History matching of complex infectious disease models using emulation

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Joint work with: I.Vernon, N.McCreesh, TJ McKinley, J.Oakley, R.Nsubuga, M.Goldstein and R.White

Outline

- What is calibration?
- The challenge.
- History matching.
- Emulation.
- Sources of uncertainty.
- Implausibility.
- Case study.
- Conclusion.

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Calibration of computer models

Simulator

A simulator is a computer model that describes a physical process.

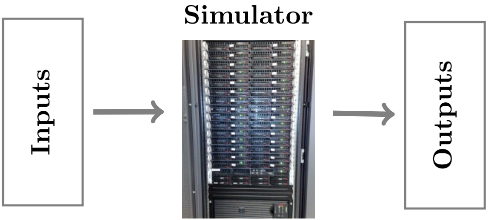
Calibration of computer models

Simulator

Inputs →

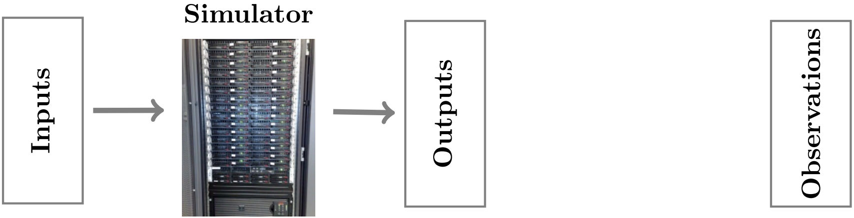
It has a number of inputs...

Calibration of computer models



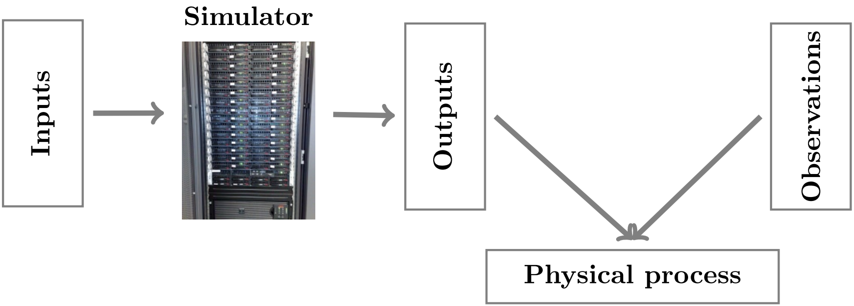
...and a number of outputs.

Calibration of computer models



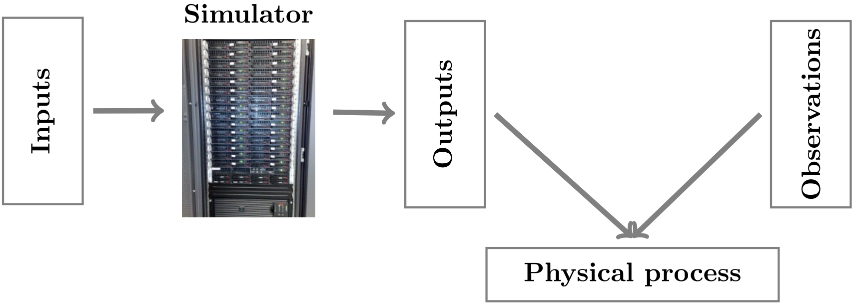
Some observations of the physical process are often available...

Calibration of computer models



... which are measurements of the same physical process the simulator tries to describe.

Calibration of computer models

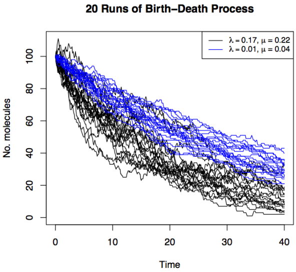


Calibration objective:

To find a set of input values so that the simulator represents best the physical process as this is described by observations.

Why Calibrate?

- Learn model parameters:
  - e.g. the decay rate of a birth-death process.



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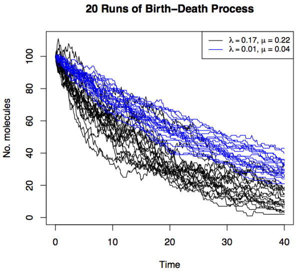
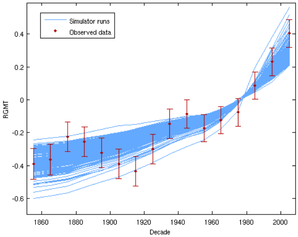


- Make predictions:
    - e.g. calibrate a climate model with observations to predict temperatures in the future.



The 'Mukwano' simulator

- A dynamic, stochastic, individual based model that simulates heterosexual sexual partnerships and HIV transmission.
- 22 inputs inc. contact rates, concurrency parameters, relationship duration, 2 sexual activity groups (high/low), 2 concurrency groups (high/low), 3 discrete behaviour periods.
- 18 outputs inc. population size, HIV prevalence, prevalence of men and women in long/short duration partnerships with one or more partners.
- Run time varied from 10 mins to >3 hours for 1 simulator run.
- Scenarios investigated were based on McCreesh 2012[1].

[1] McCreesh et al. 'Exploring the potential impact of a reduction in partnership concurrency on HIV incidence in rural Uganda: a modelling study. Sex.Transmitted diseases, 39(6):407-413,2012

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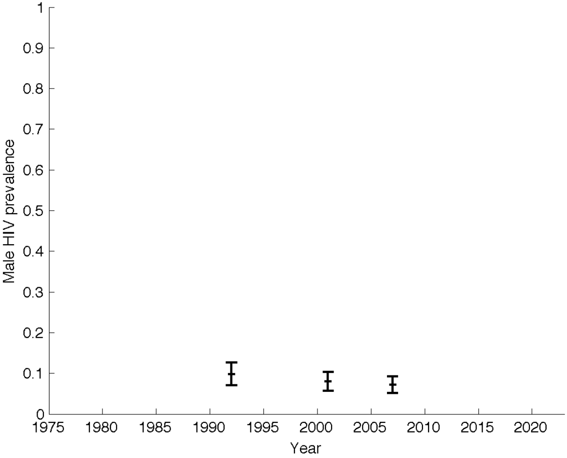
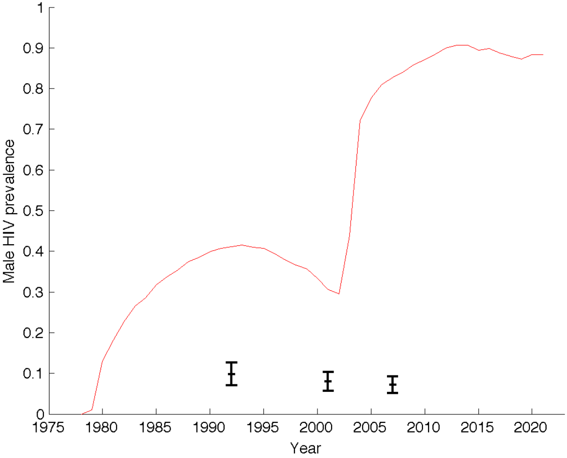
A manual approach

Suppose we want to match male HIV prevalences at 3 points in time.



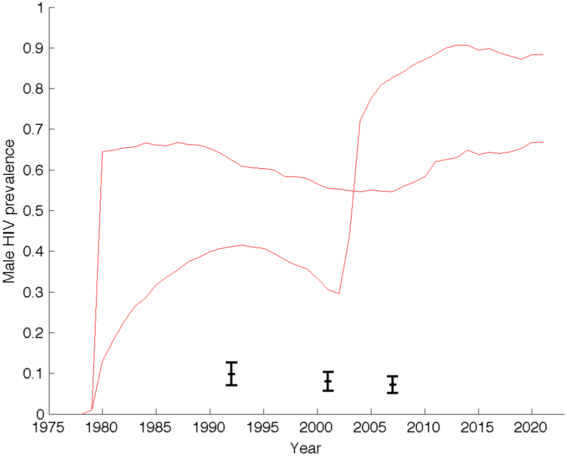
A manual approach

We choose a set of inputs run the model and...



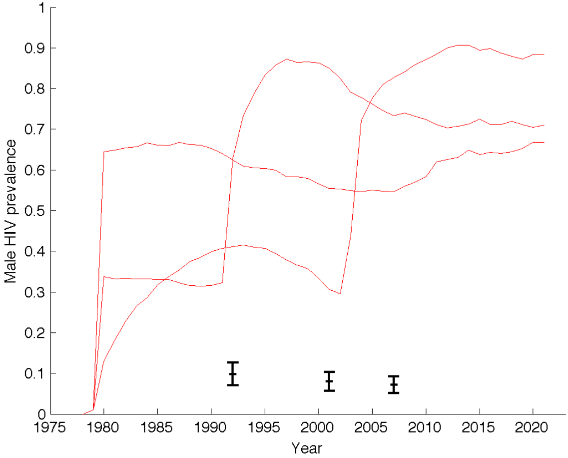
A manual approach

...we try again...



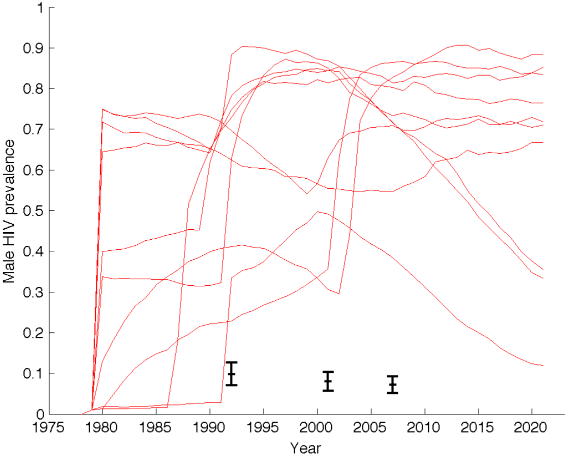
A manual approach

...and again...



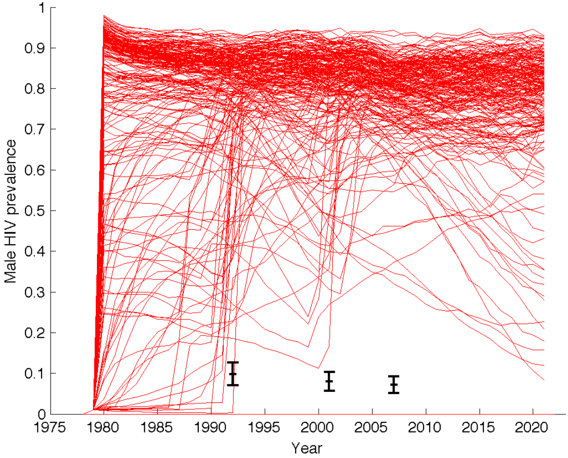
A manual approach

...after 10 runs...



A manual approach

...after 250 runs.



Existing calibration approaches

- Advanced statistical methodologies, such as MCMC and ABC, have been applied to the model calibration problem.
- Some of them require the model likelihood, which is unavailable for this model.
- Some require a large number of simulator evaluations.
- Most of them would struggle with the input/output dimensionality of this model.

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History matching

- Instead of looking for the best input values, history matching identifies and discards those unlikely to provide a match to the empirical data.

- The *implausible* input space is discarded in iterations known as waves.

- Not all inputs/outputs need to be considered at once.

- The simulator is often 'better behaved' in smaller areas of input space.

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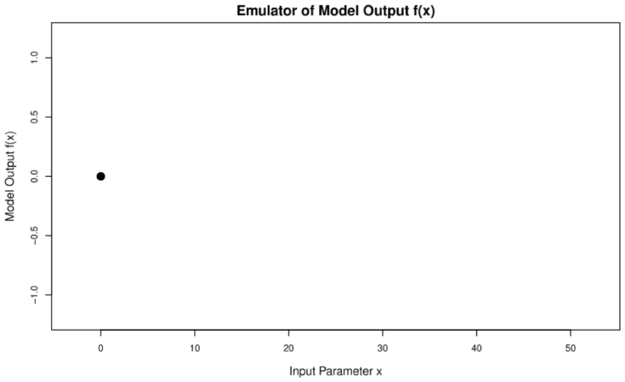
Emulation

- An emulator is a statistical representation of the simulator (meta-model).
- It does not substitute the simulator, but rather complements it.
- Once trained, emulators can predict the behaviour of the simulator, for any input parameters, almost instantaneously.
- They can simplify the calibration, uncertainty and sensitivity analysis of very complex models.
- Emulators can be built using Gaussian Processes (GP).
- The MUCM Toolkit is a good reference point for the emulation technology.

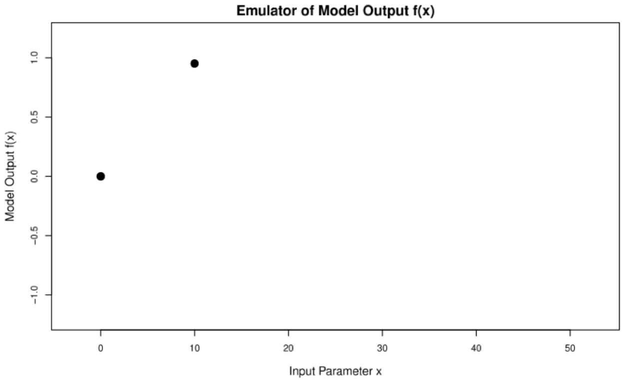
An emulator example

Suppose we want to emulate the function $f(x) = \sin(x)$



An emulator example

We only have a discrete number of model runs.



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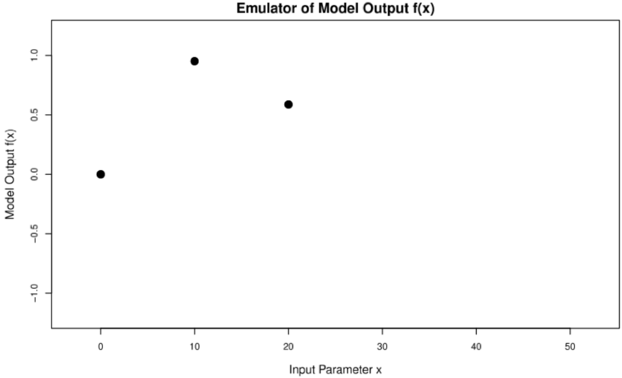

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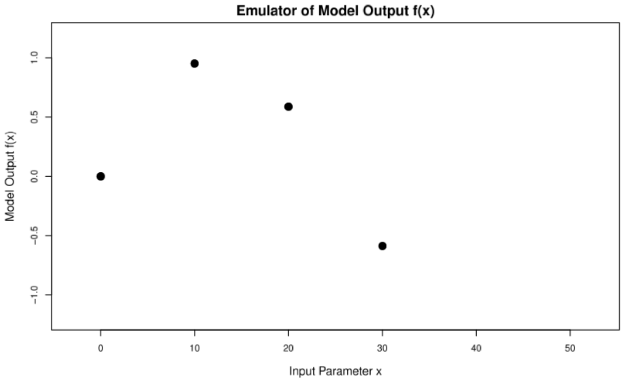

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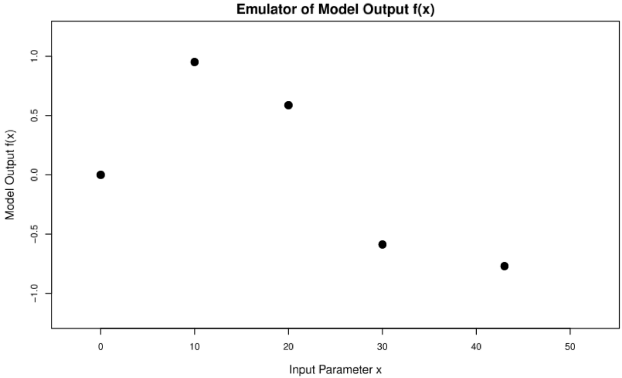

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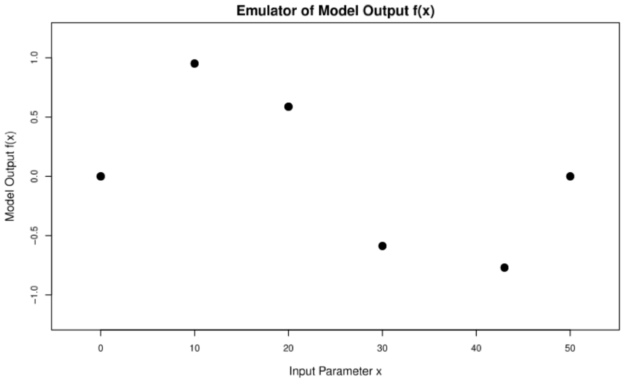
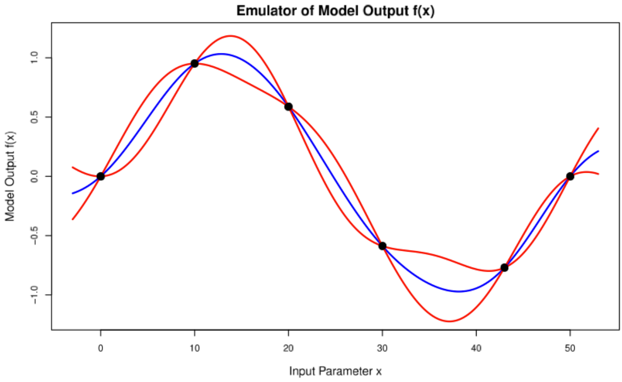
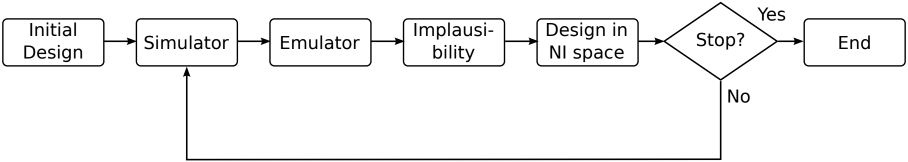


An emulator example

The emulator gives a posterior distribution for the model output, conditioned on the model runs we have seen so far.

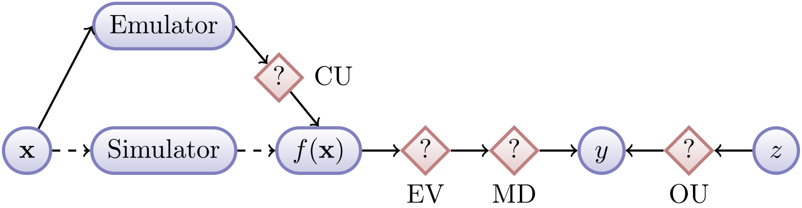


Workflow



The above schematic describes a history matching workflow.

Uncertainty structure



z : Observations

y : Physical process

$f(\mathbf{x})$: Simulator's output

$\mathbf{x}$: Simulator's input

OU: Observation Uncertainty

MD: Model Discrepancy

EV: Ensemble Variability

CU: Code Uncertainty

The implausibility measure

- The implausibility measure compares how far the model output is from the data for a given value of the input $\mathbf{x}$ taking into account all the uncertainties.

$$I(\mathbf{x}) = \frac{|z - \mathrm{E}^*[g(\mathbf{x})])|}{(V_o + V_c(\mathbf{x}) + V_s + V_m)^{1/2}}$$

- A large value of $I(\mathbf{x})$, indicates that $\mathbf{x}$ is unlikely to result in a good match between the model and the data.
- A small value of $\mathbf{x}$ does **not** imply that $\mathbf{x}$ is good! We do not know yet.
- The magnitude of $I(\mathbf{x})$ is often judged based on Pukelsheim's 3σ rule.
- The key point is that the emulator posterior mean $\mathrm{E}^*[g(\mathbf{x})]$ and variance $V_c(\mathbf{x})$ can be evaluated instantaneously.

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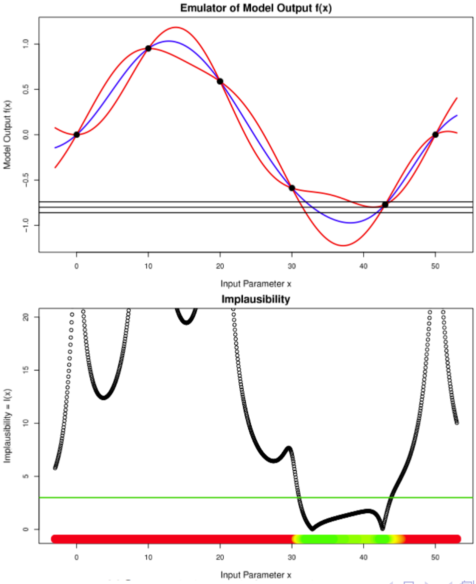
An example



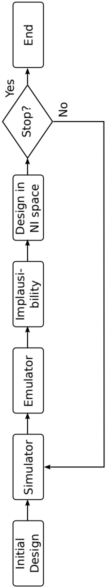
Emulator of Model Output f(x)
Model Output f(x)
1.0
0.5
0.0
-0.5
-1.0
0
10
20
30
40
50
Input Parameter x
Implausibility
Implausibility = I(x)
20
15
10
5
0
0
10
20
30
40
50
Input Parameter x

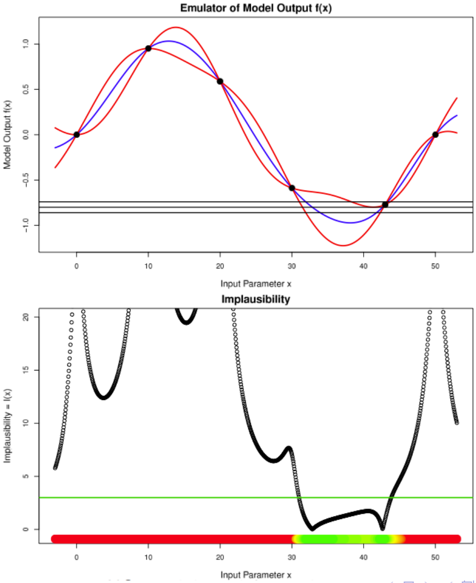
Iterative refocussing

The strength of history matching lies in that it can iteratively reduce the input space:

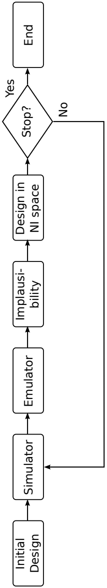
- Design a set of runs over the non-implausible region $\mathcal{X}_j$.
- Construct new emulators for $g(x)$ only over this region $\mathcal{X}_j$.
- Evaluate the new implausibility function $I_j(x)$ over $\mathcal{X}_j$.
- Define a new (reduced) non-implausible region $\mathcal{X}_{j+1}$ which should satisfy $\mathcal{X}_{j+1} \in \mathcal{X}_j$.
- Continue until a) we run out of computational resources or b) the emulators are sufficiently accurate compared with the other uncertainties present (model and observation errors).

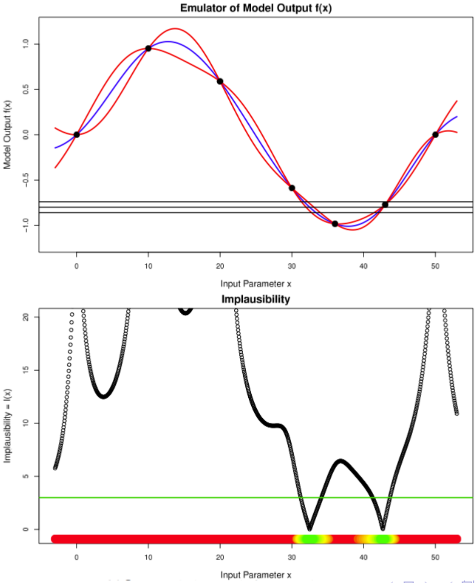
Iterative refocussing - wave 1



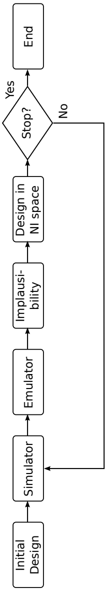


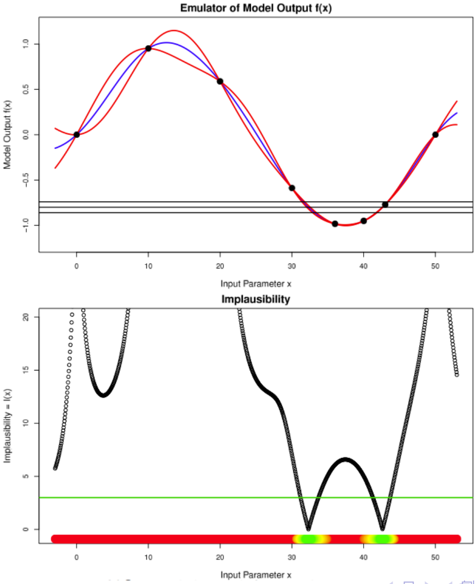
Iterative refocussing - wave 2



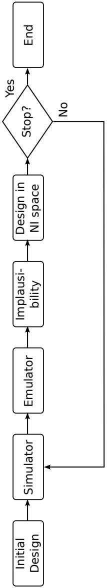


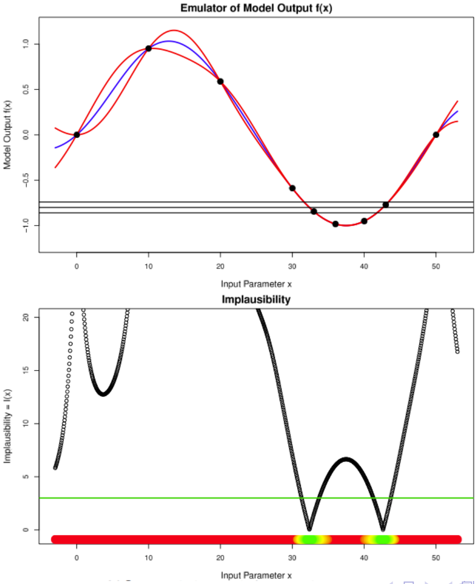
Iterative refocussing - wave 3





Iterative refocussing - wave 4





Calibration of the Mukwano simulator

- We will now present results from applying the history matching methodology to the Mukwano simulator.
- The empirical data were provided from a rural general population cohort in south west Uganda.
- We calibrate 22 inputs using 18 outputs.
- We start by running the simulator 100 times at each of the 220 input combinations (22000 runs in total).
- The exact input locations were selected using a (space filling) Latin hypercube design.
- The input ranges were suggested by our model experts.

List of inputs (1)

	Min.	Max.
Proportion of men in the high sexual activity group	0.01	0.5
Proportion of women in the high sexual activity group	0.01	0.5
Mixing by activity group [ϵ]	0	1
High activity contact rate (risk behaviour 1) [partners/yr]	0	10
Low activity contact rate (risk behaviour 1) [partners/yr]	0	2
Start year for risk behaviour 2	1986	1992
High activity contact rate (risk behaviour 2) [partners/yr]	0	10
Low activity contact rate (risk behaviour 2) [partners/yr]	0	2
Start year for risk behaviour 3	1998	2002
High activity contact rate (risk behaviour 3) [partners/yr]	0	10
Low activity contact rate (risk behaviour 3) [partners/yr]	0	2
Mean HIV transmission probability per sex act during primary stage of infection (mean of male to female and female to male transmission probabilities)	0	1
Ratio of male to female/female to male transmission probabilities	1	3

List of inputs (2)

	Min.	Max.
Proportion of low activity men in high concurrency group	0	1
Proportion of low activity women in high concurrency group	0	1
Male concurrency parameter in high concurrency group (risk behaviour 1)	0	1
Female concurrency parameter in high concurrency group (risk behaviour 1)	0	1
Male concurrency parameter in high concurrency group (risk behaviour 2)	0	1
Female concurrency parameter in high concurrency group (risk behaviour 2)	0	1
Male concurrency parameter in high concurrency group (risk behaviour 3)	0	1
Female concurrency parameter in high concurrency group (risk behaviour 3)	0	1
Duration of long-duration partnerships [years]	5	20

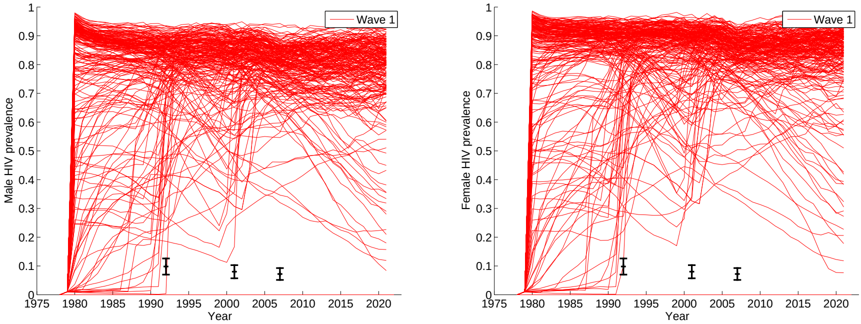
List of outputs (1)

	Min.	Max.
Population size in 2008 (male)	2986	3650
Population size in 2008 (female)	3374	4124
Average male partnership incidence in 2008 (partners/year)	0.4	0.489
HIV prevalence in 1992 (male)	0.084	0.112
HIV prevalence in 1992 (female)	0.096	0.124
HIV prevalence in 2001 (male)	0.07	0.09
HIV prevalence in 2001 (female)	0.083	0.107
HIV prevalence in 2007 (male)	0.06	0.084
HIV prevalence in 2007 (female)	0.093	0.119

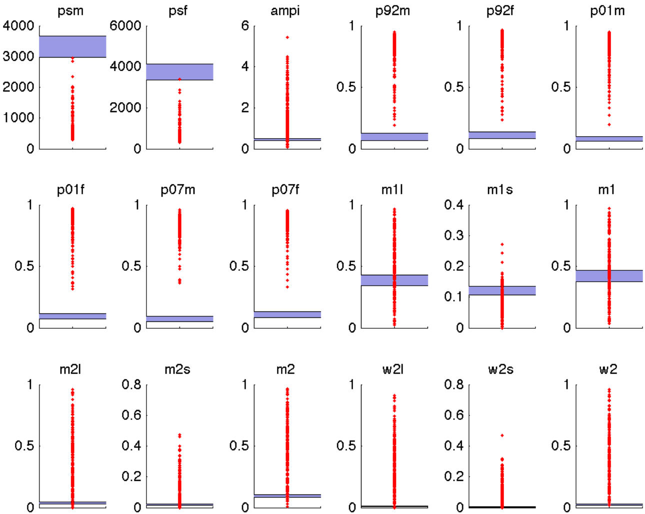
List of outputs (2)

	Min.	Max.
Point prevalence of men with 1 long duration partnership in 2008 (%)	34.62	42.31
Point prevalence of men with 1 short duration partnership in 2008 (%)	10.86	13.27
Point prevalence of men with 1 partnership (either type) in 2008 (%)	37.83	46.24
Point prevalence of men with 2+ long duration partnerships in 2008 (%)	3.38	4.13
Point prevalence of men with 2+ short duration partnerships in 2008 (%)	1.69	2.07
Point prevalence of men with 2+ partnerships (any combination) in 2008 (%)	8.66	10.59
Point prevalence of women with 2+ long duration partnerships in 2008 (%)	0.85	1.03
Point prevalence of women with 2+ short duration partnerships in 2008 (%)	0.42	0.52
Point prevalence of women with 2+ partnerships (any combination) in 2008 (%)	2.17	2.65

Results: male and female HIV prevalence in wave 1



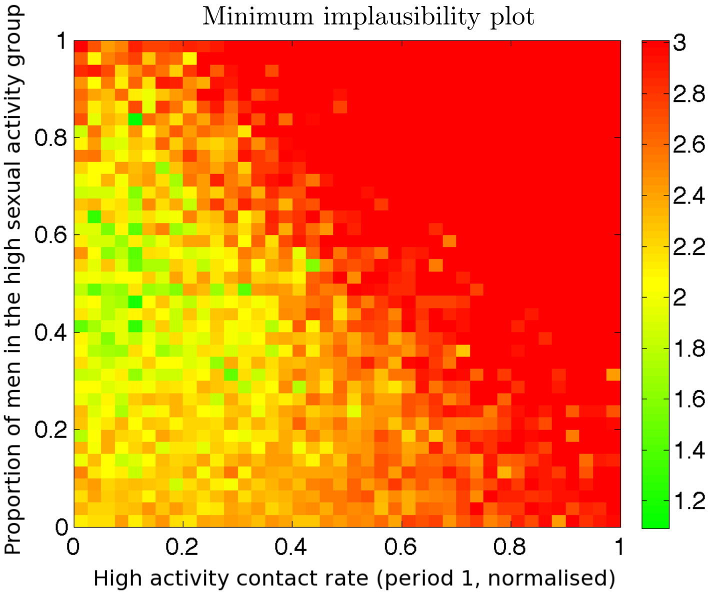
Results: best runs per scenario in wave 1



Visualising the implausible space

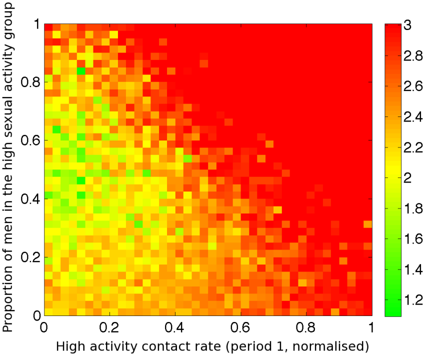
The implausible space can be visualised with minimum implausibility and optical depth plots.

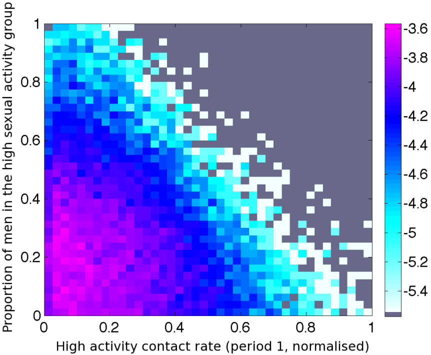
Visualising the implausible space



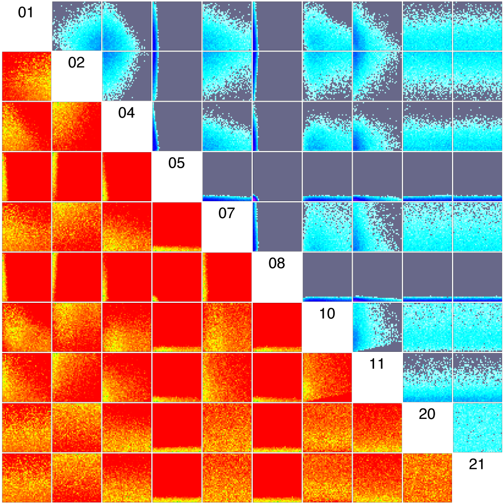
Visualising the implausible space

Optical depth plot



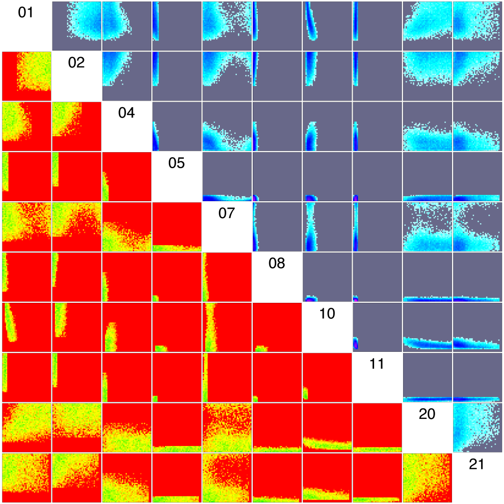


Space reduction wave 1



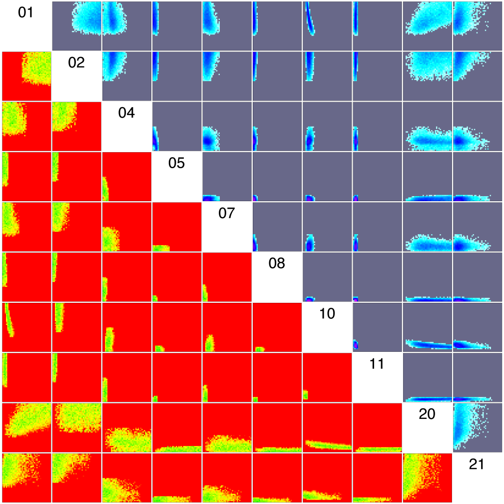
No.	Input description
01	Proportion of men in high sexual activity group
02	Proportion of women in high sexual activity group
04	High activity contact rate (period 1) [partners/yr]
05	Low activity contact rate (period 1) [partners/yr]
07	High activity contact rate (period 2) [partners/yr]
08	Low activity contact rate (period 2) [partners/yr]
10	High activity contact rate (period 3) [partners/yr]
11	Low activity contact rate (period 3) [partners/yr]
20	Male concurrency parameter in high conc. group (period 3)
21	Female concurrency parameter in high concurrency group (period 3)

Space reduction wave 4



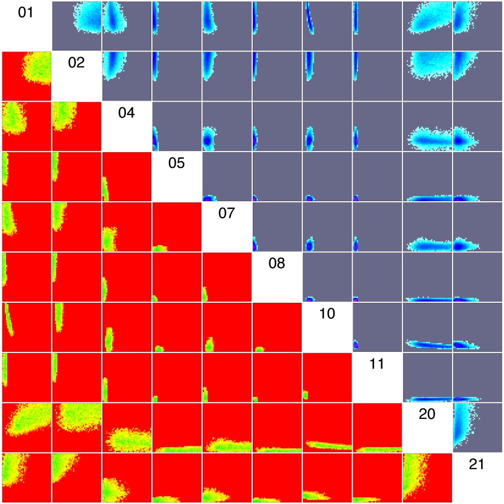
No.	Input description
01	Proportion of men in high sexual activity group
02	Proportion of women in high sexual activity group
04	High activity contact rate (period 1) [partners/yr]
05	Low activity contact rate (period 1) [partners/yr]
07	High activity contact rate (period 2) [partners/yr]
08	Low activity contact rate (period 2) [partners/yr]
10	High activity contact rate (period 3) [partners/yr]
11	Low activity contact rate (period 3) [partners/yr]
20	Male concurrency parameter in high conc. group (period 3)
21	Female concurrency parameter in high concurrency group (period 3)

Space reduction wave 7



No.	Input description
01	Proportion of men in high sexual activity group
02	Proportion of women in high sexual activity group
04	High activity contact rate (period 1) [partners/yr]
05	Low activity contact rate (period 1) [partners/yr]
07	High activity contact rate (period 2) [partners/yr]
08	Low activity contact rate (period 2) [partners/yr]
10	High activity contact rate (period 3) [partners/yr]
11	Low activity contact rate (period 3) [partners/yr]
20	Male concurrency parameter in high conc. group (period 3)
21	Female concurrency parameter in high concurrency group (period 3)

Space reduction wave 9



No.	Input description
01	Proportion of men in high sexual activity group
02	Proportion of women in high sexual activity group
04	High activity contact rate (period 1) [partners/yr]
05	Low activity contact rate (period 1) [partners/yr]
07	High activity contact rate (period 2) [partners/yr]
08	Low activity contact rate (period 2) [partners/yr]
10	High activity contact rate (period 3) [partners/yr]
11	Low activity contact rate (period 3) [partners/yr]
20	Male concurrency parameter in high conc. group (period 3)
21	Female concurrency parameter in high concurrency group (period 3)

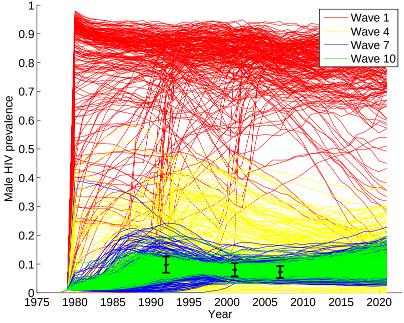
Overall space reduction

- Table shows the reduction of the non-implausible space in consecutive waves
- 'Uniform' sampling
- 'Rejection' sampling
- MCMC based sampling*

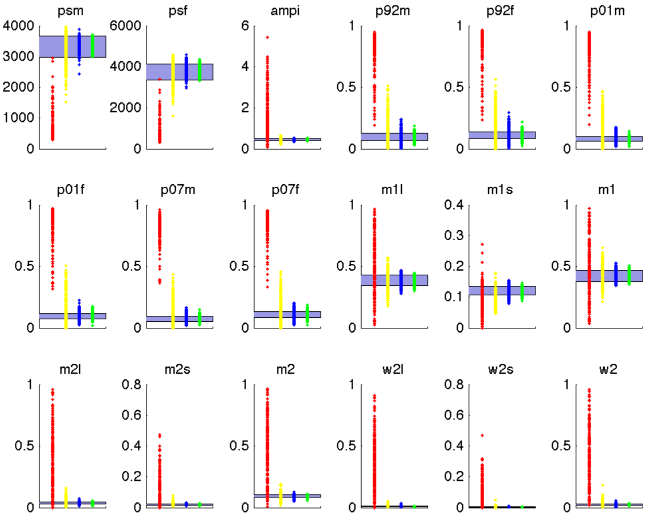
Wave 1	$4.0 \cdot 10^{-05}$
Wave 2	$1.5 \cdot 10^{-06}$
Wave 3	$4.1 \cdot 10^{-08}$
Wave 4	$2.2 \cdot 10^{-09}$
Wave 5	$2.5 \cdot 10^{-10}$
Wave 6	$8.6 \cdot 10^{-11}$
Wave 7	$5.2 \cdot 10^{-11}$
Wave 8	$2.0 \cdot 10^{-11}$
Wave 9	$1.3 \cdot 10^{-11}$

*Williamson, D and Vernon, I, *Efficient uniform designs for multi-wave computer experiments*, submitted 2013.

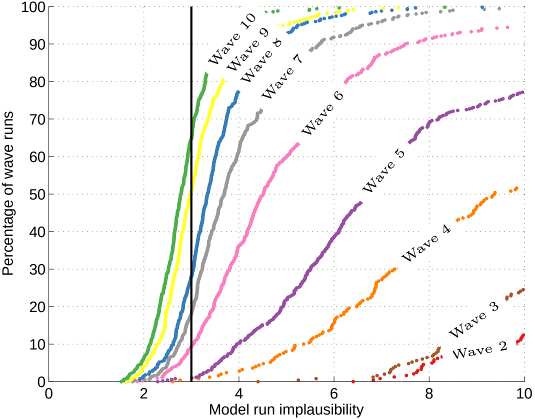
Results: male and female HIV prevalence in waves 1, 4, 7 and 10



Results: best runs per scenario in waves 1, 4, 7 and 10



Results: Implausibility of model runs



The diagram shows the implausibility of the *actual* simulator runs (no emulation involved)

$$I(\mathbf{x}) = \frac{|z - g(\mathbf{x}))|}{(V_o + V_m + V_s)^{1/2}}$$

Approximate posterior sampling

- Let $\{\mathbf{x}_{\mathrm{ni}}\}$ be the non-implausible samples from the last wave of history matching. We formulate the following proposal distribution:

$$P(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \mathrm{E}[\mathbf{x}_{\mathrm{ni}}], \kappa \mathrm{Var}[\mathbf{x}_{\mathrm{ni}}])$$

- We also define an approximate model likelihood that derives from the implausibility $I(\mathbf{x})$ and is given by

$$L(\mathbf{x}) = \mathcal{N}(z; \mathrm{E}^*[g(\mathbf{x})], V)$$

with $V = V_o + V_c(\mathbf{x}) + V_s + V_m$

- We first use the distribution $P(\mathbf{x})$ to propose a number of samples $\{\tilde{\mathbf{x}}\}$
- We then calculate a weight for each sample as $w(\tilde{\mathbf{x}}) = L(\tilde{\mathbf{x}})/P(\tilde{\mathbf{x}})$
- Finally, we draw the desired number of posterior samples $\mathbf{x_p}$ from the set of $\{\tilde{\mathbf{x}}\}$, with a probability defined by the weights $w(\tilde{\mathbf{x}})$

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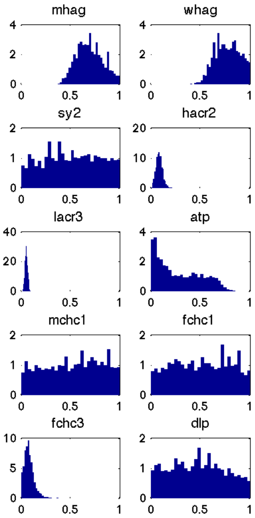
Results: approximate posterior sampling



Conclusion

- We presented an iterative method for the calibration of complex simulation models, based on emulators.
- We calibrated a dynamic, event-driven, individual-based stochastic HIV model, with 22 inputs and 18 outputs.
- The final system had a 65% probability of selecting a parameter set that fitted all 18 outputs and reduced the input space by a factor of 10^{-11}.
- Very effective in reducing the input space of slow and high dimensional models.
- Can be combined with other methods to produce posterior distributions.

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Thank you!