Bayesian uncertainty analysis for complex physical models

Michael Goldstein
Durham University*

*Work with Ian Vernon, Allan Seheult, Jonathan Cumming, and many others!

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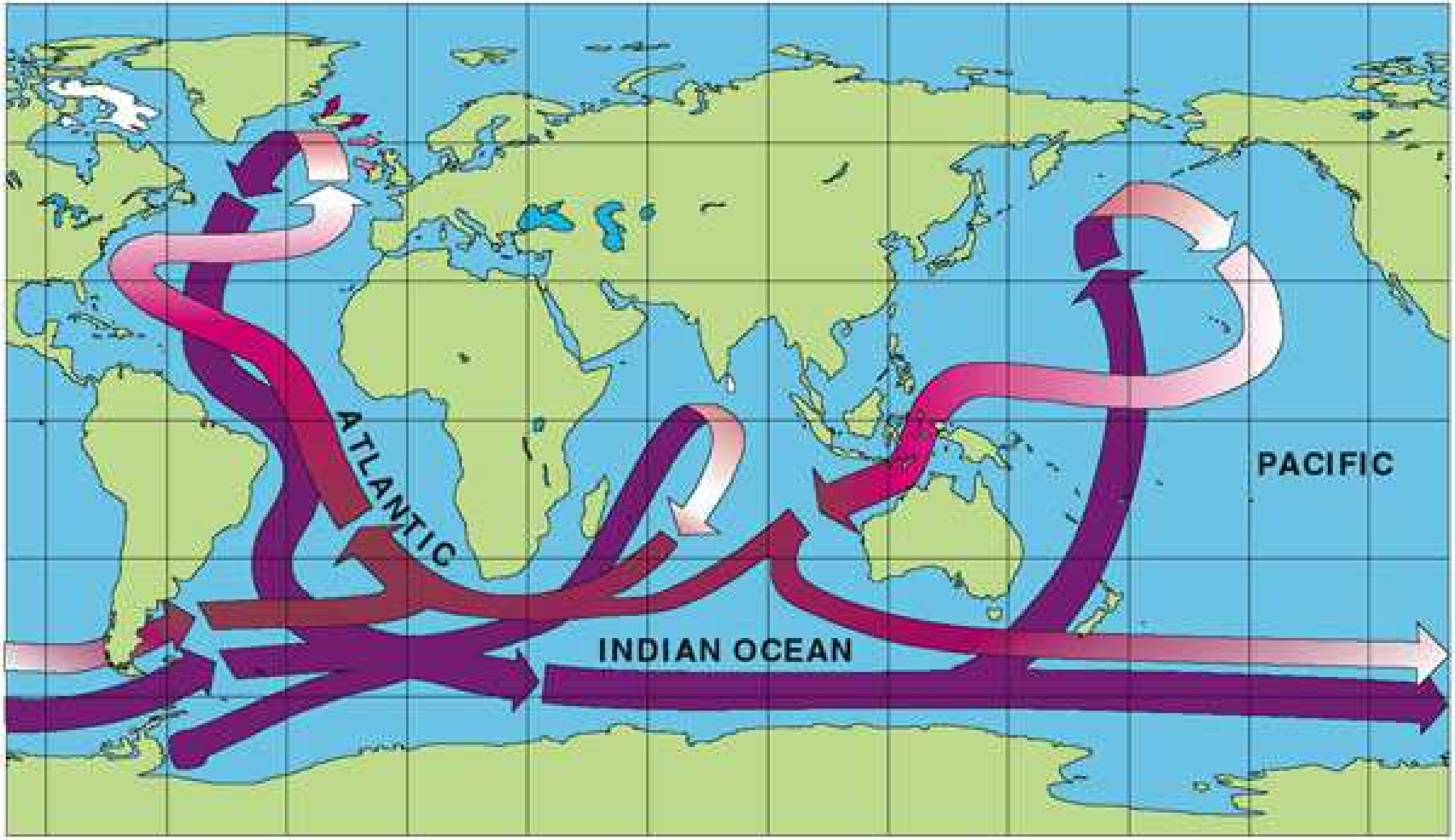
- On their journey, the water masses transport heat energy around the globe, which has a large impact on the climate of our planet.

References

Wikipedia (and see also:
Seager,R., 2005,'The Source of Europe's Mild Climate',American Scientist)

Global circulation



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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 real physical systems from the analysis of (necessarily imperfect) models?

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

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- **Thermo-haline shutdown?** Tentative prediction shown by simple models and paleo records, but not by many of the large models (so far).

The state of the art

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

Leading climate models

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The climate model has about 100 uncertain parameters, including:

1. *Large scale cloud.* Six parameters
2. *Convection.* Six parameters
3. *Sea ice.* Two parameters
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We have a few hundred evaluations of the mode, made over a period of about three years. These evaluations are one of the main resources for the UK Climate Projections Programme 2009, which is intended as a fairly definitive statement about how climate change will impact the UK.

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aims to allow users to make more robust decisions.

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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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Actual system

System observations

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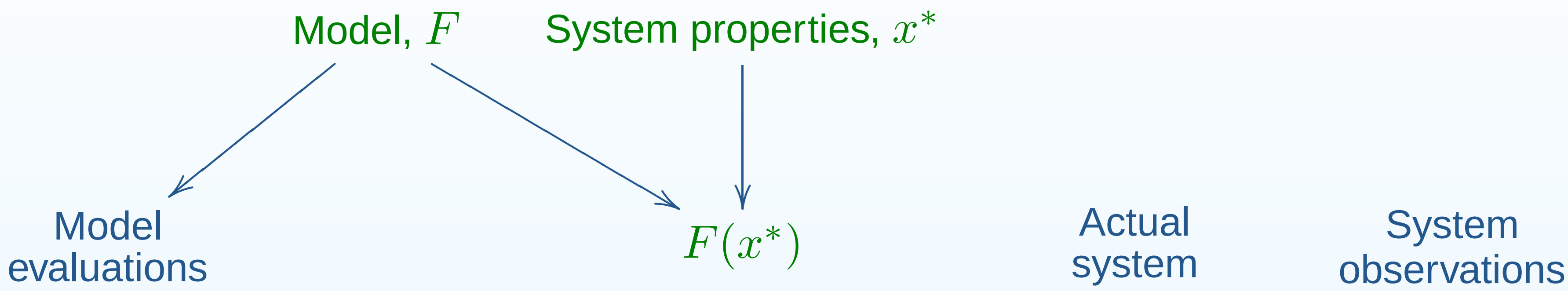

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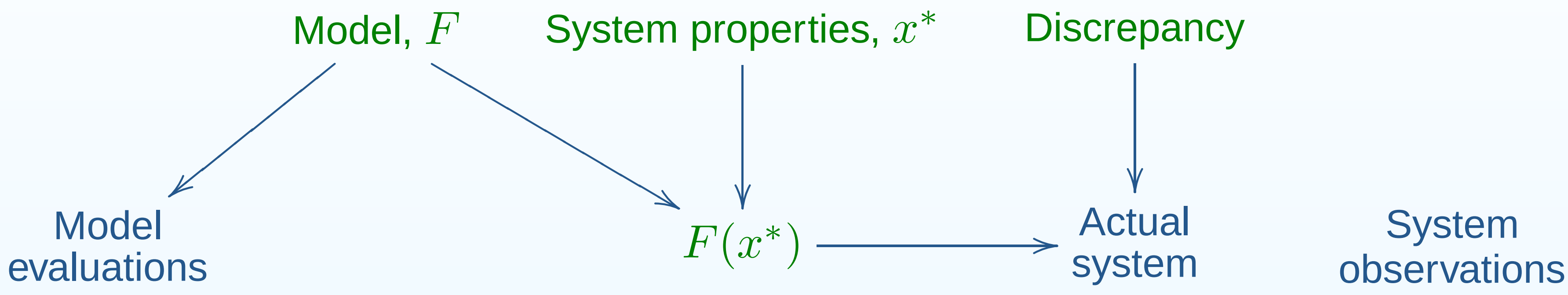

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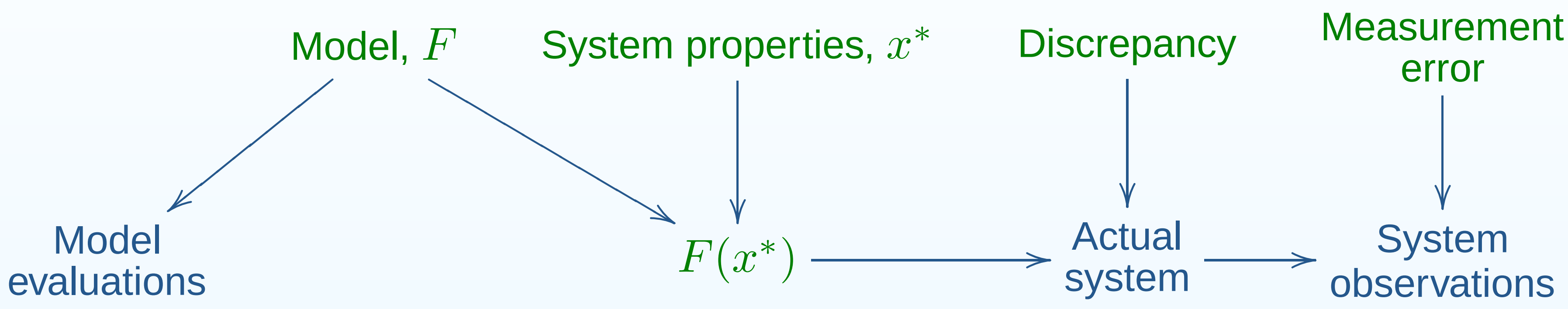

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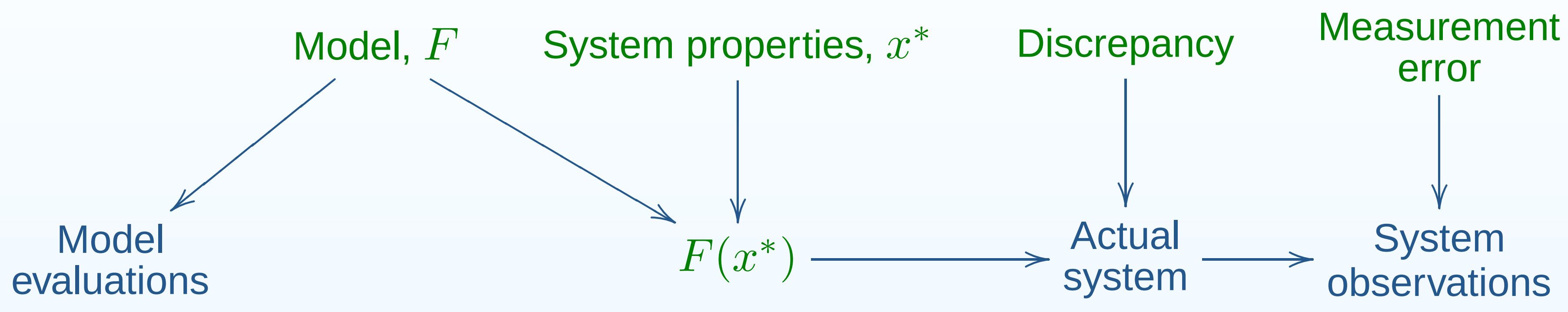

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So, we need careful experimental design to choose which evaluations of the model to make, and detailed diagnostics, to check emulator validity.

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- to "optimise" the performance of the system

Bayes linear approach

For very large scale problems a full Bayes analysis is very hard because
(i) it is difficult to give a meaningful full prior probability specification over high dimensional spaces;
(ii) the computations, for learning from data (observations and computer runs) and choosing informative runs, may be technically difficult;
(iii) the likelihood surface is extremely complicated, and any full Bayes calculation 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, (see de Finetti “Theory of Probability”, Wiley, 1974), we take as primitive.
For a full account, see
Michael Goldstein and David Wooff (2007) Bayes Linear Statistics: Theory and Methods, Wiley.

Bayes linear adjustment

Bayes Linear adjustment of the mean and the variance of y given z is

$$\mathrm{E}_z(y) = \mathrm{E}(y) + \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}(z - \mathrm{E}(z)),$$
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[6] a formal subjective framework accounting for all uncertainties (recognising Bayesian analysis itself as a model).

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We can therefore calculate, for each output $F_i(x)$, the “implausibility” if we consider the value x to be the best choice x^*, which is

$$I_{(i)}(x) = |z_i - \mathrm{E}(F_i(x))|^2 / [\mathrm{Var}(F_i(x)) + \mathrm{Var}(\epsilon_i) + \mathrm{Var}(e_i)]$$

[Large values of $I_{(i)}(x)$ suggest that it is implausible that $x = x^*$.]

Using Implausibility measures

The implausibility calculation can be performed univariately, or by multivariate calculation over sub-vectors. The implausibilities are then combined, such as by using $I_M(x) = \max_i I_{(i)}(x)$, and can then be used to identify regions of x with large $I_M(x)$ as implausible, i.e. unlikely to be good choices for x^*.

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We may find no good choices at all which give good fits and that is a clear sign of problems with our physical simulator or with our data.

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We now evaluate the adjusted mean and variance for future values y_p adjusted by z using the Bayes linear adjustment formulae.

This analysis gives system forecasts without model calibration, and therefore is tractable even for large systems.

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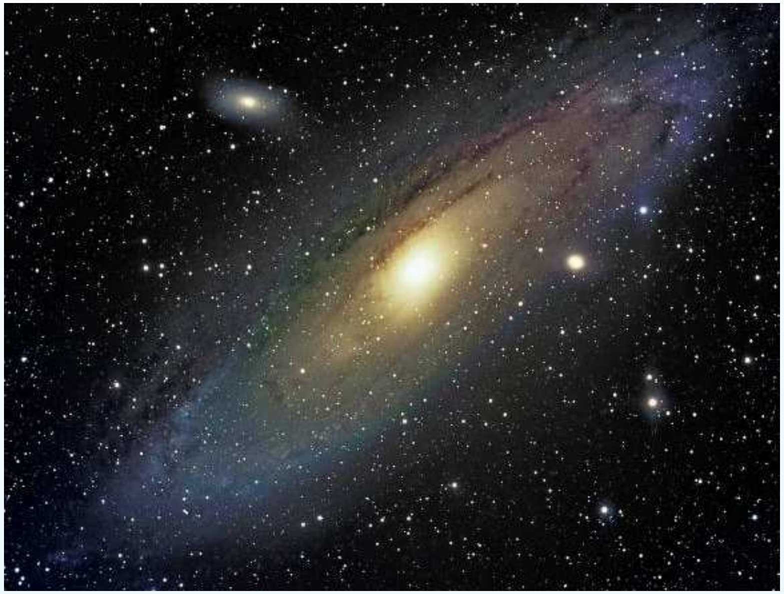
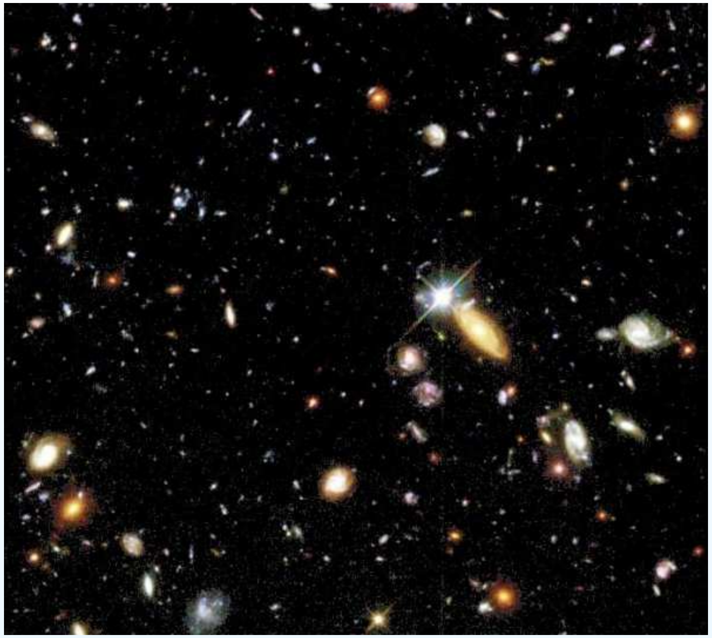
How did these galaxies form?

Andromeda Galaxy and Hubble Deep Field View





- Andromeda Galaxy: closest large galaxy to our own milky way, contains 1 trillion stars.
- Hubble Deep Field: furthest image yet taken. Covers 2 millionths of the sky but contains over 3000 galaxies.

Dark Matter and the Evolution of the Universe

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In order to study the effects of Dark Matter cosmologists try to model **Galaxy formation**

- Inherently linked to amount of Dark Matter
- Of fundamental interest as tests cosmologists' knowledge of a wide range of complicated physical phenomena

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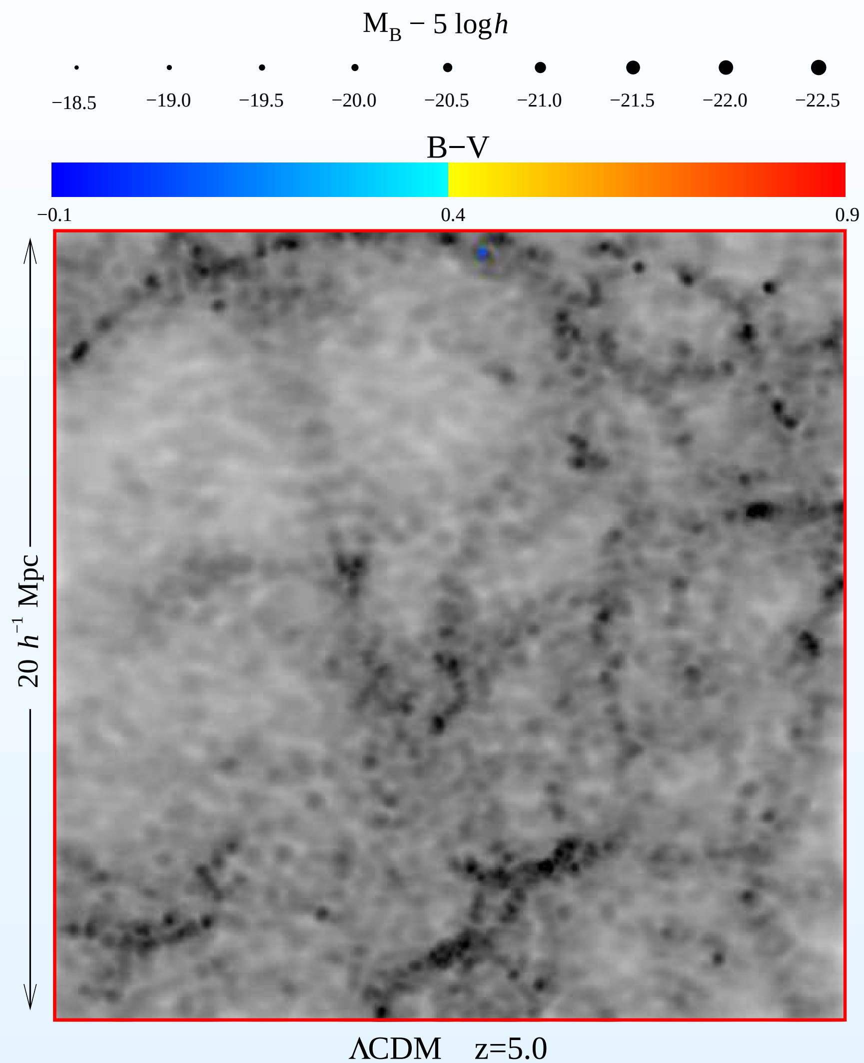
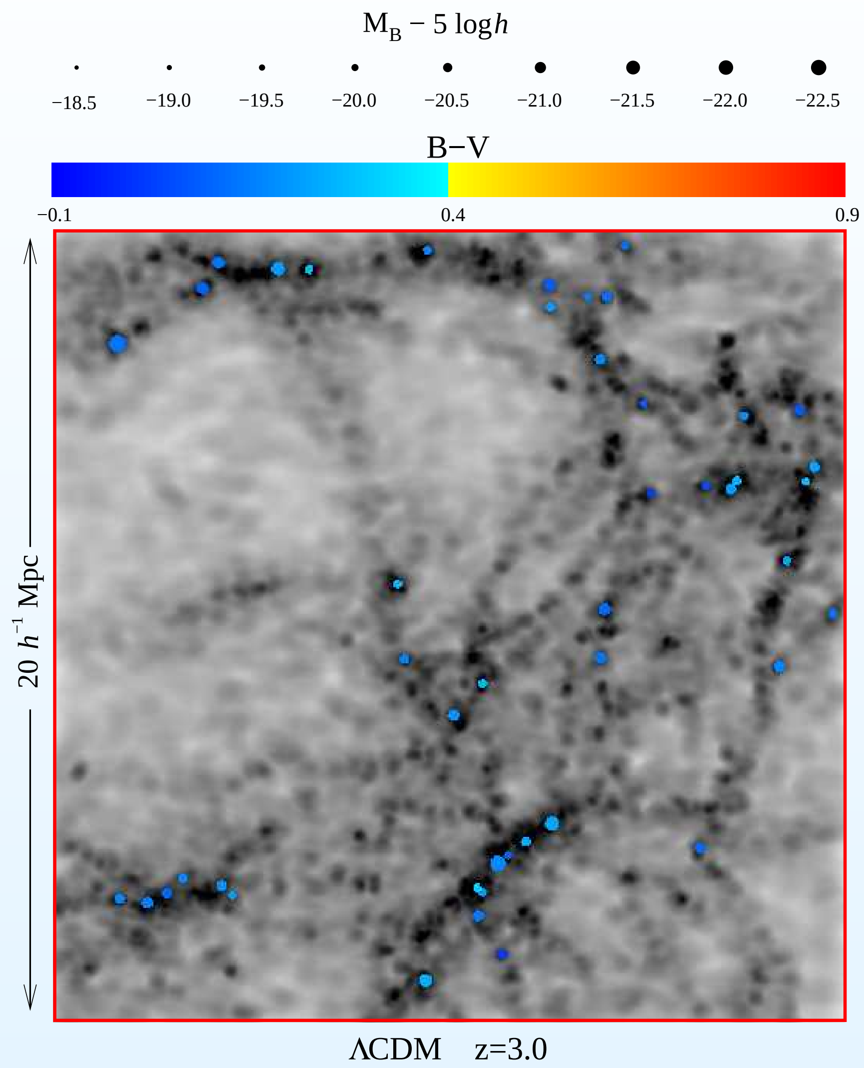
This volume is split into 512 sub-volumes which are independently simulated using the second model GALFORM. This simulation is run on upto 256 parallel processors, and takes 20-30 minutes per sub-volume per processor

Universe at $<$ 100 million years



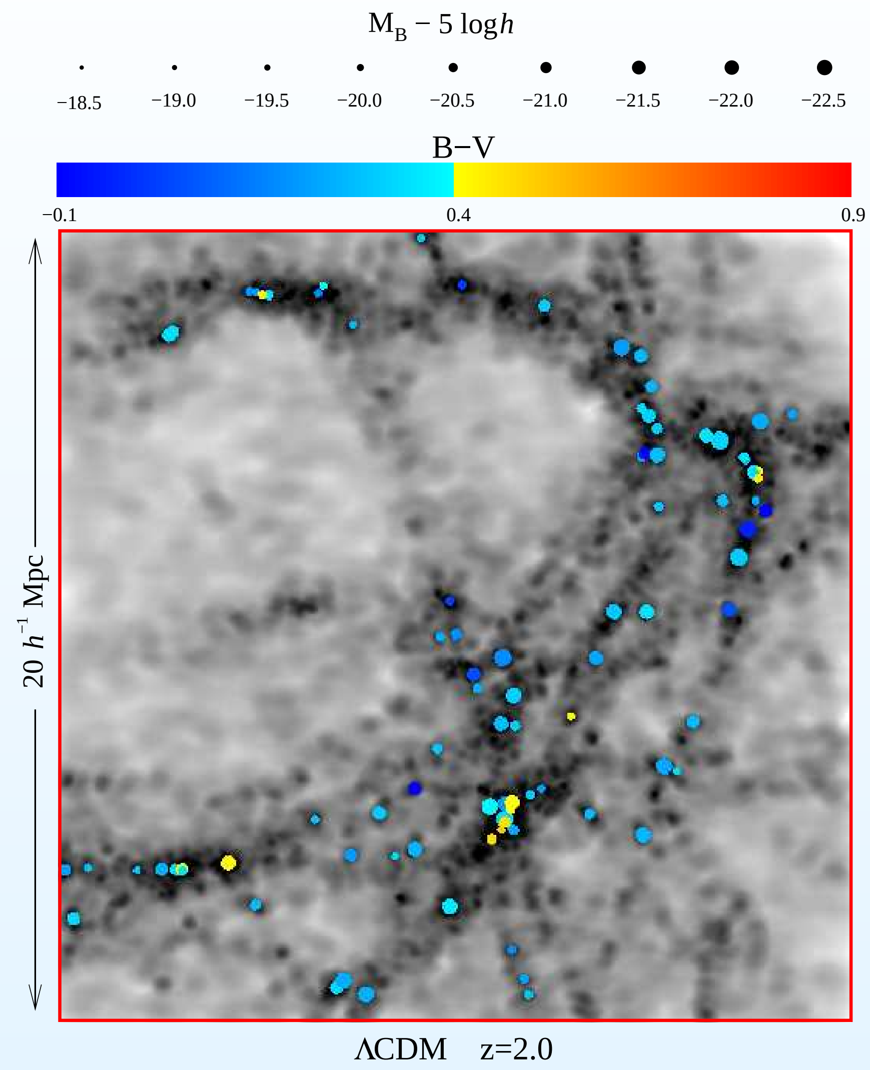
Benson, Frenk, Baugh, Cole & Lacey (2001)

Universe at $\sim$ 1 billion years



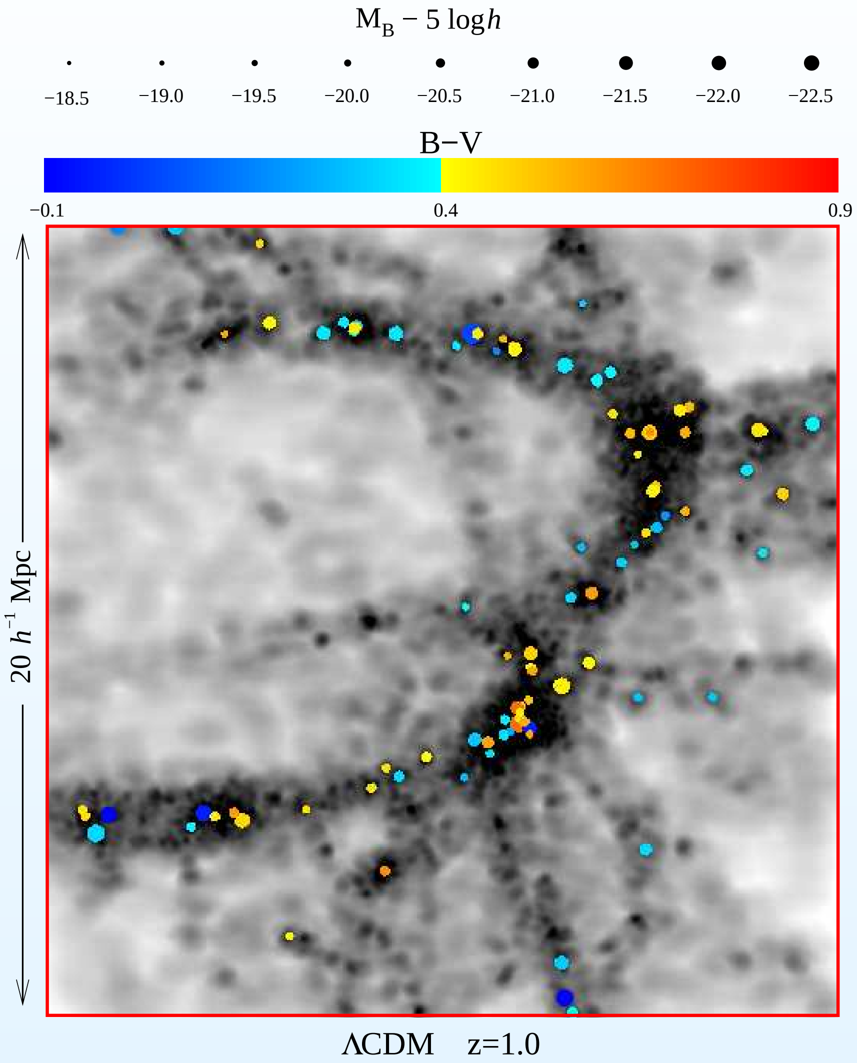
Benson, Frenk, Baugh, Cole & Lacey (2001)

Universe at $\sim$ 2 billion years



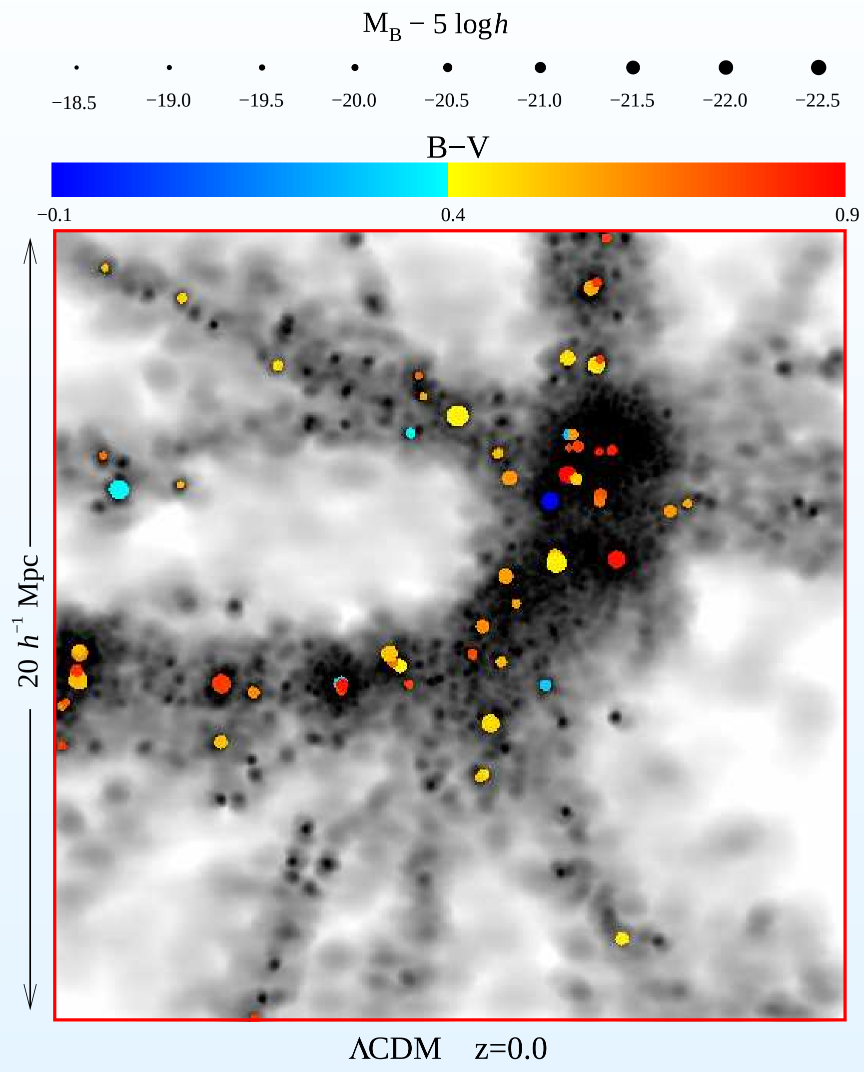
Benson, Frenk, Baugh, Cole & Lacey (2001)

Universe 4 billion years



Benson, Frenk, Baugh, Cole & Lacey (2001)

Universe 13 billion years (Today)



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Galform: Inputs and Outputs

Outputs: Galform provides many outputs but we start by looking at the bj and K luminosity functions

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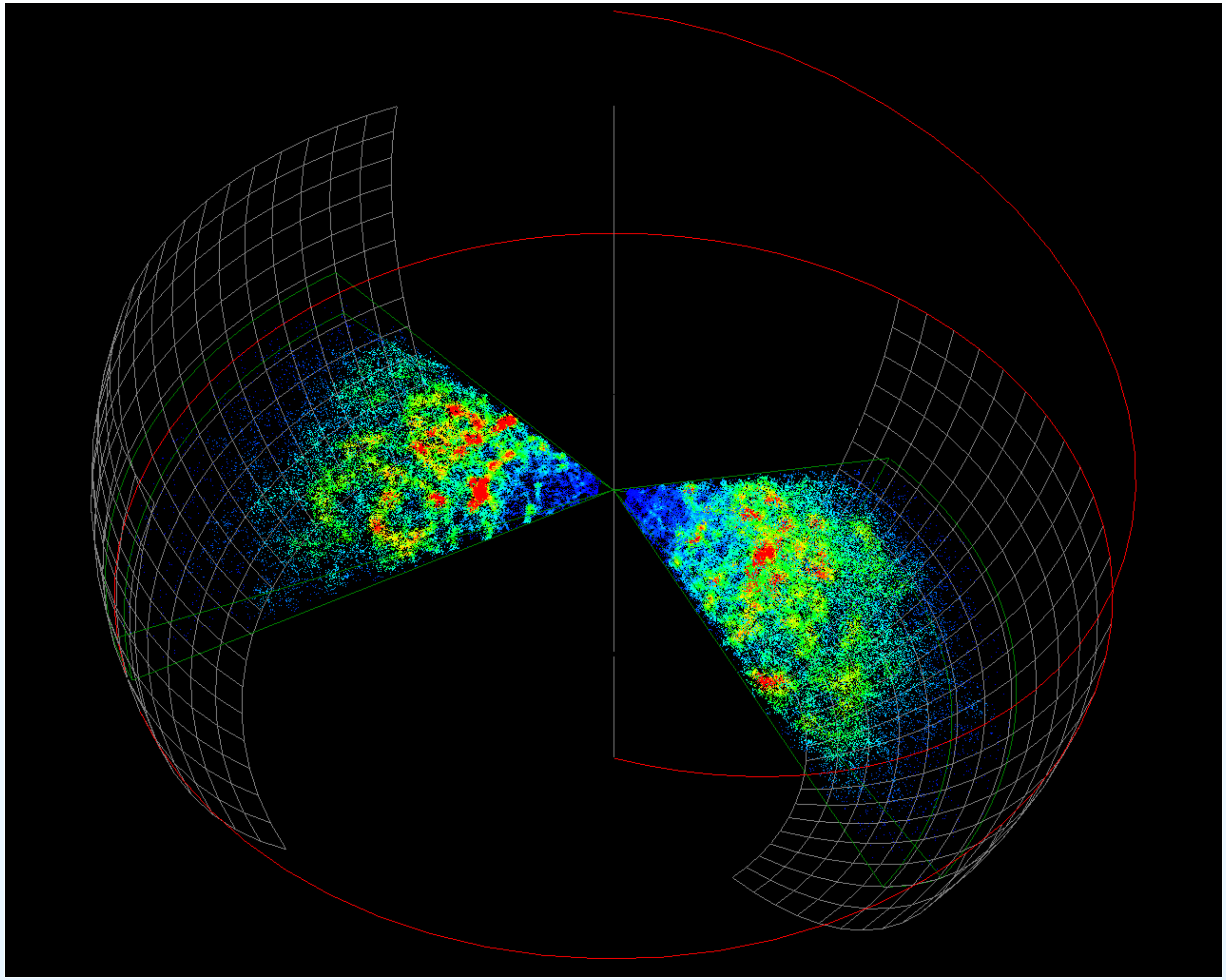
Inputs: 17 input variables reduced to 8 after expert judgements. These include:

- **vhotdisk**: relative amount of energy in the form of gas blown out of a galaxy due to star formation
- **alphacool**: regulates the effect the central black hole has in keeping large galaxies 'hot'
- **yield**: the metal content of large galaxies

and five others: alphahot, stabledisk, epsilonStar, alphareheat and vhotburst

Observational Data: Galaxy Surveys



Earth at centre of image. Data taken by telescopes looking in two seperate directions. Galaxies observed up to a distance of 1.2 billion light years.

Galaxy Formation: Main Issues

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Fundamental Sources of Uncertainty

- We only observe the galaxies in our ‘local’ region of the Universe: it is possible that they are not representative of the whole Universe.
- The output of the simulation is a ‘possible’ Universe which should have similar properties to ours, but is not an exact copy.
- The output of the simulation is 512 different computer models for “slices” of the universe which are **exchangeable** with each other and (hopefully) with slices of our universe.
- We are uncertain which values of the input parameters should be used when running the model

History matching and Galaxy Formation

We want to history match the Galaxy Formation model Galform using the emulation and implausibility techniques that we have outlined.

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This process is then repeated. This is **refocusing**. As we are now in a reduced input volume, outputs may be of simpler form and therefore easier to emulate.
As we have reduced the variation in the ouputs arising from the most important inputs, this also allows us to assess variation due to secondary inputs.

Galform: Stage 1

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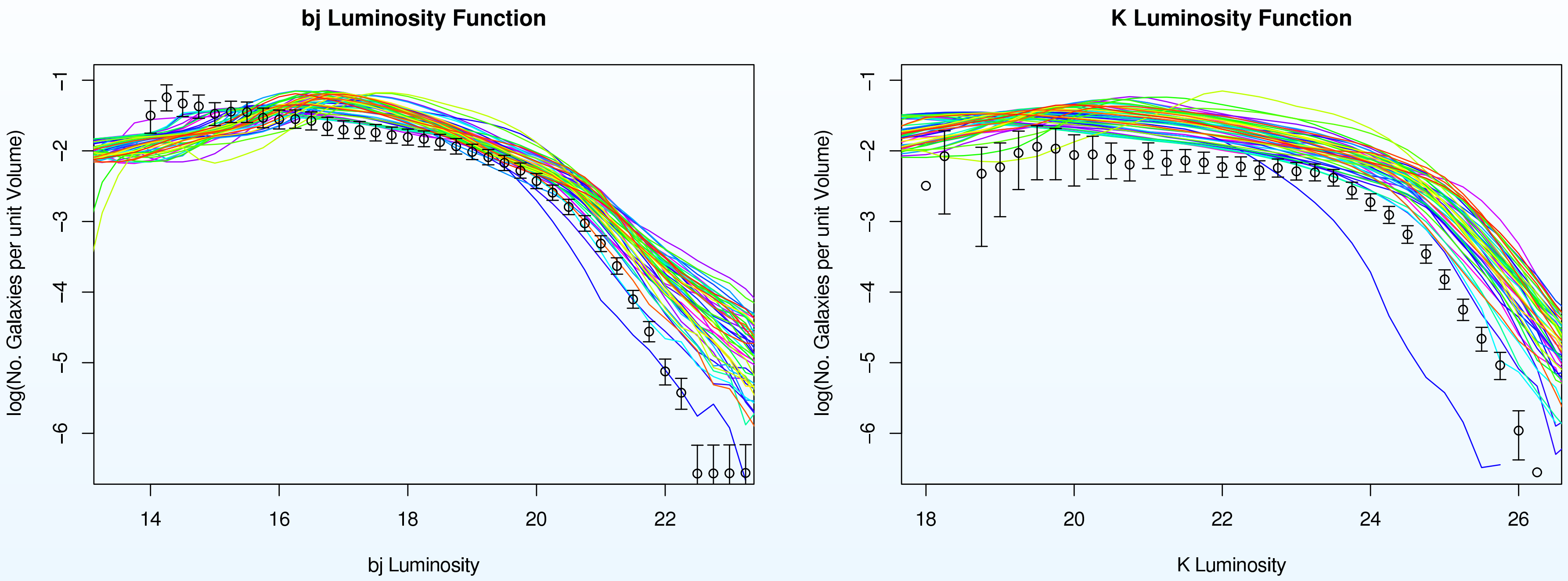
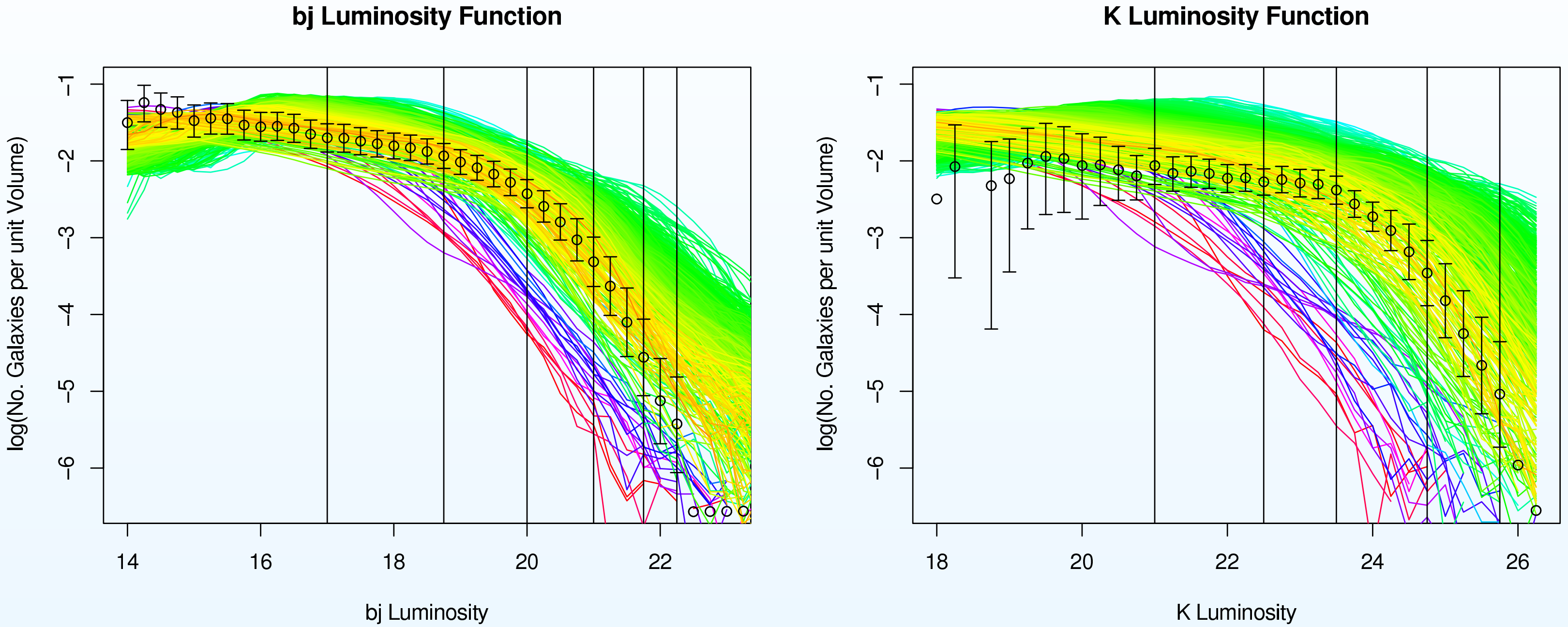
Active Variables: For each output we choose 5 active variables x^A, i.e. those inputs which are the most important for explaining variation in the output.

Galform Outputs: The Luminosity Functions



- Bj Luminosity: young (blue) galaxies
- K Luminosity: old (red) galaxies
- Circles are observed
- Coloured lines are example outputs for different input parameter choices

11 Output points Chosen



Outputs chosen to be informative enough to allow us to cut down the parameter space, but simple enough to be emulated easily.

Galform: Stage 1

We then emulate each of the 11 outputs univariately using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

where now $B = \{\beta_{ij}\}$ are unknown scalars, g_{ij} are now monomials in x^A of order 3 or less, and $u(x^A)$ is a gaussian process. The nugget $\delta_i(x)$ models the effects of inactive variables as random noise.

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Here the Adjusted R^2 for the polynomial fits were between 0.79 and 0.92

The Emulators give the expectation $\mathrm{E}(f_i(x))$ and variance $\mathrm{Var}(f_i(x))$ at point x for each output given by $i = 1, ..., 11$.

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- Φ_{12}: As we have neglected 9 parameters (due to expert advice) we need to assess effect of this (by running latin hypercube design across all 17 parameters)

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- Poisson Error: assumed Poisson process to describe galaxy production (not very accurate assumption!)

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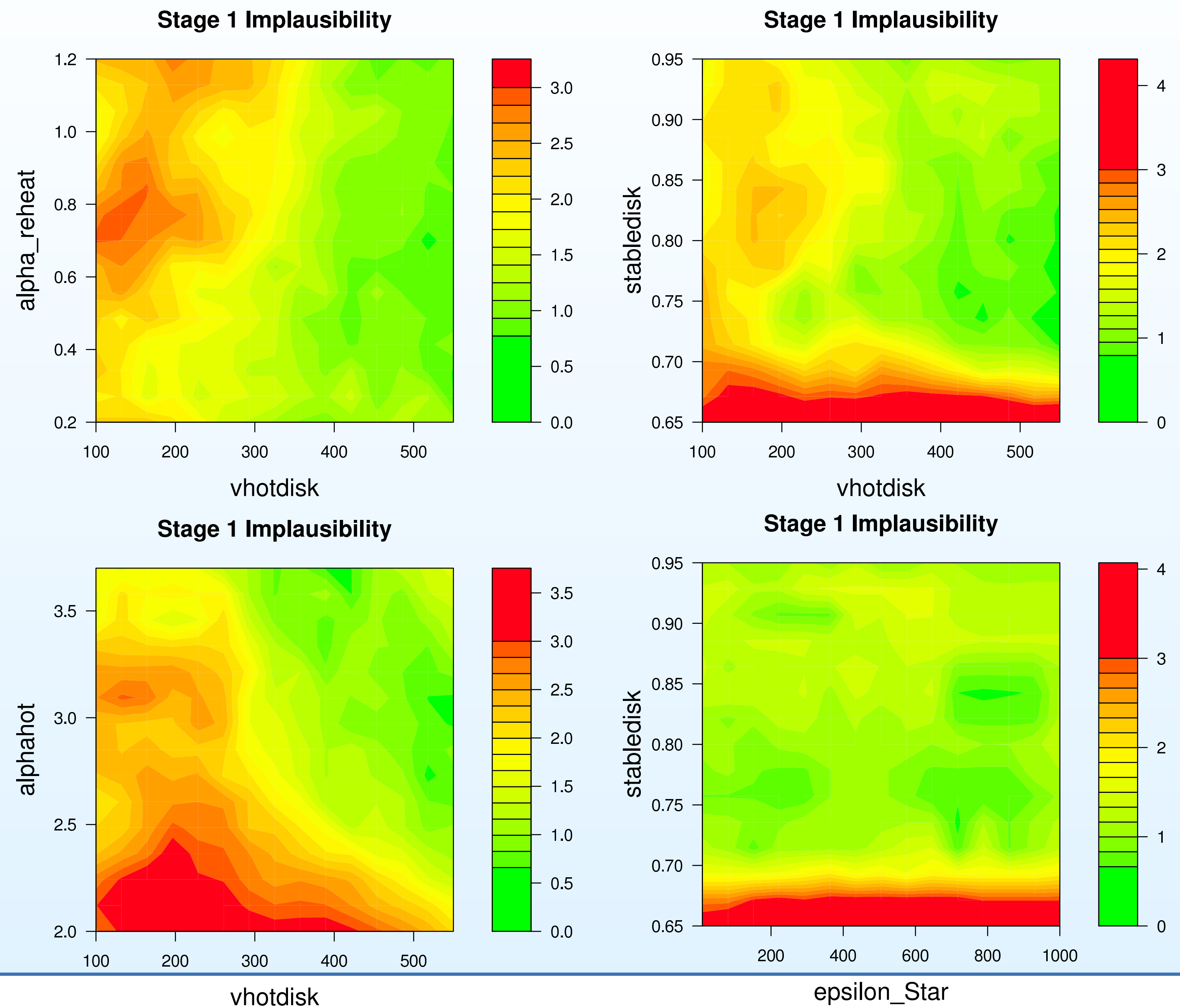
2-Dimensional Projection For each of the 28 pairs of active variables we minimize the implausibility across the remaining active variables

If a point on these plots is implausible then it will be implausible for any choice of the other active variables.

2D Implausibility Projections: Stage 1 (8%)



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We used Cluster Analysis on points in the reduced volume to determine connectedness.

In this case the region was found to be simply connected.

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- We can now calculate the implausibility as before. As our emulator accuracy improves, we may further reduce the input parameter space.

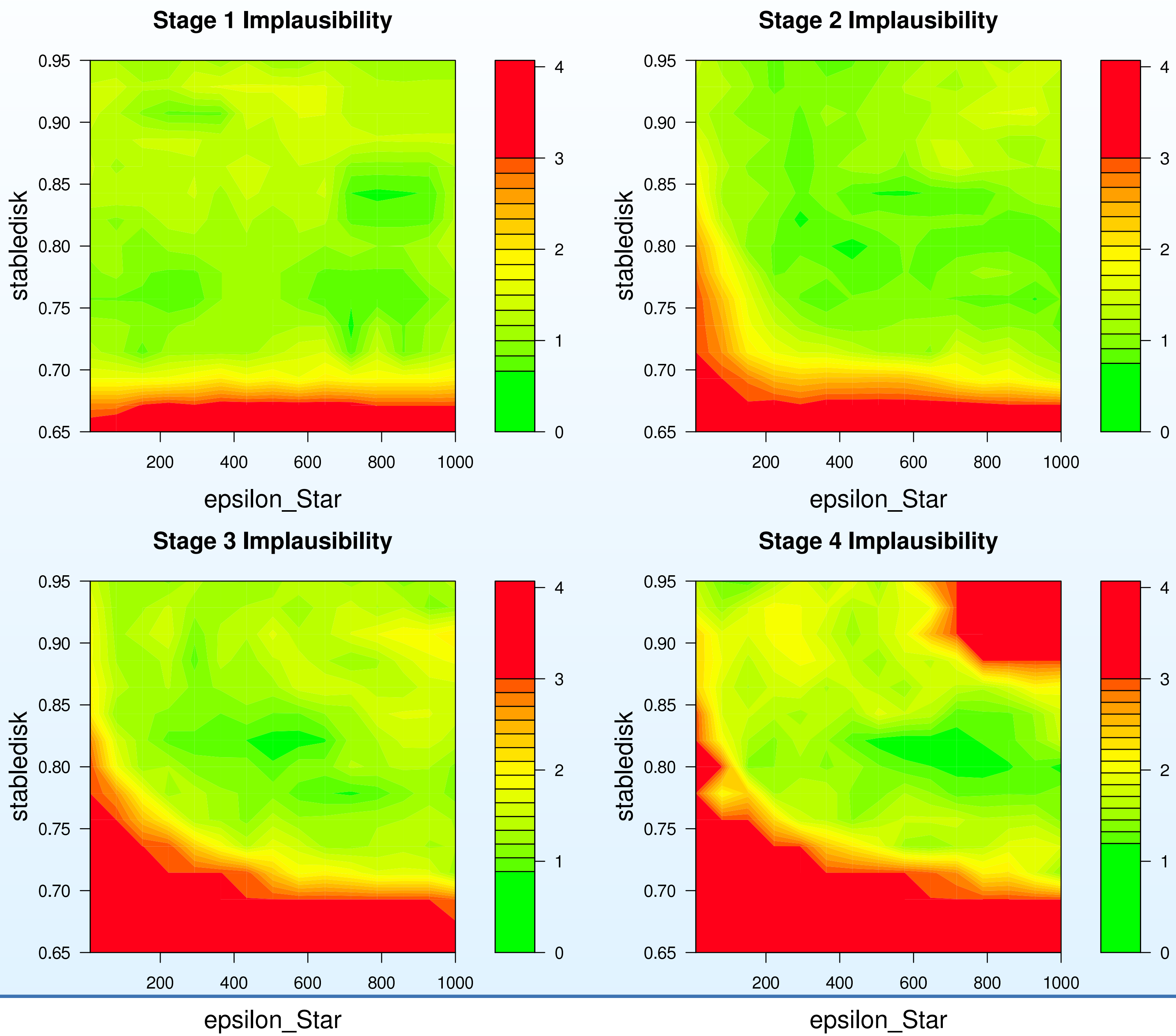
Summary of Results

- We have completed Four Stages:

	No. Model Runs	No. Active Vars	Adjusted $R2$	Space Remaining
Stage 1	1000	5	0.58 - 0.90	8.0 %
Stage 2	1916	8	0.83 - 0.98	2.9 %
Stage 3	1487	8	0.79 - 0.99	1.2 %
Stage 4	1899	10	0.75 - 0.99	0.12 %

- In Stages 3 and 4 we used a Multivariate Implausibility measure to help reduce space further.
- In Stage 4 we included 2 more active input variables that had previously been inactive.

2D Implausibility Projections: Stage 1 (8%) to Stage 4 (0.12%)



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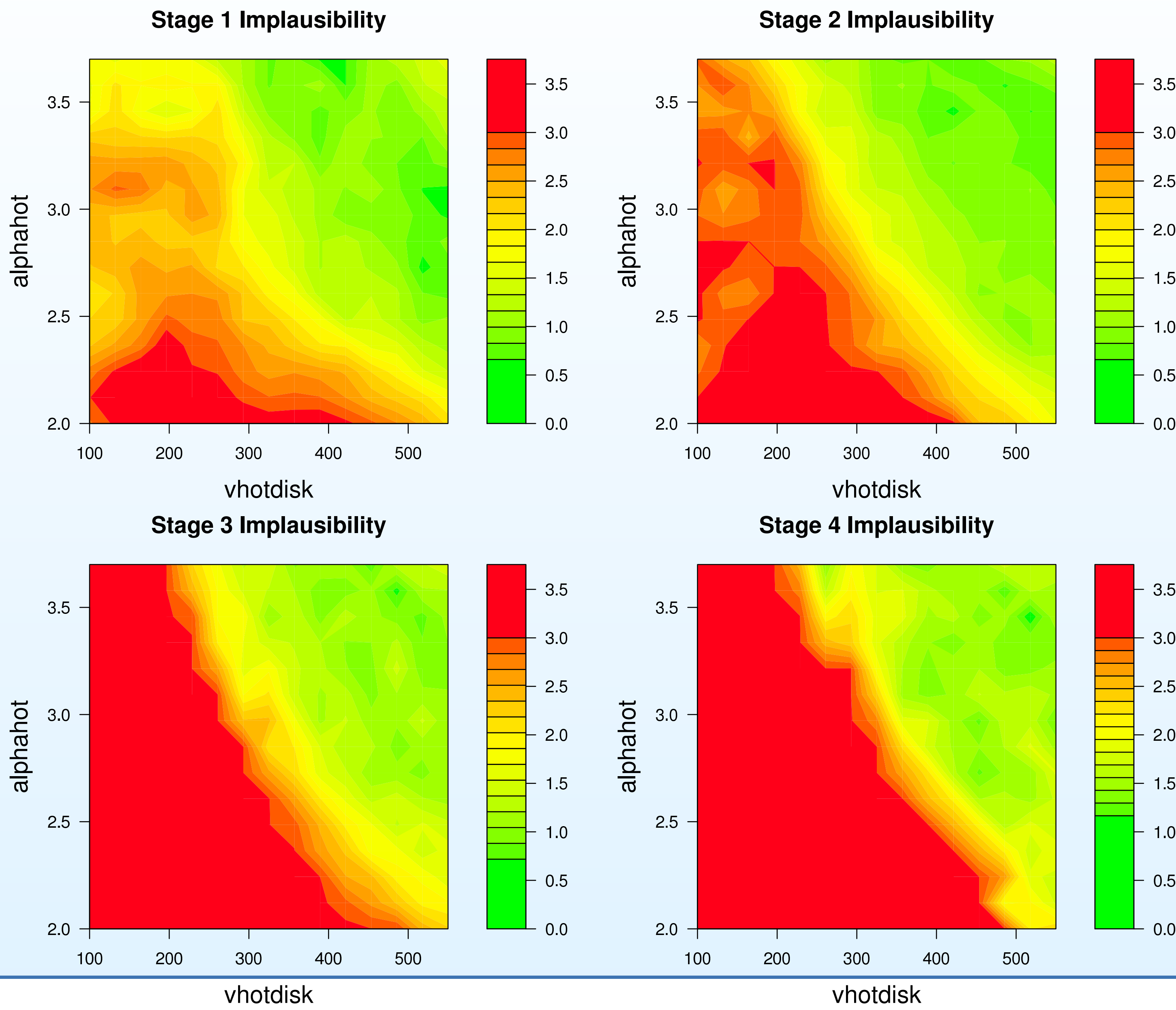

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History matching often is the first stage of a larger methodology which applies the uncertainty models that we have described for activities such as system forecasting and optimisation.

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  If we account for all uncertainties (which may be difficult), then we obtain a full uncertainty analysis for the behaviour of the physical system.

References

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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.]