Computational Models and Simulations,

MDSC 689.11

Dr. Matthias Walle

Mar 25th 2024

Lecture Overview

- **Introduction to Numerical Simulations**
  - Brief overview of numerical simulations
  - Importance in solving complex problems
  - Brief history and evolution
  - Physics-based vs data-driven
- **General Principles in Computational Modelling**
  - Complexity**,** Scaling, Hierarchical modelling, Mathematical principles (Differential equations)
- **Finite Element Analysis (FEA)**
  - Idea behind FEA modelling, Process of conducting FEA, Challenges, Examples, Tools, Common Mistakes
- **Case Study: Stress shielding in total hip replacements**
- **Q&A and Discussion**

Brief Overview of (numerical) Simulations

Simulation process

Real-World-Problem

↓

Mathematical Model

↓

Computation

↓

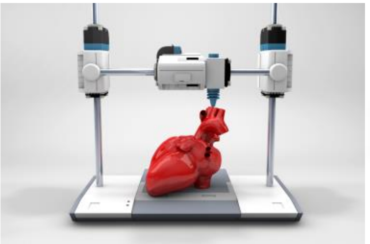
Quantification/ Visualisation

1. Definition

   "Numerical simulations are computer-based models that solve complex mathematical problems to predict the behaviour of systems in the real world."

2. Key Components
   - **Mathematical Modelling**: Real-world problems to mathematical form
   - **Computational Algorithms**: Methods to numerically solve mathematical models
   - **Visualization**: Graphical representation of simulation results

3. Other types of Simulations:
   - Physical models (e.g. mock-ups, 3D printing, animal models)

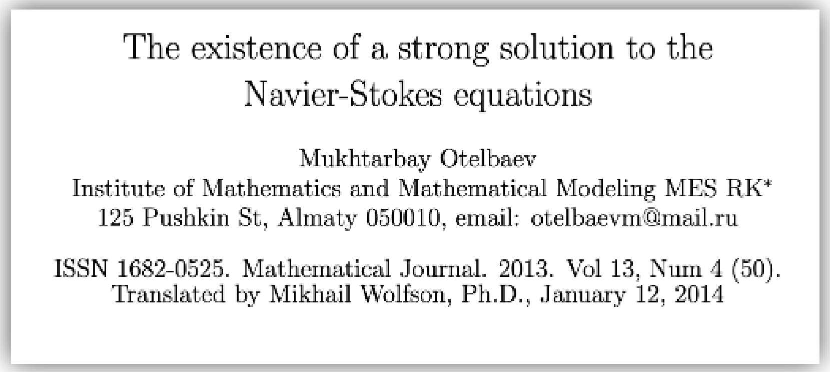


4. Applications
   - physical sciences, mathematics, economics, engineering, and biomedical fields

Importance of Simulations in Solving Complex Problems

1. Solving the Unsolvable
   - Solve complex problems that are (currently) analytically too complicated
2. Cost-Effectiveness
   - Reduce physical prototypes and experiments
3. Precision and Predictability
   - System behaviours based on physical principles, e.g. different temperatures, material properties, external loads
4. Innovation and Design
   - Rapid prototyping, e.g. devices, implants, stents, surgeries,
5. Decision Making
   - Providing data-driven insights, e.g. simulation of failure load of implants

Navier–Stokes Millennium Problem



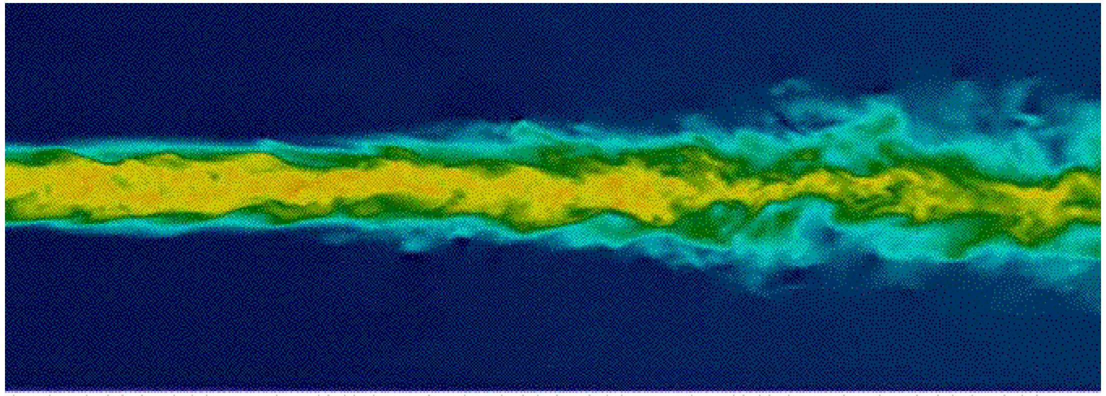
The existence of a strong solution to the Navier-Stokes equations

Mukhtarbay Otelbaev
Institute of Mathematics and Mathematical Modeling MES RK*
125 Pushkin St, Almaty 050010, email: otelbaevm@mail.ru

ISSN 1682-0525. Mathematical Journal. 2013. Vol 13, Num 4 (50).
Translated by Mikhail Wolfson, Ph.D., January 12, 2014

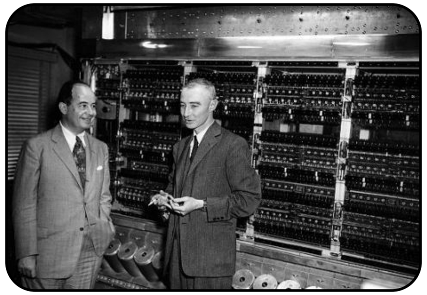
Otelbaev, 2013

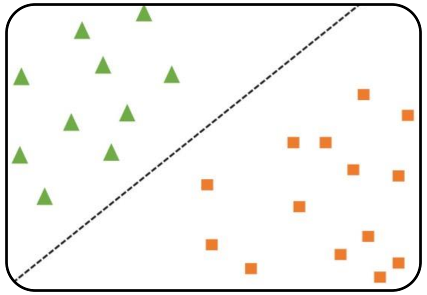
Fluid Dynamics Simulation



https://vbt.ebi.kit.edu/

Brief history and evolution





1940s: Birth of Computer Simulations

- Monte Carlo simulation by von Neumann and Ulam during the Manhatten Project

1960s: Rise of Digital Computing

- Use of computers to solve differential equations

1970s: Physics-Based Modelling

- Simulations become standard for engineering systems from aerospace to biomedical applications

1990s: Data-Driven Models

- Emergence of Machine Learning

Present: Generative AI

- Generative Adversarial Networks, Transformer Architecture (ChatGPT), Large Language Models (Llama, PaLM, Gemini), Diffusion Models (Sora)

Physics-based and data-driven Simulations

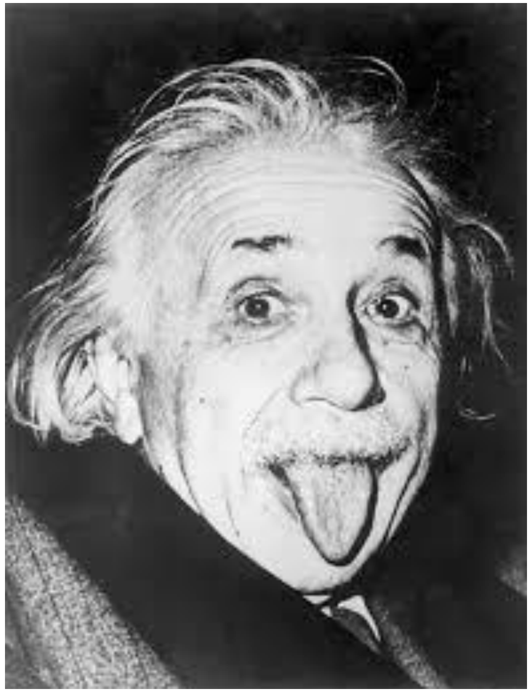
UNIVERSITY OF CALGARY

	Data-Driven: Machine Learning	Physics-Based: Numerical Modelling
Foundation	Data patterns	Physical laws
Data Need	Large datasets	Minimal to none
Predictive Scope	Within training data range	Beyond observed data
Insight	Limited to data patterns	Deep causal mechanisms
Complex Conditions	Limited by training data	Adaptable to new scenarios
Efficiency	Data-dependent costs	High initial cost, efficient long-term
Applications	Data-rich applications, explore patterns and data correlations, e.g. lung cancer detection in CT or MRI scans, fracture risk assessment in bone	Data-scarce applications, understand complex systems, predict and explore new scenarios, e.g. bone strength calculations, implant integration in bone

Underlying principle of Simulations

- Einstein's razor:

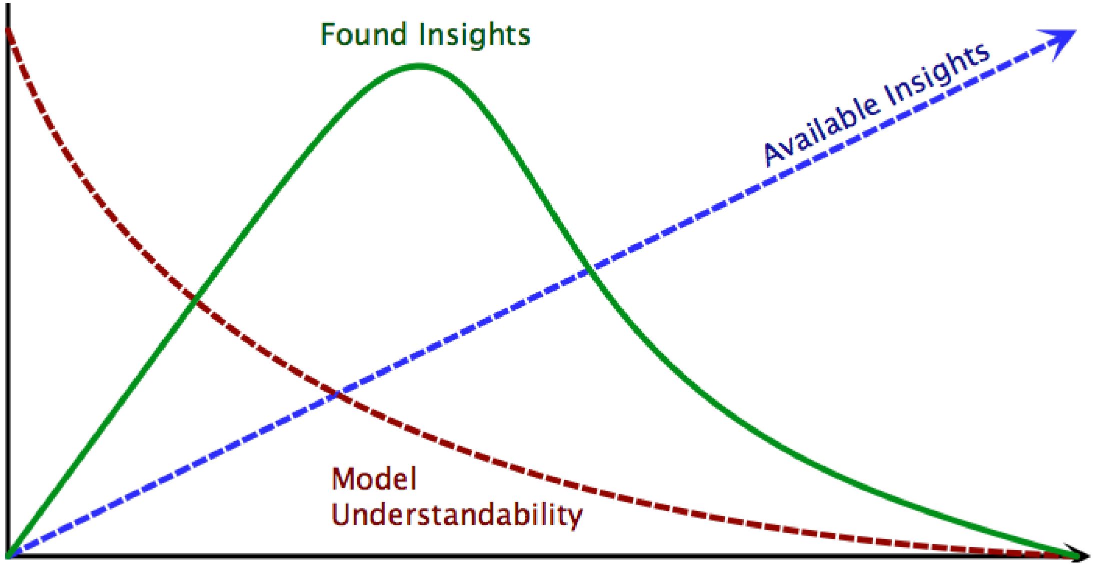
"The supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience."



Make things as simple as possible, but no simpler.

The cost of complexity

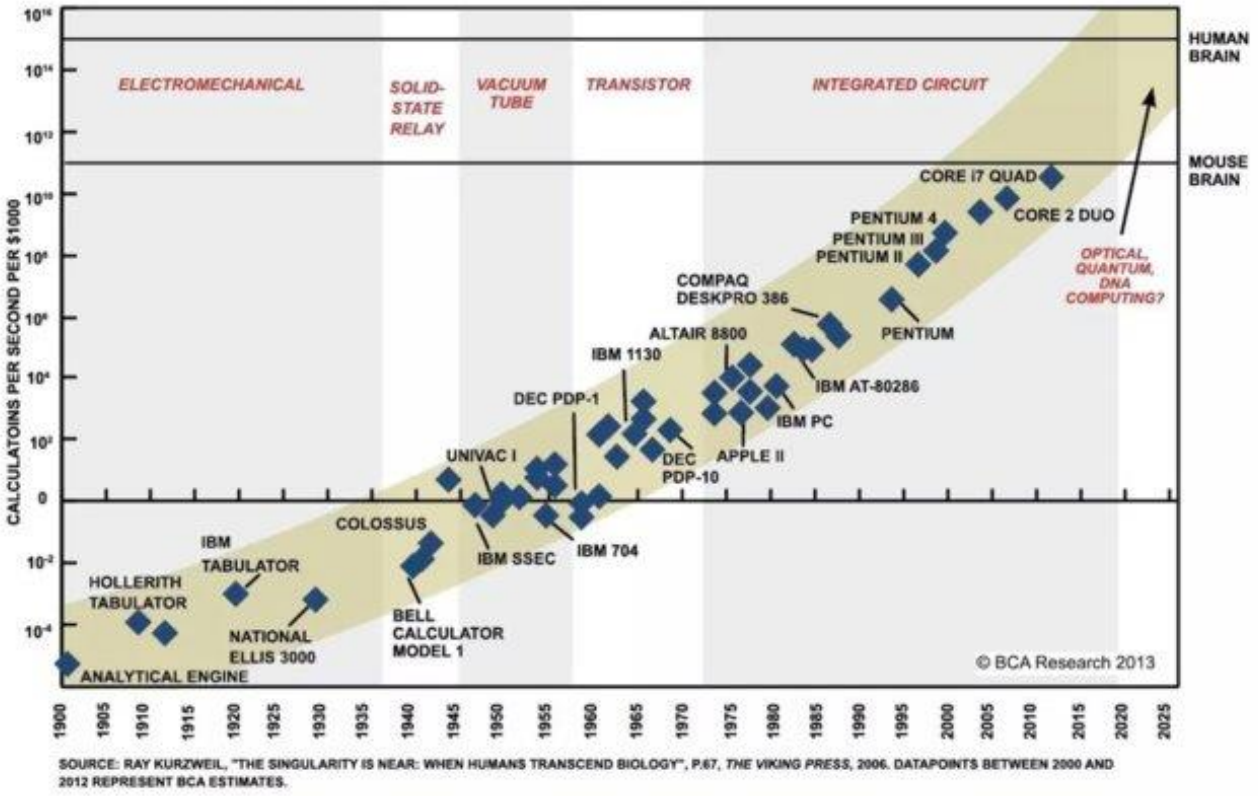
- Complex models are more expensive…
  1. as they take longer to simulate,
  2. as they are harder to interpret (cognitive costs),
  3. as they may not generalise well (e.g. overfitting in data-driven simulations)



realkm.com

The exponential progress of computing power

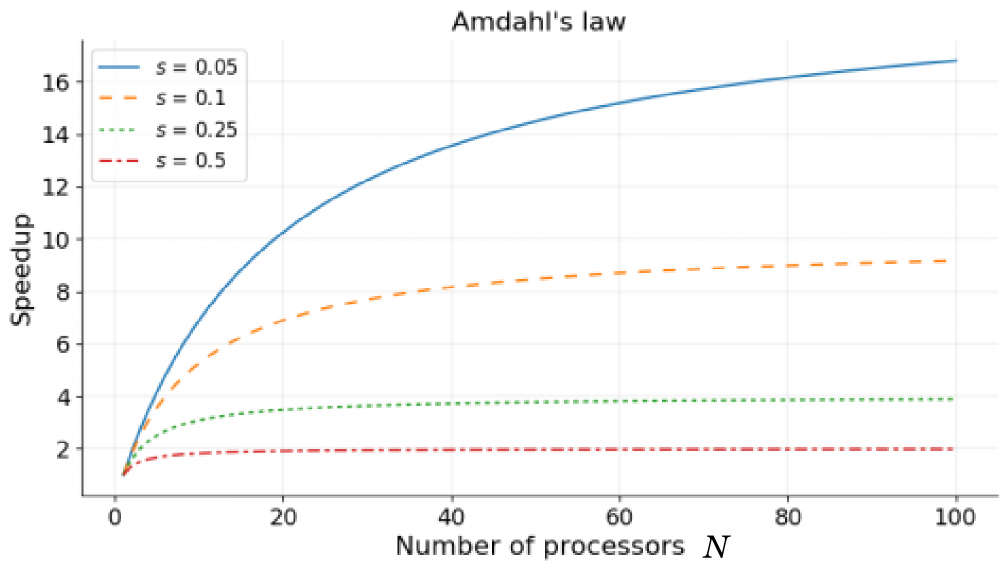
- Increasing computing power → increased model complexity and problem size



Kurzweil, 2005

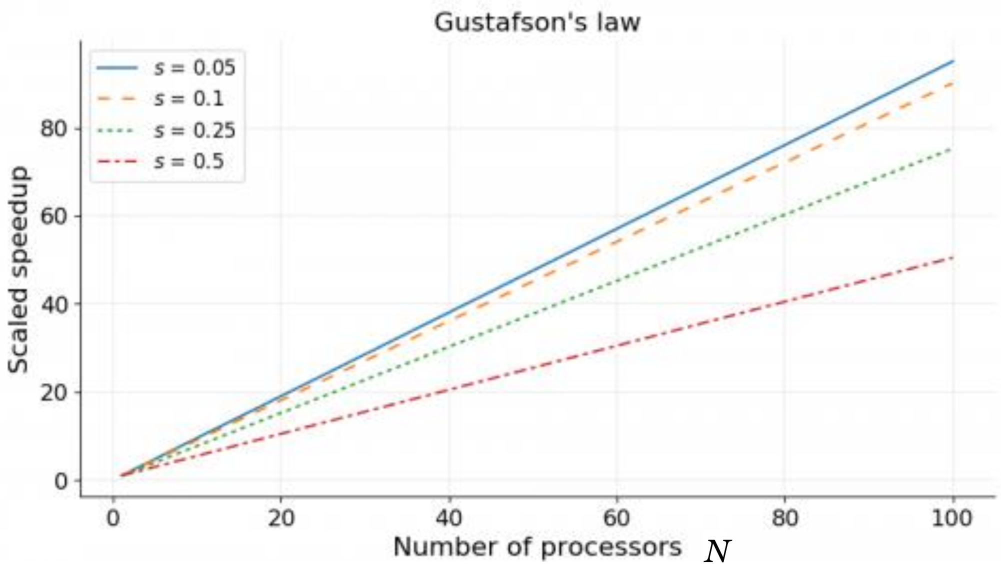
Weak and strong scalability

- Weak scaling



speedup = 1 / (s + p / N)

- Strong scaling



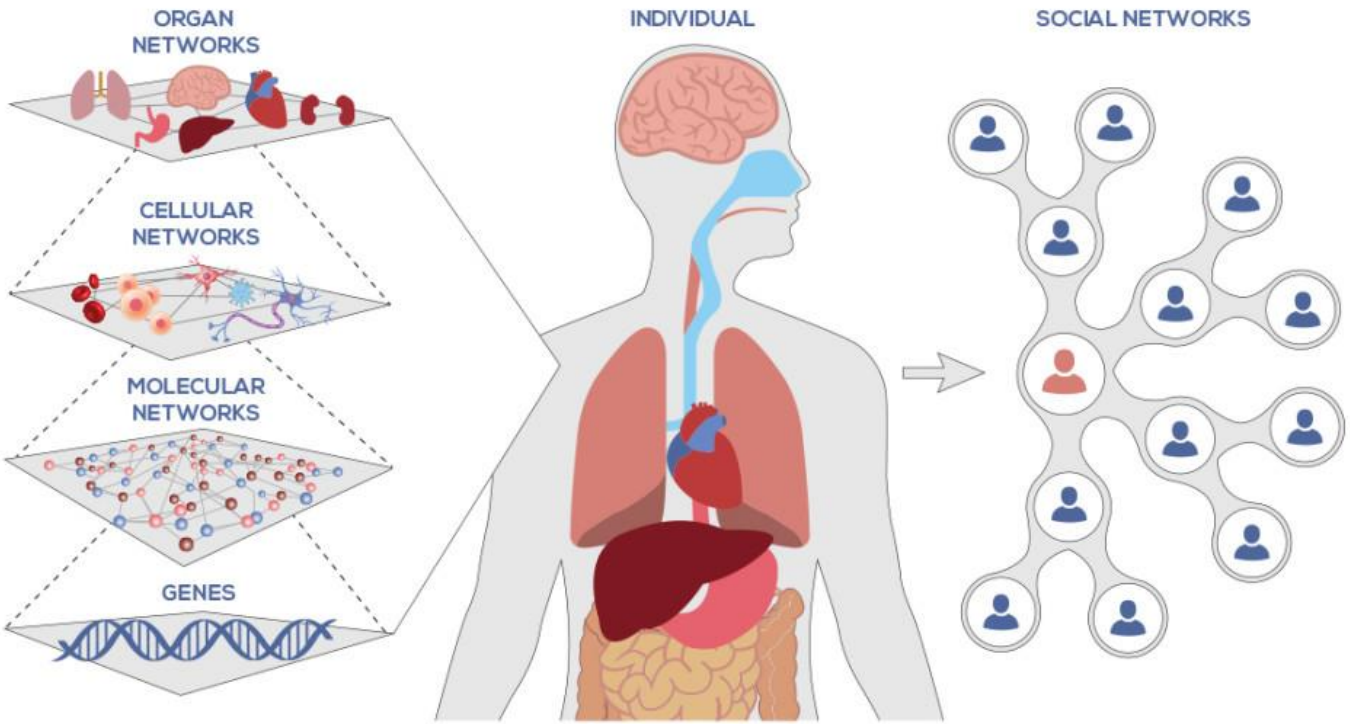
scaled speedup = $s + p \times N$

Parallelisation of mathematical models is key for large scale simulations!

p = parallel proportion
s = serial proportion

Simulations of biological systems

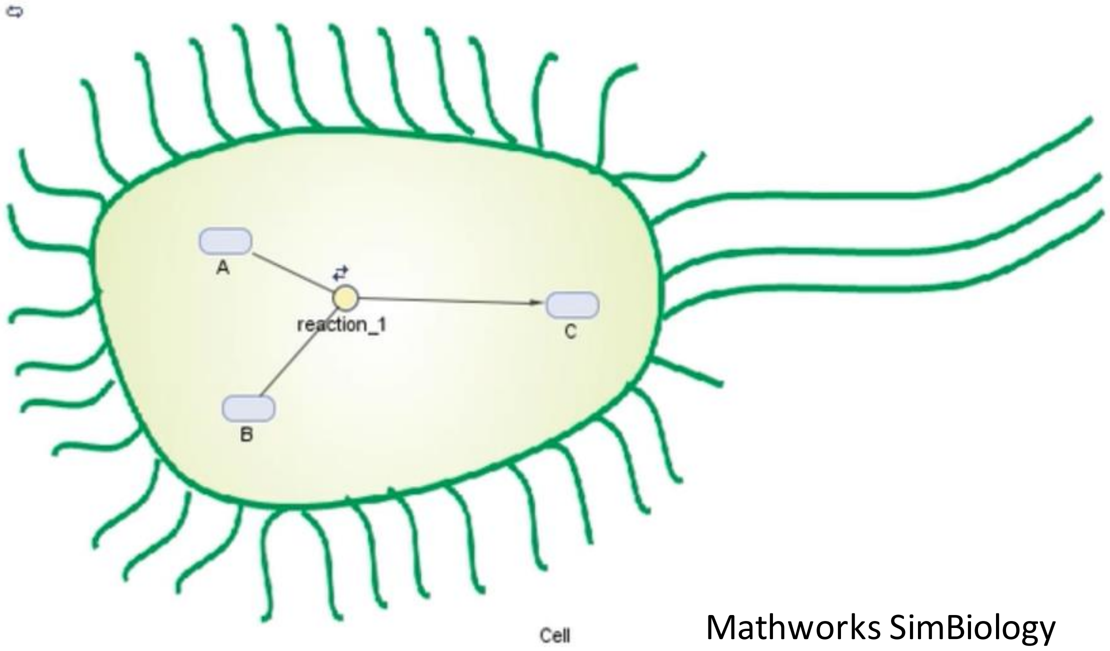
- Biological systems: Network of Networks



https://isbscience.org/

Hierarchical modelling

- **Hierarchical Modelling**: Dividing a complex system into simpler subsystems
- Two approaches:
  - **Top-down**: Begins with the broad overview or system-level perspective, breaking it down into smaller parts
  - **Bottom-up**: Starts at the most detailed and basic level, assembling these components to build more complex systems



Mathworks SimBiology

Choosing the right approach

Bottom-Up Approach

- **Mechanistic Understanding**
  - **Example**: To understand how diseases affect bones, researchers model individual cells, uncovering the disease's impact from the cellular level upwards.
- **Synthetic Biology**
  - **Example**: Constructing new biological systems or organisms from the ground up, often without a prior understanding of the system.

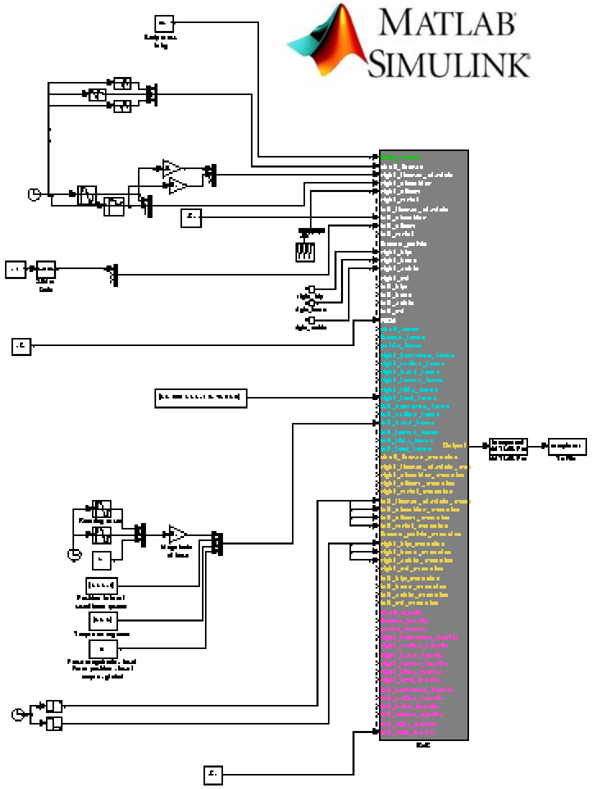
Top-Down Approach

- **Ecology and Evolutionary Biology**
  - **Example**: Examining how climate change affects certain organisms, starting from an ecosystem-wide perspective.
- **Systems Biology**
  - **Example**: Simulating the dynamic interactions within biological systems to understand how different components interact on a systemic level.

real-world scenarios approaches are typically hybrid
(no clear separation possible)

MathWorks Simulink

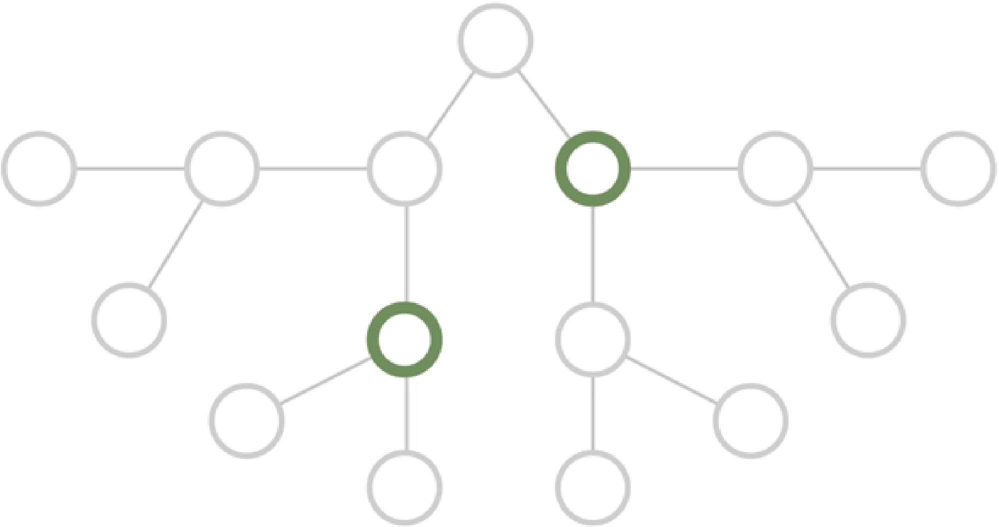
Can be used for hierarchical modelling



https://www.bob-biomechanics.com/

Key Mathematical Principles in Numerical Simulations

Differential equations



$$\frac{dI(t)}{dt} = k * I(t)$$

- Equations that describe how quantities change over time or space, involving derivatives with respect to a variable
- **Applications**: modelling the dynamics of systems, including motion, growth, decay, and changes in physical properties.

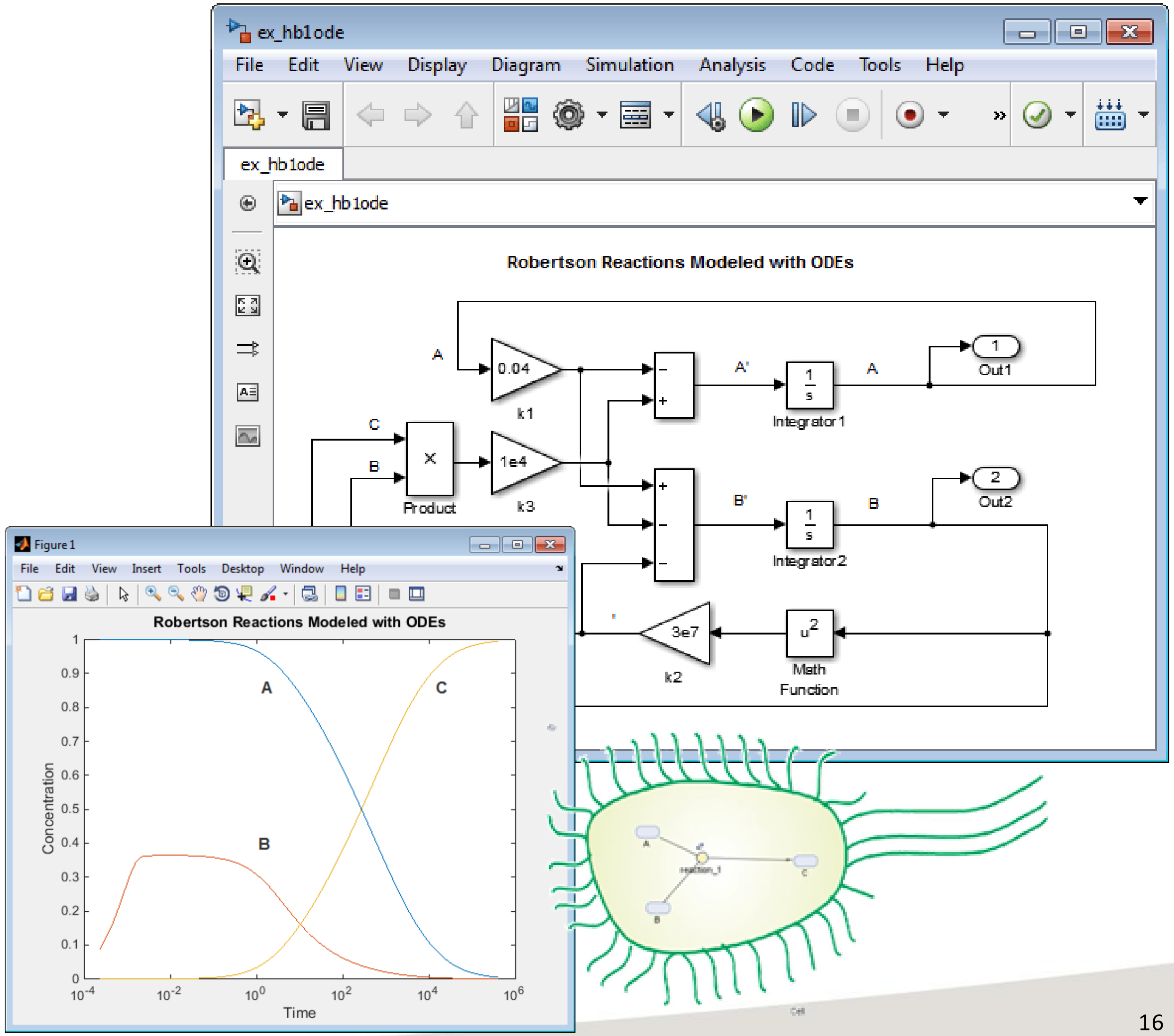
Solving differential equations using Simulink

Robertson Problem

- Set of chemical reactions among

$$
\begin{array}{llll}
A \xrightarrow{k_1} B & k_1 = 0.04 & V_1 = k_1[A] \\
B + B \xrightarrow{k_2} C + B & k_2 = 3 \cdot 10^7 & V_2 = k_2[B][B] \\
B + C \xrightarrow{k_3} A + C & k_3 = 1 \cdot 10^4 & V_3 = k_3[B][C]
\end{array}
$$

1. Initial conditions: A=1, B=0, and C=0.



Nature operates via gradients

Solid Mechanics

$$\frac{\partial \sigma_{xx}}{\partial x_1} + \frac{\partial \tau_{xy}}{\partial x_2} + \frac{\partial \tau_{xz}}{\partial x_3} + F_x = 0,$$
$$\frac{\partial \tau_{xy}}{\partial x_1} + \frac{\partial \sigma_{yy}}{\partial x_2} + \frac{\partial \tau_{yz}}{\partial x_3} + F_y = 0,$$
$$\frac{\partial \tau_{xz}}{\partial x_1} + \frac{\partial \tau_{xz}}{\partial x_2} + \frac{\partial \sigma_{zz}}{\partial x_3} + F_z = 0,$$

Fluid Mechanics

$$\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = \nu\nabla^2\mathbf{u} - \frac{1}{\rho}\nabla p + \mathbf{g}.$$

Thermodynamics/ Biology

$$\frac{\partial c}{\partial t} = \nabla\cdot(D\nabla c - \mathbf{v}c) + R$$

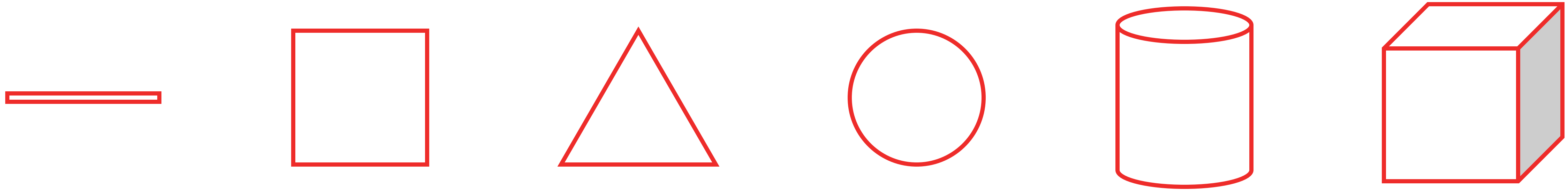
Electromagnetics

$$\nabla\times\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}$$
$$\nabla\times\mathbf{B} = \mu_0\left(\mathbf{J} + \varepsilon_0\frac{\partial \mathbf{E}}{\partial t}\right) \qquad \nabla\cdot\mathbf{B} = 0$$

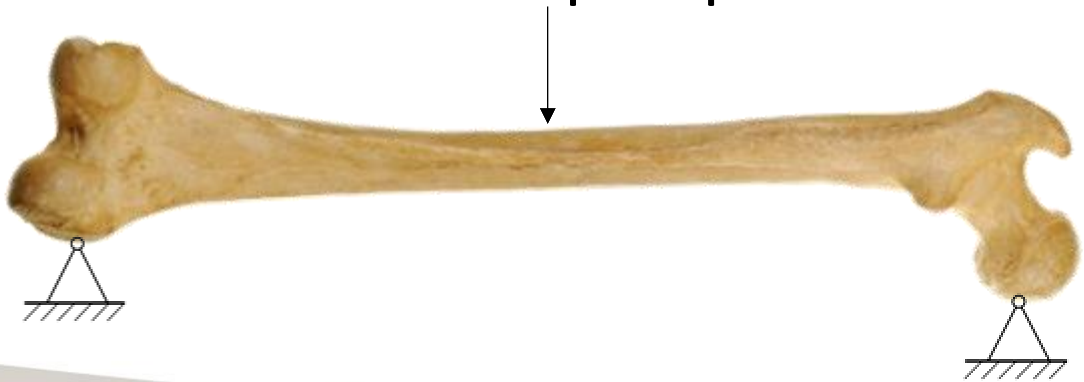
- Along with these equations with additional constraints called the boundary conditions (BCs)
- Differential equations + BC → **Boundary value problem**

Solutions to boundary value problems

- Analytical methods (Integration, Laplace transform, etc.) are only valid for certain geometries



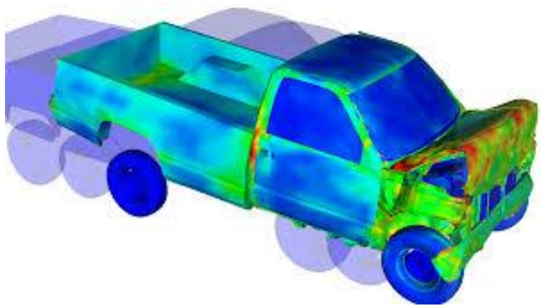
- How do we handle complex problems?



Finite element analysis (FEA)

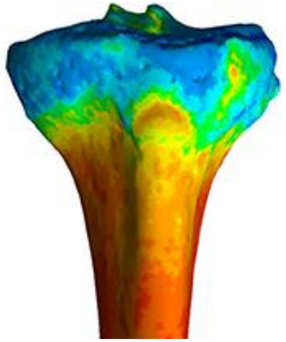
- FEA is a numerical method used to obtain an approximate solution for a given boundary value problem

Automotive Industry
Crash test

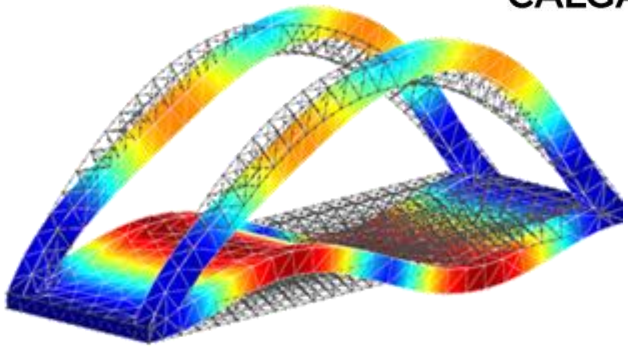


Aerospace Industry
Space Shuttle

Biomedical Engineering
Fracture risk

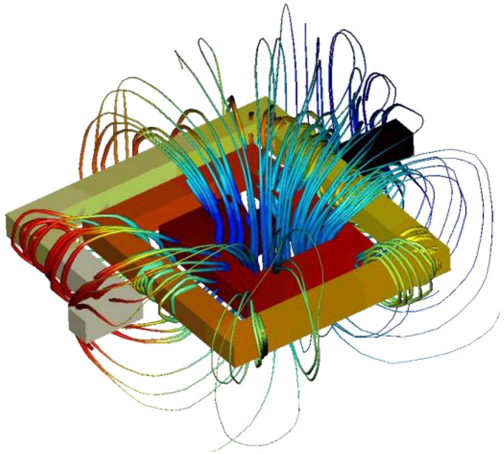


Civil Engineering
Bridge modes

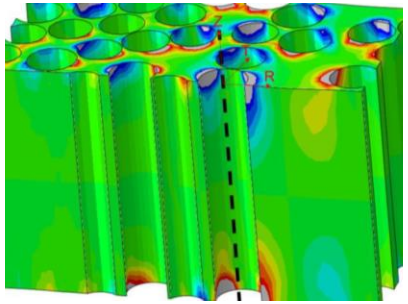


UNIVERSITY OF CALGARY

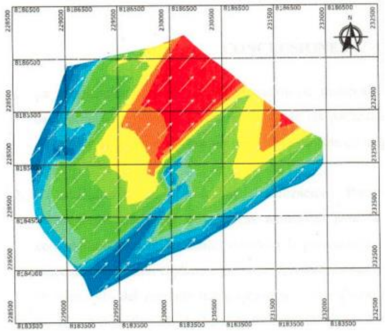
Manufacturing
Magnetic Fields



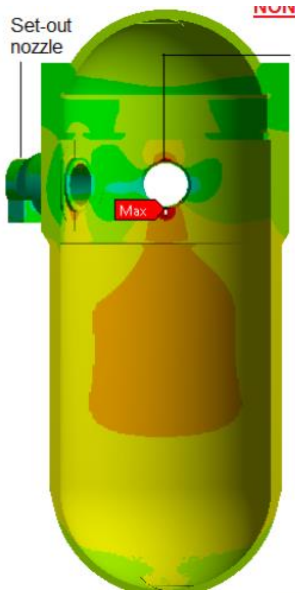
Material Science
Carbon Fibre



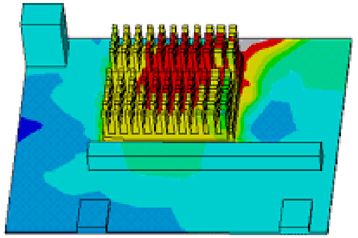
Environmental Engineering
Air Pollution



Energy Sector
Nuclear Reactor



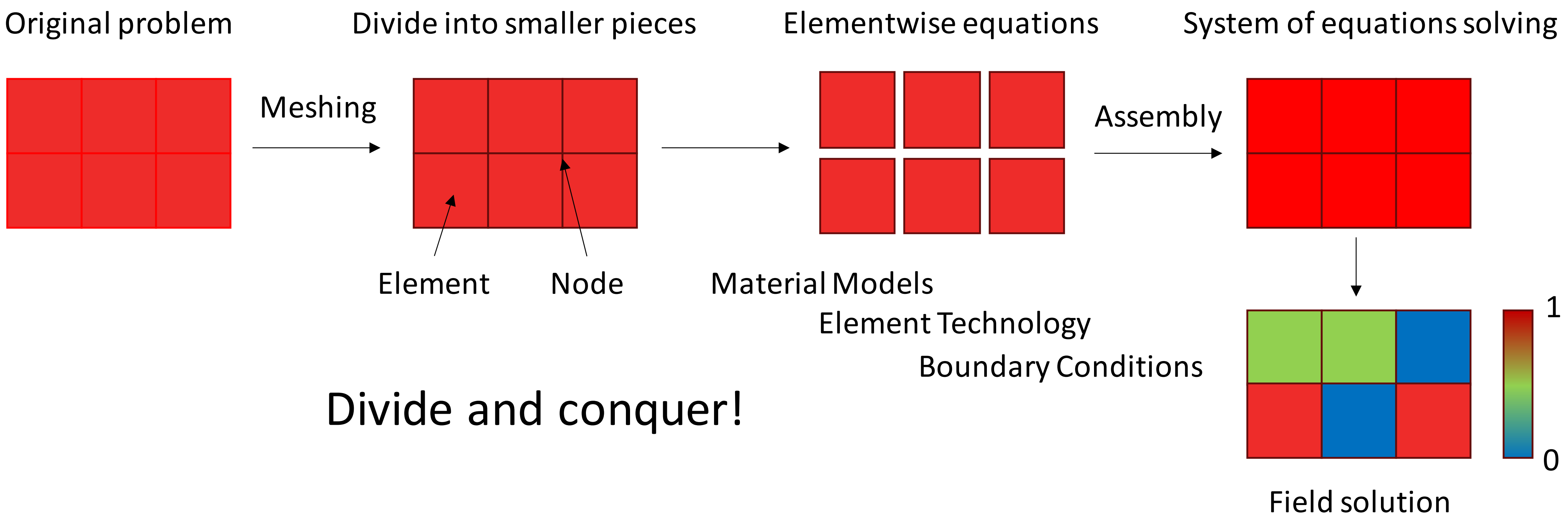
Consumer Electronics
Heat Transfer



The Power of Finite Element Analysis

Process of Finite Element Analysis

- Objective is to find the approximate solution to the boundary value problem!



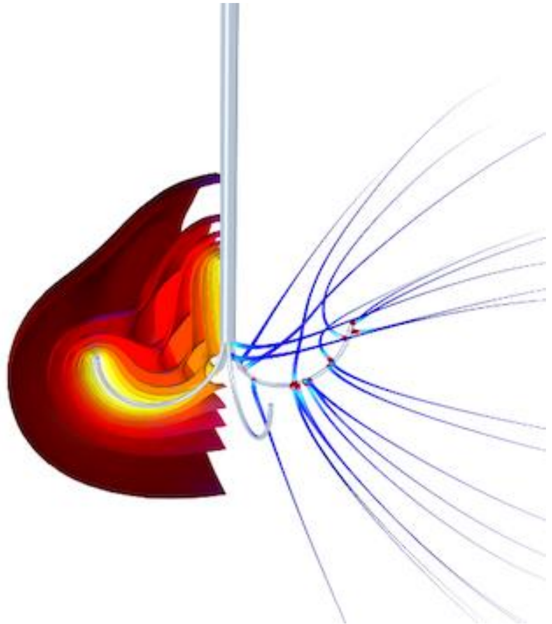
Divide and conquer!

Set up a Finite Element Analysis

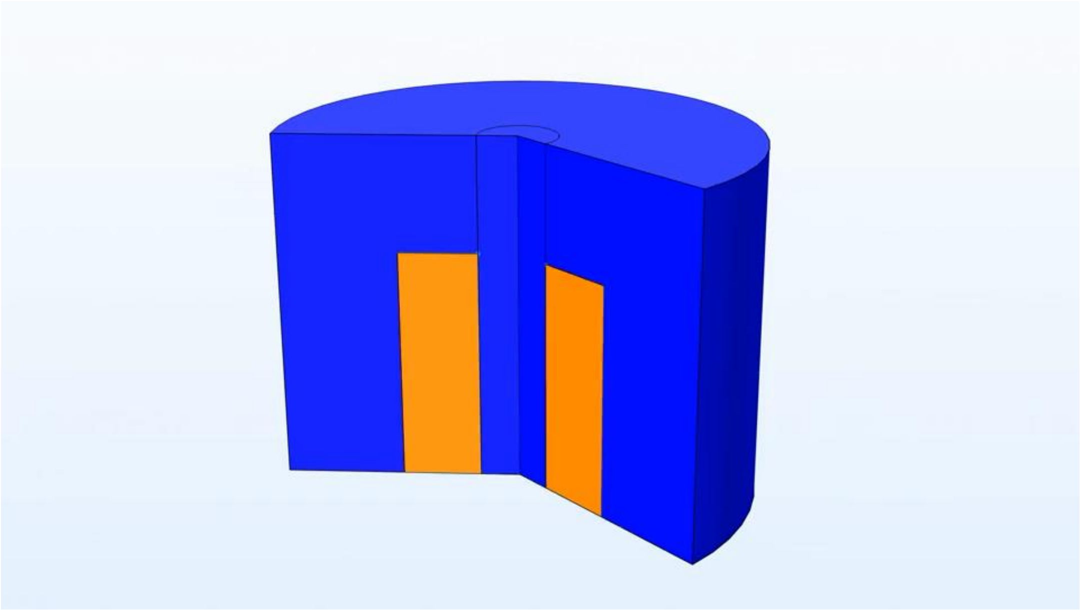
1. **Define Problem** - Objectives, Scope (e.g. Predict bone fracture load)
2. **Create Model** - Geometry Simplification (e.g. Use CT scans for 3D bone structure)
3. **Select Materials** - Properties, Behaviour (e.g. Bone material properties from literature)
4. **Meshing** - Element Type, Density (e.g. tetrahedral, hexahedral)
5. **Apply Conditions** - Constraints, Loads (e.g. Apply physiological loads and constraints mimicking joint forces)
6. **Solve** - FEA Solver (e.g. Linear static analysis to estimate failure load)
7. **Analyse Results** - Convergence, Sensibility (e.g. Evaluate stress distribution to predict potential fracture sites)

Simulations to ensure Patient Safety

Heat generated during a tumor ablation

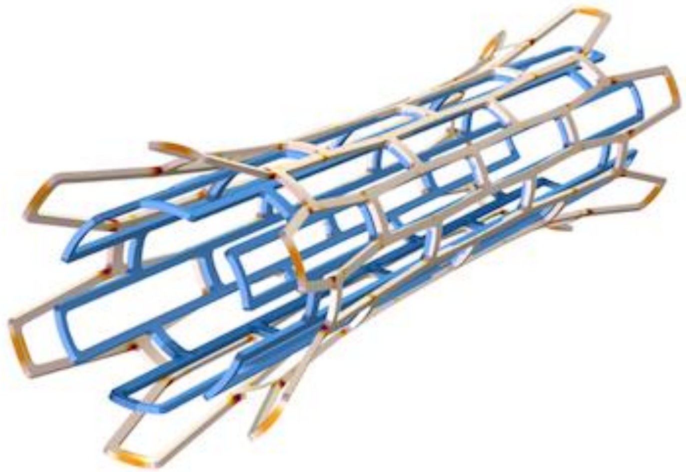


Drug delivery from a biomatrix

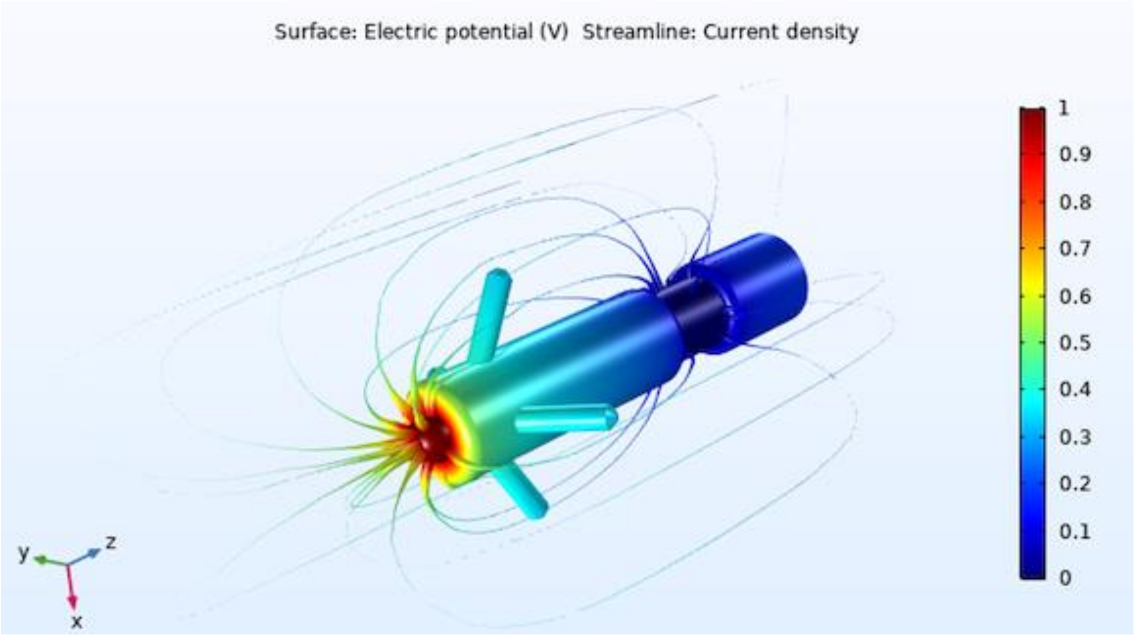


Simulations to accelerate Product Development

Biomedical stent

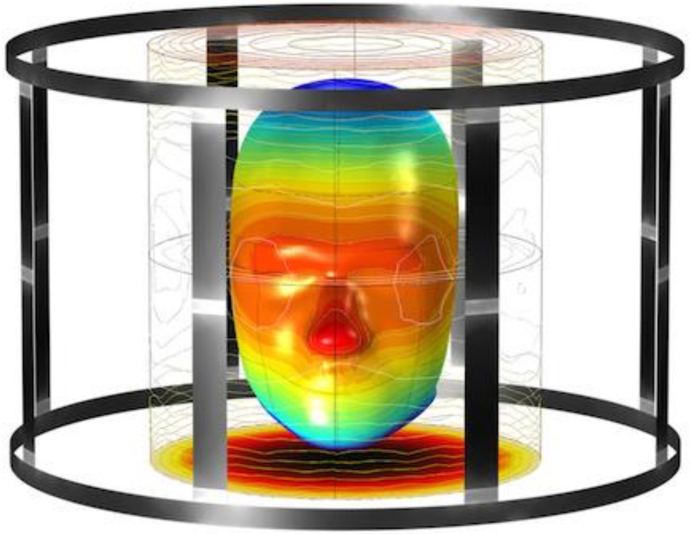


Pacemaker electrode

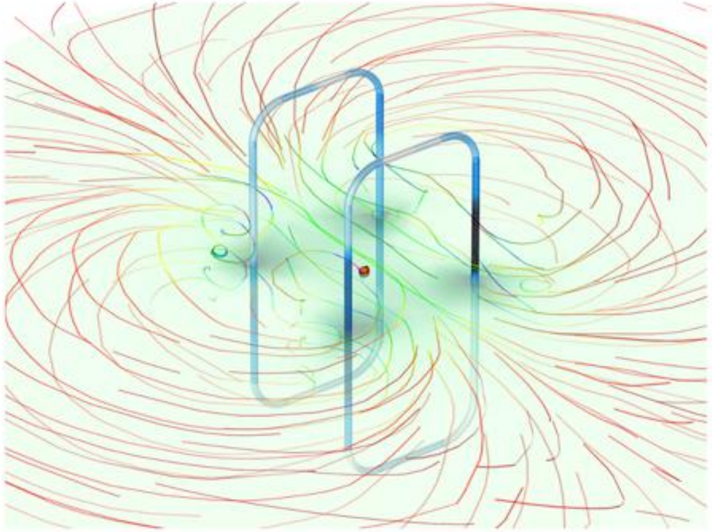


Simulations to develop medical devices

Electromagnetic field MRI birdcage coil

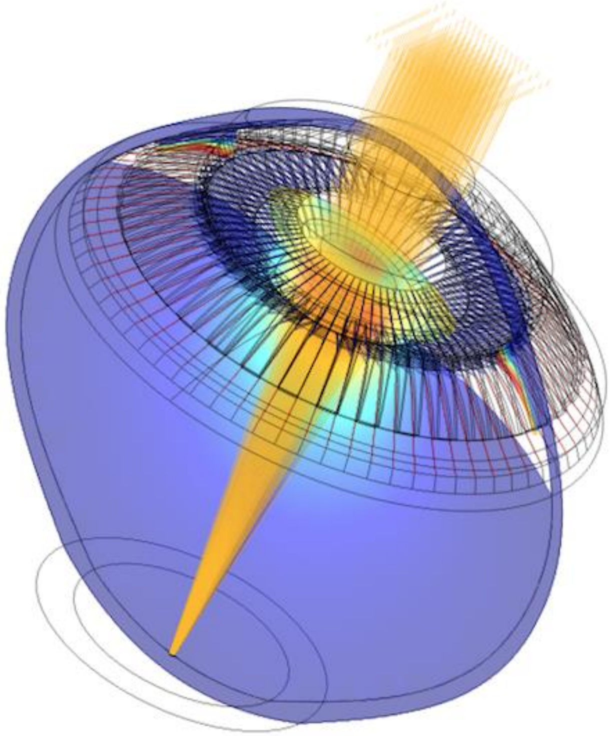


Electromagnetic interference RFID tag

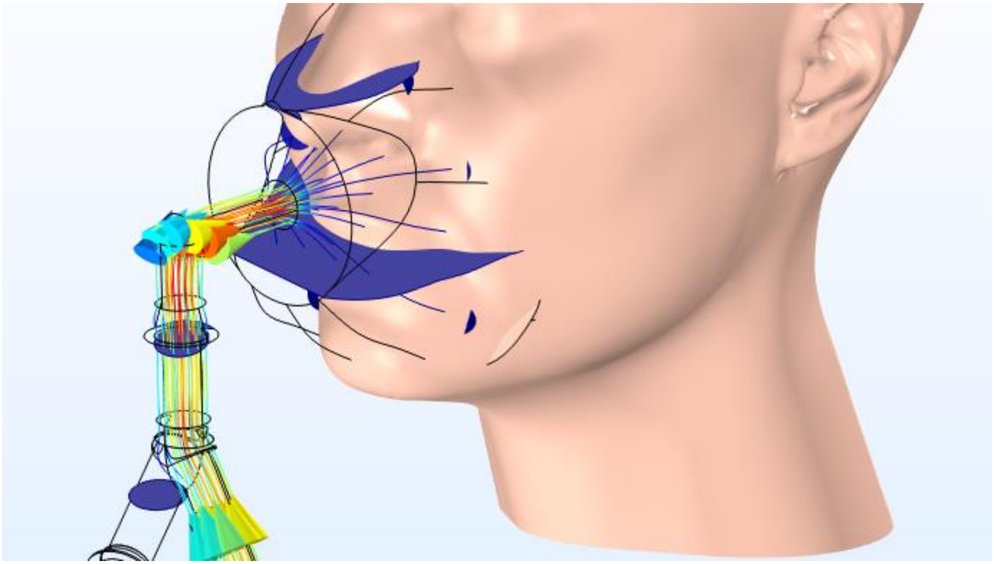


Growing field: Multiphysics simulations

Optomechanical model of the human eye

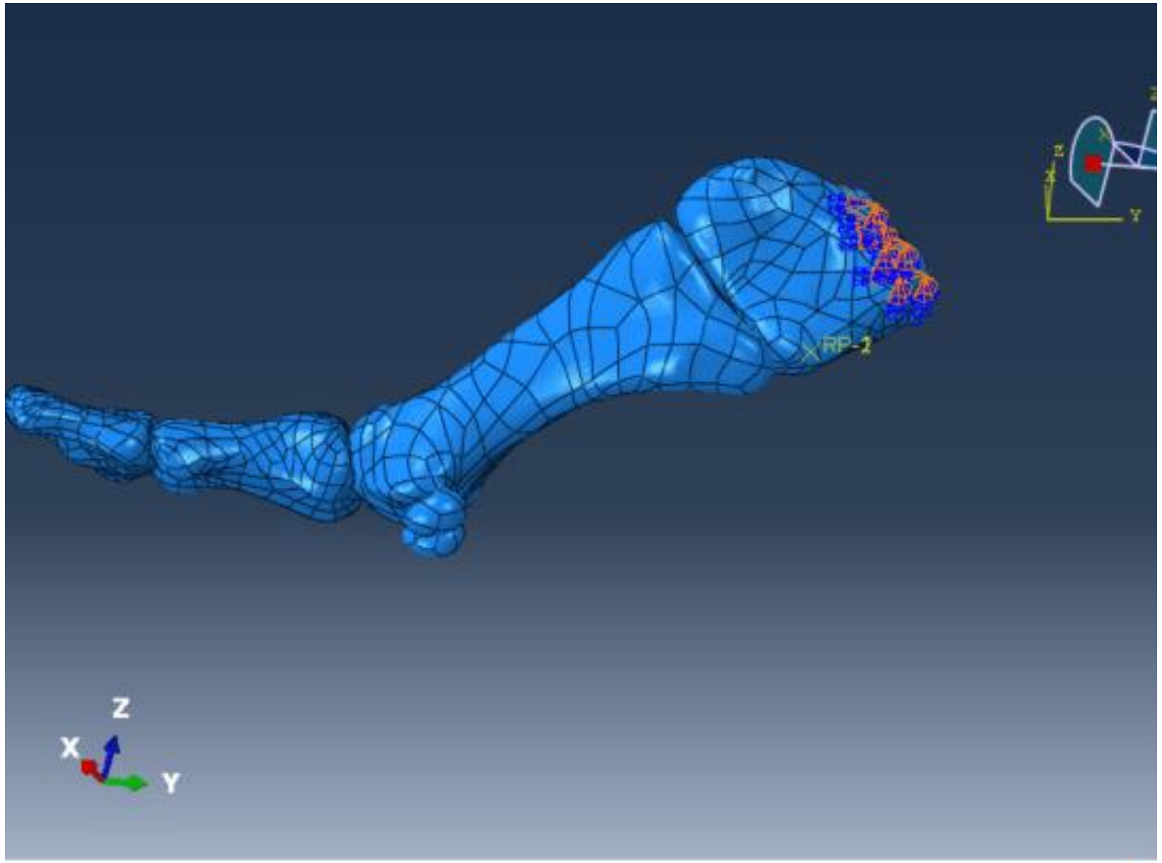


Non-invasive ventilation (NIV) mask



Tools for Finite Element Analysis

- ANSYS
  - Advanced simulations across multiple physics.
- Abaqus
  - Specialized in nonlinear problems, material failure.
- COMSOL Multiphysics
  - Multiphysics problems, user-friendly interface.
- SolidWorks Simulation
  - Integrated with CAD, user-friendly for designers.
- Custom Solvers:
  - For: Bone (FAIM, ParOsol), Soft tissue (BACI)



Connected bones using Abaqus

Common problems in FEA

UNIVERSITY OF CALGARY

1. Watch Out for Stress Concentrations
   - Are there any artefacts? High stress at the boundary conditions or sharp corners may be artefacts!
2. Ensure Adequate Mesh Quality
   - Is my solution accurate enough? Conduct mesh convergence studies!
3. Account for Material and Geometric Nonlinearities
   - Was the right material model chosen? Consider nonlinear models for large deformations (e.g. soft tissues)
4. Apply Boundary Conditions and Loads Correctly
   - Do boundary conditions accurately mimic the physical setup?
5. Validate FEA Results
   1. Always compare FEA outcomes with experimental data

Case: Finite Element Analysis to assess Bone Implants

UNIVERSITY OF CALGARY

Problem → Model → Materials → Meshing → Boundary Conditions → Solver → Results

Wolff's law[1]:

- Bone adapts to the loads under which it is placed

Problem:

Simulate stress shielding in a femoral implant

wallematthias.github.io/teaching

[1]Wolff, J. 1892

Questions?

Matthias Walle

McCaig Institute

matthias.walle@ucalgary.ca

@walle_Matthias

https://wallematthias.github.io/