

# Introduction to dynamical system modelling

Shan He

School for Computational Science  
University of Birmingham

Module 06-23836: Computational Modelling with MATLAB

# Outline of Topics

Dynamical systems

Concepts about modelling

How to model?

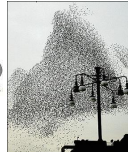
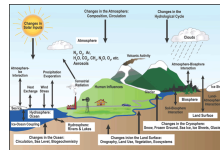
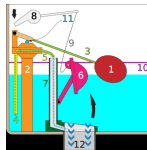
How to use models for scientific research

# What is a system?

**A System:** consisting of interconnected components, built or evolved with a desired purpose.

**Examples:**

- Toilet tank.

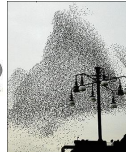
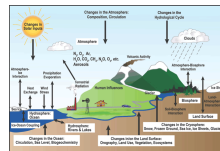
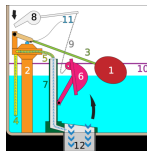


# What is a system?

**A System:** consisting of interconnected components, built or evolved with a desired purpose.

**Examples:**

- ▶ Toilet tank.
- ▶ Car engine.

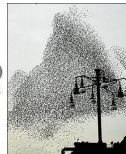
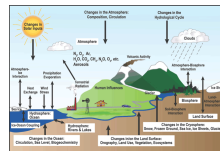
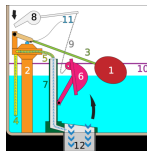


# What is a system?

**A System:** consisting of interconnected components, built or evolved with a desired purpose.

**Examples:**

- ▶ Toilet tank.
- ▶ Car engine.
- ▶ Brain.

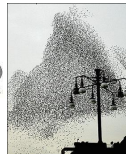
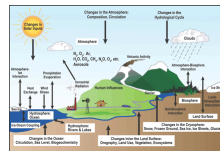
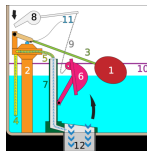


# What is a system?

**A System:** consisting of interconnected components, built or evolved with a desired purpose.

**Examples:**

- ▶ Toilet tank.
- ▶ Car engine.
- ▶ Brain.
- ▶ Bird flock.

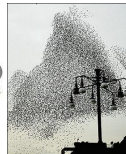
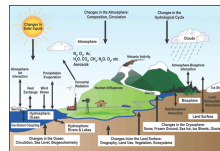
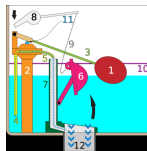


# What is a system?

**A System:** consisting of interconnected components, built or evolved with a desired purpose.

**Examples:**

- ▶ Toilet tank.
- ▶ Car engine.
- ▶ Brain.
- ▶ Bird flock.
- ▶ Climate system.



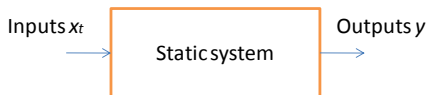
# What is a dynamical system?

- ▶ Static vs. Dynamical.



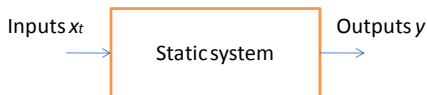
# What is a dynamical system?

- ▶ Static vs. Dynamical.
- ▶ **Static system:** current inputs  $\implies$  outputs.

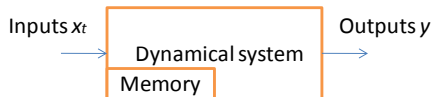


# What is a dynamical system?

- ▶ Static vs. Dynamical.
- ▶ **Static system:** current inputs  $\implies$  outputs.



- ▶ **Dynamical system:** history + current inputs  $\implies$  outputs.



# What is a dynamical system?

- ▶ Outputs depend on the present and past values of the inputs.

# What is a dynamical system?

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Changes over time.

# What is a dynamical system?

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Changes over time.
- ▶ Sometimes called dynamic systems or sequential systems.

# What is a dynamical system?

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Changes over time.
- ▶ Sometimes called dynamic systems or sequential systems.
- ▶ Mathematically described with differential or difference equations.

# Which one is a dynamical system?

## Which one is a dynamical system?

- ▶ Toilet tank.
- ▶ Car engine.
- ▶ Brian.
- ▶ Bird flock.
- ▶ Climate system.

## Which one is a dynamical system?

### Which one is a dynamical system?

- ▶ Toilet tank.
  - ▶ Car engine.
  - ▶ Brian.
  - ▶ Bird flock.
  - ▶ Climate system.
- ▶ X



## Which one is a dynamical system?

### Which one is a dynamical system?

- ▶ Toilet tank.
  - ▶ Car engine.
  - ▶ Brian.
  - ▶ Bird flock.
  - ▶ Climate system.
- ▶ X
  - ▶ ✓

# Which one is a dynamical system?

## Which one is a dynamical system?

- |                   |     |
|-------------------|-----|
| ▶ Toilet tank.    | ▶ X |
| ▶ Car engine.     | ▶ ✓ |
| ▶ Brian.          | ▶ ✓ |
| ▶ Bird flock.     |     |
| ▶ Climate system. |     |

## Which one is a dynamical system?

### Which one is a dynamical system?

- |                   |     |
|-------------------|-----|
| ▶ Toilet tank.    | ▶ X |
| ▶ Car engine.     | ▶ ✓ |
| ▶ Brian.          | ▶ ✓ |
| ▶ Bird flock.     | ▶ ✓ |
| ▶ Climate system. |     |

## Which one is a dynamical system?

### Which one is a dynamical system?

- |                   |     |
|-------------------|-----|
| ▶ Toilet tank.    | ▶ X |
| ▶ Car engine.     | ▶ ✓ |
| ▶ Brian.          | ▶ ✓ |
| ▶ Bird flock.     | ▶ ✓ |
| ▶ Climate system. | ▶ ✓ |

## Biological systems

- ▶ Outputs depend on the present and past values of the inputs.

# Biological systems

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Biological systems change over time.

# Biological systems

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Biological systems change over time.
- ▶ Biological systems are dynamical systems.

## Biological systems

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Biological systems change over time.
- ▶ Biological systems are dynamical systems.
- ▶ Biological systems are complex: emergence.



## Biological systems

- ▶ Outputs depend on the present and past values of the inputs.
- ▶ Biological systems change over time.
- ▶ Biological systems are dynamical systems.
- ▶ Biological systems are complex: emergence.
- ▶ Reductionism might not work well
- ▶ System point of view on biological systems is new - **Systems Biology**.

# What are models?

When we say models, we usually mean computational/mathematical models.

- ▶ Model: a description of a system using mathematical/computational concepts and language.

# What are models?

When we say models, we usually mean computational/mathematical models.

- ▶ Model: a description of a system using mathematical/computational concepts and language.
- ▶ **Mathematical model**: a set of variables and a set of equations that establish relationships between the variables.

# What are models?

When we say models, we usually mean computational/mathematical models.

- ▶ **Model:** a description of a system using mathematical/computational concepts and language.
- ▶ **Mathematical model:** a set of variables and a set of equations that establish relationships between the variables.
- ▶ **Computational model:** a computer program that implements computational techniques, e.g., rules, automata, petri nets or artificial neural networks to describe a system.

# What are models?

When we say models, we usually mean computational/mathematical models.

- ▶ **Model:** a description of a system using mathematical/computational concepts and language.
- ▶ **Mathematical model:** a set of variables and a set of equations that establish relationships between the variables.
- ▶ **Computational model:** a computer program that implements computational techniques, e.g., rules, automata, petri nets or artificial neural networks to describe a system.
- ▶ Can be hybrid: Mathematical models + Computational models.

# Why use models?

We use model to describe phenomena and understand phenomena.

More specifically:

- ▶ **Predict:** Make testable prediction

# Why use models?

We use model to describe phenomena and understand phenomena.

More specifically:

- ▶ **Predict:** Make testable prediction
- ▶ **Explain:** Reveal underlying mechanisms or rule out particular explanations

## Why use models?

We use model to describe phenomena and understand phenomena.

More specifically:

- ▶ **Predict:** Make testable prediction
- ▶ **Explain:** Reveal underlying mechanisms or rule out particular explanations
- ▶ **Discover:** Propose new questions



## Why use models?

We use model to describe phenomena and understand phenomena.

More specifically:

- ▶ **Predict:** Make testable prediction
- ▶ **Explain:** Reveal underlying mechanisms or rule out particular explanations
- ▶ **Discover:** Propose new questions
- ▶ **Guide:** Data collection or experiments design

## Example: Climate models

By building climate models, we can:

- ▶ **Predict:** How temperature changes in the next few days?

## Example: Climate models

By building climate models, we can:

- ▶ **Predict:** How temperature changes in the next few days?
- ▶ **Explain:** How the global atmosphere is operating?

## Example: Climate models

By building climate models, we can:

- ▶ **Predict:** How temperature changes in the next few days?
- ▶ **Explain:** How the global atmosphere is operating?
- ▶ **Discover:** How the carbon dioxide affects our climate?

## Example: Climate models

By building climate models, we can:

- ▶ **Predict:** How temperature changes in the next few days?
- ▶ **Explain:** How the global atmosphere is operating?
- ▶ **Discover:** How the carbon dioxide affects our climate?
- ▶ **Guide:** Collect climate data.

## Modelling methods

- ▶ Equation based methods:

## Modelling methods

- ▶ Equation based methods:
  - ▶ Differential equation: Ordinary Differential Equation, Partial differential equation.

## Modelling methods

- ▶ Equation based methods:
  - ▶ Differential equation: Ordinary Differential Equation, Partial differential equation.
  - ▶ Statistical methods: linear regression, multilevel model and Structural equation model.



## Modelling methods

- ▶ Equation based methods:
  - ▶ Differential equation: Ordinary Differential Equation, Partial differential equation.
  - ▶ Statistical methods: linear regression, multilevel model and Structural equation model.
  - ▶ Game theoretic methods.

## Modelling methods

- ▶ Equation based methods:
  - ▶ Differential equation: Ordinary Differential Equation, Partial differential equation.
  - ▶ Statistical methods: linear regression, multilevel model and Structural equation model.
  - ▶ Game theoretic methods.
- ▶ Agent-based methods.

## Modelling methods

- ▶ Equation based methods:
  - ▶ Differential equation: Ordinary Differential Equation, Partial differential equation.
  - ▶ Statistical methods: linear regression, multilevel model and Structural equation model.
  - ▶ Game theoretic methods.
- ▶ Agent-based methods.
- ▶ Other methods: data driven methods.

## Modelling principles

- ▶ Question: How to build the best model to model a system?

## Modelling principles

- ▶ Question: How to build the best model to model a system?
- ▶ No answer, even no a single definition to 'the best model'.

## Modelling principles

- ▶ Question: How to build the best model to model a system?
- ▶ No answer, even no a single definition to 'the best model'.
- ▶ One good attempt is Minimum Description Length principle, or Occam's razor.

## Modelling principles

- ▶ Question: How to build the best model to model a system?
- ▶ No answer, even no a single definition to 'the best model'.
- ▶ One good attempt is Minimum Description Length principle, or Occam's razor.
  - ▶ *"The best model is the one that is the smallest."*

## Modelling principles

- ▶ Question: How to build the best model to model a system?
- ▶ No answer, even no a single definition to 'the best model'.
- ▶ One good attempt is Minimum Description Length principle, or Occam's razor.
  - ▶ *"The best model is the one that is the smallest."*
- ▶ Einstein's razor' (Better!):



## Modelling principles

- ▶ Question: How to build the best model to model a system?
- ▶ No answer, even no a single definition to 'the best model'.
- ▶ One good attempt is Minimum Description Length principle, or Occam's razor.
  - ▶ *"The best model is the one that is the smallest."*
- ▶ Einstein's razor' (Better!):
  - ▶ *The model should be made as simple as possible, but no simpler.*

## How to put into practice?

I found this paper very useful: 5 Simple principles of modelling by Professor Mike Pidd. Here are the 5 principles:

- ▶ Model simple, think complicated.

## How to put into practice?

I found this paper very useful: 5 Simple principles of modelling by Professor Mike Pidd. Here are the 5 principles:

- ▶ Model simple, think complicated.
- ▶ Be parsimonious, start small and add.

## How to put into practice?

I found this paper very useful: 5 Simple principles of modelling by Professor Mike Pidd. Here are the 5 principles:

- ▶ Model simple, think complicated.
- ▶ Be parsimonious, start small and add.
- ▶ Divide and conquer, avoid mega models.

## How to put into practice?

I found this paper very useful: 5 Simple principles of modelling by Professor Mike Pidd. Here are the 5 principles:

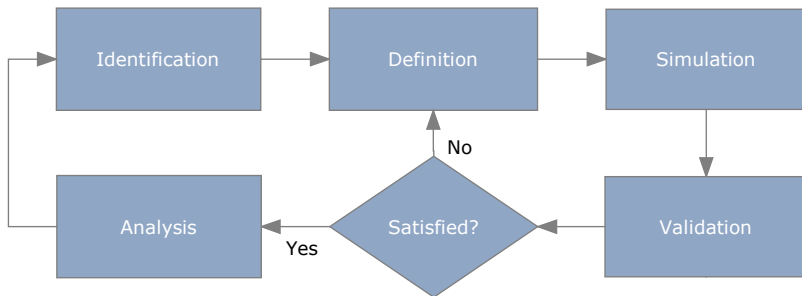
- ▶ Model simple, think complicated.
- ▶ Be parsimonious, start small and add.
- ▶ Divide and conquer, avoid mega models.
- ▶ Don't fall in love with data.

## How to put into practice?

I found this paper very useful: 5 Simple principles of modelling by Professor Mike Pidd. Here are the 5 principles:

- ▶ Model simple, think complicated.
- ▶ Be parsimonious, start small and add.
- ▶ Divide and conquer, avoid mega models.
- ▶ Don't fall in love with data.
- ▶ Model building may feel like muddling through.

## Modelling process



## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)



## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.

## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.

## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.
  - ▶ Prey-predator interaction.

## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.
  - ▶ Prey-predator interaction.
- ▶ Or more importantly, identify the problems to answer (**Why**).

## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.
  - ▶ Prey-predator interaction.
- ▶ Or more importantly, identify the problems to answer (**Why**).
- ▶ For example, if we model prey-predator interaction, we wish to answer:

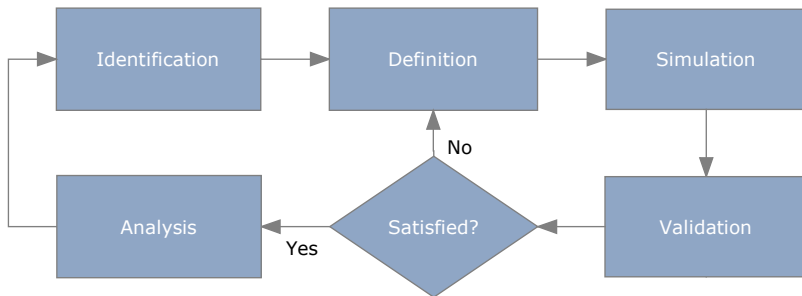
## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.
  - ▶ Prey-predator interaction.
- ▶ Or more importantly, identify the problems to answer (**Why**).
- ▶ For example, if we model prey-predator interaction, we wish to answer:
  - ▶ How predators affect prey populations, and vice-versa?

## Modelling process: **Identification**

- ▶ Identify the system to model (**What**)
  - ▶ Gene regulatory networks.
  - ▶ Cellular signalling networks.
  - ▶ Prey-predator interaction.
- ▶ Or more importantly, identify the problems to answer (**Why**).
- ▶ For example, if we model prey-predator interaction, we wish to answer:
  - ▶ How predators affect prey populations, and vice-versa?
  - ▶ Whether a prey-predator system is stable or collapse?

## Modelling process: **Definition**





## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.
- ▶ Check literature:

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.
- ▶ Check literature:
  - ▶ Any descriptions about the components?

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.
- ▶ Check literature:
  - ▶ Any descriptions about the components?
  - ▶ Any relations reported?

## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.
- ▶ Check literature:
  - ▶ Any descriptions about the components?
  - ▶ Any relations reported?
  - ▶ What parameters and variables used in similar studies?

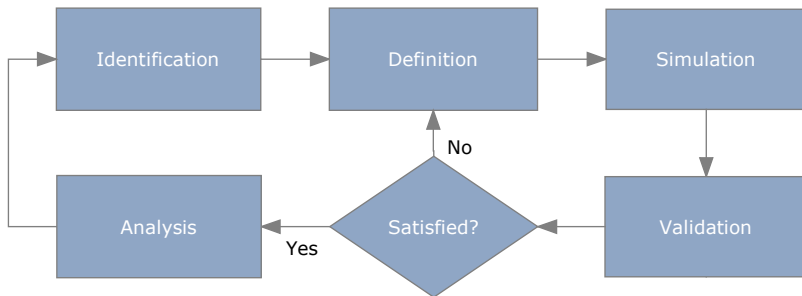


## Modelling process: **Definition**

The most important step. General suggestions are:

- ▶ Draw a detailed picture:
  - ▶ Defines all components.
  - ▶ Defines the relations between components.
- ▶ Define the parameters and variables to be used in the model.
- ▶ Check literature:
  - ▶ Any descriptions about the components?
  - ▶ Any relations reported?
  - ▶ What parameters and variables used in similar studies?
- ▶ You might need to simplify your assumptions.

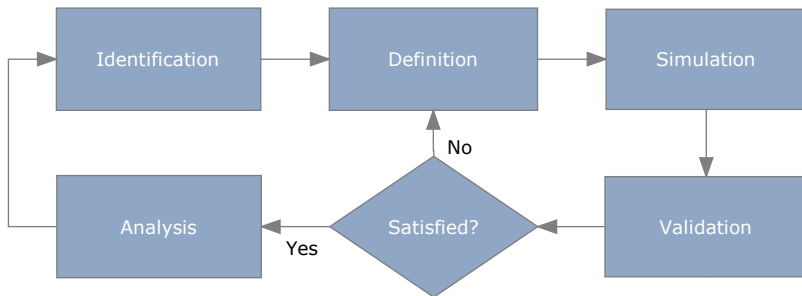
## Modelling process: **Simulation**



## Modelling process: **Simulation**

This simply means, in our module, to execute your MATLAB program ;)

## Modelling process: **Validation**



## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.

## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?

## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis

## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis
- ▶ Answer: No  $\implies$  Definition. We need to check:



## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis
- ▶ Answer: No  $\implies$  Definition. We need to check:
  - ▶ Simple typos?

## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis
- ▶ Answer: No  $\implies$  Definition. We need to check:
  - ▶ Simple typos?
  - ▶ Oversimplified assumptions?

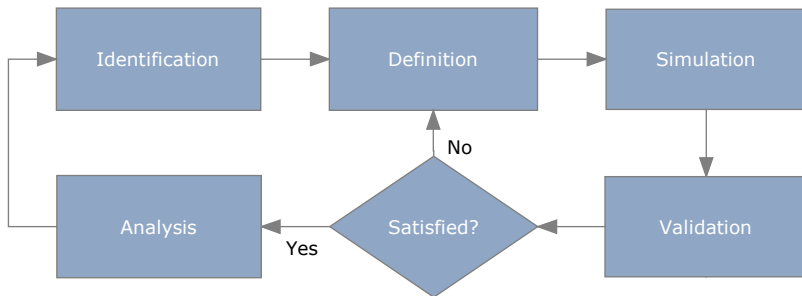
## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis
- ▶ Answer: No  $\implies$  Definition. We need to check:
  - ▶ Simple typos?
  - ▶ Oversimplified assumptions?
  - ▶ Missing components?

## Modelling process: **Validation**

- ▶ This simply means compare the outputs from your MATLAB program with experimental data.
- ▶ Decision time: Do the results match the experimental data?
- ▶ Answer: Yes  $\implies$  Analysis
- ▶ Answer: No  $\implies$  Definition. We need to check:
  - ▶ Simple typos?
  - ▶ Oversimplified assumptions?
  - ▶ Missing components?
  - ▶ Incorrect parameters?

## Modelling process: **Analysis**



## Modelling process: **Analysis**

- ▶ By analysing the results, we aim to answer:

## Modelling process: **Analysis**

- ▶ By analysing the results, we aim to answer:
  - ▶ What do the results imply or suggested?

## Modelling process: **Analysis**

- ▶ By analysing the results, we aim to answer:
  - ▶ What do the results imply or suggested?
  - ▶ What is new and what did not know?



## Modelling process: **Analysis**

- ▶ By analysing the results, we aim to answer:
  - ▶ What do the results imply or suggested?
  - ▶ What is new and what did not know?
  - ▶ What prediction can we make?

## Modelling process: **Analysis**

- ▶ By analysing the results, we aim to answer:
  - ▶ What do the results imply or suggested?
  - ▶ What is new and what did not know?
  - ▶ What prediction can we make?
- ▶ If the analysis proposes new questions, we need to go back to identification.

## Modelling process and *scientific method*

We should always put modelling into the context of scientific method:

1. Make general observations of phenomena

## Modelling process and *scientific method*

We should always put modelling into the context of scientific method:

1. Make general observations of phenomena
2. Formulate a hypothesis that is consistent with your observations.

## Modelling process and *scientific method*

We should always put modelling into the context of scientific method:

1. Make general observations of phenomena
2. Formulate a hypothesis that is consistent with your observations.
3. Use the hypothesis to make predictions.

## Modelling process and *scientific method*

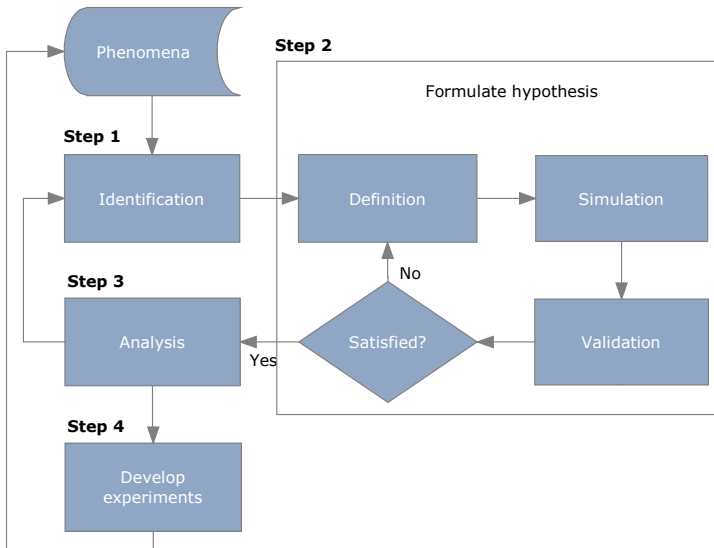
We should always put modelling into the context of scientific method:

1. Make general observations of phenomena
2. Formulate a hypothesis that is consistent with your observations.
3. Use the hypothesis to make predictions.
4. Develop experiments to test your hypothesis and modify the hypothesis in the light of your results.

## Modelling process and *scientific method*

We should always put modelling into the context of scientific method:

1. Make general observations of phenomena
2. Formulate a hypothesis that is consistent with your observations.
3. Use the hypothesis to make predictions.
4. Develop experiments to test your hypothesis and modify the hypothesis in the light of your results.
5. Repeat steps 3&4 until there are no discrepancies between hypothesis and phenomena.





## Too abstract?

After learning MATLAB next week, in week 4, I will follow the process to model predator-prey interactions using Ordinary Differential Equations.