Análise Estatística de Simuladores
Lecture 1: Introduction to Computer Experiments

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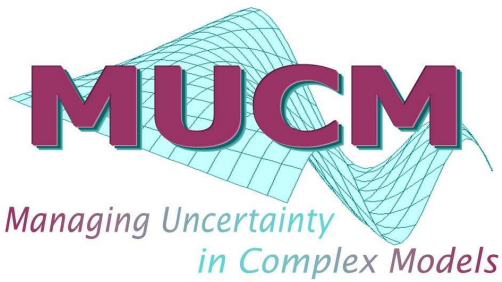

Computer experiments

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The gold-standard of empirical research is the designed experiment, studied in depth by R.A. Fisher, and involves concepts such as

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In the past three decades, computer experiments (*in silico* experiments) have become commonplace in nearly all areas of human endeavour.

Although the statistical challenges posed by physical experiments are well known, the challenges posed by computer experiments are somewhat different and have only recently begun to be tackled by statisticians.

Computer experiments

For example, for deterministic computer experiments, the concepts of replication, randomization and blocking are irrelevant because a computer model will give identical answers if run multiple times.

Methods to quantify, analyse and reduce uncertainty in the application of computer experiments are attracting increasing attention amongst users of simulation, and in this course we will describe some of the challenges faced, and introduce some of the developing methodology for dealing with these issues.

Plan of lectures

1. Lecture 1: Introduction to computer experiments
2. Lecture 2: Introduction to meta-modelling
3. Lecture 3: Design of experiments and multidimensional emulators
4. Lecture 4: Calibration
5. Lecture 5: Validation and Sensitivity Analysis
6. Lecture 6: Approximate Bayesian computation (ABC)

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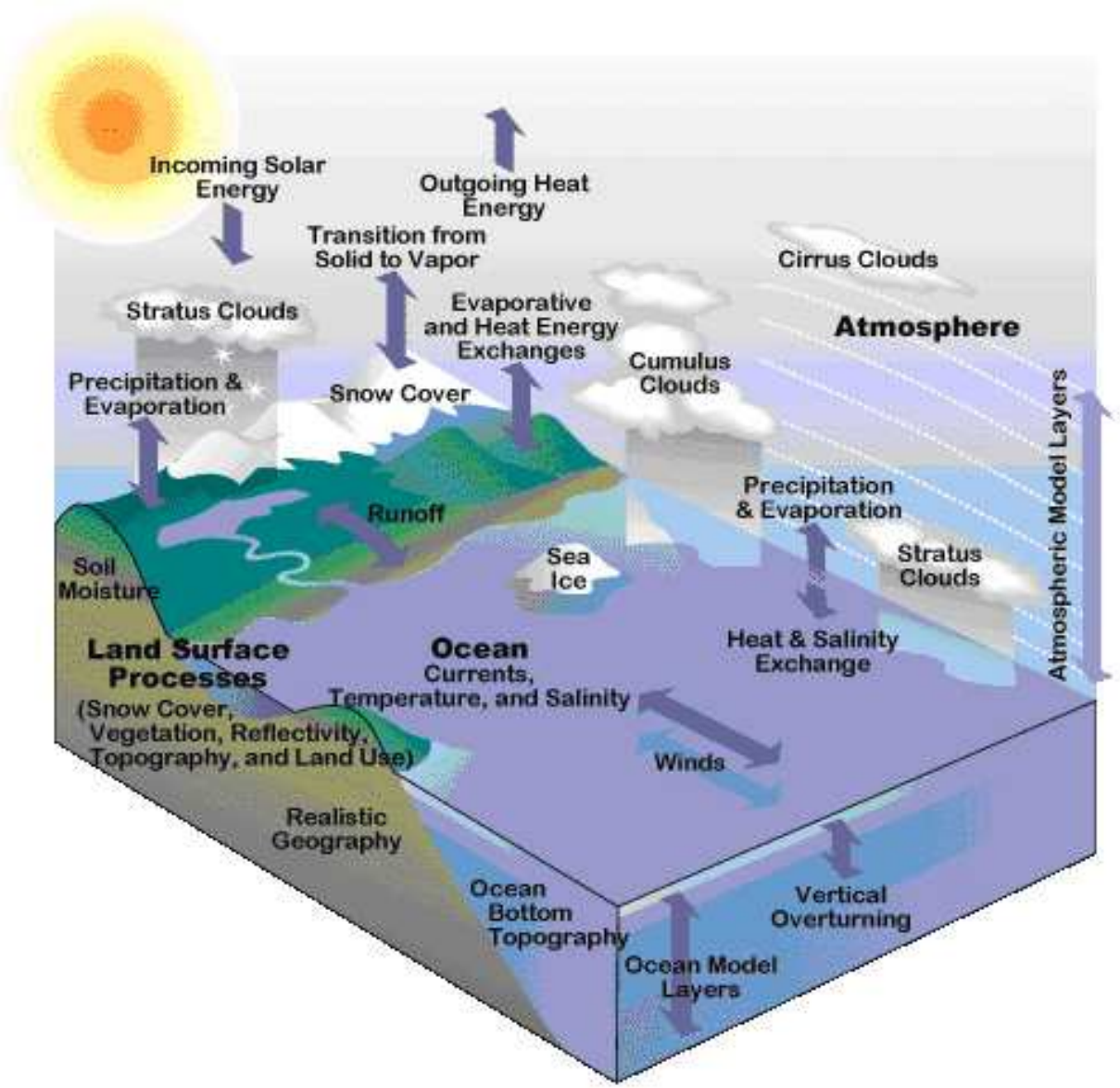
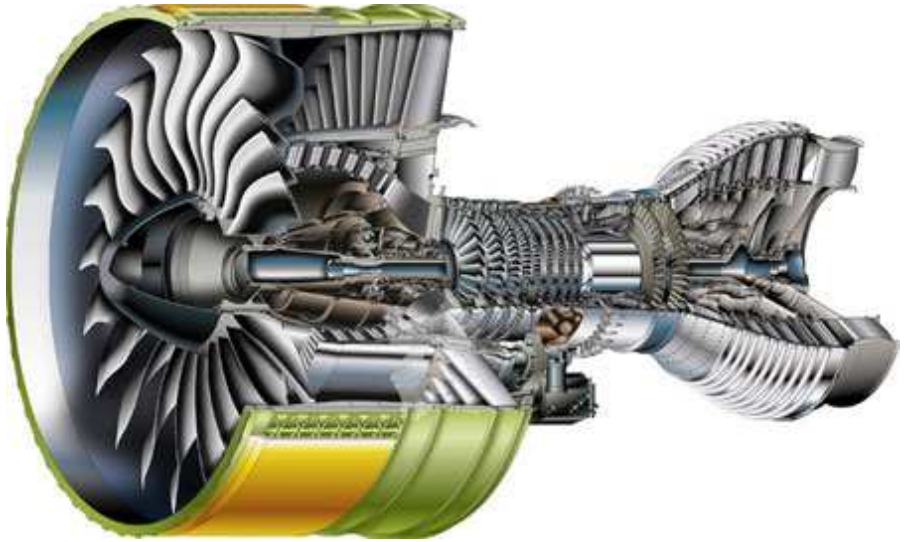
Climate Science

Predicting future climate



Engineering

Engine Health System Monitoring - Rolls Royce



We can't monitor the internals of the engine - only the outputs.

Public policy decisions

NHS drug funding decisions

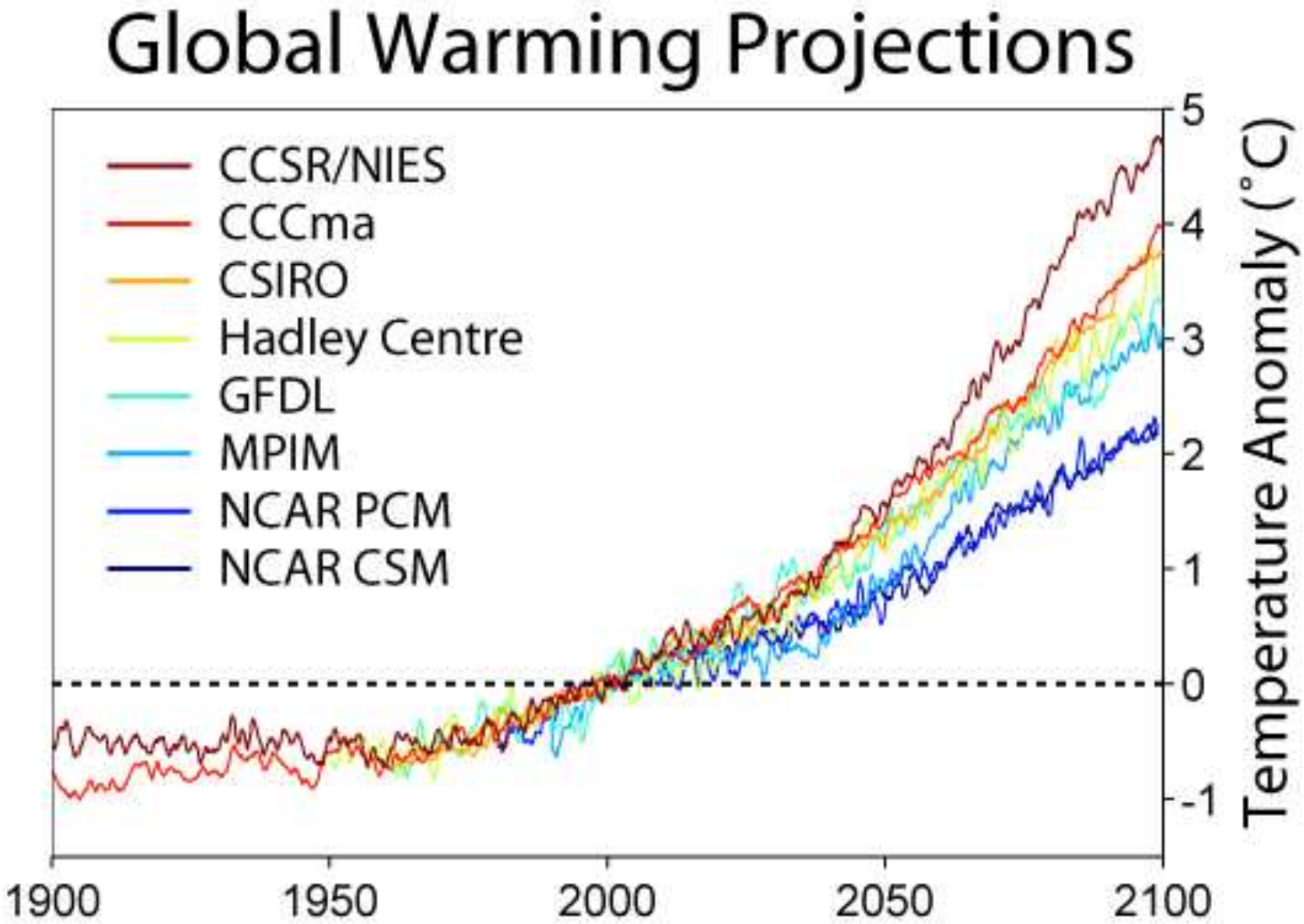
The National Health Service in the UK is a publically funded health care system. It has a finite amount of money and must decide what drugs to provide.
Complex models are used which simulate

- efficacy
- cost
- usage

and this feeds into a decision problem.
The process receives a lot of media attention and so must be transparent and carefully account for possible errors.

Challenges of computer experiments

Climate Predictions



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- Because each model can take several months to run on a supercomputer, it is not known whether the different models could all similar predictions if the right parameter value was used.

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- Because each model can take several months to run on a supercomputer, it is not known whether the different models could all similar predictions if the right parameter value was used.
- No model is perfect - all models are wrong to a certain degree. None of the predictions have accounted for model error.

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Models for climate change produce different predictions for the extent of global warming and other consequences

- Which predictions should we believe?
- What error bounds should we put around the predictions?
- Are model differences consistent with the error bounds?

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There is increasing concern about uncertainty in model outputs (cf. swine flu and climate predictions etc)

- particularly where model predictions are used to inform scientific debate or environmental policy

Methods that can be used to assess whether model predictions are robust enough for high stakes decision-making are being developed in the statistics community - we shall present a few ideas that are becoming increasingly popular.

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$$\eta : \mathcal{X} \to \mathcal{Y}$$

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The model output will sometimes be univariate $y = \eta(x, \theta) \in \mathbb{R}$, but will often be multivariate, such as a spatial temporal field.

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- Dealing with long runs times
  - If a model takes a week to run, we can't use a brute force Monte Carlo approach.

Incorporating and accounting for uncertainty

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Types of uncertainty we will consider are

- Parametric uncertainty
- Model inadequacy
- Observation errors
- Code uncertainty

Before we look at these different sources, we shall make a few comments on the Bayesian approach to uncertainty.

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  - Even unknown function will be described by probability distributions across a class of unknown functions
- We shall use the principle of conditionality, and always (where possible) condition on our data.

Bayesian Inference

The basics of Bayesian inference are very simple.

- If quantity θ is unknown we describe our uncertainty by prior distribution $\pi(\theta)$.
- Suppose we have data D from model $\pi(D|\theta)$
- Then conditional on observing this data, our posterior distribution is

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Given a model and prior the entire Bayesian statistical approach is fully specified. In practice, computational difficulties add interest!

Parametric uncertainty

Suppose we have computer model $\eta(\theta)$ which depends on unknown parameters θ.
We can describe any beliefs about θ using a distribution $\pi(\theta)$ - for example,

- we may have previous experimental evidence to suggest θ takes a particular value (within some confidence interval) and decided that $\theta \sim N(\hat{\theta}, \sigma^2)$
- we may know hard physical bounds on the value of θ but not know where it lies within these bounds and thus decide a uniform distribution is the best description of our uncertainty $\theta \sim U[a, b]$
- we may have no knowledge at all and wish to use a flat improper prior $\pi(\theta) \propto 1$ - although in practice we are rarely in this situation.
- ...

Elicitation is the process of extracting distributions for unknown quantities from experts. Garthwaite *et al.* provides a good introduction to elicitation.

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  - Given $\theta \sim \pi(\theta)$ what is $\pi(\eta(\theta))$
  - i.e., what is the distribution of the simulator output given a distribution for the input.

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  - However to predict a physical system from a simulator, we need to relate the simulator to the system by including a specification of the model error. More on this in lecture 4.
  - Sometimes we can just use the average prediction $\mathbb{E}(Y|\mathcal{D}) = \int \eta(\theta)\pi(\theta|\mathcal{D})\mathrm{d}\theta$ or perhaps a plug-in estimate $\eta(\hat{\theta})$ where $\hat{\theta} = \arg\max \pi(\theta|\mathcal{D})$.

Code uncertainty

These tasks can be computed using a brute force approach (Monte Carlo) as long as sufficient computational resources are available.
For example, to perform UA

- draw a sample of parameter values from the prior $\theta_1, \ldots, \theta_N \sim \pi(\theta)$,
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However, for complex simulators, run times might be long.
Consequently, we will only know the simulator output at a finite number of points.

We call this *code uncertainty*.

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The design of computational experiments is an active field in statistics (see lecture 3).

Meta-modelling

Idea: If the simulator is expensive, build a cheap model of it and use this in any analysis.

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We use the emulator as a cheap approximation to the simulator.

- ideally an emulator should come with an assessment of its accuracy
- rather just predict $\eta(\theta)$ it should predict $\pi(\eta(\theta)|\mathcal{D}_{sim})$ - our uncertainty about the simulator value given the ensemble $\mathcal{D}_{sim}$.

There are many ways to build emulators, but we will focus on the most popular type, the Gaussian process emulator.

Summary

Computer experiments are increasingly being used to learn about the world and to make decisions.

The statistical analysis of computer experiments is vitally important in many cases, yet the theory is only just being developed.

This is an exciting and fast moving research area with lots of opportunities for methodological development and collaborative research with other research communities.

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