TESTING HIGHER–ORDER LAGRANGIAN PERTURBATION THEORY AGAINST NUMERICAL SIMULATIONS –

2. HIERARCHICAL MODELS

by

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Summary: We present results showing an improvement of the accuracy of perturbation theory as applied to cosmological structure formation for a useful range of scales. The Lagrangian theory of gravitational instability of Friedmann–Lemaitre cosmogonies investigated and solved up to the third order in the series of papers by Buchert (1989, 1992, 1993), Buchert & Ehlers (1993), Buchert (1994), Ehlers & Buchert (1994), is compared with numerical simulations.

In this paper we study the dynamics of hierarchical models as a second step. In the first step (Buchert, Melott and Weiß 1994) we analyzed the performance of the Lagrangian schemes for pancake models, i.e., models which initially have a truncated power spectrum. We here explore whether the results found for pancake models carry over to hierarchical models which are evolved deeply into the non-linear regime. We smooth the initial data by using a variety of filter types and filter scales in order to determine the optimal performance of the analytical models, as has been done for the “Zel’dovich–approximation” – hereafter TZA – (as a subclass of the irrotational Lagrangian first-order solution) in previous work (Melott et al. 1994a). We study cross–correlation statistics employed in previous work for power–law spectra having indices in the range $(-3, +1)$.

We find that for spectra with negative power–index the second–order scheme performs considerably better than TZA in terms of statistics which probe the dynamics, and slightly better in terms of low–order statistics like the power–spectrum. In cases with much small–scale power the gain from the higher–order schemes is small, but still measurable. However, in contrast to the results found for pancake models, where the higher–order schemes get worse than TZA at late non–linear stages and on small scales, we here find that the second–order model is as robust as TZA, retaining the improvement at later stages and on smaller scales. In view of these results we expect that the second–order truncated Lagrangian model is especially useful for the modelling of standard dark matter models such as Hot–, Cold–, and Mixed–Dark–Matter.
1. Introduction

The non-linear modelling of inhomogeneities initiated by small-amplitude fluctuations at the time of decoupling of matter and radiation has been, for a long time, the privilege of numerical N-body simulations. Recently, the interest in the question has grown how well this modelling can be achieved by analytical or semi-numerical methods. Most of those efforts concentrate on Lagrangian methods introduced in a pioneering work on the Zel’dovich (1970, 1973) approximation (hereafter ZA). Here, we pursue a systematic analysis of analytic solutions obtained in the framework of the Lagrangian instability picture investigated by one of us (Buchert 1989, 1992). Lagrangian perturbation solutions are available up to the third order (Buchert 1994). In this paper we restrict the presentation of results to the first and second-order schemes (Buchert & Ehlers 1993, Buchert 1993a).

Parallel efforts in this direction, though less systematic, have been undertaken by Moutarde et al. (1991), Bouchet et al. (1992), Gramann (1993), and Lachièze-Rey (1993a,b). Other approximations are also built in a similar spirit, for instance the “adhesion model” (Gurbatov et al. 1989) introduces an artificial viscosity term into Zel’dovich’s formalism, the “frozen-flow-approximation” (Matarrese et al. 1992) assumes constancy of the velocity field, the “frozen-potential-approximation” (Brainerd et al. 1994, Bagla & Padmanabhan 1994) assumes constancy of the gravitational potential. All of these approaches are able to some extent to mimic the results of N-body simulations (for the first see Kofman et al. 1992 and Melott et al. 1994c, for the second, Melott et al. 1994b, for the third see either reference). All of them attempt to repair a major shortcoming of ZA which predicts uncomfortably thick pancakes after shell-crossing: In the “adhesion model” a viscosity term mimics a ‘sticking’ of pancakes. In the “frozen-flow-approximation” only the first-generation pancakes are reached and only asymptotically. The “frozen-potential-approximation” (as a semi-numerical model) counteracts the thickening of pancakes by modelling secondary shell-crossings, a feature which is observed in numerical simulations as well as in the higher-order Lagrangian schemes analyzed here (compare Buchert & Ehlers 1993), and can therefore be attributed to part of the “true” effect of self-gravity. However, it is almost as time consuming as a full (Particle-Mesh) N-body simulation. Other work to be mentioned in this context are the articles by Matarrese et al. (1993), Kasai (1993), Croudace et al. (1994), Bertschinger & Jain (1994), Bertschinger & Hamilton (1994), Kofman & Pogosyan (1994), Salopek et al. (1994), dealing with the corresponding equations of General Relativity, or their Newtonian limit, respectively, and Giavalisco et al. (1993), Munshi & Starobinsky (1994), Munshi et al. (1994). Matarrese et al. (1994) presented a general relativistic second-order Lagrangian solution.
There are two major problems with most of the tests (if there were any tests) of various schemes discussed here: (1) Some of them were tested by different techniques for accuracy, and against different simulations. This makes it impossible to compare their accuracy. (2) Often CDM spectra were used (e.g., Bagla & Padmanabhan 1994). Since the spectral index of CDM is negative on scales going non-linear (more so with biasing), it is not hard to get it more or less correct with ZA or ZA–based approximations.

Coles, Melott and Shandarin (1993) (hereafter CMS) and Melott, Pellman and Shandarin (1994a) (hereafter MPS) conducted a series of tests of analytical approximations by cross–correlating them with N–body simulations. They tested the Eulerian linear perturbation solution and ZA, i.e., the Lagrangian linear solution. They found that the latter is considerably more successful than the former. Considerable further improvement is made if ZA is applied not to the full power spectrum, but only to a truncated body of the spectrum (TZA). The truncation removes unwanted non–linearities, which are evolved beyond the range of applicability of the model. The shape of high–frequency filters imposed on the power–spectrum was found to be important (MPS). Most successful in respect of improvement of the cross–correlation statistics was the use of Gaussian filters, but if one wishes to work backwards from evolved to initial state, a sharp truncation (step function) in $k$ is preferable (Melott 1993).

Most recent work has applied these tests to compare TZA with the “adhesion model” and the “frozen–flow–approximation”. The result was that those procedures provide reasonable statistical toy models, however, they are both dynamically less accurate than TZA as demonstrated by the comparison of their cross–correlation statistics in the fully developed non–linear regime (Melott et al. 1994b,c). The comparison of higher moments – skewness and kurtosis – of the density contrast in the weakly non–linear regime (Bernardeau 1994, Munshi & Starobinsky 1994, Munshi et al. 1994) has also demonstrated that the “frozen–flow–” and “frozen–potential–” approximations are dynamically less accurate than ZA. However, the results of the latter tests cannot be extrapolated to late non–linear stages, where also ZA has to be replaced by TZA.

Because of the success of TZA it is worthwhile to study higher–order corrections to ZA as a subclass of the first–order Lagrangian perturbation solution (Buchert 1992) and also truncate the initial data in these models to see whether the performance of TZA can be further improved. We here continue our study on the Lagrangian perturbation schemes begun by Buchert, Melott and Weiß (1994a), henceforth BMW. In that paper we concentrated on pancake models, i.e., models which do not involve small–scale power in the initial conditions. We did this as a first step in understanding the limitations of higher–order corrections to Zel’dovich’s mapping. Also, pancake models can be understood as generic
archetype of hierarchical models which involve pancaking on all spatial scales (Kofman et al. 1992). In a second step, we here analyze (in the spirit of MPS) various power–spectra which are evolved deeply into the non–linear regime in order to probe the performance of the Lagrangian approximations in the case of hierarchical models. Although, it is not expected that a perturbation approach can be used to model highly non–linear stages, we here demonstrate that one can obtain good agreement with the N–body simulation by smoothing the initial data before evolving them.

BMW found that the second–order approximation provides in pancake models a definite and useful improvement upon the first–order approximation (ZA). We explore now whether this improvement carries over to hierarchical models.
2. Numerical realization, Lagrangian perturbation schemes
and cross–correlation statistics

2.1. Numerical realization

We specify initial data in terms of the power–spectrum \( P(k) \) (as a function of comoving wavenumber \( k = |\vec{k}| \)) of Gaussian density perturbations of the form:

\[
P(k) = \langle |\delta_k|^2 \rangle \propto |\vec{k}|^n,
\]

where \( \delta_k \) is the discrete spatial Fourier transform of the density contrast \( \delta \), and \( \langle ... \rangle \) denotes ensemble average over the entire distribution, assumed to be equivalent to the spatial average. We consider the range of indices \(-3 \leq n \leq +1\); for all spectra we use the same set of random phases, so that the overall structure is similar in all realizations.

We emphasize that we have to give initial data early in order to fairly estimate the effect of the higher–order schemes and to guarantee an objective modelling of the collapse of first objects in the model (see the discussion in BMW). For the spectra with indices \( n = -3, -1 \) and \( n = +1 \) we give initial data at the r.m.s. density contrast of \( \sigma_i(k_{Ny}) = 0.05 \), where \( k_{Ny} \) is the Nyquist frequency. For the other two indices we have taken a larger amplitude \( \sigma_i(k_{Ny}) = 0.2 \), which is about that amplitude people normally use. This we did in order to see, whether there is any detectable effect. Indeed we found an effect which will be reported in Section 3 (see also Melott et al. 1994c).

In order to let the concrete normalization of the spectra open, we define the evolution stages of the realizations in terms of the non–linearity scale \( k_{nl}(t) \):

\[
a^2(t) \int_0^{k_{nl}(t)} d^3k \ P(k) = 1 ,
\]

where \( k_{nl}(t) \) is decreasing with time as successively larger scales enter the non–linear regime; \( a(t) \) is the scale factor of the homogeneous background \( a(t_i) := 1 \). The evolution of inhomogeneities is modelled in a flat Einstein–de Sitter background \( a(t) = (\frac{t}{t_i})^{2/3} \). We shall study two stages corresponding to \( k_{nl} = 8k_f \) and \( k_{nl} = 4k_f \), where \( k_f \) is the fundamental mode of the simulation box. Thus, our models studied here have been evolved for expansion factors of 240 to 5100, depending on spectral index and \( k_{nl} \). We shall present all statistical results for both stages.

We evolve the fields with an enhanced PM (Particle–Mesh) method (Melott 1986) using \( 128^3 \) particles each on a comoving \( 128^3 \) mesh with periodic boundary conditions.
This method makes the code resolution–equivalent to a traditional PM code with $128^3$ particles on a $256^3$ mesh (see Park 1990, 1991, and Weinberg et al. 1994). We then bin the data into a $64^3$ mesh using the CIC scheme. Due to our controls (the same initial phases in all simulations) it is not necessary to do an ensemble of simulations with each power spectrum. One of each spectral type is sufficient to uncover systematic effects due to changing approximations. For more details see CMS.
2.2. Lagrangian perturbation schemes

For the Lagrangian perturbation schemes up to the third order and their realization see Buchert (1994) and BMW. However, we here restrict the presentation of results to the first– and second–order schemes, the second–order scheme is expected to contain the major effects on large scales according to the results of BMW for the present purpose. But, we also made a consistency test by going to the third order.

Denoting comoving Eulerian coordinates by $\vec{q}$ and Lagrangian coordinates by $\vec{X}$, the field of trajectories $\vec{q} = \vec{F}(\vec{X}, t)$ up to the second order reads:

$$\vec{F} = \vec{X} + q_1(a) \nabla_0 S^{(1)}(\vec{X}) + q_2(a) \nabla_0 S^{(2)}(\vec{X}) ,$$

with the time–dependent coefficients expressed in terms of the expansion function $a(t) = (\frac{t}{t_i})^{2/3}$:

$$q_1 = \left(\frac{3}{2}\right) (a - 1) ,$$

$$q_2 = \left(\frac{3}{2}\right)^2 \left( -\frac{3}{14} a^2 + \frac{3}{5} a - \frac{1}{2} + \frac{4}{35} a^{-\frac{4}{3}} \right) .$$

The perturbation potentials have to be constructed by solving iteratively the 2 Poisson equations:

$$\Delta_0 S^{(1)} = I(S_{i,k}) t_i ,$$

$$\Delta_0 S^{(2)} = 2 II(S_{i,k}^{(1)}) ,$$

where $I$ and $II$ denote the first and second principal scalar invariants of the tensor gradient $(S_{i,k}^{(1)})$:

$$I(S_{i,k}^{(1)}) = tr(S_{i,k}^{(1)}) = \Delta_0 S^{(1)} ,$$

$$II(S_{i,k}^{(1)}) = \frac{1}{2} [ (tr(S_{i,k}^{(1)}))^2 - tr((S_{i,k}^{(1)})^2) ] .$$

The general set of initial data is restricted according to the assumption of parallelism of the peculiar–velocity field and the peculiar–acceleration field at the initial time $t_i$ (see Buchert 1994 and ref. therein for a discussion of this restriction). Therefore, the initial fluctuation field can be specified to the peculiar–velocity potential $S$ alone. We can set $S^{(1)} = S t_i$ (which is the unique solution of the first Poisson equation (3c) for periodic initial data, see Buchert 1992, Ehlers & Buchert 1994). Doing this, the flow–field (3) reduces to $ZA$ if restricted to the first order.
We realize the solution by first solving Poisson’s equation for $S$ via FFT (Fast Fourier Transform) from the initial density contrast $\delta$ generated as initial condition for the numerical simulation. In an Einstein–de Sitter model we have:

$$\Delta_0 S = -\frac{2}{3t_i} \delta .$$

(4)

We then calculate the second principal invariant $II$ directly from $S$ and solve the second Poisson equation (3d) using FFT. The density in the analytical models is calculated by collecting trajectories of the Lagrangian perturbation solutions at the different orders into a $64^3$ pixel grid with the same method (CIC binning) as in the N–body simulation.

The CPU times on a CRAY YMP are for the first–order scheme 25 seconds, and for the second–order scheme 60 seconds; the corresponding CPU times on a CONVEX C220 are 2 and 5 minutes. Thus, even the second–order scheme is competitive with one step in a corresponding PM–type N–body simulation.
2.3. Cross–correlation statistics

For the presentation of the cross–correlation statistics we refer the reader to CMS, MPS
and BMW for details. We use four statistics. Firstly, the usual cross–correlation coefficient
$S$ to compare the resulting density fields:

$$S := \frac{\langle \delta_1 \delta_2 \rangle}{\sigma_1 \sigma_2}, \quad (5)$$

where $\delta_\ell, \ell = 1, 2$ represent the density contrasts in the analytical and the numerical
approximations, respectively, $\sigma_\ell = \sqrt{\langle \delta_\ell^2 \rangle - \langle \delta_\ell \rangle^2}$ is the standard deviation in a
Gaussian random field; averages $\langle ... \rangle$ are taken over the entire distribution. We believe
this is the most important statistical test, because it measures whether the approximation
is moving mass to the right place, with an emphasis on dense regions. We allow for small
errors by presenting $S$ for the two density arrays smoothed at a variety of smoothing
lengths.

Secondly, the power spectrum (eq. (1)) of the evolved N–body model and the analytic
approximations were calculated. Thirdly, the mass density distribution for both of them
are also shown. Both of these are widely displayed diagnostics in cosmology.

MPS found that the primary reason for the superiority of one window function over
another (equations (6) below) lay not in the final power spectral amplitudes but in the
phase angle accuracy. We therefore follow MPS and will display $\langle \cos \theta \rangle_k$, where $\theta =
\phi_1 - \phi_2$ is the difference in the phase angle of the Fourier coefficients of mass density
between the approximation and the simulation. The averaging is over all coefficients with
the same magnitude of wave vector, as in the power–spectrum.
3. Filtering the initial data

For the analytical realizations we filter the power–spectrum on various scales $k_c$ using a set of “trial windows”. The use of Gaussian windows proved to yield the best cross–correlation with the N–body simulations in previous work on TZA (see MPS). We here again test three main types, sharp $k$–truncation (a), Gaussian windows (b), and tophat–smoothing (c). The filters (a) and (b) are described in Fourier space, whereas the filter (c) is applied in real space (but the computing for (c) is done in Fourier space). The initial data are modified to $\delta_k^* = W \delta_k$, where the different filters $W$ are:

\begin{align*}
W_{tr}(k; k_{tr}) &= \begin{cases} 1, & k \leq k_{tr} \\ 0, & k > k_{tr} \end{cases} \quad (6a) \\
W_G(k; k_G) &= e^{-k^2/2k_G^2} \quad (6b) \\
W_{th}(k; R_{th}) &= \left( \frac{\sin(R_{th}k)}{(R_{th}k)^3} - \frac{\cos(R_{th}k)}{(R_{th}k)^2} \right) \quad (6c)
\end{align*}

We explored a wide range of values for the scale of each possible filter to find the optimum scale $k_{opt}$ for each type, as done for first–order (ZA) by MPS.

In Figs.1 we display the cross–correlation coefficient (eq. (5)) as obtained from a comparison of the truncated analytical schemes with the raw data of the numerical simulations against the truncation scale for all spectra and for all filter types. This shows how the optimal truncation (defined as the scale with the largest cross–correlation coefficient) is varying with scale. In the cases with negative power index we notice that the variation in $S$ with scale is much smaller towards higher $k$ than in the cases with positive power index. The variation effect is very weak in cases with small–scale power index less than $n = -1$.

While type (c) gives much better agreement with the N–body results than simple $k$–truncation (a), we find as in MPS that the best filter type is always (b). Although the values for $S$ for the best truncation are numerically similar for type (b) and (c), the truncation scale for the best agreement is always larger for type (c), thus erasing more non–linear information. We therefore concentrate our further analysis on type (b) and recommend generic use of Gaussian filtering.

In Table 1 we display the values of $S$ for the optimal truncation scales $k_{opt}$ for the different power–spectra and Lagrangian schemes. In Fig.2 we illustrate this table by plotting $S$ versus the power index $n$. We see an almost constant (but small) improvement of the second–order scheme over first–order for positive indices. As soon as the index drops negative we find increasing improvement with decreasing power. Fig.2 also shows that
we obtained slightly different performance for the models with spectral index \( n = 0 \) and \( n = -2 \). These models have been started at a later stage (compare 2.1). We think that this could be an indication for inaccuracies of the numerical evolution code for low–amplitude initial conditions, which we want to test in future work (see also Melott et al. 1994c).

We have used discrete steps in \( k \) to find the optimal truncation lengths. If we express the optimal scales in terms of the non–linearity scale, e.g., \( k_{nl} = 8k_f \), we find that the arithmetic mean (used here as a spectrum independent estimate) lies for the first–order scheme at \( 1.45k_{nl} \), for second–order at \( 1.2k_{nl} \), i.e., at a slightly larger scale. This difference almost vanishes at the later stage \( (k_{nl} = 4k_f) \), where the arithmetic means are \( 1.5k_{nl} \) for first–order and \( 1.4k_{nl} \) for second–order. Still, within the uncertainty bounds involved in the determination of the optimal scale we can recommend generic use of a \( k \)–scale close to, but larger than the non–linearity scale as suggested by MPS. In real space this means that the comoving truncation scale \( \lambda_T < \lambda_{nl} \). It is interesting that, although the second–order scheme requires slightly larger truncation scales, the dependence of that scale on the spectrum is weaker than in the first–order scheme. We emphasize that for negative–sloped spectra the truncation scale \( \lambda_T \) is especially small; in view of Fig.1 a truncation of models with negative spectral slope is not as important as in the other models. For spectra \( n \leq -2 \) the differences in \( S \) on the small–scale end are negligible. These models perform well even without truncation as will become evident from the Figs.4 below.

We proceed by statistically analyzing the optimally truncated models only, with \( k_{opt} \) according to Table 1. The results are presented and discussed in the next section.
4. Discussion of the results

We first concentrate on the first stage corresponding to $k_{nl} = 8k_f$.

Fig. 3 presents the cross–correlation coefficient with the N–body simulation as a function of scale for the optimally truncated and untruncated first– and second–order schemes together with two versions of the (still widely used) Eulerian linear approximation: (1) linear density contrast, and (2) (following CMS): “chopped” linear density contrast, i.e.: $1 + \delta_{\text{chopped}} = \alpha(1 + \delta)$, if $\delta > -1$ and 0 otherwise, where $\alpha$ is the normalization constant keeping the total mass the same. We have chosen the spectra with indices $n = -1$ and $n = +1$ for the illustration of the differences among the different approximations. This comparison again demonstrates that the Lagrangian schemes (even in their untruncated form) perform substantially better than the Eulerian solution with or without “chopping”. In comparison with the following figures this demonstration should teach that the Eulerian approach is almost useless to describe even slightly non–linearly evolved density fields.

In Figs. 4 we display slices of the density contrast field as predicted by the N–body simulations and the two optimally truncated Lagrangian perturbation schemes. We also display the evolved fields for the untruncated perturbation schemes to illustrate the effect of truncation, and for the “chopped” Eulerian first–order model. The structures for different power–spectra bear family resemblance due to our phase controls.

Generally, we appreciate a reasonable correspondence of the numerical density fields with those of the truncated Lagrangian schemes. Although, in the cases with small amount of power on small scales (especially $n = -2, -3$) the pictures for the untruncated models might suggest better coincidence with the numerical density fields, the cross–correlation statistics with the raw numerical data (shown in Figs. 1) prove that the truncated models agree slightly better. However, in these models the truncation plays a peculiar role, since the cross–correlation coefficient only varies weakly as a function of scale by going to smaller scales. The small numerical differences in the coefficients can be seen in Figs. 1. Already small differences in the N–body computing can yield different “optimal” truncation scales. Within this uncertainty, it is a matter of standards we want to apply, whether we truncate the models $n = -2, 3$ or not. But, clearly for models with spectra $n > -2$, truncation of the initial data is indispensible.

The contours of the optimally truncated first– and second–order models are quite similar; visually manifest differences only occur for the cases $n = -2$ and $n = -3$. Note that this is also due to the presentation in terms of grey–scale plots which are truncated at small density levels (density contrast 5), where both schemes predict similar contours. The higher cross–correlation coefficient of the second–order scheme reported below is the result of sharper and higher density peaks at second order, visible at higher density levels.
In Figs. 5 we show the r.m.s. density contrast of the N–body simulations together with that of the analytical schemes as a function of scale. In the following figures we shall use the r.m.s. density contrast of the N–body simulations as a scale parameter.

Figs. 6 show the most important result of this paper: the cross–correlation coefficient for different smoothing scales (smoothed with a Gaussian window) for different power–spectra and the two truncated Lagrangian schemes. We infer that the second–order approximation shows higher cross–correlation with the N–body density field for all spectra and for all scales. However, at this stage the improvement is small in cases with non–negative power index, but it grows substantially with decreasing small–scale power. This result can already be seen in Fig. 2. In general, we find that for negative power indices the agreement with the N–body field is very good, especially on scales which are relevant for modelling large–scale structure (i.e., above the scale of galaxy clusters), bearing in mind that both the numerical simulations and the analytical schemes are assumed to be approximations to the unknown exact solution of the problem. On scales far below the non–linearity scale, where the r.m.s. density contrast of the N–body simulation assumes the value 2, the cross–correlation coefficient generally lies close to $S = 0.8$ in the first–order scheme, while the second–order scheme is closer to $S = 0.9$ for negative–sloped power–spectra.

While the cross–correlation test yields information on the dynamical capabilities of the models, the following statistics show whether they are useful in reproducing statistical properties of the density field.

In Figs. 7 we display the power–spectra as calculated from the final distributions. We confirm the results by MPS who found a weak representation of the power–spectrum on scales below the non–linearity scale in TZA for positive power–spectra slopes. Here, the second–order result does not improve upon first–order. Again, for negative slopes, the agreement is reasonably good for both approximation schemes also below the non–linearity scale. In summary, for much small–scale power the power–spectrum is weakly represented below the non–linearity scale and especially below the comoving truncation scale $\lambda_T$. This is evident, since a truncation of the spectrum removes power which cannot be compensated by non–linear evolution.

The power–spectrum provides low–order statistical information. Figs. 8 and 9 present statistics which probe higher–order information of the density distribution. We find that phase–information is represented much better in the second–order scheme in the cases $n = -2 - 3$, while in all other cases the performance of second–order is moderately better than the first–order model. Also here we see that the positive second–order effect is counteracted by a large amount of small–scale power at this stage which erases phase–
information present in the weakly non-linear regime.

The density distribution functions (Figs.9) show excellent agreement with the N–body result for all cases with negative power index; for \( n = 0, +1 \) the number of high–density cells is underestimated and the number of low–density cells is overestimated by both schemes. The improvement due to the second–order correction is still measurable.

For the sake of showing consistency of our results, we made two further studies: (1) we evolved the fields to a later non–linear stage, where the non–linearity wavenumber has dropped to half the value of the stage analyzed above; (2) we also calculated the statistics for the third–order model (see BMW).

In Figs.10–14 the statistics corresponding to Figs.5–9 are displayed for the later stage with \( k_{nl} = 4k_f \).

One of the striking results obtained by MPS concerning the cross–correlation analysis is that TZA has proved to be very robust, i.e., the good performance of this model remains stable by going to later stages, or to smaller scales, respectively. In the context of the Lagrangian perturbation solutions, BMW attributed this property to the fact that TZA is the principal first part of a perturbation sequence, while higher–order corrections display a “blow–up” phenomenon at and after the stage when the perturbation theory breaks down. Interestingly, we here find that the improvement found for the second–order Lagrangian scheme is also robust, i.e., at later stages and on small scales the truncated second–order model does not become worse than TZA as observed for pancake models by BMW. This feature can be traced back to the optimal filtering employed here which compensates the “blow–up” of the higher–order coefficients by the choice of a different optimal scale for each order. Moreover, the improvement of second– upon first–order is even larger at the later stage, especially with respect to the cross–correlation coefficients, the phase–errors, and the density distribution functions. In particular, also the spectra with positive power–index show improvement, especially on small scales.

Since from previous comparisons with other approximations we know that it is hard to improve on the dynamical performance of TZA, we consider this as a definite and useful success of the second–order model. It is remarkable that, although the second–order scheme needs truncation at a slightly smaller frequency than first–order, thus erasing more information initially (compare Fig.1), the non–linear evolution overcompensates that.

We could not confirm the same property of ‘robustness’ for the third–order scheme. In BMW we already noted that differences between second– and third–order are smaller than the difference found for second– upon first–order, a result which is expected for a perturbation approach which converges to the exact solution (if it does). However, the break–down phenomenon at and after the perturbation schemes are evolved beyond
the range of validity after shell-crossing, i.e. the behavior observed in pancake models by BMW, could be compensated by optimized filtering of initial data for second-order perturbations. This seems not to work for the third-order scheme. Here, we have to stress that the numerical realization of the third-order scheme by iteratively solving Poisson equations should be very accurate in order to draw definite conclusions, especially for models with much small-scale power. We think that much more numerical effort has to be added in order to treat the third-order effect reliably. Remember that in the third-order model 7 Poisson equations have to be solved, 4 of them based on solutions of the second-order Poisson equation, while in the second-order model only 2 Poisson equations have to be solved (directly from the initial data). Buchert et al. (1994b) therefore pursue a different way to overcome numerical problems by solving Poisson equations analytically up to the third order. With this method one can obtain analytical expressions for all 7 perturbation potentials, and realize the Lagrangian scheme for random fields with up to about 100 Fourier modes at reasonable CPU speed. First results of this comparison are discussed by Buchert (1993b).

We emphasize that a breakdown of higher than second-order solutions at late non-linear stages does not contradict the result that third-order clearly improves upon second-order in the weakly non-linear regime before shell-crossing, e.g. in comparison with the exact spherically symmetric solution, or the skewness and kurtosis moments of the density field (Munshi et al. 1994); here we tested the extreme situation of going to stages which involve a large number of shell-crossings.

We finally remark that that we were using the exact expressions for second- and third-order solutions for initial conditions, where the peculiar-velocity potential $S$ and the peculiar-gravitational potential $\phi$ are initially proportional ($S = -\phi t_i$). The expressions used by other authors on higher-order Lagrangian schemes refer to different initial conditions and do not involve terms other than the leading term. The solutions we use involve growing parts (even with different signs than the leading terms) due to second- and third-order homogeneous solutions of the basic differential equations. The leading terms are the particular solutions of these equations only. Of course, at late non-linear stages analyzed here, only the leading terms matter, which we confirmed by dropping all terms other than the leading terms. We found that for expansion factors $a < 25$ differences with the calculations presented here become significant (compare, e.g., the second-order coefficient of the particular solution of the displacement field $-3/14a^2$ with the growing homogeneous solution $+3/5a$; at $a \approx 25$ the difference still is a 10% effect in the time-coefficients).
5. Conclusions

We have analyzed a family of hierarchical models with different amount of power on small scales, and evolved deeply into the non–linear regime of structure formation. We have compared the results from N–body simulations with those from Lagrangian perturbation schemes, where for the latter we have filtered the initial data before evolving them. The filter scale was determined by optimization of the cross–correlation coefficient with the corresponding N–body simulation.

We can report two striking advantages of going to second order in perturbation theory. Firstly, especially the statistics which probe the gravitational dynamics of the models show improvement due to second–order corrections. This success is found for a considerably higher non–linearity than is expected from a perturbation approach. Secondly, the improvement (although small for much small–scale power) is robust by going to later stages and to smaller scales.

We conclude that the second–order scheme with truncated power–spectra will be especially useful for modelling large–scale structure. In particular, the second–order scheme is computationally simple to realize with a CPU speed comparable to that of TZA. Since the second–order corrections to TZA provide noticeable improvement of dynamical accuracy for initial data with negative sloped power–spectra, we expect that the truncated second–order scheme will be useful for the modelling of standard cosmogonies (like Hot–, Cold–, and Mixed–Dark–Matter). This modelling will be especially effective for large sample calculations, since in numerical realizations of ‘fair’ samples in excess of 300 h$^{-1}$Mpc, performed with the same resolution as the simulations reported here, the truncation scale is close to the Nyquist frequency of the N–body computing. Thus, shortcomings of the analytical schemes become negligible which puts them in an ideal position for the purpose of simulating the environment of galaxy formation down to scales, where other physical effects start to affect models which are based on the description of self–gravity alone. Our method can be effective down to galaxy group mass scales ($10^{13} M_{\odot}$), or better if we include biasing or go to epochs earlier than the present.

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Figure Captions

**Figure 1:** The variation of the cross-correlation coefficient $S$ (eq. (5)) against the truncation scale $k_c$ imposed on the initial data for the evolved analytical schemes ($k_{nl} = 8k_f$) for different filter types (sharp $k-$truncation (kc; eq. (6a)), Gaussian truncation (gs; eq. (6b)), and (real space) top–hat truncation (th; eq. (6c))), for spectral indices $n = +1, 0, -1, -2, -3$ (Fig.1a,b,c,d,e). The first–order model is shown as a dotted line, the second–order model as a dashed line.

**Table 1:** The cross–correlation coefficient $S$ for the optimal truncation scale $k_{opt}$ in units of $k_{nl} = 8k_f$ (stage f), and $k_{nl} = 4k_f$ (stage g) for different spectral indices and the two Lagrangian perturbation schemes.

**Figure 2:** Illustration to Table 1. Shown is the cross–correlation coefficient $S$ for the optimal truncation scale $k_{opt}$ according to Table 1 for stage f (left) and stage g (right) as a function of spectral index. The first–order scheme is shown with squares, the second–order scheme with diamonds.

**Figure 3:** The cross–correlation coefficient $S$ for the stage $k_{nl} = 8k_f$ and the cases $n = -1$ (upper) and $n = +1$ (lower) as a function of scale. Displayed is the cross–correlation of the N–body simulation with the Eulerian linear extrapolation of the initial data (dashed–dotted), the “chopped” Eulerian linear approximation (thick dashed–dotted), the untruncated first– (dotted) and second–order (dashed) approximations, and the optimally truncated first– (thick dotted) and second–order (thick dashed) approximations.

**Figure 4:** A thin slice (thickness $L/64$) of the density field is shown for the numerical (upper–left), the “chopped” Eulerian linear (upper–right), the optimally truncated first–order (middle–left) and second–order (lower–left), the untruncated first–order (middle–right), and the untruncated second–order (lower–right) approximations for the evolution stage corresponding to $k_{nl} = 8k_f$, and for different power–spectra with index $n = +1, 0, -1, -2, -3$ (Figs. 4a,b,c,d,e). The grey–scale is linear, and the maximum density contrasts are adapted to give a satisfactory visual impression, except for the optimally truncated models for which the upper truncation is the same (density contrast 5) as for the numerical simulation to allow for an objective comparison.

**Figure 5:** The standard deviations of the density contrast as a function of smoothing scale (given in grid units $R_G$ of a $64^3$ grid) in the optimally truncated first-order (dotted), the optimally truncated second–order (dashed), and the numerical (full line) approximations, for the different power–spectra $n = -3, -2, -1, 0, +1$ (Figs. 5a,b,c,d,e).
**Figure 6:** The cross-correlation coefficient $S$ as a function of the standard deviation $\sigma_\rho$ of the numerical simulation for the different power-spectra $n = -3, -2, -1, 0, +1$ (Figs. 6a,b,c,d,e). The cross-correlation of the N-body with the optimally truncated first-order model is shown as a dotted line; with the optimally truncated second-order model a dashed line.

**Figure 7:** The power-spectra of the N–body simulations (solid line) compared with the optimally truncated first– (dotted) and second–order (dashed) approximation schemes for the different power-spectra $n = -3, -2, -1, 0, +1$ (Figs. 7a,b,c,d,e).

**Figure 8:** The relative phase–errors. Notation and labelling like in Figure 6.

**Figure 9:** The density distribution functions. Notation and labelling like in Figure 7.

**Figure 10:** Same as Fig.5 for a later stage when the non–linearity scale has dropped to half the value of the former stage ($k_{nl} = 4k_f$).

**Figure 11:** Same as Fig.6 for the later stage.

**Figure 12:** Same as Fig.7 for the later stage.

**Figure 13:** Same as Fig.8 for the later stage.

**Figure 14:** Same as Fig.9 for the later stage.
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