

Science and Simulation:

Whatever Happened to Conjecture and Refutation?

On Models, Theories and Understanding

Geoffrey K. Vallis

University of Exeter

Exeter, 2014

Science and Simulation:

Whatever Happened to Conjecture and Refutation?

On Models, Theories and Understanding

Geoffrey K. Vallis

University of Exeter

Exeter, 2014

Caution!

'It is a safe rule to apply that, when a mathematical or philosophical author writes with a misty profundity, he is talking nonsense.'

Alfred North Whitehead.

Why do we do Science?

Just one answer: For the betterment of society, in its broadest meaning.

Why do we do Science?

Just one answer: For the betterment of society, in its broadest meaning.

Two aspects of that:

1. To increase the material quality of life: from the elimination of poverty and having clean drinking water, to having nicer racing yachts.

Why do we do Science?

Just one answer: For the betterment of society, in its broadest meaning.

Two aspects of that:

1. To increase the material quality of life: from the elimination of poverty and having clean drinking water, to having nicer racing yachts.
2. Increasing the non-material quality of life: intellectual and aesthetic pleasures, the quest to understand the universe and the planet on which we live. The human adventure.
 - ▶ *Mathematics is not important because it enables us to build machines. Machines are important because they give us more time for mathematics.*
Henri Poincaré, Science and Method, 1908.

But note: funding comes mainly for task one!

Also, personal motivation can be different from societal motivation, and may be purely aesthetic.

Scientific Knowledge

Hypotheses and Theories

- ▶ Logical Positivism: Essentially that all knowledge (justified true belief) comes from either:
 1. Things that are true by definition, e.g., mathematical truths and theorems, deductions. (Analytic, a priori.)
 2. Things that we observe to be the case, e.g., I am giving a lecture at this moment. Experiential knowledge. (Synthetic, a posteriori.)

Scientific Knowledge

Hypotheses and Theories

- ▶ Logical Positivism: Essentially that all knowledge (justified true belief) comes from either:
 1. Things that are true by definition, e.g., mathematical truths and theorems, deductions. (Analytic, a priori.)
 2. Things that we observe to be the case, e.g., I am giving a lecture at this moment. Experiential knowledge. (Synthetic, a posteriori.)
- ▶ This fails to account for many things we rationally believe to be true, including scientific truths (like Newton's laws of mechanics).

Scientific Knowledge

Hypotheses and Theories

- ▶ Logical Positivism: Essentially that all knowledge (justified true belief) comes from either:
 1. Things that are true by definition, e.g., mathematical truths and theorems, deductions. (Analytic, a priori.)
 2. Things that we observe to be the case, e.g., I am giving a lecture at this moment. Experiential knowledge. (Synthetic, a posteriori.)
- ▶ This fails to account for many things we rationally believe to be true, including scientific truths (like Newton's laws of mechanics).
- ▶ *There also exist hypotheses (or conjectures).* Most scientific knowledge takes the form of hypotheses, sometimes refined into theories, then tested by experiment. Hypotheses come from constrained intuition.
- ▶ Theories can eventually become *laws of nature* after sufficient refinement and testing (e.g., Newton's laws of mechanics).
 - ▶ IMHO, scientific laws are simply hypotheses that have become canons. They are extremely useful and we know their limitations well. We know them to be wrong, and we know in what ways they are wrong.
- ▶ All laws and theories are hypotheses, but not vice versa.

Classical Scientific Method

Although relatively recent. c 1930's, 1950's.

Popper, Kuhn, Quine, others

1. There is a state of affairs that is unsatisfactory in some regard.
2. A hypothesis is made to overcome this.
3. It is tested by experiment.
4.
 - (i) If falsified, back to item 2. Make a new hypothesis.
 - (ii) If confirmed, then carry on.
5. Either the subject stagnates (all problems solved!) or item 1 eventually returns to haunt us.

Above sequence is:

1. Sometimes regarded as over-simplistic, and not reflecting what scientists do:
 - ▶ In actuality, scientists flail around, draw inspiration from anywhere, use inductive reasoning, faulty logic, etc etc.
 - ▶ 'Normal science' just gets on with the job, and is not concerned with paradigm shifts.
2. Still, the above *is a useful framework*, a way to look back and organize progress.
3. Does this algorithm also address complex science, like climate?

The Science of Complex Things

Examples: Climate science, evolutionary biology, material physics, molecular modelling.

The basic laws may be known, and we seek an understanding of the behaviour of the system. How and what kind?

- ▶ Based simply on microscopic laws (a 'Direct Numerical Simulation').
- ▶ Directly predict some emergent phenomena (a 'theory').
- ▶ Theories don't necessarily reduce everything to 'atoms'. We shouldn't try to reduce evolutionary biology to quantum physics. There are natural plateaus where we stop.
- ▶ Natural selection is independent of the microscopic laws. Biology is not a branch of chemistry, nor is chemistry a branch of physics (perhaps).

Models are often some combination microscopic laws, empirical fudge factors and elegant theories.

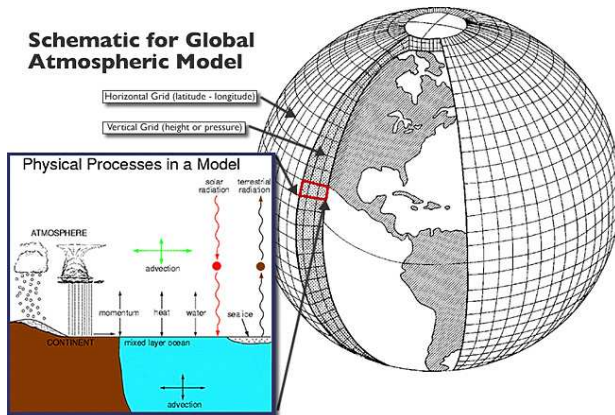
- How does simulation relate to theories? Is a good simulation a theory? Can we simulate without understanding?

The Practice of Climate Science

How is it studied?

- ▶ A very complex dynamical system, with aspects of physics, chemistry, biology and a flavour unto itself.
- ▶ Study using:
 1. General Circulation Models on large computers. Incorporate all of the 'microscopic' laws of nature we know, plus ad hoc aspects. The computer model integrates this, in both time and in concept.
 2. 'Theory' – some kind of simpler models. Try to predict macroscopic behaviour ab initio.
- ▶ Test using observations (present and past): from daily tests (weather forecasts!) to paleorecords.

General Circulation Models

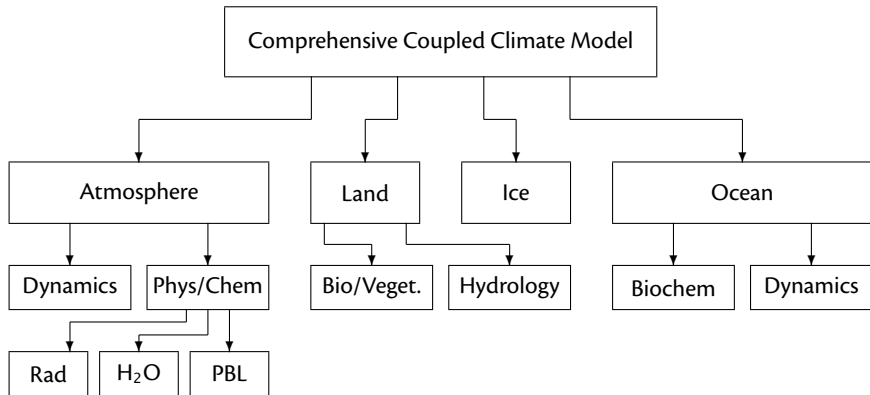


Fluid equations of motion are typically finite-differenced or expressed in spherical harmonic functions. Add 'physics' (radiation, precipitation etc) at each grid point.

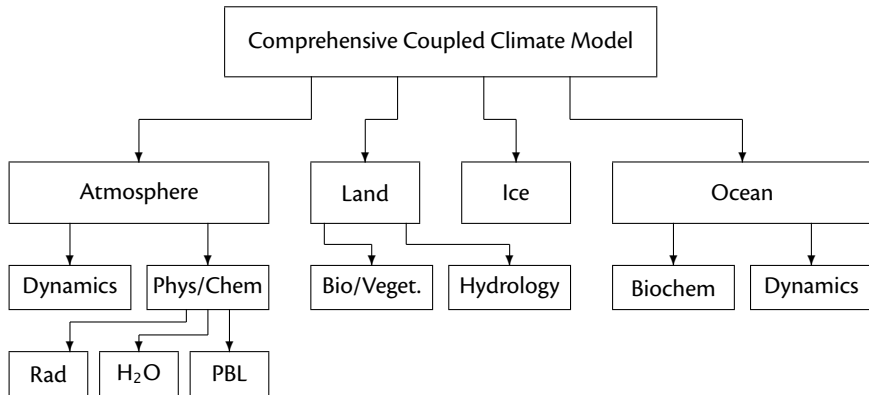
- ▶ Climate research (or at least its funding) is becoming dominated more and more by large models, so called 'General Circulation Models' (GCMs) and now by 'Earth System Models' (ESMs). Some of the largest and most complex computer code ever developed.
- ▶ Similar developments are occurring in other branches of science: ecology and evolutionary biology, astrophysics, condensed matter physics.
- ▶ 'Theory', in the traditional sense, seems to be playing a smaller role. Is such 'theory' still relevant to our scientific enterprise?
- ▶ Perhaps GCMs, as the embodiment of our collective understanding, *are* our modern-day theory of climate?

The Very Model of a Modern Major General

The Very Model of a Modern Major General Circulation Model



The Very Model of a Modern Major General Circulation Model



Theory:

$$\frac{Dq}{Dt} = 0, \quad q = \nabla^2 \psi + \beta y \quad (\text{in a doubly-periodic domain!})$$

Models and Theories. What are they?

Models and Theories. What are they?

A Model

A *model* is a representation ('re-presentation') of some phenomena. It may be empirical, or based on physical laws, laboratory or numerical, analog or digital.

Examples

- ▶ Rotating tank in the laboratory.
- ▶ Computer model of a virtual reality (the video game SimCity, the Holodeck from Star Trek, the Matrix movie).
- ▶ Conceptual/mathematical models (e.g., the Ising model, the Big Bang and Steady State models in cosmology).
- ▶ Complicated numerical models (e.g., GCM)

Properties

- ▶ Comprehensiveness and verisimilitude are often virtues.
- ▶ Predictive power is a virtue
- ▶ Parsimony is not a requirement.
- ▶ Generality is not a requirement.
- ▶ A priori nature not a requirement.

Models and Theories. What are they?

A Theory

Examples: Darwinian evolution, Relativity, Plate Tectonics.

A scientific *theory* is a set of principles or a framework that explains some phenomena, and that is:

(i) Testable

- ▶ Otherwise it is not scientific. (Karl Popper argues a theory should be *falsifiable*.)

(ii) Economical, or parsimonious

- ▶ A theory should be in some sense simpler than the phenomena it explains, or it is merely a description.

(iii) General

- ▶ A theory should be able to explain a class of phenomena, not just a single instance.
- ▶ Ideally based on some a priori foundation, at some level.
- ▶ Theories are subsets of models: A theory is a model, but not all models are theories.
- ▶ No need for a theory to be based on equations.

The Chasm

A sociological phenomenon



The Chasm

A sociological phenomenon



Modellers think that theory is:

1. Overly simple, and quantitatively poor.
2. Irrelevant in the modern scientific enterprise.
3. Theoreticians, RIP!

The Chasm

A sociological phenomenon



Modellers think that theory is:

1. Overly simple, and quantitatively poor.
2. Irrelevant in the modern scientific enterprise.
3. Theoreticians, RIP!

Theorists think that modelling is:

1. Overly complicated, ad hoc, and so not truly scientific
2. A distraction to the true scientific enterprise.
3. Modellers, be gone!

Understanding

What is that? — Is that what we seek?

I shall not today attempt further to define the kinds of material...embraced within that shorthand definition.... But I know it when I see it.

Potter Stewart, Supreme Court Associate Justice, *Jacobellis vs. Ohio*, 1964.

Understanding

What is that? — Is that what we seek?

I shall not today attempt further to define the kinds of material...embraced within that shorthand definition.... But I know it when I see it.

Potter Stewart, Supreme Court Associate Justice, *Jacobellis vs. Ohio*, 1964.

Understanding is a subjective concept that is almost undefinable. It is being able to grasp all sides and all levels of a problem simultaneously. It is not the same as having a theory, because

- ▶ You can intuitively understand something without being able to formalize it.
- ▶ You can have a theory that you don't understand!
- ▶ A good simulation does not imply understanding.

Understanding might be regarded as knowing the *meaning* of a theory.

Arguably understanding is not the end point of science, just a means to the end.

Understanding aids the construction of new theories...and better models.

Thoughts on Theory and Understanding

Theories are not permanent:

No fairer destiny [has] any physical theory, than that it should of itself point out the way to the introduction of a more comprehensive theory, in which it lives on as a limiting case.

Albert Einstein

We don't really care about understanding:

The only object of theory is to calculate results that can be compared to experiment... it is unnecessary to give the whole course of the phenomenon.

Paul Dirac

Indeed, it may be hubris to think that we actually construct theories or understand:

The sciences do not try to explain... they mainly make models. The justification [of a model] is solely and precisely that it is expected to work.

John von Neumann

Thoughts on Theory and Understanding

Theories are not permanent:

No fairer destiny [has] any physical theory, than that it should of itself point out the way to the introduction of a more comprehensive theory, in which it lives on as a limiting case.

Albert Einstein

We don't really care about understanding:

The only object of theory is to calculate results that can be compared to experiment... it is unnecessary to give the whole course of the phenomenon.

Paul Dirac

Indeed, it may be hubris to think that we actually construct theories or understand:

The sciences do not try to explain... they mainly make models. The justification [of a model] is solely and precisely that it is expected to work.

John von Neumann

Galileo might have been well advised to agree. He might have been freed had he agreed his ideas about heliocentrism were just “instruments” or useful calculating tools. But he thought they actually represented reality.

Theories — Good and Bad

Chris Garratt (U. Victoria):

Q. Do you want to hear my theory of the Gulf Stream?

Theories — Good and Bad

Chris Garratt (U. Victoria):

Q. Do you want to hear my theory of the Gulf Stream?

A. It's the Navier-Stokes equations.

Theories — Good and Bad

Chris Garratt (U. Victoria):

Q. Do you want to hear my theory of the Gulf Stream?

A. It's the Navier-Stokes equations.

So our theory of climate is

- (i) The Navier-Stokes equations
- (ii) Thermodynamical laws
- (iii) Radiative transfer (EM) equations
- (iv) Boundary conditions

This is what a GCM is — so these are our theory? Yes, in some sense. Or at least GCMs are a messy hypothesis. But GCMs are

1. low level, and so not very economical;
2. in parts ad hoc, and so not very general.

and therefore, perhaps, not a good theory. Is there a better, 'higher level' theory?

Theories at Different Levels and Emergent Phenomena

- ▶ A theory may try to predict 'emergent phenomena' directly, without reducing it to the detailed behaviour of its constituent parts.
- ▶ A simulation is a calculation from which phenomena naturally emerge from the basic building blocks, maybe as a by-product. Reductionist.

Emergent Phenomena - examples

- Temperature.
- The Gulf Stream, the Hadley Cell.
- Galaxies, clusters of galaxies, solar systems.
- Species in biological evolution. Consciousness.

Explicit Large Numerical Calculations

- Numerical calculations of colliding molecules, Maxwellian distributions.
- GCMs simulating the Gulf Stream and the Hadley Cell.
- Smoothed particle hydrodynamics for galaxies, cosmological N-body codes etc.
- Species in evolutionary biology? Consciousness? (*Not yet!*)

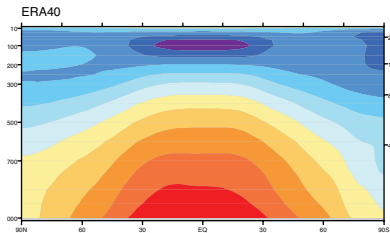
Some Differences Between Fields

- ▶ In biology, theories about some emergent phenomena (e.g., Darwin's theory of species) came first.
 - ▶ No accepted 'equations of motion' for constituent parts. A few explicit calculations been attempted (evolutionary dynamics) with synthetic equations.
 - ▶ There are natural hierarchies — simpler systems (drosophila, e coli) — to help understand.
- ▶ In statistical physics, the scale separation between macrophysical phenomena (e.g., temperature) and microphysics (e.g., bouncing molecules) is very large.
 - ▶ Sensible to have theories of both: thermodynamics and kinetic theory.
- ▶ In astrophysics
 - ▶ Similar to geosciences in some ways. Well accepted equations of motion, complicated phenomena.
 - ▶ Sometimes use numerics just to flesh out a theory and make it testable (e.g., general relativity). No parameterizations in that case.
- ▶ In geosciences and climate, large computers allow direct computation of complex phenomena (e.g., the climate system, the Gulf Stream).
 - ▶ Well accepted equations of motion.
 - ▶ No natural hierarchies — just one climate system. So we must construct our own synthetic hierarchies.

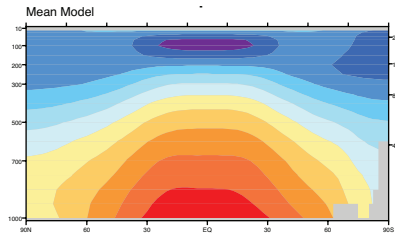
GCMs are Pretty Darned Good for some things

Zonally Averaged Temperature

Observations



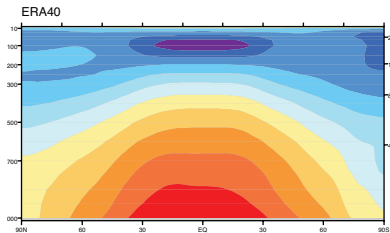
Model



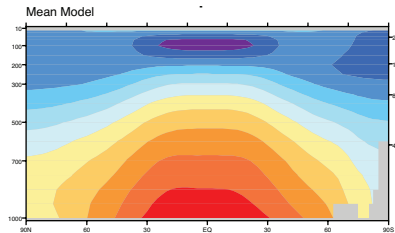
GCMs are Pretty Darned Good for some things

Zonally Averaged Temperature

Model

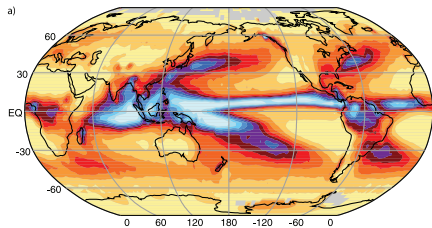


Observation

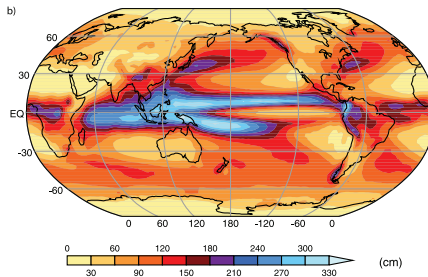


Global Rainfall

Observations



Model
(Multi-model ensemble,
IPCC AR 4)



So what's wrong with complicated models?

1. They are very complex, and not an economical theory of large-scale phenomena.
An aesthetic objection.
2. They have empirical components (so not wholly a theory).
 - ▶ They work by cancellation of errors.
3. They are imperfect — don't always agree with observations.
4. Sometimes they work very well, but we don't understand why!
 - ▶ Good simulation, poor understanding. (The MJO.)

Corollary and Practical Consequence

- ▶ They are not always trusted.
- ▶ They are hard to improve.

The Crux of the Matter

If models (simulations) were perfect, then conceptual theory and understanding would be an indulgence, a mere intellectual conceit, of little value beyond personal satisfaction.

What's wrong with Conceptual Theories?

- ▶ They doesn't always connect with the real world; they are a theory of some idealization, like a western boundary in a square ocean.
- ▶ For many problems, theory does a *worse* job of describing, and providing a basis for understanding, a phenomenon than does a direct simulation.
 - ▶ Polewards transport of heat in the atmosphere. Turbulence in general.

Consequence

- ▶ Theory is often ignored by modellers (and especially by funding agents!).
- ▶ Some theory is in danger of being irrelevant.

A Theory of Climate

(or Theory in Climate?)

Is there an underlying theory of the 'whole thing', rather like in evolution?

No: In the sense that there are no easily stated grand principles that underpin the enterprise, aside from the basic laws of physics, chemistry etc.

But simpler theory is important:

- ▶ Improving GCMs. Tomorrow's generation of numerical models will depend on today's theory.
- ▶ As an end in itself, as part of scientific progress.

Two particular classes of theory are needed:

1. Subgrid processes where models are imperfect.
2. The behavior of the system as a whole.

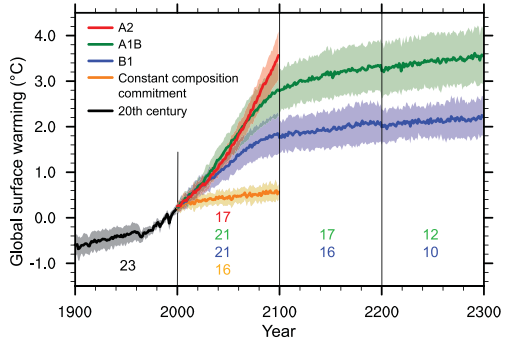
If there comes a time when theory is permanently stalled, then progress in the field halts and the subject stagnates. The end of that branch of science.

Uncertainty

Simulation of 20 and 21 Century

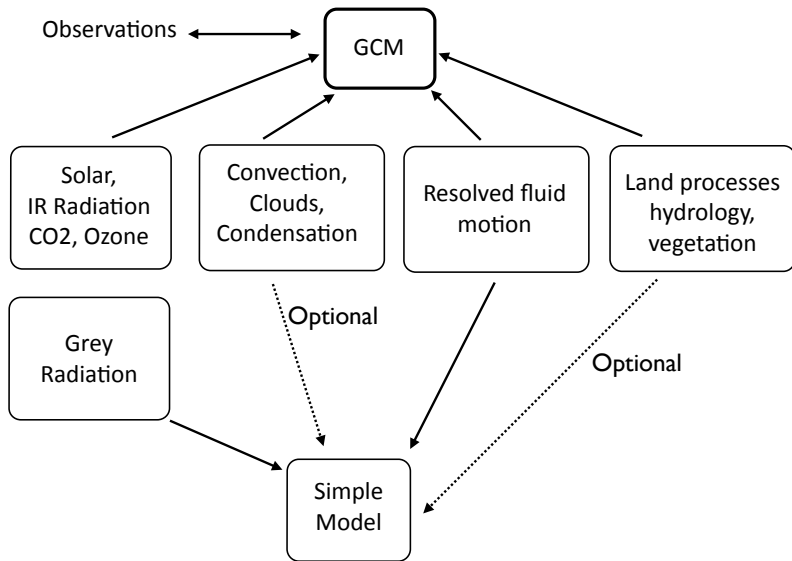
Uncertainty of future climate is greater than our seeming ability to simulate past climate.

- ▶ What level of uncertainty can be expected?
- ▶ Is the climate structurally stable?

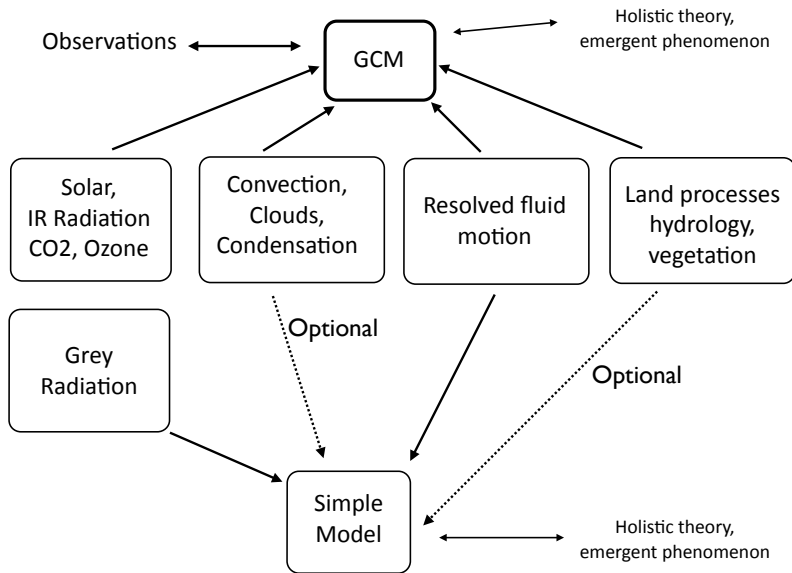


We have no good theory for climate sensitivity!

Example Traceable Hierarchy For Modelling Complex Systems



Example Traceable Hierarchy For Modelling Complex Systems



Whither Research?

- ◇ Big, complicated models are useful, messy hypotheses. Arguably even a theory, but not in the classical sense.
 - ▶ Big numerical models are here to stay. They provide benefit. That's life.
 - ▶ A good simulation is not the same as understanding.
 - ▶ We don't need understanding if the simulation is perfect (but it never is).

- ◇ We (scientists) have to set models up to be testable, or else we aren't doing science.
 - ▶ The tests may not be as clean as we would like. That's life.
 - ▶ Complex modelling is not necessarily unscientific, but it is easy to drift that way.

- ◇ The way forward:
 - ▶ Complicated simulations are blind without conceptual theory.
 - ▶ Theory can be irrelevant without models and simulations.
 - ▶ We need both, and a range in between.