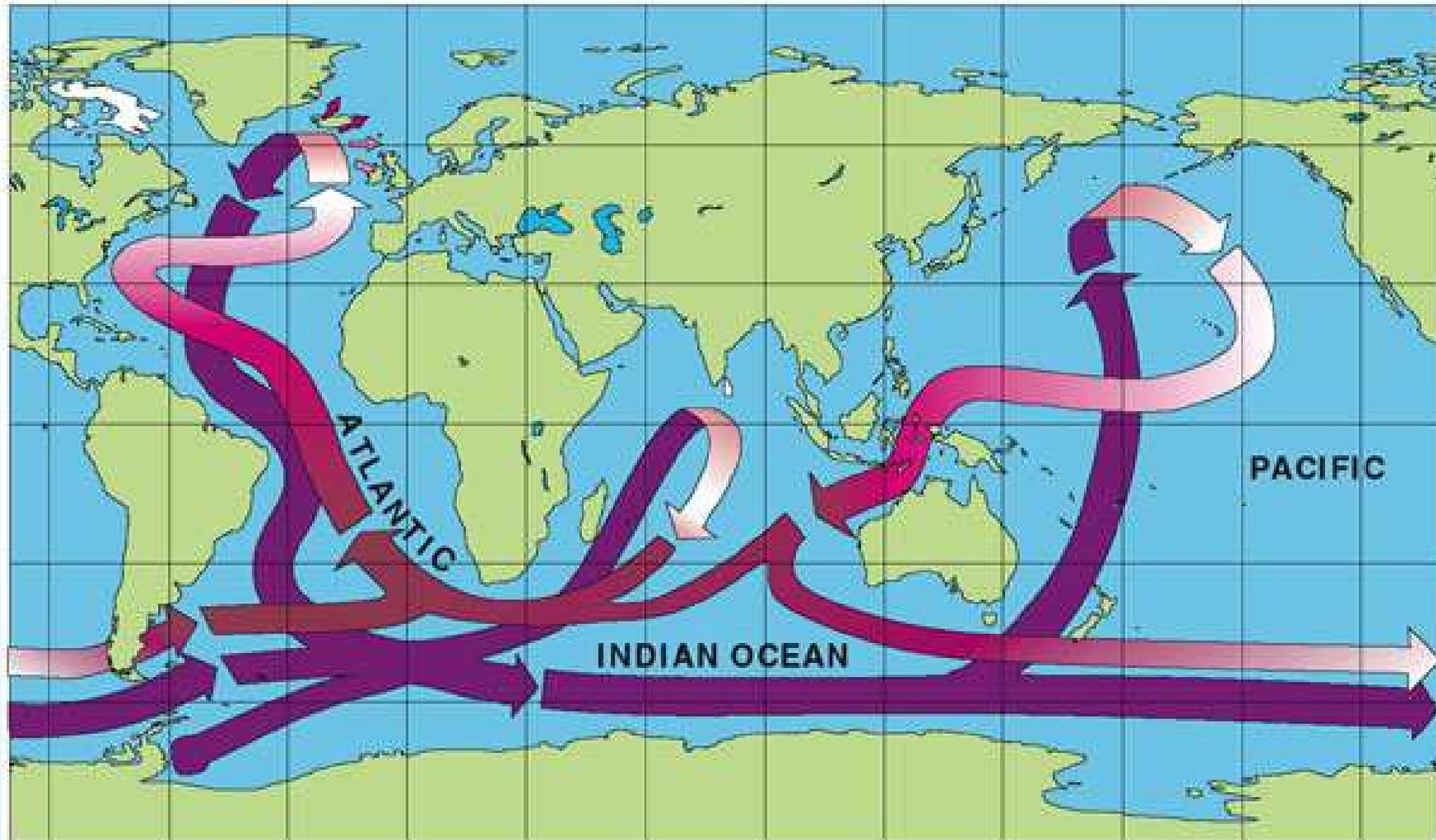


# General Issues in Uncertainty Analysis for Complex Models

Michael Goldstein  
Department of Mathematical Sciences,  
Durham University

# Global circulation



## Thermohaline shutdown

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“ The weight of evidence makes it clear that climate change is a real and present danger. The Exeter conference was told that whatever policies are adopted from this point on, the Earth’s temperature will rise by 0.6F within the next 30 years. Yet those who think climate change just means Indian summers in Manchester should be told that **the chances of the Gulf stream - the Atlantic thermohaline circulation that keeps Britain warm - shutting down are now thought to be greater than 50%.**”

[**Burying carbon** Leader Column Thursday February 3, 2005 The Guardian]

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- What do we learn about physical systems from the analysis of (necessarily imperfect) models?

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Such analysis results in our **Best Current Judgements** as to future system behaviour, expressed as **uncertainties**.

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**Stage 3** An analysis so clear and compelling that it would command agreement from all knowledgeable experts.

(This is an **objective** Bayes analysis (note non-standard use of “objective”!), and the only case where we can talk about, eg THE probability of THC collapse. )

## Model analyses in practice

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'Best current judgements' is a high standard to set (though why aim for less?). What we require is care and clarity. This is challenging, but no more challenging, in principle, than the process of collecting system data and building and analysing models themselves. However, this does require a different tool-set and proper resources to carry through.

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To understand the tool-set, we first need to look at the tool-set for individual models, and then consider how this tool-set extends to collections of models.

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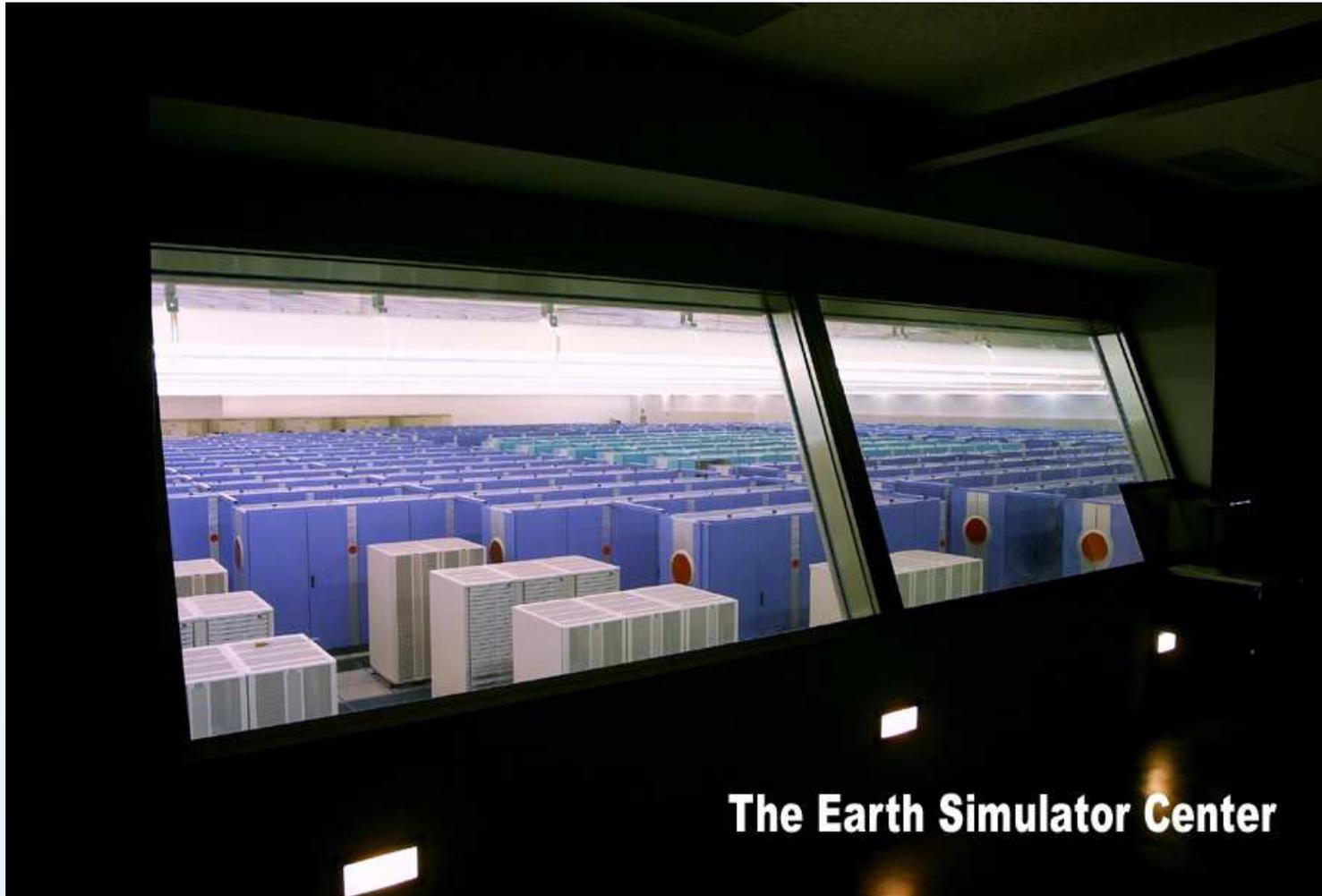
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**Issues** Serious assessment of model discrepancy is hard.

## The state of the art in climate modelling

Large climate models take months to run on supercomputers. The biggest computer in the world is the Earth Simulator in Japan, which is often used for running climate models.



**The Earth Simulator Center**

## Leading climate models

One leading climate model at the moment is HadCM3, based at the UK Met Office. One component of this model is HadAM3, the atmospheric module. In a simple experiment to study the effect of CO<sub>2</sub>-doubling (Murphy et al, 2004, Nature), this is coupled with simple mixed-layer ocean sea-ice models.

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4. *Radiation.* Four parameters
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We have a few hundred evaluations of HadSM3, made over a period of about three years. These evaluations will be one of the main resources for the UK Climate Impacts Programme 2008 (UKCIP08), which is intended as a fairly definitive statement about how climate change will impact the UK.

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- In particular, input and output very high dimensional and evaluating  $f(x)$  for any  $x$  may be VERY expensive.

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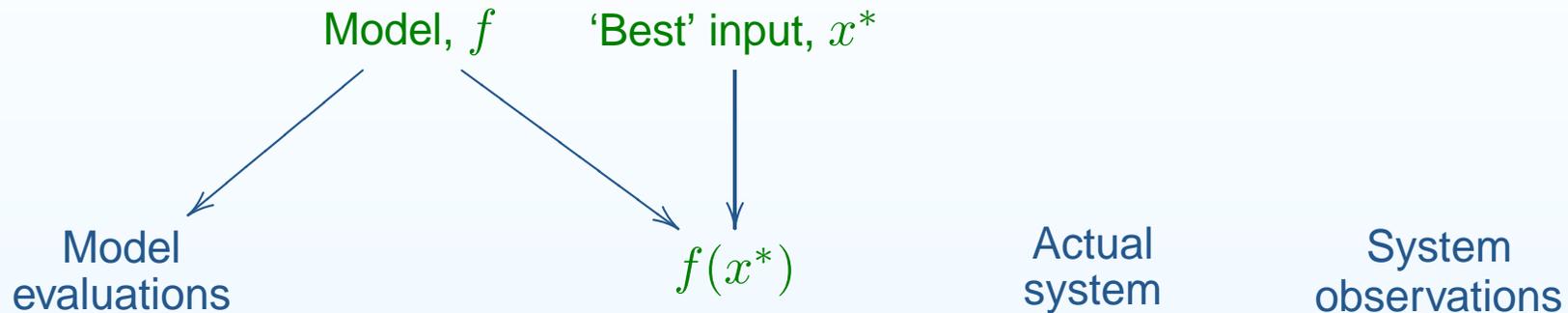
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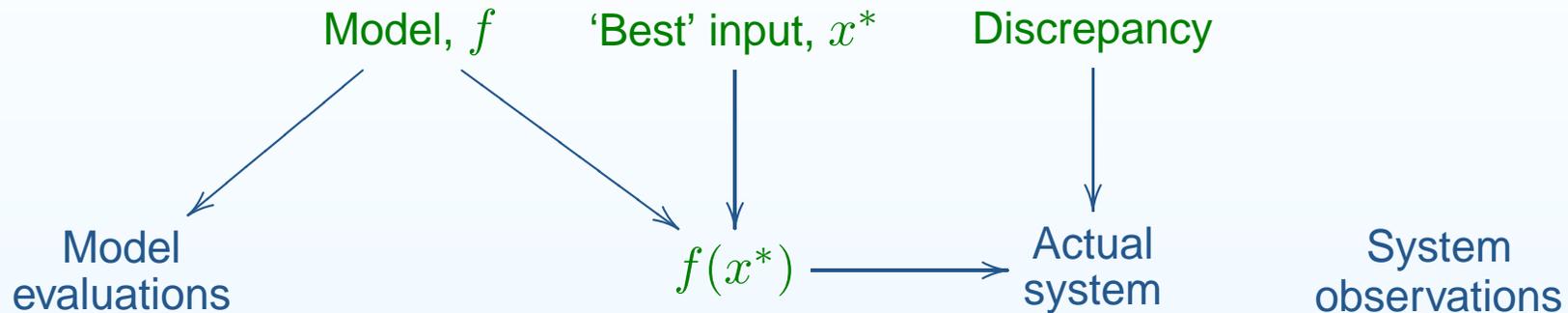
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2. We link the evaluations to the notion of a 'best' evaluation
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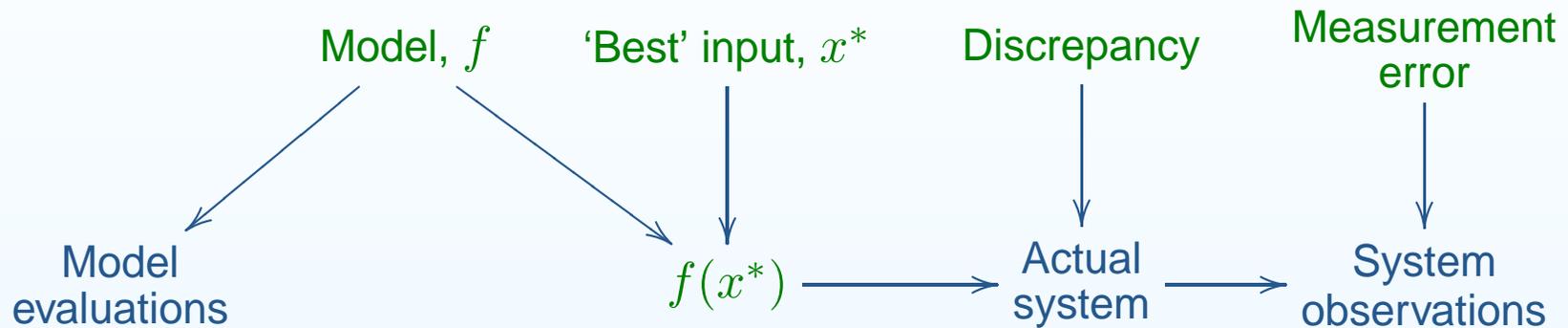
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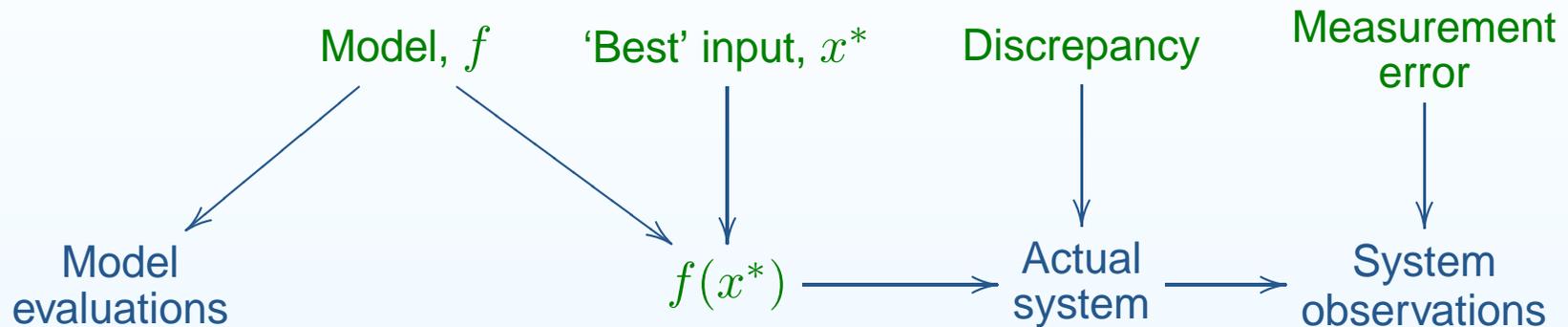
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An *emulator* is a probabilistic belief specification for a deterministic function. Our emulator for component  $i$  of  $f$  might be

$$f_i(x) = \sum_j \beta_{ij} g_{ij}(x) + u_i(x)$$

where  $B = \{\beta_{ij}\}$  are unknown scalars,  $g_{ij}$  are known deterministic functions of  $x$ , and  $u(x)$  is a weakly stationary stochastic process. [A simple case is to suppose, for each  $x$ , that  $u(x)$  is normal with constant variance and  $\text{Corr}(u_i(x), u_i(x'))$  is a function of  $\|x - x'\|$ .]

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When the input dimension is high, relative to the number of function evaluations we can make, then most of what we may learn about the function comes through the global component. For simplicity, we therefore often suppose that the simulator behaviour can be summarised by the global behaviour (as we don't learn much about local behaviour).

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The emulator expresses prior uncertainty judgements about the function.

These are modified by function evaluations. From the emulator, we may extract uncertainty statements for the function, at each input value  $x$ , e.g.

$$\begin{aligned}\mu_i(x) &= \mathbb{E}(f_i(x)) \\ \kappa_i(x, x') &= \text{Cov}(f_i(x), f_i(x')), \end{aligned}$$

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- to “optimise” the performance of the system (control).

## Uncertainty analysis for complex models

$$f(x) = Bg(x) + u(x), \quad y = f(x^*) + \epsilon, \quad z = y + e$$

The Bayesian treatment of this structure involves:

- a prior distribution for best input  $x^*$
- a probabilistic emulator for the computer function  $f$
- a probabilistic discrepancy measure relating  $f(x^*)$  to the system  $y$
- a likelihood function relating historical data  $z$  to  $y$

This full probabilistic description provides a formal framework to synthesise expert prior judgement, historical data and a careful choice of simulator runs. We may then use our collection of computer evaluations and historical observations to analyse the physical process

- to determine “correct” settings for simulator inputs (calibration);
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For problems of medium size, this approach is very powerful and effective.

## Bayes linear approach

For very large scale problems a full Bayes analysis is very hard because

- (i) it is difficult to make meaningful probability specifications over high dimensional spaces;
- (ii) the computations, for learning from data (observations and computer runs), particularly when choosing informative runs, may be technically difficult;
- (iii) the likelihood surface is extremely complicated, and any full Bayes calculation (based on emulation) may be extremely non-robust.

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The Bayes Linear approach is (relatively) simple in terms of belief specification and analysis, as it is based only on the mean, variance and covariance specification which, following de Finetti, we take as primitive.

For a full account, see

Michael Goldstein and David Wooff (2007) *Bayes Linear Statistics: Theory and Methods*, Wiley.

## Calibration via history matching

History Matching is concerned with learning about best inputs,  $x^*$ , using simulator evaluations and data,  $z$ . Using the emulator we obtain, for each input choice  $x$ , the adjusted values of  $\mathbf{E}(f(x))$  and  $\mathbf{Var}(f(x))$ . We rule out regions of  $x$  space for which  $f(x)$  is likely to be a very poor match to observed  $z$ .

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We iteratively refocus on the 'non-implausible' regions of the input space, by further model runs and refitting our emulator over the sub-region and repeating the analysis. This process is a form of iterative global search aimed at finding all choices for  $x^*$  which would give acceptable fits to historical data.

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If all values of  $x$  are implausible, this is important diagnostic information!

## Forecasting without calibration

For the computer model emulator, the mean and variance of  $f^* = f(x^*) = Bg(x^*) + u(x^*)$  are obtained from the mean function and variance function of the emulator for  $f(x)$ . Therefore, we can compute the mean and variance of  $f^*$  by conditioning on  $x^*$  and then integrating with respect to a prior distribution on  $x^*$ .

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Where appropriate, we can improve accuracy by adding a Bayes linear calibration stage to the forecasting (while retaining tractability).

## The Best input

How does learning about  $f$  inform us about  $y$ ?

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The simplest (and therefore most popular) way to relate uncertainty about the simulator and the system is the so-called “Best Input Approach”.

We proceed as though there exists a value  $x^*$  independent of the function  $f$  such that the value of  $f^* = f(x^*)$  summarises all of the information that the simulator conveys about the system. This means that we consider the model discrepancy,  $\epsilon = y - f^*$ , to be independent of  $f, x^*$ .

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Further, surprising contradictions arise when we try to construct joint specifications linking collections of models to the physical system in this way.

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Consider both our inputs  $x$  and the simulator  $f$  as abstractions/simplifications of real physical quantities and processes (through approximations in physics, solution methods, level of detail, limitations of current understanding) to a much more realistic simulator  $f^*$ , for which real, physical  $x^*$  would be the best input, in the sense that  $(y - f^*(x^*))$  would be judged independent of  $(x^*, f^*)$ .

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### Reifying principle

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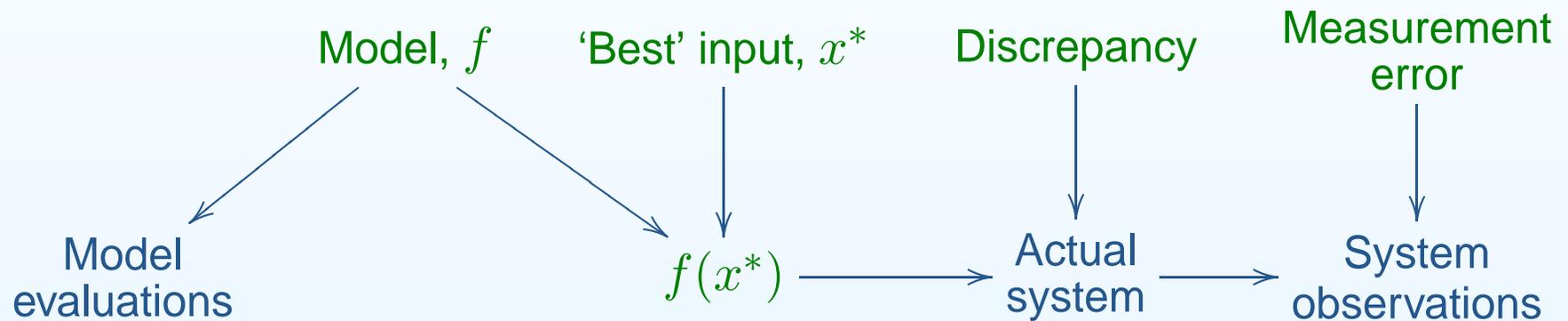
[2] A collection of simulators  $f_1, f_2, \dots$  is jointly informative for  $y$ , as the simulators are jointly informative for  $f^*$ .

## Relating the model and the system (2)

Our model  $f$  is informative for  $y$  because  $f$  is informative for a more elaborate model  $f^*$

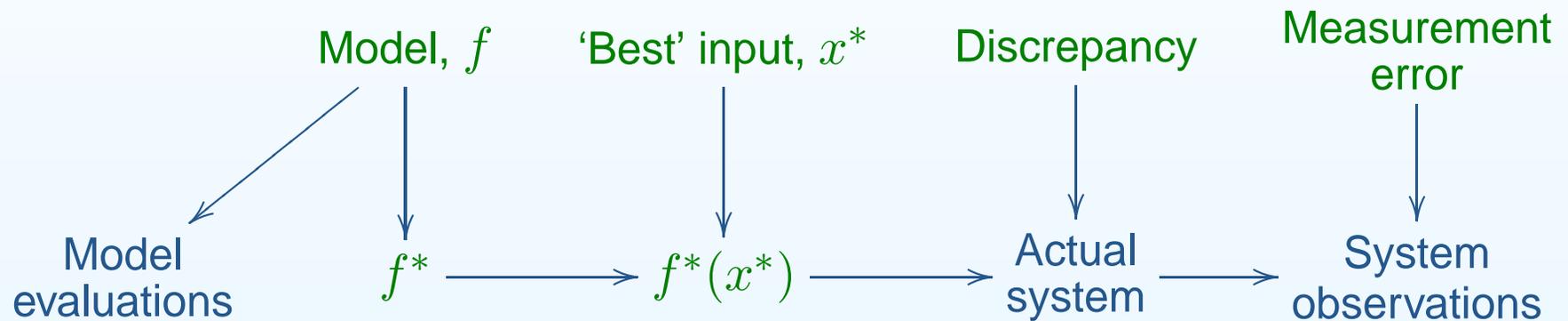
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where we might model our judgements as  $B^* = CB + \Gamma$  for known  $C$  and uncertain  $\Gamma$ , correlate  $u(x)$  and  $u^*(x)$ , but leave  $u^*(x, w)$ , involving any additional parameters,  $w$ , uncorrelated.

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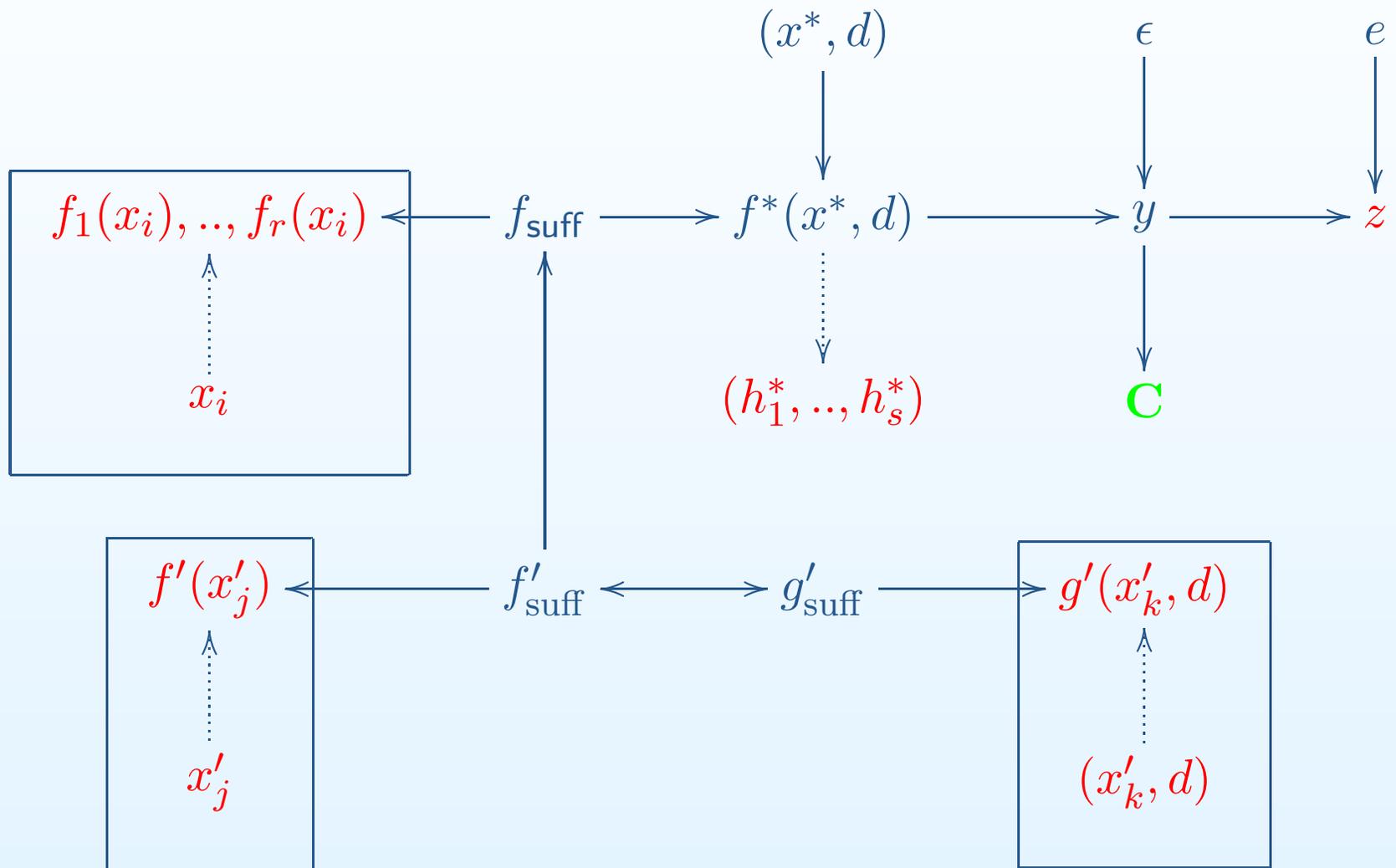
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Structured reification: systematic probabilistic modelling for all those aspects of model deficiency whose effects we are prepared to consider explicitly.

Comment: All our previous methods are unchanged - all that has changed is our description of the joint covariance structure.

## A reified influence diagram



Reified simulator  $f^*$ ;  $f_1, \dots, f_k$  are exchangeable refinements of  $f'$ ;  $g'$  is a simulator at level of  $f'$  adding decision variables  $d$ ;  $(h_i^*)$  is ensemble of tuned model runs.  $C$  is cost to the planet.

## Best current judgements for complex systems

To assess best current judgements about complex systems, it is enormously helpful to have an overall framework to unify all the uncertainties arising from

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We have suggested a conceptual/graphical framework for unifying our qualitative and quantitative knowledge about all such uncertainties within a structure which is both logical and tractable, so that we can focus on science rather than technical/computational issues.

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Such analysis poses serious challenges, but they are no harder than all of the other modelling, computational and observational challenges involved with studying large scale physical systems.

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- And don't forget to check out the website for the **Managing Uncertainty in Complex Models (MUCM)** project [A consortium of Aston, Durham, LSE, Sheffield and Southampton all hard at work on developing technology for computer model uncertainty problems.]