Bayesian Uncertainty Analysis for Tipping Points in Systems Modelled by Computer Simulators

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Simulators and physical systems

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- Denote y as the actual system behaviour. For a perfect model,

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  where x^* is an "appropriate choice" or "best input".
- Models are rarely (never?) perfect so we write

$$y = f(x^*) + \epsilon$$

  where ϵ is a correlated random vector corresponding to structural discrepancy between the simulator and the real system.

Simulators and physical systems

- Furthermore, we can only have observations $\mathbf{z}$ of this system on a historical subvector $y_{\mathbf{h}}$ of y corresponding to output subvector $f_{\mathbf{h}}(x^*)$. We then write

  $$z = y_{\mathbf{h}} + \eta$$

  where η corresponds to measurement errors often taken to be independent of $y_{\mathbf{h}}$.

Box models

What are box models?

- Simplification of large environmental system, e.g. ocean circulation
- Assumption of homogeneity within each box
- Represented by systems of differential equations

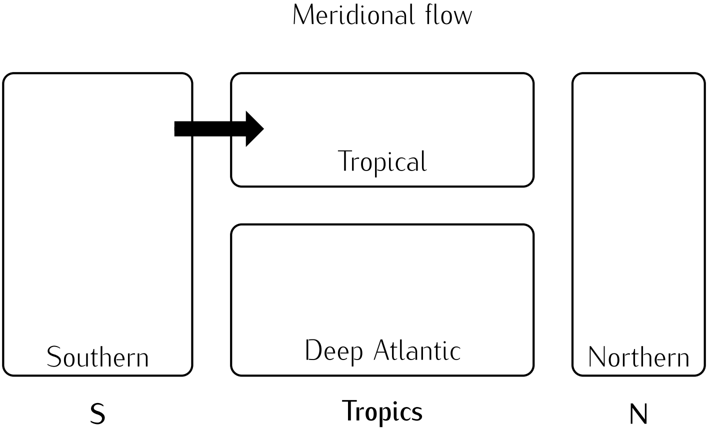
Why use ocean box models?

- Navier-Stokes equations are complicated
- GCMs are highly complex, computationally expensive and obscure the fundamental system dynamics
- Better idea of how the system behaves before equilibrium

Downfalls

- Not as complex as N-S but can't usually be solved analytically
- Numerical solvers for ODEs become unstable near bifurcations
- Still quite expensive computationally

Four-box model - Zickfield et al (2004)



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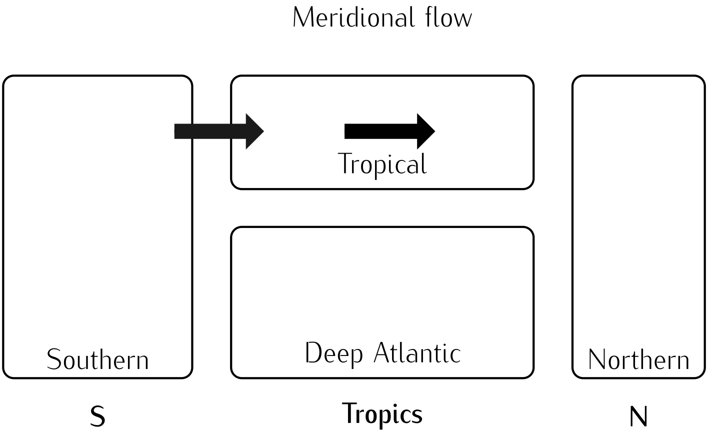

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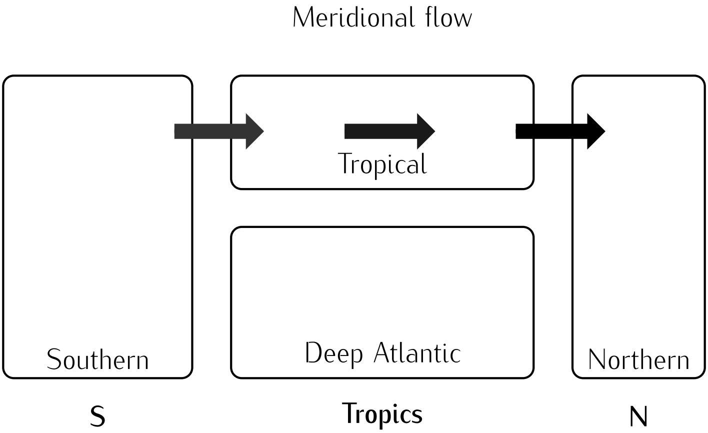

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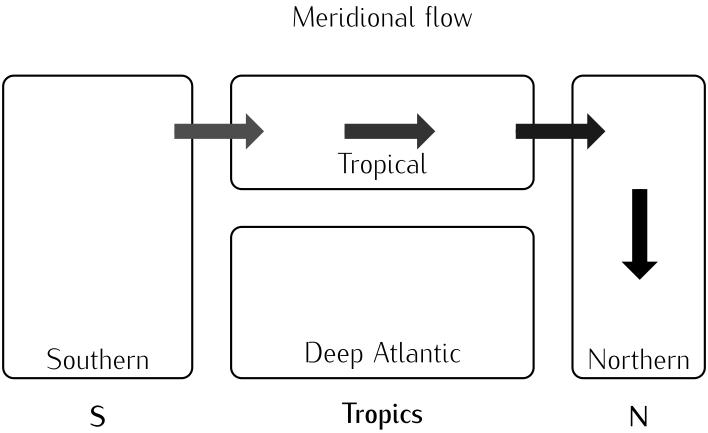

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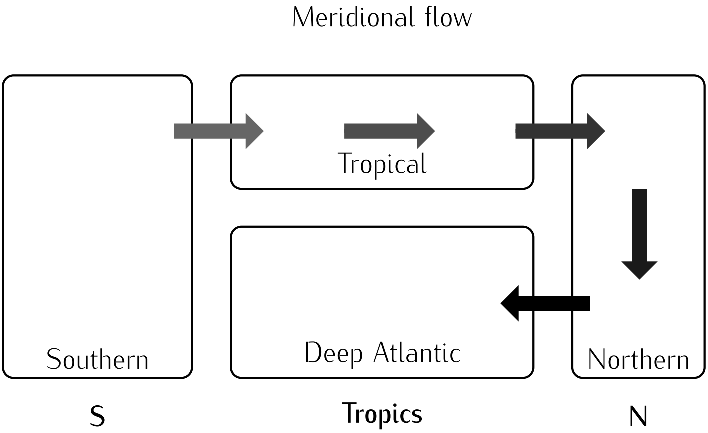

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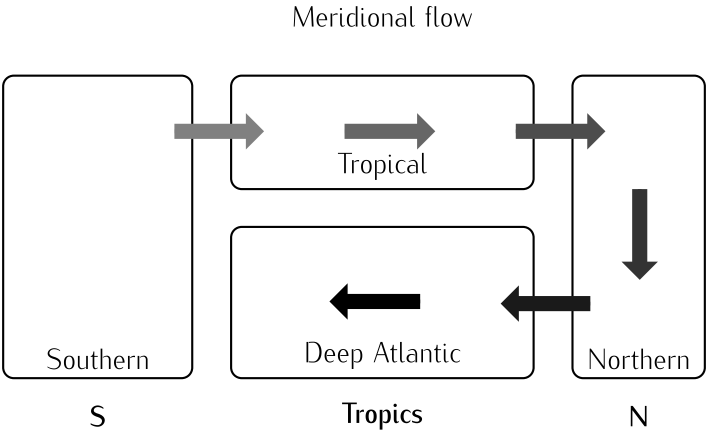

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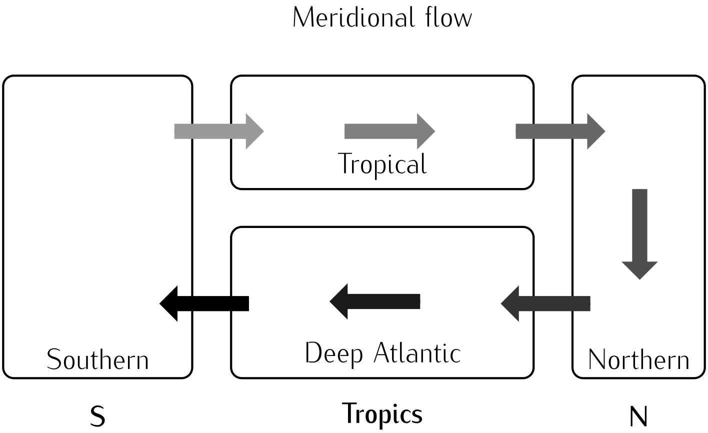

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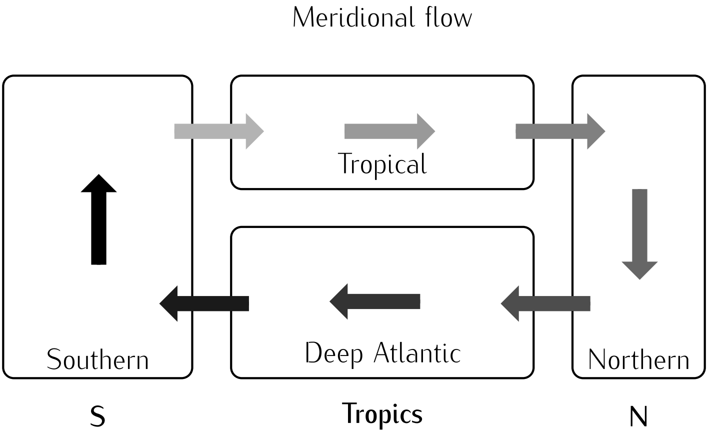

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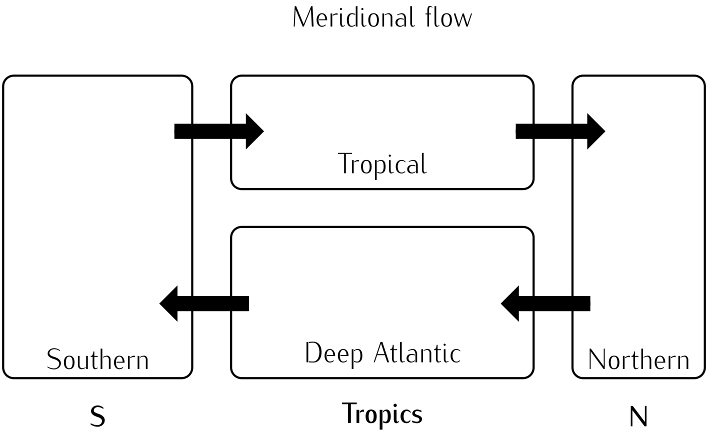

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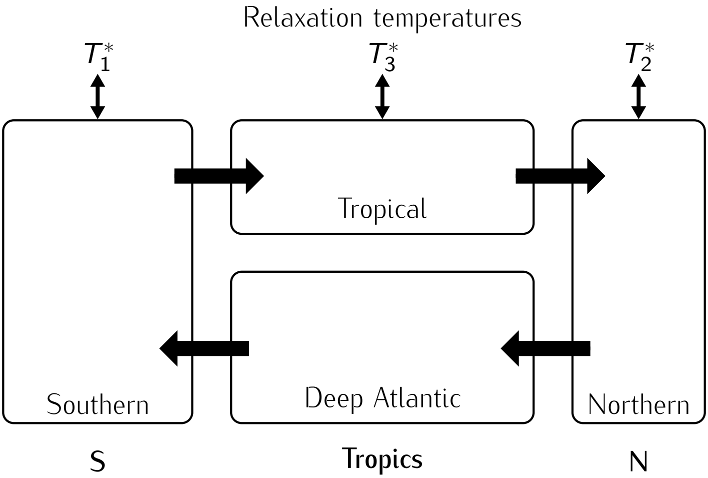

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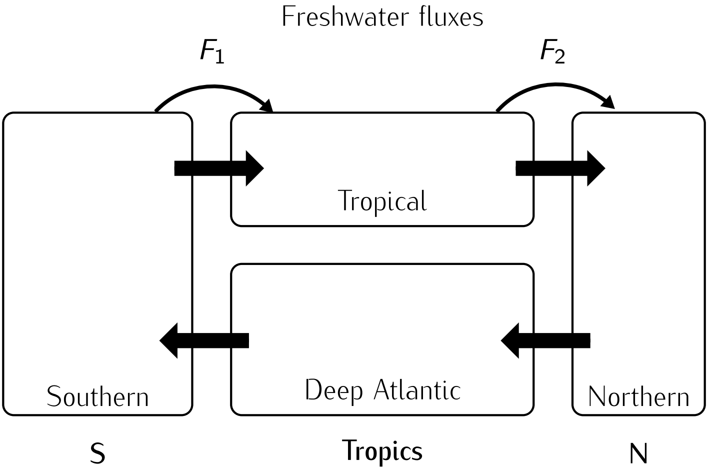

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The remaining variables are defined as follows:

- 'Overturning': $m = k\left[\beta(S_2 - S_1) - \alpha(T_2 - T_1)\right]$
- Individual coupling constants: $\lambda_i = \dfrac{\Gamma}{c\rho_0 z_i}$

where

k : Empirical flow constant

α : Thermal expansion coefficient

β : Haline expansion coefficient

c : Specific heat capacity of sea water

z_i : Depth of box i

Γ : Thermal coupling

Four-box model - Zickfield et al (2004)

The 'overturning' m responds mainly to

- the freshwater flux from the southern box into the tropical box F_1
- thermal coupling Γ (radiative relaxation and atmospheric heat diffusion)

For present day climate, there are two possible equilibria:

R_1 : $m > 0$ vigorous overturning (ideal)

R_2 : $m \leq 0$ reverse mode (water masses in southern box sink and northern box up-wells)

We treat m as a function of F_1 and Γ

$$x = (F_1, \Gamma)$$
$$m(t) = s(x, t), \ \ t \geq 0$$
$$m_{eq} = \lim_{m \to \infty} m(t)$$

Representing beliefs about f using emulators

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- An emulator is a probabilistic belief specification used to express uncertainty judgements for f. Often emulators are constructed as:

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

where $B = \{\beta_{ij}\}$ are unknown scalar, g_{ij} are known deterministic functions of x, and $u(x)$ is a stationary stochastic process (e.g. a Gaussian process).

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$$E_z(y) = E(y) + Cov(y,z)Var^{-1}(z)(z - E(z))$$
$$Var_z(y) = Var(y) - Cov(y,z)Var^{-1}(z)Cov(z,y)$$

Classification and Emulation

Setup

- Let s be a simulator such that $s : X \to Y$
- There are two qualitatively different regimens for s, R_1 and R_2 (e.g. collapse/non-collapse)
- Each regimen maps back to a subspace in X, RX_1 and RX_2

Process

- Choose a training sample $X_t = \{\mathrm{x}_1, \ldots, \mathrm{x}_\mathrm{m}\}$, run s for all x in X_t
- Separate X_t into $X_{t,1}$ and $X_{t,2}$ depending on regimen
- Construct a probabilistic classifier, $P(x \in R_1)$, based on the training sample
- Divide the input space X into 3 regions, RX_1, RX_2 and RX_0, depending on whether the classifier assigns high, low or medium probability that $\mathrm{x} \in R_1$, for each $\mathrm{x} \in X$.
  - $f_1(\mathrm{x})$ for $\mathrm{x} \in RX_1^* = RX_1 \cup RX_0$
  - $f_2(\mathrm{x})$ for $\mathrm{x} \in RX_2^* = RX_2 \cup RX_0$
- Increase training sample if $X_{t,1}$ or $X_{t,2}$ are small

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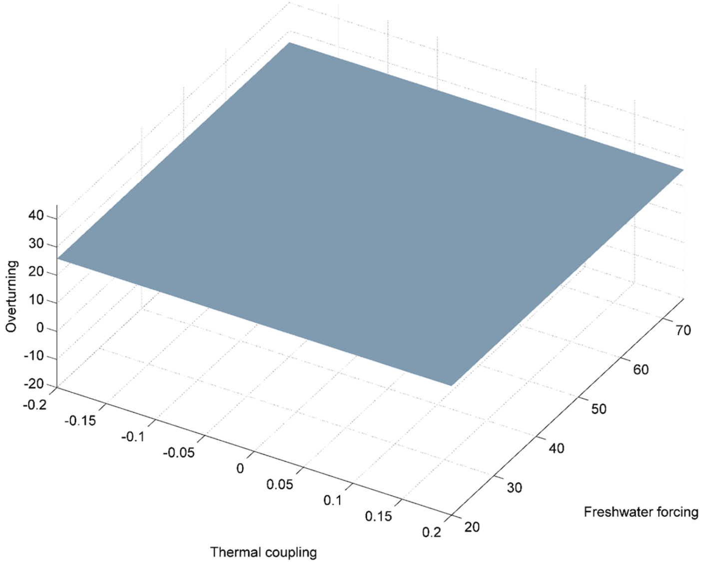
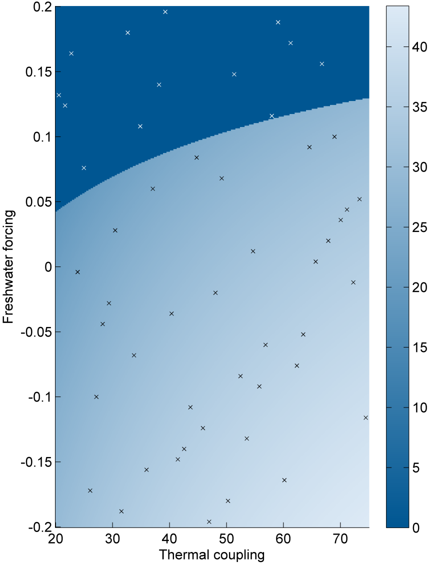


Training set

40 samples: 27 in R_1 (non-collapse) and 13 in R_2 (collapse)



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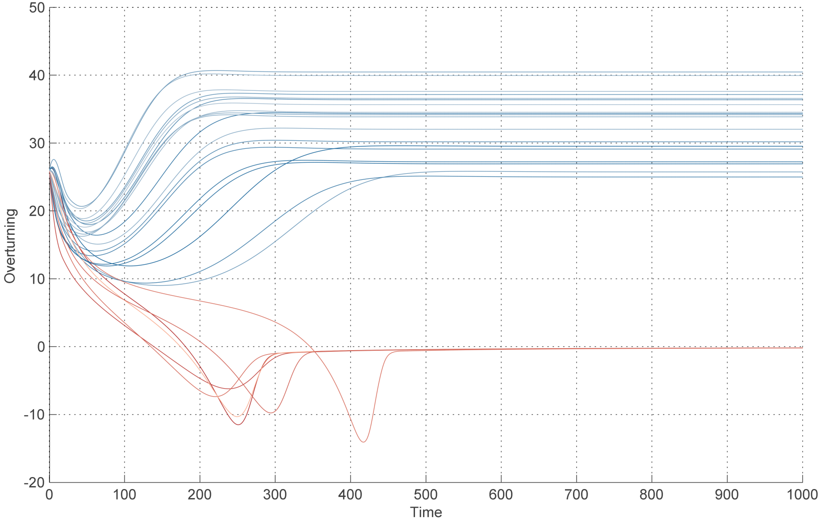
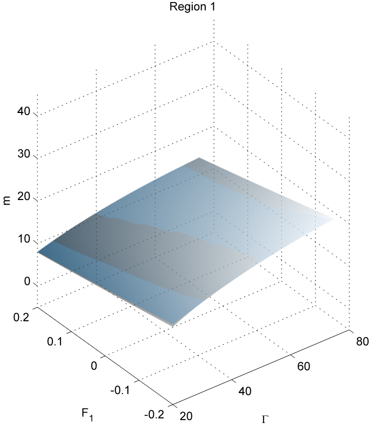
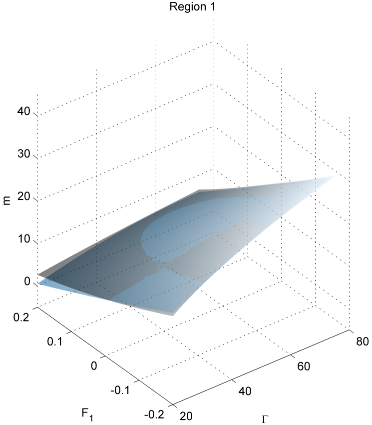


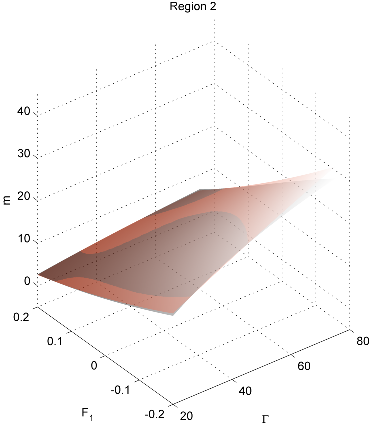
Posterior mean surfaces at $t = 40$



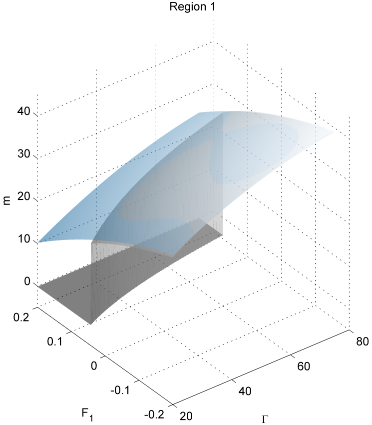
At each time t, the simulator surfaces are smooth within each region, including equilibrium. So we build the emulators $f_i(x, t)$, for a given time t, such that $f_i(x, t) \sim GP(m_i(x), \Sigma_i(x))$ where m_i is a quadratic polynomial and Σ_i is a squared-exponential covariance function.

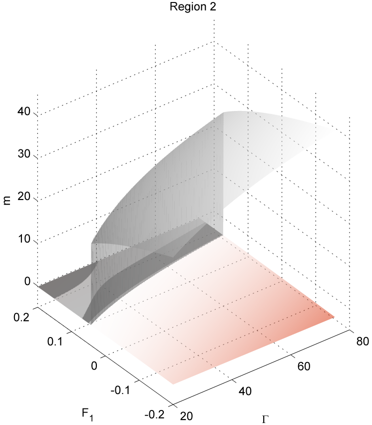
Posterior mean surfaces at $t = 90$



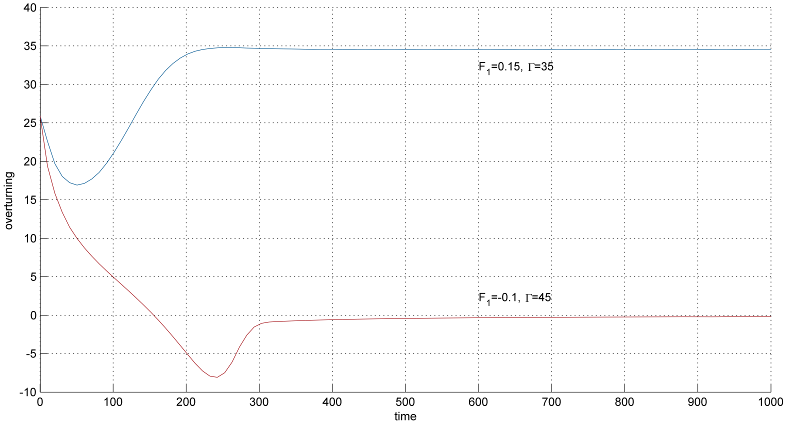


Posterior mean surfaces at equilibrium





Two test samples



Implausibility measures

- The implausibility $I_{(i)}(x)$ at any input x for the i-th output is given by

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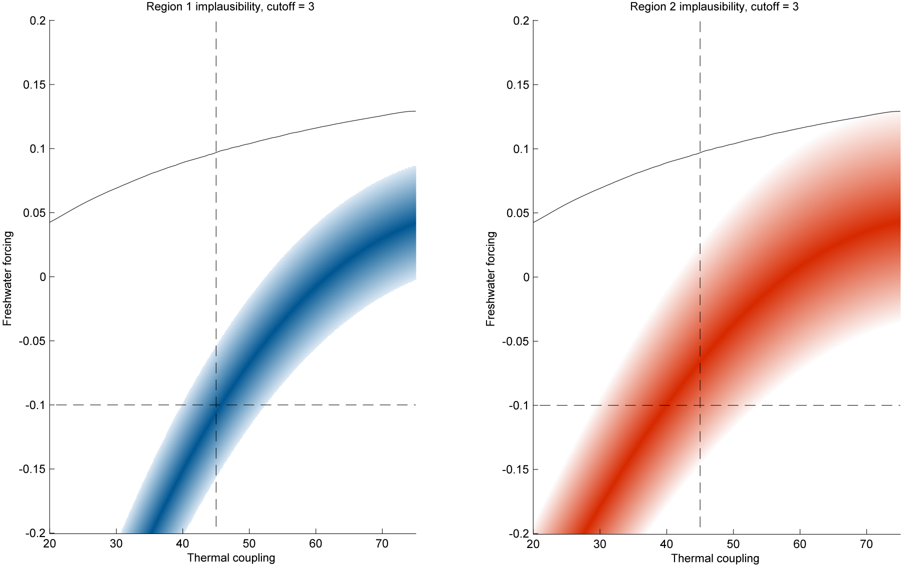
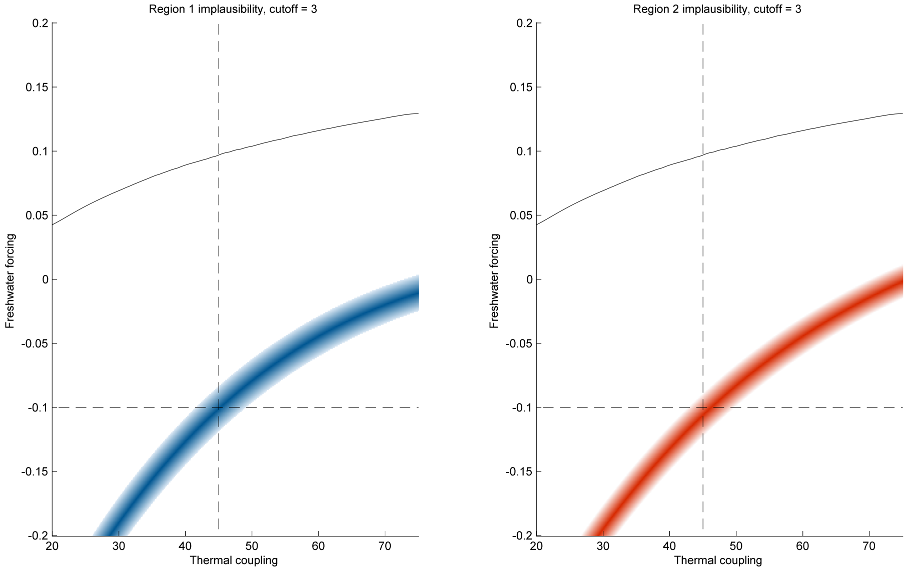
- Large values of $I_{(i)}(x)$ imply highly unlikely matches between model output and observed data at input x. However, small values do not imply good matches.
- Cutoff criteria: $I_M(x) = max_i I_{(i)}(x) < c_M$. The cutoff c_M is often set based on Pukelsheim's 3-sigma rule.

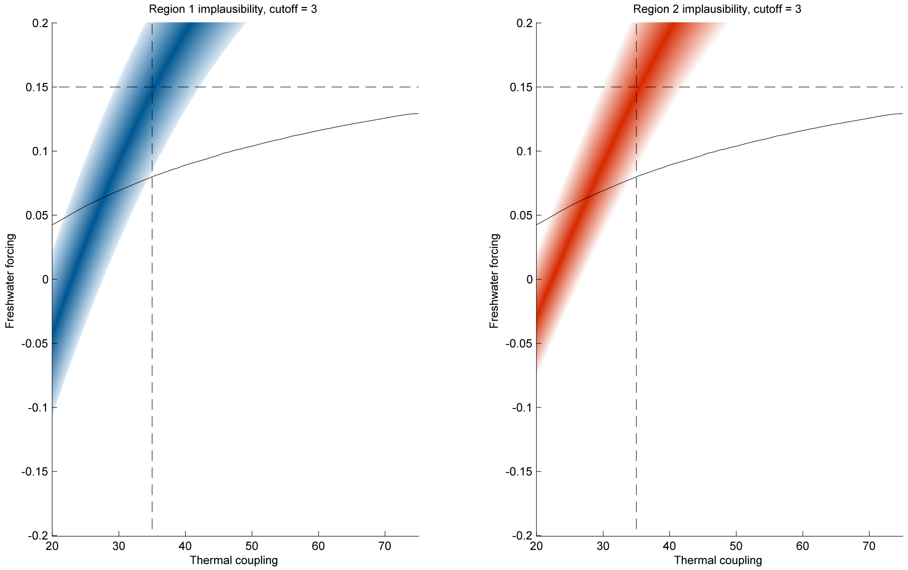
Observe at $t = 40$, find plausible regions for sample 1



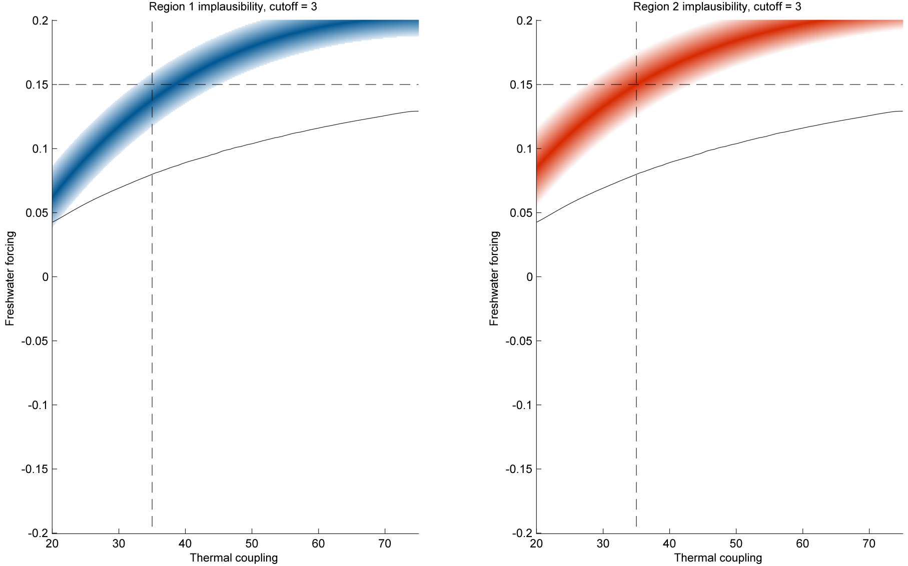
Observe at $t = 90$, find plausible regions for sample 1



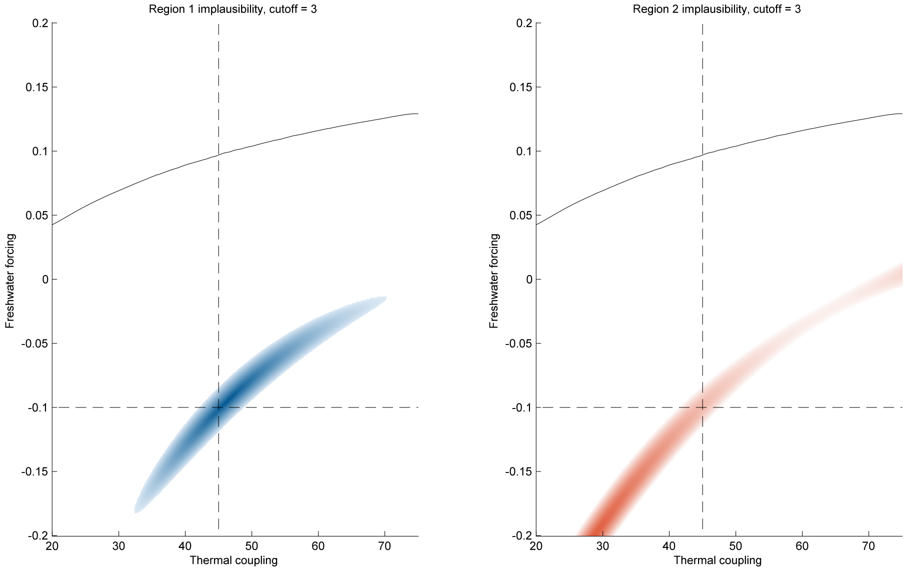
Observe at $t = 40$, find plausible regions for sample 2



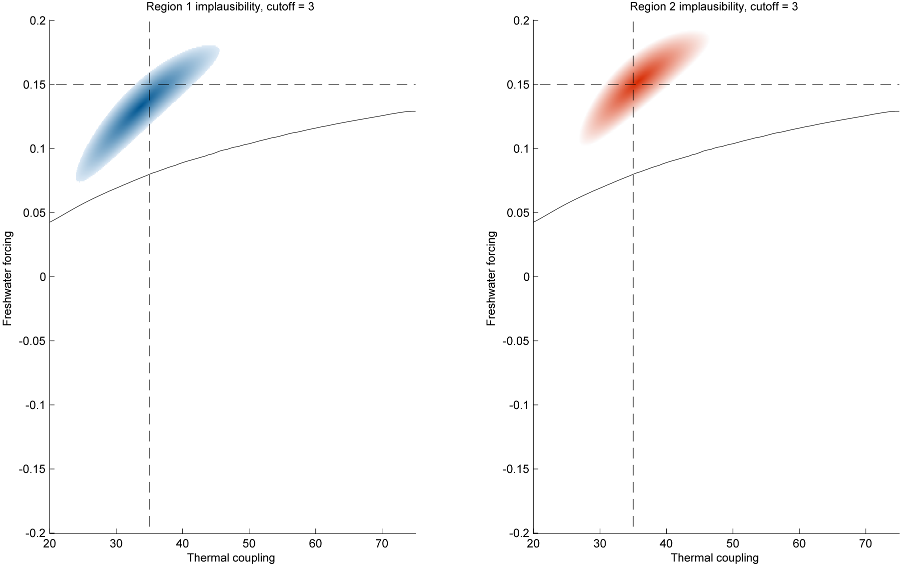
Observe at $t = 90$, find plausible regions for sample 2



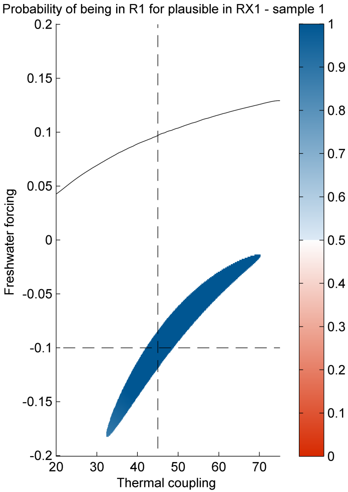
Joint emulation for $t = 40$ and $t = 90$, sample 1

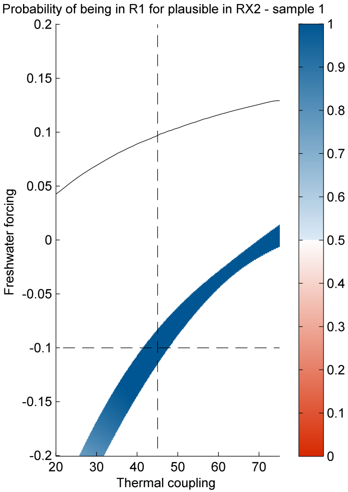


Joint emulation for $t = 40$ and $t = 90$, sample 2

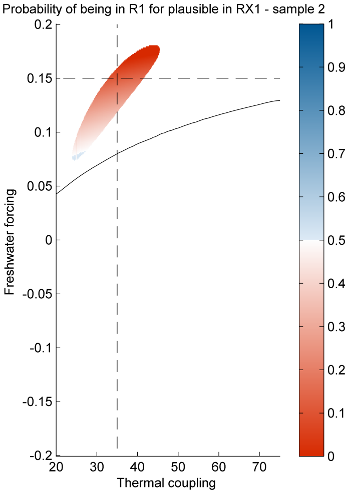


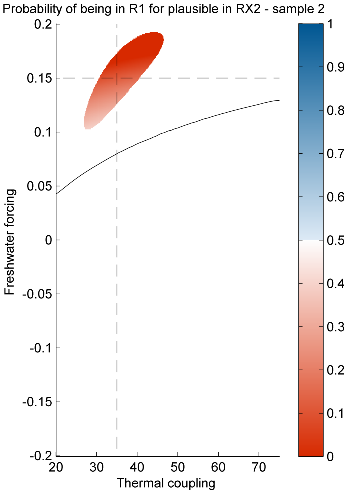
Probability maps for sample 1



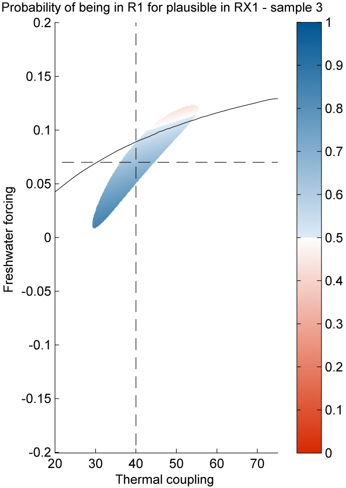


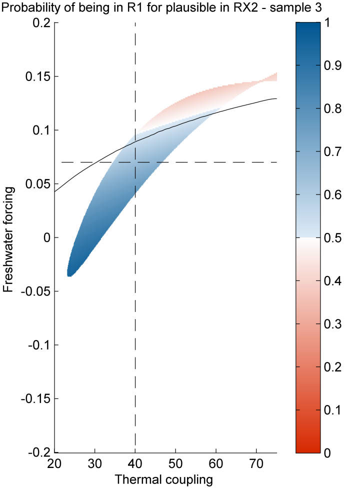
Probability maps for sample 2



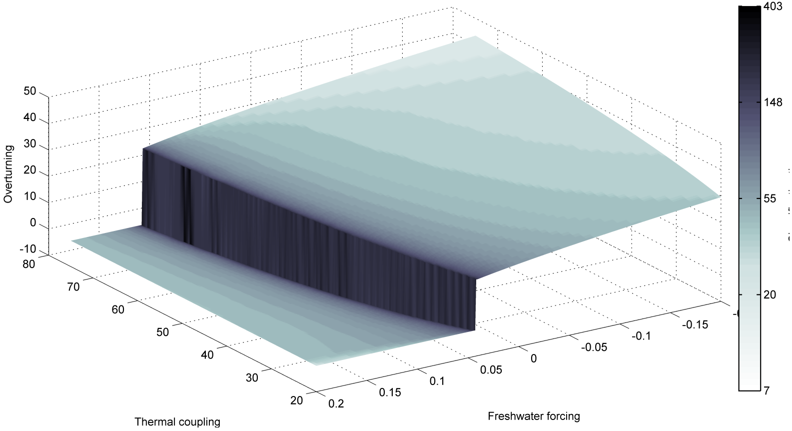


Probability maps for sample near boundary

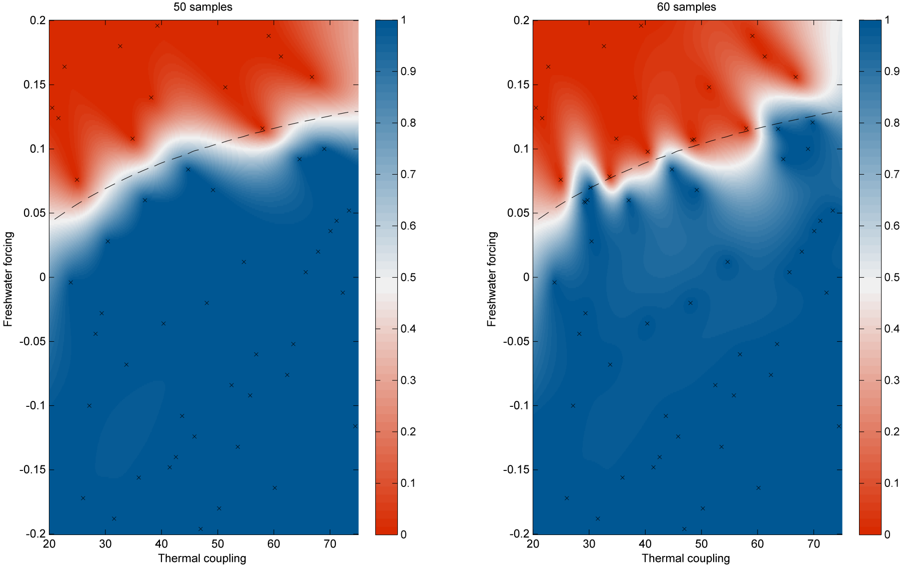




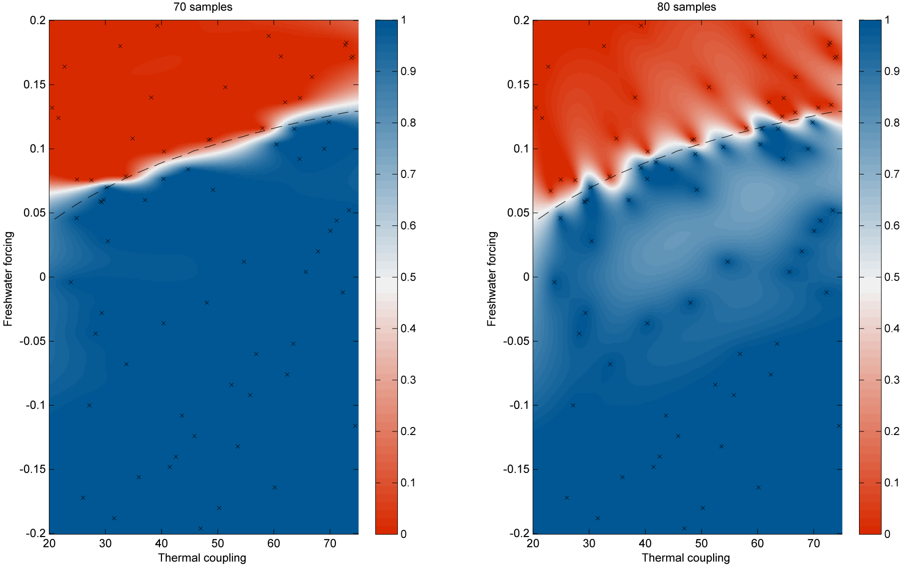
Classification time by region elimination



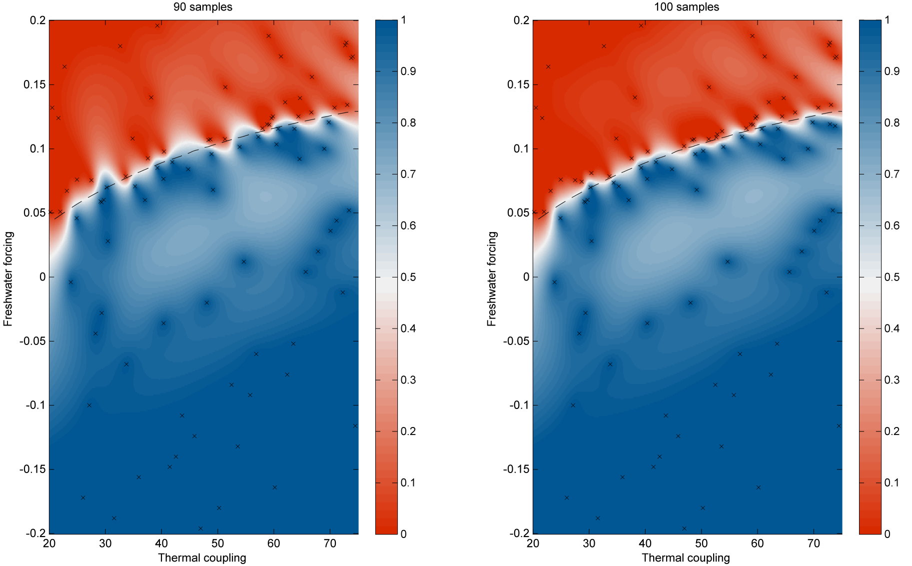
Boundary emulation



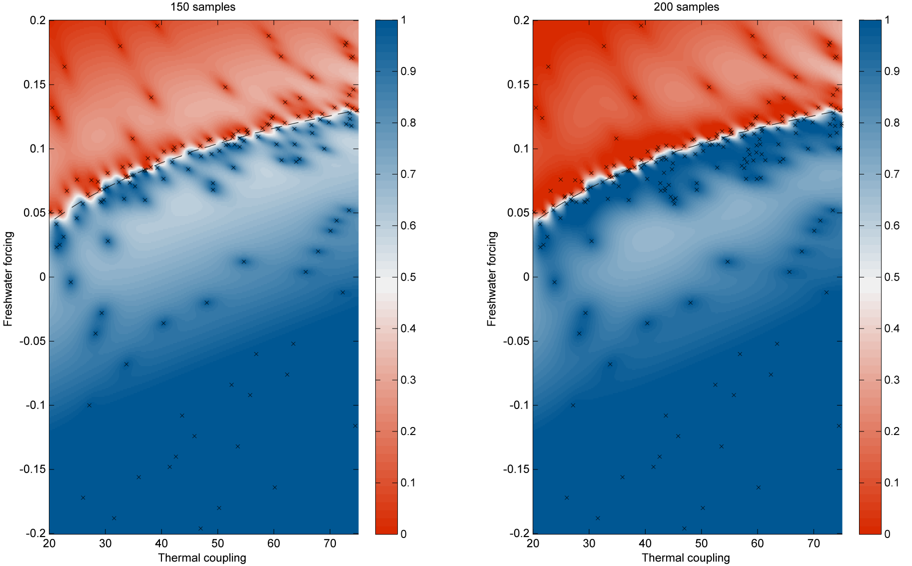
Boundary emulation



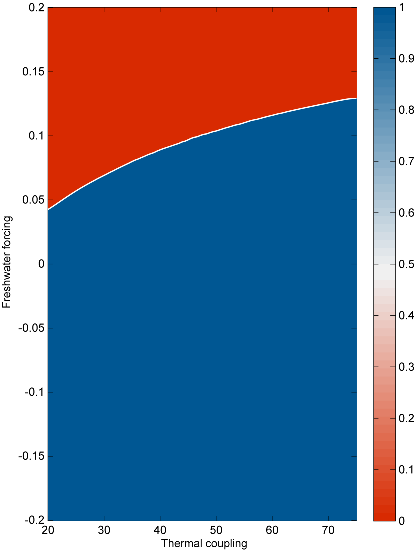
Boundary emulation



Boundary emulation



Boundary emulation



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