Multilevel Emulation and History Matching of EAGLE: an expensive hydrodynamical Galaxy formation simulation.

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PEN Emulator Workshop, 21st July, 2017

Joint work with: Richard G. Bower, Aaron Ludlow, Alejandro B Llambay, Dept. of Physics
With thanks to the VIRGO consortium

Outline

- The EAGLE model.
- The multilevel structure of EAGLE.
- Multilevel Emulation: taming heavy simulators.
- History Matching (provisional results)

- Andromeda Galaxy: closest large galaxy to our own milky way.
- Hubble Deep Field: covers approximately 2 millionths of the sky but contains thousands of galaxies.

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The EAGLE Model

- EAGLE (Evolution and Assembly of GaLaxies and their Environments) is a simulation aimed at understanding how galaxies form and evolve.
- See http://icc.dur.ac.uk/Eagle/ for details.
- It models the formation of structures in a cosmological volume of size (100 Megaparsecs)^3, approximately (326 million light-years)^3.
- This volume contains approximately 10,000 galaxies of the size of the Milky Way or bigger, enabling a comparison with detailed galactic surveys.
- The simulation starts soon after the Big Bang, when the Universe is still very uniform - no stars nor galaxies had formed yet.

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- Dark matter enables structures like galaxies to form, even while the Universe is expanding rapidly: gas falling into these dark matter structures cools and forms stars and hence galaxies.
- However core collapse supernovae (exploding massive stars), and Active Galactic Nuclei (bursting supermassive black holes), severely limit what fraction of the gas forms stars.
- Modelling these aspects accurately is key to produce a virtual universe that looks like the real one.
- The EAGLE simulation is one of the largest cosmological hydrodynamical simulations ever, using nearly 7 billion particles to model the physics.
- It took more than one and a half months of computer time on 4064 cores of the DiRAC-2 supercomputer in Durham (about 5 million hours of CPU time).

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- EAGLE has less flexibility than previous models, e.g. semi-analytic models such as Galform (17-20 input parameters), as it instead relies on fundamental physics to model many processes directly, without requiring many tuning parameters.
- However, it still has 7 uncertain input parameters x, that relate to the core collapse supernovae and supermassive black holes.
- EAGLE output $f(x)$ can be compared to a variety of observed galaxy data z: Stellar Mass Function, Galaxy Sizes, ...
- We have just been awarded 60 million hours of processor time in Switzerland (CSCS, via PRACE) to do a single run 15 times larger than the current volume.
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History Matching

- Primary Scientific Question: what is the region $\mathcal{X}$ of 7-dimensional input space that produces model outputs consistent with the observed data?
- We will use the computer model technique of “history matching" to identify $\mathcal{X}$ by cutting out implausible regions of input space (and find out whether $\mathcal{X}$ is empty: different from usual Bayesian calibration).
- This will involve emulation (of course) and the assessment of many relevant uncertainties (observation error, model discrepancy etc).
- Primary statistical question: we obviously cannot hope to cover 7-dimensional space with such a slow model, but how can we even emulate it?
- Thankfully, EAGLE has been set up to run at 4 levels of accuracy, with each level approximately 8 times faster than the previous level: we will hence setup multilevel emulators, and use these in the history match.

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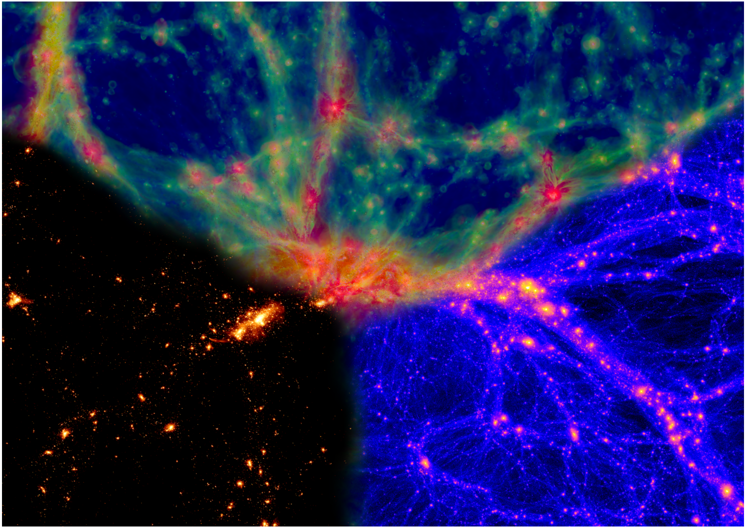
EAGLE Outputs

Gas Temperature



Visual spectrum

Dark Matter density

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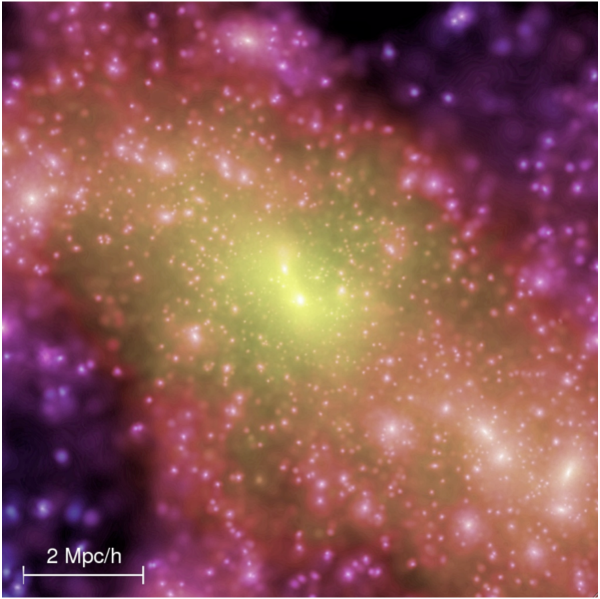

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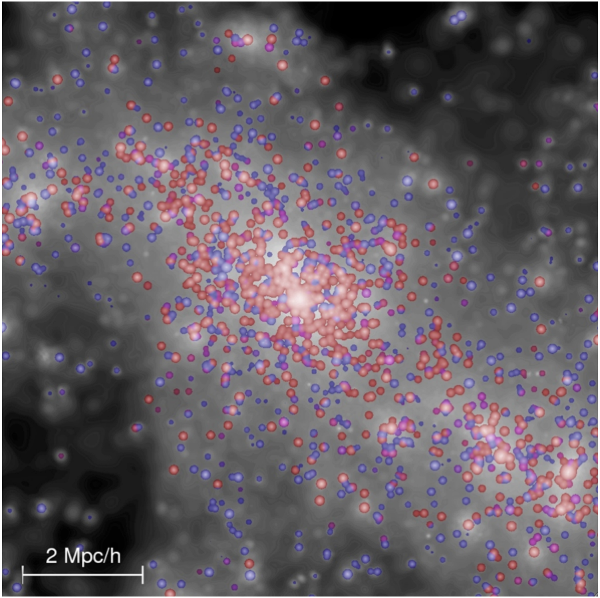
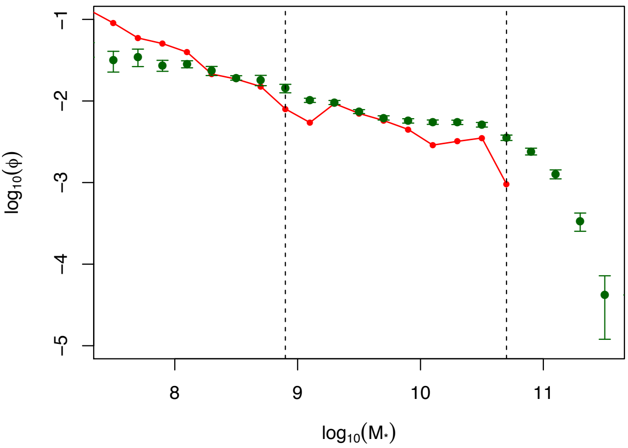


EAGLE Observed data Stellar Mass Function



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- Very important for any Galaxy simulation to match this data set.

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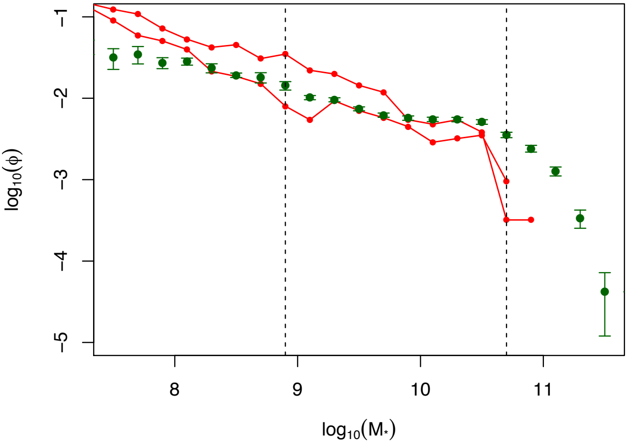

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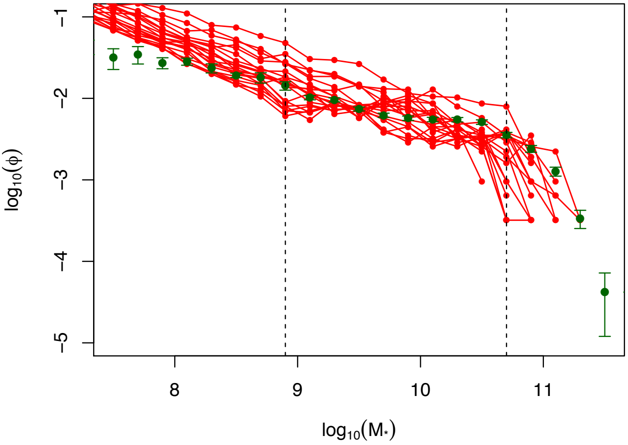

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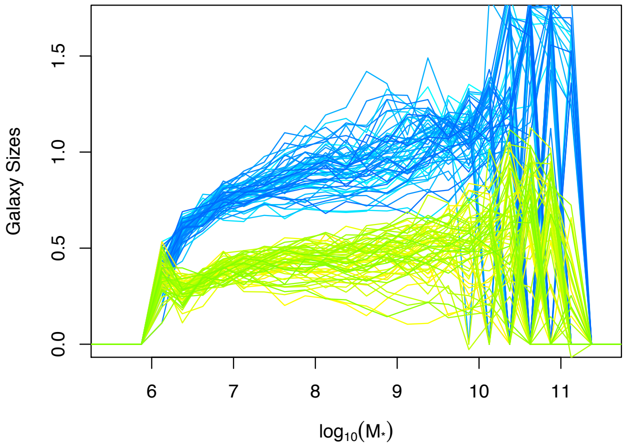
EAGLE Observed data Galaxy Sizes



- We have just begun the analysis of Galaxy sizes...

EAGLE Input Parameters

- To perform one run, we need to specify numbers for each of the following 7 inputs:

Input Parameter	min	max	Transform	Process
SNII_MinEnergyFraction	0.1	1.0	-	Supernova
SNII_MaxEnergyFraction	1.0	5.0	-	"
SNII_rhogas_power	0.1	3.0	-	"
SNII_rhogas_physdensnormfac	1	50	log_{10}	"
SNII_Width_logTvir_dex	0.1	3	log_{10}	"
BlackHoleViscousAlpha	10^3	10^8	log_{10}	Blackholes
BH_ConstantHeatTemp	10^8	10^9	log_{10}	"

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- However, thankfully EAGLE has been designed to run at 4 different levels of accuracy, with each level approximately 8 times faster than the previous one.
- These levels correspond to smaller volumes of the Universe:

Level	Volume$^{1/3}$	Approximate Evaluation Time
1	12.5 Mpc	1/512
2	25 Mpc	1/64
3	50 Mpc	1/8
4	100 Mpc	1

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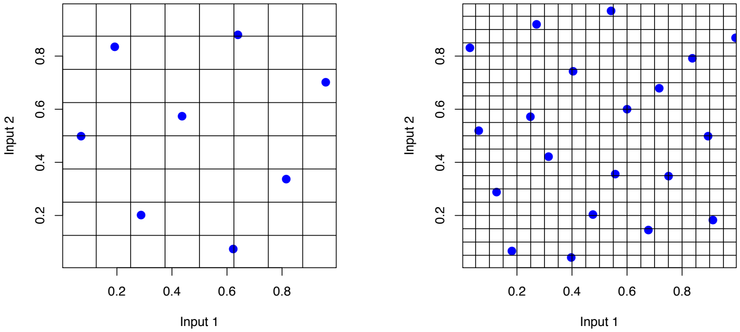

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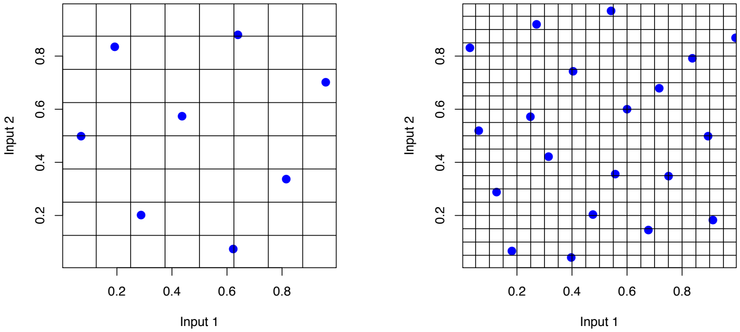

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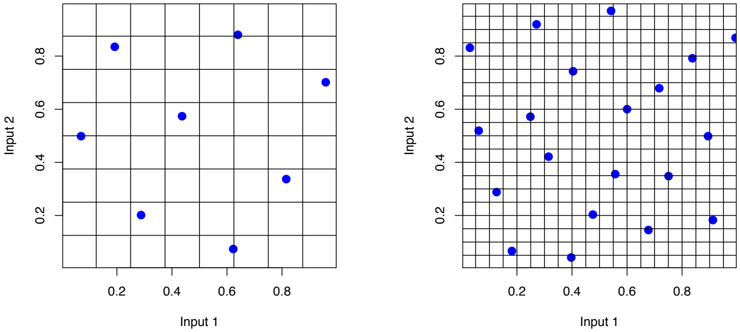

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Initial Design of EAGLE runs

- First Question: are the fast but noisy level 1 runs (at 12.5 Mpc), which we can run in 2 days on 32 processors, informative for higher levels at all?
- We constructed a 20 point LHC design, which was a) maxmin across the 7 inputs, b) maximin across 4 inputs thought to be strongest, and c) had no large holes in those 4 inputs.
- We ran this design at level 1 and at level 2 (each level 2 run takes about 8 days on 64 processors).
- Result: after smoothing, the level 1 runs are very informative for a subset of (low/medium mass) stellar mass function outputs: can use in history matching.
- We were then allowed to run 20, possibly followed by another 20, level 1 runs.
- We hence designed two more 20pt LHCs such that the first 40pts also formed a LHC with the above properties, as did the total 60pts.

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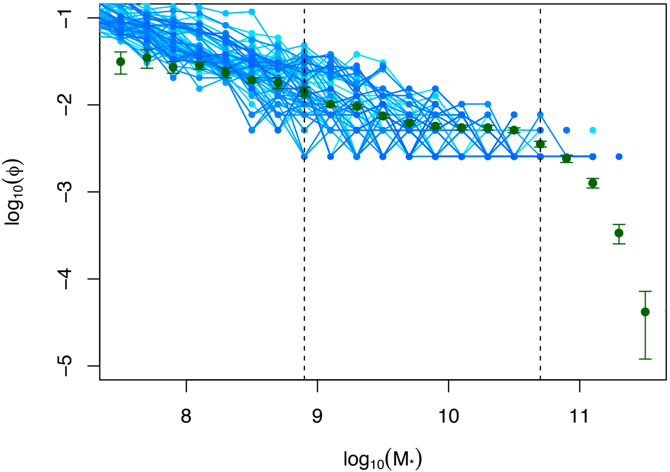
- We hence designed two more 20pt LHCs such that the first 40pts also formed a LHC with the above properties, as did the total 60pts.

Initial Design of EAGLE runs

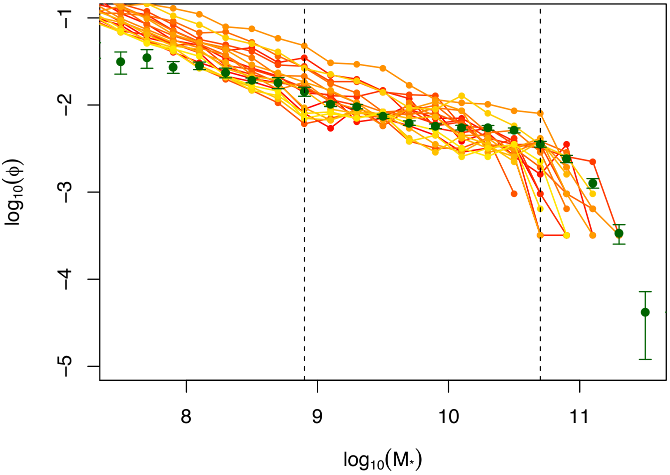
- First Question: are the fast but noisy level 1 runs (at 12.5 Mpc), which we can run in 2 days on 32 processors, informative for higher levels at all?
- We constructed a 20 point LHC design, which was a) maxmin across the 7 inputs, b) maximin across 4 inputs thought to be strongest, and c) had no large holes in those 4 inputs.
- We ran this design at level 1 and at level 2 (each level 2 run takes about 8 days on 64 processors).
- Result: after smoothing, the level 1 runs are very informative for a subset of (low/medium mass) stellar mass function outputs: can use in history matching.
- We were then allowed to run 20, possibly followed by another 20, level 1 runs.
- We hence designed two more 20pt LHCs such that the first 40pts also formed a LHC with the above properties, as did the total 60pts.

Initial Design: 60 runs at level 1 for 12.5Mpc



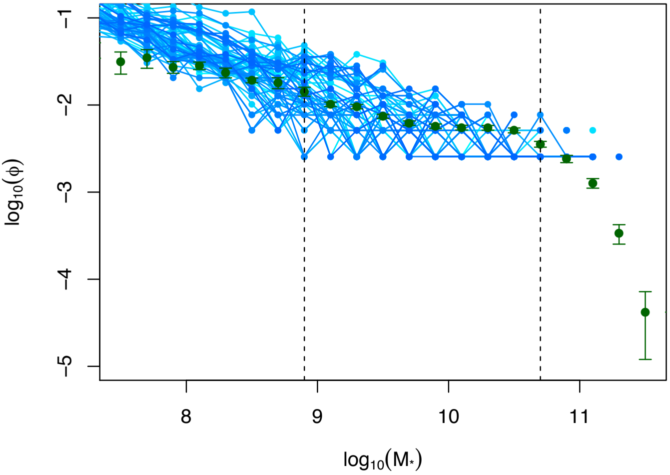
- Level 1: 60 runs of the 12.5 Mpc simulator.

Initial Design: 20 runs at level 2 for 25Mpc



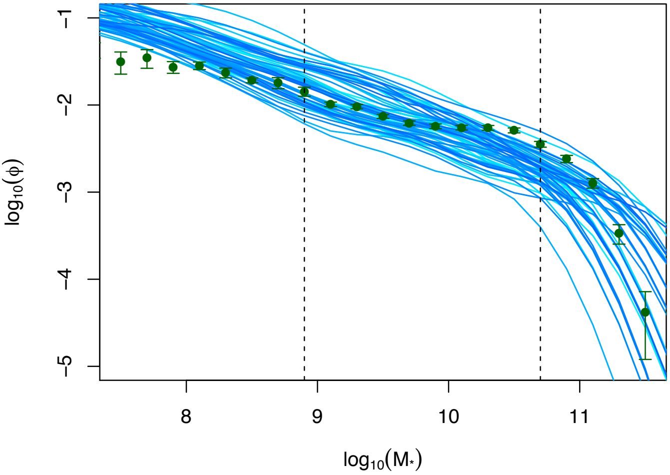
- Level 2: 20 runs of the 25 Mpc simulator.

Initial Design: 60 runs at level 1 for 12.5Mpc



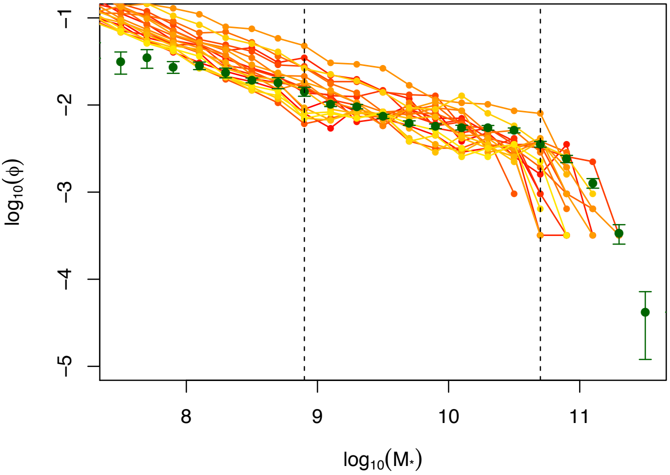
- Level 1: 60 runs of the 12.5 Mpc simulator.

Initial Design: 60 smoothed runs at level 1 for 12.5Mpc



- Level 1: 60 runs of the 12.5 Mpc simulator, smoothed.

Initial Design: 20 runs at level 2 for 25Mpc



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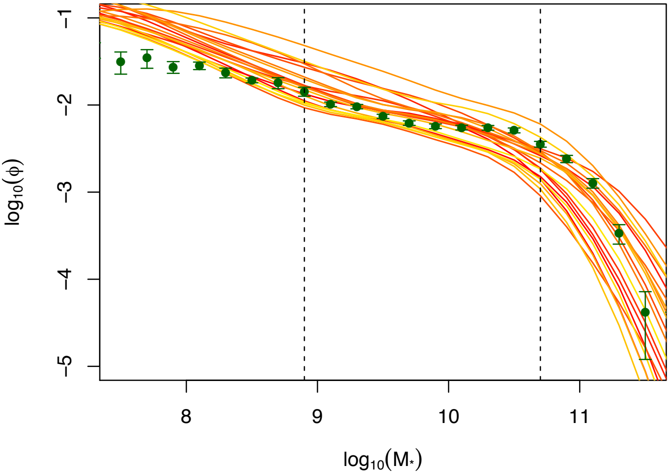
Initial Design: 20 smoothed runs at level 2 for 25Mpc



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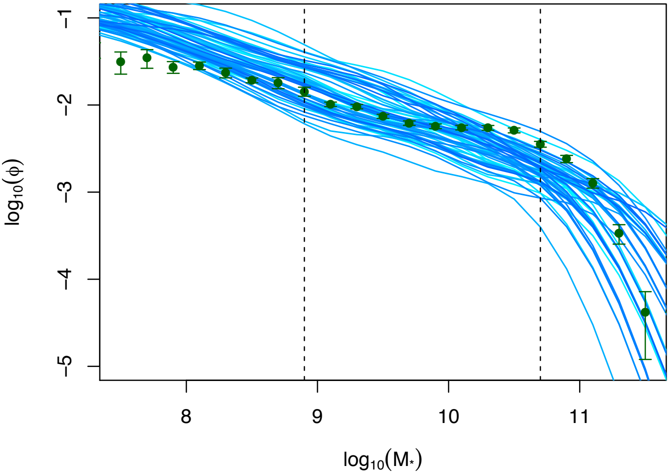

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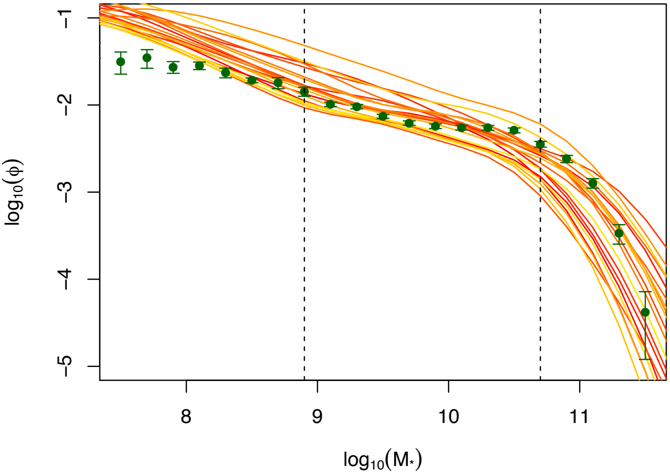

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Linking EAGLE to the Real Universe

- A common major problem is caused by not acknowledging the difference between model $f(x)$ and the system or reality y, and failing to embed them and the observations z into a statistical model.
- Our goal will be to link the real Universe y with EAGLE at the 4th level $f^{(4)}(x)$

$$y = f^{(4)}(x^*) + \epsilon^{(4)}$$

where we define $\epsilon^{(4)}$ to be the Model Discrepancy, which represents the difference between $f^{(4)}(x)$ and the Universe y at some 'best input' x^*.

- (Actually, we will explore linking at different levels using $y = f^{(k)}(x^*) + \epsilon^{(k)}$, with $k = 1, \ldots, 5$).
- We relate the true system y to the observed data z via observation errors e:

$$z = y + e$$

- If we assert probabilistic relations between the random vectors $f^{(4)}, \epsilon^{(4)}, e$ and x^* e.g. independence, we can proceed.
- Often, scientists may be able to specify say $\mathrm{E}[\epsilon^{(4)}]$, $\mathrm{E}[e]$ (often zero), and $\mathrm{Var}[\epsilon^{(4)}]$, $\mathrm{Var}[e]$. Remember $\epsilon^{(4)}$ and e are vectors.

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Emulation Theory: Single Level

- To emulate at the lowest level, i.e. for $f^{(1)}(x)$ we proceed as follows.
- For each of the outputs of interest $f_i^{(1)}(x)$, we pick active variables x_{A_i} then emulate univariately (at first) using:

$$f_i^{(1)}(x) = \sum_j \beta_{ij}^{(1)} g_{ij}(x_{A_i}) + u_i^{(1)}(x_{A_i}) + v_i^{(1)}(x)$$

- The $\sum_j \beta_{ij}^{(1)} g_{ij}(x_{A_i})$ is a 3rd order polynomial in the active inputs, with $\beta_{ij}^{(1)}$ unknown constants: very important to include such global structure here.
- $u_i^{(1)}(x_{A_i})$ is a Gaussian process representing local variation, with covariance:

$$\text{Cov}[u_i^{(1)}(x_{A_i}), u_i^{(1)}(x'_{A_i})] \;=\; (\sigma_i^{(1)})^2 \exp[-|x_{A_i} - x'_{A_i}|^{p_i} / \theta_i^{(1)p_i}]$$

- The nugget $v_i^{(1)}(x)$ models the effects of inactive variables as random noise.
- The Emulators give the expectation $\text{E}[f_i^{(1)}(x)]$ and variance $\text{Var}[f_i^{(1)}(x)]$ at point x for each output of interest and are **fast** to evaluate.

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Emulation Theory: Bayes Theorem

- Quick Aside: to emulate a general function $f_i(x)$ we have a choice of approaches.
- We perform an initial wave 1 set of n runs at input locations $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ giving a column vector of model output values

$$D_i = (f_i(x^{(1)}), f_i(x^{(2)}), \dots, f_i(x^{(n)}))^T$$

- If we had provided prior distributions for each part of the emulator we could use Bayes Theorem to update our beliefs $\pi(f_i(x))$ about $f(x)$:

$$\pi(f_i(x)|D_i) = \frac{\pi(D_i|f_i(x))\pi(f_i(x))}{\pi(D_i)}$$

  where $\pi(f_i(x))$ and $\pi(f_i(x)|D)$ are the prior and posterior pdfs for $f_i(x)$.

- This follows the standard Bayesian statistics paradigm, however this involves a detailed, full specification of the joint prior distribution: a complex and difficult task, and is hard to calculate.

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Emulation Theory: Bayes Linear Methods

- There is a better way: if we are instead prepared to specify just the expectations, variances and covariances of the parts of the emulator, we can use Bayes Linear methodology.

- This is an alternative version of Bayesian statistics that is easier to specify and far easier to calculate with.

- Instead of Bayes Theorem we use the Bayes linear update:

$$\begin{aligned} \mathrm{E}_{D_i}(f_i(x)) &= \mathrm{E}(f_i(x)) + \mathrm{Cov}(f_i(x), D_i)\mathrm{Var}(D_i)^{-1}(D_i - \mathrm{E}(D_i)) \\ \mathrm{Var}_{D_i}(f_i(x)) &= \mathrm{Var}(f_i(x)) - \mathrm{Cov}(f_i(x), D_i)\mathrm{Var}(D_i)^{-1}\mathrm{Cov}(D_i, f_i(x)) \end{aligned}$$

  where $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the Bayes Linear adjusted expectation and variance for $f_i(x)$ at new input point x, and are all that are needed for the subsequent implausibility measures and history match.

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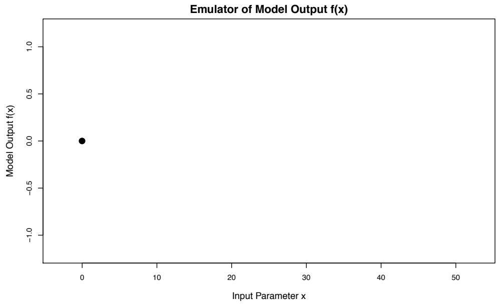
Emulation: a 1D Example



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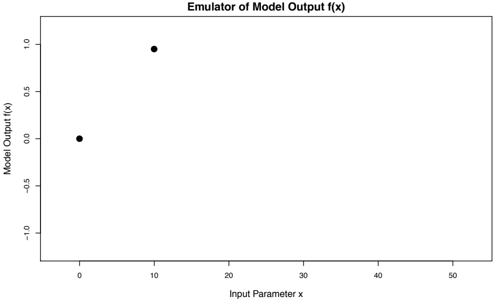

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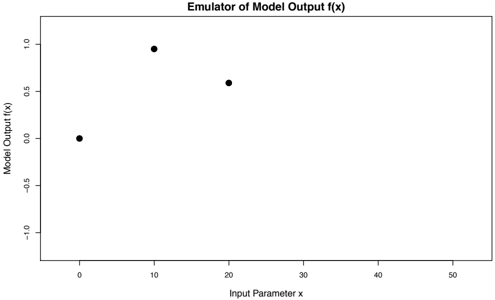

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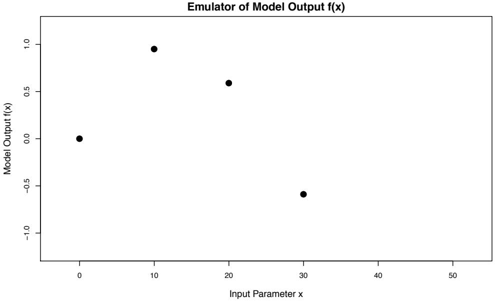

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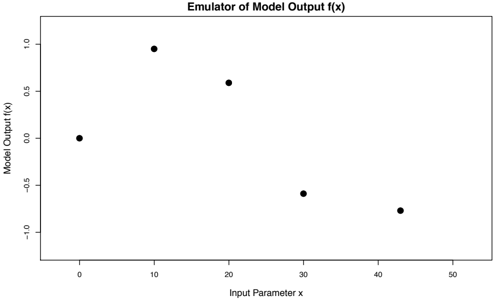

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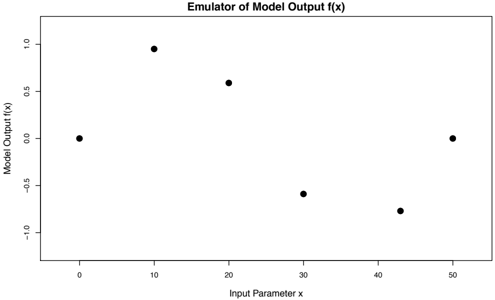

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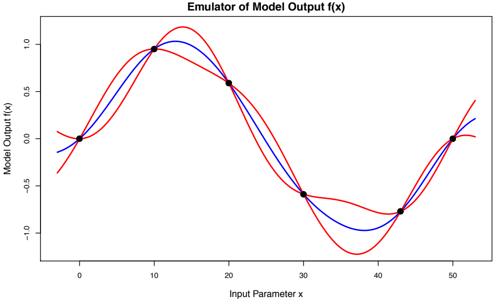

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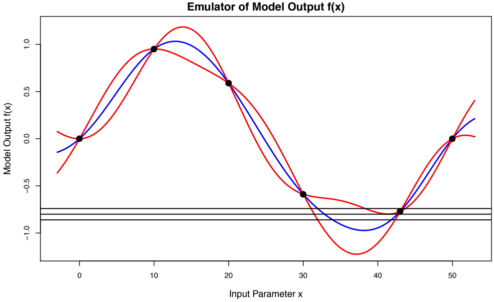

Multilevel Emulation

- Once we have constructed the emulator for level 1, we can use it to construct a highly informed prior for the level 2 emulator.
- We have for a univariate emulator at level 1, dropping the i index for simplicity so that $f_i^{(1)}(x) \to f^{(1)}(x)$:

$$f^{(1)}(x) = \sum_j \beta_j^{(1)} g_j(x_A) + u^{(1)}(x_A) + v^{(1)}(x)$$

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with $a_j, b_{ij}, \beta_{ij}^{(2)}$ uncorrelated, and give a simple BL specification:

$$\mathrm{E}[a_j] = 1, \quad \mathrm{Cov}[a_j, a_k] = \sigma_{a_j}^2 \delta_{jk}$$

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- So the a_j describe a multiplicative uncertainty, and the b_j an uncertain offset.

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- Therefore the expectation and covariance of $\beta^{(2)}$ becomes

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- Finally, we decompose the nugget $v_i^{(1)}(x)$ into two uncorrelated pieces:

$$v^{(1)}(x) = v_I^{(1)}(x) + v_S^{(1)}(x)$$

where $v_I^{(1)}(x)$ represents the inactive variables and $v_S^{(1)}(x)$ the stochasticity due to finite galaxy counts. We have that

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and make the judgement that $\sigma^2_{v_I^{(2)}} \simeq \sigma^2_{v_I^{(1)}}$ but that

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- We now have all the pieces needed to construct the prior for the level 2 emulator.
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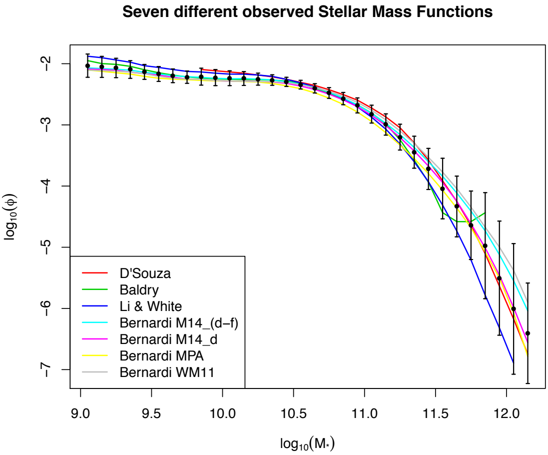

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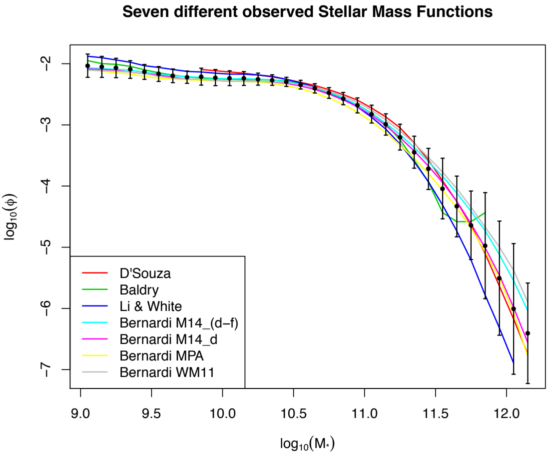

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- The cosmologists have performed one good run, called the reference run, at all 4 levels.
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- First identify set of outputs $i \in Q_j$ that are good to emulate.
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- We can combine the univariate implausibilities across the outputs in Q_i by maximizing over outputs:

$$I_M(x) = \max_{i \in Q_j} I_{(i)}(x) \quad (1)$$

- We can then impose a cutoff

$$I_M(x) < c_M \quad (2)$$

in order to discard regions of input parameter space x that we now deem to be implausible.

- The choice of cutoff c_M is often motivated by Pukelsheim's 3-sigma rule, which does not require precise distributions.

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Multivariate Implausibility Measure

- If we have constructed a multivariate model discrepancy, we can define a multivariate Implausibility measure, using only the outputs in Q_i:

$$I^2(x) = (\mathrm{E}_{D_i}(f_i(x)) - z)^T \mathrm{Var}[f(x) - z]^{-1} (\mathrm{E}_{D_i}(f_i(x)) - z),$$

  which becomes:

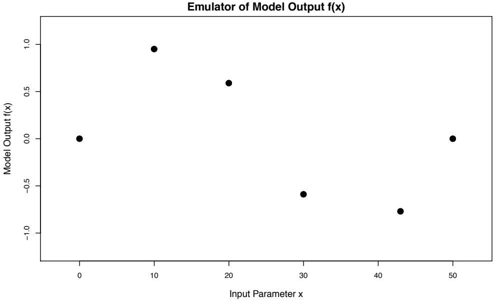
$$I^2(x) = (\mathrm{E}_D(f(x)) - z)^T (\mathrm{Var}_D(f(x)) + \mathrm{Var}[\epsilon] + \mathrm{Var}[e])^{-1} (\mathrm{E}_D(f(x)) - z)$$

- where $\mathrm{Var}[f(x)]$, $\mathrm{Var}[\epsilon]$ and $\mathrm{Var}[e]$ are now the multivariate emulator variance, multivariate model discrepancy and multivariate observational errors respectively (all matrices).

- We now have two implausibility measures $I_M(x)$ and $I(x)$ that we can use to reduce the input space.

- We impose suitable cutoffs on each measure to define a smaller set of non-implausible inputs.

History Matching via Implausibility: a 1D Example



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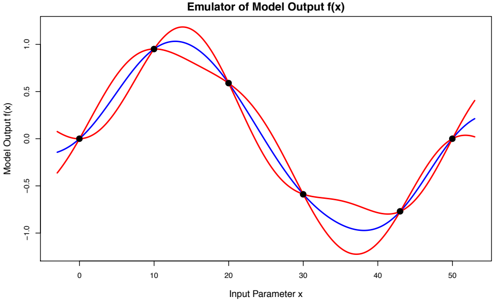

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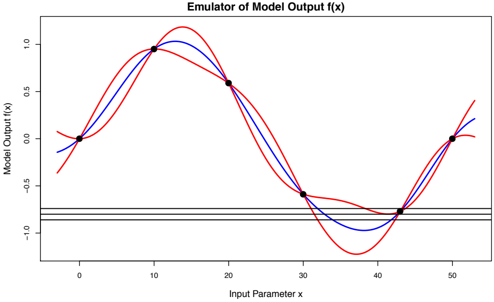

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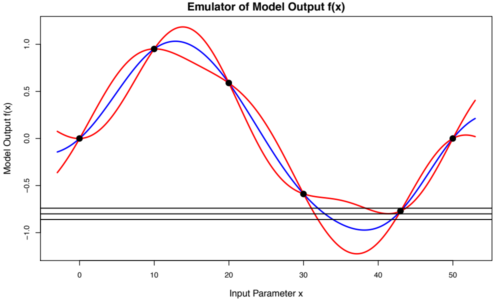

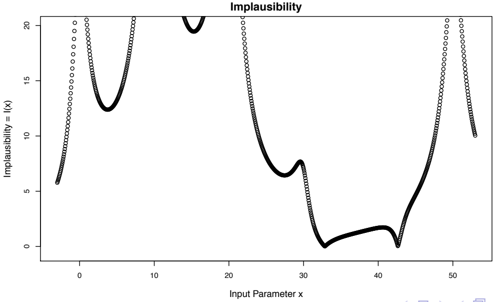

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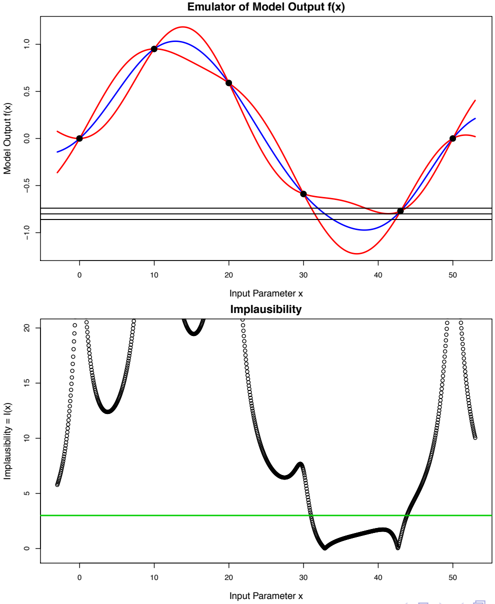

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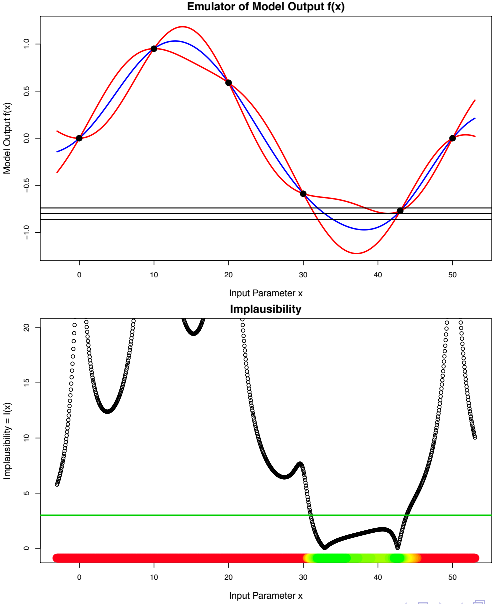

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- Often the set of acceptable inputs $\mathcal{X}$ only occupies a tiny fraction of the original input space.
- Therefore we do not want to use a single one shot space filling design, as this would waste a lot of runs in implausible parts of the space.
- Instead we perform a series of iterations or waves, designing in ever smaller non-implausible regions of the input space (i.e. batch sequentially). Fairly obvious.
- However, we would also not want to use the same statistical form for the emulator across all waves, as the model will most likely behave very differently over the original input space $\mathcal{X}_1$ compared to $\mathcal{X}$ which may be a billion times smaller. Less obvious.
- Therefore we must fit emulators of possibly different structure and complexity at each iteration: to forget this is a mistake (it also has important implications for the full design calculation).
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Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
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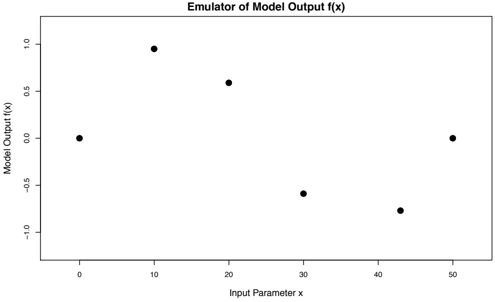

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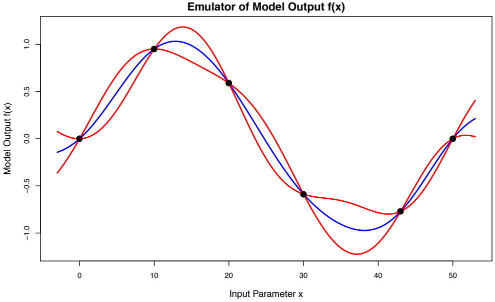

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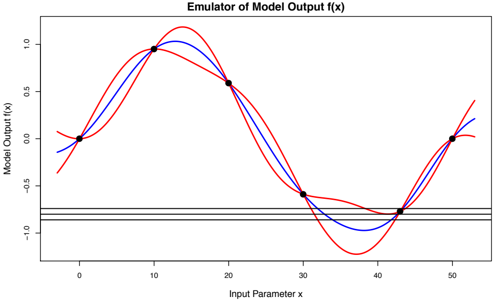

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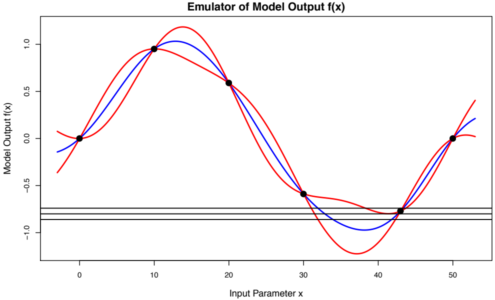

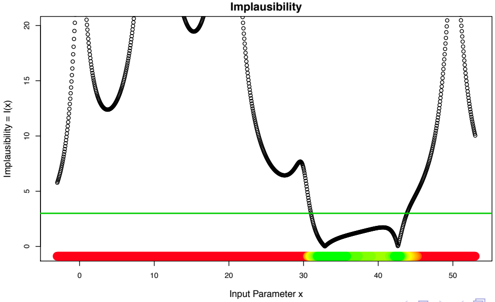

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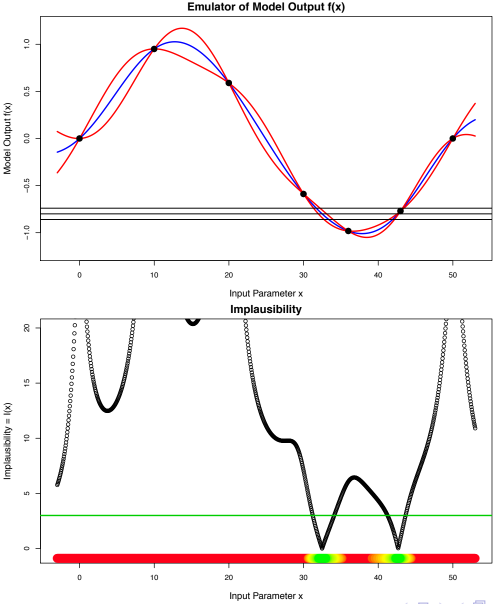

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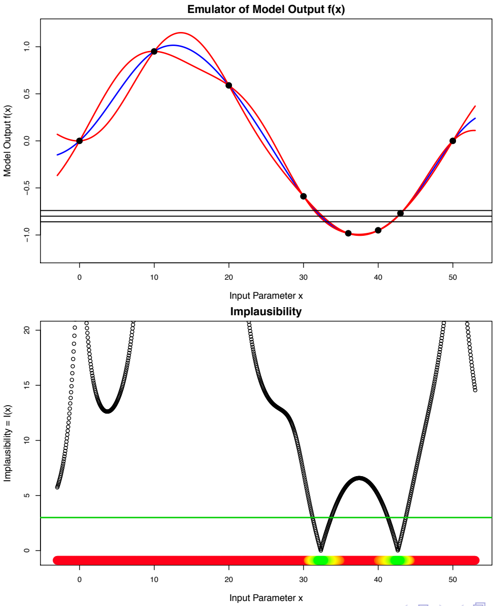

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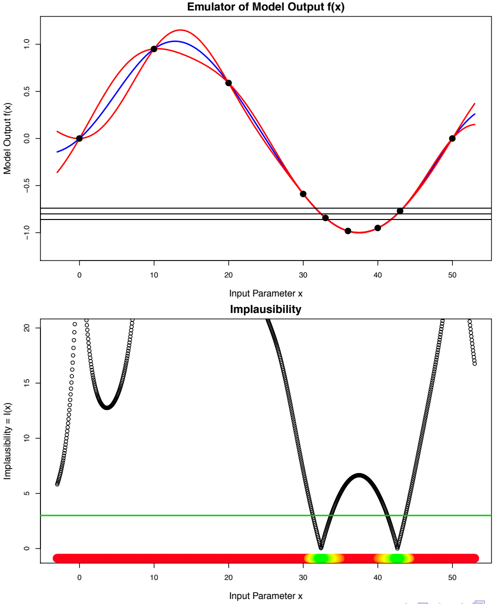

Minimised Implausibility Plots

- Using the speed of the emulators, we can now blitz the input space by evaluating the implausibility

$$I_M(x) = \max_{i \in Q_j} I_{(i)}(x)$$

across a huge latin hypercube, where

$$I^2_{(i)}(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

- To visualise this, we can project down into 2 dimensions, by minimising the implausibility.

$$I_P(x') = \min_{x''} I_M(x', x'')$$

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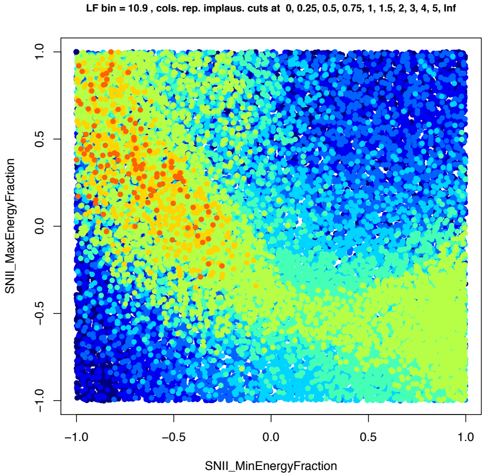

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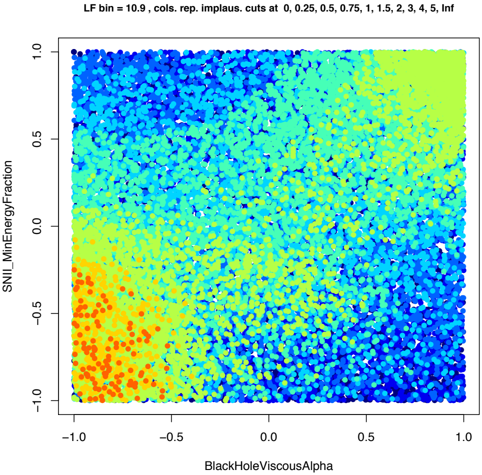

Zero Emulator Variance Implausibility Plots

- Low implausibility at x can be due to the emulators predicting a good match at x, or just due to high emulator uncertainty there.
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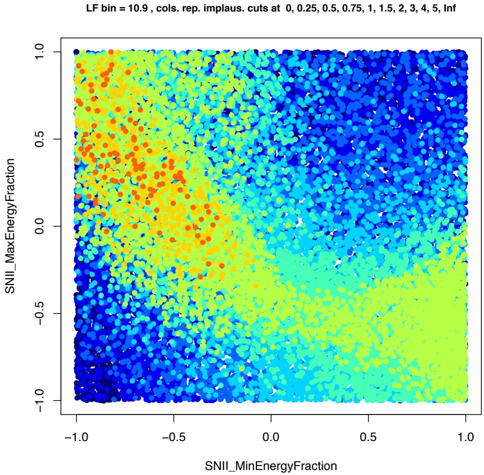

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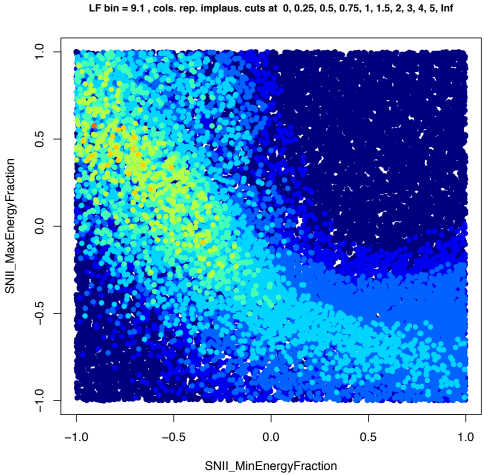

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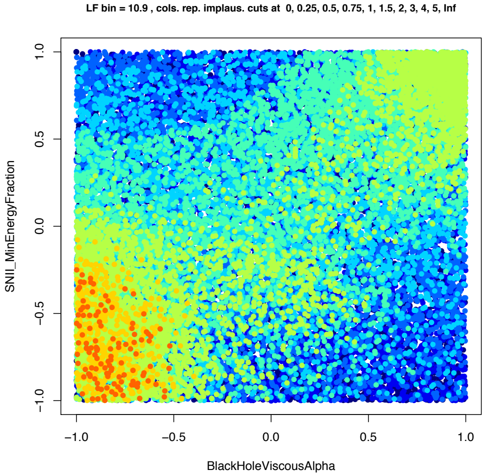

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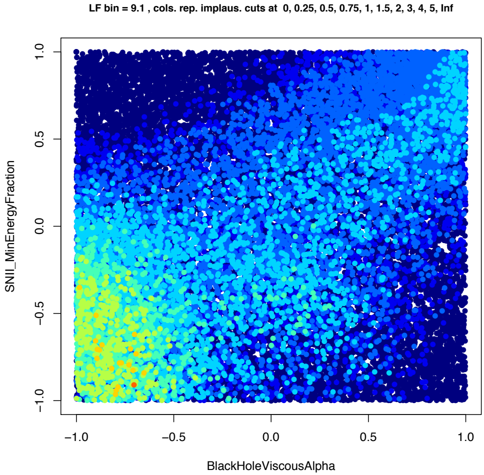

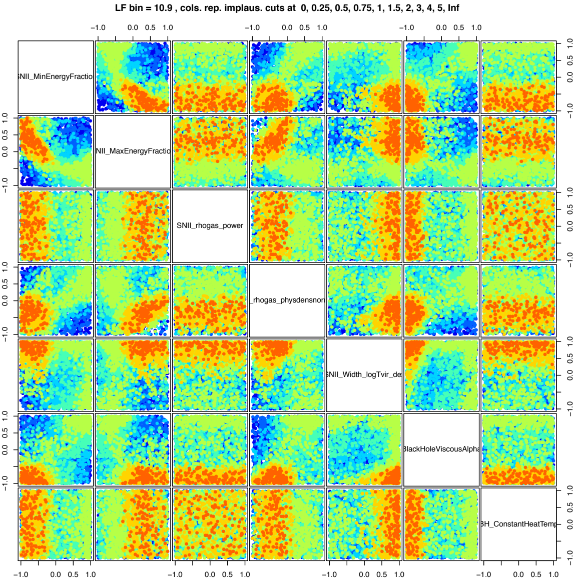
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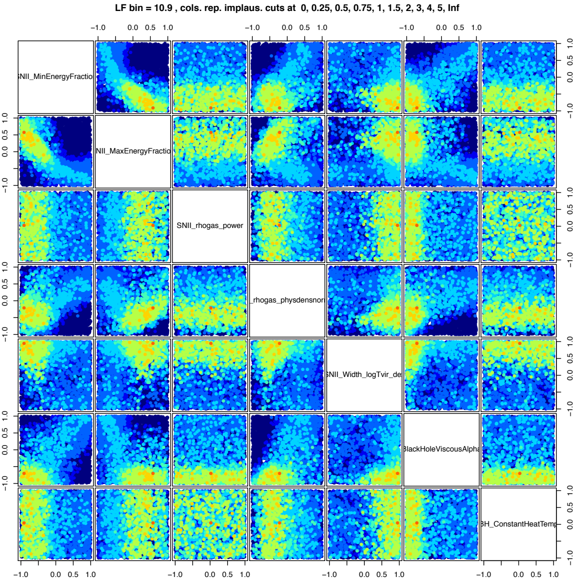
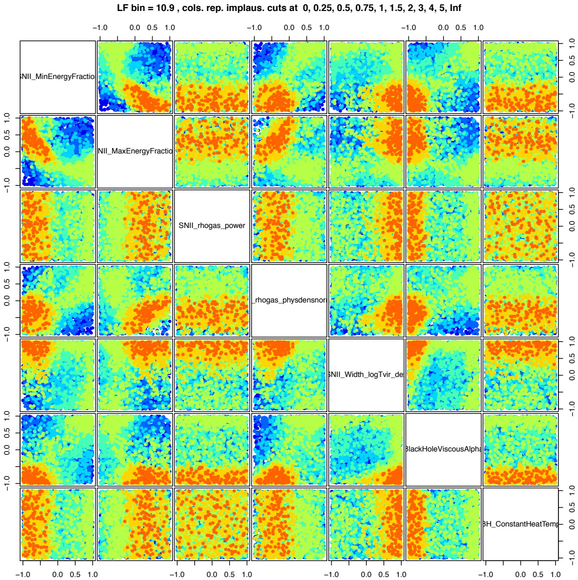
BlackHoleViscousAlpha
BH_ConstantHeatTemp
−1.0
0.0
0.5
1.0

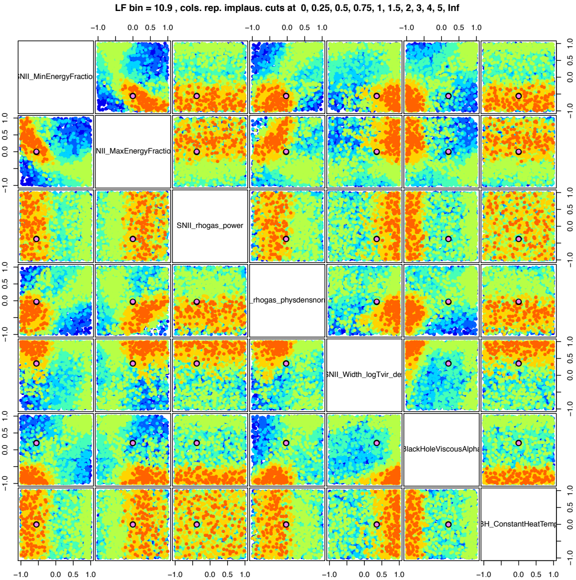
Results: Level 2, Zero Emulator Variance Implausibility



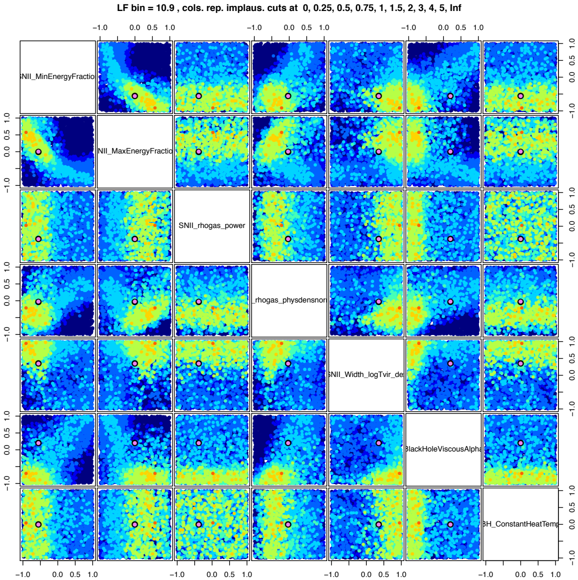
Results: Level 2, Minimised Implausibility



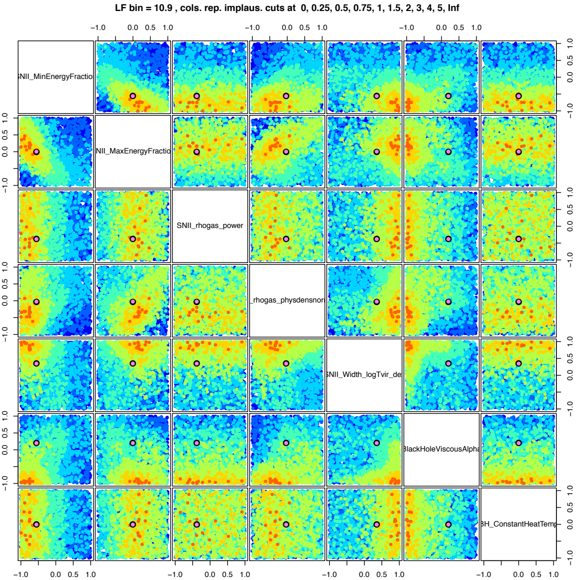
Results: Level 2, Minimised Implausibility, with Ref Run



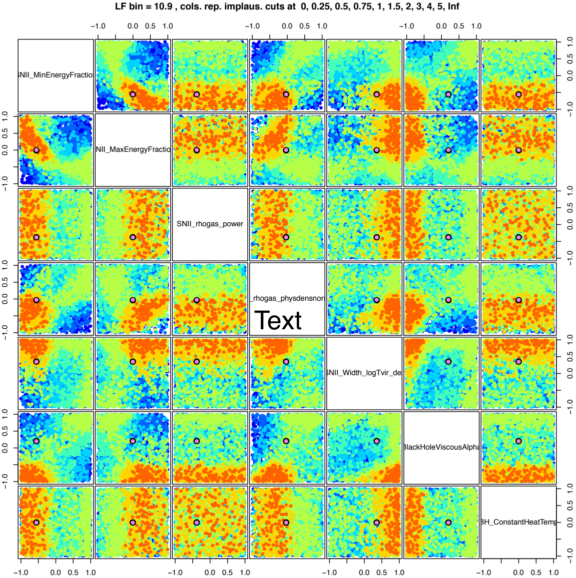
Results: Level 2, Zero Emulator Variance Implausibility, with Ref Run



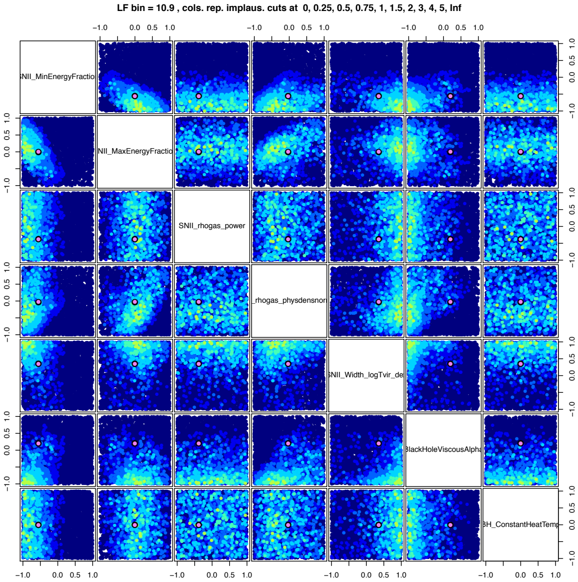
Results: Level 1, Minimised Implausibility, with Ref Run



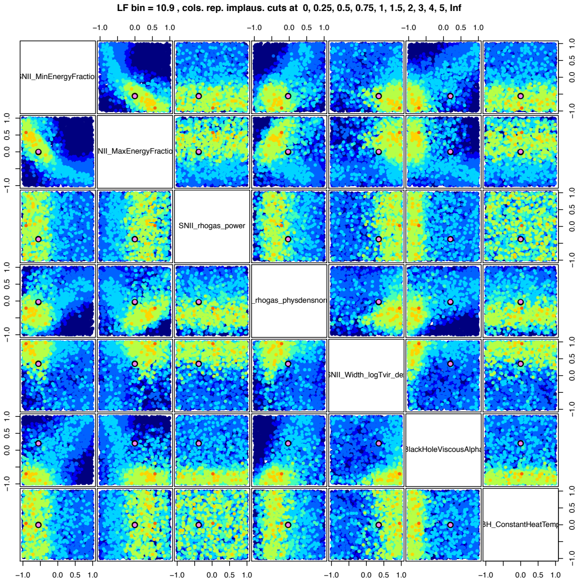
Results: Level 2, Minimised Implausibility, with Ref Run



Results: Level 1, Zero Emulator Variance Implausibility, with Ref Run



Results: Level 2, Zero Emulator Variance Implausibility, with Ref Run



Conclusion

- We have constructed a multilevel emulator for the EAGLE simulation.
- We have emulated at levels 1 and 2 and history matched to rule out bad parts of the input space.
- Current results suggest we may be able to do better than the previous best run.
- We are now in a position to design runs at level 3, and possibly level 4 (or do more runs at levels 1 and 2).
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Goldstein, M., Seheult, A., Vernon, I.: "*Assessing Model Adequacy*". In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, (2013)

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Andrianakis, I., McCreesh, N., Vernon, I, McKinley, T. J. Oakley, J. E. Nsubuga, R. Goldstein, M. & White, R. G. (2016). "History matching of a high dimensional individual based HIV transmission model". JUQ (Accepted).

McCreesh, N., Andrianakis, I, Nsubuga, R., Strong, M., Vernon, I., McKinley, T.J. Oakley, J.E., Goldstein, M., Hayes, R. & White, R.G. "Universal Test, Treat, and Keep: Improving ART Retention is Key in Cost-effective HIV Control in Uganda. BMC Infectious Diseases (2017) 17:322

Trevelyan J. McKinley, Ian Vernon, Ioannis Andrianakis, Nicky McCreesh, Jeremy E. Oakley, Rebecca N. Nsubuga, Michael Goldstein, Richard G. White (2016). "Approximate Bayesian Computation and simulation-based inference for large-scale stochastic epidemic models. Statistical Science (to appear).

Vernon, I. & Gosling, J.P. (2017). "Bayesian computer model analysis of a Robust Bayesian analysis. Bayesian Analysis" (in submission), arXiv:1703.01234

References

Rodrigues, L.F.S., Vernon, I., Bower, R.G.: *Constraints to galaxy formation models using the galaxy stellar mass function, stronger feedback during starbursts?*, MNRAS (2017) 466 (2): 2418-2435. arXiv:1609.06922v3

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: "*Bayesian History Matching for the Observable Universe*". *Statistical Science* 29 (2014), no. 1, 81–90.

Vernon, I., Goldstein, M., and Bower, R. G. (2010), "*Galaxy Formation: a Bayesian Uncertainty Analysis*", *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), "*The Parameter Space of Galaxy Formation*", *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: *Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in Uganda*. PLoS Comput Biol. 11(1), 1003968 (2015)

Goldstein, M., Seheult, A., Vernon, I.: "*Assessing Model Adequacy*". In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, (2013)

Vernon, I, Goldstein, M, Rowe, J, Liu, J and Lindsey, K, "*Bayesian uncertainty analysis for complex systems biology models: emulation, global parameter searches and evaluation of gene functions.*", *in submission, BMC Systems Biology*, arXiv:1607.06358v1 [q-bio.MN].

Andrianakis, I., McCreesh, N., Vernon, I, McKinley, T. J. Oakley, J. E. Nsubuga, R. Goldstein, M. & White, R. G. (2016). "History matching of a high dimensional individual based HIV transmission model". JUQ (Accepted).

McCreesh, N., Andrianakis, I, Nsubuga, R., Strong, M., Vernon, I., McKinley, T.J. Oakley, J.E., Goldstein, M., Hayes, R. & White, R.G. "Universal Test, Treat, and Keep: Improving ART Retention is Key in Cost-effective HIV Control in Uganda. BMC Infectious Diseases (2017) 17:322

Trevelyan J. McKinley, Ian Vernon, Ioannis Andrianakis, Nicky McCreesh, Jeremy E. Oakley, Rebecca N. Nsubuga, Michael Goldstein, Richard G. White (2016). "Approximate Bayesian Computation and simulation-based inference for large-scale stochastic epidemic models. Statistical Science (to appear).

Vernon, I. & Gosling, J.P. (2017). "Bayesian computer model analysis of a Robust Bayesian analysis. Bayesian Analysis" (in submission), arXiv:1703.01234

References

Rodrigues, L.F.S., Vernon, I., Bower, R.G.: *Constraints to galaxy formation models using the galaxy stellar mass function, stronger feedback during starbursts?*, MNRAS (2017) 466 (2): 2418-2435. arXiv:1609.06922v3

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: "*Bayesian History Matching for the Observable Universe*". *Statistical Science* 29 (2014), no. 1, 81–90.

Vernon, I., Goldstein, M., and Bower, R. G. (2010), "*Galaxy Formation: a Bayesian Uncertainty Analysis*", *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), "*The Parameter Space of Galaxy Formation*", *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: *Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in Uganda*. PLoS Comput Biol. 11(1), 1003968 (2015)

Goldstein, M., Seheult, A., Vernon, I.: "*Assessing Model Adequacy*". In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, (2013)

Vernon, I, Goldstein, M, Rowe, J, Liu, J and Lindsey, K, "*Bayesian uncertainty analysis for complex systems biology models: emulation, global parameter searches and evaluation of gene functions.*", *in submission, BMC Systems Biology*, arXiv:1607.06358v1 [q-bio.MN].

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McCreesh, N., Andrianakis, I, Nsubuga, R., Strong, M., Vernon, I., McKinley, T.J. Oakley, J.E., Goldstein, M., Hayes, R. & White, R.G. "Universal Test, Treat, and Keep: Improving ART Retention is Key in Cost-effective HIV Control in Uganda. BMC Infectious Diseases (2017) 17:322

Trevelyan J. McKinley, Ian Vernon, Ioannis Andrianakis, Nicky McCreesh, Jeremy E. Oakley, Rebecca N. Nsubuga, Michael Goldstein, Richard G. White (2016). "Approximate Bayesian Computation and simulation-based inference for large-scale stochastic epidemic models. Statistical Science (to appear).

Vernon, I. & Gosling, J.P. (2017). "Bayesian computer model analysis of a Robust Bayesian analysis. Bayesian Analysis" (in submission), arXiv:1703.01234