Optimizing higher order Lagrangian perturbation theory for standard CDM and BSI models

Arno G. Weiβ,1* Stefan Gottlöber2* and Thomas Buchert3*

1 Max-Planck-Institut für Astrophysik, Karl-Schwarzschild-Straße 1, D-85748 Garching, Germany
2 Astrophysikalisches Institut Potsdam, An der Sternwarte 16, D-14482 Potsdam, Germany
3 Theoretische Physik, Ludwig Maximilians Universität, Theresienstraße 37, D-80333 München, Germany

Accepted 1995 September 8. Received 1995 August 29; in original form 1995 May 22

ABSTRACT

We investigate the performance of Lagrangian perturbation theory up to the second order for two scenarios of cosmological large-scale structure formation, standard cold dark matter (SCDM) and broken scale invariance (BSI). We study the latter model as a representative of COBE-normalized CDM models which fit the small-scale power of galaxy surveys. In this context, we optimize the performance of the Lagrangian perturbation schemes by smoothing the small-scale fluctuations in the initial data. The results of the Lagrangian mappings obtained are computed for a set of COBE-normalized SCDM and BSI initial data of different sizes and at different times. We compare these results with those obtained with a numerical particle mesh (PM) code. We find an excellent performance of the optimized Lagrangian schemes down to scales close to the correlation length. This is explained by the counterintuitive fact that non-linearities in the model can produce more small-scale power, if initially such power is removed. The optimization schemes can be expressed in a way that is independent of the type of fluctuation spectrum and the size of the simulations.

Key words: dark matter – large-scale structure of Universe.

1 INTRODUCTION

Zel'dovich's celebrated approximation (Zel'dovich 1970) has largely improved the qualitative understanding of how large-scale structure forms in the Universe. The reason why this approximation is so useful can be traced back to the fact that it can be understood as a subset of the first-order solution in a Lagrangian perturbation approach (Buchert 1989, 1992), which allows us to follow the evolution of gravitational instabilities into the weakly non-linear regime of structure formation, i.e. where the rms fluctuation of the density contrast is of order unity. This value roughly corresponds to the limit of application of Lagrangian perturbation theory at any order. The quantitative demonstration of this limitation, in comparison with N-body simulations, actually restricts its application to so-called 'pancake models' (Buchert, Melott & Weiss 1994) which lack power on small scales similar to the traditional hot-dark-matter picture of structure formation. The 'Zel'dovich-approximation' has been applied only to initialize N-body codes, or to model structures at mildly non-linear stages down to scales of $10^{13} \, M_\odot$.

Meanwhile, Zel'dovich's original model has developed into a powerful tool for the modelling of structure formation also on smaller spatial scales, with the implication that models with a substantial amount of small-scale power can be accessed. The basic idea of improvement relies on the smoothing of small-scale power in the initial conditions, i.e. the main failure of the model to describe the gravitational collapse after shell crossing is effectively compensated. Recent work (see: Coles, Melott & Shandarin 1993; Melott, Pellman & Shandarin 1994), and the summary by Melott (1994 and references therein), Bouchet et al. (1995) and Sathyaprakash et al. (1995) have exploited this idea with the result that the first-order Lagrangian perturbation scheme, in a truncated form, is capable of modelling structure formation down to galaxy group mass-scales ($10^{13} \, M_\odot$) in any model, including hierarchical cosmogonies at fully developed non-linear stages. Going to higher order Lagrangian perturbation schemes improves the performance of such models only up to the second-order approximation, which appears to be remarkably robust and consistently better than the first-order scheme as measured by various statistics (Melott, Buchert & Weiβ 1995).

The present paper is motivated by the need to apply this tool to realistic dark matter models, since earlier systematic
analyses were limited to case studies, e.g. power spectra of power-law form. It is designed to uncover, also, universal properties of truncation of initial data, i.e. rules that may apply to any initial data set. For example, a Gaussian type of smoothing window and a truncation slightly below the non-linearity scale was suggested by the earlier systematic studies and will be confirmed for the dark matter spectra analysed in this work. Therefore, this paper forms the final step to achieve a reliable modelling of large-scale structure with simple analytical tools, which can guide and meet the contemporary efforts of understanding the formation of galaxies in the large-scale environment. Here, we emphasize that a statistically 'fair' domain of the Universe can be modelled fast, effectively and reliably down to those scales which - for a large realization - coincide with the Nyquist frequency of standard N-body runs. There is no need for N-body computing on these scales, while smaller scales are no longer ruled by the gravitational interaction alone, and must be accessed by more complex methods such as hydrodynamical simulations.

The second-order scheme employed in this work is easy to implement as the first-order scheme. The CPU times on a CRAY YMP are, for the first-order scheme, 25 s, and for the second-order scheme 60 s; the corresponding CPU times on a CONVEX C220 are 2 and 5 min, respectively. Thus, even the second-order scheme is competitive with one step in a corresponding PM-type N-body simulation.

The paper is organized as follows. In Section 2 we describe the Lagrangian perturbation theory up to the second order, and present the optimizing technique used. In Section 3 we discuss N-body simulations of large-scale structure formation in a universe dominated by cold dark matter. We use both the primordial Harrison–Zel'dovich perturbation spectrum and a primordial spectrum with broken scale invariance (BSI). The latter was introduced (Gottlöber, Müller & Starobinsky 1991; Gottlöber, Mücket & Starobinsky 1994) in order to solve a discrepancy in the COBE-normalized SCDM model, which shows too much structure on small scales. Both in the SCDM and BSI model, the universe is dominated by cold dark matter. In Section 4 we present the results of our optimizing procedure and compare the performance of the optimized Lagrangian perturbation theory against our numerical simulations. In Section 5 we compare the performance of the optimized Lagrangian perturbation theory with that of the Eulerian linear perturbation theory. In Section 6 we present our conclusions from these results. Throughout this paper we assume that the Hubble constant is 50 km s⁻¹ Mpc⁻¹, however, for comparison with other works, we present our results in terms of a Hubble constant $H_0 = 100$ km s⁻¹ Mpc⁻¹ with $h = 1/2$.

## 2 LAGRANGIAN THEORY AND OPTIMIZATION

The Lagrangian perturbation schemes which we employ in the present work together with a description of their realization can be found in Buchert (1993, 1994), Buchert et al. (1994) and Melott et al. (1995). As in the latter work, we restrict the presentation of results here 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 Buchert et al. (1994) for the present purpose.

Denoting comoving Eulerian coordinates by $q$ and Lagrangian coordinates by $X$, the field of trajectories $q = F(X, t)$ up to the second order on an Einstein–de Sitter background is

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

(1)

with the time-dependent coefficients expressed in terms of the expansion function $a(t) = (t/t_0)^{2/3}$,

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

(2)

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

(3)

The perturbation potentials have to be constructed by solving iteratively the two non-local boundary value problems,

$$\Delta_0\mathcal{S}^{(1)} = I(\mathcal{S}^{(1)}_{i,k}),$$

(4)

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

(5)

where $I$ and $II$ denote the first and second principal scalar invariants of the tensor gradient $\left[\mathcal{S}^{(1)}_{i,k}\right]$, $I(\mathcal{S}^{(1)}_{i,k}) = \text{tr}(\mathcal{S}^{(1)}_{i,k}) = \Delta_0\mathcal{S}^{(1)}$, $II(\mathcal{S}^{(1)}_{i,k}) = \frac{1}{2} \left[\text{tr}(\mathcal{S}^{(1)}_{i,k})^2 - \text{tr}[(\mathcal{S}^{(1)}_{i,k})^2]\right]$. 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 $t_0$ (see Buchert 1994 and references therein for a discussion of this restriction). Therefore, the initial fluctuation field can be specified by the peculiar-velocity potential $\mathcal{S}$ alone. We can set $\mathcal{S}^{(1)} = \mathcal{S}_t$ (which is the unique solution of the first Poisson equation (4) for periodic initial data, see Buchert 1994, appendix B). Doing this, the flow-field (1) reduces to Zel'dovich's approximation if restricted to the first order.

We realize the solution by first solving Poisson's equation for $\mathcal{S}$ via fast Fourier transform (FFT) from the initial density contrast $\delta$ generated as initial data for the numerical simulation. In an Einstein–de Sitter model we have

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

(8)

We then calculate the second principal invariant $II$ directly from $\mathcal{S}$ and solve the second Poisson equation (7) using FFT. The density in the analytical models is calculated by collecting trajectories of the Lagrangian perturbation solutions at the different orders into a 64³-pixel grid with the same method (CIC binning) as in the N-body simulation.

The optimization of these approximations is performed as proposed by Coles et al. (1993) by smoothing the high-frequency part of the Fourier transform of the initial density field. In previous work (Melott et al. 1995), we found that convolving the initial density field, with a Gaussian, consistently gives the best results for both first and second order. The characteristic smoothing scale can best be given as the
width \(k_{ps}\) of the Gaussian window function in \(k\)-space
\[ W_{ps}(k) = \exp\left(-\frac{k^2}{2k_{ps}^2}\right), \tag{9} \]
in units of the scale of non-linearity \(k_{nL}\), defined as the scale on which the integral of the linearly evolved power spectrum of the initial data becomes unity, i.e.
\[
\frac{a^2(r)}{2\pi^3} \int_0^{R_{c}} d^3k P(k) = 1. \tag{10}
\]
The error that is introduced here, by setting the lower bound of the 'loop' over the smoothing scale \(k_{ps}\) for the different models, box sizes and times. We run both the numerical simulation and the analytical approximation schemes with a resolution of 128\(^3\) particles, which we collect at the final stages into a density grid of 64\(^3\) cells, using the clouds-in-cells algorithm. A comparison of the density fields obtained by the different algorithms is then performed by evaluating the cross-correlation coefficient
\[
S = \frac{\left< \delta_1 \delta_2 \right>}{\sigma_1 \sigma_2}, \tag{11}
\]
where \(\langle ... \rangle\) denotes spatial averaging over the whole volume of the simulation, and \(\sigma_1, \sigma_2\) are the rms-density contrasts of the density contrast fields, \(\delta_1\), of the numerical simulation and \(\delta_2\) of the analytical schemes, respectively. The cross-correlation coefficient \(S\) measures whether mass is moved to the right place. For the optimization procedure, we run a loop over different smoothing lengths, \(k_{ps}\), for the initial data of the Lagrangian approximations. Then we compare the resulting set of final density fields obtained by the Lagrangian approximations with that obtained by evolving the unsmoothed initial data with the PM code. The smoothing length \(k_{ps}\) that maximizes the cross-correlation coefficient \(S\) on a cell-to-cell basis is recognized as the optimum smoothing length \(k_{opt}\). In a latter analysis, we compare only those final density fields obtained by the Lagrangian approximations, with the optimum filter scale, against those obtained by the PM code (without filtering of the initial data). For a scale-sensitive procedure, we smooth the final density fields of both the optimized Lagrangian perturbation theory and the PM code with a set of Gaussian window functions in real space. From this we obtain a scale-dependent cross-correlation coefficient \(S(R_{h})\).

Other statistics we consider here for a comparison of our analytical schemes against the numerical simulations include the power-spectral analysis of the final density fields, the density distribution functions, and the two-point correlation functions. For a more detailed discussion of the statistics suitable for a comparison of the density fields obtained by different algorithms see, e.g. Melott et al. (1994, 1995).

3 NUMERICAL SIMULATIONS WITH COBE-NORMALIZED SCDM AND BSI INITIAL DATA

In order to follow the non-linear evolution of the formation of structure, we have performed \(N\)-body calculations using a standard PM code (Kates, Kotok & Klypin 1991) with 128\(^3\) particles on a 256\(^3\) grid (Kates et al. 1995). The Universe is assumed to be spatially flat \((\Omega = 1)\). It is dominated by cold dark matter. We consider here simulations which were performed in boxes of 500, 200 and 75 \(h^{-1}\) Mpc. The simulations were started with the power spectrum \(P(k)\) of density perturbations calculated at \(z = 25\),
\[
P(k) = \left(\frac{\delta_0}{\rho} \right)^2 = \frac{4}{9} \left(\frac{kR_{h}^3}{2}\right)^4 \Phi^2(k) T^2(k), \tag{12}
\]
where \(R_{h} = 2 \, h^{-1}\) Mpc denotes the horizon. The primordial perturbation spectrum \(\Phi\) is either the Harrison–Zel’dovich spectrum \((\Phi = \text{constant})\) of the SCDM model, or the spectrum with broken scale invariance calculated from a double inflationary model (Gottlöber et al. 1991). In the BSI model, the spectrum is of Harrison–Zel’dovich type, both in the limit of very large and very small scales.

We have used the CDM transfer function \(T(k)\) of Bond & Efstathiou (1984). For all simulations we have normalized our spectra using the 10° variance of the CMB fluctuations \(\sigma_{_1} = (30 \pm 7.5) \mu K\) of the first year COBE data (Smoot et al. 1992). Thus the power spectrum of the BSI model shows less power on small scales than the SCDM model. The scales of non-linearity defined in equation (10) are \(\lambda_{nL}^{SCDM} = 27 \, h^{-1}\) Mpc and \(\lambda_{nL}^{BSI} = 7 \, h^{-1}\) Mpc. In Fig. 1 we show the linear BSI and SCDM spectra and indicate the box sizes and the resolution of our simulations.

The first and second year COBE data were analysed by many authors using different statistical techniques. The new normalization of Górski et al. (1994) is about 25 per cent higher than the normalization that we used in the simula-

![Figure 1. The linear power spectrum of the SCDM model (dashed line) and the BSI model (solid line).](https://example.com/figure1.png)
sections. Consequently, in this normalization, the scales of non-linearity would increase to \( \lambda_{\text{NL,SCDM}} = 33 \, h^{-1} \text{Mpc} \) and \( \lambda_{\text{NL,BSI}} = 11 \, h^{-1} \text{Mpc} \).

4 RESULTS

In Fig. 2 we have collected the results of our optimization procedure in a scatter plot of \( k_{\text{gal}}/k_{\text{ad}} \) against the effective power index \( n(k_{\text{gal}}) \) on the scale of non-linearity, which is obtained as the tangent to \( P(k) \) in a log-log plot. Interestingly, the optimum smoothing scales, for both first and second order, show no significant variation with \( n(k_{\text{gal}}) \) over the whole range of \( n(k_{\text{gal}}) \) investigated here, ranging from \( n = 2.4 \) to \( -0.4 \). A linear-regression fit of the data shows only a slightly negative slope of \( k_{\text{gal}}/k_{\text{ad}} \) with respect to \( n(k_{\text{gal}}) \).

However, the second-order scheme requires a stronger smoothing with \( k_{\text{gal}}/k_{\text{ad}} = 1.2 \) than the first-order scheme, which requires \( k_{\text{gal}}/k_{\text{ad}} = 1.45 \). But the second-order scheme has much less scatter in the optimum smoothing length for the different models than the first-order scheme.

The cross-correlation function \( S(R_g) \) for different smoothing scales \( R_g \) applied to the final density fields in real space is shown in Fig. 3. Here we measure the smoothing scale \( R_g \) in units of \( 1/128\text{th} \) of the simulation's size, i.e. in grid units of the resolution of the initial data.

For the stage \( z = 0 \), according to COBE normalization of BSI initial data, the cross-correlation coefficient indicates an excellent performance, already, on scales of the resolution limit \( (R_g = 1) \). This remains true for all three sizes of the simulations that we have investigated, although for the smallest box \( (75 \, h^{-1} \text{Mpc}) \), the performance of the analytical schemes is worse than for the two larger boxes. At earlier times \((z = 1 \text{ and } z = 2)\) the performance of the analytical schemes for the two smaller boxes \( (75 \, h^{-1} \text{Mpc} \text{ and } 200 \, h^{-1} \text{Mpc}) \) is better than for \( z = 0 \).

For COBE-normalized standard CDM, the performance of the analytical schemes at time \( z = 0 \) is not as good as for BSI; for the \( 75 \, h^{-1} \text{Mpc} \) box we get an acceptable performance (comparable to that for BSI at \( R_g = 1 \)) only on scales of \( R_g \geq 2.5 \ldots \). The performance on the larger boxes is comparable to that on the next-smallest ones for BSI. At the earlier times \((z = 1 \text{ and } z = 2)\), the performance of the optimized perturbation schemes with standard CDM is not as good as for BSI initial data, in a way that is similar to the results for \( z = 0 \).

Owing to the Gaussian smoothing applied to the initial data in Fourier space, the power spectrum of the final density distribution for the optimized Lagrangian schemes (Figs 4 and 5) is not even as high as that of the linearly evolved power-spectra, both for SC defense and BSI initial density distributions, although for the latter - owing to its higher \( k_{\text{gal}} \) - the Lagrangian approximations differ much less from the linearly evolved power spectrum, even at the late stage \( z = 0 \).

This is an inherent disadvantage of the smoothing of the initial data. However, a comparison to Eulerian linear theory (see below) will show that the Lagrangian perturbation schemes are less affected by such a smoothing of the initial data than is the Eulerian theory. Remarkably, though, is the fact that at later stages, when the density field is evolved more non-linearly, the optimized Lagrangian perturbation schemes show more small-scale power than the Lagrangian schemes without a smoothing of the initial data.

The density distribution functions (Fig. 6) show an over-representation of low-density cells and an under-representation of high-density cells for the optimized Lagrangian approximation schemes in comparison with the numerical simulations, consistently for both kinds of initial data and for each step in the temporal evolution. The density values, where the density distribution functions of the Lagrangian schemes intersect with the density distribution functions of the numerical simulations, decrease with earlier times. Consistently throughout all of our simulations, the density distribution functions of the second-order optimized Lagrangian perturbation theory lie closer to the numerical ones than those of the first-order scheme.

Finally, a look at the two-point correlation function at \( z = 0 \) (Fig. 7) confirms the high quality of the optimized Lagrangian perturbation theory. While the correlation function of the optimized schemes on scales below the correlation length \( r_0 [\xi(r_0) = 1] \) lies well below that of the numerical simulations, the correlation length itself is underestimated only slightly (by less than \( 1 \, h^{-1} \text{Mpc} \)) by the optimized Lagrangian schemes. For the largest boxes (500 \( h^{-1} \text{Mpc} \)), the somewhat larger error in \( r_0 \) is mainly determined by the resolution limit of the initial data. Above the correlation length, the correlation functions of optimized Lagrangian perturbation theory and numerical simulations come into good agreement. In contrast to this, the Lagrangian perturbation theory without a smoothing of the initial conditions yields an estimate of the correlation length that is much too low, especially for standard CDM initial data (having a higher \( \xi(r) \) at small scales than the BSI initial data).

©1996 RAS, MNRAS 278, 953–964
Figure 3. Density cross-correlations for SCDM and BSI. Dash-dotted lines: OLPT1; dashed lines: OLPT2, dash-dot-dot-dotted lines: chopped linear theory. Thick lines: $500 \, h^{-1}\text{Mpc}$; medium lines: $200 \, h^{-1}\text{Mpc}$; thin lines: $75 \, h^{-1}\text{Mpc}$ boxes.
Figure 4. Power spectra for SCDM and BSI at $z=0$. Thin solid lines: linear spectrum. Dotted lines (except vertical): linear evolution of initial data smoothed with optimum second-order window. Thick solid lines: numerical simulation. Dash-dotted lines: first order; dashed lines: second order. Thick lines: OLPT; thin lines: Lagrangian perturbation theory without optimization (LPT). Vertical bars denote the Nyquist frequency of the initial data. The dotted vertical line shows the non-linearity scale $k_{nl}$. 

©1996 RAS, MNRAS 278, 953-964
5 COMPARISON TO THE EULERIAN LINEAR PERTURBATION THEORY

Looking at the convolution of the linearly evolved power spectrum with the square of the window function (9) (Figs 4 and 5, dotted lines) we see that the optimized Lagrangian schemes do not only produce more small-scale (large $k$) power than those without optimization, but that their power spectra show, at the small-scale end, considerably more power than expected for a linear evolution of the smoothed initial density distributions. This feature is especially prominent for the SCDM initial data, whose non-linear evolution at each stage reaches larger length scales than that of the BSI initial data. In view of the fact that the convolved linear spectra lie nearly above each other, one can also see that our procedure consistently yields comparable smoothing lengths in physical units, which are almost independent of the size of the simulation box.

The prediction of the Eulerian linear theory for the two-point correlation function (dotted line in Fig. 7) shows no noticeable difference to the Lagrangian schemes in the case of BSI initial data evolved to $z=0$, which is to be seen in light of the less non-linear state of this model. Only for the more non-linearly evolved SCDM model at $z=0$, the differences between Eulerian linear perturbation theory and optimized Lagrangian perturbation theory become significant. Compared to the numerical simulations, the Eulerian theory overestimates the correlation length about as much as it is underestimated by the optimized Lagrangian theory. This, however, could be due to the uncertainty in the two-point correlation function at small scales. On scales below the correlation length, the Eulerian theory does not underestimate correlations as much as the Lagrangian schemes do.

For an investigation of the density field predicted by the Eulerian linear theory, we use a modification of this theory, called the chopped linear theory (Coles et al. 1993). This is an improvement on Eulerian linear theory which complies to both conditions $\delta_{\text{lin}} \geq -1$ and $\langle \delta_{\text{lin}} \rangle = 0$, even at late times. In terms of the linearly evolved $\delta_{\text{lin}}$, we set $1 + \delta_{\text{cin}} = a(1 + \delta_{\text{lin}})$ if $\delta_{\text{lin}} > -1$ and 0 otherwise, where $a$ is

![Figure 5. The same as in Fig. 4, for times $z=1$ and $z=2.$](image)
Figure 6. Density distribution functions for SCDM and BSI. Solid lines: numerical simulations; dash-dotted lines: OLPT1; dashed lines: OLPT2, dash-dot-dot-dotted lines: chopped linear theory. Thick lines: 500 $h^{-1}$ Mpc; medium lines: 200 $h^{-1}$ Mpc; thin lines: 75 $h^{-1}$ Mpc boxes.
Figure 7. Two-point correlation function for $z=0$ SCDM and BS1. Solid lines: numerical simulations; dash-dotted lines: first order; dashed lines: second order. Thin lines: LPT; thick lines: OLPT. Dotted lines: Eulerian linear theory.
a normalization constant, keeping the total mass the same. The cross correlation function of the chopped linear theory (Fig. 3 dash-dot-dot dotted lines) shows that this scheme reproduces the density field much worse than the Lagrangian schemes, except when the models are still quite near to the linear regime (as the BSI model is at $z = 2$). Especially at later stages in the non-linear evolution, as the BSI model at $z = 0$, and the SCDM model at all stages investigated here, the chopped Eulerian linear theory performs considerably worse than the optimized Lagrangian perturbation theory. This is also true for the density distribution function (dash-dot-dot dotted lines in Fig. 6 denote the prediction of the chopped linear theory). The number of high-density cells produced by Eulerian linear theory is much lower than that produced by the optimized Lagrangian schemes.

6 CONCLUSIONS

Overcoming the problem of runaway evolution of small-scale modes in Lagrangian perturbation models by filtering out these modes in the initial data seems, at first glance, counterproductive. However, earlier work, as well as the results of this work, show that a genuine gain in performance on small scales can be obtained by such an optimizing approach. These and the present investigations clearly show the following.

(i) The smoothing scale in the initial data for a set of (in their amount of small-scale power) quite different models can be consistently connected to the scale of non-linearity, equation (10). Over a broad range of effective power indices,
larger smoothing lengths in real space than the first-order scheme shows much less scatter in \( n(k_h) \) (given in terms of the scale of non-linearity \( k_h \)) can be fitted to be nearly constant for varying \( n(k_h) \) for both first- and second-order Lagrangian schemes. Here the second-order scheme shows much less scatter in \( k_h/k_0(n) \) and requires larger smoothing lengths in real space than the first-order scheme. For the latter, a Gaussian smoothing window of width \( k_h/k_0 = 1.45 \) seems to lie close to the optimum for most of the models considered here, while for second-order \( k_h/k_0 = 1.2 \) is close to the optimum for virtually all models and times considered here. This is consistent with the results of Melott et al. (1994, 1995), obtained for an even broader range of \( n(k_h) \). Thus, for a given initial power spectrum and time evolution, the optimal smoothing can be given by an absolute physical length scale and is independent of the scale of the simulations.

(ii) The performance of the optimized Lagrangian approximation schemes, with respect to the evolution of the density field, is excellent for larger boxes down to their resolution limit (see Fig. 8 for slices through our largest SCDM and BSI models). For smaller boxes, which resolve smaller physical scales, the approximation of the density field is satisfactorily modelled only on scales above the resolution limit; for SCDM initial data, the density cross-correlation coefficient at \( z = 0 \) shows that the Lagrangian schemes differ from the numerical simulations by about 2 per cent on scales of \( \sim 1.5-2.0 \, h^{-1} \text{Mpc} \), for BSI initial data this difference occurs on scales in the range \( 1.0-1.5 \, h^{-1} \text{Mpc} \).

(iii) The performance of the optimized Lagrangian approximation schemes, with respect to the clustering point process, is very good down to scales close to the correlation length \( r_0 \) of the two-point correlation function. The correlation length \( r_0 \) itself is underestimated at the time \( z = 0 \) by about 10–20 per cent, for BSI and SCDM. Especially for models with a high amount of small-scale power in the initial data, like SCDM, the Lagrangian schemes display a considerable gain in performance by introducing an optimized smoothing of the initial data.

(iv) The removal of small-scale power in the initial density fluctuation field actually causes the Lagrangian perturbation schemes to produce more power on small scales. Although optimized Lagrangian perturbation schemes still produce less power on small scales than predicted by Eulerian linear theory, they do not only produce more power than Lagrangian perturbation theory without an optimized smoothing of the initial data (which is confirmed in an analytical calculation in Schneider & Bartelmann 1995), but also introduce large amounts of small-scale power in the initial data, like SCDM, the Lagrangian schemes display a considerable gain in performance by introducing an optimized smoothing of the initial data.

(v) Compared to the Eulerian linear theory, the Lagrangian perturbation schemes perform worse in the modelling of the power spectrum and two-point correlation function, two low-order statistics which are sensitive to small-scale clustering. This is true even for the optimized Lagrangian schemes, although they perform better than those without optimization for these statistics, especially at later stages, which show more non-linear evolution. The discrepancy between the Lagrangian schemes and the Eulerian linear theory for these statistics increases with decreasing, more non-linearly evolved, scales. The optimized Lagrangian schemes have an advantage over the Eulerian linear theory for modelling statistics that are more closely related to the accuracy of positions, values and shapes of density peaks, such as cross correlation of the density field with numerical simulations and the density distribution function. These statistics are modelled better by the optimized Lagrangian schemes than by the Eulerian linear theory, even on quite small scales in the non-linear regime, where the comparison concerning small-scale clustering properties favours the Eulerian linear theory.

These results clearly indicate that, at least in cases where one is interested in the formation of large-scale structure on scales above the correlation length, the optimized approximations considered here are a viable way to replace numerical simulations. This is especially true when one is interested in the simulation of the large-scale distribution of matter, as in the analysis of the cluster distribution (see e.g. Borgani et al. 1995). These authors have chosen, for the first-order scheme, a smoothing which uses a smaller physical smoothing length-scale, which is still near to the optimal one determined by this work. In this context, we wish to emphasize that an increase of the smoothing length-scale, i.e. a decrease of \( k_g \), beyond the optimal one, soon significantly decreases the performance of the Lagrangian perturbation schemes, while, at least for negative \( n(k_h) \), a decrease of the smoothing length-scale shows a much smaller effect. Numerical simulations, however, still remain the optimal tool in the range \( 1 \, h^{-1} \text{Mpc} \), both precision-wise and cost-wise. Only below this range do hydrodynamic effects contribute significantly to the evolution of structures (see e.g. Frenk et al. 1995). Also, in the domain of the numerical simulations, the predictions of the Eulerian linear theory for measuring the small-scale clustering of the point process, like power spectrum and two-point correlation function, are better than those of the optimized Lagrangian perturbation theory. However, the situation is reversed when one considers the accuracy of the density field. Positions, heights and shapes of density maxima are reproduced much better by the optimized Lagrangian perturbation theory than by the Eulerian linear theory, even on these small scales. On larger scales, the modelling of the point process by the optimized Lagrangian perturbation theory becomes as accurate as that by the Eulerian linear theory. The scale, where optimized Lagrangian perturbation theory is at least as good as the Eulerian linear theory in all of the statistics here, lies somewhere between the correlation length and the scale of non-linearity.

Another interesting application of the Lagrangian perturbation schemes lies in the simulation of sparse surveys such as, e.g., pencil beams. Here the analytic nature of the solution (1) allows the running of higher absolute particle densities by interpolation of the mapping (1). This higher particle density, in comparison with numerical simulations of the same resolution, is especially beneficial when introducing a high selection effect in the post-processing of the particle distribution, as is necessary for the simulation of galaxy surveys. For an example of the possibilities offered by such a procedure see Weiß & Buchert (1993). In addition to this, it is notable that the time needed to realize the mapping (1) corresponds to roughly one time-step of a numerical particle-mesh simulation; the gain in execution time of the simulations is considerable. Thus, our analytical schemes provide a useful
tool for the simulation of large-scale and very large-scale observations, as well as for a quick checking of, e.g., the large-scale behaviour of newly constructed initial data.

ACKNOWLEDGMENTS

We thank Adrian L. Melott (University of Kansas) for valuable remarks as well as for the permission to use his programs for the cross-correlation statistics, which were also used in Buchert et al. (1994) and Melott et al. (1995). AGW wishes to thank the AIP in Potsdam for the opportunity to work on this project during a stay at the AIP. TB acknowledges support of the Sonderforschungsbereich 375-95 für Astro-Teilchenphysik der Deutschen Forschungsgemeinschaft. SG thanks the MPA in Garching for its hospitality. We thank the referee for constructive comments.

REFERENCES

Bond J. R., Efstathiou G., 1984, ApJ, 285, L45
Borgani S., Plionis M., Coles P., Moscardini L., 1995, MNRAS, 277, 1191
Bouchet F. R., Colombi S., Hivon E., Juszkiewicz R., 1995, A&A, in press
Buchert T., 1989, A&A, 223, 9
Buchert T., 1992, MNRAS, 254, 729
Buchert T., 1993, A&A, 267, L51
Buchert T., 1994, MNRAS, 267, 811
Buchert T., Melott A. L., Weiss A. G., 1994, A&A, 288, 349
Coles P., Melott A. L., Shandarin S. F., 1993, MNRAS, 260, 765
Frenk C. S., Evrard A. F., White S. D. M., Summers F. J., 1995, ApJ, submitted
Görski K. M., Hinshaw G., Banday A. J., Bennett C. L., Wright E. L., Kogut A., Smoot G. F., Lubin P., 1994, ApJ, 430, L89
Gottlöber S., Müller V., Starobinsky A. A., 1991, Phys. Rev. D, 43, 2510
Gottlöber S., Mücket J. P., Starobinsky A. A., 1994, ApJ, 434, 417
Kates R., Kotok E., Klypin A., 1991, A&A, 243, 295
Kates R., Müller V., Gottlöber S., Mücket J. P., Retzlaff J., 1995, MNRAS, 277, 1254
Melott A. L., 1994, ApJ, 426, L19
Melott A. L., Pellman T. F., Shandarin S. F., 1994, MNRAS, 269, 626
Melott A. L., Buchert T., Weiss A. G., 1995, A&A, 294, 345
Sathyaprakash B. S., Sahni V., Munshi D., Pogosyan D., Melott A. L., 1995, MNRAS, 275, 463
Schneider P., Bertelmann M., 1995, MNRAS, 273, 483
Smoot G. F. et al., 1992, ApJ, 396, L1
Weiß A. G., Buchert T., 1993, A&A, 274, 1
Zel’dovich Y. B., 1970, A&A, 5, 84