TMA 4195
MATHEMATICAL MODELLING
AUTUMN 2009

Philosophy, Contents and Examples

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OUTLINE OF PRESENTATION:

- Industrial Mathematics
- What the Industry Asks For
- Mathematical Modelling
- Traditional and Current Tools

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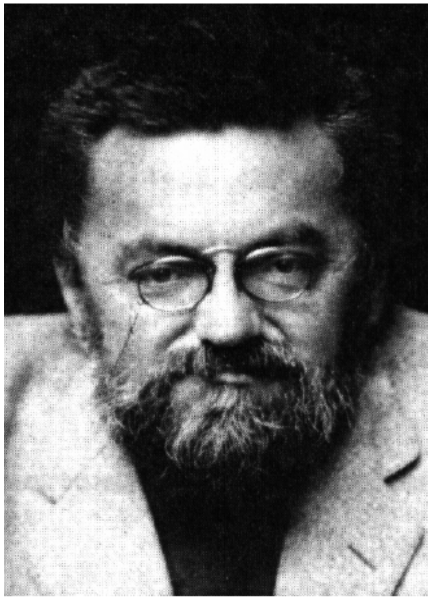
The Start of Industrial Mathematics (?)



Charles Proteus Steinmetz (1865 -1923)

... **his formulation ... simplified *alternating current theory* to the point where it could be understood and used by all engineers**

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Society for Industrial and Applied Mathematics' report on
Mathematics in Industry (1998)
http://www.siam.org/about/mii/

Key elements of the study:

- Role of mathematics outside academia
- Working environments of nonacademic mathematicians
- Views of nonacademic mathematicians and their managers
- Skills needed for success vs. traditional education
- Strategies for enhancing graduate education

IMPORTANT SKILLS OF NON-ACADEMIC MATHEMATICIANS:

- formulating, modeling, and solving problems from diverse areas
- interest in and knowledge of applications
- knowledge of and experience with computations
- communication skills, spoken and written
- adeptness at working with colleagues (''teamwork'')

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THE MATHEMATICAL FUNCTIONS OF GREATEST VALUE (AS SEEN BY THE MANAGERS):

- modeling and simulation;
- mathematical formulation of problems;
- algorithm and software development;
- problem-solving;
- statistical analysis;
- verifying correctness;
- analysis of accuracy and reliability.

SUMMARY:

Most needed skill:

- *mathematical formulation of problems*
- *modelling and simulation*

Most important lesson:

”*Problems never come formulated as mathematical problems!*”

MATHEMATICAL MODELLING

MODELS

Descriptive

Regression
PCA/PLS
Neural nets
ARMA/ARIMA/…
Fractal geomertry

Explanatory

Dimensional analysis
Conservation principle-based
Dynamic models
Averaging models

Hybrids

Controlled systems
Markov models with basis in reality
Diff. Eqns. with stochastic input
Stochastic Diff. Eqns.
Geophysical models
Homogenisation models

MATHEMATICAL MODELLING - *OBJECTIVES*

The main objective is to give the students

- a professional attitude towards problem solving

- how to ask colleagues the right questions, - questions that force *them* to think again about what is really the problem!

- simple techniques to check model consistency and do the important primary analysis

- to think *before* (and *while*) starting to compute!

SOME GENERIC MODELLING TOOLS

Technique	Importance	Related mathematical techniques
Dimensional analysis • reduce the number of parameters • check model reasonability	• lab. work • experimental design • numerical experiments • data analysis	
Conservation laws • basic requirement of models!	• models conform to nature • develop numerical models • understand shock behaviour	• hyperbolic PDEs • diffusion equations • shock tracking num. schemes
Averaging • macroscale behaviour	• models of multi-scale stochastic phenomena (porous media, turbulence)	• stochastic processes/fields • homogenisation techniques
Scaling • systematic model analysis • important/not important	• forces the modeller to think!	• perturbation/multiple scale/asymptotic techniques • selection of numerical techniques

DIMENSIONAL ANALYSIS

- ❑ based on a fundamental law in *physics*!
- ❑ requires all valid relations to be unit independent
- ❑ gives a minimal number of parameters to be used in experimental and numerical work
- ❑ may prove that a suggested model is impossible
- ❑ suggests suitable dimensionless parameters

There are phenomena in nature where dimensional analysis gives information we have not yet been able to explain directly!

Example from Minitab™

What is the volume of a tree (Black American Cherry tree) given its height (h) and root diameter (d)?

Diameter (*d*) (inch)	Height (*h*) (ft)	Volume (*v*) (ft^3)
8.3	70	10.3
8.6	65	10.3
8.8	63	10.2
10.5	72	16.4
10.7	81	18.8
10.8	83	19.7
11.0	66	15.6
11.0	75	18.2
11.1	80	22.6
…	…	..

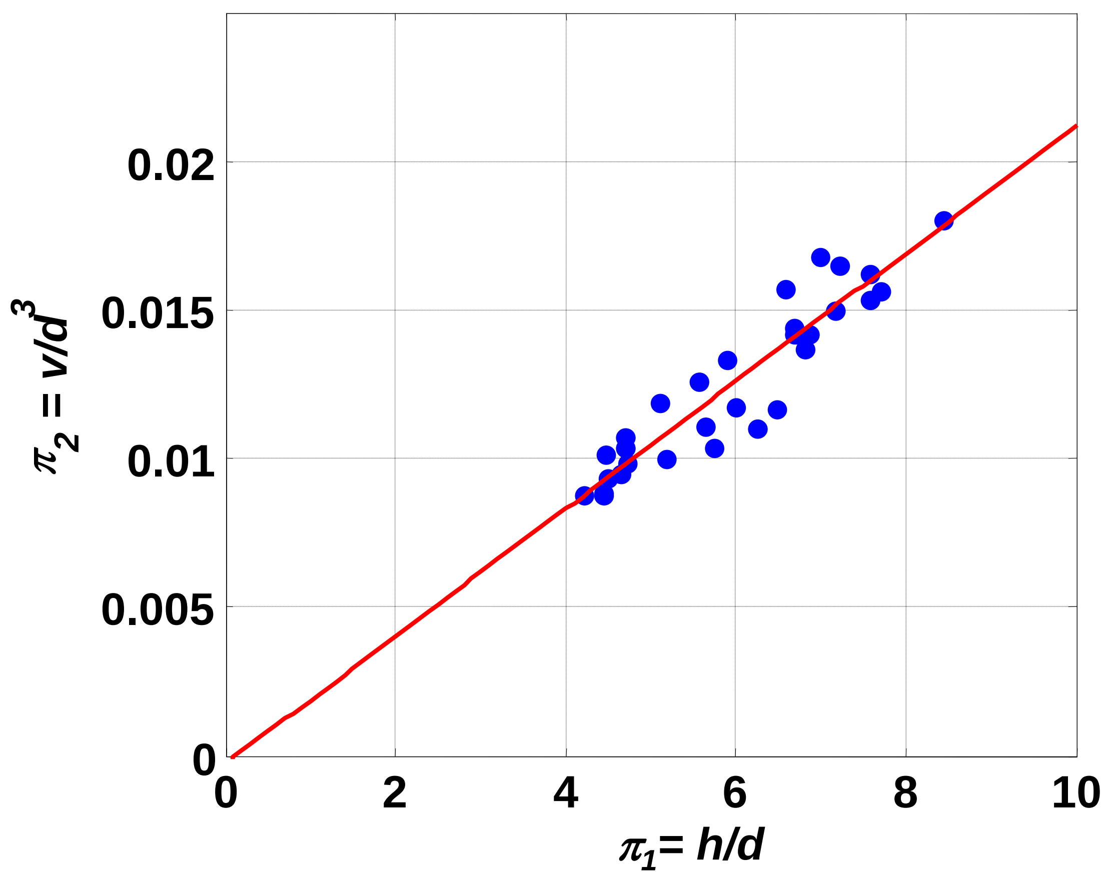
Minitab suggests:

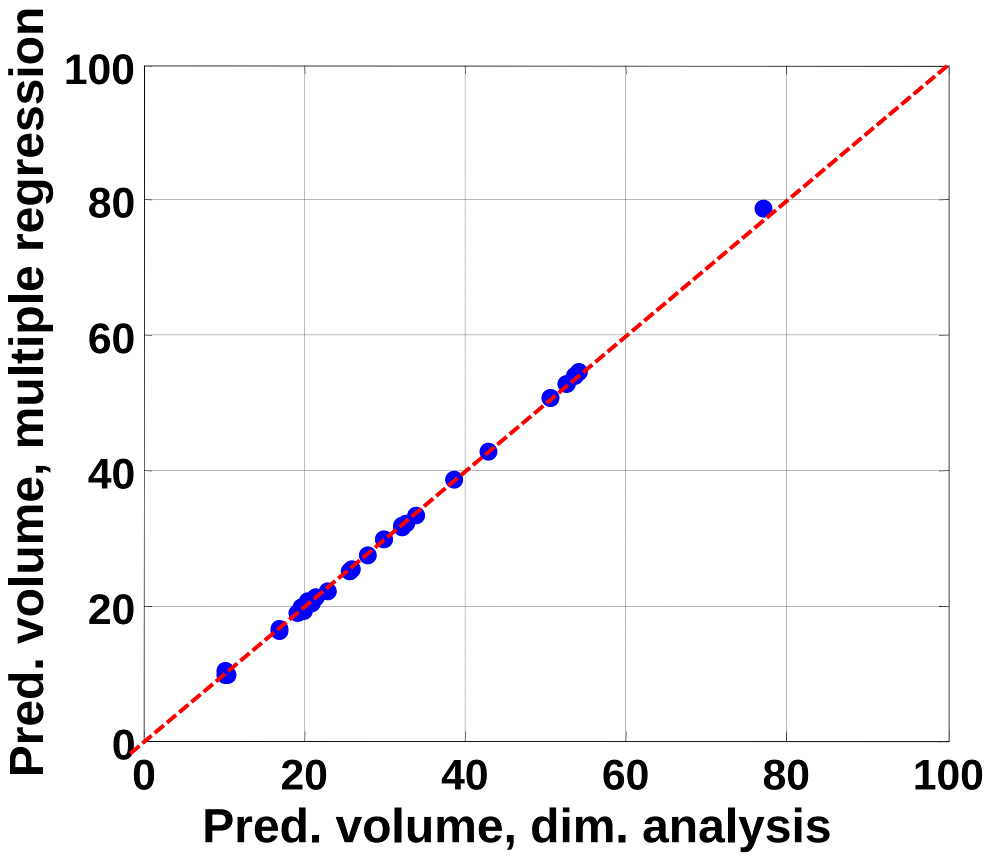
$$v^{1/3} = \beta_0 + \beta_1 d + \beta_2 h + \beta_3 d^2$$

Dimensional analysis suggests (e.g.):

$$\boxed{\frac{v}{d^3} = \phi\left(\frac{h}{d}\right)}$$

Dimensional Analysis Regression




Pred. volume, multiple regression
100
80
60
40
20
0
0
20
40
60
80
100
Pred. volume, dim. analysis

Minitab suggests:

$$v^{1/3} = \beta_0 + \beta_1 d + \beta_2 h + \beta_3 d^2$$

Dimensional analysis suggests:

$$\boxed{\frac{v}{d^3} = \phi\left(\frac{h}{d}\right)}$$

For a "cone"-shaped tree:

$$\phi(x) = \frac{\pi}{12} x$$

What about a Fractal Tree?

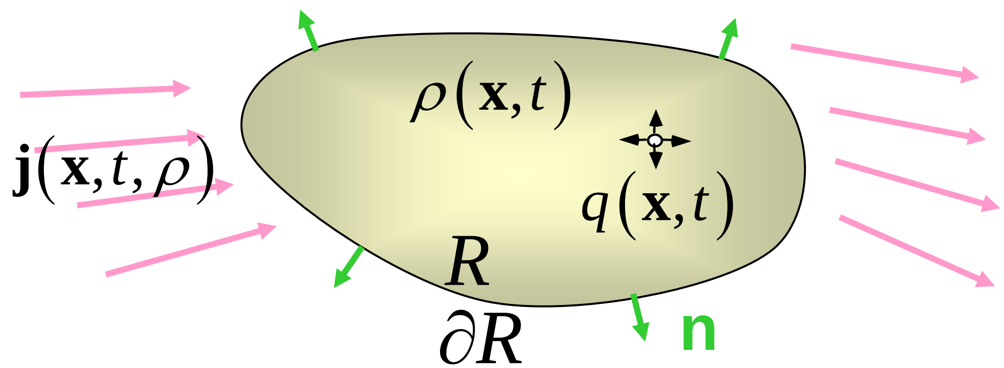
THE UNIVERSAL CONSERVATION LAW

$$\frac{d}{dt}\int_R \rho(\mathbf{x},t)dV + \int_{\partial R} \mathbf{j}(\mathbf{x},t,\rho)\cdot\mathbf{n}d\sigma = \int_R q(\mathbf{x},t)dV$$

Change of content in control volume

Transport across the boundary

Production (q>0) or destruction (q<0)



1. Identify density, flux, and sources

2. Use Reynold's Transport Theorem to transform the first term when necessary.

INTEGRAL FORM | **DIFFERENTIAL FORM**

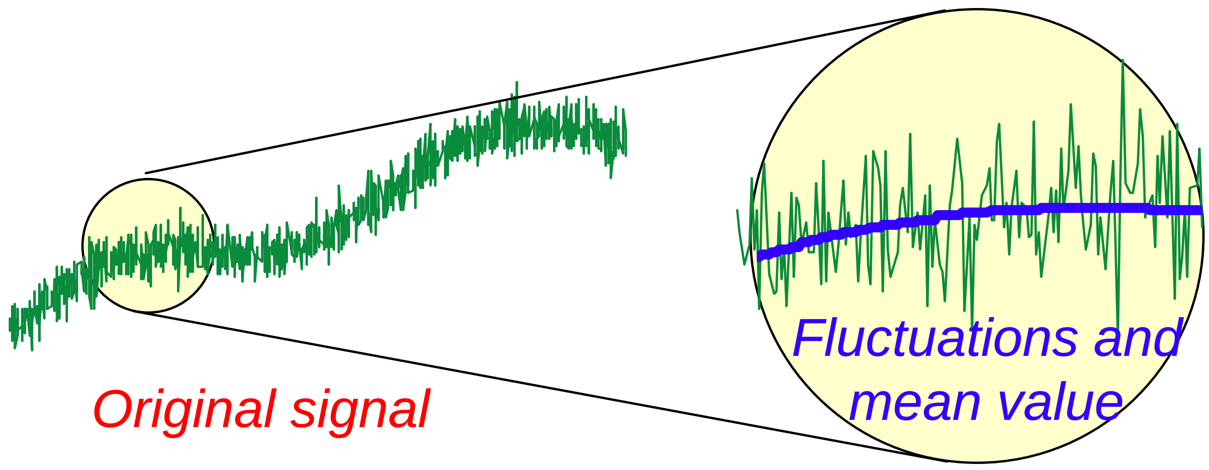
Gauss' theorem etc.

$$\frac{d}{dt}\int_R \rho(\mathbf{x},t)\,dV + \int_{\partial R} \mathbf{j}(\mathbf{x},t,\rho)\bullet\mathbf{n}\,d\sigma = \int_R q(\mathbf{x},t)\,dV \;\Rightarrow\; \frac{\partial\rho(\mathbf{x},t)}{\partial t} + \nabla\cdot\mathbf{j}(\mathbf{x},t,\rho) = q(\mathbf{x},t,\rho)$$

- independent of coordinate system
- direct connection to physics
- required for discontinuous solutions
- basis for conservative numerical schemes

- classic theory of differential equations (analytical solutions, series expansions, integral transforms, perturbation techniques)
- conventional numerical algorithms
- cannot treat discontinuous solutions properly

THE AVERAGING PRINCIPLE



Get rid of fast, *microscopic* fluctuations by averaging

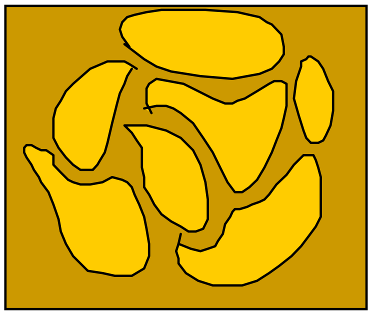
- obtain a *macroscopic* model for the mean values!

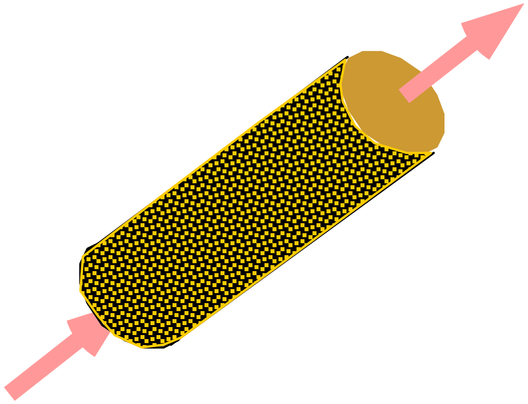
MODELS REQUIRING AVERAGING

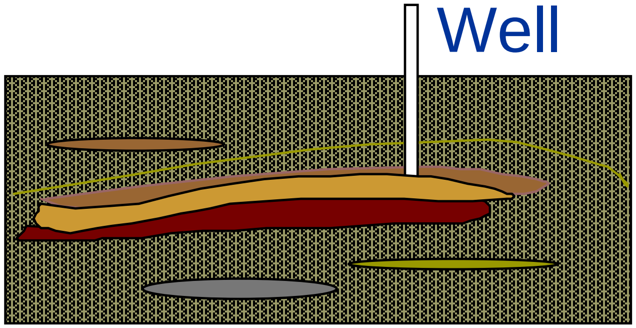
- **Turbulence, diffusion etc.**
  - Atmospheric models
  - Ocean circulation
  - Heat convection in fluids
  - Pollution spreading
  - Epidemics
- **Porous media flow**
  - Ground water
  - Oil/gas reservoirs
- **Geophysical modelling**
  - Atmospheric modelling
  - Climate modelling
- **Traffic flow**
- **Material science**

OIL RESERVOIR MODELLING

Pores	Core samples	Full reservoir
~10^{-5}m	~10^{-1}m	~1000m







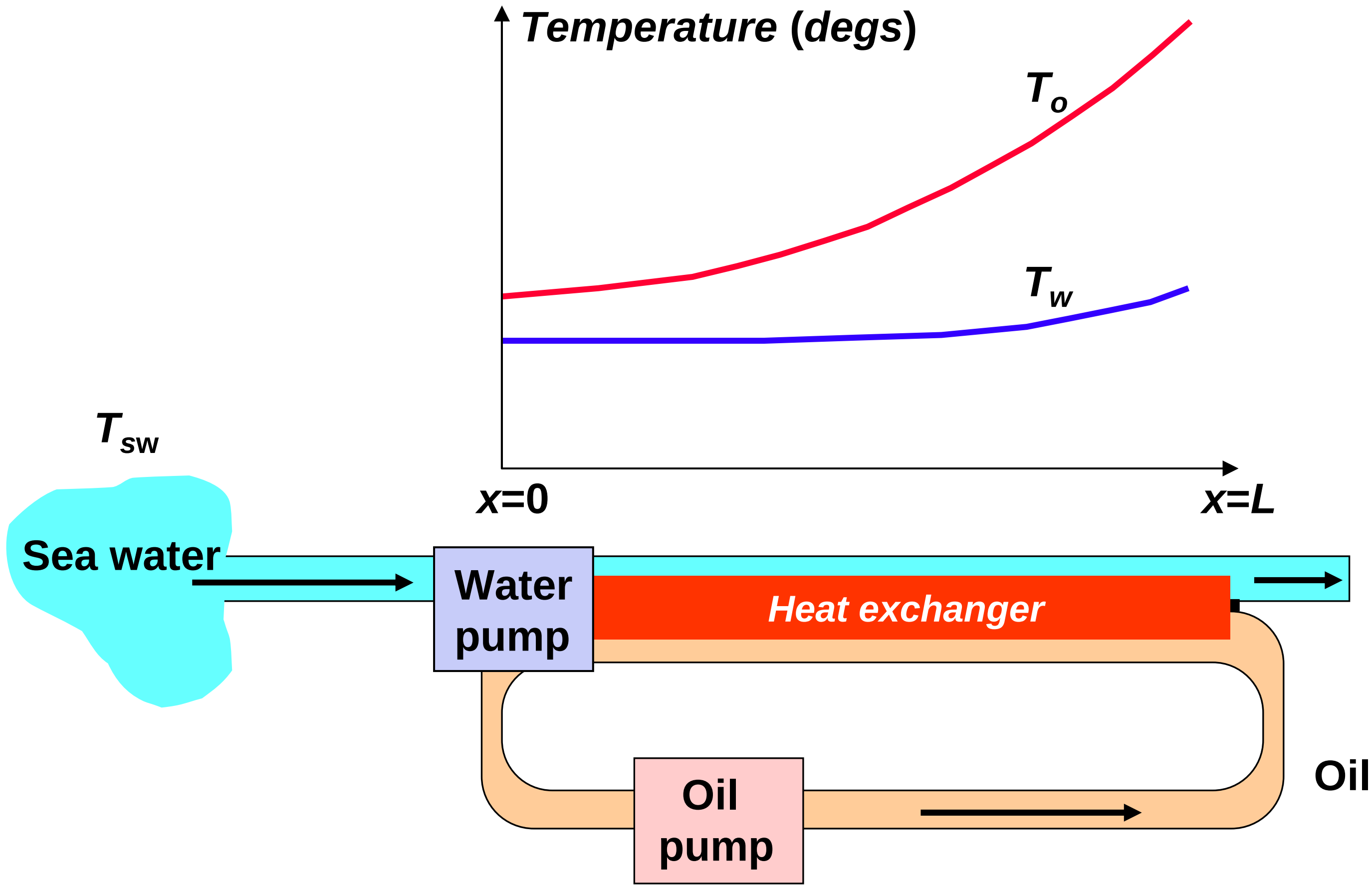
The "upscaling" problem:

How to get from properties of the small scale samples to large scale models of the full reservoir

SCALING

- The *scale* is a *natural measuring stick* for the variable
- Scaling forces problem insight!
- Scaled equations show what is important and what is not
- Scaled equations are important for revealing the behaviour of numerical algorithms
- No scales? - similarity solutions!

OIL COOLING OF A WATER PUMP



What determines the maximum oil temperature?

VARIABLES AND PARAMETERS

x	*position*
t	*time*
$T_{o,w}$	*oil/water temperatures*
L	*length of heat exchanger*
T_{sw}	*sea water temperature*
$c_{o,w}$	*oil, water specific heats*
$A_{o,w}$	*oil, water tube cross sections*
$\rho_{o,w}$	*oil, water densities*
$k_{o,w}$	*oil/water turbulent heat diffusivities*
W	*water velocity*
U	*oil velocity*
α	*heat exchange coefficient*
Q	*heat production in the water pump*

4 variables and 14 parameters !

After *scaling* and showing that *turbulent heat diffusion is negligible*, we end up with a *linear* system and 3 dimensionless parameters for the stationary temperature distribution:

$$\frac{dT_o}{dx} = \mu(T_o - T_w)$$

$$\frac{dT_w}{dx} = \varepsilon\mu(T_o - T_w)$$

$$T_w(1) = \varepsilon\Delta T,\ T_w(0) = 0$$

$$\mu = \frac{\alpha L}{A_o U \rho_o c_o}$$

$$\varepsilon = \frac{A_o U \rho_o c_o}{A_w W \rho_w c_w}$$

$$\Delta T = \frac{Q}{A_o U \rho_o c_o}$$

Exact solution:

$$T_o(1) = \frac{e^{\mu(1-\varepsilon)} - \varepsilon}{e^{\mu(1-\varepsilon)} - 1}\Delta T$$

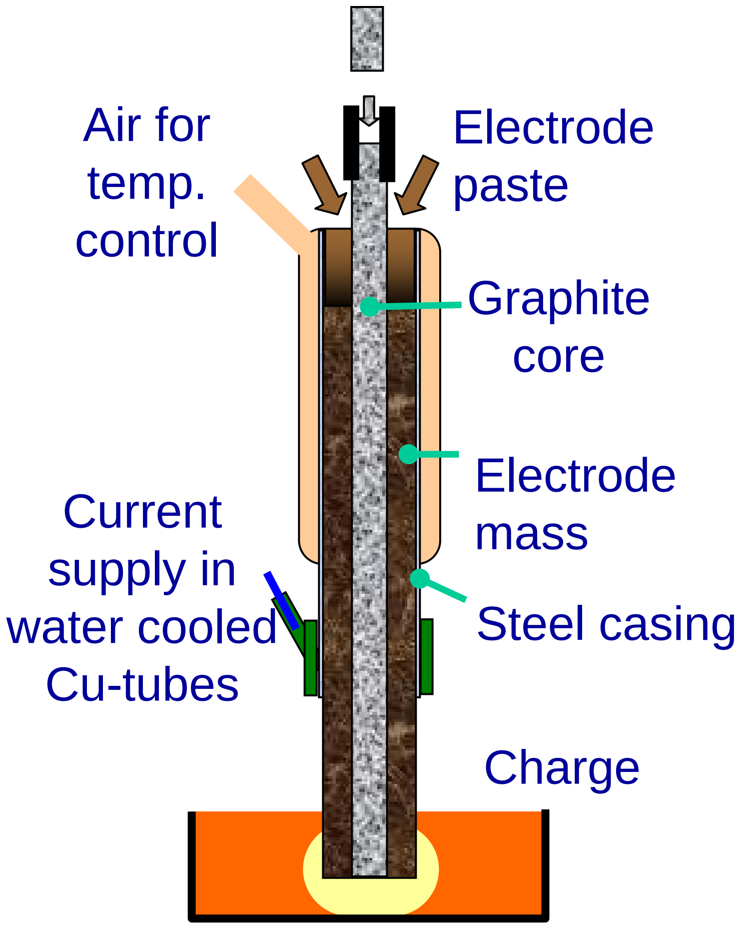
EXAMPLES OF PREVIOUS MODELLING SEMINARS

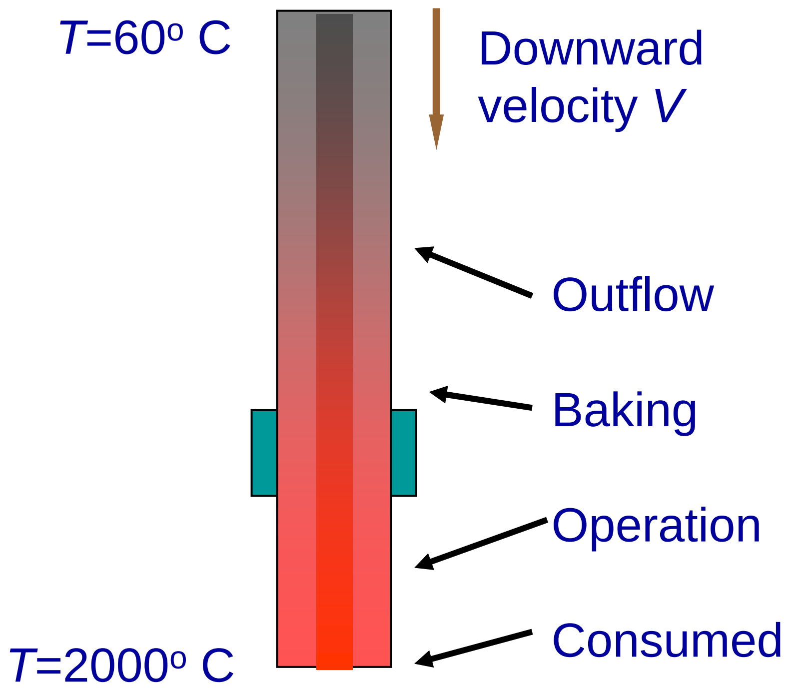
TRAFFIC MODELLING

- The “1001-1002-1003” gap rule
- Optimal pedestrian crossings
- Modelling of a roundabout
- “The green wave”
- Modelling of multi-lane traffic
- Changing winter conditions
- Road capacity under icy conditions
- Studded tire friction modelling

THE SELF-BAKING ELECTRODE

(Provided by *Elkem Research, Norway)*





Elkem asked us to consider the following two main problems:

(A) How can we “shape” the temperature isotherms in the upper region of the electrode by changing the slip velocity, *V*, and the temperature on the circulating air?

(B) The current is entered radially into the electrode. Since the electric conductivity of the electrode paste is strongly temperature dependent, is it possible that this arrangement becomes unstable, that is, that one develops hot and cold regions in the electrode?

(For more info: See the *Proc. ECMI Modelling Week 2000* from Lund)

2006 MODELLING SEMINAR

Models Related to Climatic Change

- Is it really possible to determine ancient temperatures by measuring the temperatures in Greenland ice-cores?
- Dynamics of glaciers in a changing climate
- Modelling of the earth's radiation balance
- Will melting polar ice destroy the North Atlantic Coastal Current and trigger a new ice age?

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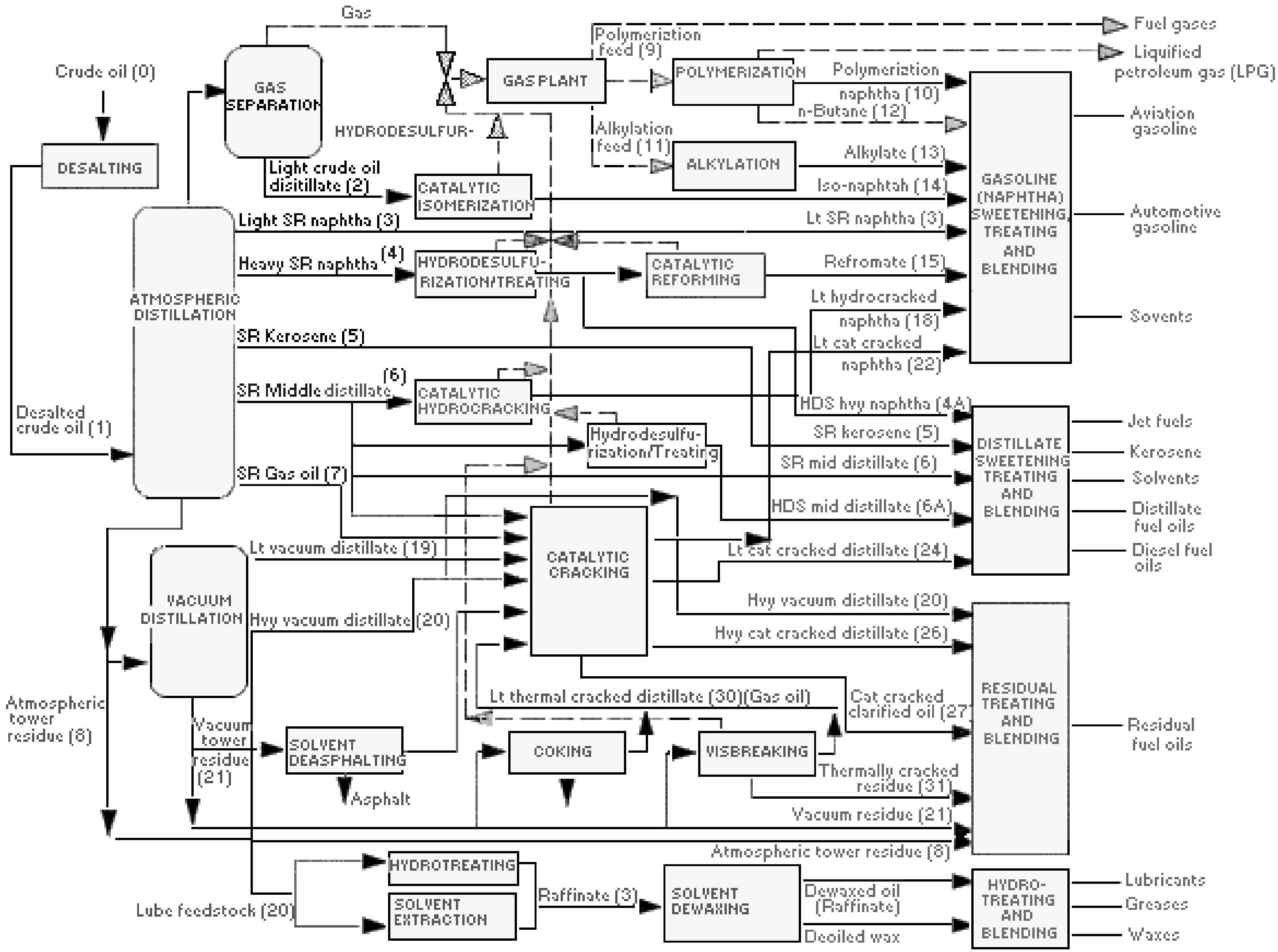
MODELLING SEMINAR 2007

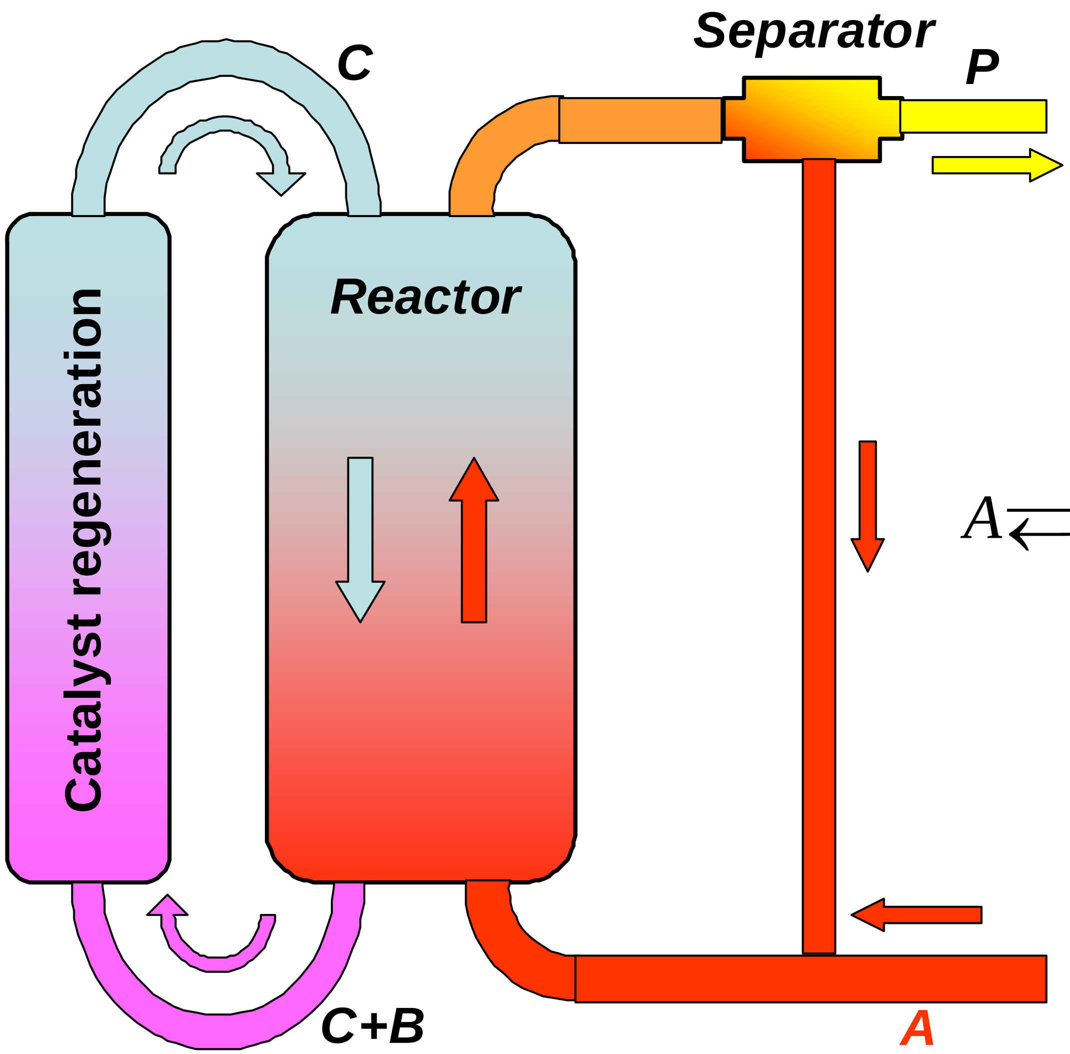
Modelling of Biological Systems

- Population models with delayed response
- Optimal fish harvesting (-or bear hunting)
- Improved models for interacting species
- Migration of King Crab along the Norwegian coast
- Spreading of epidemics
- Models for the world’s population

Nice field, interesting results, easy to do numerical experiments


Mathematical Modelling Seminar
Autumn 2008
MATHEMATICAL MODELLING OF A
CATALYTIC COUNTER-CURRENT
CHEMICAL REACTOR


Crude oil (0)
DESALTING
Desalted crude oil (1)
Gas
GAS SEPARATION
Light crude oil distillate (2)
GAS PLANT
HYDRODESULFUR-
CATALYTIC ISOMERIZATION
ATMOSPHERIC DISTILLATION
Light SR naphtha (3)
Heavy SR naphtha (4)
HYDRODESULFU-RIZATION/TREATING
CATALYTIC REFORMING
SR Kerosene (5)
SR Middle distillate (6)
CATALYTIC HYDROCRACKING
Hydrodesulfu-rization/Treating
SR Gas oil (7)
Polymerization feed (9)
POLYMERIZATION
Alkylation feed (11)
ALKYLATION
Polymerization naphtha (10)
n-Butane (12)
Alkylate (13)
Iso-naphtah (14)
Lt SR naphtha (3)
Refromate (15)
Lt hydrocracked naphtha (18)
Lt cat cracked naphtha (22)
GASOLINE (NAPHTHA) SWEETENING, TREATING AND BLENDING
Fuel gases
Liquified petroleum gas (LPG)
Aviation gasoline
Automotive gasoline
Sovents
HDS hvy naphtha (4A)
SR kerosene (5)
SR mid distillate (6)
HDS mid distillate (6A)
Lt cat cracked distillate (24)
DISTILLATE SWEETENING TREATING AND BLENDING
Jet fuels
Kerosene
Solvents
Distillate fuel oils
Diesel fuel oils
VACUUM DISTILLATION
Lt vacuum distillate (19)
Hvy vacuum distillate (20)
CATALYTIC CRACKING
Hvy vacuum distillate (20)
Hvy cat cracked distillate (26)
Atmospheric tower residue (8)
Vacuum tower residue (21)
SOLVENT DEASPHALTING
Asphalt
Lt thermal cracked distillate (30)(Gas oil)
Cat cracked clarified oil (27)
COKING
VISBREAKING
Thermally cracked residue (31)
Vacuum residue (21)
Atmospheric tower residue (8)
RESIDUAL TREATING AND BLENDING
Residual fuel oils
HYDROTREATING
SOLVENT EXTRACTION
Lube feedstock (20)
Raffinate (3)
SOLVENT DEWAXING
Dewaxed oil (Raffinate)
Deoiled wax
HYDRO-TREATING AND BLENDING
Lubricants
Greases
Waxes



$$A \underset{k_d}{\overset{k_a}{\rightleftarrows}} B \xrightarrow{k_r} P$$

Sketch of the Reactor Arrangement

A: Substrate to be transformed

B: Intermediate product. Stick to the catalyst's surface

P: Product

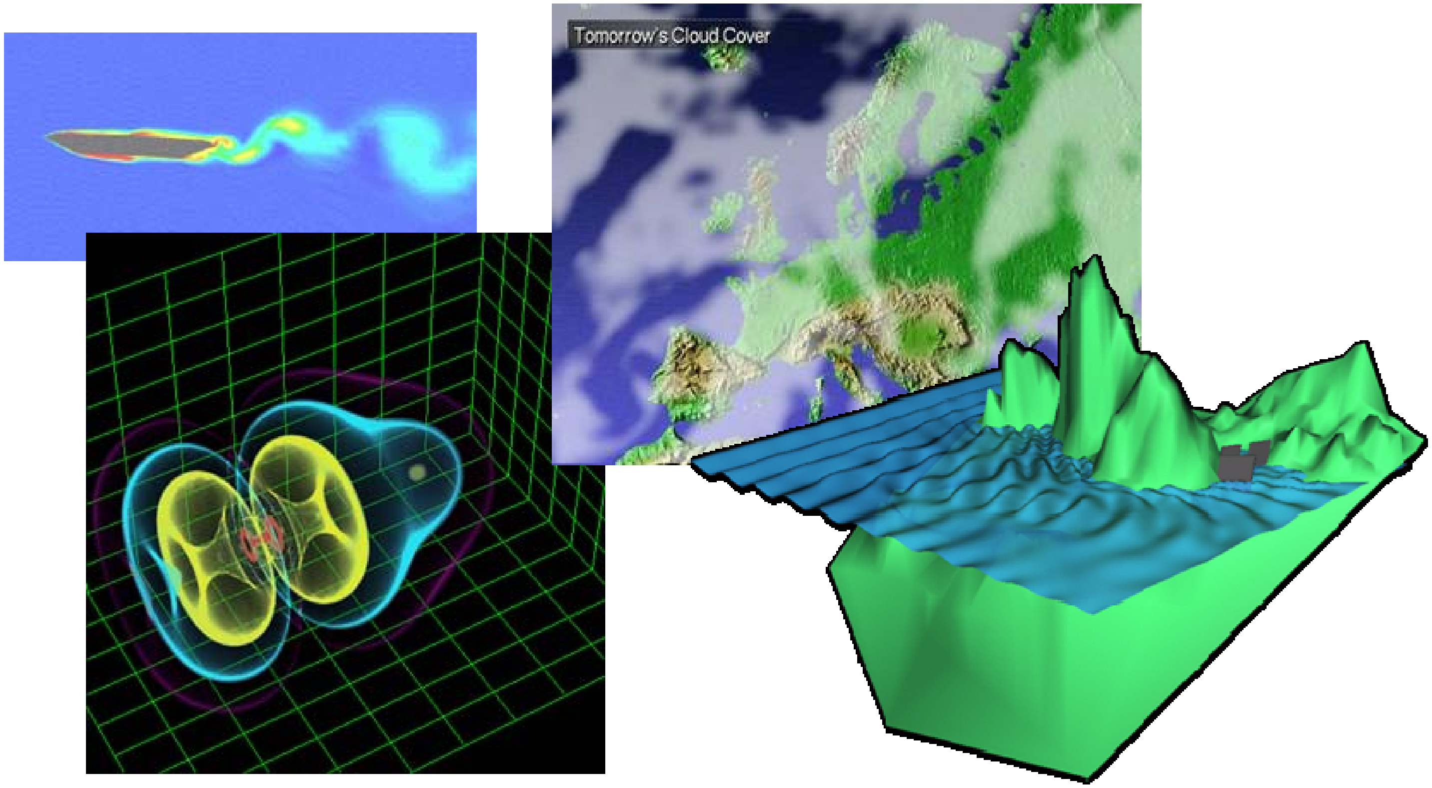
$$A \underset{k_d}{\overset{k_a}{\rightleftarrows}} B \xrightarrow{k_r} P$$

Reaction equations:

$$\begin{aligned}
\phi \frac{da^*}{dt^*} &= -k_a \phi a^* \left(1-\phi\right)\left(B_0 - b^*\right) + k_d \left(1-\phi\right) b^*, \\
\left(1-\phi\right) \frac{db^*}{dt^*} &= k_a \phi a^* \left(1-\phi\right)\left(B_0 - b^*\right) - k_d \left(1-\phi\right) b^* - k_r \left(1-\phi\right) b^*, \\
\phi \frac{dp^*}{dt^*} &= k_r \left(1-\phi\right) b^*.
\end{aligned}$$

ϕ : Porosity

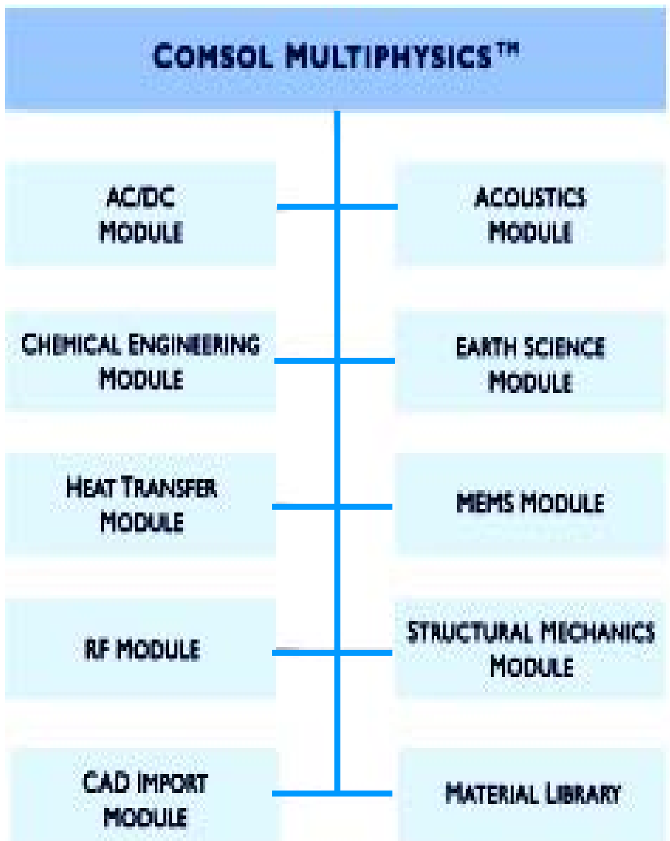
MATHEMATICAL MODELLING AND THE NEW TOOLS

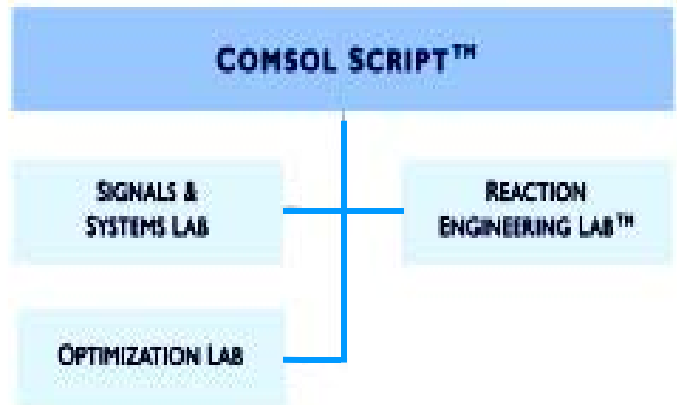


Computational Science and Engineering

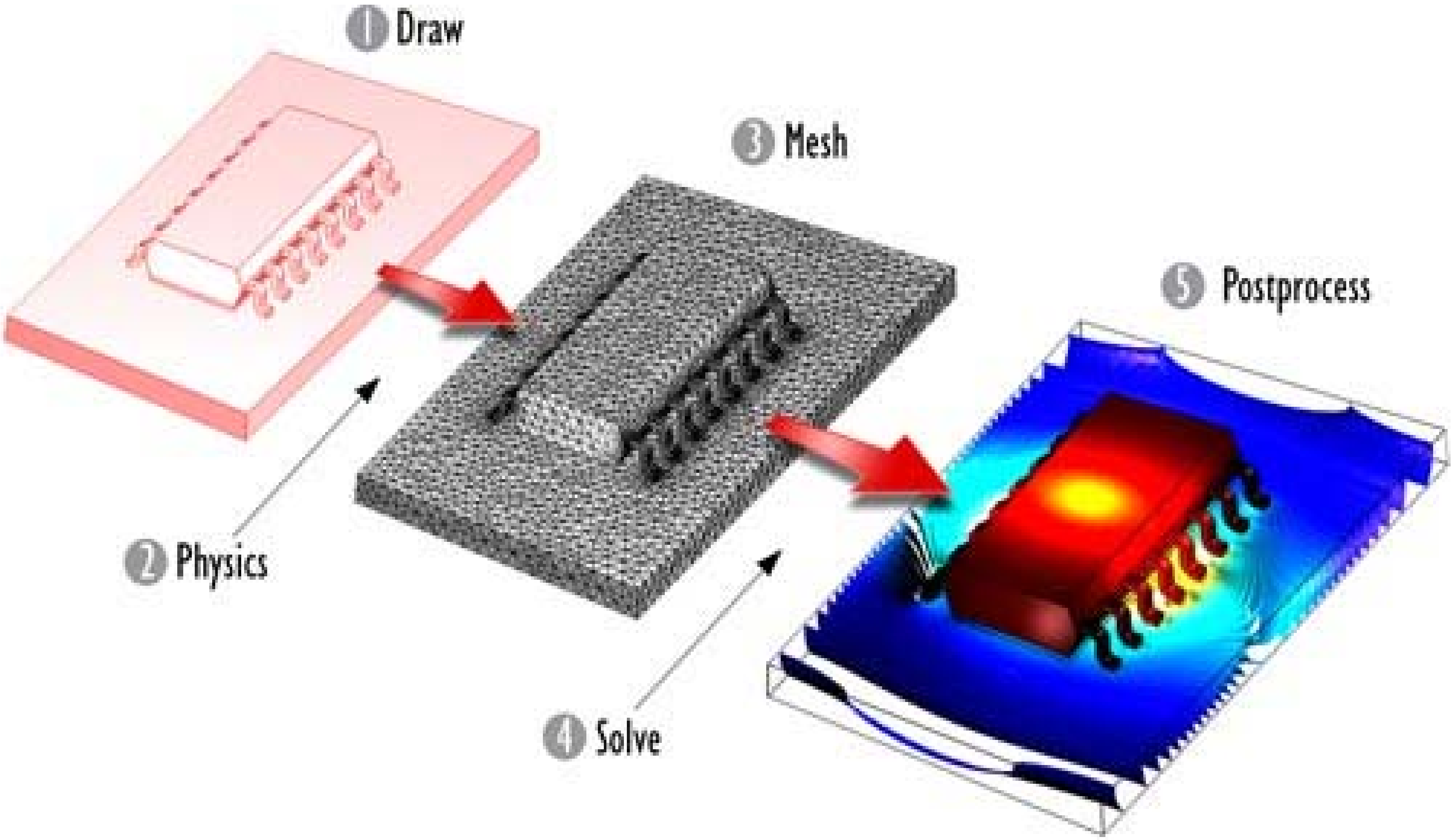
THE COMSOL MULTIPHYSICS^{TM} SYSTEM

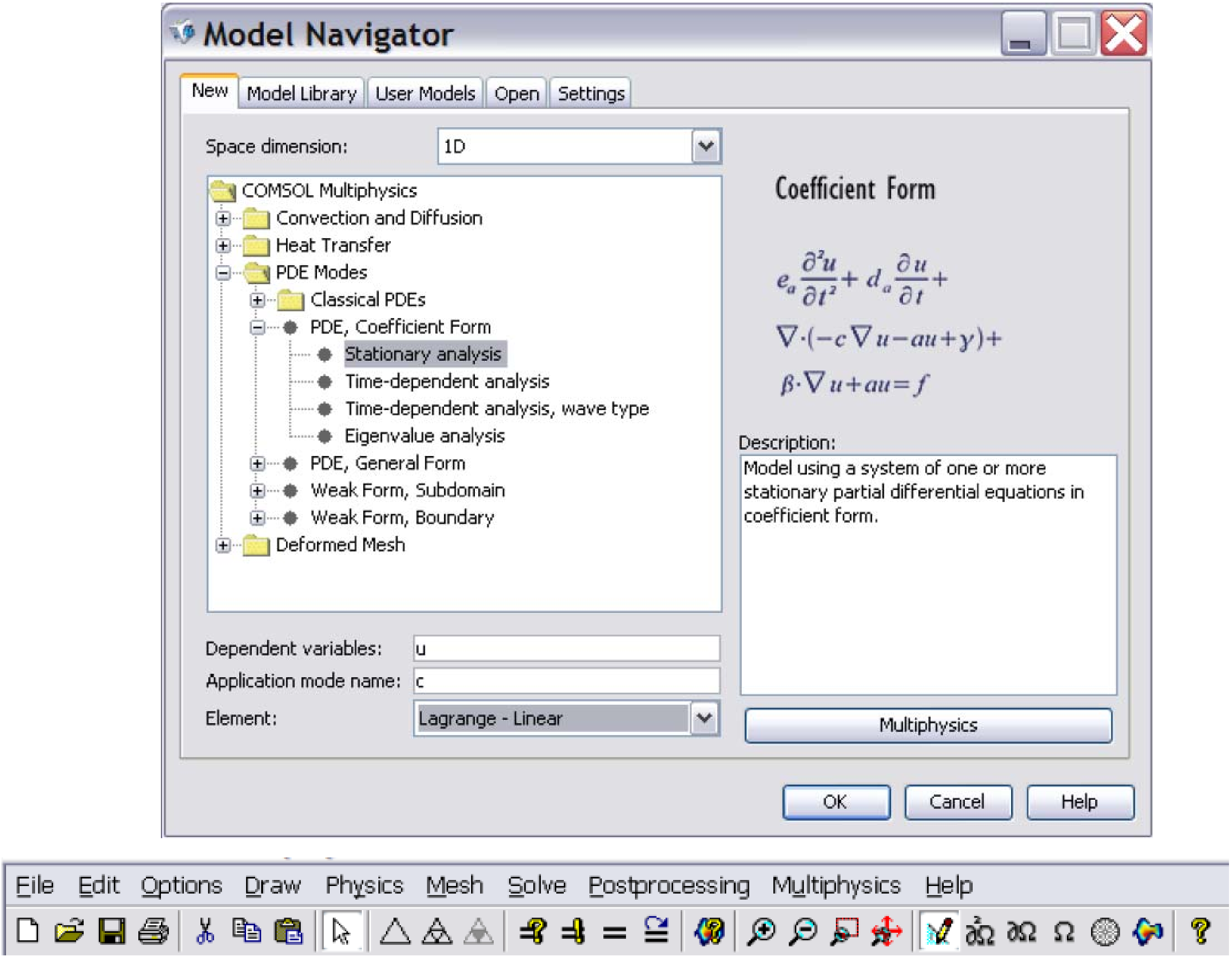
Matlab → PDE Toolbox →
FEMLAB → COMSOL MULTIPHYSICS

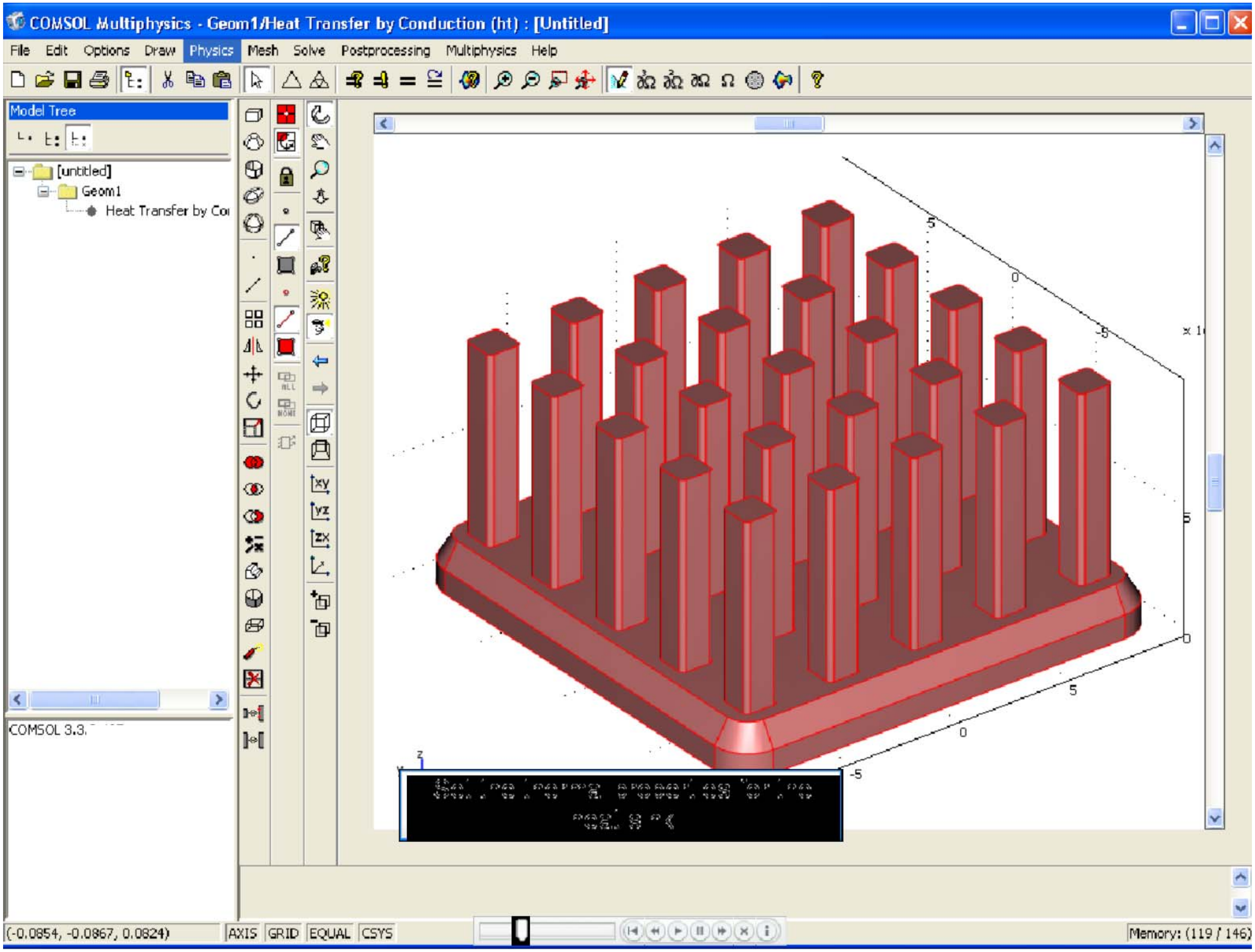




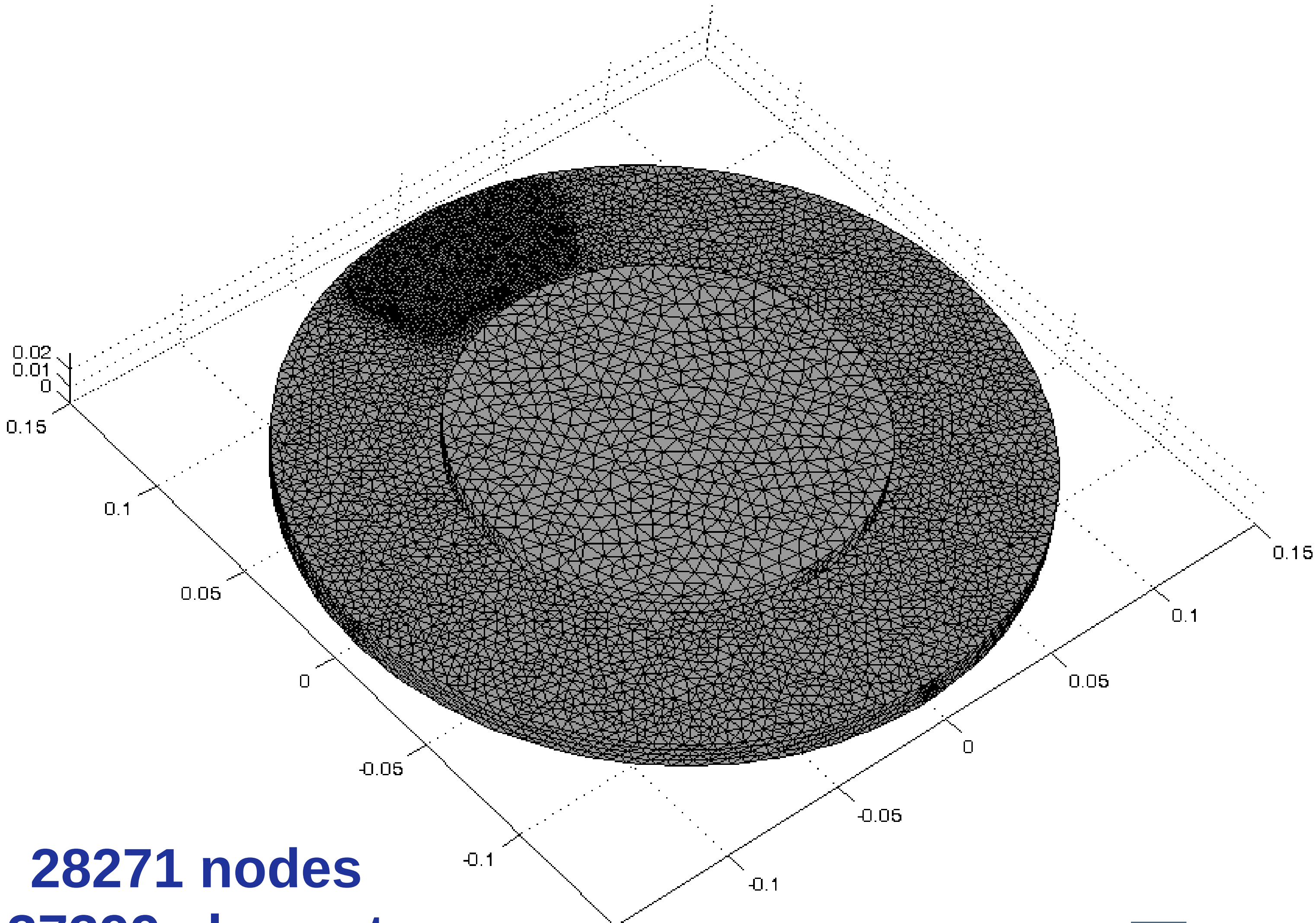
MODELLING WORKFLOW:




Model Navigator
New
Model Library
User Models
Open
Settings
Space dimension:
1D
COMSOL Multiphysics
Convection and Diffusion
Heat Transfer
PDE Modes
Classical PDEs
PDE, Coefficient Form
Stationary analysis
Time-dependent analysis
Time-dependent analysis, wave type
Eigenvalue analysis
PDE, General Form
Weak Form, Subdomain
Weak Form, Boundary
Deformed Mesh
Coefficient Form
$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla \cdot (-c \nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + au = f$
Description:
Model using a system of one or more stationary partial differential equations in coefficient form.
Dependent variables:
u
Application mode name:
c
Element:
Lagrange - Linear
Multiphysics
OK
Cancel
Help
File
Edit
Options
Draw
Physics
Mesh
Solve
Postprocessing
Multiphysics
Help

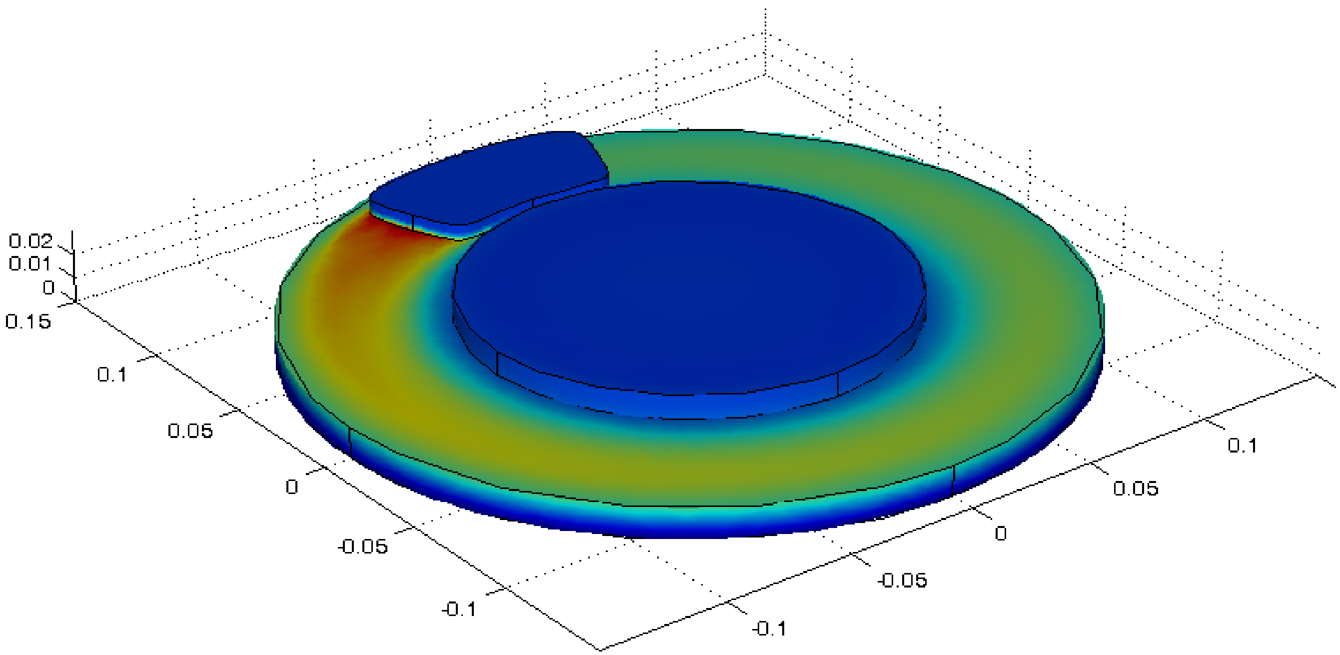

COMSOL Multiphysics - Geom1/Heat Transfer by Conduction (ht) : [Untitled]
File Edit Options Draw Physics Mesh Solve Postprocessing Multiphysics Help
Model Tree
[untitled]
Geom1
Heat Transfer by Co
(-0.0854, -0.0867, 0.0824)
AXIS GRID EQUAL CSYS
Memory: (119 / 146)

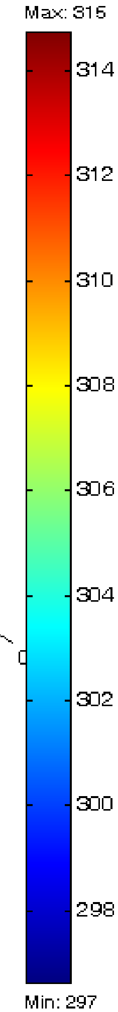
MODELLING OF HEAT IN A DISK-BRAKE



28271 nodes
137399 elements

TEMPERATURE DISTRIBUTION





$$\rho C \frac{\partial T}{\partial t} - \nabla \bullet \left(k \nabla T \right) = \rho C \omega \left(y \frac{\partial T}{\partial x} - x \frac{\partial T}{\partial y} \right)$$

THE STUDENTS' EXPERIENCE:

***Mathematics*: Difficult methods applied to simple problems!**

***Modelling*: Simple methods applied to difficult problems!**

Today it is

- ❑ easy to measure
- ❑ easy to compute
- ❑ easy to visualize
- ❑ easy to write

… *but still hard to understand what is really going on!*

Knowledge and use of mathematics is and will probably forever be the best way to understand the world around us.