Introduction to emulators

- the what, the when, the why

Dr Lindsay Lee

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What is a simulator?

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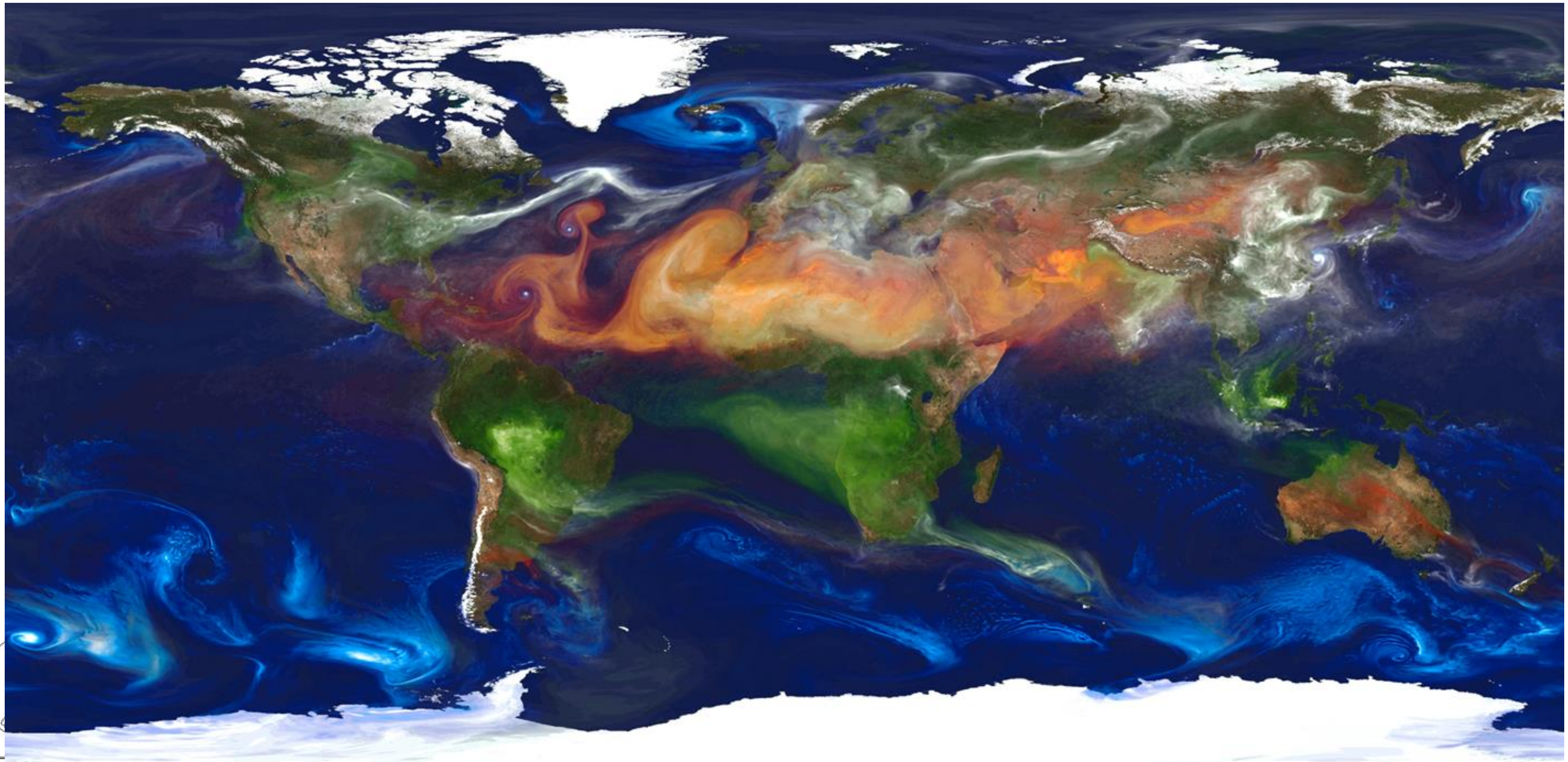
A simulator is a computer code used to represent some real world process



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Why simulate?

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Understand

Which aerosol are most effective at cooling the climate?

Predict

Could aerosol be used to cool the climate for geoengineering?

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Notation

- $y = f(x)$ represents the simulation process
- y is the simulator output
- x is the simulator input
- f is the simulator

Uncertainty in simulation

$$\boldsymbol{Y} = f(\boldsymbol{X})$$

Computer codes are imperfect representations of the real world.

How do these imperfections affect our understanding and predictions?
What is the effect on $\boldsymbol{Y}$?

Uncertainty in climate simulators

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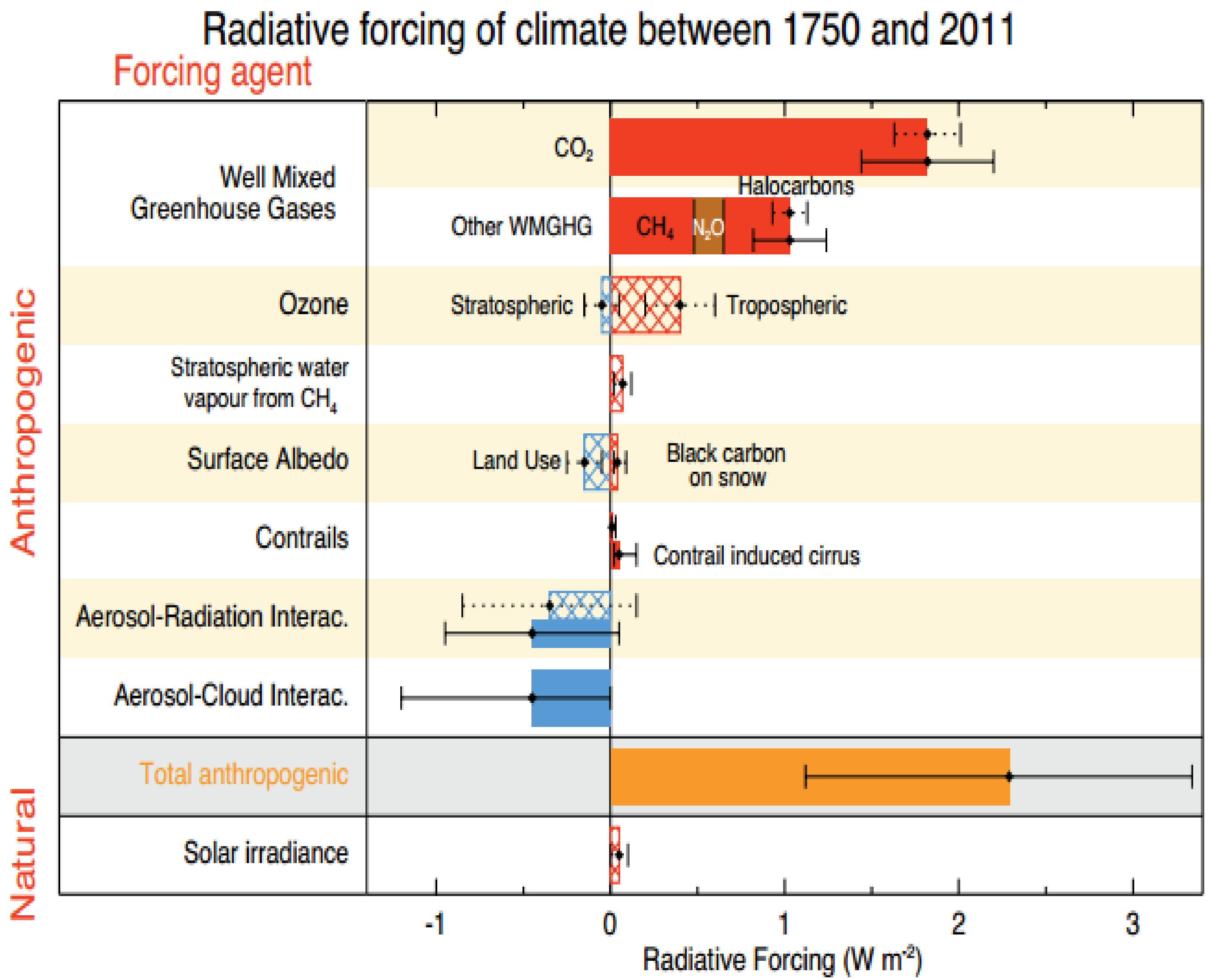

Figure 8.15 | Bar chart for RF (hatched) and ERF (solid) for the period 1750–2011, where the total ERF is derived from Figure 8.16. Uncertainties (5 to 95% confidence range) are given for RF (dotted lines) and ERF (solid lines).

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What is X?

- $\boldsymbol{X}$ are ‘model inputs/parameters’
- They may be spatial fields/time series
- They may be single values used globally or regionally

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Where X is a spatial field or series…

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We will represent the uncertainty in $\boldsymbol{X}$ by a single value to perturb the whole field, or series (maybe regionally, but mostly globally)

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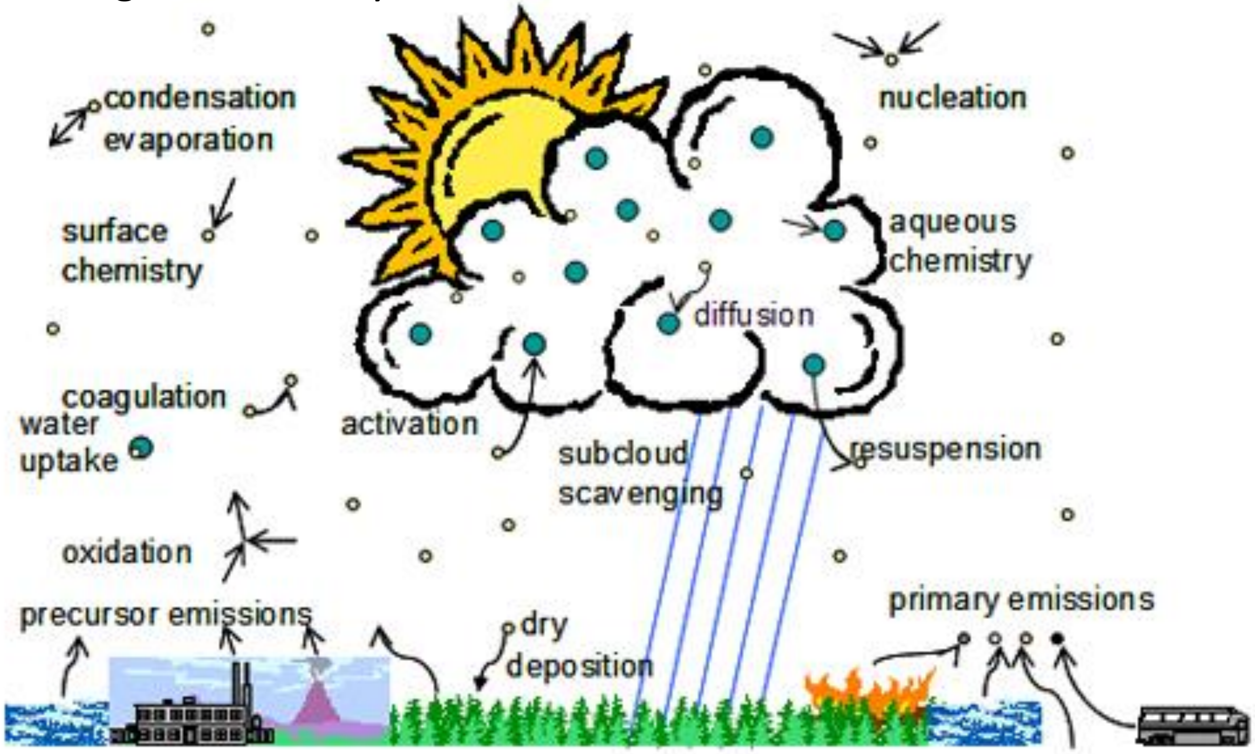
Uncertainty in aerosol simulator inputs

Diagram courtesy of PNNL



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Uncertainty in simulator inputs

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- $\boldsymbol{X}$ is uncertain $\rightarrow$ $\boldsymbol{Y}$ is uncertain
- $\boldsymbol{x}$ can be given uncertainty distribution $\boldsymbol{G}$
- Marginally x_k has distribution G_k

Obtain $\boldsymbol{y}_i = f(\boldsymbol{x}_i)$ for given $\boldsymbol{x}_i$ from $\boldsymbol{G}$

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Simulator complexity

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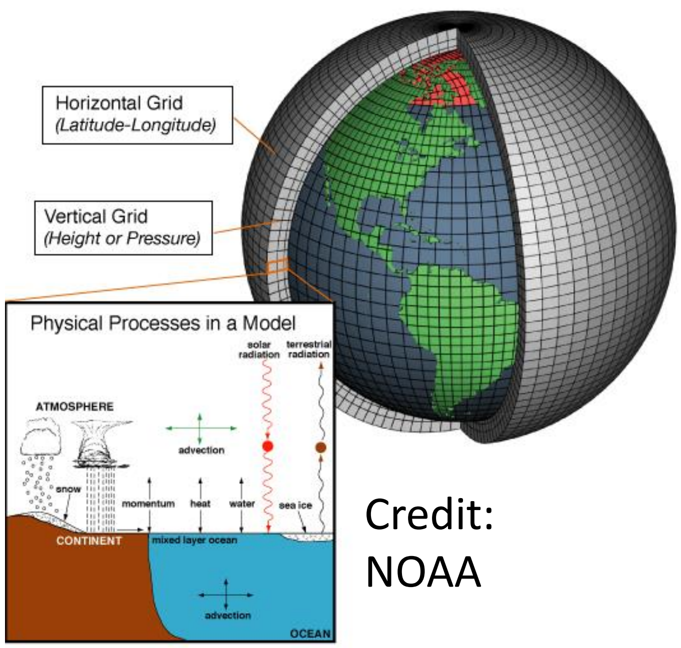
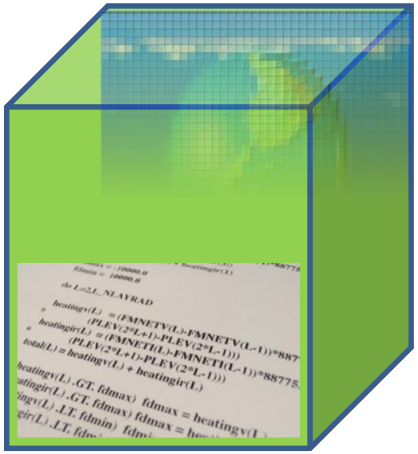
- Simulators contain lots of equations (hundreds of lines of code)

- Simulator resolution increases with computer power



Credit: NOAA



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Bottom line…

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f is often too complex to simulate many $\boldsymbol{x}_i$ from $\boldsymbol{G}$ to characterise the effect of uncertainty on $\boldsymbol{y}$

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Emulation

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- Replace f with $\hat{f}$
- $\hat{f}$ is the emulator
- $\hat{f}$ is much quicker to run but accurately represents f

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More accurately…

- Replace $y_k = f(x)$ with $y_k = \hat{f}(x)$

Define an output (or selection of) to be emulated

- doesn't replace the whole simulator for all research

What is $\mathbf{y}$?

- From the simulator $\boldsymbol{y}$ can be any/all model output/diagnostics
- For emulation $\mathbf{y}$ must be more restricted
- y is often a scalar representing a single model output, at a particular time and location
  - Eg.
    - global mean temperature for 2000
    - total number for particulate matter aerosol > 2.5um in a model grid box
- $\boldsymbol{y}$ could be a spatial field, or a time series, or EOF/PCAs, or a selection of model outputs

Emulator complexity

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The complexity of the emulator is dependent on the complexity of the model output to be emulated

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Continuing…..

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- We will carry on assuming y is scalar and $\boldsymbol{x}$ is a collection of scalar values

- $\boldsymbol{x} = x_1, x_2, x_3, \ldots, x_p$ for p uncertain parameters

- Use a selection of $\boldsymbol{x}_i, \boldsymbol{y}_i$ from f to 'build' $\hat{f}$

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When is an emulator useful?

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uncertainty analysis

Quantify the impact of uncertainty on model output

sensitivity analysis

Understand model response to uncertain inputs

And the model is too complex to do the sampling required

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A statistical emulator

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An emulator that gives estimates of its own uncertainty

We tend to use the Gaussian process

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The Gaussian process emulator,
(Rasmussen and Williams, 2006 & O'Hagan 2006).

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- Each point in space has a Gaussian distribution
- Each collection of points has a multivariate Gaussian distribution
- The whole collection is a Gaussian process
- In its basic form requires 'smooth output'

Does not require the output to be Gaussian

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The GP prior

Set up the Gaussian process prior function

$$f(\boldsymbol{x})|\beta,\sigma \sim GP(h(\boldsymbol{x})^T\beta, \sigma^2 c(\boldsymbol{x},\boldsymbol{x}'))$$

$h(\boldsymbol{x})^T\beta$ is the mean function

$c(\boldsymbol{x},\boldsymbol{x}')$ is the covariance function

β,σ are hyperparameters

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Specifying the GP mean

- Use the mean function to specify any functional form known to exist

- In the absence of prior information we tend to specify it as constant or a linear regression formula

$$h(x) = 1$$

$$h(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p$$

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What does the prior mean function do?

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- When there are very few simulator runs to give information the function is weighted towards the prior mean

- Outside the bounds of the simulator runs the emulator tends towards the prior mean

- With more (well-chosen) simulator runs the hyperparameters β are better estimated

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β hyperparameters

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- Can be plugged in if a particular regression model is required

- Usually use maximum likelihood to estimate them and ‘plug-in’

- Could use a Bayesian approach but time-consuming

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Specifying the GP covariance

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- The covariance function should reflect $c(\boldsymbol{x}, \boldsymbol{x}) = \mathbf{1}$ and that $c(\boldsymbol{x}, \boldsymbol{x}')$ decreases as $|\boldsymbol{x} - \boldsymbol{x}'|$ increases

- Includes further hyperparameters δ that specify the speed of covariance decrease with increasing $|\boldsymbol{x} - \boldsymbol{x}'|$

$$cov\{f(\boldsymbol{x}), f(\boldsymbol{x}')|\sigma\} = \sigma^2 \, c(\boldsymbol{x}, \boldsymbol{x}')$$

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Typical choices for $c(x, x')$

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Gaussian:

$$c(x, x')|\delta = \exp\{-\frac{(x - x')^2}{2\delta^2}\}$$

Matern 5/2:

$$c(x, x')|\delta =$$

$$\left(1 + \frac{\sqrt{5}|x-x'|}{\delta} + \frac{5(x-x')^2}{3\delta^2}\right) exp(-\frac{\sqrt{5}|x-x'|}{\delta})$$

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Effect of covariance

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- The uncertainty at simulator runs is 0
  - unless a nugget is used

- The uncertainty between points decreases as it gets closer to simulator suns

- The width of bounds between points increases as δ decreases

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The posterior distribution

- A Gaussian process, with parameters estimated by the training data

- Any point can be estimated

- Uncertainty in the estimate can also be estimated

Emulator uniqueness

- The emulator is non-unique
- Hyperparameters will be different if you re-run
  - Unless you set the seed
- Using prior information can help stability
- Often, it's not actually a problem…

Building an emulator

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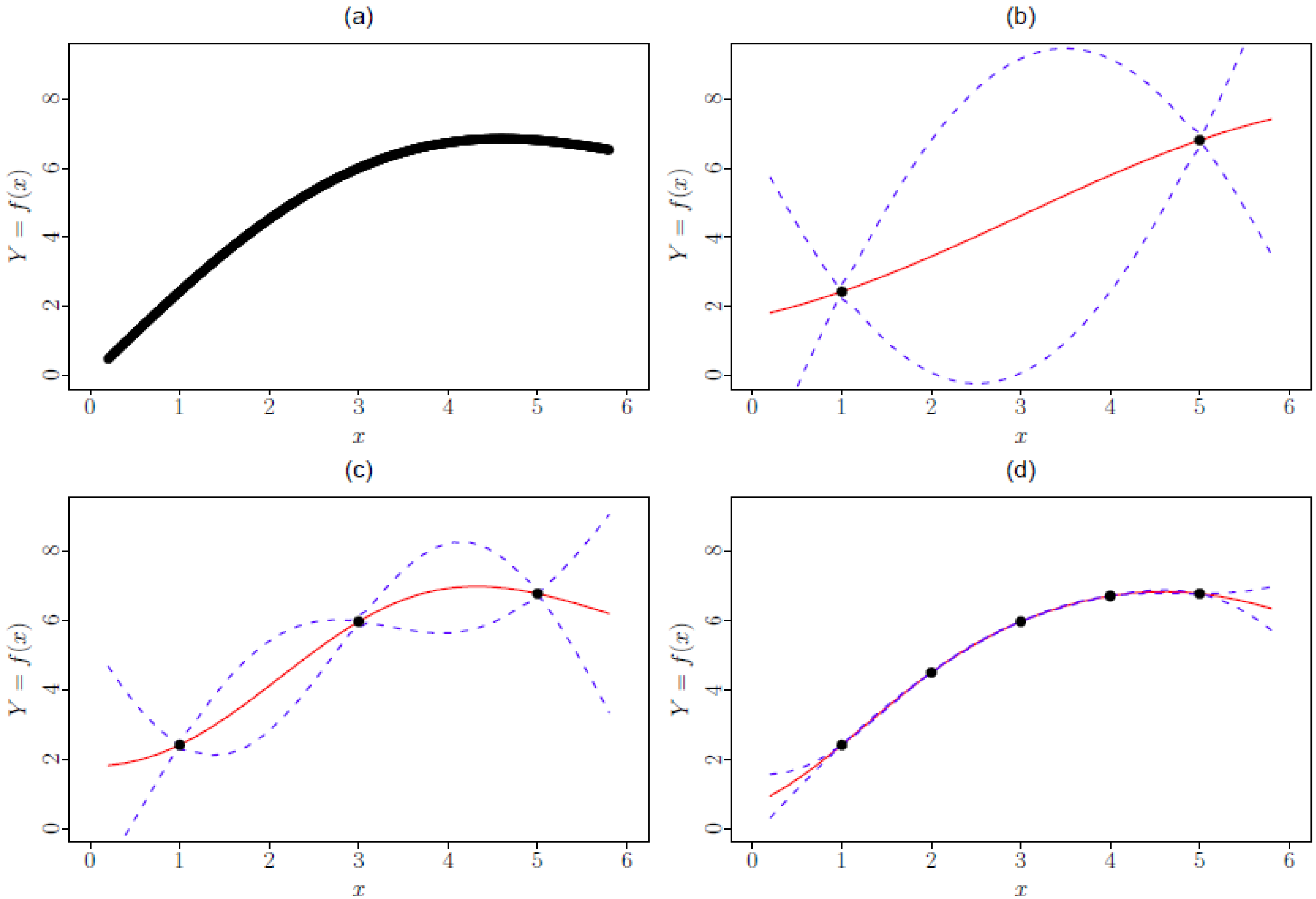

From Jill Johnson following O’Hagan (2006)

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Aerosol model emulation with DiceKriging (Roustant et al., 2012 & Lee,at al, 2013)

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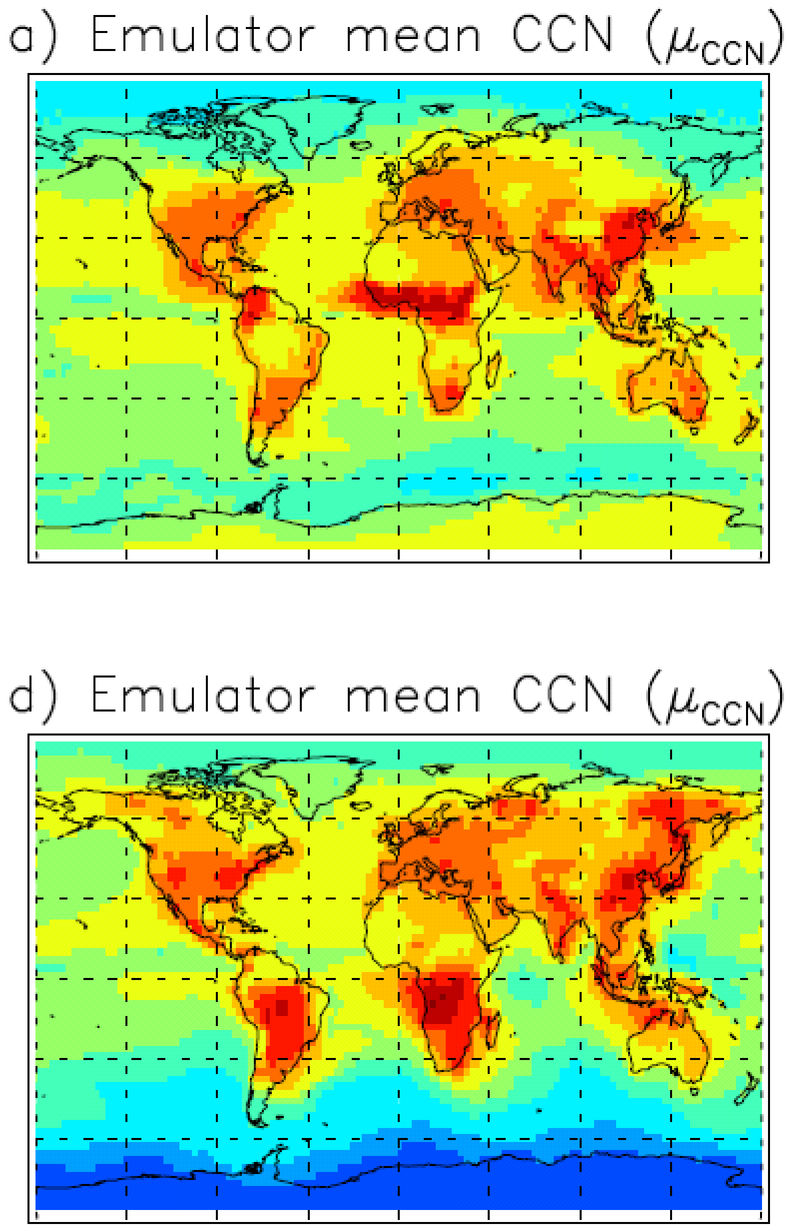

Emulation done gridbox by gridbox for sensitivity analysis

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Training data

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- Need to update the prior with simulator points
- Require these points to provide good information about the function through uncertain space
- Often consider no prior information regarding particular parts of the space

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Design for training data
(McKay et al., 1979)

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Latin hypercube sampling

- Good for inactive dimensions
- Use optimum or maximin
- May want piecewise LHS

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Latin hypercube sampling

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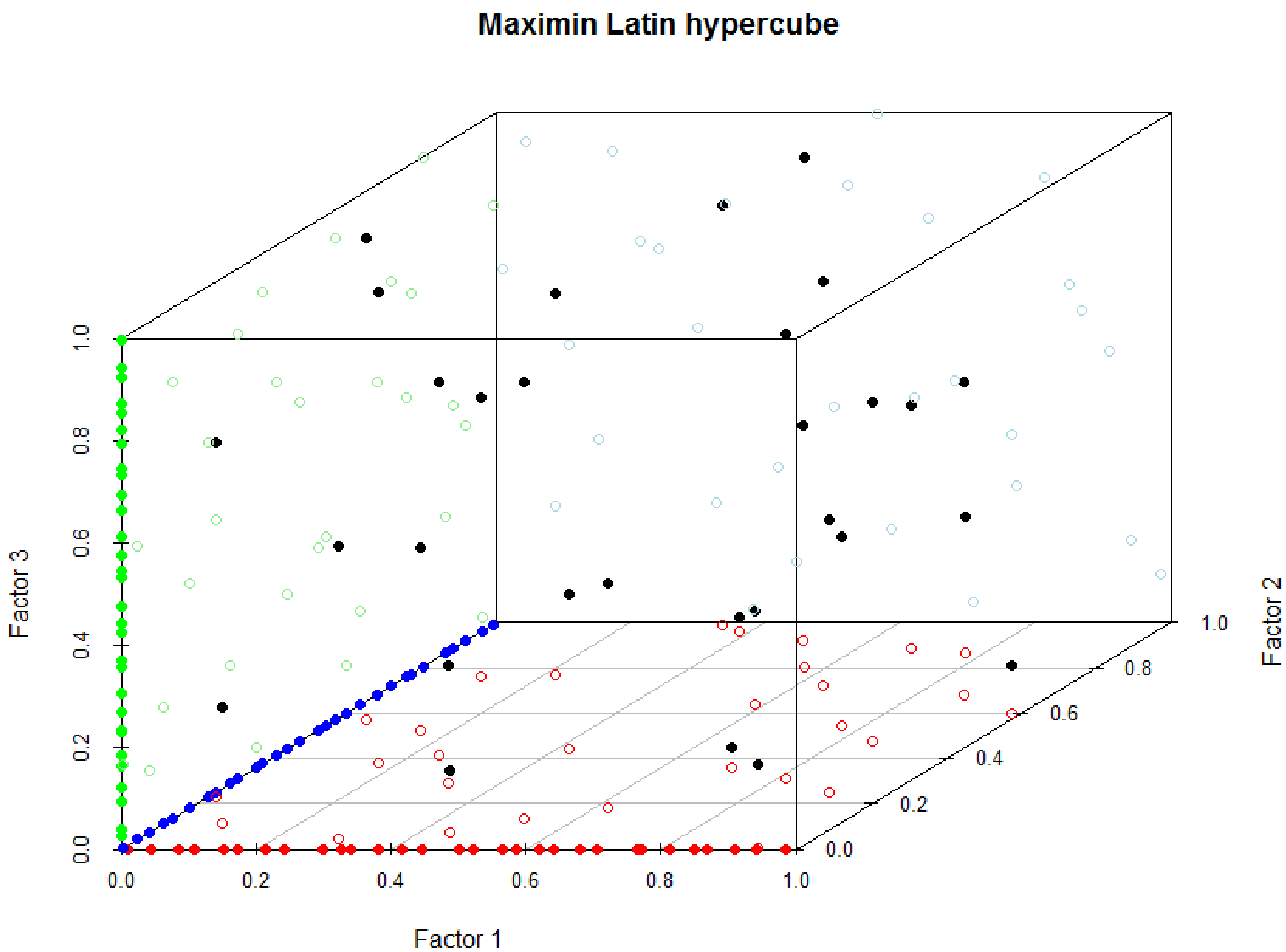

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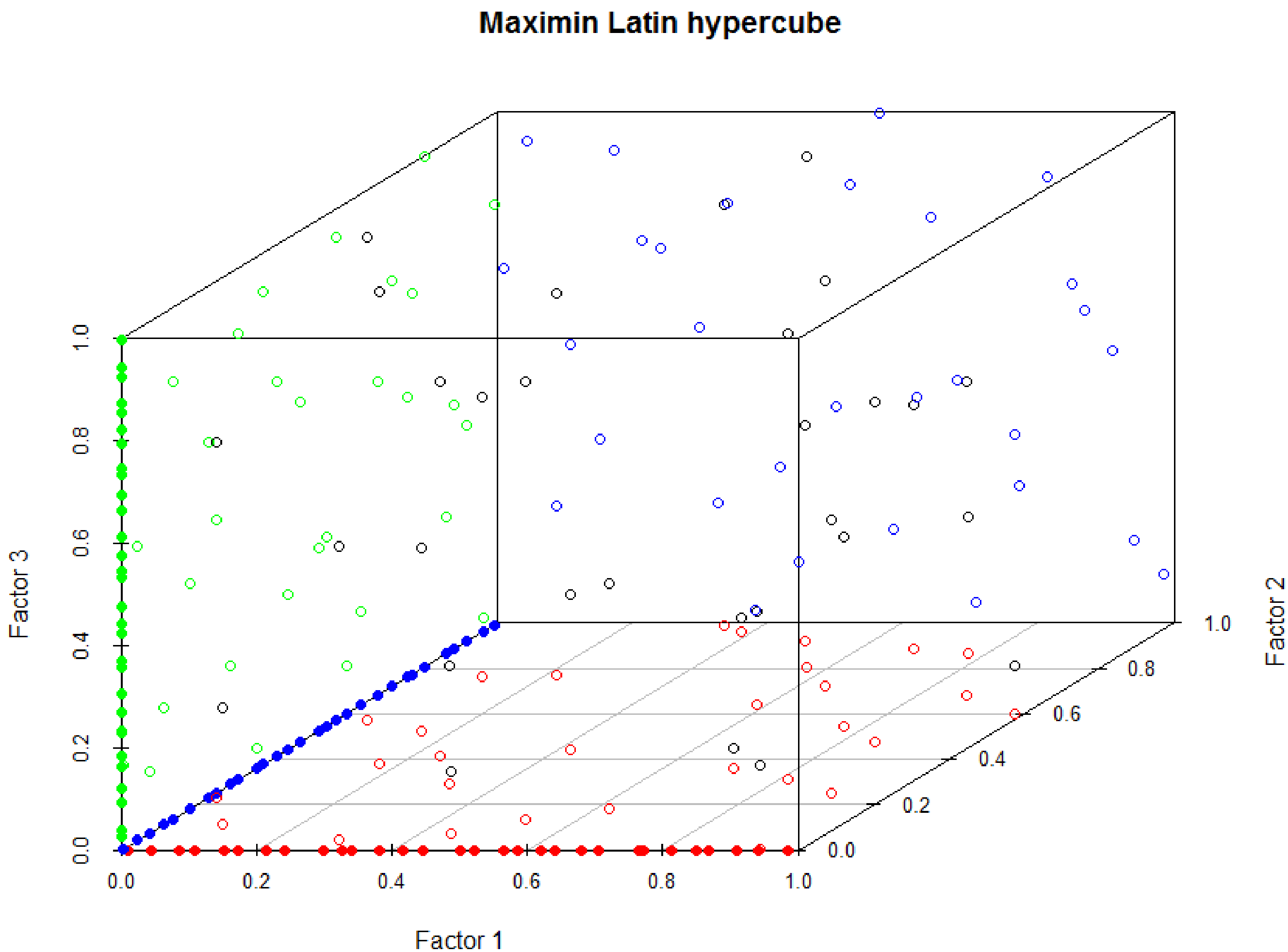
The marginals



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Sequential design

- When emulator validation suggests can update the design sequentially
- If no reason to search particular region, augment the design
- Can add points sequentially, perhaps Sobol, to particular regions

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Factorial designs

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- These are not recommended
- The covariance function is better estimated using a variety of distances between points
- Uncertainty between training points will be very high

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Validation of emulators

- Have to check the emulator can predict what the emulator would say

- Usually want to check ‘out of sample’

- Can use leave one out when circumstances dictate

Aims of validation

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Prediction value

Ensure emulator predictions are close to simulator

Prediction uncertainty

Ensure uncertainty in emulator is small enough for further inference

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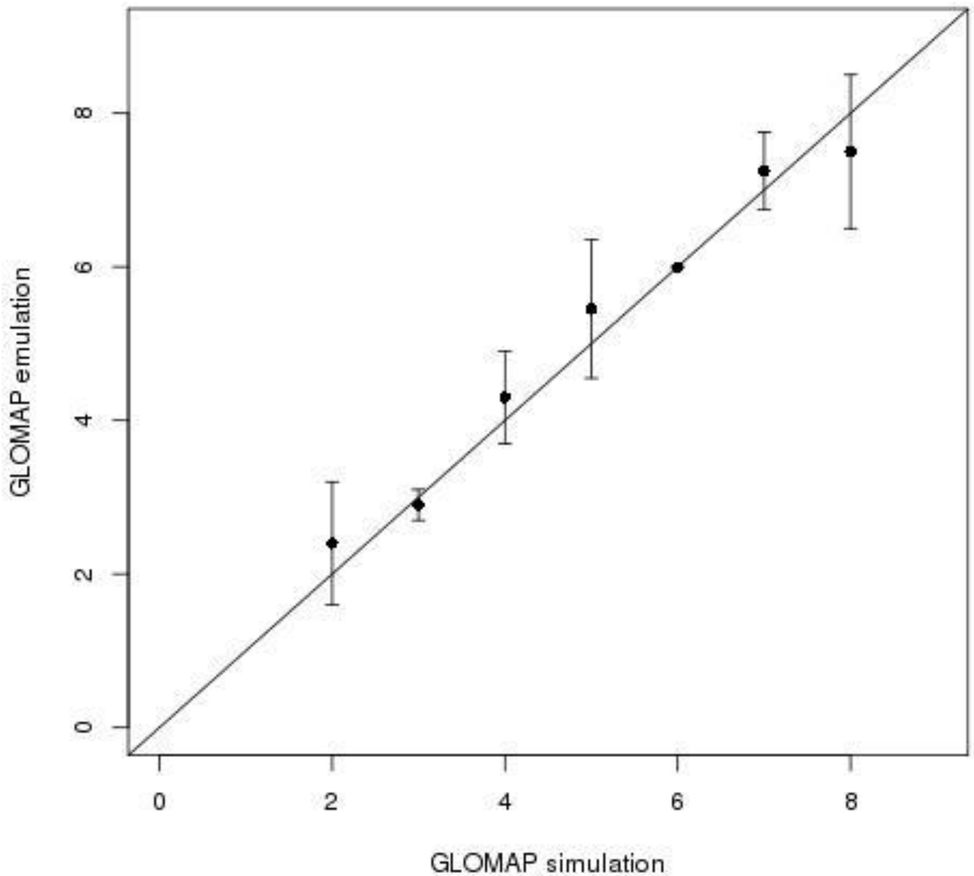
GLOMAP emulation
0
2
4
6
8
0
2
4
6
8
GLOMAP simulation

Validation design

- When out-of-sample tend to design two groups, as per Bastos & O'Hagan (2009)

- 1/3 close to simulated points and 2/3 spaced out
  - Helps reveal particular difficulties

Validation statistics

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- Individual prediction errors
  - Treat like regression errors, approximately Gaussian and <|2| standardised
- Mahalanobis distance
  - single summary of individual prediction errors
  - extreme values indicate emulator/simulator mismatch
- Pivoted Cholesky errors
  - following variance decomposition
  - particular patterns aid interpretation of mismatch

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Validation plots

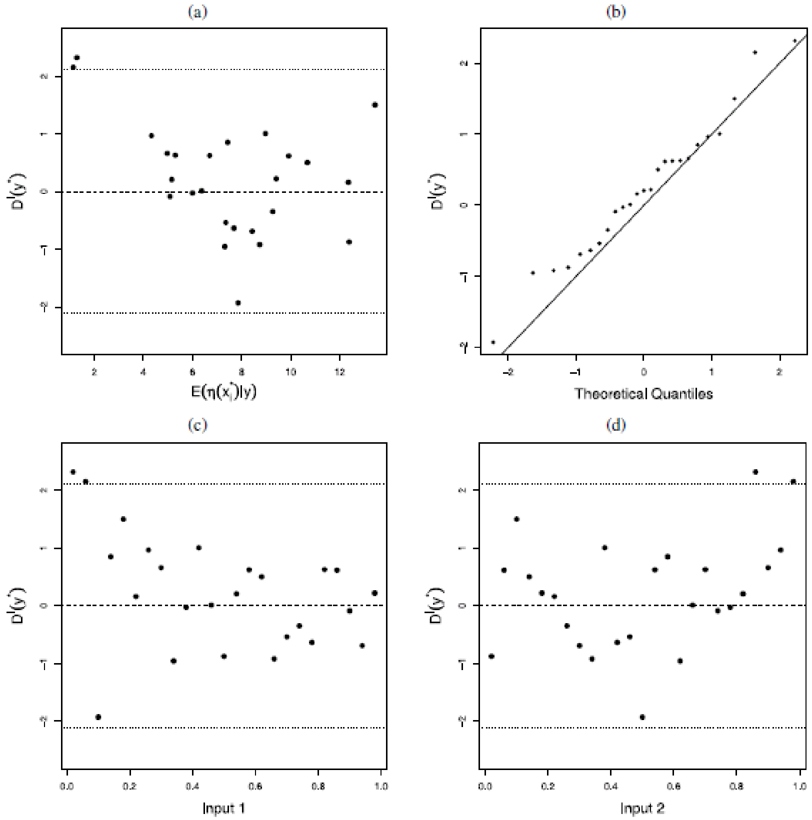
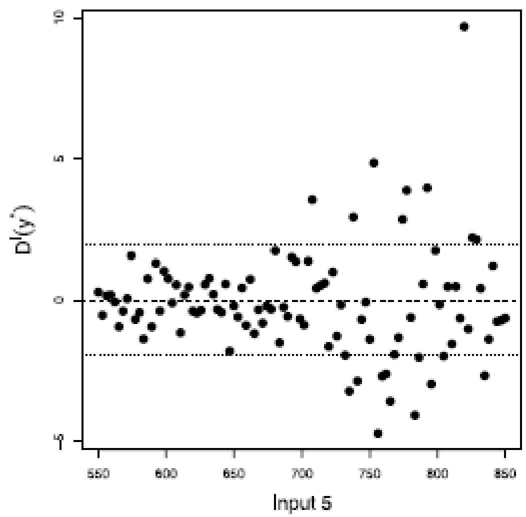
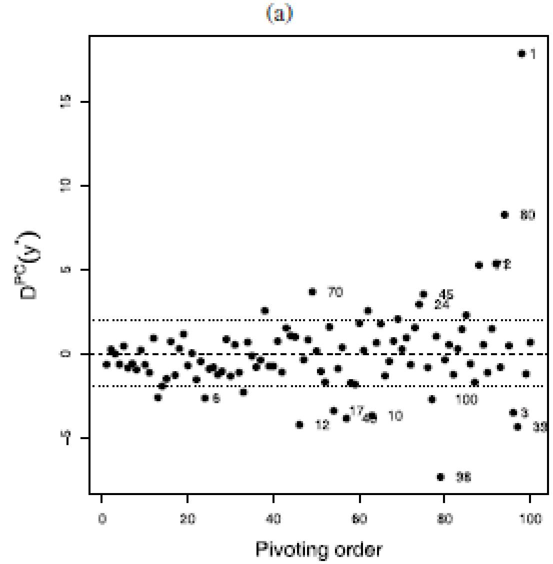


Figure 1. Graphical diagnostics for the toy example using the individual standardized errors: (a) $D^I(\mathbf{y}^*)$ against the emulator predictions; (b) QQ-plot; (c) $D_i(\mathbf{y}^*)$ against input 1; and (d) $D_i(\mathbf{y}^*)$ against input 2.





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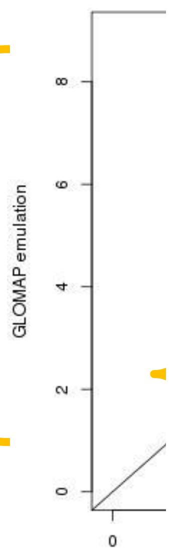
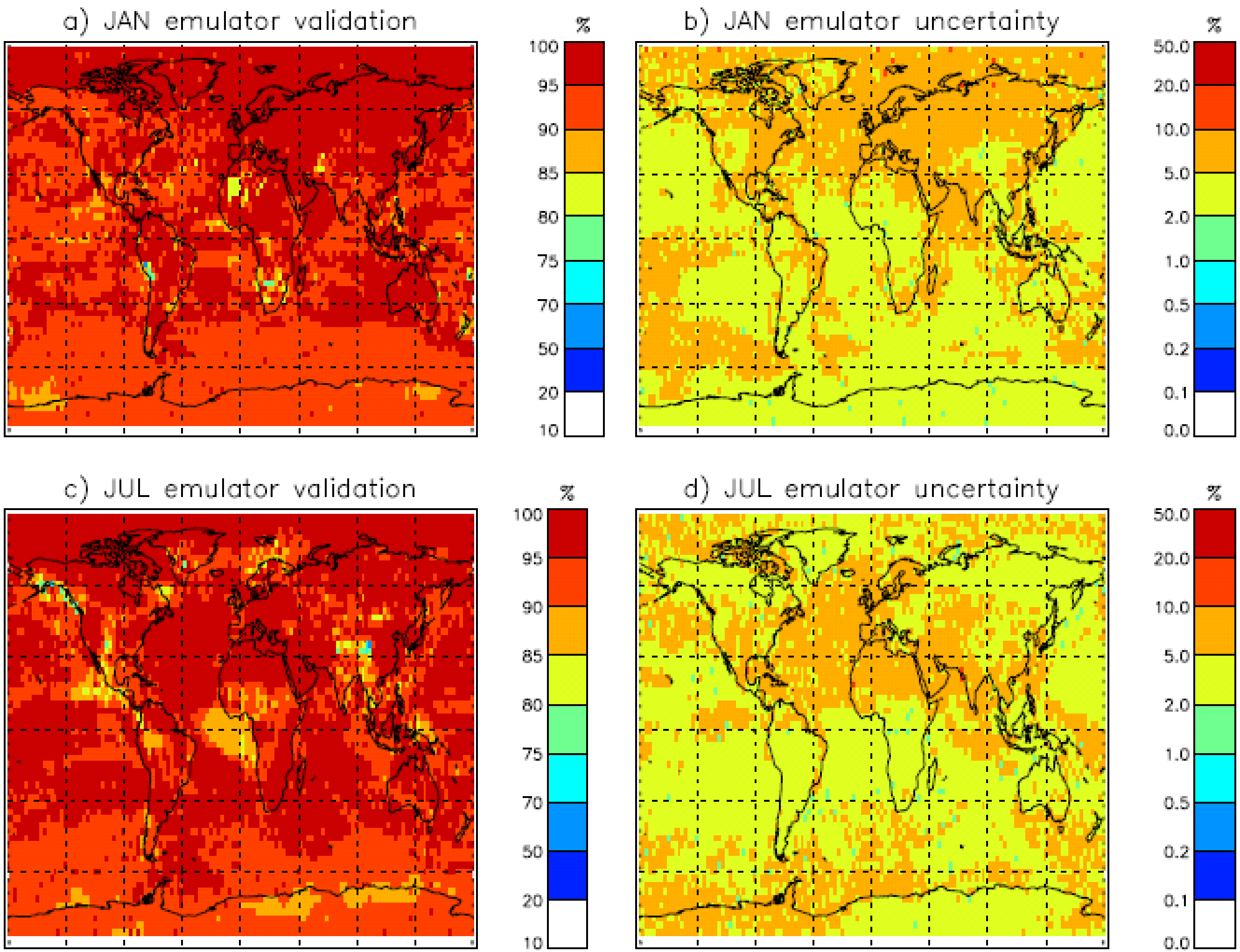
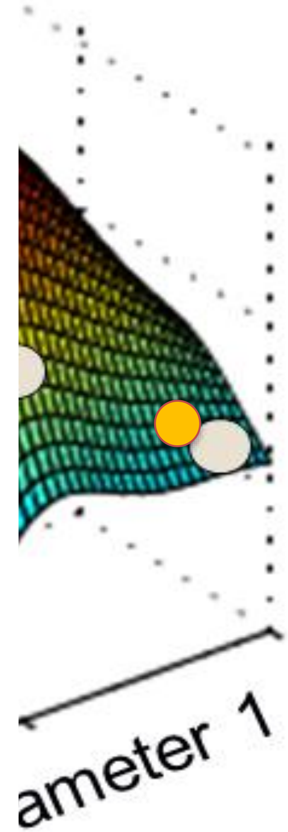
Aerosol emulator validation







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Leave one out

- When out-of-sample is not possible
- Leave a point out, build emulator, produce validation statistics
- Repeat for all points and compare statistics
- Any points with extreme statistics indicate problems

Emulation for understanding

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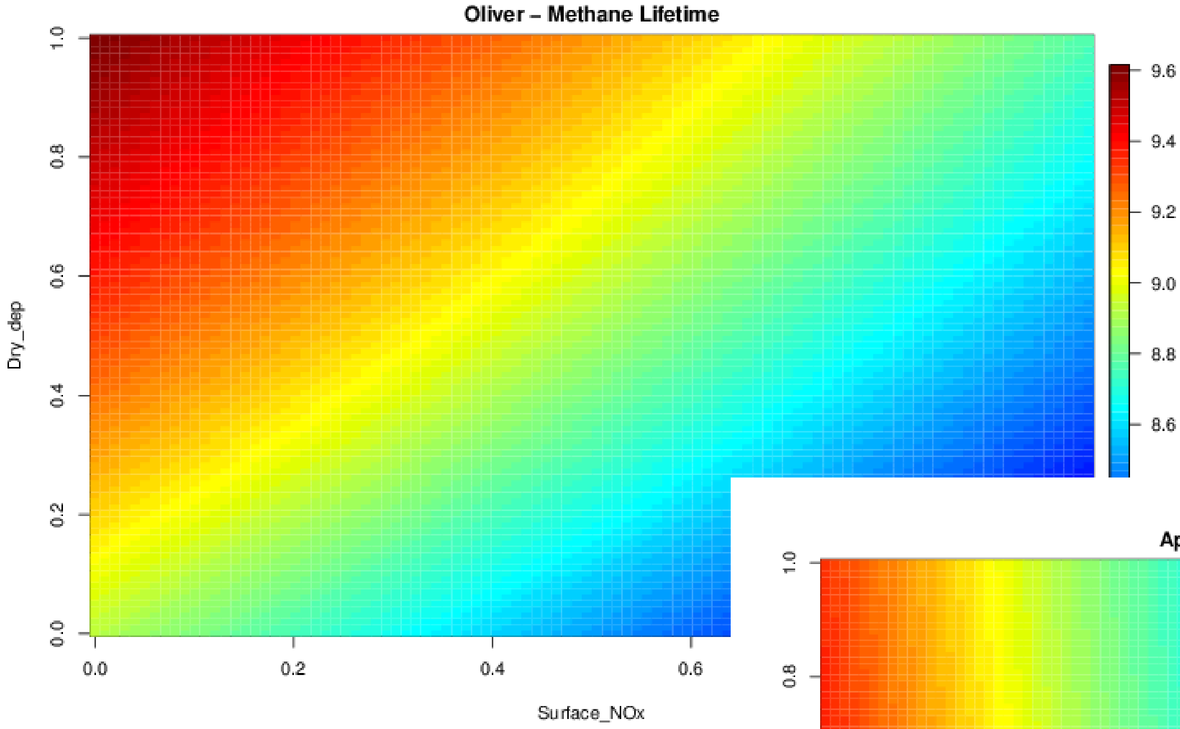

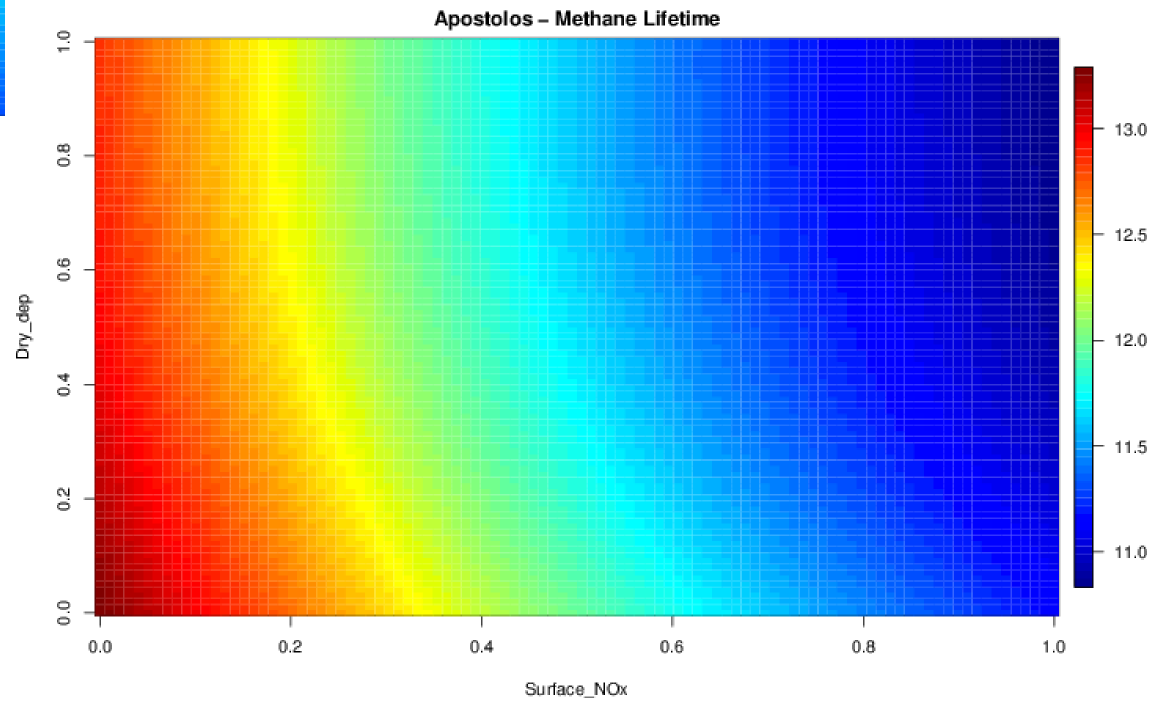

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Emulation for uncertainty analysis

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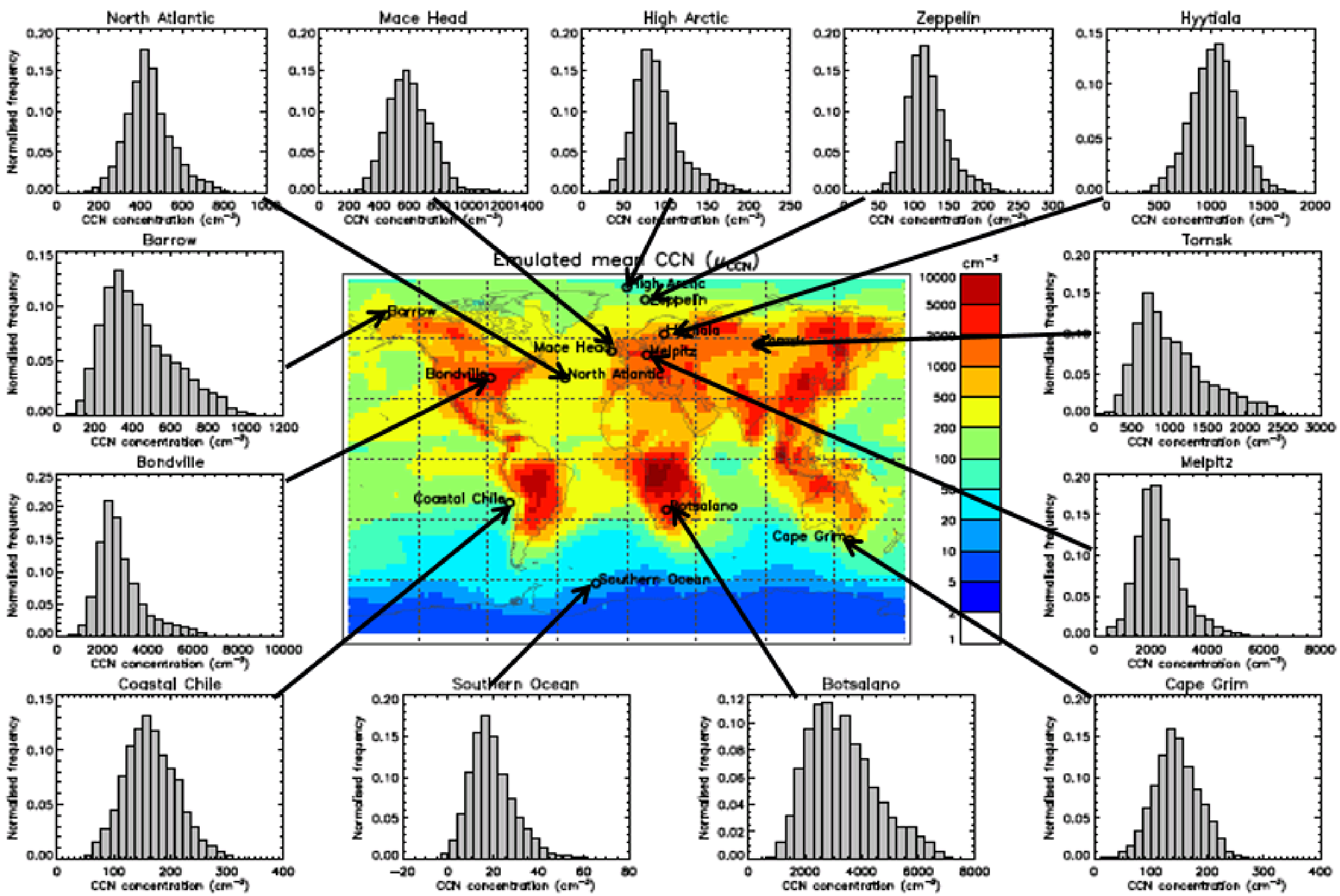

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Emulation for sensitivity analysis (Saltelli et al., 2000) using R sensitivity (Pujol et al., 2008)

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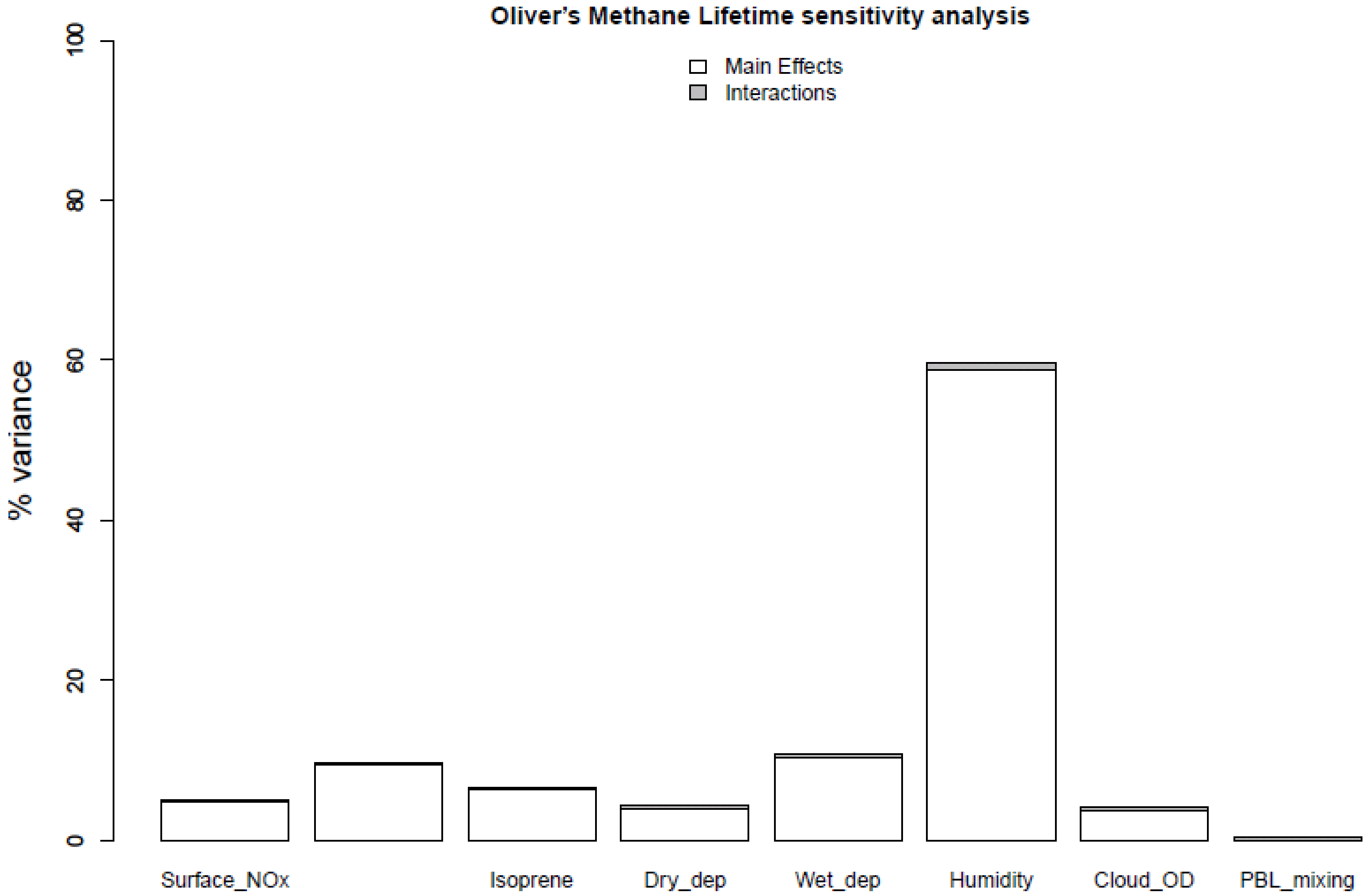

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Aerosol model sensitivity analysis

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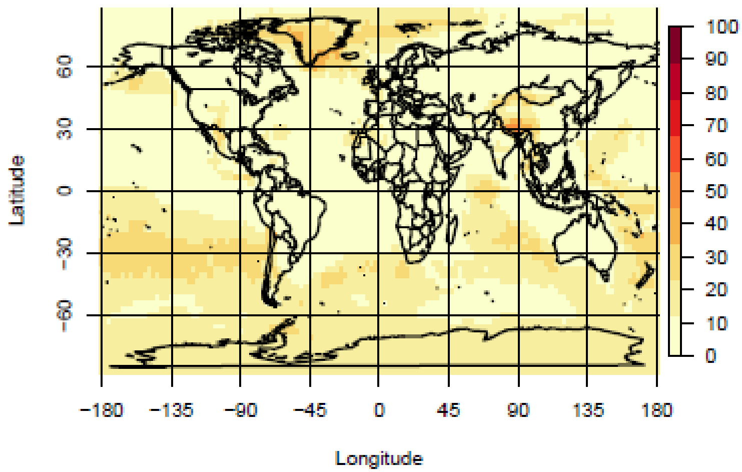
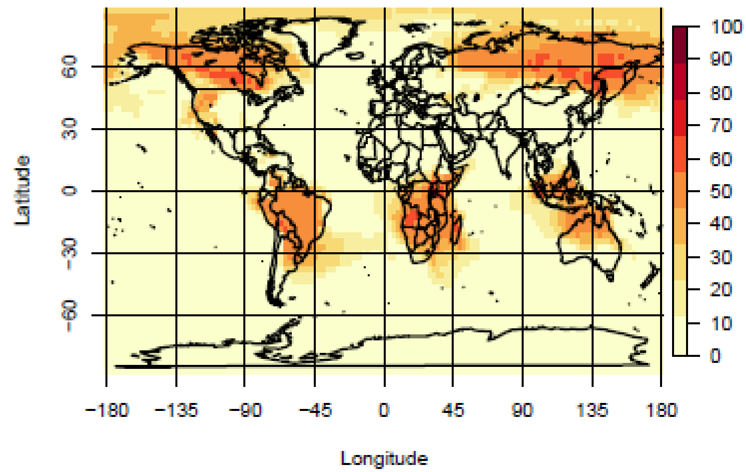
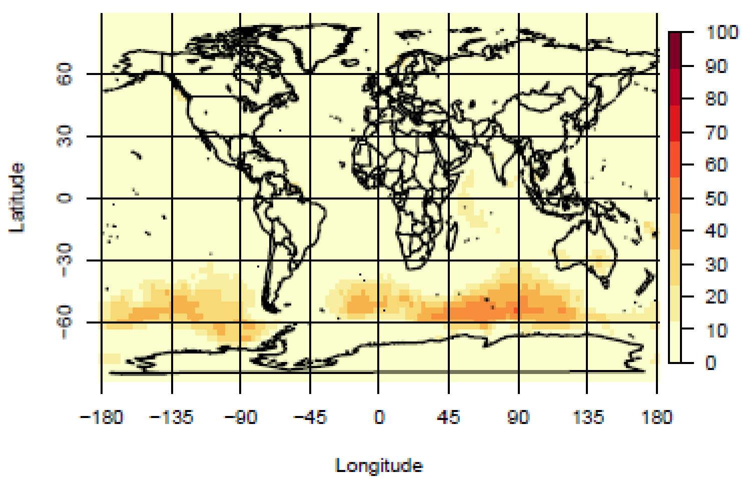
AIT_WIDTH JULY



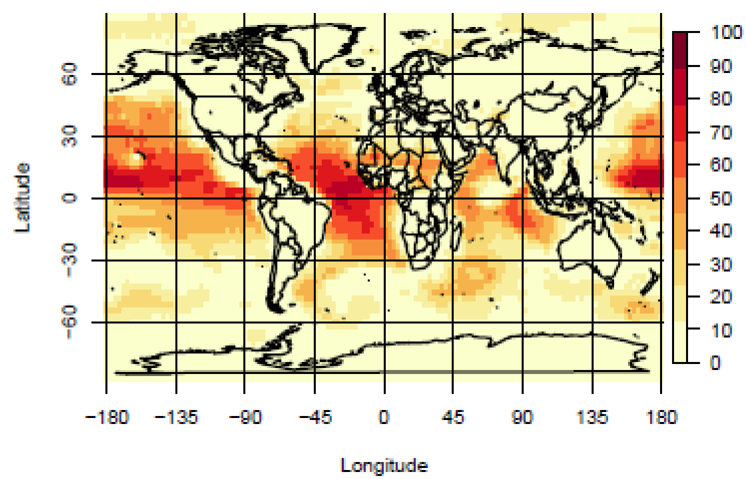
BB_DIAM JULY



SS_ACC JULY



DRYDEP_AER_ACC JULY



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Aerosol model sensitivity analysis II

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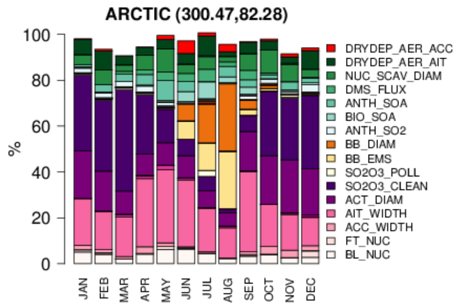

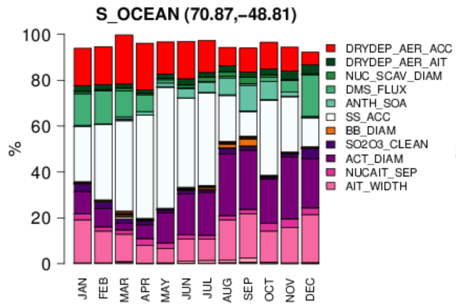

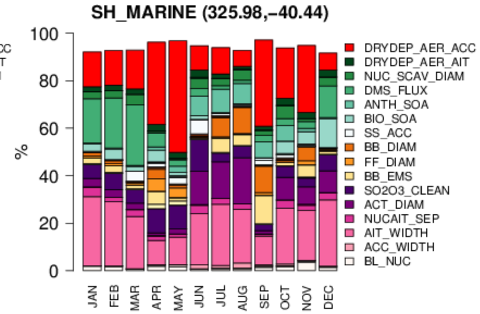

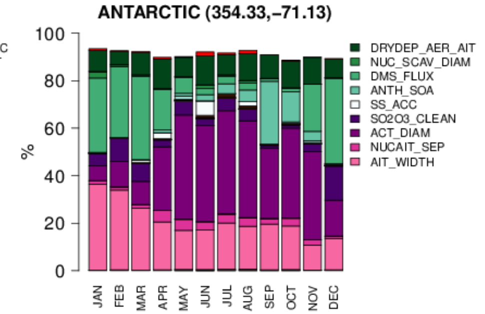

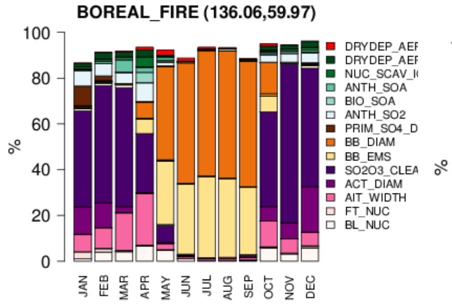

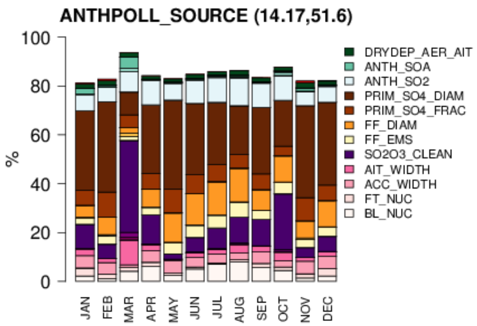

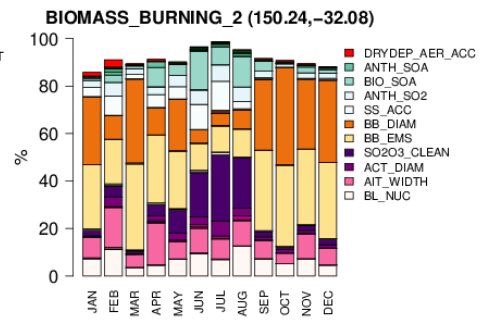

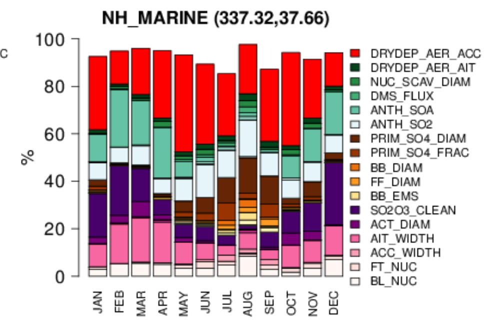

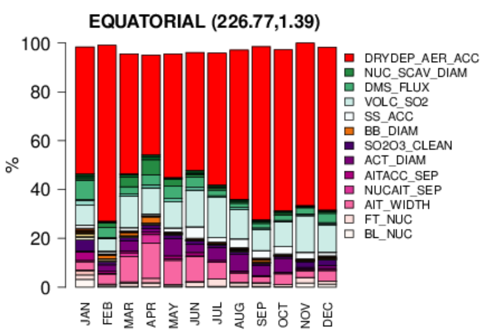

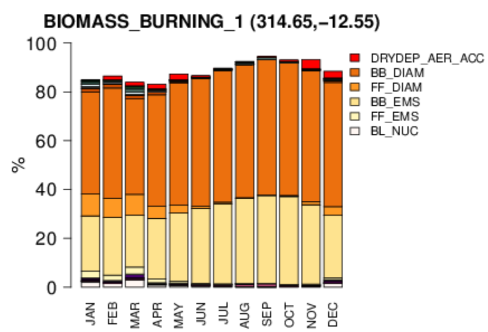

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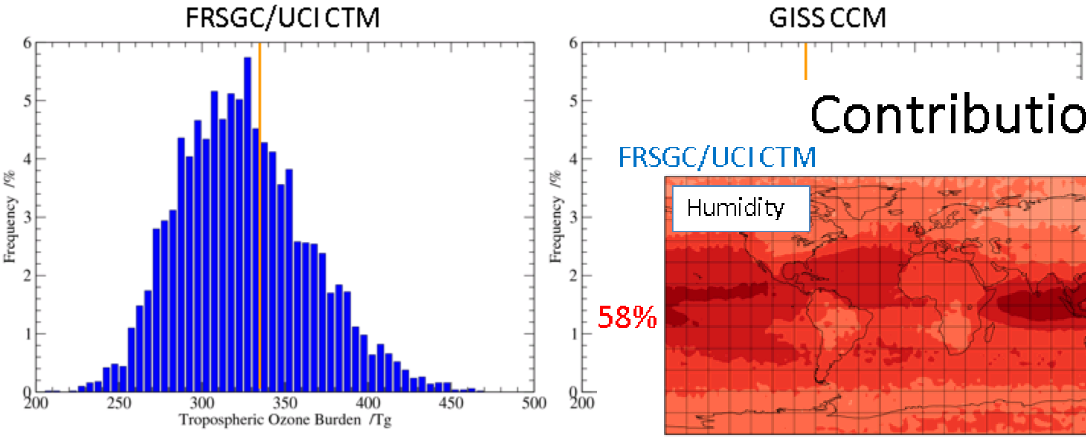
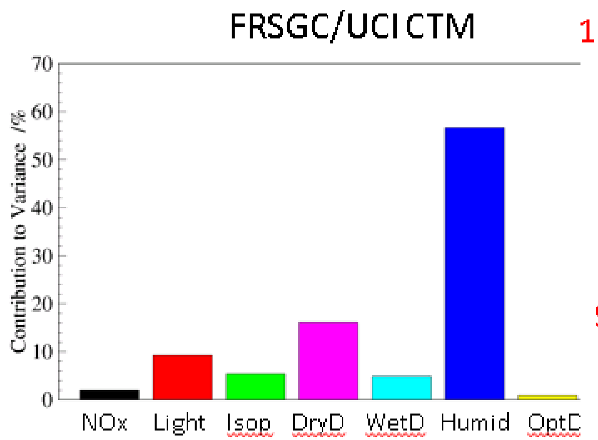
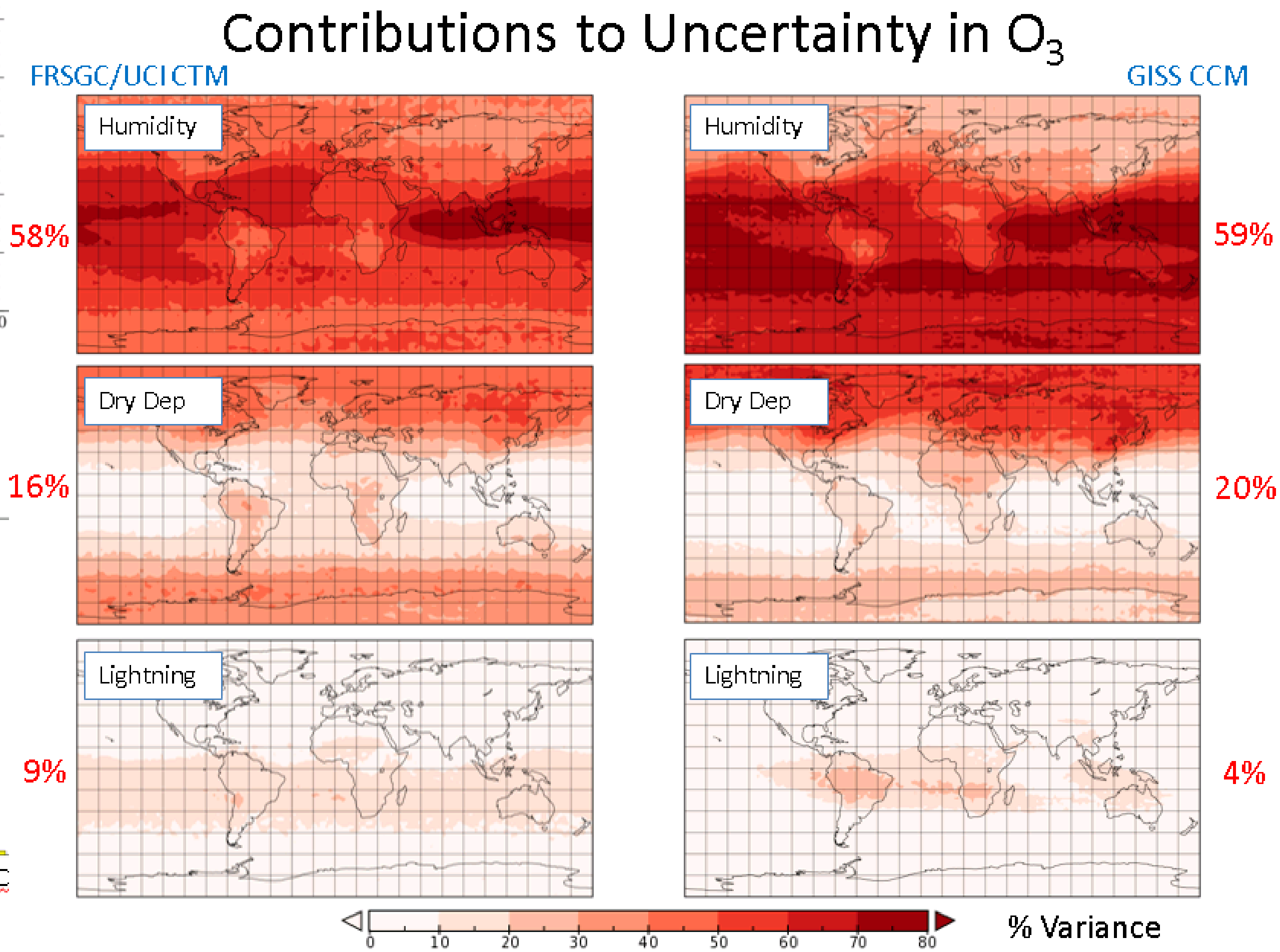
Multiple model sensitivity analysis I



FRSGC: 325 ± 39 Tg





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Multiple model sensitivity analysis II

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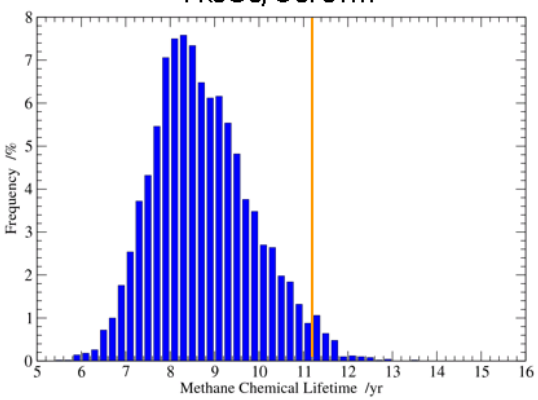
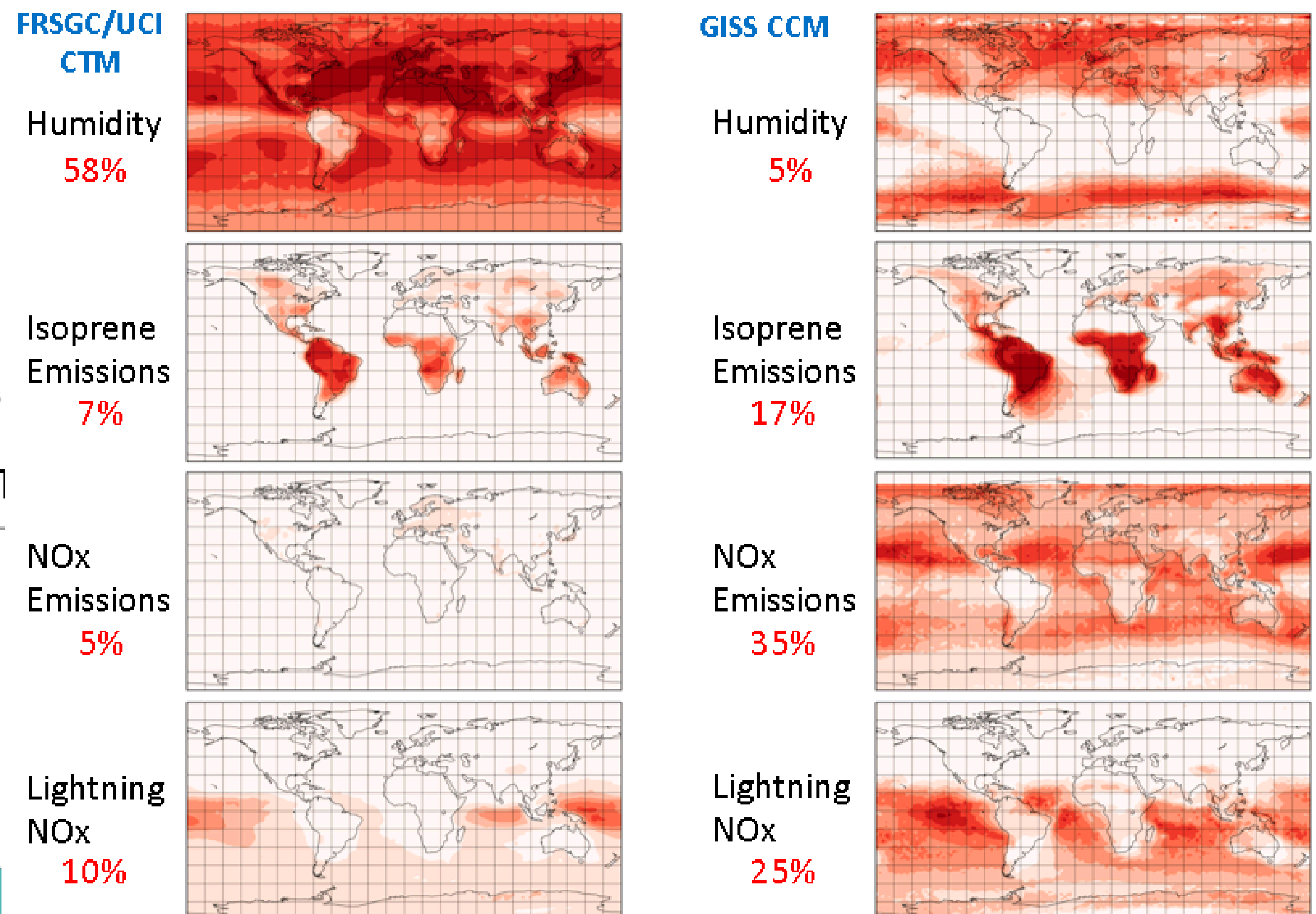
Tropospheric

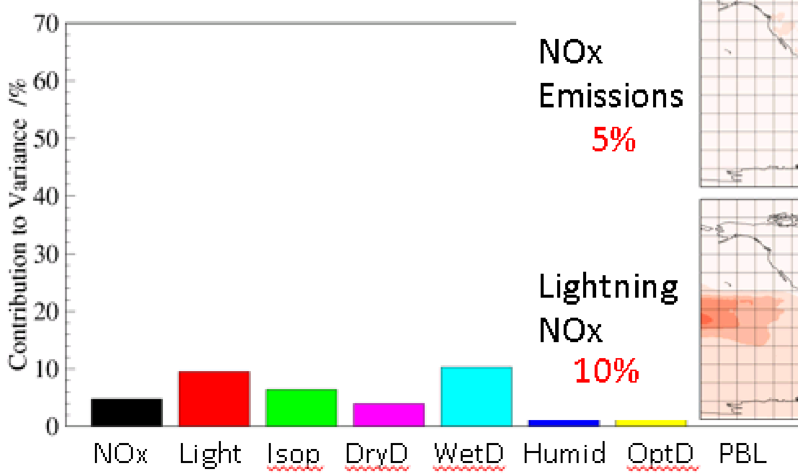
Contributions to Uncertainty in CH_4 Loss Rate

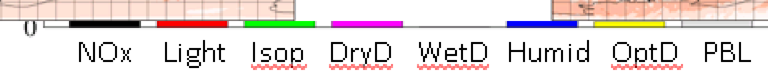
FRSGC/UCI CTM





FRSGC/UCI CT





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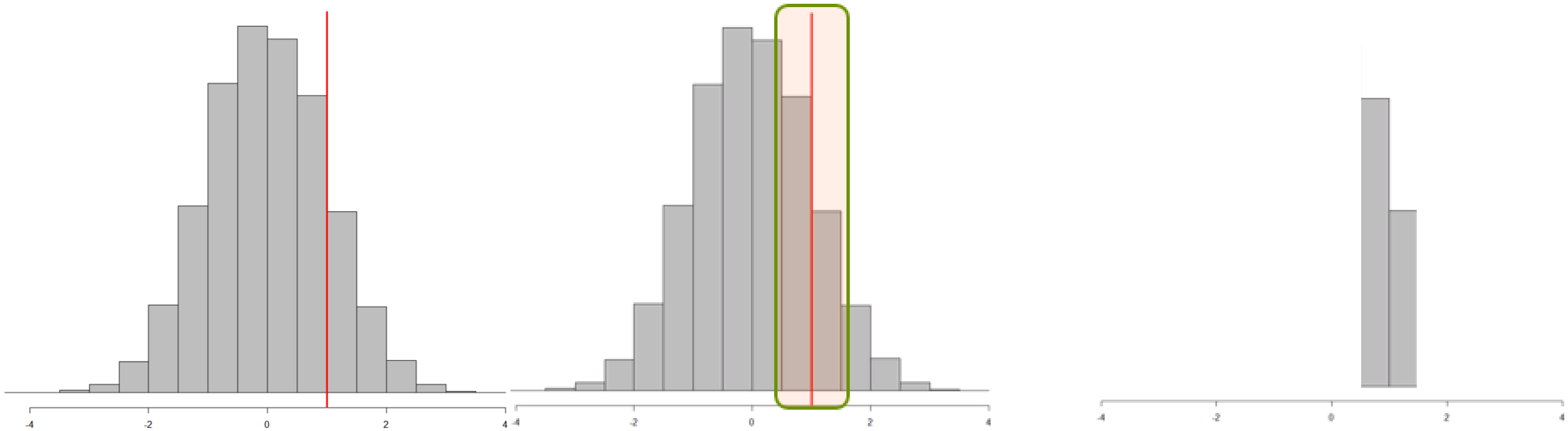
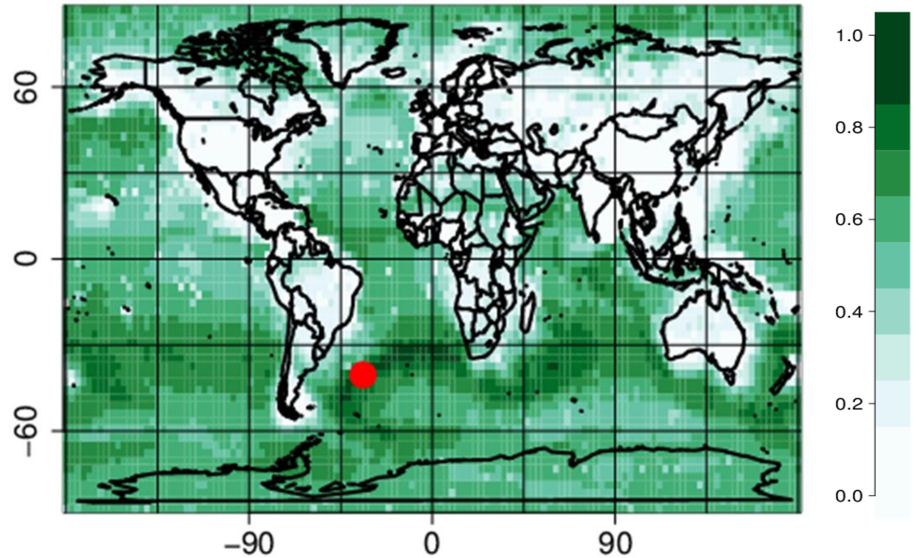
Emulators for model constraint I





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Emulators for model constraint II

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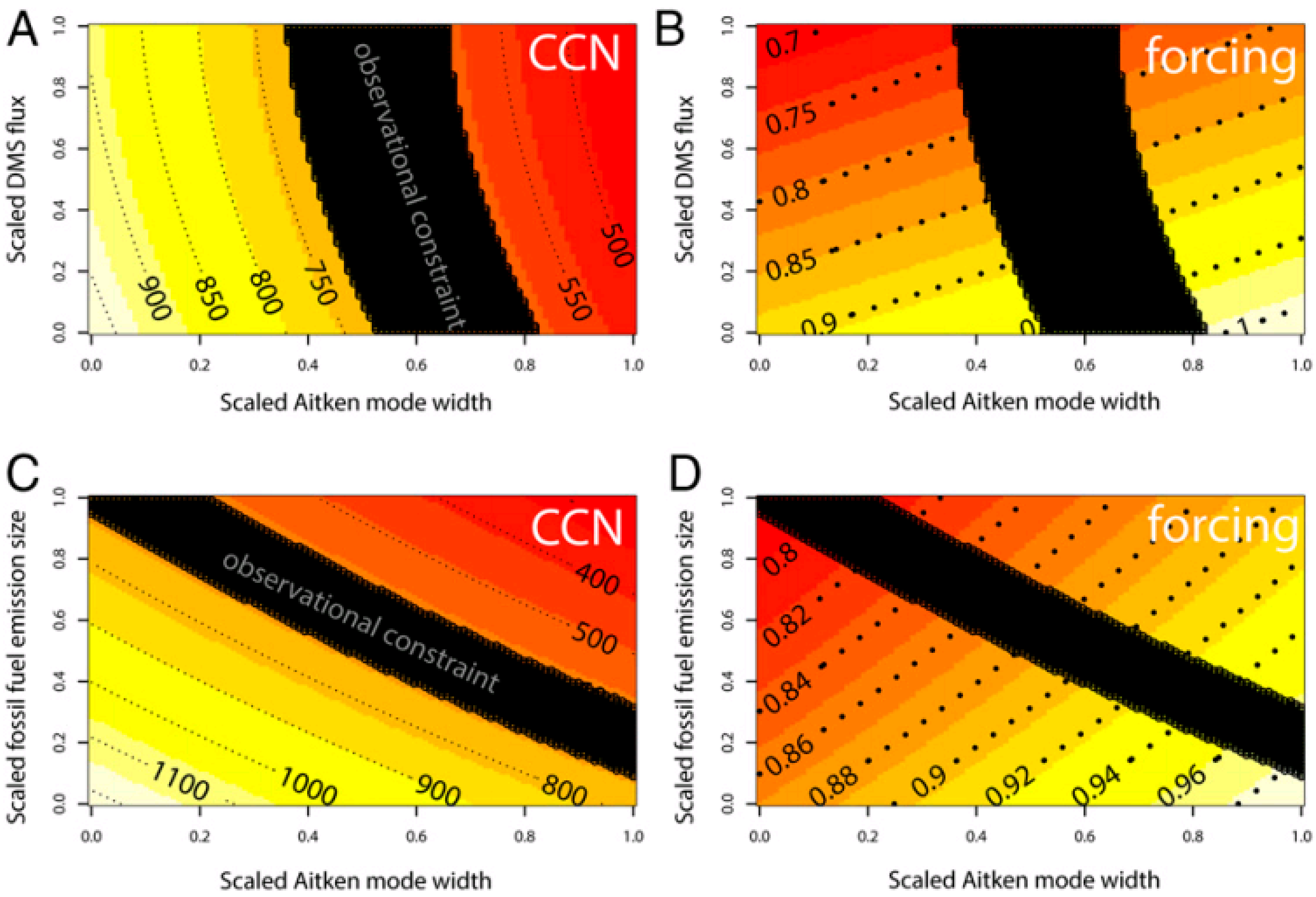

Extension to GP emulators

- Stochastic simulator – add an estimated nugget to covariance
- Multivariate emulator – must characterise the covariance between multiple outputs
- Discontinuities – could build multiple emulators, perhaps multivariate

What an emulator can't do

- Extrapolate too far with confidence
- Estimate a simulator output it's not trained to
- Replace the simulator

When not to use an emulator

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- When the simulator is very cheap to run
- When it won’t validate
- When you haven’t got a good set of simulator runs for training
- When you aren’t sure what you’ll use it for

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Methodology references

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