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Tailoring triaxial *N*-body models via a novel made-to-measure method

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ABSTRACT

The made-to-measure *N*-body method slowly adapts the particle weights of an *N*-body model, whilst integrating the trajectories in an assumed static potential, until some constraints are satisfied, such as optimal fits to observational data. I propose a novel technique for this adaption procedure, which overcomes several limitations and shortcomings of the original method. The capability of the new technique is demonstrated by generating realistic *N*-body equilibrium models for dark matter haloes with prescribed density profile, triaxial shape and slowly outwardly growing radial velocity anisotropy.

Key words: stellar dynamics – methods: *N*-body simulations – galaxies: haloes – galaxies: kinematics and dynamics – galaxies: structure.

1 INTRODUCTION

A standard problem in contemporary galaxy dynamics is the interpretation of kinematic observations of galaxies in terms of their orbital structure as well as their dark and luminous matter distribution. There are several methods one can employ for this problem. First, moment-based methods find solutions of the Jeans equations (or higher order velocity moments of the collisionless Boltzmann equation) that best fit the observed moments, such as density and velocity dispersion. Secondly, distribution-function-based methods directly fit the distribution function to the data, which can be more general than mere moments, e.g. the line-of-sight velocities of many individual objects. Both techniques are usually restricted to spherical or, under certain simplifying assumptions, axisymmetric systems (though for different reasons[1]). However, distribution-function models are technically much more challenging (since an integral equation has to be solved instead of differential equations) and hence much less used than the moment-based approach. In both cases, astrophysically unjustified assumptions, such as velocity isotropy, are often made in order to make the problem tractable.

Thirdly, Schwarzschild's (Schwarzschild 1979, 1993) orbit-based method constructs a dynamical model by first integrating many orbits over many orbital times in an assumed gravitational potential, whereby recording their properties in an orbit library, and then superposing them such that a best fit to the data is obtained. This is a powerful method, since it comes, in principle, without restrictions on the symmetry, and one may even obtain the distribution function (Häfner et al. 2000). However, in practice most applications are restricted to axisymmetry, since there are several technical subtleties to overcome when applying the method to potentials with a complex phase-space structure, the typical situation for triaxial or barred systems (though this is not impossible and has been done, e.g. Häfner et al. 2000).

Fourthly, in 1996, Syer & Tremaine (hereafter ST96) introduced the 'made-to-measure (hereafter M2M) *N*-body method', which slowly adapts an *N*-body model to fit the data. The first application of this method came as late as 2004, when Bissantz, Debattista & Gerhard used it to construct a dynamical model for the Milky Way's barred bulge and inner disc. More recently, De Lorenzi et al. (2007, hereafter DL07) refined the method to incorporate observational errors; this has since been applied for modelling elliptical galaxies to assess their dark matter content (De Lorenzi et al. 2008a,b). The M2M method is as powerful as Schwarzschild's orbit-based method, and in fact is closely related. Whereas in Schwarzschild's approach orbits are first separately integrated and then superimposed, these two steps are merged in the M2M method: trajectories are integrated and their weights adapted at the same time. As a consequence, there is no need for an orbit library and all the technical difficulties associated with it. However, with the M2M method as proposed by ST96 and DL07 some problems remain, as I shall discuss, in particular the appropriate time-scale for adapting the particle weights of the *N*-body model.

Finally, Rodionov, Athanassoula & Sotnikova (2009) introduced a variation of the M2M technique (though the authors did not make this association), which they dubbed the 'iterative method'. Their method starts from a near-equilibrium dynamical model (constructed by any other method), which is alternately relaxed under self-gravity (to evolve towards equilibrium) and adapted to

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[1] For moment-based models, symmetry reduces the number of independent moments and enables simple assumptions necessary to close the Jeans equations. For non-spherical distribution-function models, knowledge of isolating integrals of motion other than energy is necessary, and angular momentum is available only for axial symmetry.

prescribed properties. In practice, this method too employs the N-body approach and, like the traditional M2M technique, suffers from the time-scale problem.

Another application of all the aforementioned techniques is the generation of N-body initial conditions representing a galaxy or galaxy component (though moment-based models additionally require the incorrect assumption of a Gaussian velocity distribution and should not be used for this purpose). However as mentioned above, distribution-function models, which are the most commonly employed technique for generating N-body galaxy models, are restricted to spherical (or, under simplifying assumptions, axial) symmetry, which seriously limits their realism. Since the M2M technique works directly with N-body data, it offers a simple and natural way to generate N-body initial conditions with prescribed properties (ST96), in particular non-spherical shape and non-isotropic velocity structure. As we shall see, however, this requires some modification to the traditional M2M technique.

In this paper, I revisit the M2M method and propose several modifications aimed at improving it, in particular in view of its application for tailoring N-body initial conditions. I present the traditional ST96 and DL07 version of M2M in Section 2 and my modifications to the method in Section 3, while Section 4 presents some tests of tailoring non-spherical and/or velocity-anisotropic N-body models. Finally, Section 5 discusses the results and concludes.

2 TRADITIONAL M2M

In this section, the M2M method as laid out by DL07 (which in turn was based on ST96) is outlined, though with slightly different notation and conventions.

The fitting of the N-body model to the data is expressed as maximization problem: the N-body model shall maximize the *merit function*

$$Q = \mu S - \frac{1}{2} C. \tag{1}$$

Here, C is the *constraint function*, which measures the goodness of fit of the N-body model to some target. There are many possible choices for C, but for now let us follow DL07 and consider a χ^2-like measure of the deviation of moments of the N-body model from target values

$$C = \sum_{j=1}^{n} \left(\frac{Y_j - y_j}{\sigma_j} \right)^2. \tag{2}$$

Here,

$$y_j = \sum_i w_i K_j(\boldsymbol{x}_i, \boldsymbol{v}_i) \tag{3}$$

are some *moments* of the model defined via the *kernel* $K_j(\boldsymbol{x}_i, \boldsymbol{v}_i)$ and the particle weights $w_i \equiv m_i/M_{\rm tot}$, while Y_j are the *targets* for those moments and represent the observed data[2] with uncertainties σ_j.

Simply minimizing C is not a well-defined procedure for two reasons: first, there is no point in reducing C well below the expectation value even if this were possible (this would amount to 'fitting the noise'); secondly, minimizing C may not be uniquely constraining the N-body model: there are, for instance, many possible equilibrium models with the same density. Thus, in order to yield a well-defined problem, one has to *regularize* the merit function by a penalty functional S times a Lagrange multiplier μ, which controls the amount of regularization. The penalty function is traditionally taken to be the pseudo-entropy

$$S = -\sum_i w_i^\star \log \frac{w_i^\star}{\hat{w}_i}, \tag{4}$$

with $w_i^\star \equiv w_i / \sum_j w_j$ the normalized weights and $\{\hat{w}_i\}$ a predetermined set of normalized weights, the so-called priors. For general priors, S defined in this way is the Kullback & Leibler (1951) information distance (also known as 'K–L divergence') of the model corresponding to $w_i = \hat{w}_i$ from the actual N-body model, i.e. S penalizes against deviations of the normalized weights from the priors. Only for $\hat{w}_i \propto f_i^{-1}$, where f_i denotes the value of the equilibrium distribution function corresponding to $w_i = 1/N$, does S reduce to the true entropy of the N-body model (plus a constant; this corrects statements made by ST96 and DL07).

The idea of the M2M method is now to adjust the weights slowly such that Q is maximized. The standard method is to evolve the weights according to

$$\dot{w}_i = \epsilon\, w_i\, U_i \tag{5}$$

with some *rate of change* ϵ and the *velocity of change*[3]

$$U_i = \frac{\partial Q}{\partial w_i}. \tag{6}$$

For the particular choice (2) of the constraint function, this gives

$$U_i = \mu \frac{\partial S}{\partial w_i} - \sum_{j=1}^{n} \frac{Y_j - y_j}{\sigma_j^2} K_j(\boldsymbol{x}_i, \boldsymbol{v}_i). \tag{7}$$

For sufficiently small ϵ, integrating (5) will increase Q and eventually result in an N-body model for which Q is maximal and the w_i no longer change. This method is similar to (and was in fact inspired by) Richardson (1972)–Lucy (1974) iteration, though with a much reduced step size.

Unfortunately, it is not as simple as that, because the merit function, being a function of the randomly sampled particle trajectories, is itself a random variable and fluctuates even with fixed weights. In order to suppress these fluctuations, traditional M2M replaces the model moments y_j in (2) with their time-averaged values $\bar{y}_j$, which are obtained by integrating the differential equation

$$\dot{\bar{y}}_j = \alpha(y_j - \bar{y}_j) \tag{8}$$

starting with[4] $\bar{y}_j = y_j$ at $t = 0$. If fitting to observed data with finite uncertainties σ_j, this method has the virtue that the model uncertainties due to N-body shot noise (which have been ignored in the definition of the constraint function) are much reduced.

A problem with this time averaging is that the computation of the derivatives required for the velocity of change (6) is no longer straightforward. In fact, $\partial \bar{y}_j / \partial w_i$ is simply the time-averaged kernel

[2] This standard practice restricts the data to be just moments of the distribution function, and excludes, for example, the line-of-sight mean and dispersion velocity, which are functions of moments. However, this restriction is not fundamental and the method can easily be extended to fit any function of moments, see Section 4.2 for an example.

[3] Unfortunately, ST96 dubbed $\epsilon w_i U_i$ the 'force of change', which is an inaccurate analogy since it is proportional to the first time derivative of the dependent variable. Below I introduce a method which indeed uses the second time derivative, for which the expression 'force of change' is much more appropriate.

[4] Corresponding to $\bar{y}_j(t) = y_j(0)\,\mathrm{e}^{-\alpha t} + \alpha \int_0^t \mathrm{e}^{\alpha(t'-t)} y_j(t')\,\mathrm{d}t'$; ST96 and DL07 give $\bar{y}_j(t) = \alpha \int_{-\infty}^t \mathrm{e}^{\alpha(t'-t)} y_j(t')\,\mathrm{d}t'$ which results from integrating (8) from $t = -\infty$, a practical impossibility.

– the quantity which in Schwarzschild's method is stored in the orbit library. In traditional M2M, one simply replaces y_j with $\bar{y}_j$ directly in equation (7). Even though, this means that weight adaption is not strictly along the gradient of the merit function, it appears that the method still converges in practice, though it is not completely obvious that it always does (DL07 introduce the time averaging only after they argue for convergence), in particular for other forms of the constraint function than simple χ^2 expressions on model moments.

3 A NOVEL M2M METHOD

In this section, I criticize the traditional M2M method and propose alternatives and/or modifications, which ultimately cumulate in a novel method.

3.1 Time-scales

An important issue is the appropriate choice for the adjustment rate ϵ. The velocity of change (6) varies on the orbital time-scale of the ith trajectory, because different parts of the orbit contribute differently to the merit function. Clearly, the weight adaption should happen adiabatically, i.e. $\epsilon < \Omega_i$ with Ω_i the natural (orbital) frequency of trajectory i. Unfortunately, the orbital frequencies of the N trajectories may easily vary by many orders of magnitude, such that meeting this condition for all of them becomes a serious problem. In traditional M2M, this is not really solved: using a very low adaption rate ϵ ensures that the weights for all but the outermost trajectories are adapted adiabatically.

One may think that using individual adjustment rates $\epsilon_i \propto \Omega_i$ would solve the problem. However, this is not the case: the method no longer converges (it does initially, but eventually convergence stalls well before reaching the optimum), presumably because such an alteration changes the direction of adjustment away from the gradient of Q. Instead, I turn the tables and achieve $\omega_i \propto \epsilon$ by integrating each trajectory on its own dynamical time-scale. To this end, I introduce the dimensionless time

$$\tau = t/T_i \tag{9}$$

with $T_i = 2\pi/\Omega_i$ the orbital period, such that with respect to this new dimensionless time each trajectory has natural frequency $\omega = 2\pi$. The equations of motion for the N-body system expressed in τ are

$$\boldsymbol{x}_i'' = -T_i^2\, \nabla\Phi(\boldsymbol{x}_i), \tag{10}$$

where a prime denotes derivative with respect to τ. Conversely, the M2M equation remains

$$w_i' = \epsilon w_i U_i \tag{11}$$

such that now ϵ is a dimensionless rate per orbit for *each* particle. In practice, a rough estimate for the orbital period, e.g. based on the epicycle approximation, is sufficient for T_i.

3.2 Enforcing total-weight conservation

With the traditional M2M formulation, conservation of the total weight is not guaranteed, as the maximum of Q may occur at $\sum_i w_i \neq 1$. This problem has not been discussed by ST96 and DL07, and I assume that it is dealt with by simply renormalizing the weights after each step.

While this may be a viable method, I propose a somewhat different approach which incorporates the total-weight constraint into the adjustment step. I start by observing that the unconstrained maximum of the modified merit function

$$Q^\star(\boldsymbol{w}) \equiv Q(\boldsymbol{w}^\star) + \ln \textstyle\sum_k w_k - \sum_k w_k \tag{12}$$

maximizes $Q(\boldsymbol{w})$ subject to the constraint $1 = \sum_k w_k$ (e.g. Dehnen 1998). Thus, the total-weight constraint can be incorporated by replacing Q with $Q^\star$ in equation (6). Note that since $Q^\star$ depends on the constraints only through the $w_i^\star$, the N-body system must still be renormalized after each adaption step, but the step hardly carries the system away from normalization.

Alternatively, the total weight of the N-body system may be allowed to float freely and be constrained only by the data via the constraint function.

3.3 An alternative adjustment

As discussed in the last paragraph of Section 2, the traditional time-averaging procedure interferes with the computation of the gradient of the merit function. Moreover, as I shall discuss in the next subsection, the time averaging is particularly undesirable when using the M2M method for tailoring N-body initial conditions. These considerations lead me to consider a different time-averaging approach: instead of averaging the moments, I consider suppressing fluctuations in the merit function by averaging $Q^\star$ (or Q) itself and its derivatives. In analogy to the moment-averaging equation (8), this would yield

$$U_i' = \eta\left(\frac{\partial Q^\star}{\partial w_i} - U_i\right)$$

with the dimensionless averaging rate η. Combining this with the weight-adjustment equation (11) results in a second-order differential equation for $\varphi_i \equiv \ln w_i$:

$$\varphi_i'' = \epsilon\eta \frac{\partial Q^\star}{\partial w_i} - \eta\,\varphi_i'.$$

Thus, $\partial Q^\star/\partial w_i$ acts like a force for the φ_i. I now take this analogy even further and replace it with the gradient of $Q^\star$ with respect to the dependent variable φ_i:

$$\varphi_i'' = \lambda \frac{\partial Q^\star}{\partial \varphi_i} - \eta\,\varphi_i' \tag{13}$$

(where I have substituted λ for $\epsilon\eta$), corresponding to

$$U_i' = \eta\left(w_i \frac{\partial Q^\star}{\partial w_i} - U_i\right). \tag{14}$$

For $\eta = 0$, equation (13) is equivalent to the familiar equation of motion under the influence of the 'potential' $-\lambda Q^\star$. Thus, if the time dependence of $Q^\star$ were solely due to temporal changes in the weights, then the energy-like quantity

$$\mathcal{E} \equiv \tfrac{1}{2} \textstyle\sum_i \varphi_i'^2 - \lambda\, Q^\star \tag{15}$$

is conserved. The frictional term proportional to η in equation (13) in fact ensures that $\mathcal{E}$ is not conserved but decreases, thus ultimately leading to the maximum of $Q^\star$, as desired. Thus, unlike the situation for traditional M2M, where the time averaging of model moments may interfere with the convergence (see the discussion in the last paragraph of Section 2), the time averaging in my approach provides the damping term required for convergence.

3.4 Tailoring N-body initial conditions

As already mentioned in the introduction, the M2M technique offers a natural and powerful way to generate N-body initial conditions with prescribed properties. There is, however, a fundamental difference compared to employing M2M for fitting data: the target values Y_j now represent these prescribed properties and, unlike observed data, have no natural uncertainties. A common practice with model fits without known uncertainties is to simply set $\sigma_j = 1$ (alternatively, setting $\sigma_j = Y_j$ alters C to measure the relative error and yields ST96's original method). However, this is rather unsatisfactory here, as the value obtained for C then no longer provides insight about the goodness of fit.

Moreover, unlike most parametric model fits, an N-body model, being a Monte Carlo representation, does have its own natural uncertainties. This suggests that the σ_j should be set to the uncertainties expected from shot noise in the N-body model itself. If this is done, C retains its interpretability: a good fit corresponds to C equalling to the number of constraints. While this sounds natural and straightforward, it introduces some subtle problems. One problem with traditional M2M is that the time averaging of the model moments intentionally reduces the shot noise, which invalidates the interpretability of C.

With the alternative time averaging of the merit function itself (see Section 3.3), this is no longer the case, but the shot noise in the N-body model causes temporal variations of $Q^\star$ additional to those induced by changing the weights. This means that equation (13) corresponds to following a frictional trajectory (in N-dimensional $\boldsymbol{\varphi}$-space) in a temporally fluctuating potential. The fluctuations are of the same order as the optimal value for C and prevent the algorithm to converge in the sense that $\varphi_i' \propto U_i \to 0$. However, the examples in Section 4 suggest that this is not a serious problem.

3.5 Resampling

The adjustment of the weights in the M2M technique may lead to a wide range of weights (or for $\hat{w}_i \neq N^{-1}$ to a wide range of $w_i/\hat{w}_i$). This potentially reduces the effective resolution of the N-body model substantially and is particularly undesirable if the σ_j represent the uncertainties expected for an N-body system with weights following the priors. A wide range in $w_i/\hat{w}_i$ (corresponding to unequal masses for a flat prior) is also undesirable with N-body initial conditions. Therefore, it is useful to resample the N-body model from time to time during and after the adjustment process. This is easily done by drawing phase-space points for the new model from the original set $(\boldsymbol{x}, \boldsymbol{v})_i$ with probability proportional to the relative normalized weight

$$\gamma_i = w^\star_{i,\mathrm{old}}/\hat{w}_i, \tag{16}$$

and subsequently setting the weights to $w_i = \hat{w}_i$ if the total weight is constraint to unity and $w_i = \hat{w}_i N^{-1} \sum_k w_{k,\mathrm{old}}$ otherwise.

In this process, some trajectories of the original set will not be resampled, others get copied exactly once, yet others several times. In this latter case, I make the first copy a straight clone of the original phase-space point, but for any additional copies, I first randomize position and velocity as far as the underlying symmetry allows (for spherical symmetry, e.g. rotate them by a random angle about a random axis), and secondly add a small random velocity component. This added velocity component prevents multiple trajectories to be on identical orbits, and allows the model to explore phase-space regions of high weights.

In order for the M2M method to still maximize the same merit function, one has to alter the definition of the pseudo-entropy to

$$S = -\sum_i w^\star_i \log \frac{\Gamma_i\, w^\star_i}{\hat{w}_i}, \tag{17}$$

with Γ_i the product of the factors γ_i from each resampling so far. In this way, the contributions to S from each trajectory are on average the same before and after resampling. However, the actual value for S may increase (in particular if a trajectory with $\gamma_i \ll 1$ happens to be resampled).

3.6 Technicalities

The description of my M2M method is completed by giving some technical details. The M2M adjustment step is taken to be $\delta\tau = 2^{-6}$, which appears to be sufficiently short. Between these, the trajectories are integrated using individual adaptive time-steps (which are required despite the fact that every trajectory is integrated on its own orbital time). While this could be implemented with any type of method, I use the traditional N-body block-step scheme with a kick-drift-kick leap-frog and a time-step $\delta\tau = 2\pi f \sqrt{\boldsymbol{x}^2/|\boldsymbol{x}\cdot\nabla\Phi|}/T_i$ with $f = 1/400$. In this way, trajectories are automatically synchronized at M2M adjustment steps and the simultaneous computation of gravitational forces for many positions allows some optimization.

The M2M equations are also integrated using a kick-drift-kick leap-frog – note that equation (14) can be integrated exactly at fixed w_i. In practice, ϵ is grown slowly over $\delta\tau = 1$ to its final value, but also limited to $\epsilon \leq \eta \max\{|U_i|\}$ at any time.

The N-body model is resampled whenever the ratio between maximum and minimum $w^\star_i/\hat{w}_i$ exceeds a certain threshold (4 in the runs of Section 4) and a minimum interval has elapsed since the last resampling ($\delta\tau = 10$ in Section 4). The phase-space coordinates for the kth resampled trajectory are set to those of the ith original trajectory where

$$G_i < \bar{\gamma}\left(k - \frac{1}{2}\right) \leq G_{i+1}, \quad i, k \in [1, N], \tag{18}$$

with $\bar{\gamma} \equiv N^{-1}\sum_k \gamma_k$ the mean relative normalized weight and $G_i = \sum_{k<i} \gamma_k$ the cumulative relative normalized weight of the original model. Trajectories with $\gamma_i < \bar{\gamma}$ generate at most one copy, while those with $\gamma_i > \bar{\gamma}$ get copied once or more. The random component added to the velocities of extra copies is drawn from a normal distribution with standard deviation $0.05\exp(-\tau/10)$ times the local escape velocity (but avoiding generation of unbound trajectories). In the case of a flat prior $\hat{w}_i = N^{-1}$, which I used in Section 4, these relations simplify somewhat (in particular $\bar{\gamma} = N^{-1}$).

The M2M method is ideally suited for distributed-memory parallelization, since the gravitational potential is fixed (no interactions between trajectories) and the evaluation of the merit function and its derivatives require only minimal communications. I implemented my method using the message-passing interface (MPI) and found the resulting code to be superscaling: doubling the number of processors at fixed problem size reduces the execution time to less then half. This is presumably a result of the increase in total cache, reducing the total sum of computation times, which outweighs the small communication overhead.

4 APPLICATION: TAILORED N-BODY INITIAL CONDITIONS

Almost all published N-body simulations featuring individual galaxies use initially spherical dark matter haloes with isotropic velocity distributions. This is because for these settings distribution-function models, on which N-body initial conditions are usually based, are relatively simple to obtain. However, there is no physical justification for these simplifications and triaxial dark matter haloes with anisotropic velocity distributions are certainly more realistic.

Here, I apply my novel M2M method to tailor such N-body initial conditions.

4.1 A triaxial halo model

Let us first consider the problem of designing a triaxial equilibrium with prescribed shape and density profile, but without constraining its velocity structure. The aim is to construct a triaxial truncated Dehnen & McLaughlin (2005) model, which has density

$$\rho \propto \left(\frac{q}{r_\mathrm{s}}\right)^{-7/9}\left[\left(\frac{q}{r_\mathrm{s}}\right)^{4/9}+1\right]^{-6}\operatorname{sech}\frac{q}{r_\mathrm{t}}, \tag{19}$$

with scale radius r_s, truncation radius r_t and 'elliptical radius'

$$q^2 \equiv \frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}, \tag{20}$$

with $abc = 1$. For this model, the radius at which $-\mathrm{d}\ln\rho/\mathrm{d}\ln q = 2$, often referred to as the scale radius for dark matter haloes, equals $r_2 = (11/13)^{9/4} r_\mathrm{s} \approx 0.687 r_\mathrm{s}$. I choose $r_\mathrm{t} = 10 r_\mathrm{s}$ and axis ratios $c/a = 0.5$ and $b/a = 0.7$.

A convenient way to constrain the full three-dimensional density distribution of the model is by means of an expansion in bi-orthonormal potential-density basis functions $\psi_\mathrm{nlm}(\boldsymbol{x})$ and $\rho_\mathrm{nlm}(\boldsymbol{x})$. These satisfy the Poisson equation as well as the bi-orthonormality and completeness conditions

$$-\nabla^2\psi_{\boldsymbol{n}}(\boldsymbol{x}) = 4\pi\rho_{\boldsymbol{n}}(\boldsymbol{x}), \tag{21}$$

$$\int \mathrm{d}^3\boldsymbol{x}\;\psi_{\boldsymbol{n}}(\boldsymbol{x})\,\rho_{\boldsymbol{n}'}(\boldsymbol{x}) = \delta_{\boldsymbol{n}\boldsymbol{n}'}, \tag{22}$$

$$\sum_{\boldsymbol{n}}\psi_{\boldsymbol{n}}(\boldsymbol{x})\,\rho_{\boldsymbol{n}}(\boldsymbol{x}') = \delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{23}$$

where $\boldsymbol{n} \equiv (n, l, m)$. In this study, I use Zhao's (1996) basis set, whose lowest order functions satisfy

$$\psi_0 \propto \frac{1}{\left(|\boldsymbol{x}|^{1/a}+s^{1/a}\right)^{a}}, \quad \rho_0 \propto \frac{1}{|\boldsymbol{x}|^{2-1/a}\left(|\boldsymbol{x}|^{1/a}+s^{1/a}\right)^{2+a}} \tag{24}$$

with scale radius s and a free parameter a, which controls the density profile. The expansion coefficients

$$A_{\boldsymbol{n}} = \sum_i w_i\;\psi_{\boldsymbol{n}}(\boldsymbol{x}_i) \tag{25}$$

are moments of the model and of the form (3), such that the resulting constraint function

$$C_\rho = \sum_{\boldsymbol{n}}\left(\frac{A_{\boldsymbol{n}}-B_{\boldsymbol{n}}}{\sigma_{\boldsymbol{n}}}\right)^2 \tag{26}$$

is of the form (2). Note that the calculation of the derivative

$$\frac{\partial C_\rho}{\partial w_i} = 2\sum_{\boldsymbol{n}}\frac{A_{\boldsymbol{n}}-B_{\boldsymbol{n}}}{\sigma_{\boldsymbol{n}}^2}\psi_{\boldsymbol{n}}(\boldsymbol{x}_i) \tag{27}$$

is equivalent to computing the gravitational potential due to the coefficients $2(A_{\boldsymbol{n}} - B_{\boldsymbol{n}})/\sigma_{\boldsymbol{n}}^2$ at the position $\boldsymbol{x}_i$. This has the benefit that the functionality of an existing basis-function-based N-body force solver (dubbed 'self-consistent field code' by Hernquist & Ostriker 1992) can be readily utilized. I use $s = r_\mathrm{s}$ and $a = 9/4$ for the parameters of the expansion and include terms up to $n_\mathrm{max} = 20$ and $l_\mathrm{max} = 12$. Since the model is forced to have triaxial symmetry already by the assumed underlying gravitational potential (see below), one does not need to constrain this symmetry. This considerably reduces the number of terms in equation (26), since coefficients with odd l or m can be ignored (they vanish for triaxial symmetry) as well as those with $m < 0$ (since $A_{n\,l\,m} = A_{n\,l\,-m}$), which leaves just 588 independent constraints for $N = 10^6$ particles.

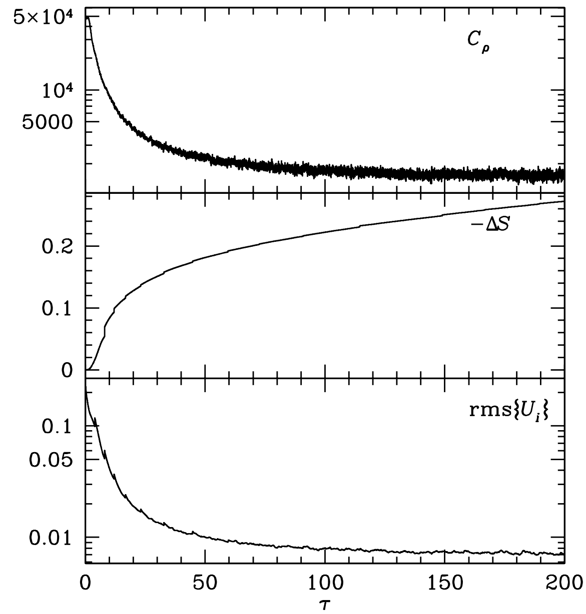

Figure 1. Triaxial model: time evolution of the constraint function C_ρ, pseudo-entropy S and rms value of the velocities of change for the M2M adjustment of $N = 10^6$ particles with $\mu = 100$, $\epsilon = 0.5$, $\eta = 0.5$.

In order to prepare for the M2M adjustment, I sample $N = 10^6$ positions from the target density model and evaluate the resulting $A_{\boldsymbol{n}}$. This is repeated many times to obtain the target values $B_{\boldsymbol{n}}$ and the expected errors $\sigma_{\boldsymbol{n}}$ from ensemble averaging. Next, also the velocities are sampled from the equivalent spherical (and velocity-isotropic) distribution-function model and scaled in each dimension such that the tensor virial theorem is satisfied (whereby correcting for unbound particles). Lastly, to achieve phase-mixing the resulting trajectories are integrated for several orbital times in the potential of the target model computed from the expansion

$$\Phi(\boldsymbol{x}) = -GM_\mathrm{tot}\sum_{\boldsymbol{n}} B_{\boldsymbol{n}}\;\psi_{\boldsymbol{n}}(\boldsymbol{x}). \tag{28}$$

I hoped this procedure already results in a model close to the target, but this was not the case at all: the resulting value for the constraint function (26) is $\sim 5\times10^4 \gg 588$.

Finally, I run the M2M scheme of equations (5) and (14) with $\epsilon = 0.5$, $\eta = 0.5$ and various values for μ, whereby integrating the trajectories in the target potential (28). Fig. 1 shows the time evolution of C_ρ, S and the rms value of U_i for an adjustment run with $\mu = 100$. After a quick reduction of the error (as measured by C_ρ), convergence becomes somewhat slower. C_ρ fluctuates with amplitude similar to its good-fit value of 588, as the discussion in Section 3.4 suggested, and does not reach this value.

In order to independently assess whether the adjustment successfully produced a stable N-body model with the desired properties, I run it for 200 time units[5] (corresponding to $\sim$6 dynamical times at the scale radius) under self-gravity, whereby monitoring shape and

[5] I use a unit system with $r_s = 1$, $G = 1$ and $M = 1$, the total halo mass.

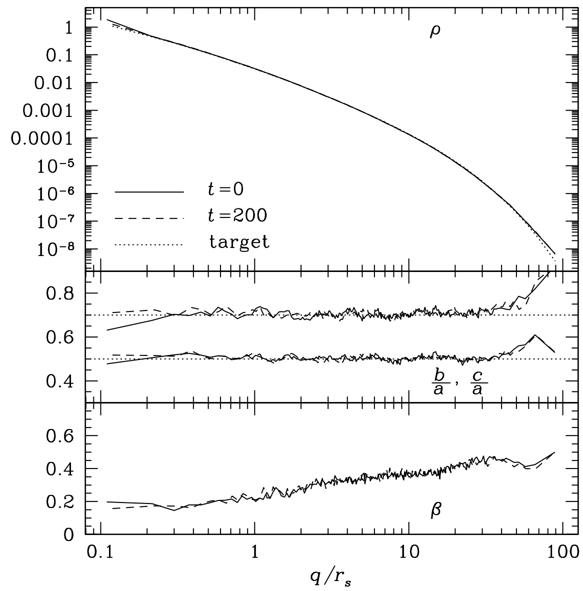

Figure 2. Triaxial model: density (top) and axis ratios (middle) plotted versus elliptical radius for the target model (dotted lines) and the N-body model just after M2M adjustment ($t = 0$) and after running them stand-alone (under self-gravity) for 200 time units. Also plotted is the velocity anisotropy parameter $\beta \equiv 1 - (\sigma_\theta^2 + \sigma_\phi^2)/2\sigma_r^2$ (bottom). Note that the density at very small and large values is overestimated: an artefact of the density estimation procedure.

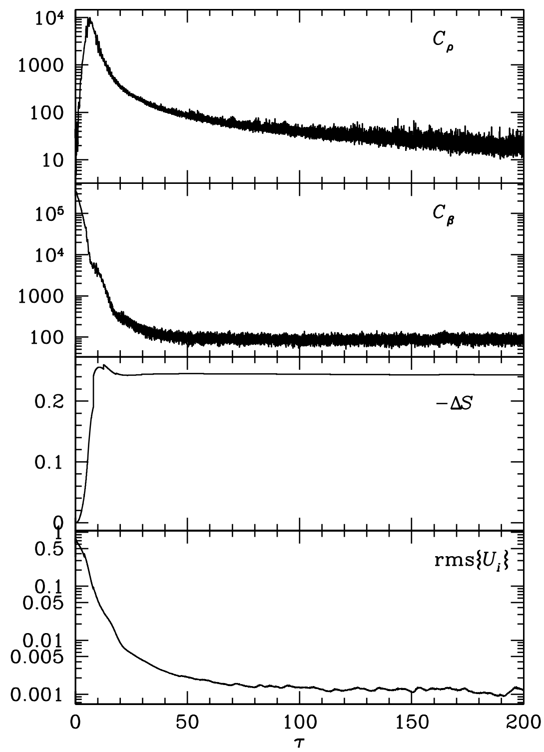

Figure 3. Similar to Fig. 1, but for the M2M adjustment of the spherical model with anisotropic velocities.

density profile. This latter is done by first estimating the density at each particle using a kernel-estimator from its 32 nearest neighbours and then binning particles in density (with 5000 per bin) to estimate the rms radius and axis ratios (from the eigenvalues of the moment-of-inertia tensor) of density shells. As evident from Fig. 2, the N-body model matches the target very well, except for too little flattening in the outermost regions. It appears thus that the failure of convergence of C_ρ close to its good-fit value is caused by the model being too round at very large radii (well outside the virial radius of a CDM halo). The model appears stable: there is no significant change over 200 time units.

4.2 A spherical halo model with anisotropic velocities

Next, I consider the problem of generating a spherical halo model with specified velocity anisotropy. I use the spherical version of the model (19) and aim to constrain Binney's anisotropy parameter $\beta \equiv 1 - (\sigma_\theta^2 + \sigma_\phi^2)/2\sigma_r^2$ to have radial profile

$$\beta_{\rm model}(r) = \beta_\infty \frac{(r/r_s)^{4/9}}{1 + (r/r_s)^{4/9}}. \tag{29}$$

This corresponds to isotropy ($\beta = 0$) in the very centre, and a slowly increasing radial anisotropy (for $\beta_\infty > 0$), reaching $\beta \to \beta_\infty$ at $r \to \infty$, which describes simulated dark matter haloes remarkably well (Dehnen & McLaughlin 2005). If one wants to retain the traditional M2M approach of constraining model moments, one must constrain the moments $\rho\sigma_r^2$, $\rho\sigma_\theta^2$ and $\rho\sigma_\phi^2$ to values obtained from solving the Jeans equation. However, this latter step requires spherical symmetry and hence cannot be generalized to non-spherical systems. Instead, I directly constrain the anisotropy via

$$C_\beta = \sum_j \left(\frac{\beta_j - \beta_{\rm model}(r_j)}{\sigma_j^2} \right)^2, \tag{30}$$

where j indexes radial bins with rms radius r_j and measured anisotropy

$$\beta_j = 1 - \frac{\sum_i w_i (v_{\theta i}^2 + v_{\phi i}^2)}{2 \sum_i w_i v_{ri}^2}, \tag{31}$$

where the sums are over all particles in the jth radial bin. Since β_j is not a moment of the model, but a function (ratio) of moments, it is not of the form (3). However, the derivatives $\partial \beta_j / \partial w_i$, needed for $\partial C_\beta / \partial w_i$, can still be easily computed. The uncertainties σ_j could be estimated from the N-body model, but since such an estimate depends on the w_i and hence adds to $\partial C_\beta / \partial w_i$, this would complicate matters unnecessarily. Instead, I simply assume (with n_j the number of particles in the bin)

$$\sigma_j = (1 - \beta) \sqrt{\frac{3}{n_j - 1}}, \tag{32}$$

which is the standard deviation expected for a multivariate normal velocity distribution[6] with anisotropy β.

Fig. 3 shows the time evolution of the various quantities for an M2M run with $N = 10^6$, $n_{\rm max} = 20$ in C_ρ (only terms with $l = m = 0$ are considered) and 100 radial bins for C_β with $\beta_\infty = 0.75$, i.e. increasing radial anisotropy. The values for the constraint functions converged to their best-fit values relatively quickly and after $\tau \sim 100$ hardly any improvement is made. This is different from the situation for the triaxial halo model in the previous subsection, which took much longer to reduce C_ρ and required much smaller μ. The reason for this difference is not clear, but possibly it is because

[6] This standard deviation also depends on the ratio $\sigma_\theta^2/\sigma_\phi^2$. The minimum occurs for $\sigma_\theta^2 = \sigma_\phi^2$ and corresponds to equation (32), while the maximum (arising at vanishing σ_θ^2 or σ_ϕ^2) is only a factor $\sqrt{4/3}$ larger.

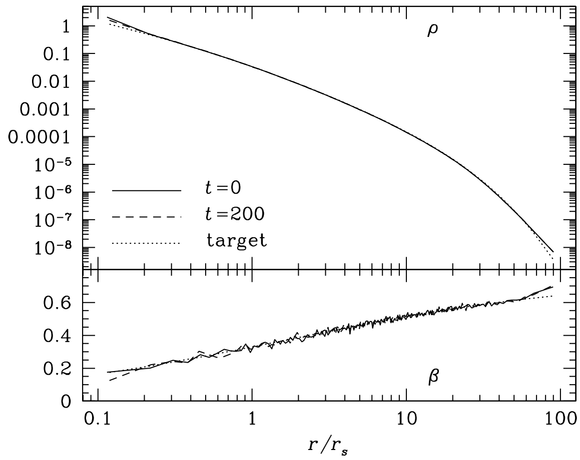

Figure 4. Spherical anisotropic model: radial profiles of density and velocity anisotropy parameter for the target model (dotted lines) and those measured for the *N*-body model just after M2M adjustment ($t = 0$) and after running them stand-alone (under self-gravity) for 200 time units.

the solution space for spherical models with anisotropic velocities is larger than that for triaxial models with the assumed axis ratios.

The resulting radial profiles for ρ and β for the *N*-body model provide an excellent match to the target values both just after the M2M adjustment and after running the model in isolation (under self-gravity) for 200 time units, as demonstrated in Fig. 4.

4.3 A triaxial halo model with anisotropic velocities

Finally, I want to generate a triaxial halo with the same triaxial density distribution as in Secton 4.1 but with the velocity anisotropy profile given by equation (29) with $\beta_\infty = 0.75$, though with r replaced with the elliptical radius q defined in equation (20). To this end, I take the *N*-body models generated in Section 4.1 as starting point for the M2M adjustment. Just as in the previous subsection, the constraint function now consists of two terms, constraining the density and velocity anisotropy, respectively. Figs 5 and 6 show, respectively, the M2M adjustment and the comparison of the final model with the target. Evidently, the model matches the target excellently, even the shape in the outermost parts, which was too round in Section 4.1.

5 DISCUSSION

The basic idea of the M2M method is to adjust the *N*-body weights until the model satisfies some constraints, expressed as maximization of a merit function. This is achieved by changing the weights slowly in the uphill direction of the merit function. While any M2M algorithm must follow this basic recipe, there is significant freedom in the details of how this is done. The purpose of this study was to improve these details compared to the original method as proposed by ST96 and slightly further developed by DL07.

A significant problem of this original method originates from the fact that the natural time-scale for the adjustment (and moment-averaging) is some small multiple of the orbital time. Since the latter varies substantially between orbits and, in particular, has no finite upper limit, any finite value for the adjustment time results in too slow or too fast an adjustment for most orbits. I solved this problem by introducing a dimensionless time variable, which effects to integrating each trajectory for the same number of orbital times. This is similar to Schwarzschild's method, where usually each orbit considered is integrated for a fixed amount of orbital times. In fact, the number of orbital time-scales in Schwarzschild's method is of the same order (~100, depending on details, such as orbital symmetries) as with my M2M technique, indicating that for typical orbits this number is required to gather sufficient information.

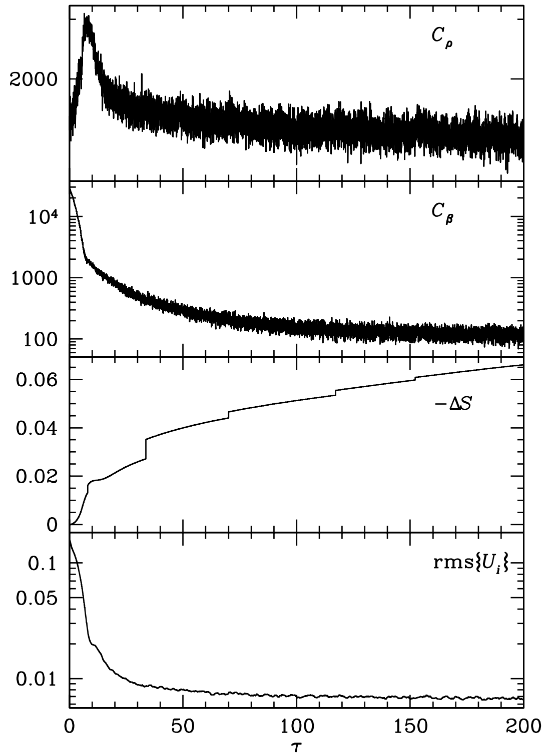

Figure 5. Similar to Figs 1 and 3, but for M2M adjustment of triaxial model with anisotropic velocities.

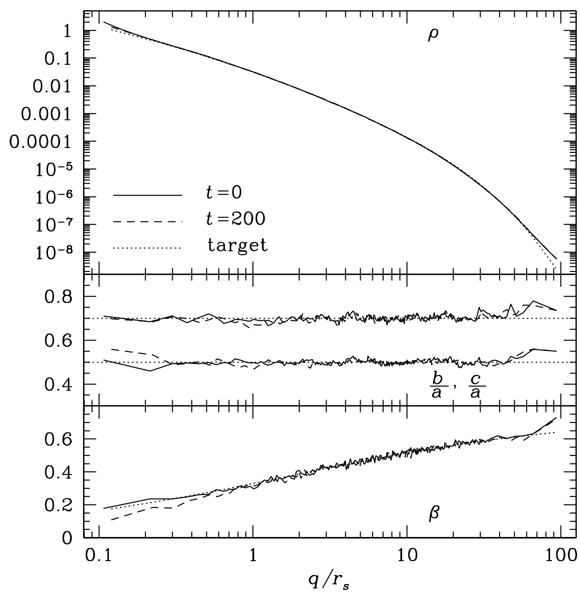

Figure 6. Triaxial model with anisotropic velocities: radial profiles of density, axis ratios and velocity anisotropy parameter for the target model (dotted lines) and those measured for the *N*-body model just after M2M adjustment ($t = 0$) and after running them stand-alone for 200 time units.

Note that the iterative method of Rodionov et al. (2009), mentioned in the introduction, suffers from the same basic problem:

evolving the model over some (short) time-scale will bring the inner parts, where the dynamical time is short, much closer to equilibrium than the outer parts. In order to gather sufficient information about the dynamics in the outer parts, one would need to integrate orbits (or evolve the model) over a considerably longer time than is often practical.

Another issue with the original M2M method is that the averaging of the model moments, required to suppress N-body shot noise, interferes with the adjustment process, though apparently this did not lead to practical problems so far. However, if the M2M method is used to tailor N-body initial conditions, the uncertainties entering the constraints are not observational errors but those due to shot noise in the N-body model itself. In this case, time averaging the model moments reduces this shot noise and renders the interpretation of the χ^2-like constraint meaningless. I have overcome both these problems by introducing a novel adjustment algorithm which effects to time averaging the merit function instead of the model moments and corresponds to following an orbit in N-dimensional weight space with the merit function representing the potential. A damping term, which emerges from the averaging, guarantees that the maximum of the merit function will be reached.

I also propose to (optionally) modify the merit function such that it automatically meets the total-mass conservation constraint. Finally, I propose to resample the N-body model from time to time during the M2M adjustment process to (1) avoid a loss of resolution because of unequal weights and (2) to allow the model to explore phase-space in regions of high weights. This latter is achieved by adding a small random velocity to extra copies of trajectories, effecting to probe another orbit close to a highly weighted one.

Certainly, one can think of further improvements to the M2M method. One issue is an automatic adaption of the parameters ϵ and η to achieve optimal convergence (a technique to adapt μ such that the constraint function obtains a certain numerical value was already proposed by ST96). The priors for the weights can be used to allow the N-body model to have different mass resolution in different phase-space regions, which is a common technique (e.g. Zemp et al. 2008; Zhang & Magorrian 2008) for increasing the resolution in, say, the inner parts of models for dark matter haloes. A significant speed-up may be achieved by starting with a relatively low number of particles and increasing N (essentially like resampling) only later after the merit function is close to maximal.

Finally, one would like to adapt not only the weights of the N-body model, but also the underlying mass distribution generating the gravitational potential, for instance when interpreting kinematic data in terms of the underlying (dark) matter distribution. Unfortunately, changes in the orbits induced by changes of the gravitational potential are not straightforward to anticipate and hence to take into account in the adjustment process. In a spherical setting, one may, for instance, rescale the phase-space coordinates of every particle such that the eccentricity, inclination and mean radius are preserved when the gravitational potential is changed. Unfortunately, however, something similar can no longer be done in the general, i.e. triaxial, case. Thus, it seems that this is a really hard problem and that one is forced to 'jump' from one mass model to the next whereby starting from the best-fit N-body model of a 'nearby' potential. In this case, convergence may be fast, i.e. only a few ten orbital times, leading to significant speed-up.

As the practical examples of the previous section demonstrated, my novel M2M algorithm is a powerful tool to construct N-body models with specified properties. One may use the method to explore possible stellar-dynamical equilibrium solutions and their properties. For instance, the triaxial models of Section 4.1 exhibit a significant radial velocity anisotropy (Fig. 2 bottom panel), even though the initial conditions fed to the M2M adjustment procedure were created from a velocity isotropic model and the velocity structure was not constrained. This strongly suggests that radial velocity anisotropy is an inevitable property of (non-rotating) triaxial equilibrium models. This can be qualitatively understood from the inevitable prevalence of box orbits, which are the only orbital family supporting a triaxial shape, but a more quantitative understanding would be desirable.

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