

COMSOL at CEMEA

Computational possibilities

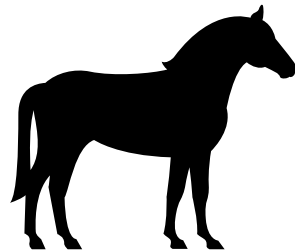
<https://www.cemea.sav.sk/>

Outline

- Hardware
- COMSOL - general introduction
- COMSOL - available modules
- COMSOL - user cases
- use politics

Hardware

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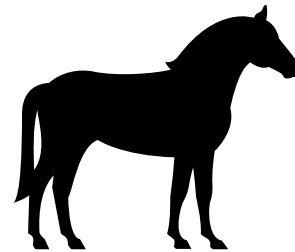
**CPU: AMD Ryzen Threadripper
PRO 3955WX 16-Cores**

Memory: 128GB

**GPU: 2x Nvidia Quadro
RTX5000,
1x Nvidia Quadro
RTX4000**

Disk: 3x1TB SSD

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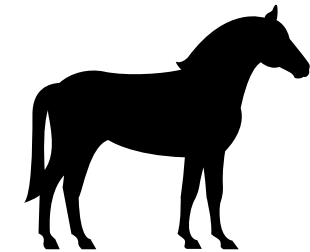
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RTX5000,
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P2200**

Disk: 2TB

COMSOL

COMSOL - Software for Multiphysics Simulation



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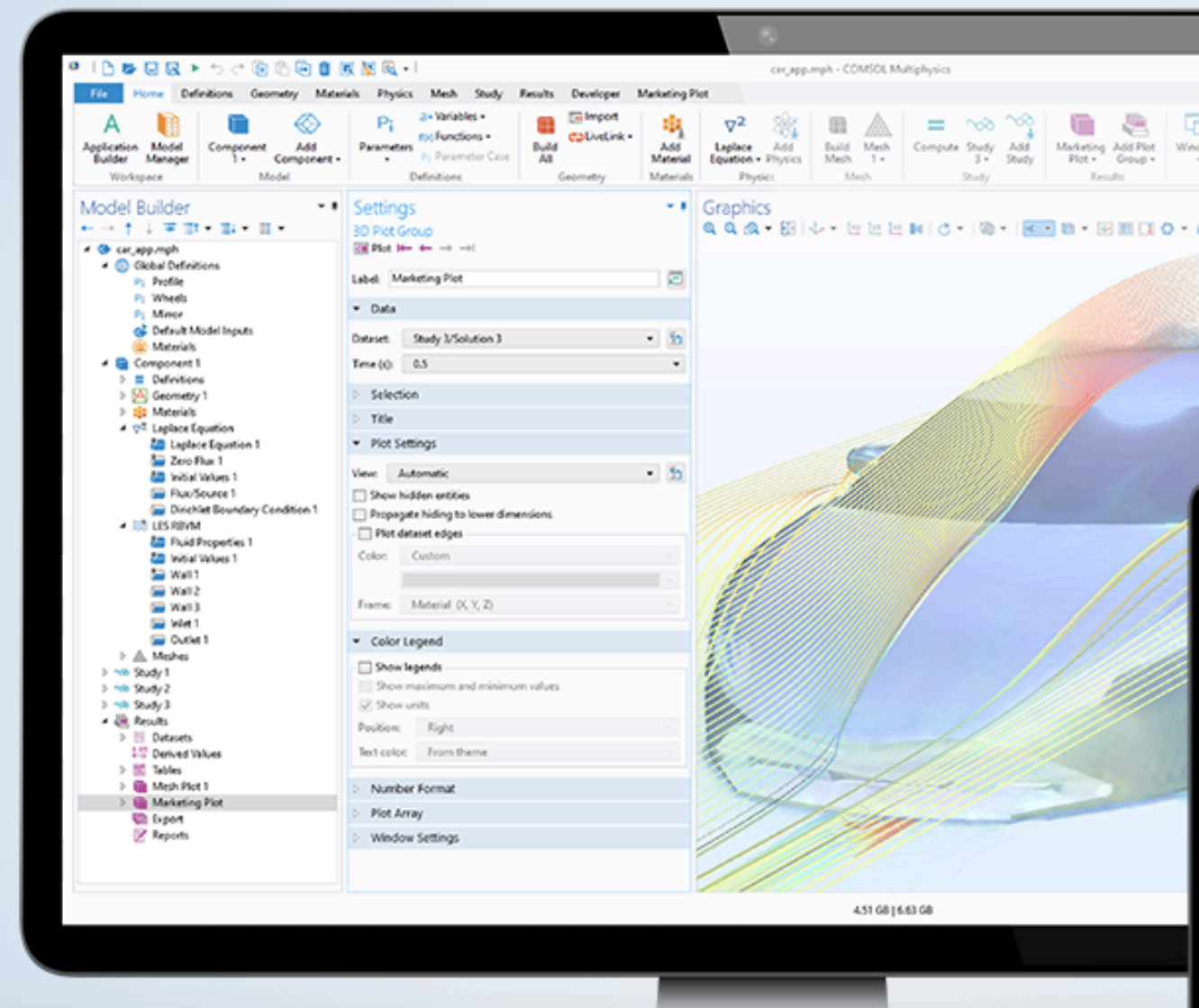
Simulate real-world designs, devices, and processes with multiphysics software from COMSOL.

- ✓ General-purpose simulation software based on advanced numerical methods.
- ✓ Fully coupled multiphysics and single-physics modeling capabilities.
- ✓ Complete modeling workflow, from geometry to results evaluation.
- ✓ User-friendly tools for building and deploying simulation apps.

[View COMSOL Multiphysics® >](#)

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Screenshot



<https://www.comsol.com>

COMSOL

COMSOL - Software for Multiphysics Simulation



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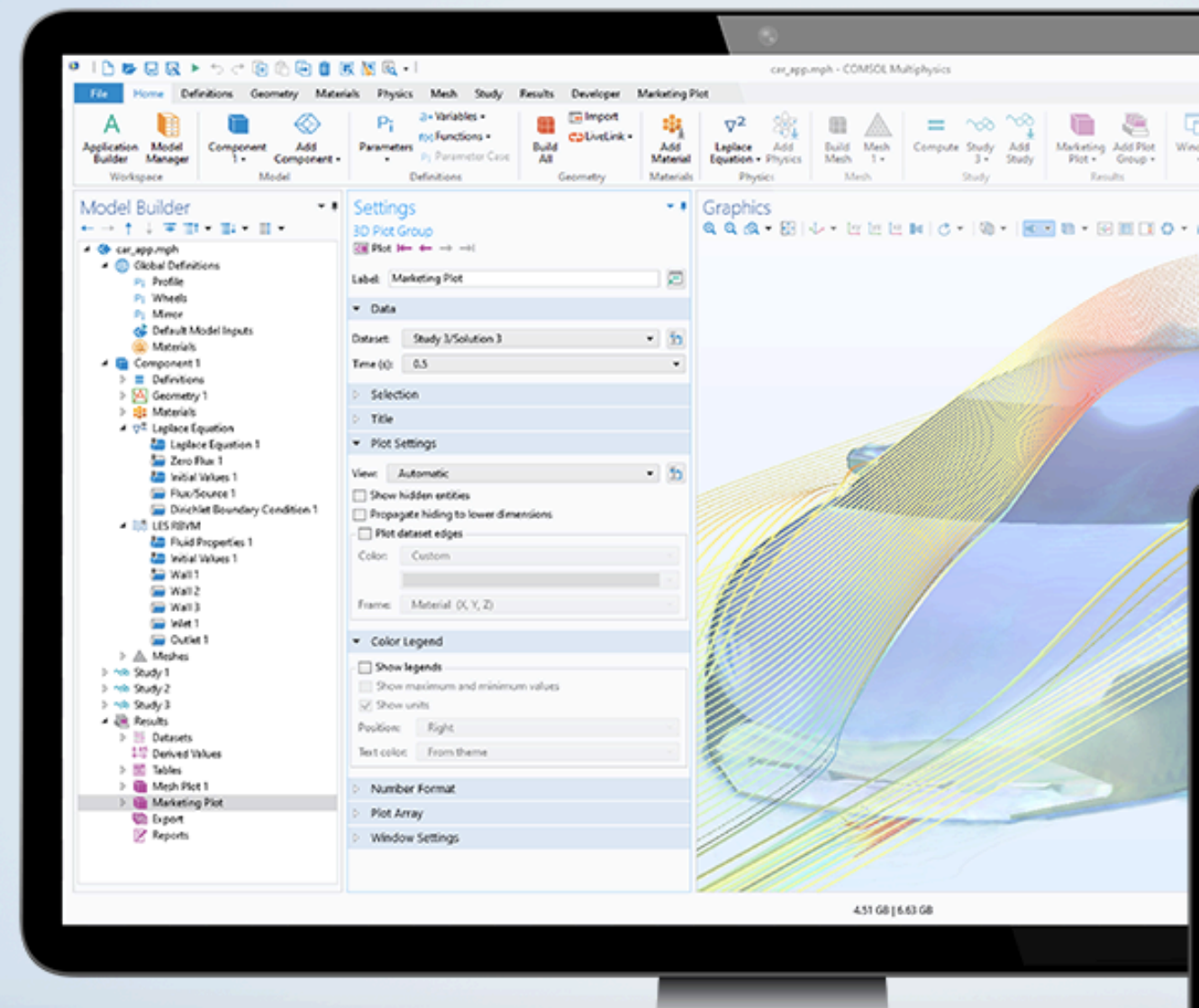
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Screenshot



<https://www.comsol.com>

Mostly, but not only PDE FEM solver

Difusion:

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = -\operatorname{div} \mathbf{j} \quad \mathbf{j} = -D \operatorname{grad} n(\mathbf{r}, t) + \dots \quad \frac{\partial n(\mathbf{r}, t)}{\partial t} - D \Delta n(\mathbf{r}, t) = \dots$$

Heat transfer:

$$\frac{\partial Q}{\partial t} = -\operatorname{div} \mathbf{j}_Q \quad \mathbf{j}_Q = -k \operatorname{grad} T \quad Q = c\rho T \quad \frac{\partial T(\mathbf{r}, t)}{\partial t} - \alpha \Delta T(\mathbf{r}, t) = \dots$$

Wave equation:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u$$

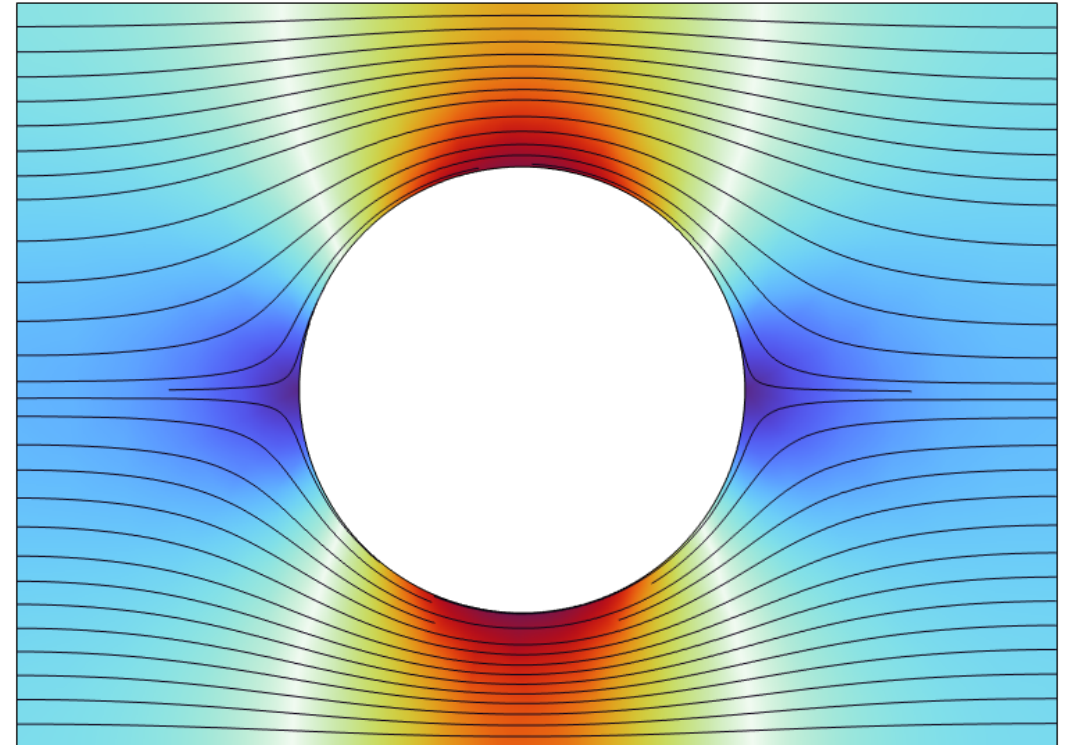
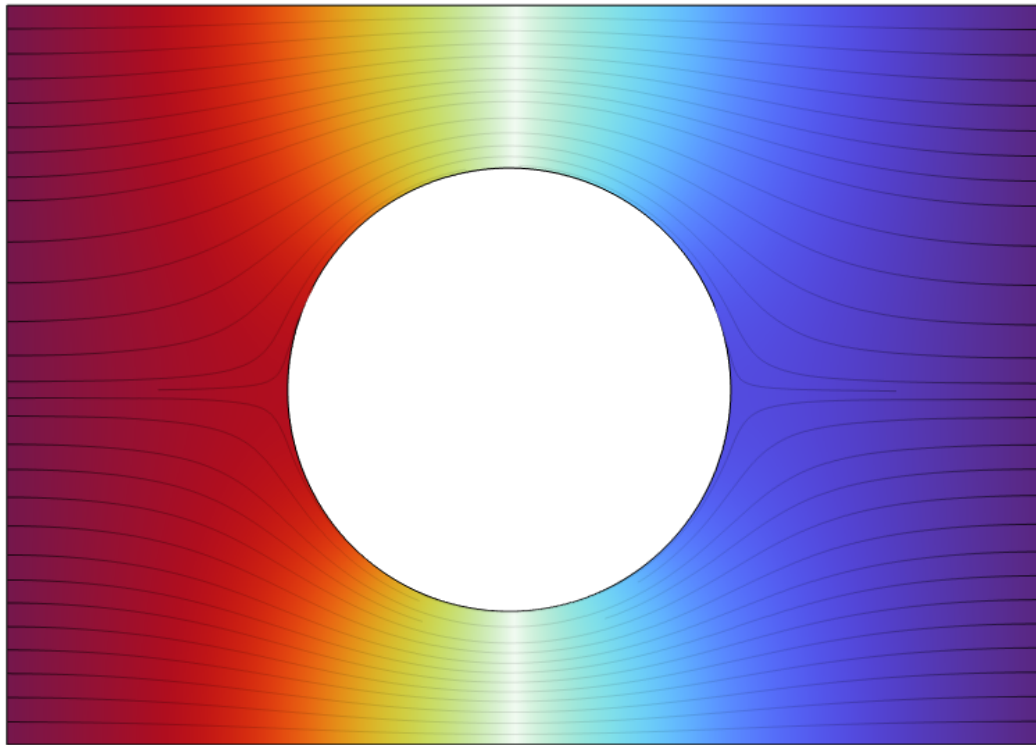
Electrostatic generated by known charge density:

$$\operatorname{div} \mathbf{E} = -\frac{\rho}{\epsilon} \quad \mathbf{E} = -\operatorname{grad} \varphi \quad \Delta \varphi = \frac{\rho}{\epsilon}$$

...and many, many more

Problems are usually connected

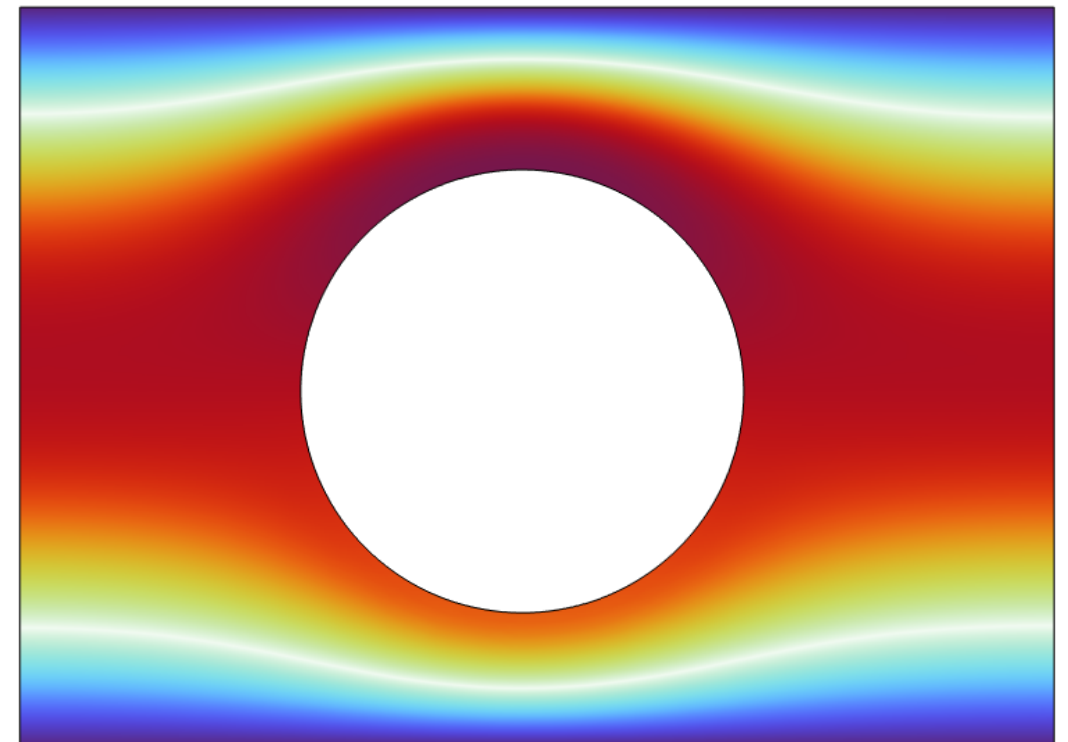
$$\mathbf{j} = \sigma \mathbf{E} \quad \mathbf{E} = -\text{grad } \varphi \quad \text{div } \mathbf{j} = 0$$



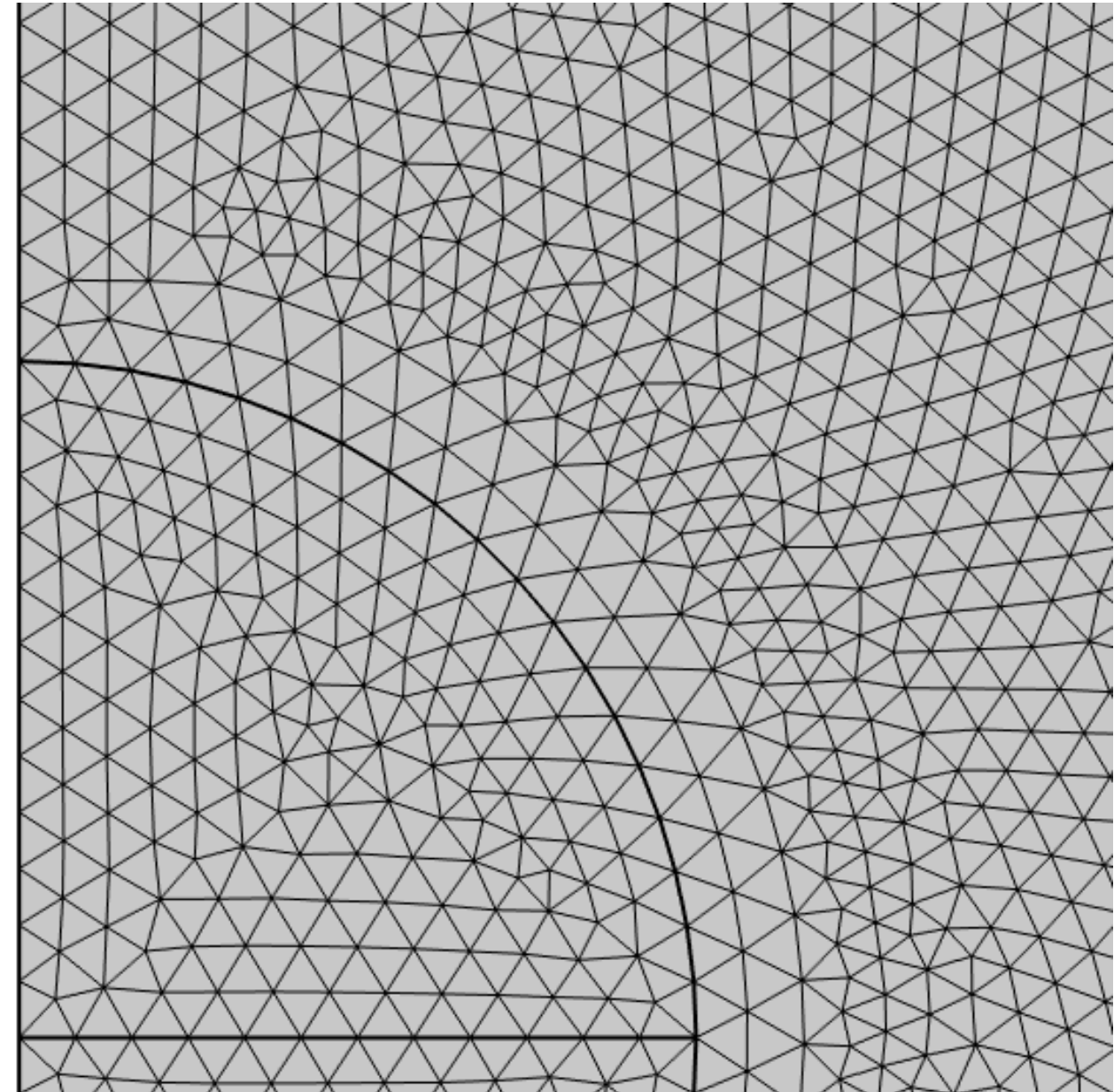
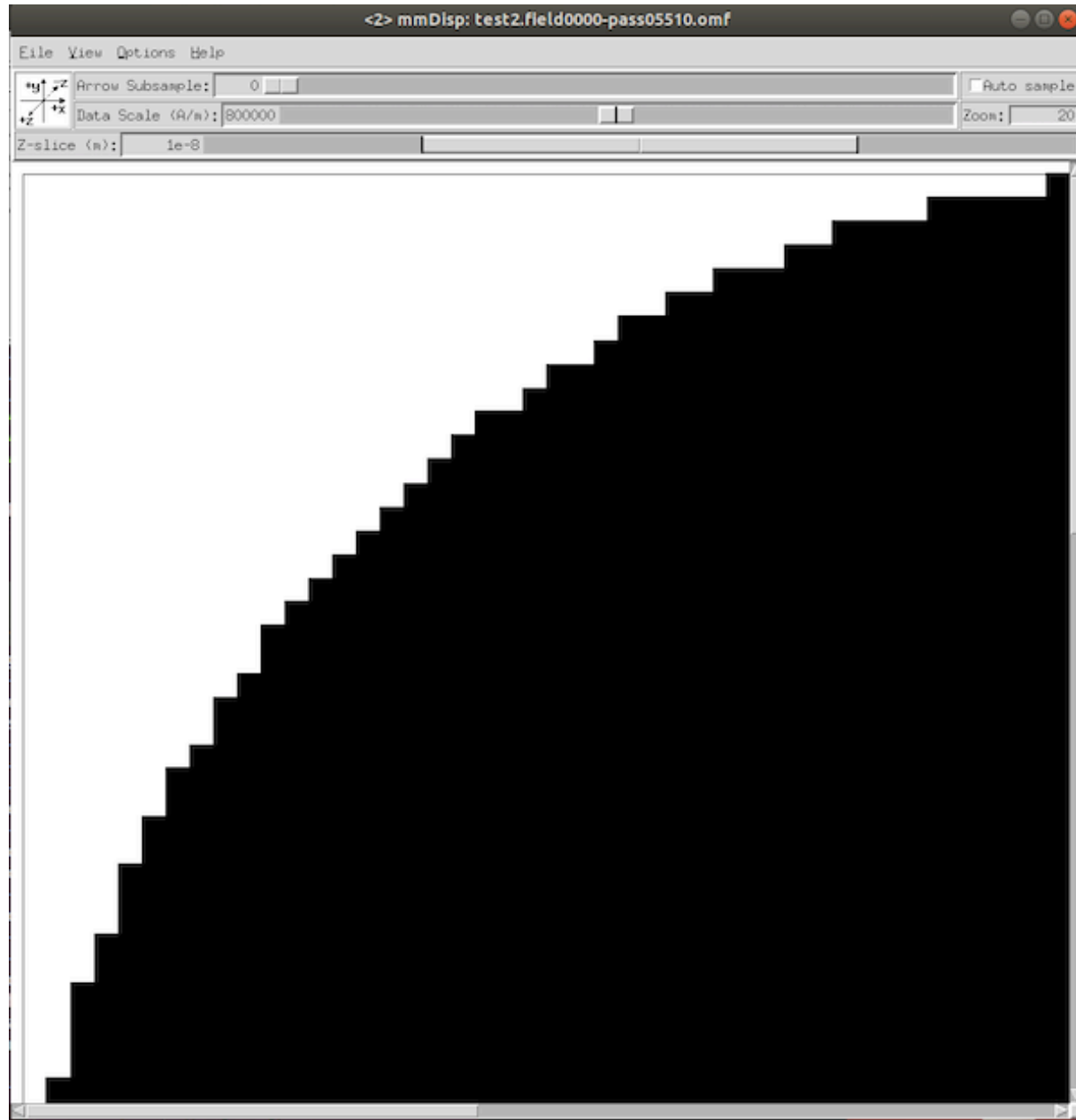
$$p = \frac{1}{\sigma} j^2 \quad \frac{\partial T}{\partial t} = c \rho p + k \alpha \Delta T$$

$(P = RI^2)$

$$\sigma = \sigma_0 + \sigma_1 (T - T_0)$$



Finite Difference vs Finite Element Methods



The screenshot shows the COMSOL website with a navigation bar at the top. The main content area is divided into six sections, each with a title and a list of modules. The sections are: Electromagnetics Modules, Fluid Flow & Heat Transfer Modules, Structural Mechanics & Acoustics Modules, Chemical Engineering Modules, Multipurpose Products, and Interfacing Products. The website is displayed in a browser window with the address bar showing 'comsol.com'.

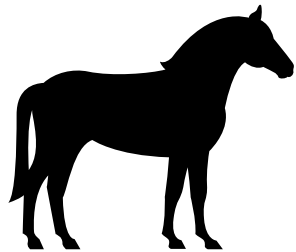
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- Electromagnetics Modules**
 - AC/DC
 - RF
 - Wave Optics
 - Ray Optics
 - Plasma
 - Semiconductor
- Fluid Flow & Heat Transfer Modules**
 - CFD
 - Mixer
 - Polymer Flow
 - Microfluidics
 - Porous Media Flow
 - Subsurface Flow
 - Pipe Flow
 - Molecular Flow
 - Metal Processing
 - Heat Transfer
- Structural Mechanics & Acoustics Modules**
 - Structural Mechanics
 - Nonlinear Structural Materials
 - Composite Materials
 - Geomechanics
 - Fatigue
 - Rotordynamics
 - Multibody Dynamics
 - MEMS
 - Acoustics
- Chemical Engineering Modules**
 - Chemical Reaction Engineering
 - Battery Design
 - Fuel Cell & Electrolyzer
 - Electrodeposition
 - Corrosion
 - Electrochemistry
- Multipurpose Products**
 - Optimization Module
 - Uncertainty Quantification Module
 - Material Library
 - Particle Tracing Module
 - Liquid & Gas Properties Module
- Interfacing Products**
 - LiveLink™ for MATLAB®
 - LiveLink™ for Simulink®
 - LiveLink™ for Excel®
 - CAD Import Module
 - Design Module
 - ECAD Import Module
 - LiveLink™ for SOLIDWORKS®
 - LiveLink™ for Inventor®
 - LiveLink™ for AutoCAD®
 - LiveLink™ for Revit®
 - LiveLink™ for PTC® Creo® Parametric™
 - LiveLink™ for PTC® Pro/ENGINEER®
 - LiveLink™ for Solid Edge®
 - File Import for CATIA® V5

<https://www.comsol.com/products>

COMSOL Modules

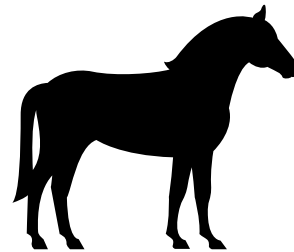
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COMSOL Multiphysics
AC/DC Module
CFD Module
Heat Transfer Module
Structural Mechanics Module
CAD Import Module
Design Module

Licence: CPU

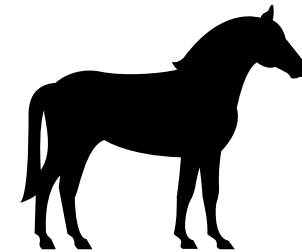
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COMSOL Multiphysics
Fatigue Module
Multibody Dynamics Module
Structural Mechanics Module
CAD Import Module
Design Module
LiveLink for Matlab

Licence: NSL (Tóbik)

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COMSOL Multiphysics
AC/DC Module
CFD Module
Heat Transfer Module
Acoustics Module
Mixer Module
Pipe Flow Module

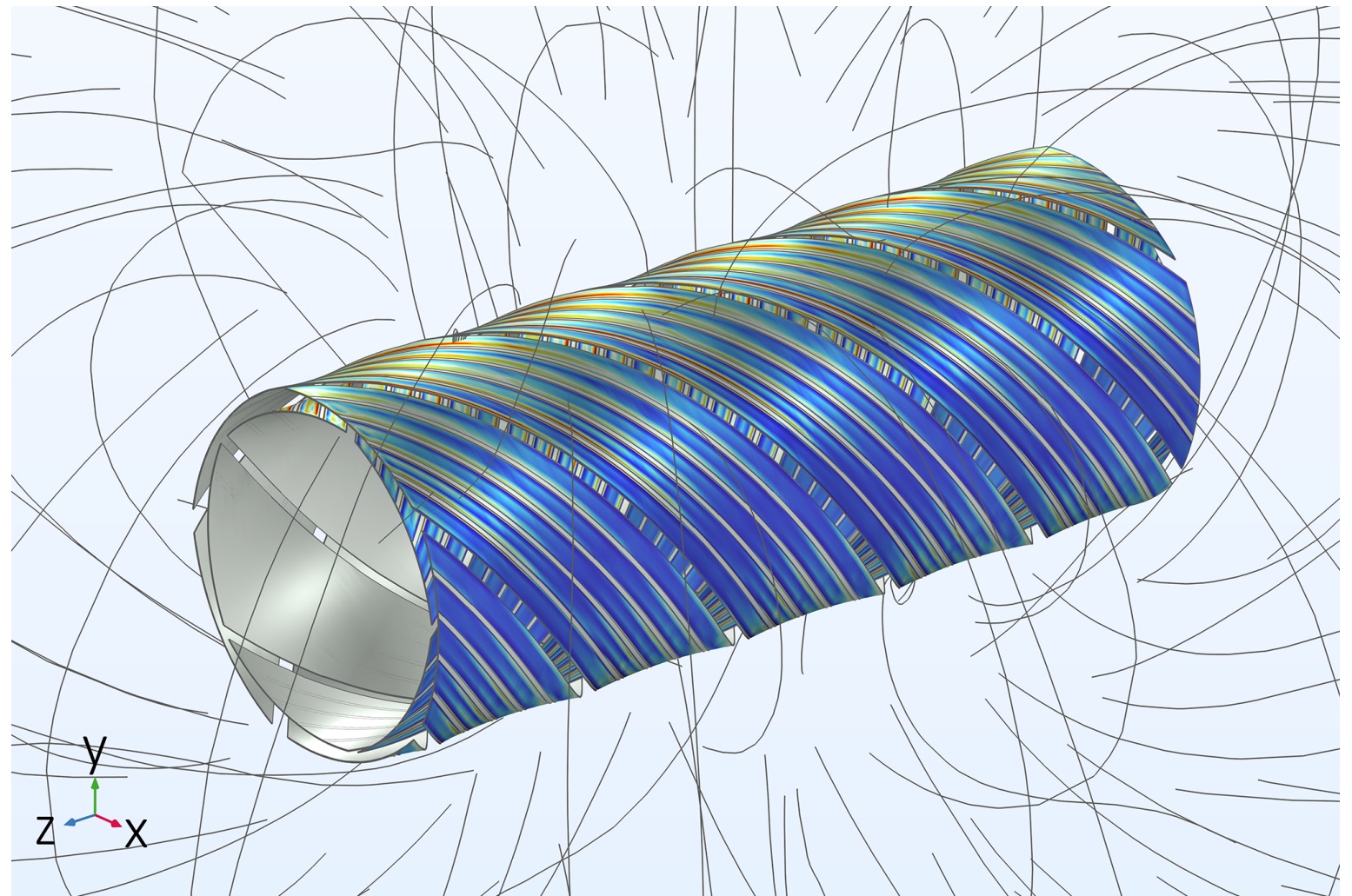
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Use cases

Juraj Feihauer



Mykola Solovyov



Use politics

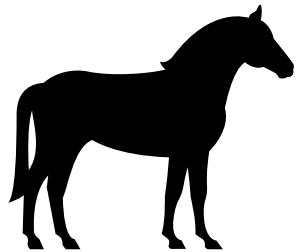
We require the acknowledgment to CEMEA project in publications:

<https://cemea.sav.sk/en/structural-funds-project/publications/>

These studies were performed during the implementation of the project Building-up Centre for advanced materials application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF.

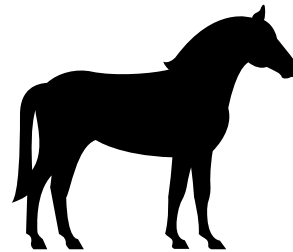
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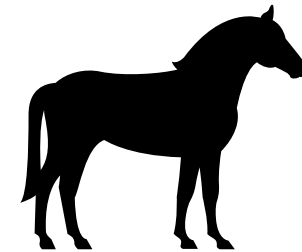
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Licence: CPU

Licence: NSL (Tóvik)

Licence: NSL (Feilhauer)

CPU - single computer, multiple users

NSL - named single user licence

<https://www.comsol.com/products/licensing>

Projects for calculations are welcomed!

Contact persons:

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Juraj Feilhauer: juraj.feilhauer@savba.sk

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