UNIVERSITAT POLITÈCNICA DE CATALUNYA

LABORATORI DE CÀLCUL NUMÈRIC

COMPUTATIONAL MECHANICS TOOLS
Introduction

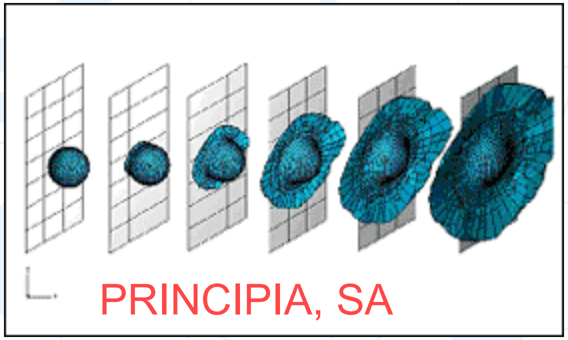
Laboratori de Càlcul Numèric (LaCàN)

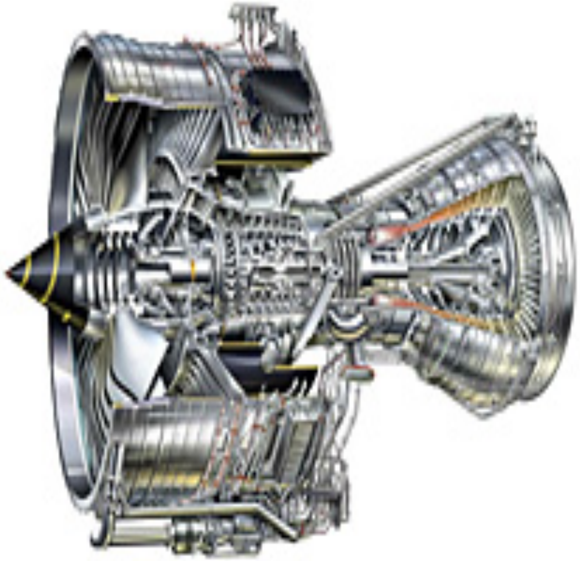
Universitat Politècnica de Catalunya (Spain)

http://www-lacan.upc.es

Motivation: Why?

- Cost effective

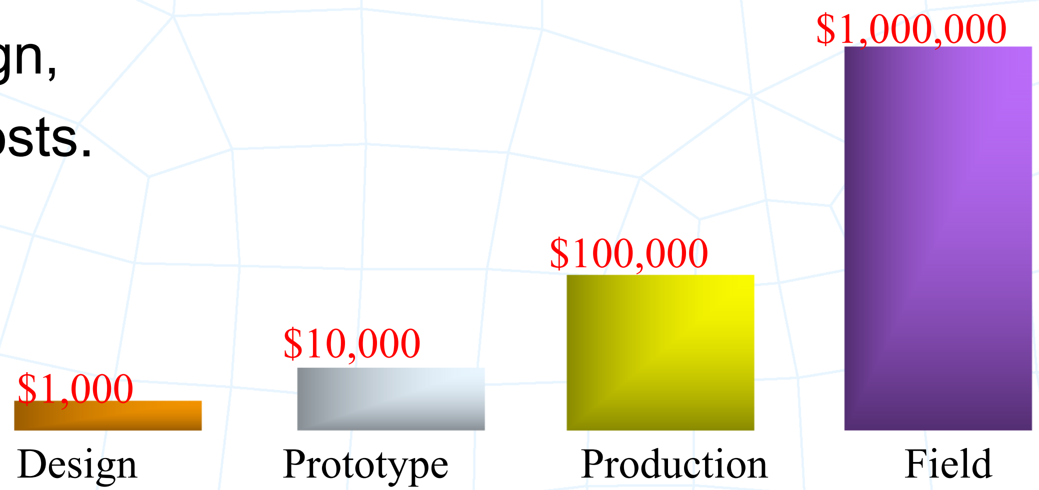




- Complements experiments
- Crucial technology at the design stage
- Identifies:
  - Suitable materials
  - Product performance
  - Process conditions

Motivation: Why?

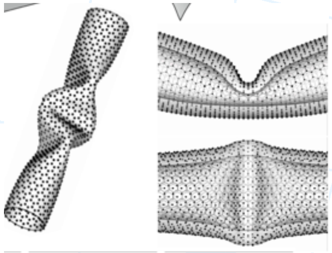
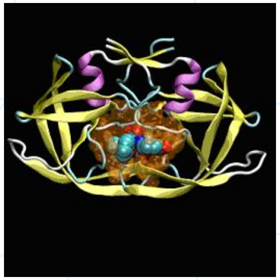
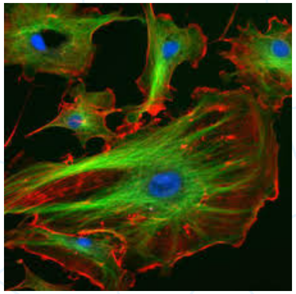
- Save money $$$$
  - field failures, redesign, rework and scrap costs.



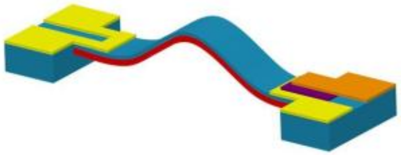
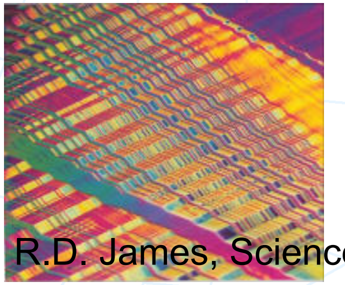
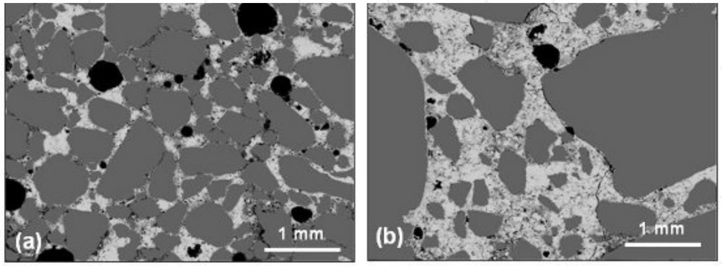
- Save time
  - Manufacturing → 80% of time
- Modelling also helps generate new knowledge

Computational Mechanics: multiple scales

- Nanomechanics: atoms, molecules, cells,…

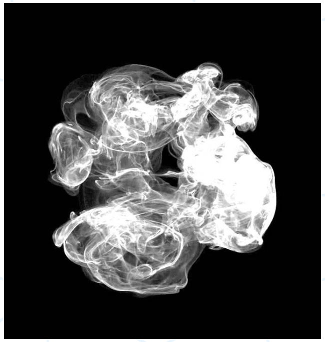
- Micromechanics: MEMS, material microstructure,…



R.D. James, Science


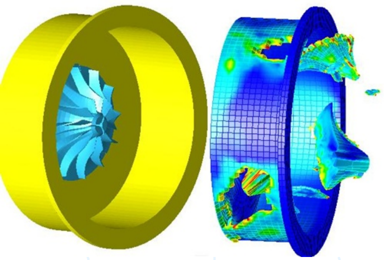
- Solids and Structures: civil engineering structures,…


Computational Mechanics: multiple physics

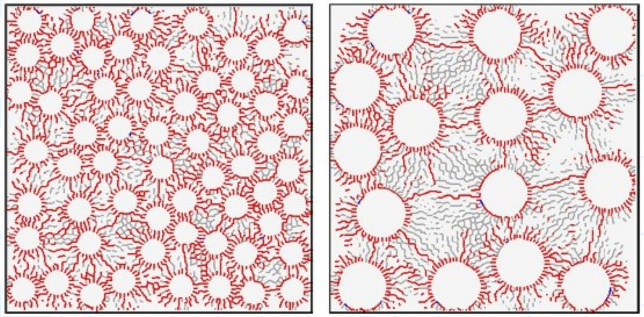
- Fluids: liquids, gases



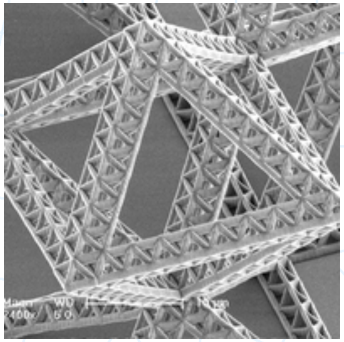
- Coupled systems: thermo-mechanical, fluid-solid



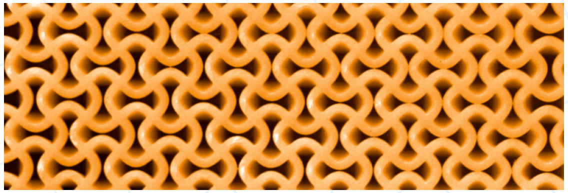
- Multi-scale: solid with microcracks or cellular structure,…



Nick Buenfeld, Imperial College

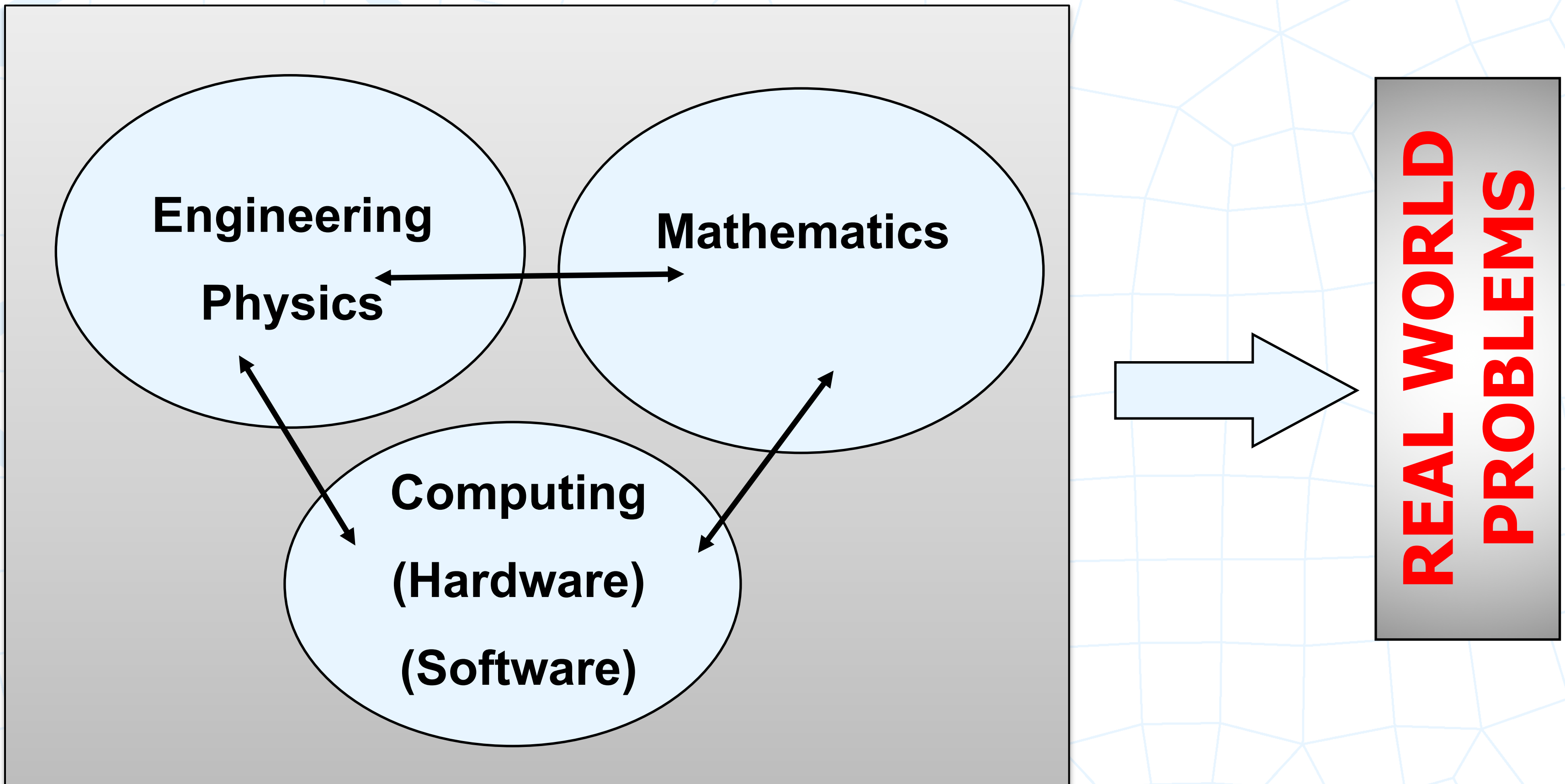


Julia Greer, CalTech

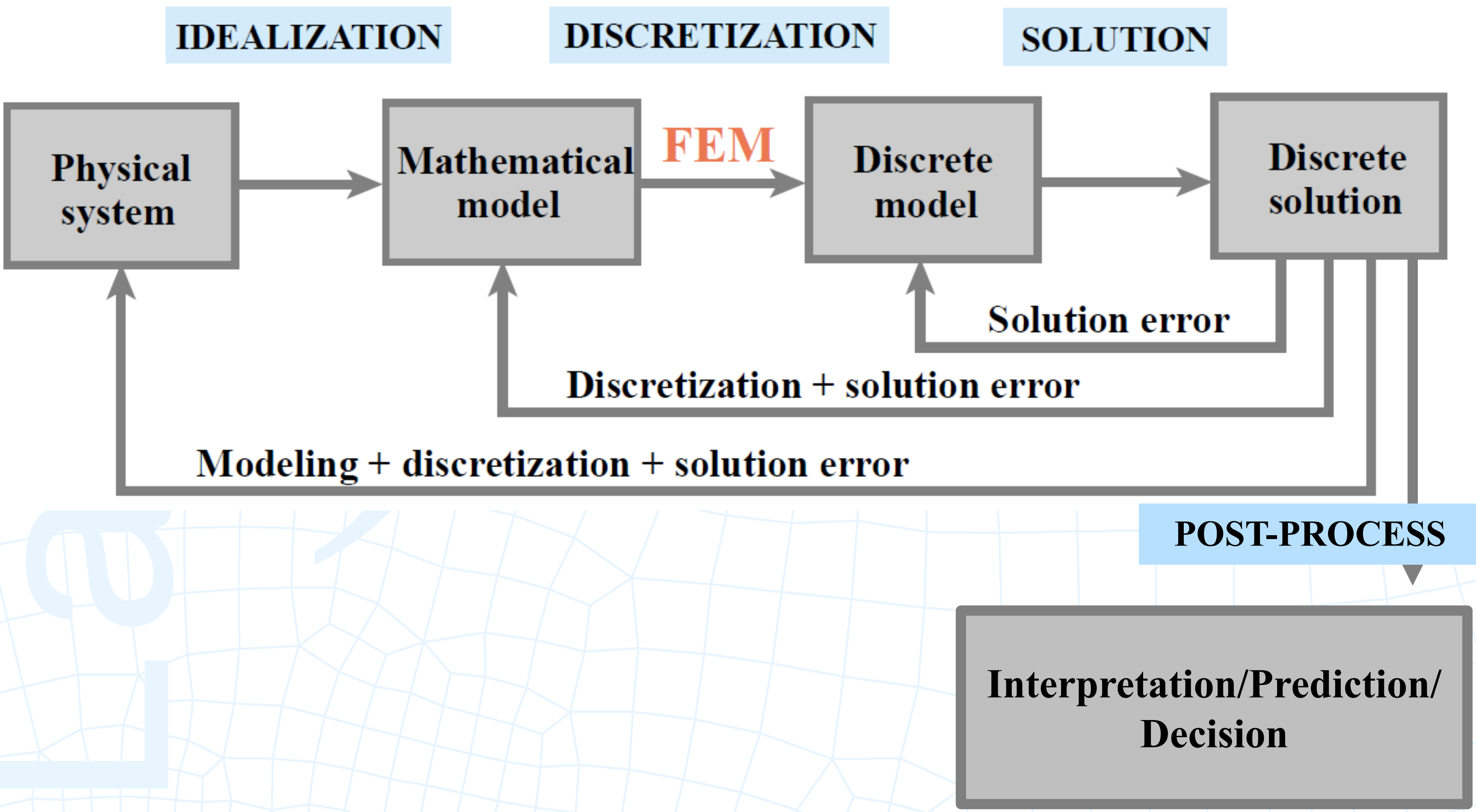


Katia Bertoldi, Harvard

Key Ingredients and Steps



Key Ingredients and Steps

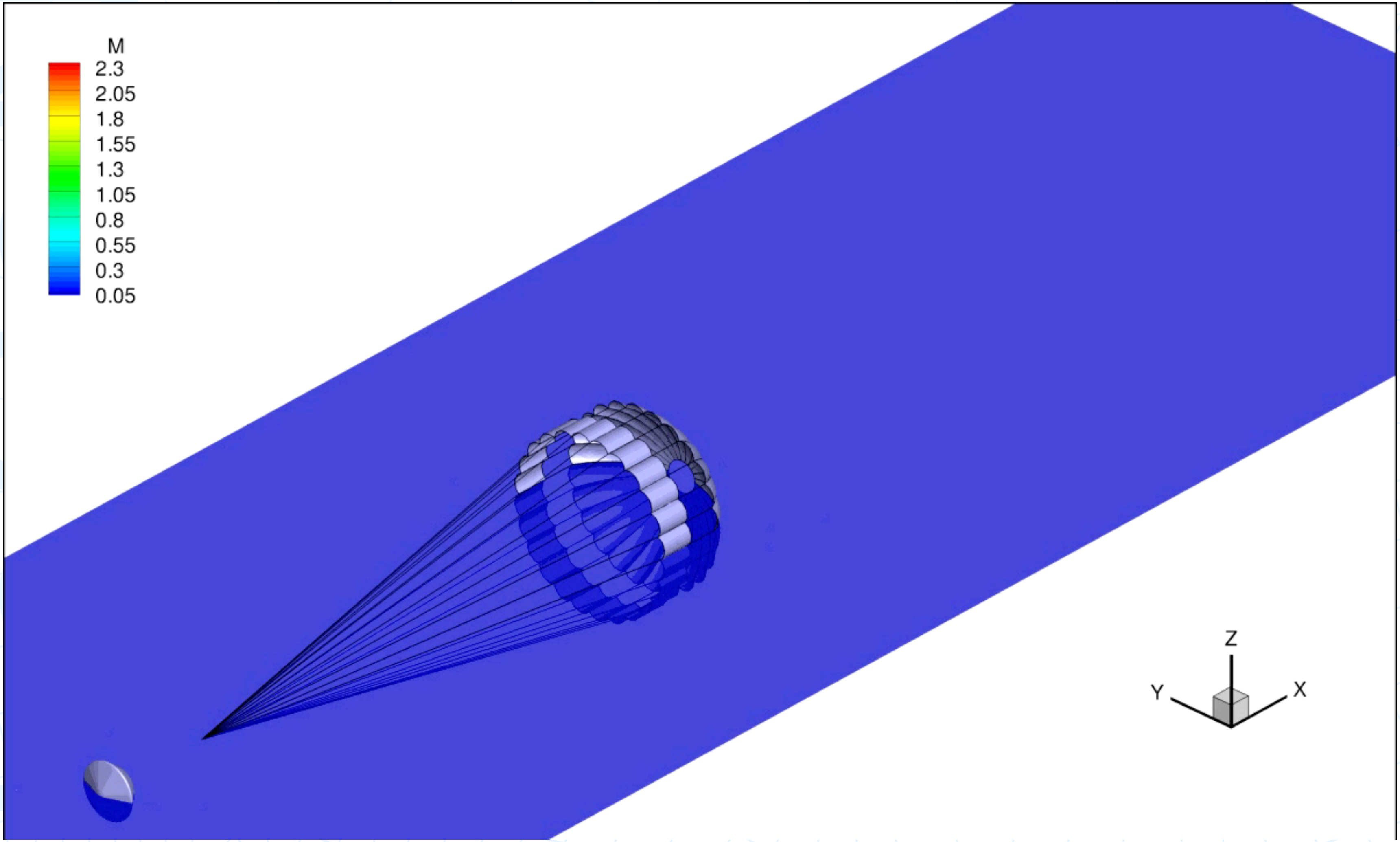


Idealization

- The aim is to encode a real engineering problem by means of a physical model. Note that, with this step, we are idealizing the real problem, but computational engineering allows us to do it in a more realistic way than classical engineering.
- Then, the physical model needs to be formulated in a mathematical way (i.e. govern equations), prior to solve it numerically
- This is a fundamental step and requires a deep knowledge of the real problem to be solved. Decisions need to be taken:
  - *Which physical phenomena are relevant?* (heat conduction, flux in porous media, solid or fluid mechanics, electromagnetism, acustics, coupling)
  - *Solid or structural model*
  - *Governing material parameters-> behavior laws*
  - *Static or dynamic model*
  - ***Boundary conditions***

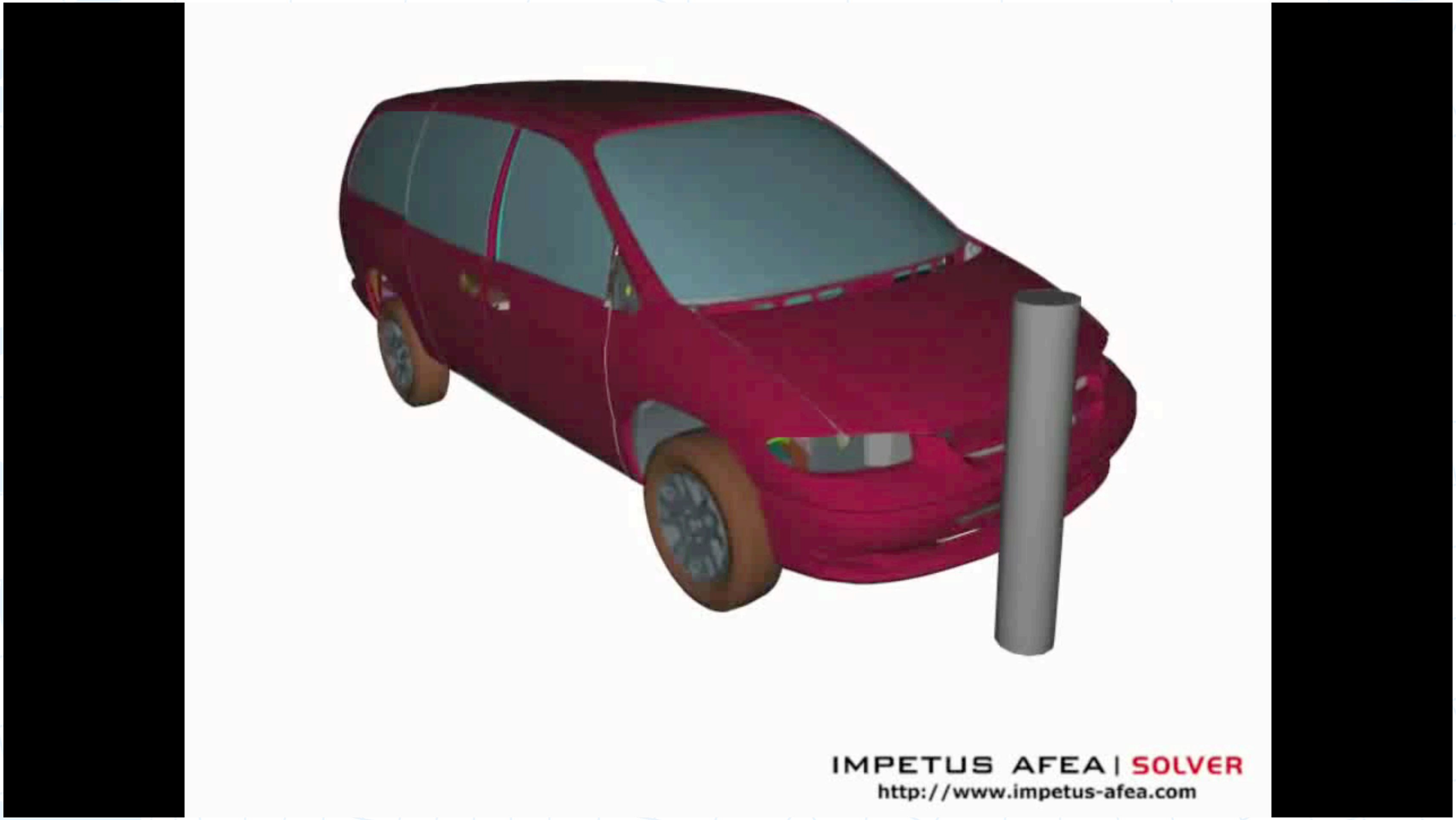
Idealization

A coupled fluid-structure problem: compressible inviscid fluid (Cirak, Cambridge)



Idealization

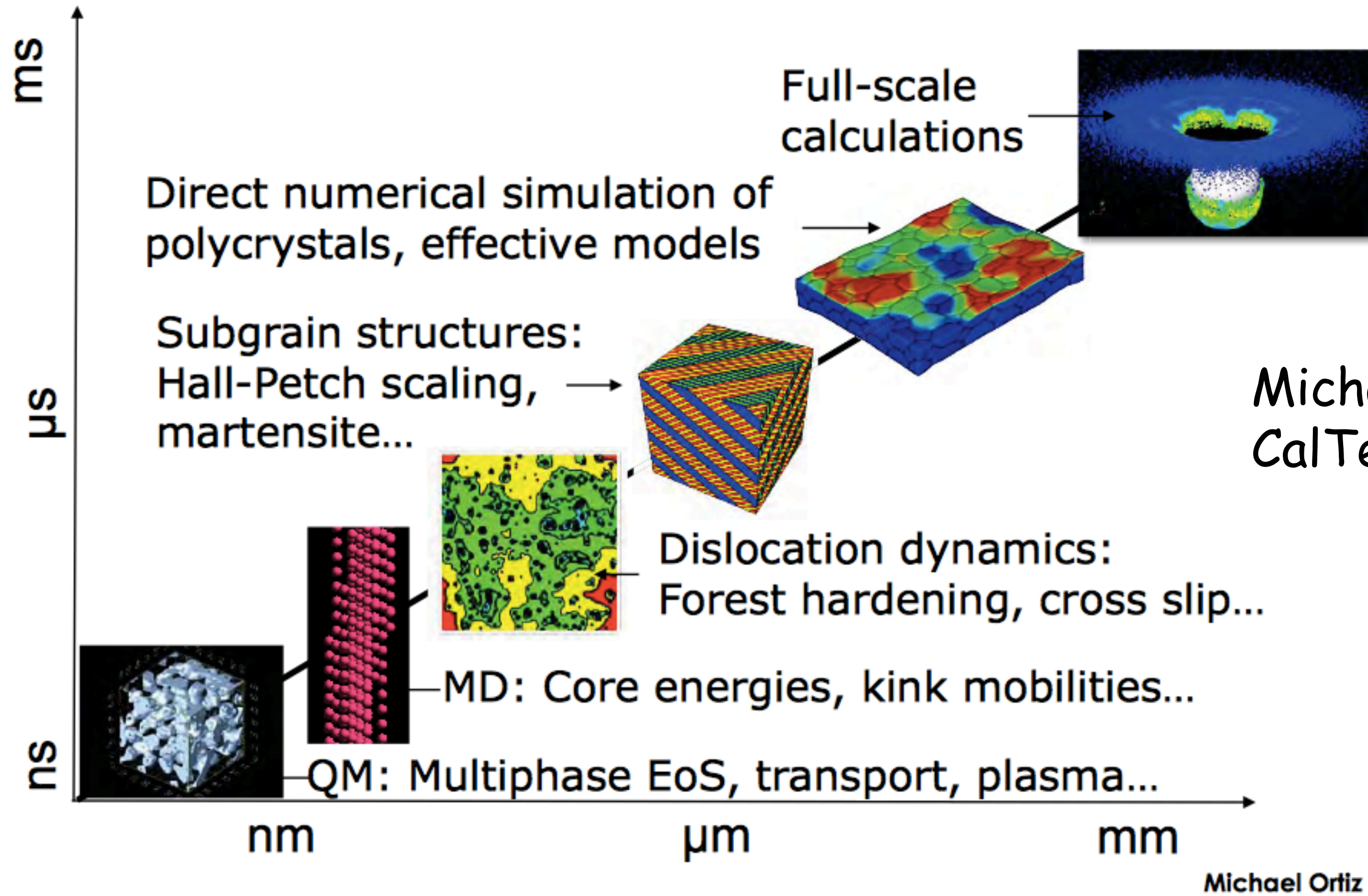
Virtual car crash analysis, pioneered by Ted Belytschko in the 80s.



Idealization

Material modeling is crucial in many cases

Unfortunately, the *homogeneous linearly elastic solid* is NOT ENOUGH in some cases.



Michael Ortiz
CalTech

Idealization

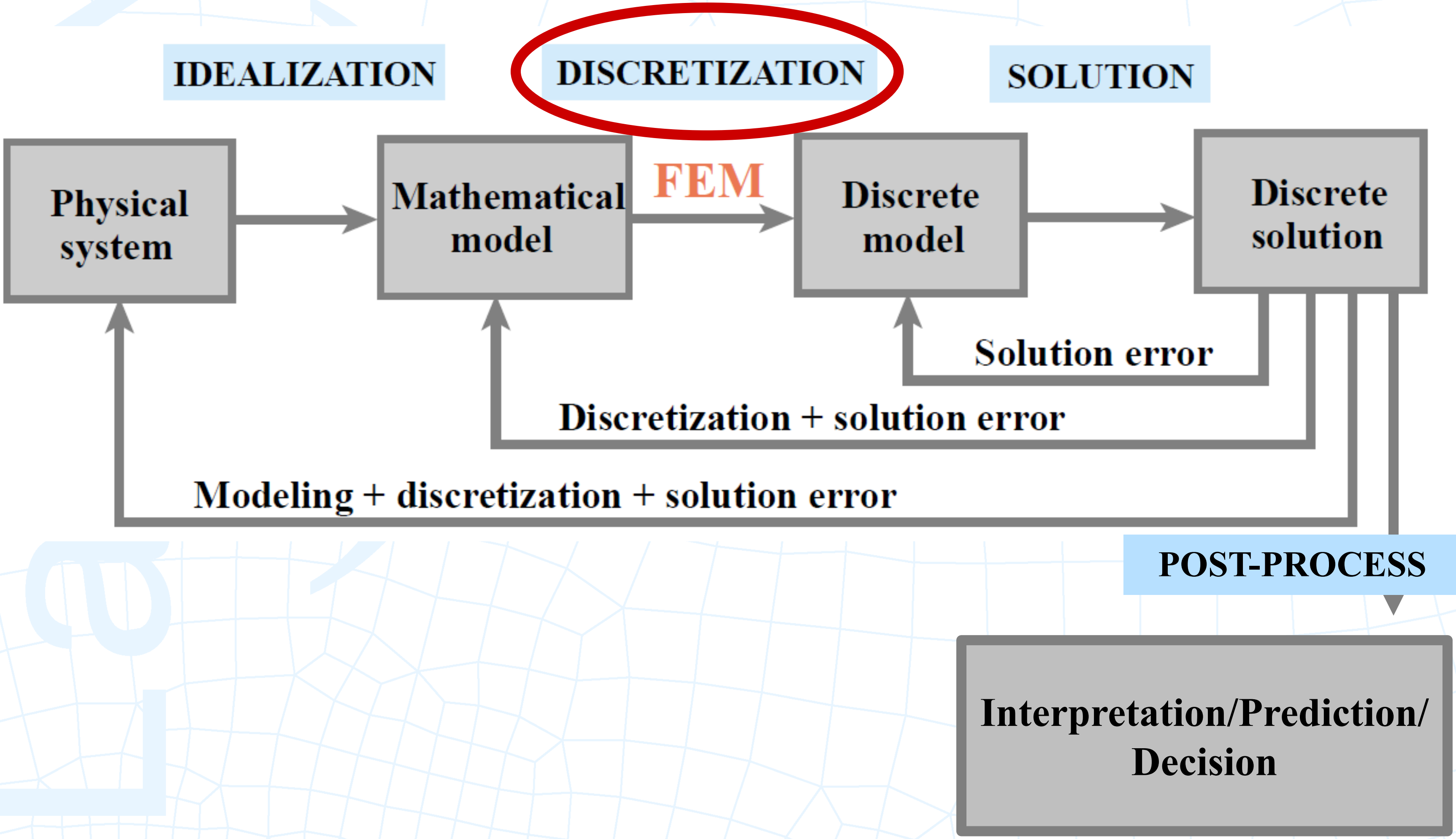
- The idealization process is obviously bound to **errors**. The control of those errors is called **VALIDATION** of the model.

Are we solving the right equations?

- Often it requires direct comparison with experiment or observation, or sometimes other models.

Arias & Arroyo

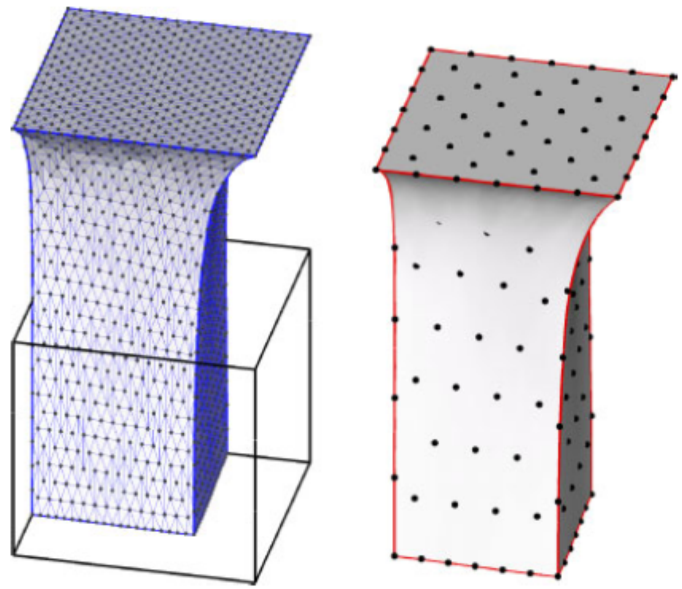
Key Ingredients and Steps



Discretization and solution

Warning: Not to use as a "black box"

- Type of method
  - Finite differences
  - Finite elements
  - Boundary elements
  - Finite volumes
  - Meshless methods



- Type of element (instabilities/locking)
- Type of *solver*
  - Linear systems of equations
  - Non-linear systems of equations
  - Time integration scheme

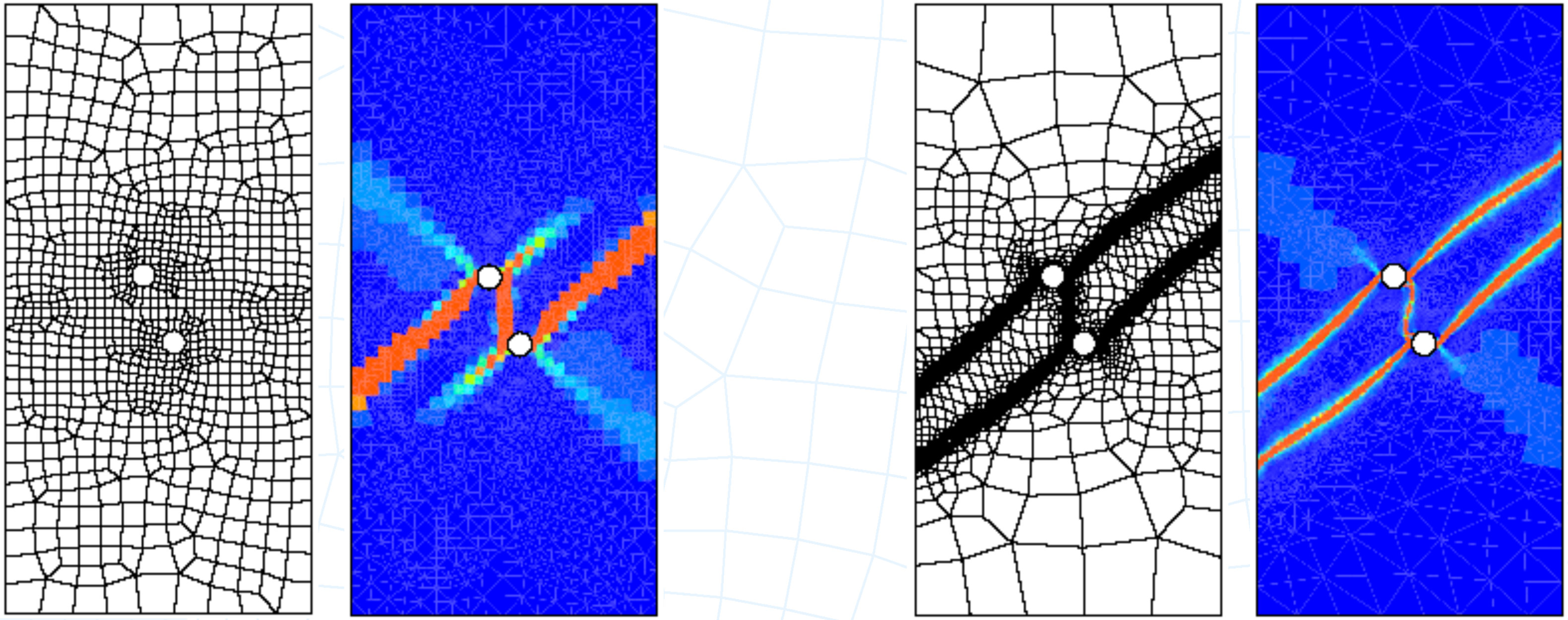
Discretization and solution

Discretization leads to numerical errors.

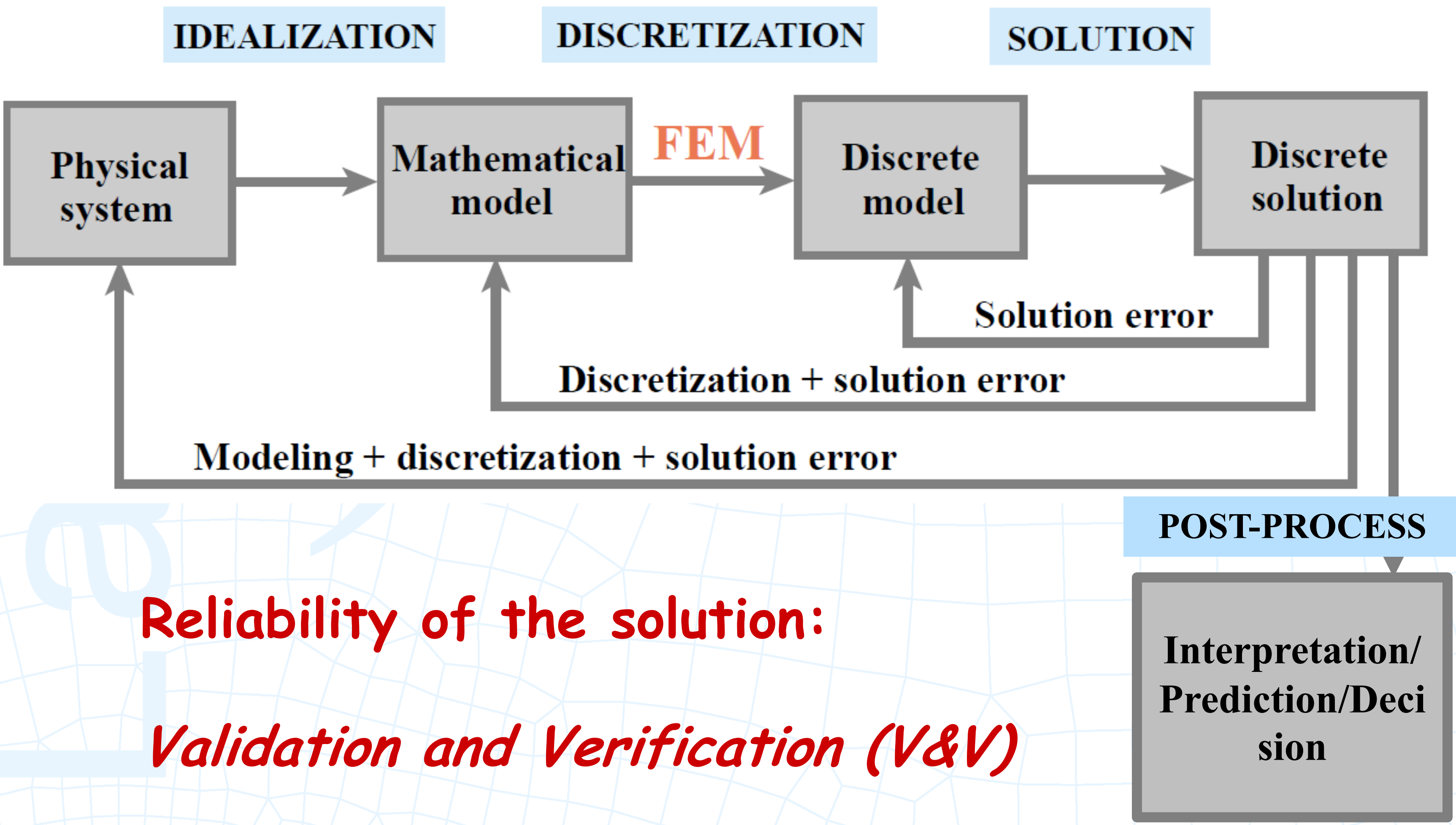
The control of those errors is called **VERIFICATION** of the numerical method.

Are we solving the equations right?

Error estimation and adaptivity



Key Ingredients and Steps



Reliability of the solution:

Validation and Verification (V&V)

Computational Engineering

The **cost** of the numerical solution depends on:

- In the whole computational engineering approach:
  - Hardware (serial/parallel computing)
  - Software
  - Know-how
- In the solution step:
  - Pre-process (preparing data)
  - Process (computation)
  - Post-process

Depending on the type of problem, one or other element becomes critical.

Problem classification: time-dependence

- **Statics**: no time dependence (steady solution), and inertial terms are negligible.

$$-\nabla \cdot \sigma(u) = f \qquad \text{in } \Omega$$

- **Quasi-static**: external forces or material properties may be time-dependent, but no inertial forces (no time-derivatives).

- **Dynamics**: time dependence is explicit, and inertial forces cannot be neglected.

$$\beta \frac{\partial^2 u}{\partial t^2} + \alpha \frac{\partial u}{\partial t} + \mathcal{L}u = f \qquad u \in \overline{\Omega} \times [0, \infty[$$

Problem classification: linearity

- Linear
  - Cause-effect proportionality
  - If the applied forced are doubled, then, displacements and internal stresses are doubled.
  - The solution of the discretised problem is found by solving a system of linear equations:

$$\mathbf{K}\boldsymbol{u}=\boldsymbol{f}$$

- Non-linear
  - All remaining cases…
  - The solution of the discretized problem is found by solving a non-linear equation:

$$\boldsymbol{g}(\boldsymbol{u},\dot{\boldsymbol{u}},\ldots)=\boldsymbol{f} \quad \text{or} \quad \mathbf{K}(\boldsymbol{u})\boldsymbol{u}=\boldsymbol{f}$$

Physical classification

1. Equilibrium problems

Steady. Defined in closed domains.

Example: heat equation

- Equilibrium: $\nabla \cdot \mathbf{q} = 0$

- Fourier's law:

$$\mathbf{q} = -\mathbf{K}\,\nabla\mathbf{T} = \begin{bmatrix} k_x & & \\ & k_y & \\ & & k_z \end{bmatrix} \begin{pmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{pmatrix}$$

$$\frac{\partial}{\partial x}\left[k_x \frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_x \frac{\partial T}{\partial y}\right] + \frac{\partial}{\partial z}\left[k_x \frac{\partial T}{\partial z}\right] = 0$$

- Non isotropic, non homogeneous and nonlinear

$$k_r = k_r(x, y, z, T)$$

- Non isotropic and non homogeneous: $k_r = k_r(x, y, z)$

$$\frac{\partial}{\partial x}\left[k_x \frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_x \frac{\partial T}{\partial y}\right] + \frac{\partial}{\partial z}\left[k_x \frac{\partial T}{\partial z}\right] = 0$$

- Non isotropic, homogeneous:

$$k_x \neq k_y \neq k_z \qquad k_x = cte;\ k_y = cte;\ k_z = cte;$$

$$k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} = 0$$

- Isotropic and homogeneous: $k_x = k_y = k_z = k$

$$k\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right] = 0 \qquad \nabla^2 T = 0$$

2. Evolution problems

Defined in infinite domains (time)

- Diffusion problems (transient heat equation)

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[k_x \frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_x \frac{\partial T}{\partial y}\right] + \frac{\partial}{\partial z}\left[k_x \frac{\partial T}{\partial z}\right]$$

- Wave problems: displacement of a vibrating membrane

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right] = c^2\, \nabla^2 T$$

- Convection problems: pollutant transport

$$\frac{\partial u}{\partial t} + v\, \frac{\partial u}{\partial x} = 0$$

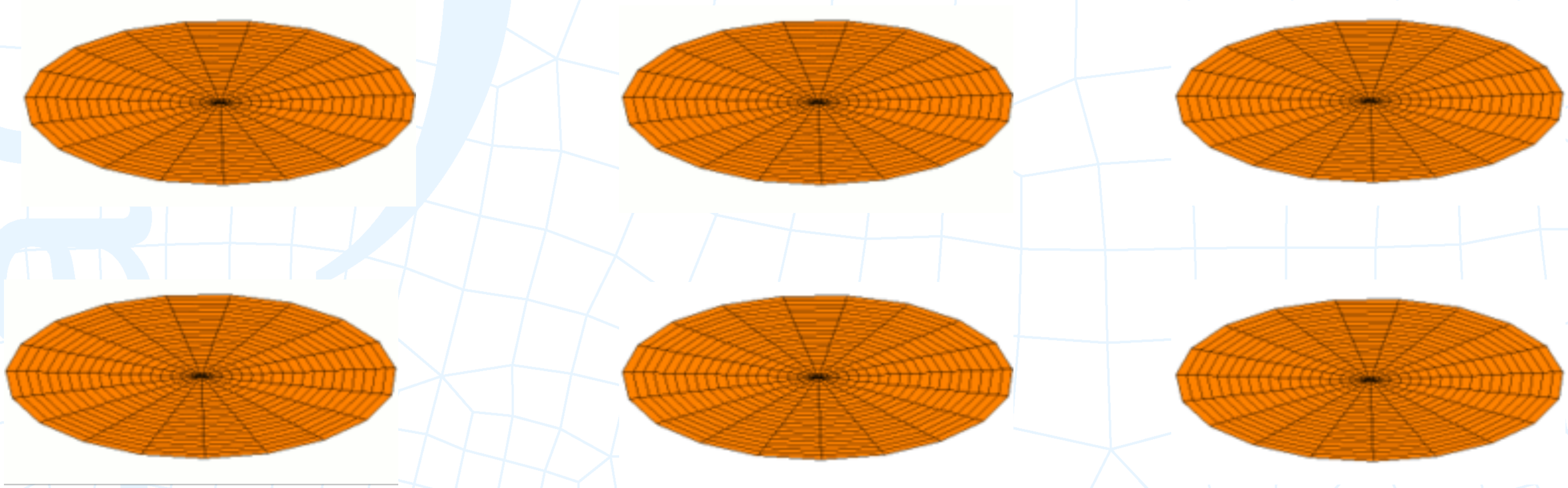
3. Eigenvalue problems

Steady problems whose solution exists only under certain conditions (for particular values of a given parameter).

Defined on closed domains.

Example: vibration of a circular drum

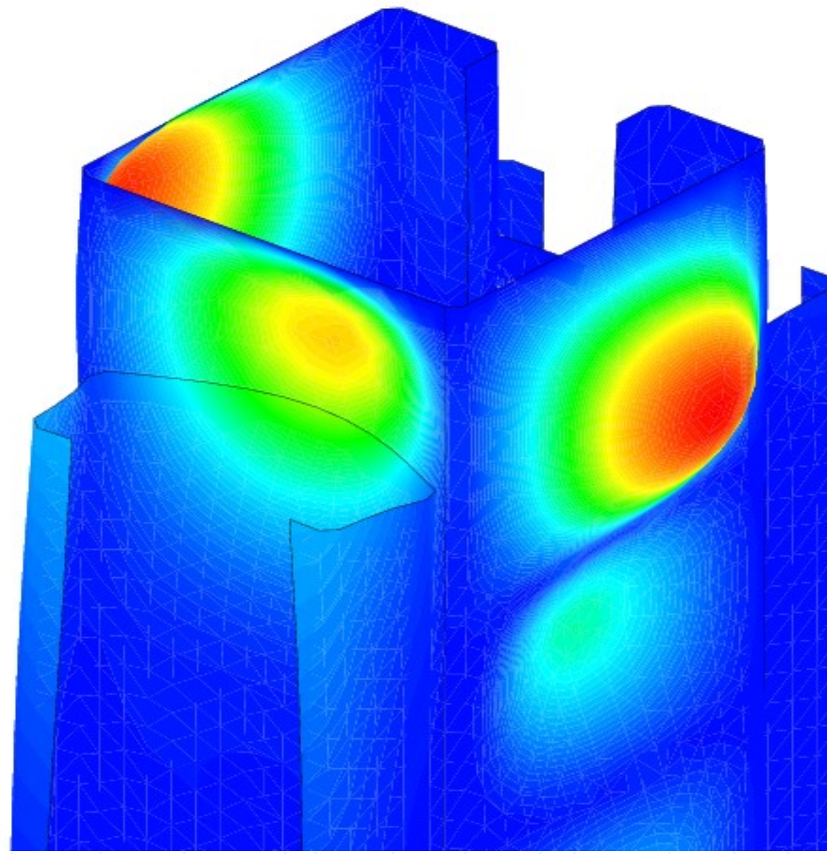
$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \lambda u = 0$$



Figures from wikipedia: Vibrations of a circular drum

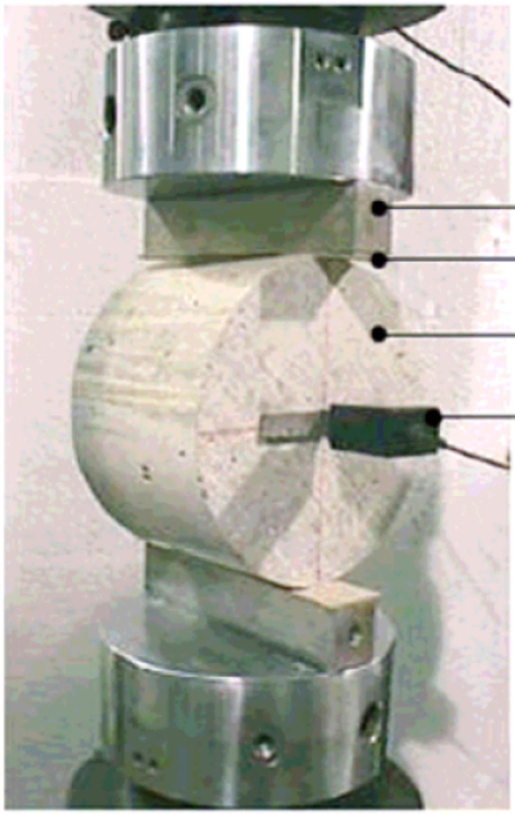
Examples: buckling in steel profiles

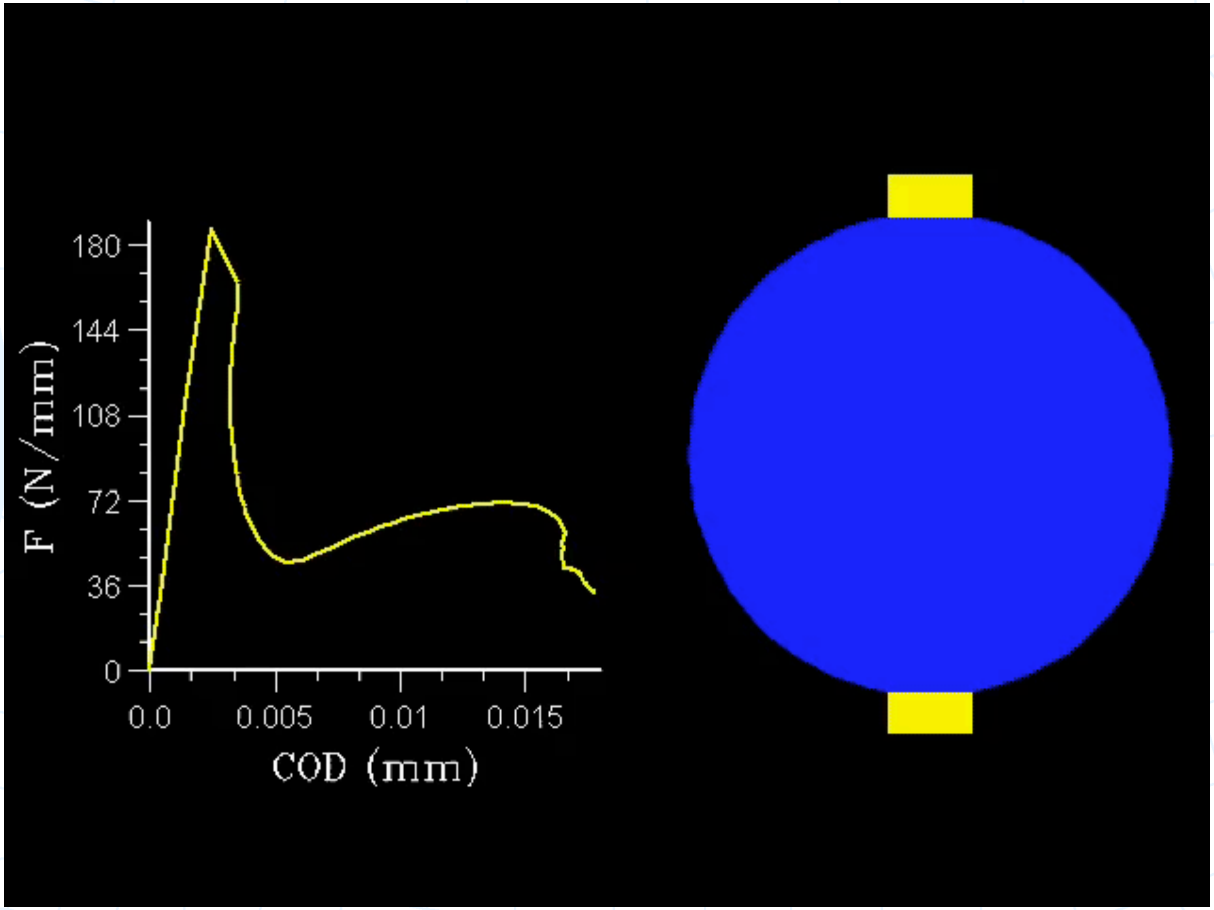
Comparison between experimental tests and numerical model



Mechanical problem: linear buckling analysis (eigenvalues)

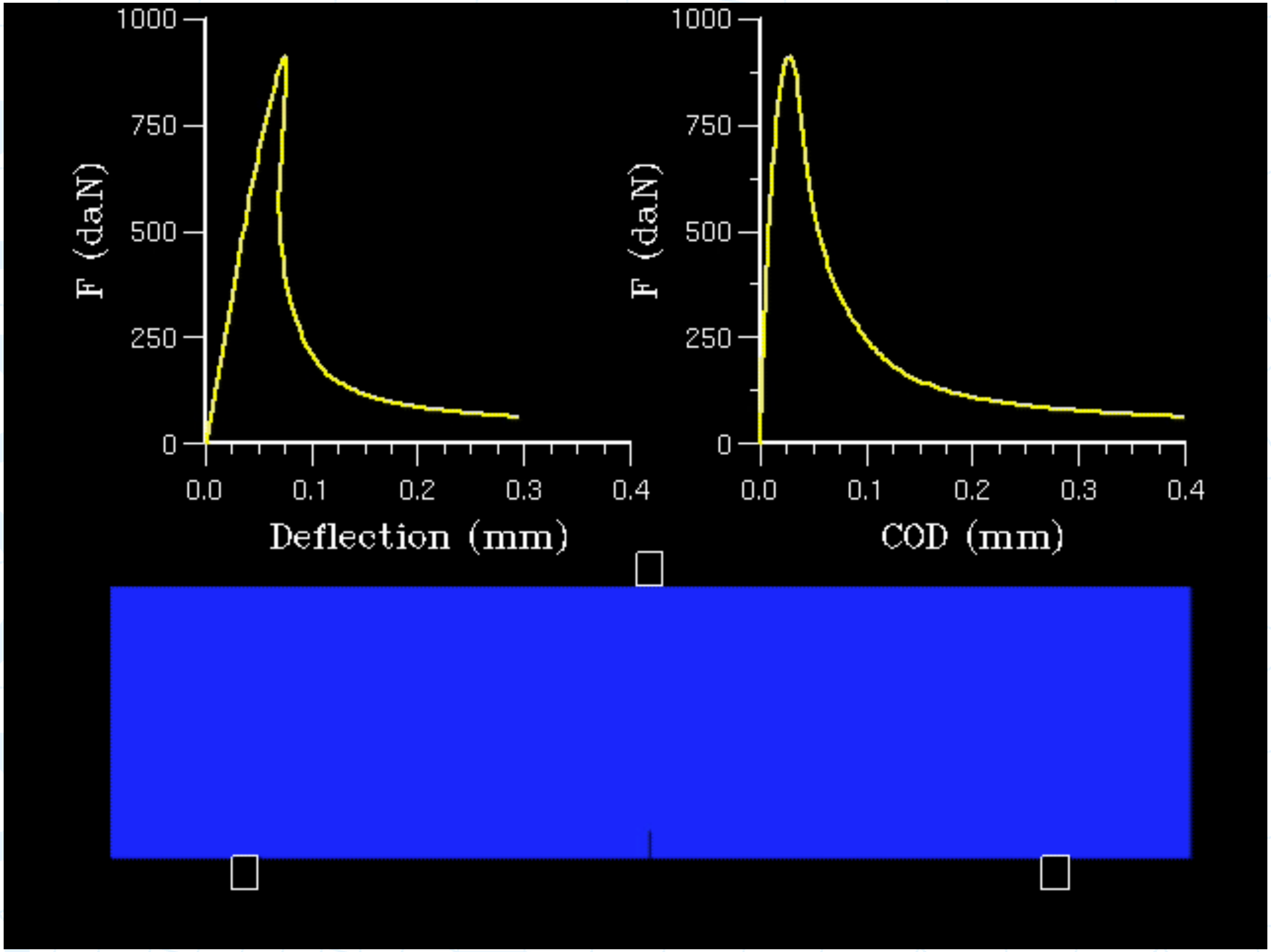
Examples: damage models





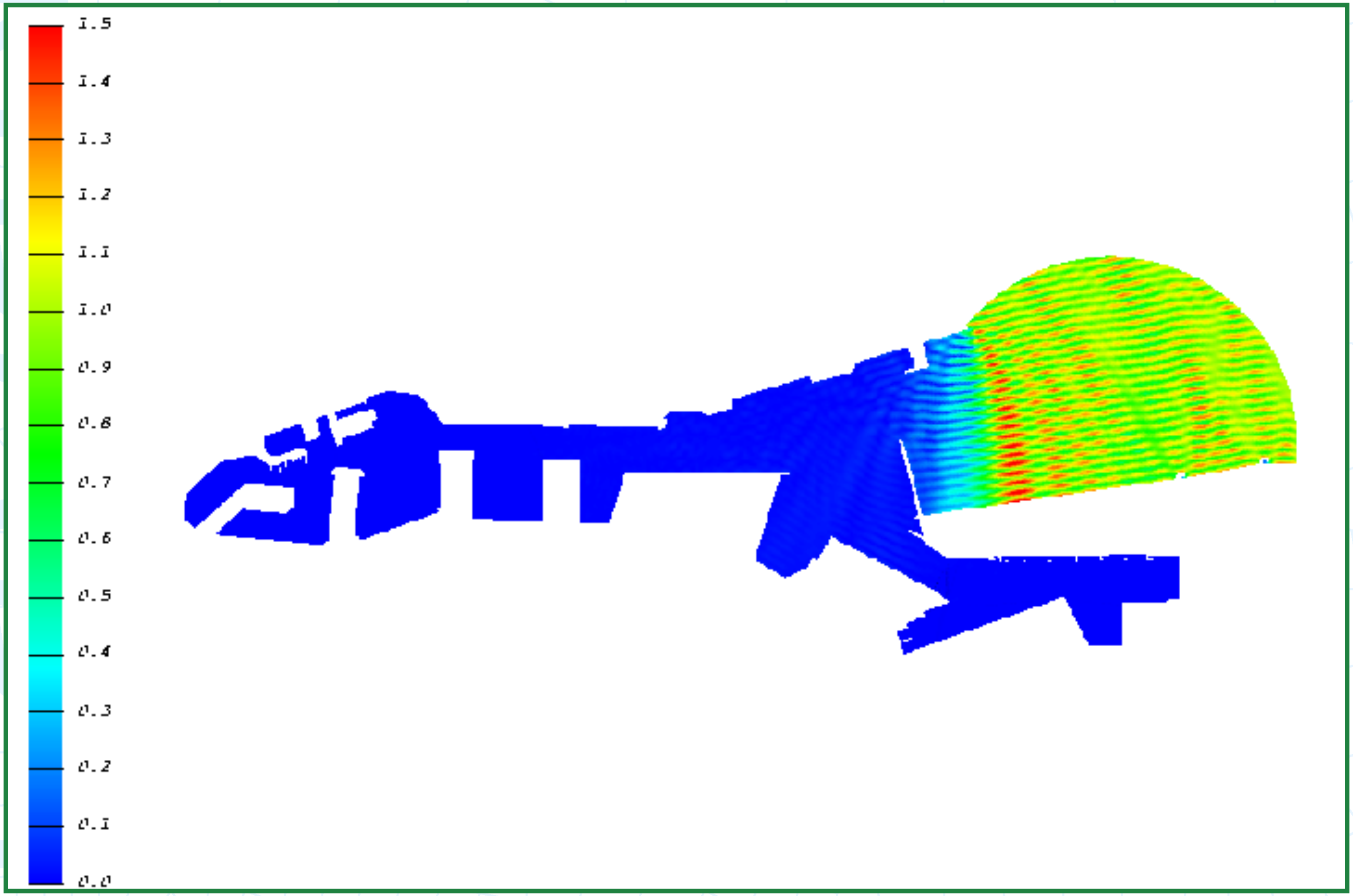
Mechanical problem: damage constitutive model (nonlinear)

Examples: Damage models



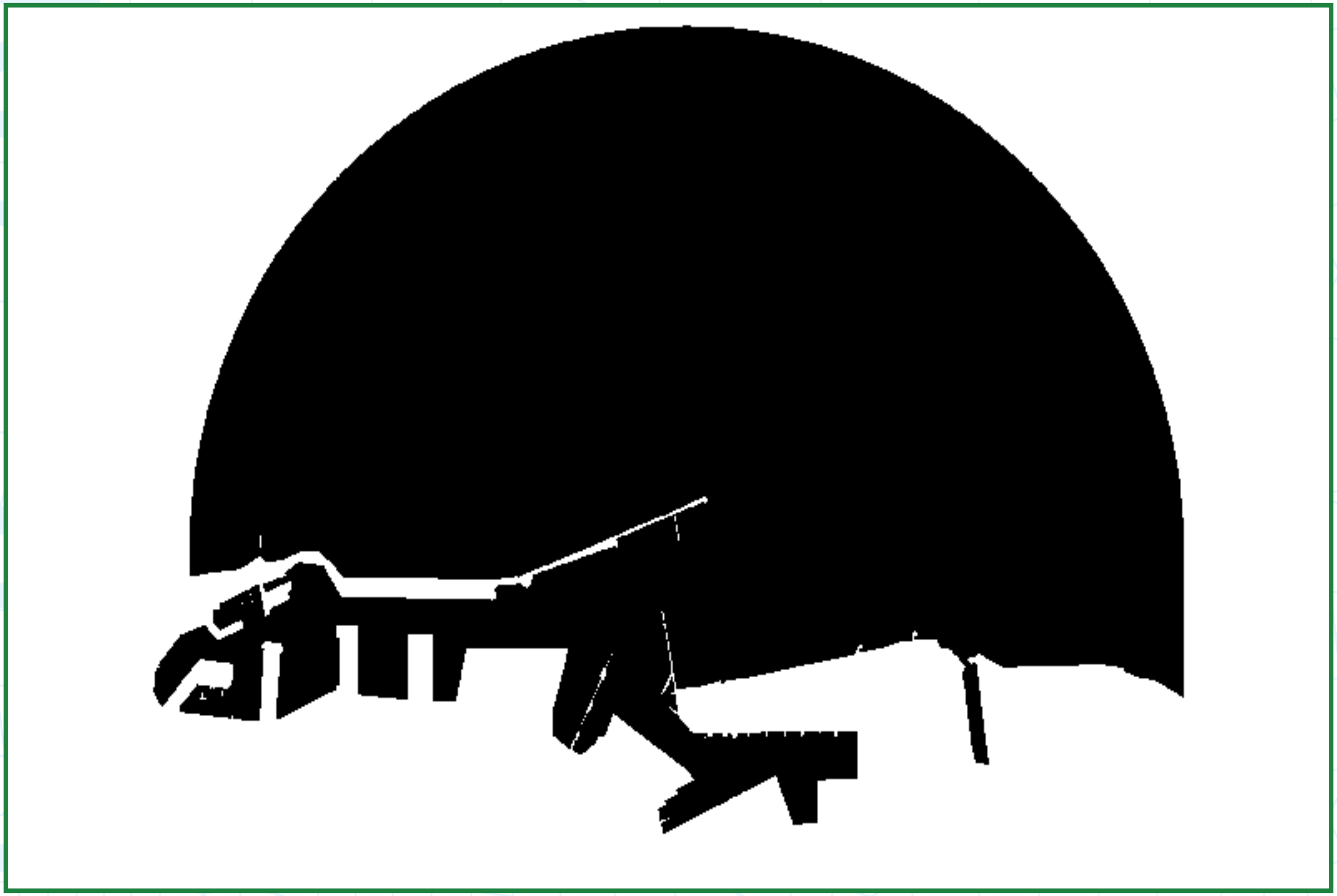
Mechanical problem: damage constiutive model (nonlinear)

Examples: wave height in Barcelona port



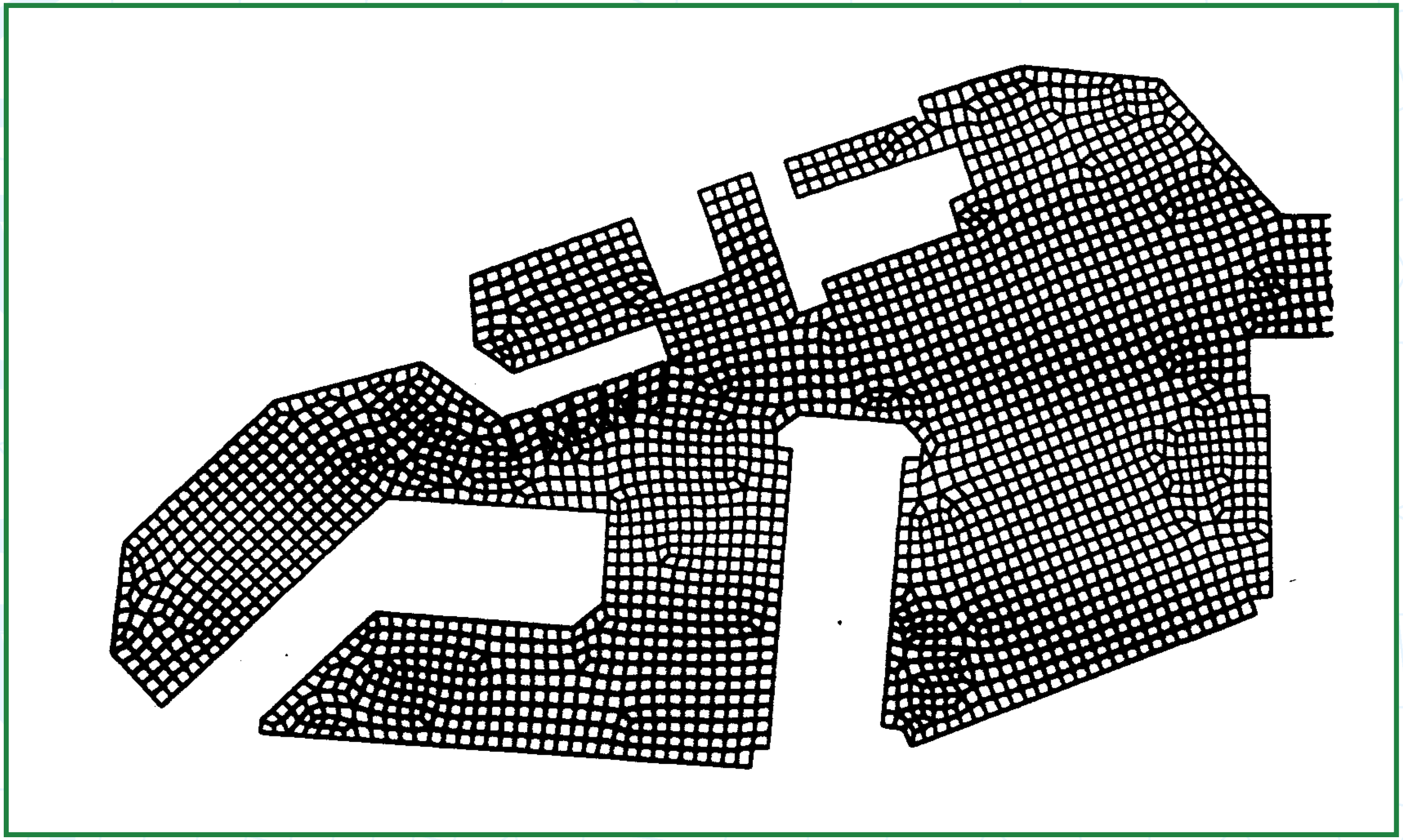
Examples: wave propagation

Calculation mesh
(1 476 014 node, 2 unknowns per node)

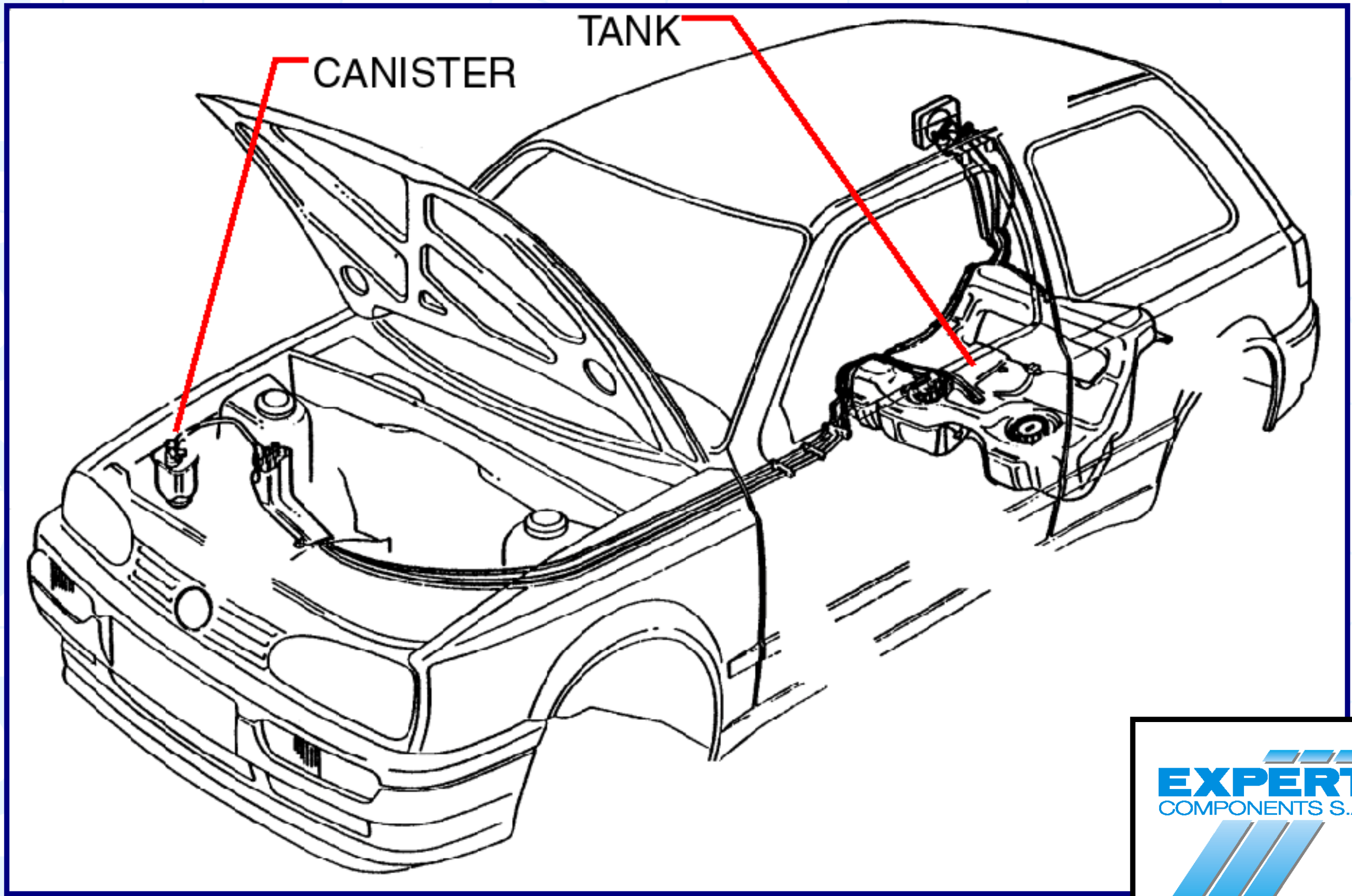


Examples: wave propagation

Mesh calculation detail



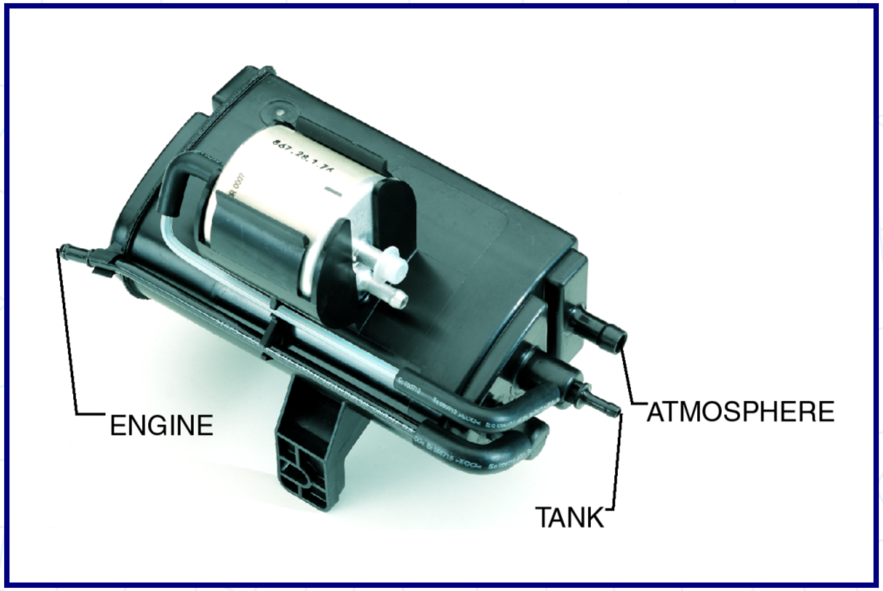
Example: active carbon filters



EXPERT COMPONENTS S.A.

Example: active carbon filters

- Car stopped, engine:
  - The volatile hydrocarbons from the gas tank evaporate
  - Inside the canister, the active carbon adsorbes the hydrocarbons to avoid that they reach the atmosphere
- Car running:
  - The carbon gets cleaned (desorption) and the HC go to the engine to be burned

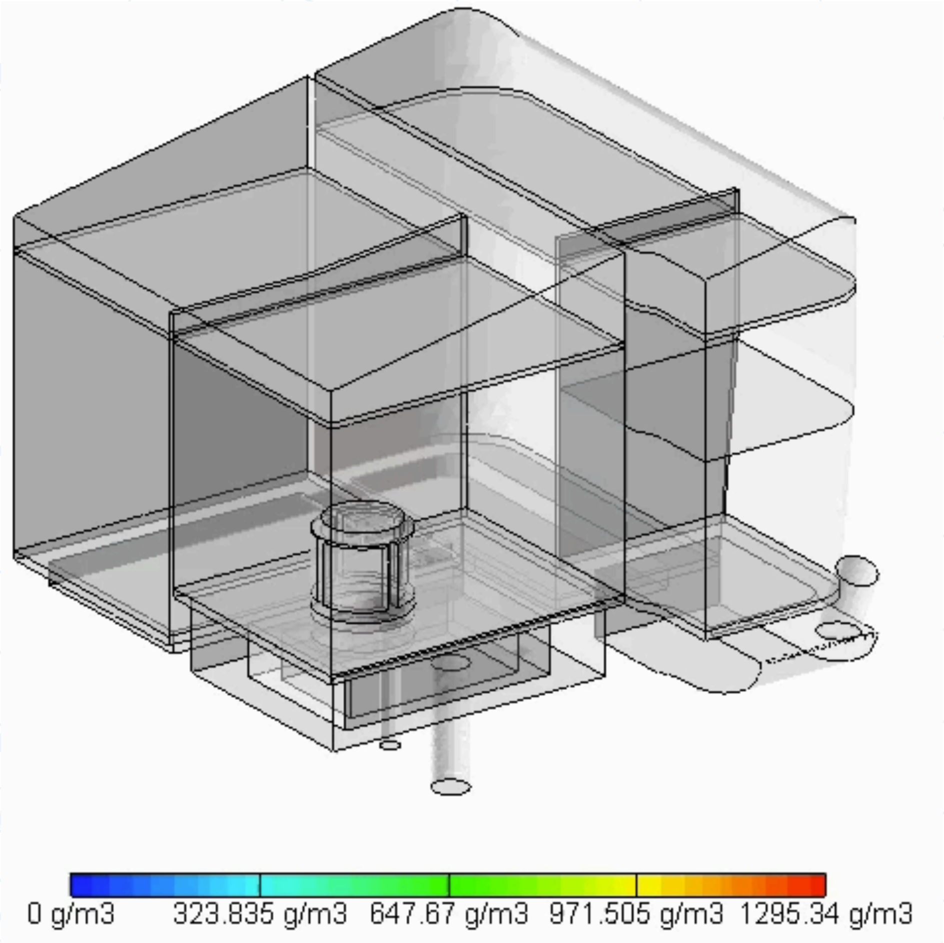


Example: active carbon filters

- Complicated 3D geometries
- Different materials:
  -plastics, active carbons,,
  -air cavities
  -foams ...

Example: active carbon filters

- Simulation:



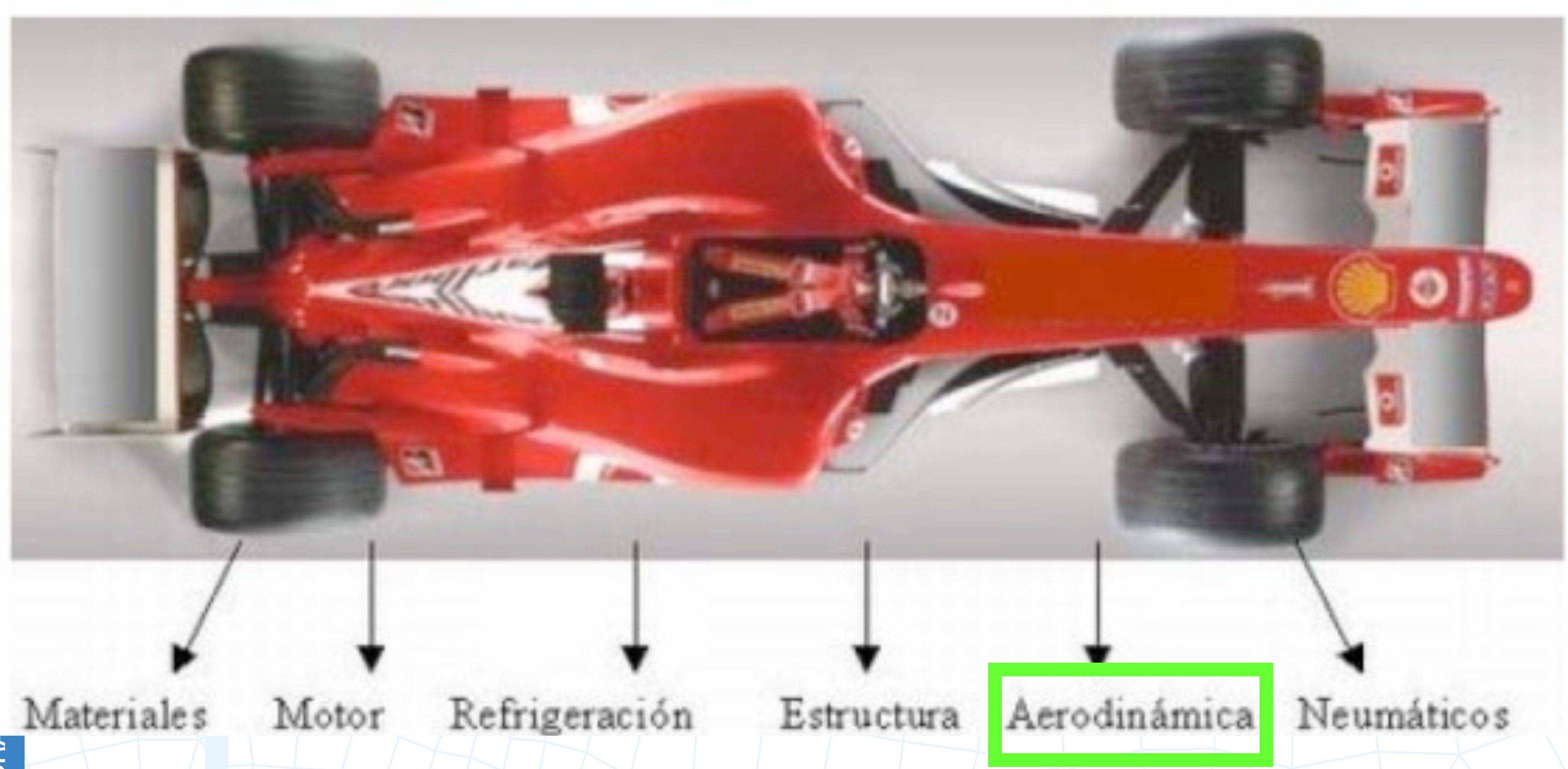
- convection-difussion-reaction equation

Convection-diffusion-reaction equation

$$\frac{\partial c}{\partial t} = \underbrace{\nabla \cdot (D\nabla c)}_{\text{Diffusion}} - \underbrace{\nabla \cdot (\vec{v}c)}_{\text{Convection}} + \underbrace{R(\mathbf{r}, t)}_{\text{Reaction}}$$

- Reaction term
  - models adsorption/desorption
  - couples local and global levels
  - is nonlinear
- Diffusion term
  - tiny (important in localized areas)
  - renders the problem parabolic
- Convection term
  - models fuel vapor motion
  - $\vec{v}$ previously computed

Example: Aerodynamics of Fórmula 1



Navier-Stokes Equations

- Isotropic incompressible viscous flow

$$\boldsymbol{v}_t + (\boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{v} - \nu\nabla^2\boldsymbol{v} + \boldsymbol{\nabla}p = \boldsymbol{b}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0$$

b: volume forces p: thermodynamic pressure

v: velocity ν: viscosity

- Non-dimensional Navier-Stokes equation

$$\boldsymbol{v}_t + (\boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{v} - \frac{1}{Re}\nabla^2\boldsymbol{v} + \boldsymbol{\nabla}p = 0$$

Reynold's Number: Re = VL/ν

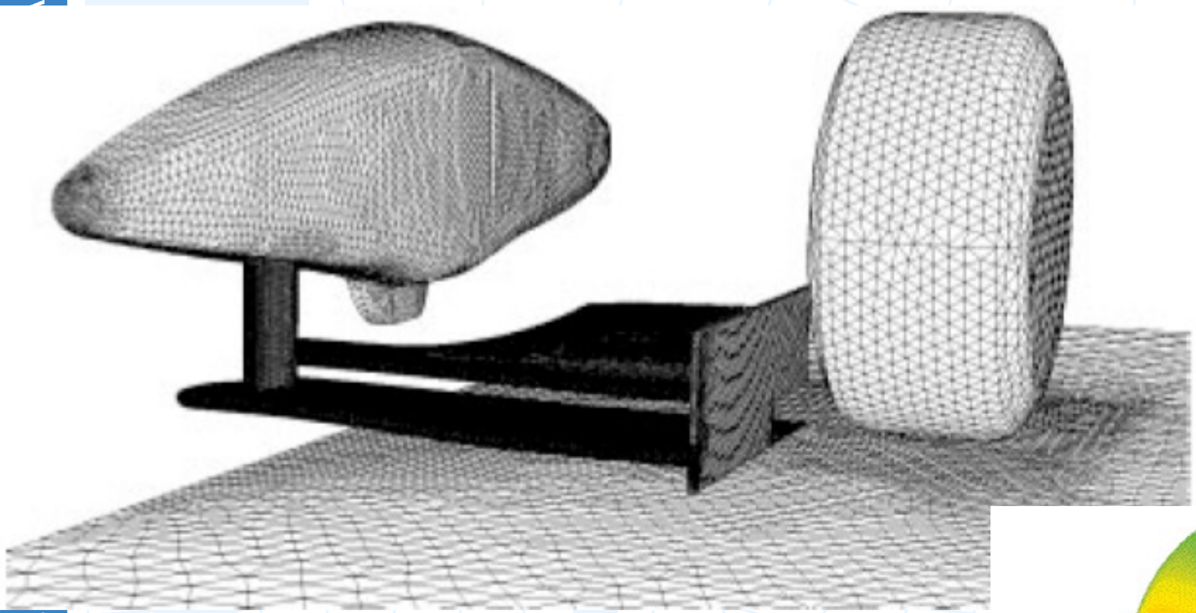
Wind tunnel

- Very high cost, e.g. Sauber's team wind tunnel experiment costs 55 million dollars.

Wind tunnel

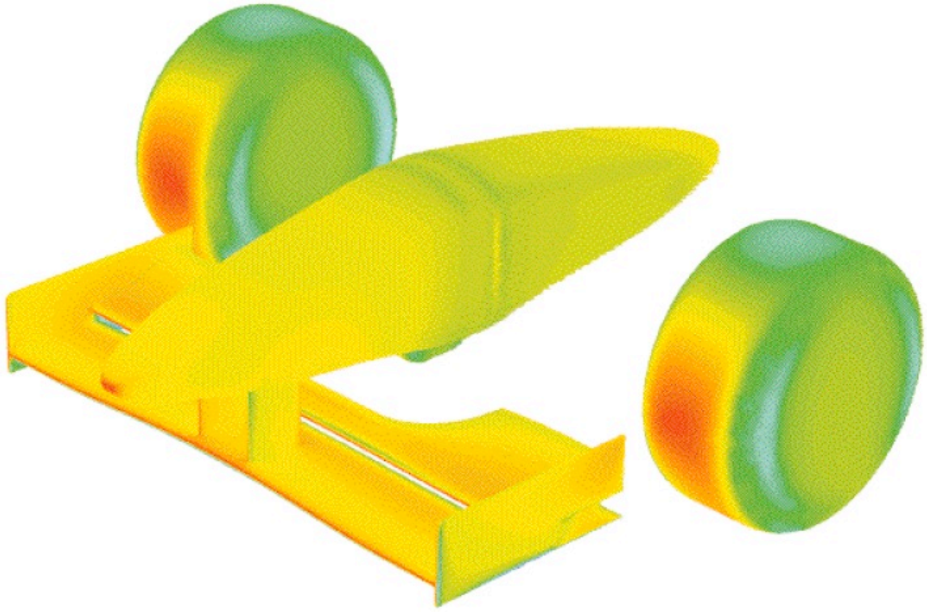
Computational Engineering

- Front wing



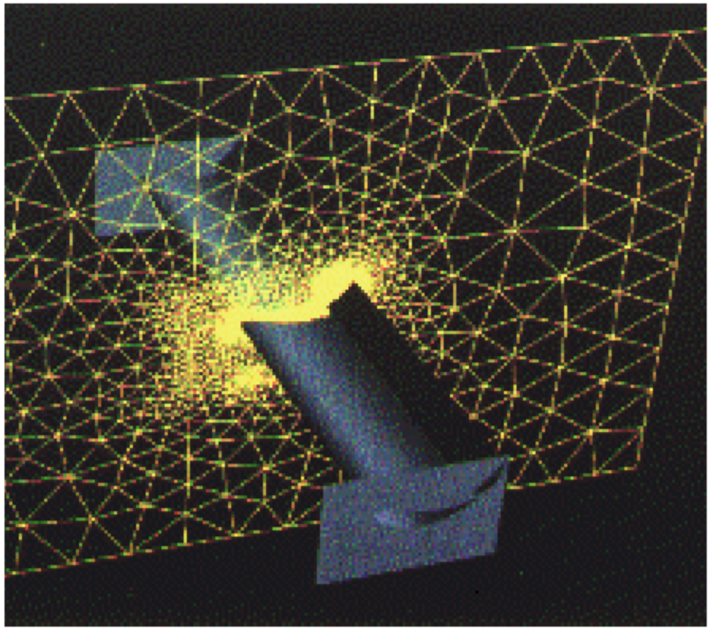
Finite element mesh (symmetry)

Pressure distribution

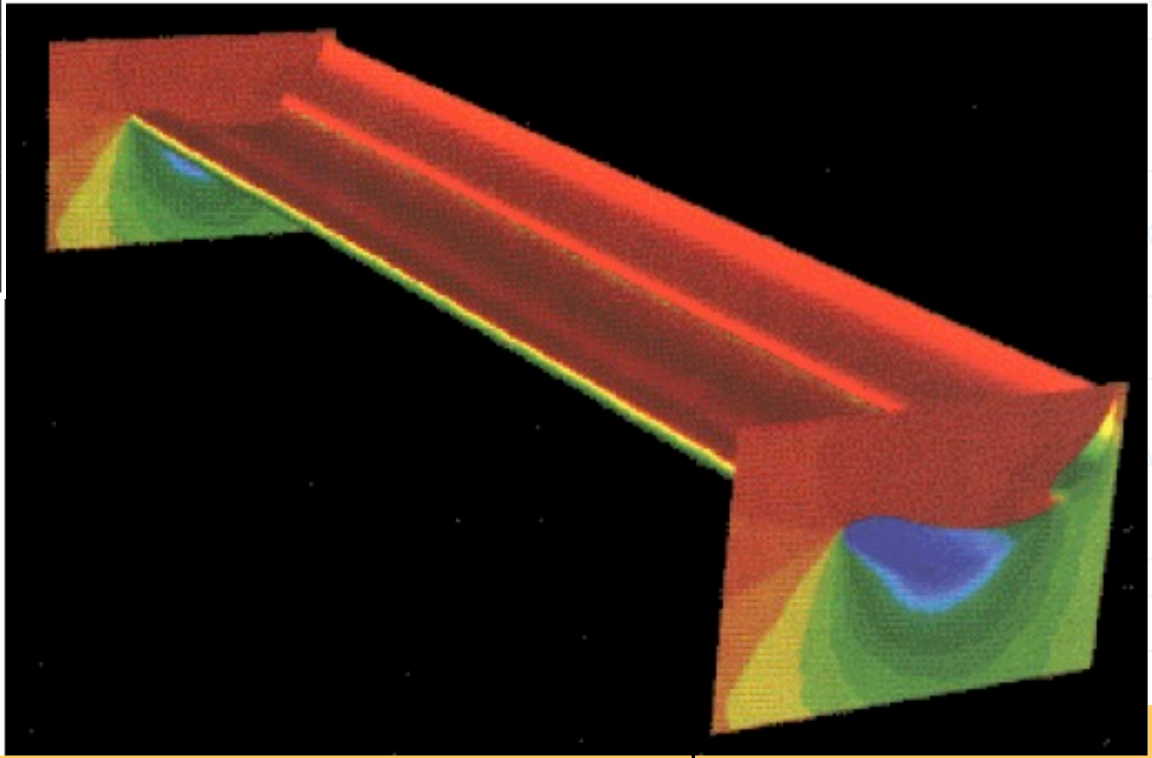


Computational Engineering

- Rear wing

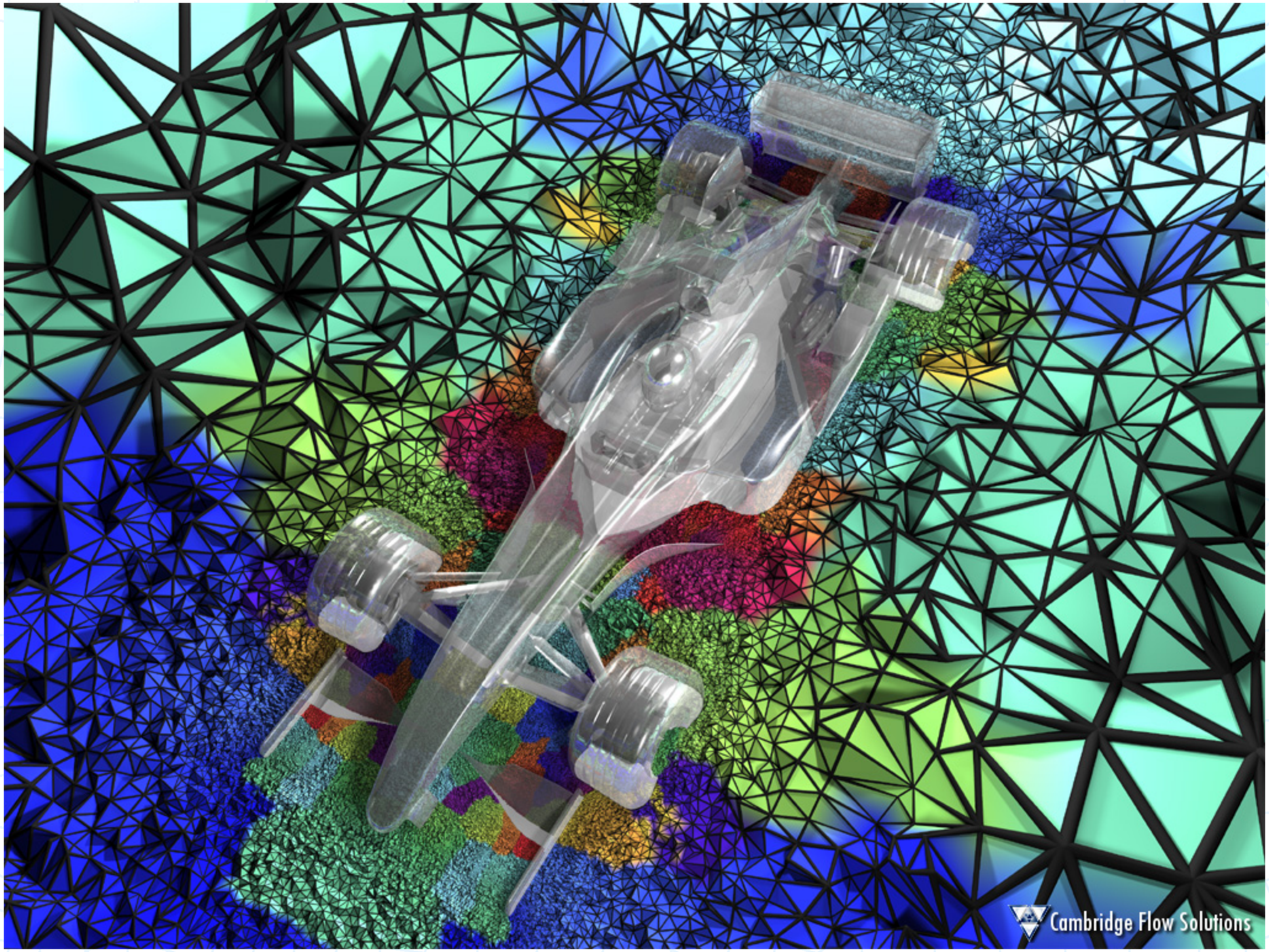


Finite element mesh (symmetry)

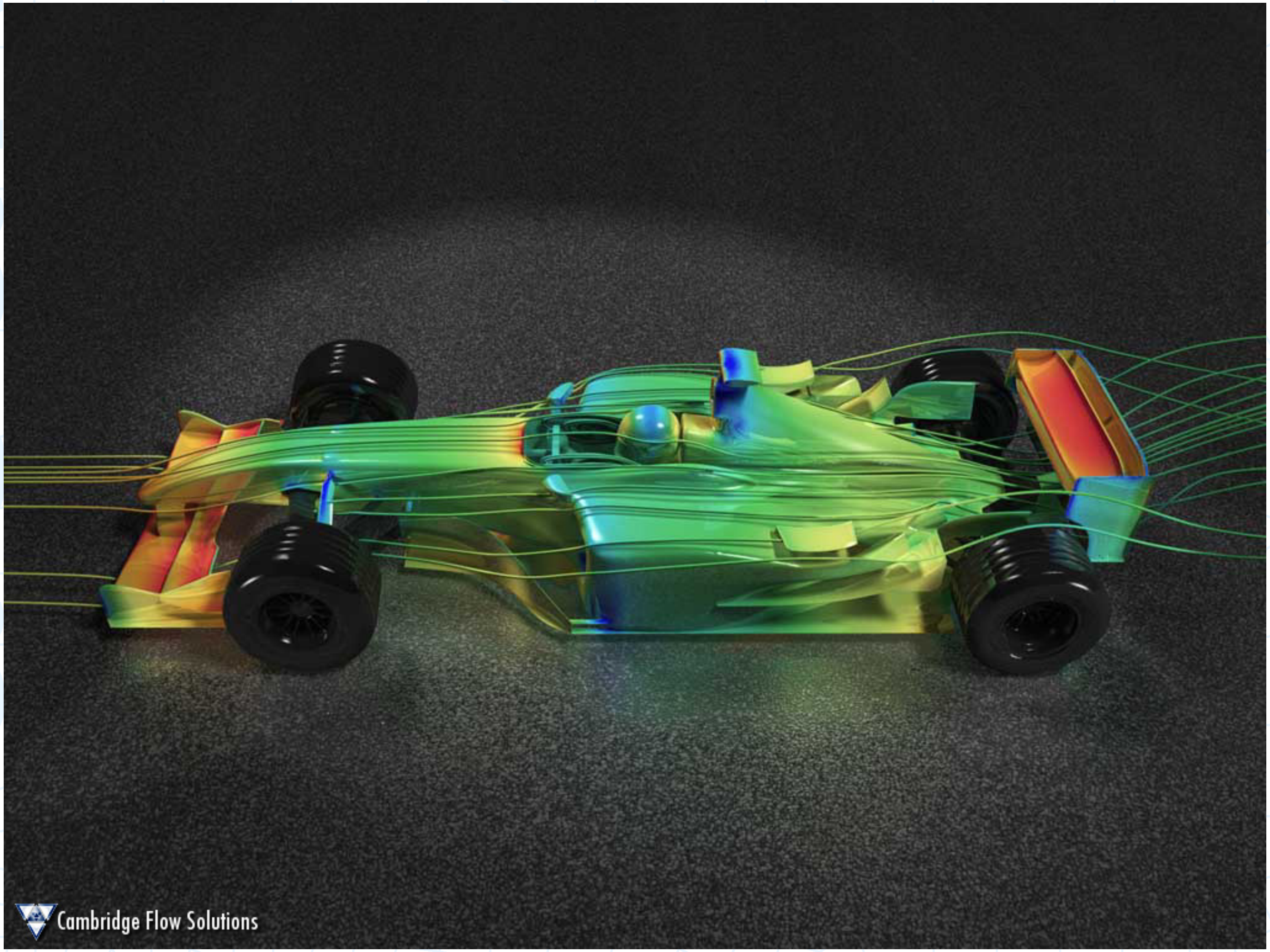


Pressure distribution

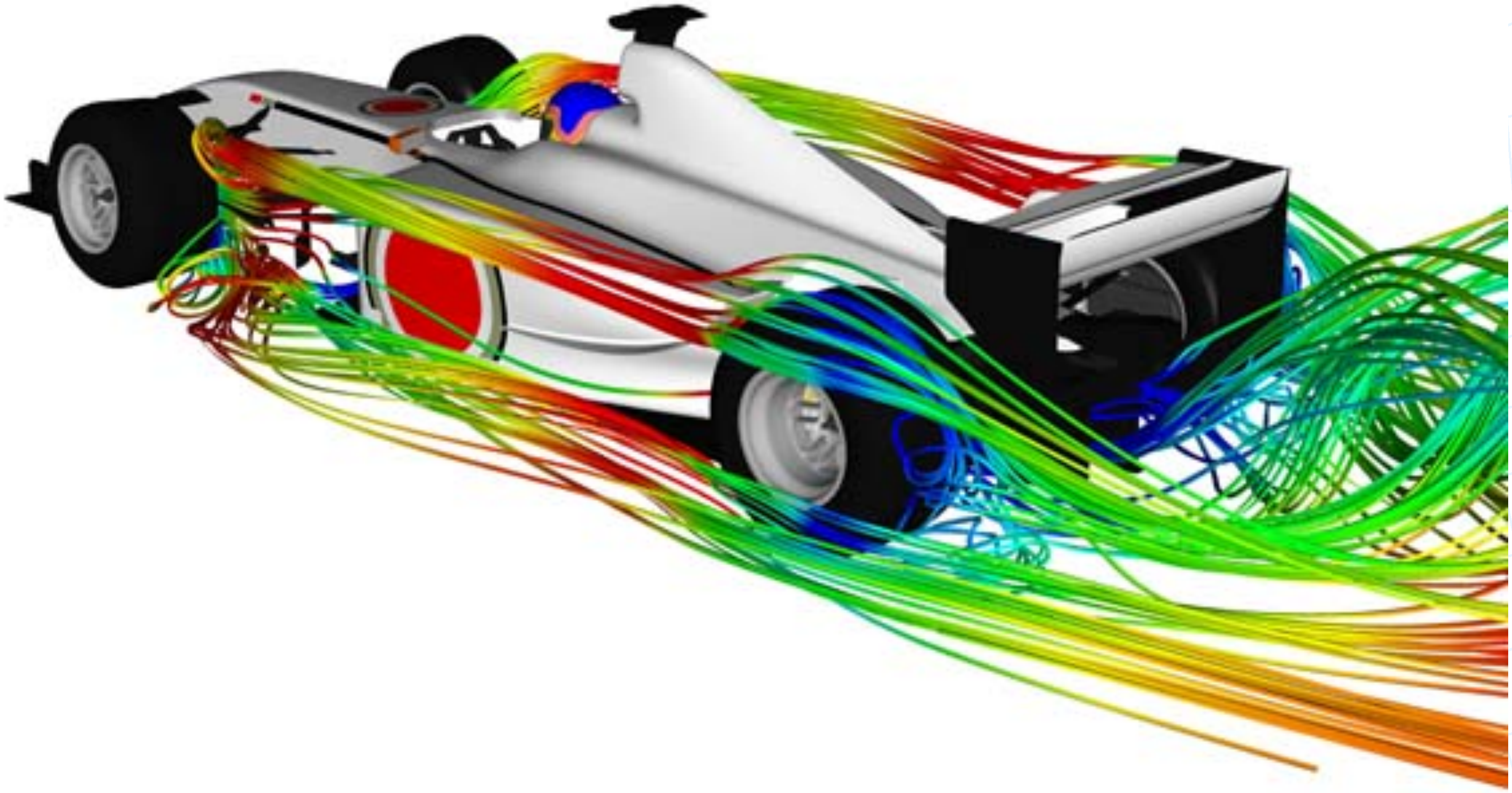
- Whole vehicle. Computational Mesh



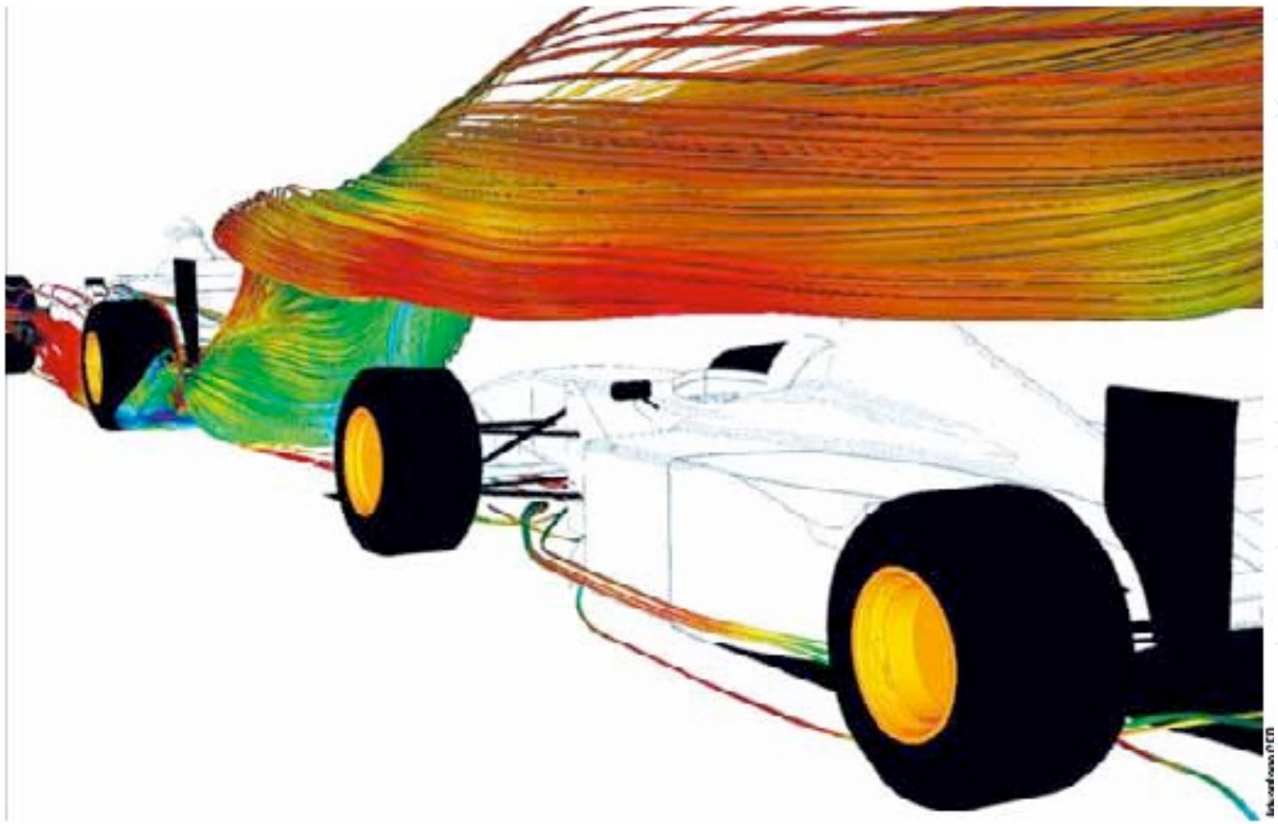
- Quantities of interest: pressure and stream lines



- Vortices formation in the back



- Vortices formation in the back (“clean air”)



Summary

- Simulating real-world phenomena on a computer involves:
  - understanding the governing physics.
  - formulating a mathematical description of the physical problem
  - writing computer software to solve the mathematical equations.
  - performing virtual tests efficiently
  - Viewing and critically analyzing the results.
- Goal:
  - assist the design process: simulation-driven design
  - assist the decision-making process
- Many commercial softwares are now available.
- Good computer-based engineering analysis requires well-trained engineers that understand the global picture of computational engineering.