Monte Carlo Markov Chain parameter estimation in semi-analytic models of galaxy formation

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ABSTRACT
We present a statistical exploration of the parameter space of the De Lucia and Blaizot version of the Munich semi-analytic (SA) model built upon the Millennium dark matter simulation. This is achieved by applying a Monte Carlo Markov Chain method to constrain the six free parameters that define the stellar and black hole mass functions at redshift zero. The model is tested against three different observational data sets, including the galaxy $K$-band luminosity function, $B-V$ colours and the black hole–bulge mass relation, separately and combined, to obtain mean values, confidence limits and likelihood contours for the best-fitting model. Using each observational data set independently, we discuss how the SA model parameters affect each galaxy property and find that there are strong correlations between them. We analyse to what extent these are simply reflections of the observational constraints, or whether they can lead to improved understandings of the physics of galaxy formation.

When all the observations are combined, we find reasonable agreement between the majority of the previously published parameter values and our confidence limits. However, the need to suppress dwarf galaxy formation requires the strength of the supernova feedback to be significantly higher in our best-fitting solution than in previous work. To balance this, we require the feedback to become ineffective in haloes of lower mass than before, so as to permit the formation of sufficient high-luminosity galaxies: unfortunately, this leads to an excess of galaxies around $L_\ast$. Although the best fit is formally consistent with the data, there is no region of parameter space that reproduces the shape of galaxy luminosity function across the whole magnitude range.

For our best fit, we present the model predictions for the $b_J$-band luminosity and stellar mass functions. We find a systematic disagreement between the observed mass function and the predictions from the $K$-band constraint, which we explain in light of recent works that suggest uncertainties of up to 0.3 dex in the mass determination from stellar population synthesis models.

We discuss modifications to the SA model that might simultaneously improve the fit to the observed mass function and reduce the reliance on excessive supernova feedback in small haloes.

Key words: methods: numerical – methods: statistical – galaxies: evolution – galaxies: formation.

1 INTRODUCTION
The combination of the well-established $\Lambda$ cold dark matter ($\Lambda$CDM) paradigm and the geometrical growth of computer power in recent years has allowed direct $N$-body simulations to give us a comprehensive picture of the formation and evolution of dark matter structure, from the primordial gravitational instabilities to the formation of massive superclusters today (The Millennium Run; Springel et al. 2005).

However, this progress is not reflected in our theoretical understanding of the behaviour of the baryons, with much of the physics governing galaxy formation and evolution still poorly understood. A combined simulation of gas and dark matter resolving small-scale galaxy evolution processes (such as gas cooling, star formation and feedback) over a cosmologically interesting volume is still
years away. Therefore, the only plausible method to construct a model galaxy population for comparison with observed large-scale surveys is using a semi-analytic (SA) formalism. Originally introduced by White & Rees (1978), this formalism treats the dark matter structure using either a Press–Schechter (Press & Schechter 1974), Monte Carlo or N-body approach, and on top of that follows galaxy evolution using parametrized equations governing the laws of sub-grid physics. The basic methodology was set by Cole (1991), Lacey & Silk (1991) and White & Frenk (1991), including the dependence of gas cooling and star formation on the dark matter halo density profile, feedback and chemical enrichment to account for the effect of supernova (SN) explosions on the properties of the hot gas, and stellar population synthesis models to convert star formation histories into observed stellar properties.

Further developments included newly derived stellar population models and improved star formation and SN feedback laws (Kauffmann, White & Guiderdoni 1993; Lacey et al. 1993; Cole et al. 1994). With the level of complexity achieved, they were able to predict a large range of galaxy properties such as star formation rates, luminosity functions and relations between circular velocity, luminosity, metallicity and mass-to-light ratios.

From this original recipe, two models started evolving separately, one mainly based in Munich and another in Durham. By the end of the decade, most of the modern-day prescriptions were already introduced (Kauffmann et al. 1999; Cole et al. 2000), including gas cooling, star formation, chemical enrichment and dust extinction, calculations of discs and bulge properties, stellar population synthesis models, merger follow up with dynamical friction and an early version of the SN feedback treatment.

In Kauffmann & Haehnelt (2000), a model for the growth of black holes (BHs) due to instabilities arising from mergers was proposed, and Benson et al. (2003) and De Lucia, Kauffmann & White (2004) studied new treatments of the SN feedback, including the current model where the SN can not only reheat the cold gas into the hot phase but also eject gas from the halo (to be reincorporated at later times). In parallel, a number of other groups began to develop independent models, to study different aspects of galaxy formation (Somerville & Primack 1999; Menci et al. 2002; Hatton et al. 2003; Daigne et al. 2004; Monaco 2004; Kang et al. 2005).

Most recently, the Munich and Durham SAs have been combined with the Millennium dark matter simulation and an additional recipe, the BH radio mode, introduced to reproduce the quenching of gas cooling star formation in the gas surrounding central cluster galaxies (Springel et al. 2005; Croton et al. 2006; Bower et al. 2006; see also Granato et al. 2004; Cattaneo et al. 2006; Menci et al. 2006; Monaco, Fontanot & Taffoni 2007; Somerville et al. 2008).

Finally, present-day studies include new dust models (De Lucia & Blaizot 2007, hereafter DLB07), the study of alternative feedback processes such as galactic winds (Bertone, De Lucia & Thomas 2007), improved recipes for the stripping of gas during galaxy mergers (Font et al. 2008) and investigation of the ability of the energy released by active galactic nuclei (AGN) feedback to reproduce the properties of the intra-cluster medium (Bower, McCarthy & Benson 2008).

With all these recipes in place, the models successfully reproduce a vast range of observable properties, from galaxy luminosities and colours, including environment dependences, to scaling relations such as Tully–Fisher diagrams. However, until now the level of agreement with observations and the relative weight of different observations in the final choice of the parameters have never been studied in a statistically consistent way.

Moreover, the large number of observational properties that the models aim to predict requires a large number of parameters (some of which are strongly correlated), producing considerable difficulties in determining how to improve the agreement with new observations without destroying the match with existing data sets. In addition, whenever reasonable agreement proves to be impossible, it is hard to know whether there is a failure in determining the right parameter configuration, whether there is a fundamental problem with the underlying model or whether the introduction of new physics is called for.

These difficulties can be overcome by combining multiple observations with proper sampling of high-dimensional parameter spaces. This has proved to be a fruitful approach in theoretical cosmology where techniques such as Monte Carlo Markov Chain (MCMC) parameter estimation have been extensively used (see Trotta 2008 for a comprehensive review). The aim of this paper is to introduce MCMC techniques into SA models of galaxy formation. While this work was being developed, a first result was produced by Kampakoglou, Trotta & Silk (2008). These authors have introduced similar tools to their own SA recipe, an extension of Daigne et al. (2004), which uses a statistical method to generate haloes. We differ from them in that we use the SA model (DLB07), in our case built upon a direct dark matter simulation of a cosmological size (the Millennium Run).

This will allow us to understand how galaxy properties are affected by individual parameters, obtain confidence limits for the parameters and verify the agreement between the model and different observations in a statistically robust way.

This paper is organized as follows. In Section 2, we briefly describe the SA model used in our study. In Section 3, we present the MCMC technique used to constrain the model parameters and explain how it is implemented into the SA recipe. Section 4 describes the observational data used in this work, clarifying which parameters are constrained by each observational galaxy property. In Section 5, we present our results including correlations between the parameters analyzed and predictions for our best-fitting model. Finally, in Section 6 we summarize our conclusions.

2 THE MODEL

In this section, we briefly describe the SA model we use for this work (DLB07), and the underlying dark matter simulation, the Millennium Simulation (Springel et al. 2005).

The Millennium Simulation traces the evolution of dark matter haloes in a cubic box of $500 h^{-1}$ Mpc on a side. It assumes a $\Lambda$CDM cosmology with parameters $\Omega_m = 0.25$, $\Omega_b = 0.045$, $h = 0.73$, $\Omega_{\Lambda} = 0.75$, $n = 1$ and $\sigma_8 = 0.9$, where the Hubble parameter is $H_0 = 100 h^{-1}$ km s$^{-1}$ Mpc$^{-1}$. The simulation follows $2160^3$ dark matter particles of mass $8.6 \times 10^8 h^{-1} M_{\odot}$. Since dark matter haloes are required to contain at least 20 particles, the minimum halo mass is $1.7 \times 10^{10} h^{-1} M_{\odot}$, with a corresponding baryonic mass of about $3.1 \times 10^{9} h^{-1} M_{\odot}$.

The coupling of the SA model on to the high-resolution N-body simulation follows the technique implemented by Springel et al. (2001). The treatment of physical processes driving galaxy evolution builds on the methodology introduced by Kauffmann et al. (1999), Springel et al. (2001) and De Lucia et al. (2004), and is a slightly modified version of that used in Springel et al. (2005) and Croton et al. (2006).

The model divides the gas content of galaxies into several distinct phases. When the galaxy first forms, the gas enters the hot halo at the virial temperature. It can then cool down to join the cold disc.
Table 1. Best-fitting parameters for the SA model from DLB07. The first six parameters are frozen in our analysis at the values shown here. A detailed description of the parameters is given in the text.

| $f_b$  | $z_0$ | $z_r$ | $T_{merger}$ | $R$ | $Y$ |
|-------|-------|-------|--------------|-----|-----|
| 0.17  | 8     | 7     | 0.3          | 0.43| 0.03|
| $a_{SF}$ | $k_{AGN}$ | $f_{BH}$ | $\epsilon_{disc}$ | $\epsilon_{halo}$ | $\gamma_{ej}$ |
| 0.03  | $7.5 \times 10^{-6}$ | 0.03 | 3.5 | 0.35 | 0.5 |

Stars form from the disc, and feedback of energy via SNe can cause gas to heat back up from the cold disc to the hot halo. Finally, it is possible to heat gas still further, ejecting it from the galaxy into an external reservoir from which it gradually leaks back into the hot halo.

From the original 12 parameters in the model, we choose to freeze six of them at the values chosen by DLB07, as shown in the top row of Table 1. The cosmic baryon fraction, $f_b$, is fixed by the cosmology,\(^1\) while the redshifts of the beginning and end of reionization ($z_0$, $z_r$) are used to modify the baryon fraction in small haloes, accounting for the effects of photo-ionizing heating (Kravtsov, Gnedin & Klypin 2004; Croton et al. 2006). $T_{merger}$ is the threshold mass ratio that defines the distinction between major and minor mergers. $R$ is the recycled fraction and $Y$ the yield, both of which depend upon the details of the stellar initial mass function (IMF). The observational data that we use in this work do not allow us to strongly constrain any of these values.

That leaves six free parameters in our study. These are the star formation efficiency, $a_{SF}$, the fraction of cold gas accreted by the central BH during mergers, $f_{BH}$, the quiescent hot gas BH accretion rate, $k_{AGN}$, the SN feedback disc reheating efficiency, $\epsilon_{disc}$, the SN feedback halo ejection efficiency, $\epsilon_{halo}$, and the ejected gas reincorporation efficiency, $\gamma_{ej}$. We briefly describe the meaning of each of these parameters below; for a full description see Croton et al. (2006) and DLB07.

The model converts cold gas into stars at a rate given by

$$m_* = a_{SF} \frac{(m_{\text{cold}} - m_{\text{crit}})}{t_{\text{dyn,disc}}}$$

where $m_{\text{cold}}$ is the mass of cold gas, $m_{\text{crit}}$ is the mass that corresponds to a critical surface density above which gas can collapse and form stars (following Kennicutt 1998) and $t_{\text{dyn,disc}}$ is the dynamical time of the disc. Note that the fraction of mass locked up in stars is $(1 - R)m_d dr$, the rest being instantaneously returned to the disc.

As massive stars complete their life cycle, SN events start injecting energy into the surrounding medium, reheating cold disc gas and even ejecting gas from the hot halo.

For each mass $\Delta m_*$ turned into stars, the amount of gas reheated from the cold disc to the hot halo is given by

$$\Delta m_{\text{reheated}} = \epsilon_{\text{disc}} \Delta m_*$$

with the canonical efficiency of 3.5 being motivated by observations by Martin (1999).

This proves insufficient to prevent star formation in dwarf galaxies as the cooling times are so short that the gas rapidly cools back down to rejoin the disc. For this reason, and motivated also by observations of galactic outflows (Martin 1996), the models allow SN to expel gas completely from low-mass galaxies.

The amount of energy released by SN during the formation of $\Delta m_*$ stars is

$$\Delta F_{\text{SN}} = 0.5 \epsilon_{\text{halo}} \Delta m_*/V_{\text{SN}}^2,$$

where $V_{\text{SN}} = 630 \text{ km s}^{-1}$. Any excess energy left over from reheating the cold gas is used to eject a mass of gas $\Delta m_{\text{ejected}}$ from the galaxy

$$\Delta m_{\text{ejected}} = \left( \frac{\epsilon_{\text{halo}} V_{\text{SN}}^2}{V_{\text{halo}}^2} - \epsilon_{\text{disc}} \right) \Delta m_*.$$

where $V_{\text{halo}}$ is the circular velocity of the dark matter halo.

This ejected gas is kept in an external reservoir and returned to the hot halo at a rate

$$m_{\text{ejected}} = -\gamma_{ej} m_{\text{ejected}}/t_{\text{dyn}},$$

where $m_{\text{ejected}}$ is the mass of ejected gas and $t_{\text{dyn}}$ is the dynamical time of the halo.

SN feedback is ineffective in large galaxies and so another form of heating must be included. Without it, central cluster galaxies appear too massive and too blue, an aspect of the cooling flow problem, well known to X-ray astronomers. The solution is thought to be mechanical heating by BHs accreting at well below the Eddington limit, with the amount of energy released depending on the mass accretion rate of the central supermassive BH, which in turn depends on the BH mass.

To describe this process, it is necessary to introduce two different modes of AGN activity: the quasar and radio modes. The former is thought to be inefficient at heating the gas but is primarily responsible for BH growth. It was originally introduced into the models simply to predict the mass of central BHs, and the corresponding SA model parameter, $f_{BH}$, regulates the BH growth by accretion associated with galaxy mergers

$$\Delta m_{\text{BH,Q}} = \frac{f_{BH} (m_{\text{crit}}/m_{\text{central}}) m_{\text{cold}}}{1 + (280 \text{ km s}^{-1}/V_{\text{vir}}^2)}.$$

The radio-mode reflects the BH growth via quiescent accretion in a static hot halo. It may represent either Bondi accretion directly from the hot phase or the accretion of small quantities of cold gas. It is described by the phenomenological model

$$m_{\text{BH,R}} = k_{AGN} \left( \frac{m_{\text{BH}}}{10^6 M_\odot} \right) \left( f_{\text{hot}}/0.1 \right) \left( \frac{V_{\text{vir}}}{200 \text{ km s}^{-1}} \right)^3,$$

where $m_{\text{BH}}$ is the BH mass and $f_{\text{hot}}$ is the mass fraction of hot gas in the halo.

The radio-mode makes a minor contribution to the growth in mass of the BH but is assumed to generate mechanical heating at a rate

$$L_{\text{BH}} = \eta \dot{m}_{\text{BH,R}} c^2,$$

where $c$ is the speed of light and the efficiency parameter $\eta$ is frozen at 0.1.\(^3\) This heating is used to reduce the rate at which gas cools from the hot halo into the cold disc.

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1 Note that, as in DLB07, we use the value of 0.17 suggested by Wilkinson Microwave Anisotropy Probe rather than the value of 0.18 used to generate the power spectrum for the Millennium Simulation.

2 Note that the reheated fraction is not reduced if this excess is negative.

3 Note that it is the combination $k_{AGN}$ that determines the heating rate so that the value of $\eta$ is unimportant.
3 MONTE CARLO MARKOV CHAIN

3.1 Bayesian Monte Carlo Markov Chain analysis

MCMC methods are a class of algorithms for sampling a multidimensional space with a probability proportional to the likelihood that the model describes the observational constraints. The following brief description follows that in Press et al. (2007).

A typical application of this method is when it is possible to calculate the probability, \( P(D|x) \), of a given data set, \( D \), given the values of some model parameters, \( x \). Bayes’ theorem says that, given a prior \( P(x) \), the (posterior) probability of the model (which will be sampled by the MCMC) is \( \pi(x) \propto P(D|x) \, P(x) \) with an unknown normalizing constant. The advantages of MCMC are that the posterior distribution and correlations for the parameters in study can be easily recovered from the sample list and the un-normalized probability, and that the computational power required scales only linearly with the number of parameters.

The MCMC method uses a Markov chain to step from one point in the sample space to the next, meaning that each point is chosen from a distribution that depends only on the preceding point (the ergodic property). The transition probability \( p(x_2|x_1) \) for stepping from point \( x_1 \) to point \( x_2 \) should satisfy the detailed balance equation

\[
\pi(x_1) \, p(x_2|x_1) = \pi(x_2) \, p(x_1|x_2).
\]

3.2 Metropolis–Hastings algorithm

There are several algorithms that can produce a chain with the required properties, the most common being the Metropolis–Hastings algorithm (Metropolis et al. 1953; Hastings 1970). This method requires a proposal distribution \( q(x_2|x_1) \) that can assume various shapes, as long as the chain reaches everywhere in the region of interest. However, an inappropriate choice can delay significantly the convergence of the chain. Considering the underlying probability distribution of our parameters we choose a lognormal proposal distribution with a width that assures that the final acceptance of the chain is between 10 and 40 per cent.

The chain is then started in a randomly selected point in parameter space \( x_1 \). A new candidate point \( x_{2c} \) is selected by drawing from the proposal distribution, and the acceptance probability \( \alpha(x_1, x_{2c}) \) calculated using the formula

\[
\alpha(x_1, x_{2c}) = \min \left[ 1, \frac{\pi(x_2)q(x_1|x_{2c})}{\pi(x_1)q(x_{2c}|x_1)} \right].
\]

The candidate point is accepted with probability \( \alpha(x_1, x_{2c}) \) and \( x_2 \) is set equal to \( x_{2c} \), or rejected and the point left unchanged (\( x_2 = x_1 \)).

The ratio \( q(x_1|x_{2c})/q(x_{2c}|x_1) \) in equation (10) represents the prior which we assume to be lognormal.

3.3 MCMC applied to the semi-analytic model

Implementing the MCMC sampling approach on the SA model parameter space raises considerable issues related not only to the copious amount of I/O (the original recipe reads in the full Millennium dark matter trees), but also to the volume of calculations required to follow the evolution of over 20 million galaxies in a cosmological volume, through more than 50 redshift slices. At each MCMC step, the SA model needs to be run with the proposed set of parameters, to compute the acceptance probability by comparing the outputted galaxy properties with the observational constraints. The size of the calculation and the number of steps required for convergence make it unfeasible to perform our analysis using the full Millennium volume.

The structure of the Millennium Simulation provides a way to circumvent this difficulty. The output is divided into 512 files which have self-contained trees, with the galaxies on each treated independently. We choose to perform our analysis in a single file with a mean density and luminosity function analogous to the full Millennium box. This assures that the parameter study done on it is representative of the full data set. Only the largest galaxies with stellar masses greater than about \( 10^{11} \, h^{-1} \, M_\odot \) are not properly sampled this way.

For our best-fitting parameters, we rerun the SA model on the full simulation: these results are presented in Section 5.

4 INDIVIDUAL OBSERVATIONAL CONSTRAINTS

4.1 Overview

The traditional SA approach is to adjust parameters only considering observations at redshift zero. Following this philosophy, we select three independent and local observational data sets: the K-band luminosity function, the colour–stellar mass relation and the BH–bulge mass relation, to fully constraint the six parameters defining galaxy masses and formation rates of stars and AGN.

In this section, we present the observations used in our analysis and show how each individual property constrains the different parameters by running the MCMC sampling with one observational data set at a time. The output is analyzed using GETDIST, part of the COSMOMC software package (Lewis & Bridle 2002), adapted to produce one- and two-dimensional maximum likelihood (profile) and MCMC marginalized (posterior) distributions. For the independent observational properties, we use different statistical tests to assess the likelihood of the model, reflecting the observational uncertainty and the nature of the relation under study.

Running our sampling technique with separate observational data sets one at a time allows us to gain insight on which degeneracies between the different parameters are broken by each additional observation. We start by studying the influence of varying the parameters on the final K-band luminosity function.

4.2 The K-band luminosity function

Despite being one of the most fundamental properties of a galaxy, stellar mass is not easily derived from observations. To get estimates for this quantity from the observed luminosities, it is necessary to assume mass-to-light (\( M/L \)) ratios based on stellar population synthesis models that include still poorly understood dust corrections, IMFs and metallicity evolution. On the other hand, SA models directly predict mass, but to produce observable luminosities the same crudely established process must be taken in the reverse direction.

This difficulty leads us to use the K-band luminosity function. The K band is known as a good mass indicator as it is relatively unaffected by dust and represents a fair sample of the stellar population. We combine three observational studies (Cole et al. 2001; Bell et al. 2003; Jones et al. 2006), respectively, from 2dFGRS, 2MASS and 6dFGRS, from which we build a final luminosity function. The final data points are given by the average of the maximum and minimum number density estimates in each magnitude bin, with errors \( \sigma_i \), equal to half the difference between them. 

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The galaxy $K$-band luminosity function at $z = 0$ for the DLB07 model (dashed red line) and our best-fitting model (solid red line). The model predictions are compared with observations from Cole et al. (2001), Bell et al. (2003), Jones et al. (2006) combined to produce a new luminosity function reflecting the scatter between them.

The comparison between the $K$-band luminosity function from the original DLB07 model (using the published parameter values) with the observations is shown in Fig. 1. The original model already shows good agreement with the combined data except for the faint end, overpredicting the number of dwarfs galaxies with magnitudes fainter than $K \approx -22$.

To compute the likelihood of the model for the $K$-band luminosity function, we use the chi-square probability function where

$$\chi^2 = \sum_i \frac{(N_i - n_i)^2}{\sigma_i^2 + n_i}$$

is summed over the observational bin range plotted in Fig. 1, and $N_i$ and $n_i$ represent the number of observational and simulated galaxies in each bin, respectively.

In Fig. 2, we plot the 1σ and 2σ preferred values from the MCMC (solid lines) and the maximum likelihood value sampled in each bin (colour contours), for the subset of the original parameters (with values plotted in log space) constrained only by the observational $K$-band luminosity function.

In interpreting this and future plots, one should bear in mind that the contours follow the MCMC sampling in parameter space, which should trace out the relative likelihoods of different regions (the posterior distribution). The colours represent the maximum likelihood projected along all the hidden dimensions in the plot (profile distribution). Usually, as in this case, the two match fairly well. The exceptions arise when there is a high-likelihood region that only occupies a small volume of parameter space.

The two lower panels of Fig. 2 show that the three parameters controlling the SN feedback are all positively correlated with each other, in a way that allows us to learn how the $K$-band luminosity function constrains the feedback model. To do this, we rewrite equation (4) as

$$\frac{\Delta m_{\text{ejected}}}{\Delta m_*} = \epsilon_{\text{halo}} \frac{V^2_{\text{vir}}}{V^2_{\text{SN}}} \left( 1 - \frac{\epsilon_{\text{disc}}}{\epsilon_{\text{halo}}} \frac{V^2_{\text{disc}}}{V^2_{\text{SN}}} \right).$$

In our analysis, this cut-off is represented by the line of maximum likelihood in the lower-left panel of Fig. 2 and corresponds to the $V_{\text{vir},0} = \left( \frac{\epsilon_{\text{halo}}}{\epsilon_{\text{disc}}} \right)^{\frac{1}{2}} V_{\text{SN}}$. From which we see that the amount of ejected gas per unit mass of star formation drops to zero for haloes with virial speed greater than

$$V_{\text{vir},0} = \left( \frac{\epsilon_{\text{halo}}}{\epsilon_{\text{disc}}} \right)^{\frac{1}{2}} V_{\text{SN}}.$$

In our analysis, this cut-off is represented by the line of maximum likelihood in the lower-left panel of Fig. 2 and corresponds to $V_{\text{vir}} \approx 140 \, \text{km} \, \text{s}^{-1}$, which translates into $M_{\text{star}} \approx 10^{10.5} M_\odot$ and $M_K \approx -23$. This cut-off virial velocity is lower than in DLB07, which means that our SN feedback stops being effective at fainter magnitudes, allowing more stars to form in $L_*$ galaxies. Since we need to assume a stronger SN feedback to decrease the faint end of the luminosity function, this is the only way to assure that enough stars will still form in brighter galaxies.

For a given value of $V_{\text{vir},0}$, the amount of ejected gas is proportional to $\epsilon_{\text{halo}}$, with the maximum likelihood solutions showing a linear relation $\gamma_{\text{ej}} \propto \epsilon_{\text{halo}}$. This corresponds to a roughly constant amount of gas being held in the external reservoir: in a steady state the external gas content is proportional to the ratio of the influx and outflux rates. Our regions of high likelihood represent a considerably higher amount of gas being in the external reservoir than in DLB07 with a corresponding reduction in star formation in faint galaxies.

The value of $\epsilon_{\text{disc}}$, controlling the reheating of cold to hot gas, has a minor impact except as a way of controlling the critical magnitude limit above which feedback is ineffective. Presumably cooling times are so short in galaxies below the magnitude limit that any gas that
is reheated will quickly cool down again. One might have expected that it could be used to control the stellar mass fraction in large galaxies where the cooling time is relatively long; however this does not seem to be the case.

The AGN feedback parameters, shown in the top-left panel of Fig. 2, have a broader acceptable region but also show a high-likelihood spine that runs diagonally down from top left to bottom right. This can be explained by combining equations (6), (7) and (8) to obtain the mechanical heating rate produced by this process,

\[ L_{\text{BH}} \propto f_{\text{BH}} \Delta \log k_{\text{AGN}} m_{\text{cold}} f_{\text{BH}}. \]

Thus, for given cold and hot gas fractions in the galaxies, the line represents a single heating rate. This degeneracy is broken if the BH masses are used as a constraint (Section 4.4), since their growth is mainly dominated by the quasar mode.

The maximum likelihood channels described above all have star formation efficiencies of \( \epsilon_{\text{SF}} \approx 0.04 \), similar to that of DLB07. This reinforces the conclusion that the SN and AGN feedback parameters act to maintain a constant mass of cold gas available for star formation.

Apart from the main band discussed above, the two upper panels in Fig. 2 show alternative regions of acceptable likelihood. These have lower star formation efficiencies, requiring a greater mass of cold gas. This, in turn, leads to a smaller product of \( f_{\text{BH}} \) and \( k_{\text{AGN}} \). We do not dwell on these solutions here as they seem to be ruled out by other observations: in particular they result in excessive BH–bulge mass ratios.

4.3 The colour–stellar mass relation

The star formation rate is another essential quantity in characterizing the galaxy population. Although this property can be directly extracted from the models, it is not easily comparable with observations. While in the models, the mass transformed into stars at each time-step is computed, only indirect observational estimators are available.

Galaxy colours are one such indirect measure of the recent star formation history of galaxies, with a clear bimodality between an old, passively evolving red population, and a young star-forming blue sequence (e.g. Kauffmann et al. 2003; Brinchmann et al. 2004; Baldry et al. 2004).

The top panel of Fig. 3 shows the colour–magnitude relation for the DLB07 model. Although it has some problems in correctly predicting the slope and fraction of each population in some mass ranges (see Baldry et al. 2006; Weinmann et al. 2006a), it clearly reproduces the bimodality.

To test the correctness of model colours, we divide the galaxies into the two populations using the selection criteria in Weinmann et al. (2006a), \( (g - r) = 0.7 - 0.032(M_r - 5 \log h + 16.5) \), converted into a cut on the colour–stellar mass relation at redshift zero, \( (B - V) = 0.065 \log (M_r h^2 / M_\odot) + 0.09 \) and shown as the solid line in the upper panel of Fig. 3. The conversion from the \( g - r \) to the \( B - V \) colour was done following Fukugita et al. (1996), \( g - r = 1.05(B - V) - 0.23 \). The fraction of red galaxies for different mass bins is then compared with observations from Baldry et al. (2004) as shown in the lower panel. The observational masses based on the ‘diet’ Salpeter IMF (Bell et al. 2003) were reduced by 0.15 dex to agree with the IMF assumed in our SA model (Chabrier 2003). The fact that a different blue band was used in the observational colour cut \((u - r)\) instead of our converted \(g - r\) could potentially lead to discrepancies in the number of objects identified in each population if the two Gaussian distributions defining each population significantly overlap. However, as Fig. 3 shows, there is a clear division between red and blue galaxies in the \( B - V \) CM diagram for model galaxies. In this way, any small differences in the number of red galaxies caused by the different colour cut used should be well within the 0.05 error assumed for the model fraction.

Following Croton et al. (2006), we take the resolution limit for model colours to be at a stellar mass of approximately \( 10^{9.5} h^{-2} M_\odot \), above which the model reproduces the red fraction reasonably well, with some minor excess for galaxies above \( L_\ast \).

The agreement between model and observational colours is calculated using a maximum likelihood method with a constant value for the errors in the model \((\sigma_{\text{model}} = 0.05)\) given by the variation in the fraction of red galaxies in a sample of 20 sub-volumes of the Millennium Simulation, similar to the one used in our analysis.

![Figure 3](https://academic.oup.com/mnras/article-abstract/396/1/535/1247858/540)
We assume that both model and observational values are Gaussian distributed around the true fraction $F$, with a likelihood

$$L_{\text{(Colour)}} = \exp \left\{ -\frac{(f_{\text{model}} - F)^2}{2\sigma_{\text{model}}} - \frac{(f_{\text{obs}} - F)^2}{2\sigma_{\text{obs}}} \right\}$$

(15)

that has a maximum value

$$L_{\text{(Colour)}} = \exp \left\{ -\frac{(f_{\text{model}} - f_{\text{obs}})^2}{2\left(\sigma_{\text{model}}^2 + \sigma_{\text{obs}}^2\right)} \right\}.$$  (16)

The DLB07 model, tuned to reproduce a different set of observational colours (the red and blue luminosity functions from 2dFGRS), correctly predicts the fraction of red galaxies at low and high masses but overpredicts the number of red galaxies at intermediate masses.

In Fig. 4, we plot the allowed regions in likelihood and posterior space. Perhaps surprisingly, the colour constraint picks out a similar relationship between $\epsilon_{\text{halo}}$ and $\epsilon_{\text{disc}}$ as does the $K$ band. This is because it also requires a cessation of SN heating in galaxies with virial speeds above 140 km s$^{-1}$ which would otherwise have an excessive red fraction.

The constraint again requires a constant mechanical heating from AGN feedback (as shown by the line of maximum likelihood in the upper-left panel of the figure) which is responsible for the elimination of blue galaxies at high masses. The line of highest likelihood lies slightly below that seen for the $K$-band constraint. Along with this, the upper-right panel of the figure shows a preference for a slightly lower star formation efficiency. However, in each case there is an acceptable region where the allowed parameter spaces overlap. This changes when we move to our third constraint.

### 4.4 The BH–bulge mass relation

We have seen in the previous section that the power of the radio-mode AGN feedback depends upon the product of the quasar and radio-mode growth factors. However, the mass growth of the BHs is dominated by the quasar mode alone. We can therefore use the BH–bulge mass relation to break this degeneracy.

If we require SA galaxies to be constrained solely by this relation, then the other parameters in the model will be free to shift into implausible values allowing any point in parameter space to have a reasonable likelihood. For this reason, we require model galaxies to follow both the BH–bulge mass relation and the $K$-band luminosity function of bright galaxies (i.e. the host galaxies of these BHs).

The BH and bulge masses for the original model are plotted in Fig. 5 and compared with local observations from Haring & Rix (2004). The model galaxies fall on top of the observational best fit (given by the blue line), with the scatter in the relation also reproduced.

In order to test the SA results against observations, we divide the data into two bins (perpendicular to the observational best fit), represented by the solid black lines on Fig. 5. $15.2 < m_{\text{BH}} + 0.90 m_{\text{bulge}} \leq 17.75$ and $17.75 < m_{\text{BH}} + 0.90 m_{\text{bulge}}$, and for each of the bins we compute the binomial probability for the observed distribution of mass ratios above and below the best-fitting line, given the fractional distribution from the model galaxies:

$$L_{(\text{BH–bulge})} = \begin{cases} 
2I_p(k, n - k + 1), & I_p \leq 0.5 \\
2(1 - I_p(k, n - k + 1)), & I_p > 0.5
\end{cases}$$

(17)

where $k$ is the number of observed galaxies above the best fit in each bin, $n$ is the total number of observed galaxies in the same bin and $p$ is the equivalent fraction, $kn$, for the model galaxies in the bin. $I_p(a, b)$ is the incomplete beta function as defined in Press et al. (2007). The two formulae are required since we need to exclude both extremes of the distribution, corresponding to an excess of points both above and below the best-fitting line.

Figure 5. The BH–bulge mass relation for DLB07 (contours and dots) is compared with local observational data from Haring & Rix (2004) (blue crosses). The best fit to the observational data points is given by the blue line running from bottom left to top right, while the two black lines perpendicular to this relation divide galaxies into the two mass bins used to compute the likelihood.
Figure 6. As for Fig. 2, but constrained only by the binomial test on the BH–bulge mass relation and by the K-band luminosity function of galaxies above $M_k = -23$. The colour scale is normalized by the maximum likelihood value of 0.86.

In Fig. 6, we plot the posterior and profile likelihood distributions of the parameters constrained only by this binomial test and the K-band luminosity function of galaxies brighter than $M_k = -23$.

It is immediately apparent that the region of high likelihood is much smaller for this test than for the first two constraints. Moreover, this region corresponds to high values for the SN feedback parameters, combined with a low AGN feedback efficiency. As such, it is incompatible with the acceptable regions in those previous tests.

However, there is a lower likelihood, but still acceptable (likelihood > 0.1) region that extends towards lower SN and higher AGN parameters. As the MCMC contours show, this occupies a much larger volume of parameter space than the high-likelihood peak (and so, in a Bayesian sense, the true solution is more likely to be found in the former than the latter).

Looking at the upper-left panel in the figure, we can see that the acceptable region runs from bottom left to top right, perpendicular to the lines seen in the previous two tests. The BH–bulge mass ratio thus breaks the degeneracy in the AGN parameters.

5 COMBINED OBSERVATIONAL CONSTRAINTS

The likelihood of the model for a given point in parameter space is computed by taking the product of the three independent observational constraints described in the previous sections.

$$\pi(x_i) = \mathcal{L}(K\text{-band}) \times \mathcal{L}(\text{colour}) \times \mathcal{L}(\text{BH–bulge}).$$

(18)

This quantity is calculated at each MCMC step and used to derive the acceptance probability (equation 10). We run our sampling over approximately 30 000 steps, excluding an initial burn-in to assure the independence of the final results from the starting point of the chain. The output is then analysed using getdist, part of the cosmomc software package (Lewis & Bridle 2002). As for the individual constraints, the code is adapted to produce one- and two-dimensional maximum likelihood (profile) and MCMC marginalized (posterior) distributions, best values and confidence limits for the parameters, convergence statistics for the chain and correlation statistics for each parameter.

Although, in our sampling we do not impose rigid limits on the parameter range, Fig. 7 shows that the preferred regions are well-constrained. Fig. 8 shows the profile distribution for each parameter, marginalized over all others. Unfortunately, the maximum likelihood is just 0.037, thus the best-fitting solution is incompatible with the three combined observations at the 2σ level.

The principal cause of the low likelihood is an incompatibility between the BH–bulge mass constraint and the K band and $B - V$ colours. As discussed in Section 6, this might be caused by observational uncertainties in the BH and bulge masses or might reflect a deficiency in the BH growth model, which is still very simplistic. Nevertheless, observational uncertainties, principally that associated with stellar population synthesis modelling, make it premature to conclude that the DLB07 formalism is ruled out.

5.1 Best-fitting parameters and confidence limits

The best fit and confidence limits for the six free parameters, together with the published values from DLB07, are shown in Table 2. All the parameter values in the original model fall within our 2σ regions except for the SN disc reheating efficiency, which we require to be larger than before.

Both the star formation efficiency and the AGN quasar mode parameters from DLB07 closely match our best-fitting values, while our AGN radio-mode efficiency is slightly lower than before.
For the SN feedback parameters, the original halo ejection efficiency, $\epsilon_{\text{halo}}$, is below our best fit, whereas the original gas reincorporation efficiency, $\gamma_{\text{ej}}$, is slightly higher. This combination acts so as to produce a higher fraction of gas trapped in the external reservoir with the new parameters, and hence a smaller mass of cold gas available for star formation in dwarf galaxies.

The DLB07 SN reheating efficiency, $\epsilon_{\text{disc}}$, is considerably lower than our best fit. As discussed earlier, the main effect of this is to raise the ratio $\epsilon_{\text{disc}}/\epsilon_{\text{halo}}$ with the new parameters and hence, from equation (13), to lower the critical virial speed above which feedback is ineffective.

5.2 Galaxy properties in our best-fitting model

The MCMC parameter estimation was carried out using only one data-file representing 1/512 of the Millennium volume. In this section, we present results using our best-fitting parameters in the full volume.

5.2.1 Galaxy luminosity functions

The requirement that star formation be inefficient in low-mass galaxies is a common problem to both sets of SA models built upon the Millennium Simulation. There is an apparent excess of dwarf galaxies that can be seen in the $K$-band luminosity function in both Croton et al. (2006) and Bower et al. (2006).

In the left-hand panel of Fig. 9, the $K$-band luminosity functions from DLB07 and our best-fitting model are plotted against the observations used to constrain the luminosities of galaxies in our MCMC parameters estimation (Cole et al. 2001; Bell et al. 2003; Jones et al. 2006).

Figure 9. Comparison of the predicted $K$-band (left-hand panel) and $b_J$-band (right-hand panel) luminosity functions at $z = 0$ from DLB07 (dashed red line) and our best-fitting model (solid red line). On the left-hand panel, the observational scatter represents the observations used to constrain the luminosities of galaxies in our MCMC parameters estimation (Cole et al. 2001; Bell et al. 2003; Jones et al. 2006). On the right-hand panel, the $b_J$-band luminosity function is compared with observations from 2dFGRS (green filled squares) and 6DFGS (blue open circles), respectively Norberg et al. (2002) and Jones et al. (2006).
observational data set used to constrain the sampling. As discussed in Section 4.2, to get a good agreement with observations, the model needs to form considerably fewer stars in low-mass galaxies. This is achieved by reducing the amount of cold gas available for star formation by increasing the SN heating efficiency and decreasing the amount of gas reincorporated at each time-step. To assure that enough \( L_\star \) galaxies are produced, the virial velocity cut-off above which SN feedback is ineffective is lowered, by raising \( \epsilon_{\text{disc}} \) relative to \( \epsilon_{\text{halo}} \) (equation 13).

In the right-hand panel of Fig. 9, the best-fitting model seems to show poorer agreement with the \( b_1 \) band than the original DLB07. The new fit does reproduce the number density of dwarf galaxies accurately, but shows a large excess around \( L_\star \). This is partly a reflection of the excess seen in the \( K \) band in the same region, but has a large magnitude. Given the good match to the colour fraction, this seems surprising and points to inconsistencies and/or uncertainties in the conversion of mass to luminosity via stellar population synthesis (see Section 5.3).

5.2.2 Galaxy colours

In Fig. 10, we show the predicted galaxy colours in our best-fitting model, the \( B - V \) colour–stellar mass relation on the top panel and the fraction of red over the total number of galaxies as a function of stellar mass in the bottom panel. Our best fit correctly reproduces the fraction of red galaxies by slightly increasing the number of blue galaxies around \( L_\star \), compared to DLB07.

The colour–stellar mass relation also shows improvements, keeping the bimodality between the red and the blue galaxies, but increasing the slope of each population as suggested by observations. Nevertheless, near the lower-mass limit we impose in our study a population of red dwarfs starts to emerge, representing the highest number density peak in the red population. This is in disagreement with observations, where the majority of the red galaxies are massive, and the dwarfs are predominately blue. We address this problem, and explore possible solutions in Section 6.

5.2.3 The BH–bulge mass relation

The best-fitting BH–bulge mass relation is almost unchanged from that shown in Fig. 5 and so we do not repeat it here. There is enough freedom in the model to allow the AGN parameters to adjust themselves to recover the correct BH masses, despite the differences in the SN parameters between DLB07 and out best fit.

5.3 The galaxy stellar mass function

As discussed in Section 4.2, the stellar mass function is one of the most fundamental properties of a galaxy population, but it is difficult to derive accurately from observations. In Fig. 11, we show how our best-fitting model and DLB07 masses compare with observationally derived stellar mass functions from Bell et al. (2003) and Baldry, Glazebrook & Driver (2008). The latter is one of the most robust mass derivations, using the New York University Value-Added Galaxy Catalogue that combines four different methods for determining galaxy masses from Sloan Digital Sky Survey data. The error bars in the figure span the maximum and minimum mass estimates from that analysis.

After all the data sets are converted into the same IMF (that of Chabrier 2003), the comparison between our best-fitting model and the masses derived from Bell et al. (2003) in Fig. 11 shows the same behaviour as the \( K \)-band luminosity function. With our more effective SN feedback, the excess of dwarf galaxies largely disappears, but there is a slight excess of \( L_\star \) galaxies. Small differences might arise when comparing both the \( k \)-band and stellar mass functions from the model and a specific observational data set, even though similar stellar population synthesis models were used. This is because, to convert stellar mass into luminosity, one should have knowledge about the age and metallicity of the galaxy stellar population. These quantities are directly available in the model, but in observations they are difficult to derive and are subject to large uncertainties.

Also shown in Fig. 11 is a comparison of the predicted masses with data from Baldry et al. (2004). A systematic difference between the model and the data is evident, with the former predicting a much larger number of galaxies on and above \( L_\star \). While the horizontal error bars plotted in Fig. 11 for Baldry et al. (2004) reflect only the
bin size, the authors refer to differences as large as 0.15 dex in mass estimates from the different methods. Another recent work (Conroy, Gunn & White 2008) points to even larger errors of up to 0.3 dex that may result from imprecise modelling of key phases of stellar evolution. If these uncertainties lead to the observationally derived masses of large galaxies being underestimated by about 0.15 dex, then our best fit and observations from Baldry et al. (2008) would be in extremely good agreement throughout the whole mass range.

The differences between data sets highlight the need for caution when galaxy formation models are compared with observations. In principle, one should expect the properties and allowed parameter ranges to change if either the stellar population synthesis or the dust model needs to be readjusted. In this paper, we have chosen to fix these so as to focus our study on the parameters controlling the most basic properties of the SA model: star formation and feedback.

6 DISCUSSION AND CONCLUSIONS

Since they were introduced as a new technique to understand galaxy formation (White & Rees 1978; Cole 1991; Lacey & Silk 1991; White & Frenk 1991), SA models have always lacked a proper statistical analysis of the allowed range of their free parameters and a consistent way to test the goodness of the fits produced.

To overcome this weakness, we have implemented an MCMC parameter estimation technique into the DLB07 SA model, to obtain the best values and confidence limits for the six free parameters in the model responsible for shaping the stellar mass function and for the colours of galaxies. Comparing the model with three different observational constraints separately: the combined BH–bulge mass relation from H09 Jones et al. (2006), galaxy colours from Baldry et al. (2004) and the luminosity function from Cole et al. (2001), Bell et al. (2003), different observational constraints simultaneously: the combined $\pi(X_i) = L_{(\text{mass})} \times L_{(\text{colour})} \times L_{(\text{BH–bulge})} = 0.037$. This value means that the best-fitting solution is incompatible with the three combined observations at the 2$\sigma$ level.

In this paper, we have used the Millennium Simulation which adopts a ΛCDM cosmology. It is possible that the Universe may be better described by an alternative cosmology with fewer low-mass haloes. However, our purpose here is to try to find an astrophysical solution that is compatible with ΛCDM.

As discussed in previous chapters, observational uncertainties, principally that associated with stellar population synthesis and dust modelling, make it premature to conclude that the DLB07 formalism is ruled out: shifting the observed BH/bulge mass ratio by 0.15 dex raises the best-fitting likelihood to 0.07, which is marginally acceptable. Nevertheless, the apparent incompatibility between the BH–bulge mass relation and the other constraints indicates that the BH growth treatment in the model might be too simplistic, in particular by assuming that there is no feedback from the quasar mode, when it seems to be required to reproduce the X-ray luminosity function of haloes (Bower et al. 2008; Short & Thomas 2008). As discussed below, some additional recipes might also need to be included for the model to better reproduce observational luminosities and colours, which could in principle increase the likelihood of the best-fitting model.

We produce a $K$-band luminosity function for our best parameter values that improves the agreement with observations at the low-luminosity end. This is achieved by taking a higher heating efficiency from SN and a lower reincorporation rate of gas ejected from the halo. This reduces the amount of cold gas available to form stars, avoiding the excess of faint galaxies in the original recipe. More effective SN feedback has been proposed in the past. For example, Bertone et al. (2007) studied a wind model that improved the number density of dwarfs for both the mass and luminosity function while improving the distribution of metals. However, the high value of ejection that is required by our model seems to be unrealistic when compared with observations (Martin 1999). This indicates that additional processes such as disruption of satellites through tidal effects might need to be included (Bullock, Kravtsov & Weinberg 2001; Taylor & Babul 2001; Benson et al. 2002; Monaco et al. 2006; Weinmann et al. 2006b; Murante et al. 2007; Henriques, Bertone & Thomas 2008; Somerville et al. 2008).

For both the luminosity-function and colour constraints, the SN reheating and ejection parameters are strongly correlated, which we interpret as an upper virial velocity limit of $140\,\text{km}\,\text{s}^{-1}$ for galaxies that can eject mass via SN heating. Since we need to assume a stronger SN feedback to decrease the faint end of the $K$-band luminosity function, this relatively low value assures that our SN feedback stops being effective for galaxies with masses above $M_r \approx 10^{10.5}\,\text{M}_\odot$. This is the only way to ensure that enough stars will form in brighter galaxies, and also produces more blue galaxies around $L_r$ than the original DLB07 parameters.

Significant correlations exist between the three parameters governing SN feedback, $f_{\text{disc}}, f_{\text{halo}}$, and $y_{\text{ej}}$ even in the combined analysis. This suggests that the model could be rewritten with one or two
fewer free parameters. However, this degeneracy could in principle be broken if the metallicity of gas and stars were to be considered.

The model with the original DLB07 parameters correctly predicts the bimodality in the colour–stellar mass relation, however, it has difficulties in matching the exact number of the blue and red sequence galaxies. Our best-fitting model correctly predicts the relative fraction of galaxies in each colour population; however, the early cut-off on SN feedback leads to an excess of galaxies with masses between $10^{10.5}$ and $10^{11.5} \, M_{\odot}$. Furthermore, as the original model, it shows a large population of small red galaxies in the $B - V$ colour–stellar mass plot in contradiction with observations.

The problems with low-mass galaxy colours in SA models have been identified in the past, particularly the excess of red dwarfs (Baldry et al. 2006; Croton et al. 2006). Possible solutions might include the delayed stripping of gas from satellites after their dark matter halo is disrupted (allowing them to cool gas, form stars and stay blue for longer; Font et al. 2008), or again, tidal disruption of dwarfs, which would affect mostly red, satellite galaxies. This would move them to even lower masses, below $10^{10.5} \, M_{\odot}$ (where an upturn in the stellar mass function is seen) and produce intra-cluster light (Weinmann et al. 2006b; Henriques et al. 2008; Somerville et al. 2008).

The purpose of this paper is to show that MCMC parameter estimation techniques, adapted from those used in cosmology, can be used to map out likelihood contours in the parameter space of SA models of galaxy formation. For this particular analysis, we chose the formalism of DLB07, but the same method could equally be applied to other models.

In the future, we would like to extend the method to undertake model selection, providing an objective measure of the relative value of models with different numbers of free parameters.

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