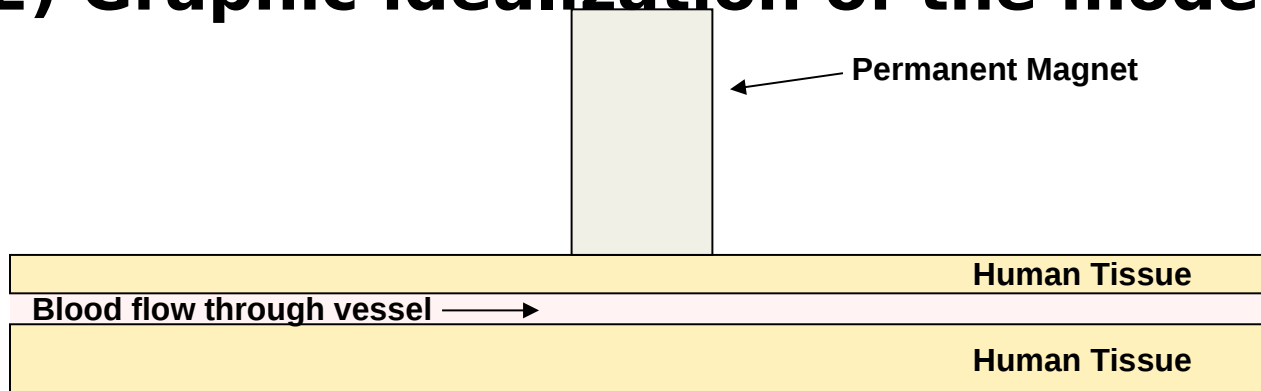
Magnetic Drug Targeting

MAGNETOSTATIC EQUATIONS

Maxwell-Ampere's law

$$\nabla \times \mathbf{H} = \mathbf{J} \qquad (1)$$

magnetic field $\mathbf{H}$ (A/m) and the current density $\mathbf{J}$ (A/m^2)

Gauss' law for the magnetic flux density $\mathbf{B}$ (Vs/m^2)

$$\nabla \cdot \mathbf{B} = 0 . \qquad (2)$$

The constitutive equations describing the relation between $\mathbf{B}$ and $\mathbf{H}$ in the different parts of the modeling domain read:

$$\mathbf{B} = \begin{cases} \mu_0 \mu_{r, mag} \mathbf{H} + \mathbf{B}_{rem} & \text{permanent magnet} \\ \mu_0 (\mathbf{H} + \mathbf{M}_{ff}(\mathbf{H})) & \text{blood stream} \\ \mu_0 \mathbf{H} & \text{tissue and air} \end{cases} \qquad (3)$$

Here μ_0 is the magnetic permeability of vacuum (Vs/(A·m)); μ_r is the relative magnetic permeability of the permanent magnet (dimensionless); $\mathbf{B}_{rem}$ is the remanent magnetic flux (A/m); and $\mathbf{M}_{ff}$ is the magnetization vector in the blood stream (A/m), which is a function of the magnetic field, $\mathbf{H}$.

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Magnetic Drug Targeting

Defining a magnetic vector potential **A** such that

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \nabla \cdot \mathbf{A} = 0, \tag{4}$$

you finally, by substitution in Equation 1 through Equation 3, arrive at the following vector equation to solve:

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{J}$$

Simplifying to a 2D problem with no perpendicular currents, this equation reduces to

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{0}. \tag{5}$$

Note that this equation assumes that the magnetic vector potential has a nonzero component only perpendicularly to the plane, $\mathbf{A} = (0, 0, A_z)$.

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the induced magnetization $\mathbf{M}_{ff}(x, y) = (M_{ffx}, M_{ffy})$ of a ferrofluid

$$M_x = \frac{\chi}{\mu_0}\frac{\partial A_z}{\partial y}$$

$$M_y = -\frac{\chi}{\mu_0}\frac{\partial A_z}{\partial x}$$

(6)

where $\chi = \alpha\beta$ is the magnetic susceptibility.

Magnetic Drug Targeting

FLUID FLOW EQUATIONS

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{F} \qquad (7)$$

$$\nabla \cdot \mathbf{u} = 0$$

where η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ the velocity (m/s), ρ the fluid density (kg/m^3), p the pressure (N/m^2), and $\mathbf{F}$ a volume force (N/m^3).
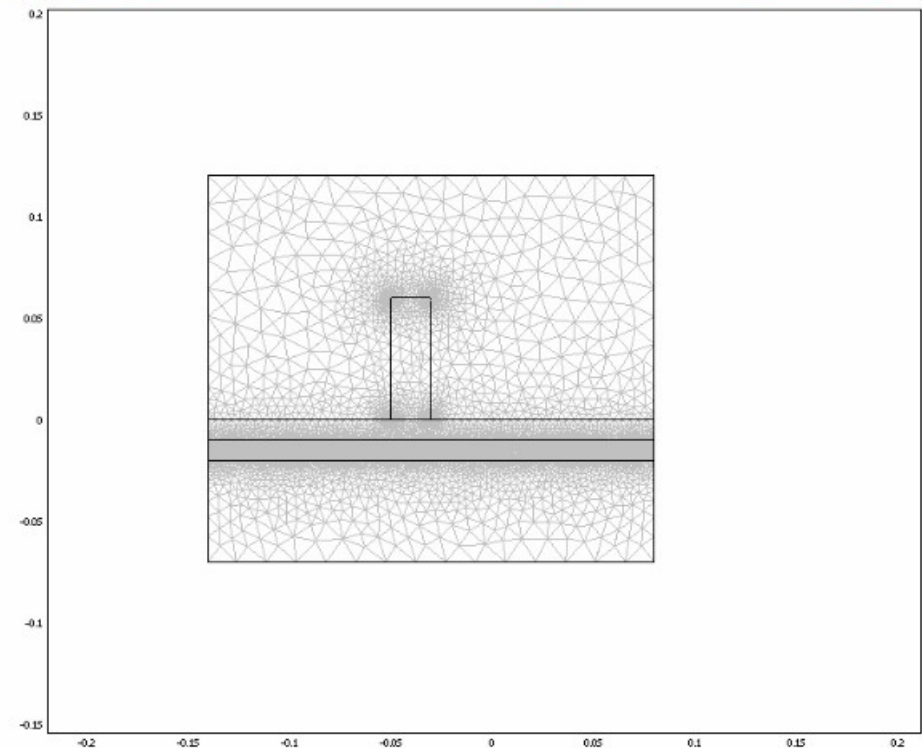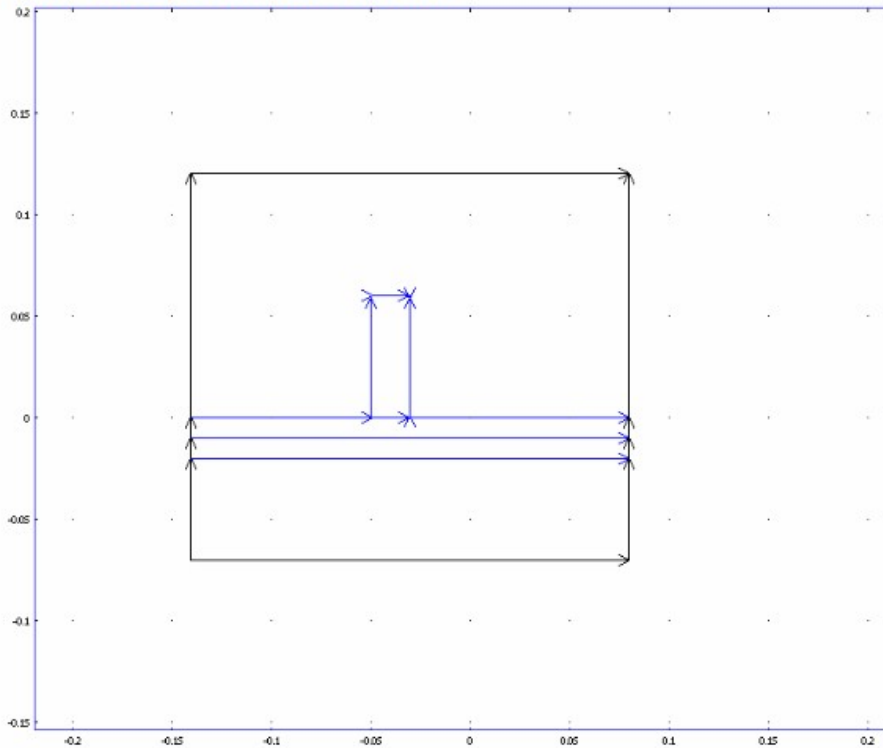
With the assumption that the magnetic nanoparticles in the fluid do not interact, the magnetic force $\mathbf{F} - (F_x, F_y)$ on the ferrofluid for relatively weak fields is given by $\mathbf{F} = |\mathbf{M}|\nabla|\mathbf{H}|$. Using Equation 3, Equation 4, and Equation 6 then leads to the expressions

$$F_x = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial x \partial y}\right)$$

$$F_y = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x \partial y} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial y^2}\right)$$
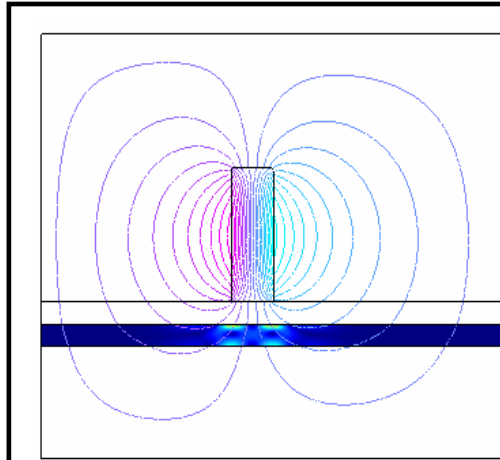
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Magnetic Drug Targeting

4) Domain definition and meshhing

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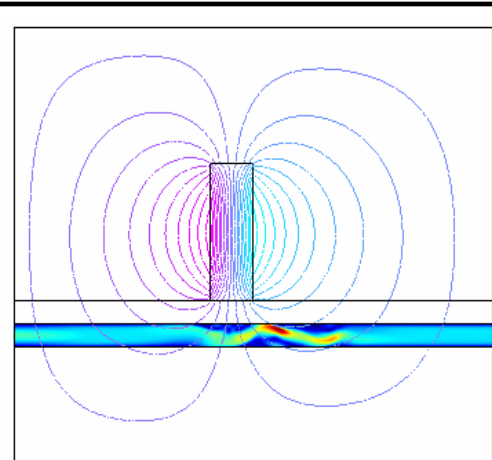
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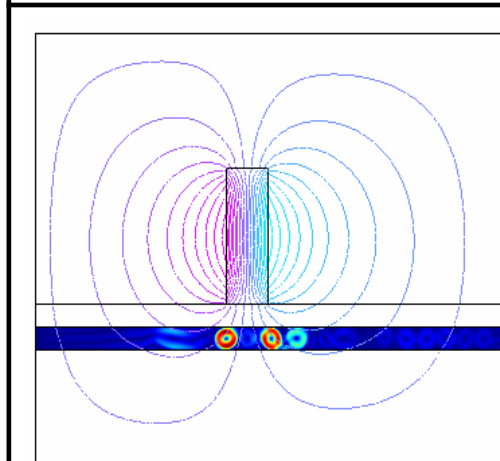
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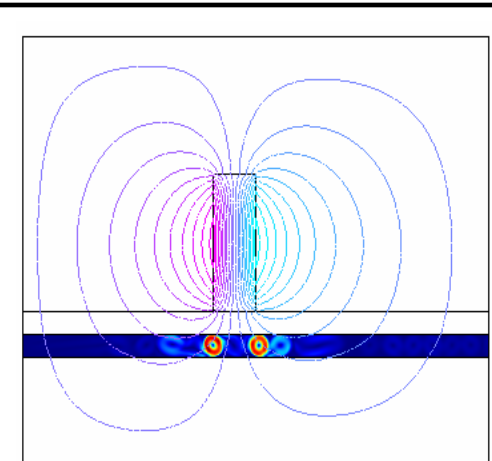# Timedependent snap-shots

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T= 0.2 sec

T= 0.7 sec

T= 1 sec

Steps

Steps to be regarded when building a simulation

1. Background of the problem
2. Graphic idealization of the model
3. Mathematical Model (underlying equations)
4. Boundary Conditions
5. Domain definition and meshing

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The END.

Next episode:

COMSOL 101. (airs on Thurs

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