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Monash Academy for Cross &
Interdisciplinary Mathematical Applications

# MATHEMATICAL MODELLING OF COMPLEX SYSTEMS


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# OUTLINE

- The importance of mathematics for modelling complex systems
  - Why we need models
  - Why complex systems require an extended and modern toolkit
  - Implications for curriculum reform and training
- Types of models
- Case studies

# THE VALUE OF MATHEMATICS

- Mathematics is an abstract language that describes properties of objects, relationships between objects, temporal dynamics, uncertainties → complex systems
- Current Priorities:
  - – Connecting the right kind of mathematical expertise relevant to a problem, since the field is so vast and deep
  - – Training young mathematicians in the kind of modern mathematical toolkit needed for complex systems

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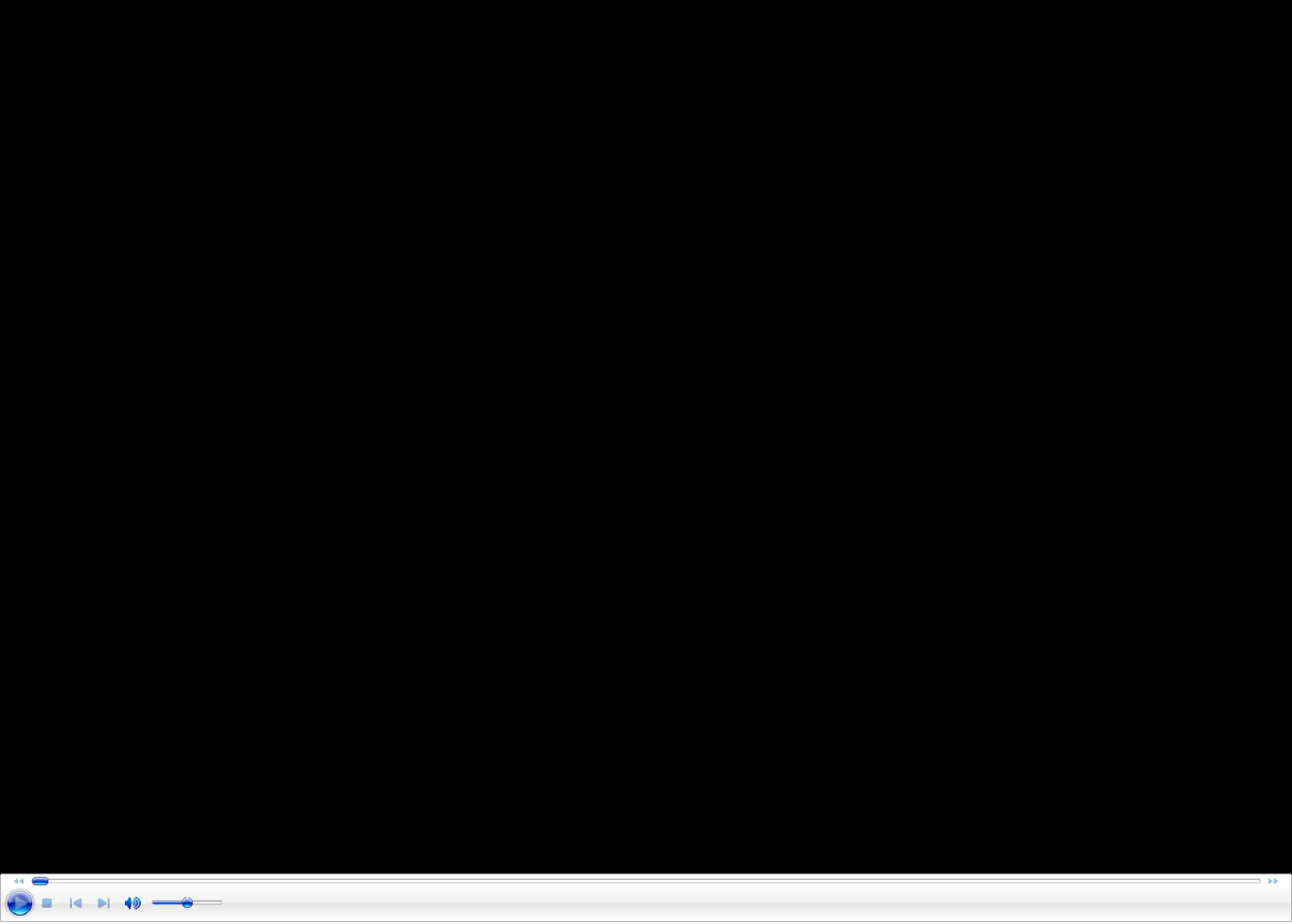

**Video at monash.edu/maxima**

# WHY WE NEED MODELS OF COMPLEX SYSTEMS

- Mathematical models help us to:
  - Describe the system (descriptive models)
  - Predict how the system will behave if we change something (predictive models)
  - Figure out how to get the optimal behaviour out of the system (prescriptive models)

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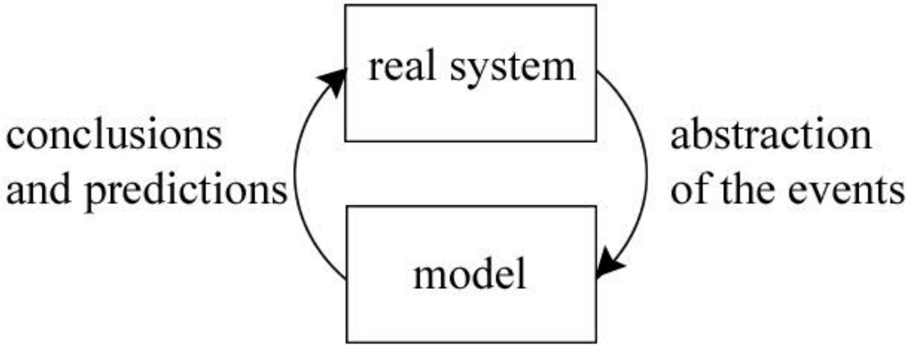
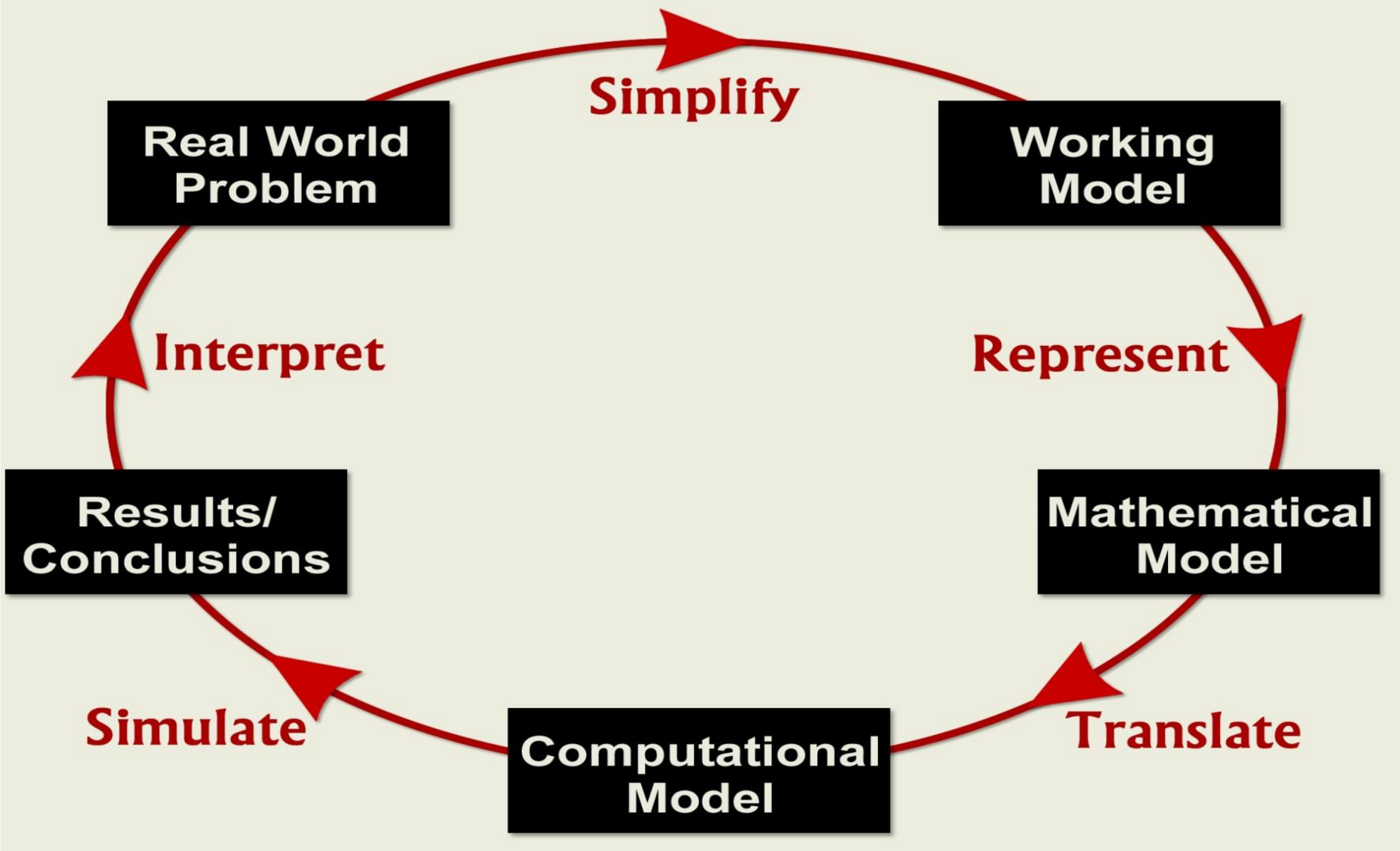
# IDEAL WORLD v REAL COMPLEX SYSTEMS

- A model is an abstraction
  - Simplifying assumptions help to make it “model-able” but also limit conclusions about the real system



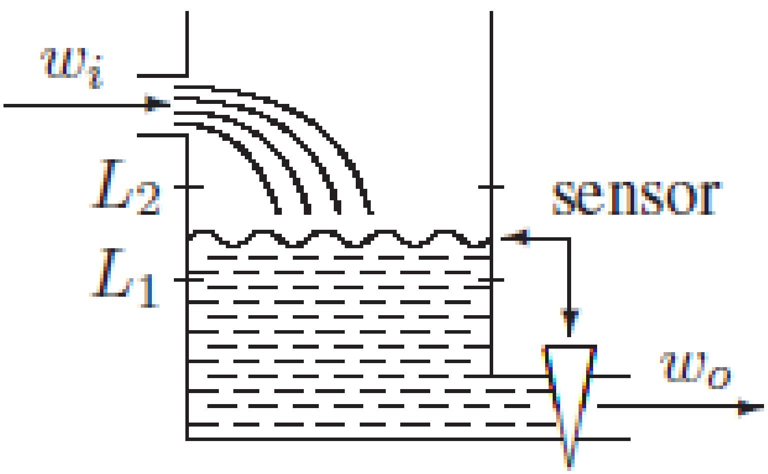

- The accuracy of the model depends greatly on the mathematical toolkit being used
  - E.g. how we choose to treat time, stochasticities, assumptions of linearity, parameter estimation methods

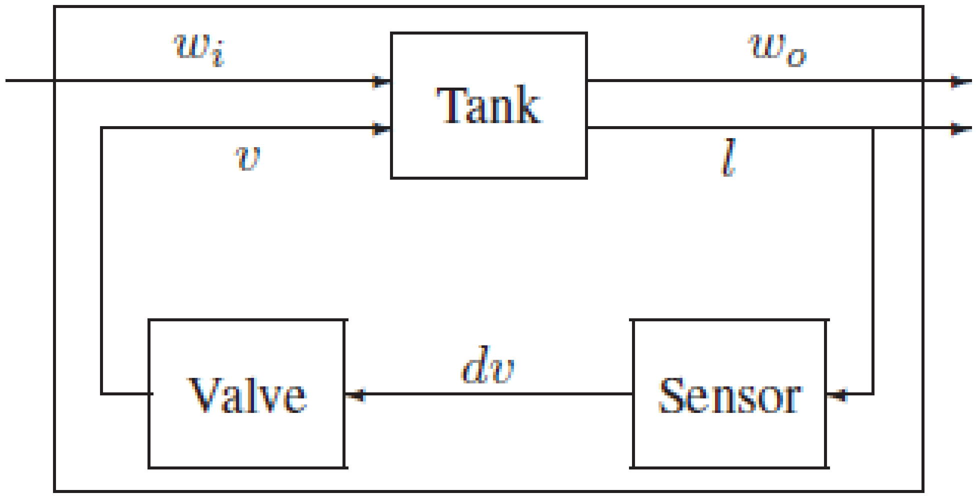
# MATH MODELLING - AN ITERATIVE PROCESS



# EXAMPLE: A SIMPLE (COMPLEX) SYSTEM

- Consider a water tank with input flow, and a sensor and release valve designed to ensure the water level is always between $L_1$ and $L_2$

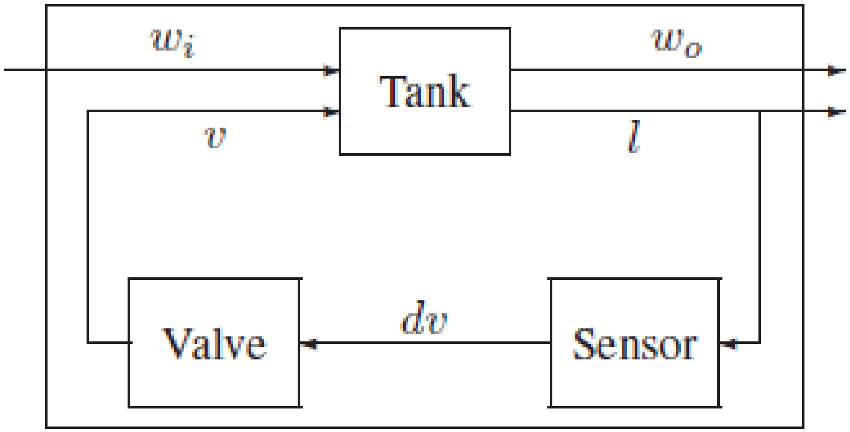



S. Bliudze and D. Krob, "Modeling of Complex Systems: Systems as Data Flow Machines", Fundamenta Informaticae, vol. 91, pp. 1-24, 2009

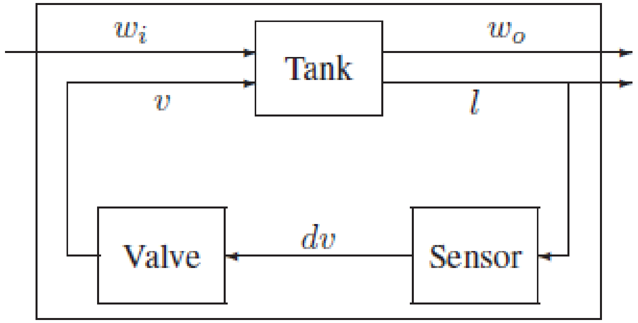
# MODELLING THE SYSTEM DEPENDENCIES

- The output flow depends on the valve position
- The valve position depends on the sensor reading
- The sensor reading depends on the water level
- The water level depends on the input flow and previous output flow
- But how?



# MATHEMATICAL DESCRIPTION

- Assumptions:
  - Time (t) advances with an infinitesimally small time step ε (t=0, ε, 2ε, 3ε, etc.)
  - $w_i(t) \geq 0$ is the arrival rate of water into the tank
  - $w_0(t) \geq 0$ is the exit rate of water out of the tank
  - c is the maximum throughput capacity of the exit pipe
  - v(t) in range [0,1] is the valve position (0=closed; 1=open; with intermediate values accepted)
  - $l_0$ is the initial water level in the tank with $l_0$ in range $[L_1, L_2]$
  - $\max(w_i(t)) \leq C$



# DERIVING GOVERNING EQUATIONS

- The output flow depends on the valve position

$$w_o(t+\varepsilon) = cv(t)$$

- The valve position depends on the sensor reading

$$v(t+\varepsilon) = v(t) + dv(t) \quad \text{if } v(t) + dv(t) \in [0,1],$$
$$\text{else} \quad v(t+\varepsilon) = v(t) \quad \text{no change}$$

- The sensor reading depends on the water level

$$dv = sign(l(t) - \frac{(L_1 + L_2)}{2})\varepsilon$$

so that if $l < mid, dv = -\varepsilon$ (close more)
$l > mid, dv = \varepsilon$ (open more)

- The water level depends on the input flow and previous output flow

$$l(t+\varepsilon) = l(t) + wi(t) - wo(t)$$

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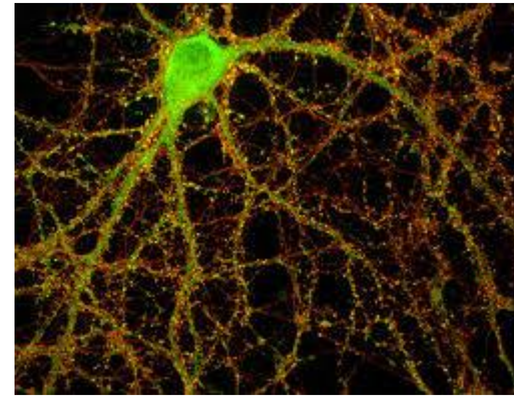
# SIMPLE v COMPLEX SYSTEMS

- This simple (complex) system can be modelled easily
  - Simple sub-systems are integrated in a direct path
  - Assumptions (linearity, known inflow) seem reasonable
- (Real world) Complex Systems are harder to model because governing equations often can't be derived, or assumptions are too unrealistic
- This creates challenges for mathematicians
  - Studying physical systems has created much of classical mathematics
  - Studying complex systems like biological and human-made systems is driving future mathematics
  - But there is still a need to modernise the math curriculum!

# COMPLEX SYSTEM PROPERTIES

- Large scale
- Feedback loops
- Nested organisation
- Nonlinear (chaotic) dynamics
- Adaptive dynamics
- Emergent organisation
- Stochasticity



# A NOBEL LAUREATE'S CAUTION

- In 1974, Friedrich von Hayek was awarded Nobel Prize in Economic Science
  - for his "penetrating analysis of the interdependence of economic, social and institutional phenomena"
- In his Nobel Lecture "The Pretence of Knowledge" he questioned the power of mathematics to model truly complex systems
  - He attacked mathematical models and the planning pretensions of the would-be "economic scientists"

The failure of the economists to guide policy more successfully is closely connected with their propensity to imitate as closely as possible the procedures of the brilliantly successful physical sciences

- Fortunately, our toolkit of mathematics is broader now than in 1974

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# MATHEMATICAL MODELS FOR COMPLEX SYSTEMS

- White-Box (mechanistic, 1st principles)
- Black-Box (data-driven observational, inference)
- Grey-Box (mixture of white and black)


- Black-box modelling involves techniques common in big data analytics: data mining/machine learning, stochastic modelling, parameter estimation, agent-based simulation, graph theory or network analysis, dynamical systems, Bayesian networks, optimisation, etc.

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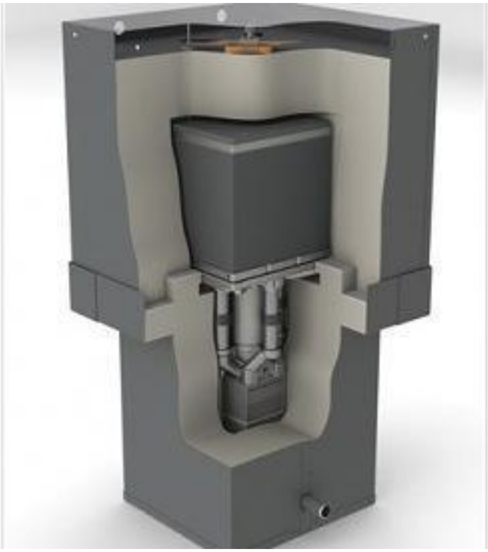
# MAXIMA’S TOOLKIT

| | |
|---|---|
| **Modelling and Simulation** | Developing a mathematical model of a real-world problem, and using computer simulation to study how the system behaves. |
| **Optimisation** | Methods to select the optimal decision amongst many choices, with various constraints limiting the choices. |
| **Probability and Stochastic Processes** | The study of uncertainty caused by random phenomena. |
| **Design of Experiments** | The development of controlled experiments that enable the maximum information to be gathered through the minimal number of experiments. |
| **Data Mining** | The process of discovering useful patterns in large datasets to assist decision making. |
| **Numerical Analysis** | The development of algorithms to find approximate solutions to continuous domain problems that can't be solved analytically. |
| **Continuum Mechanics** | The study of the motion of fluids (liquids, gases, plasmas) and solid objects, and the forces that act upon them in systems. |
| **Particle Mechanics** | The study of sets of particles or solid bodies and how they interact. |
| **Dynamical Systems** | Mathematical equations that describe the dynamics of a system in space and time. The stability of the system and its tendency to exhibit chaotic, periodic or steady state behaviours can be studied. |

# CASE STUDY: OPTIMISING EXPERIMENTAL DESIGN

- Industry Partner:
  Ceramic Fuel Cells Ltd.
- The problem:
  - 200 design variables
  - 5 objective functions
  - Complicated constraints
  - Expensive (time and cost) experiments to evaluate
  - Limited past experimental designs
  - What design should they build next to improve performance?
- Expensive Black-Box Optimisation



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# MINIMISING THE IMPACT OF INVASIVE SPECIES

- A/Prof Jon Keith
- Industry Partner:
  Biosecurity Qld

- Agent-based Bayesian modelling
- Given observations of fire-ants, where are their nests most likely to be?
- Inverse problem is also of interest

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# MINIMISING TRAFFIC CONGESTION

- A/Prof. Tim Garoni
- Industry Partner:
  VicRoads


- How do traffic light signal durations affect traffic congestion? What about clear-ways?
- Statistical mechanics, cellular automata …

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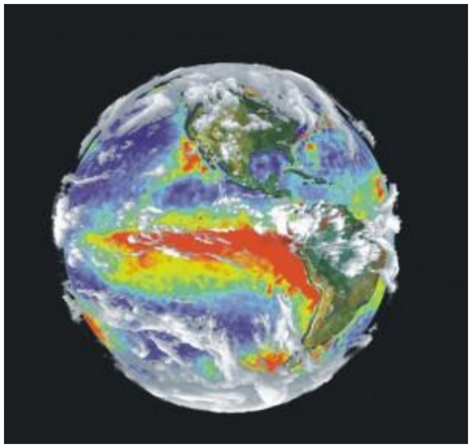
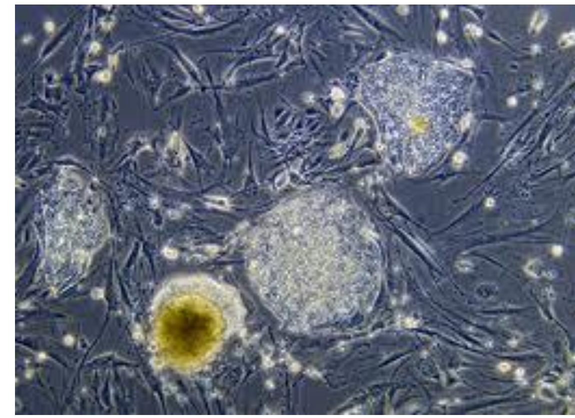
# MATHEMATICS UNDERPINS MANY OF THE GRAND CHALLENGES OF OUR TIME (ALL COMPLEX SYSTEMS)



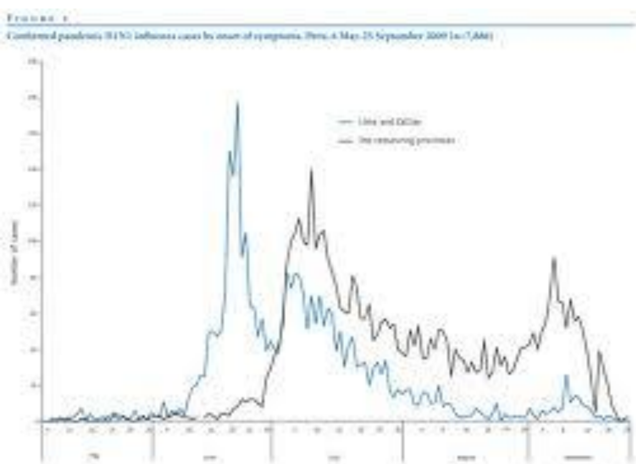
**Climate modelling**

**Traffic modelling**

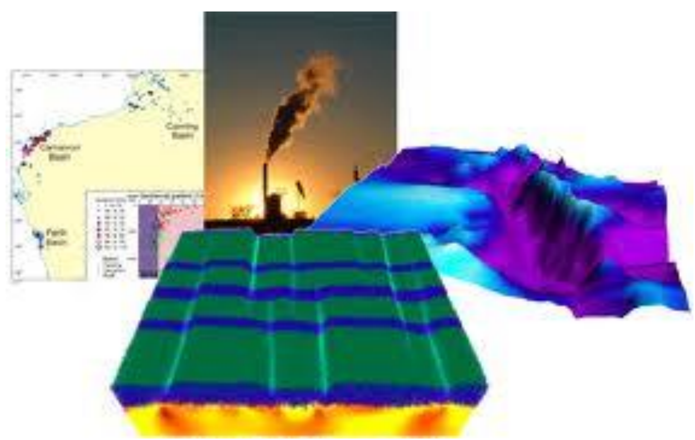


**Stem cell modelling**

**Outbreak detection**



**Fluid flow analysis**



**Biosecurity**

# SUMMARY

- Modern mathematical tools are critical for modelling complex systems
- University curricula must update to prepare young mathematicians for the vital role they will play in tackling grand challenges facing society
- Success stories show importance of collaboration between
  - Domain expert
  - Traditional Mathematicians
  - Modern mathematicians (data scientists)