Refinement of initial conditions for cosmological $N$-body simulations

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Abstract. In modern cosmology, the precision of the theoretical prediction is increasingly required. In cosmological $N$-body simulations, the effect of higher-order Lagrangian perturbation on the initial conditions appears in terms of statistical quantities of matter density field. We have considered the effect of third-order Lagrangian perturbation (3LPT) on the initial conditions, which can be applied to Gadget-2 code. Then, as statistical quantities, non-Gaussianity of matter density field has been compared between cases of different order perturbations for the initial conditions. Then, we conclude that we should apply the initial conditions with 3LPT for predictions of precision cosmology.

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1. Introduction

Based on recent observations, refinement of the cosmological scenario is under progress [1, 2, 3, 4, 5]. For example, galaxy surveys not only present large-scale structures but also evolution of such structures in the Universe [3, 4, 5]. As the evolution of large-scale structures is clarified, various dark energy models [6, 7], which explain the acceleration of the cosmic expansion, would be restricted.

As one of the useful methods to restrict cosmological models such as dark energy scenario, cosmological N-body simulations have been applied [8, 9, 10, 11, 12, 13], which describe the evolution of nonlinear structures such as cluster of galaxies. Because cosmological N-body simulations include the cosmic expansion, evolution of the nonlinear structures would be affected by the dark energy models. By the comparison between observations and the predictions by the cosmological N-body simulations, we can verify the validity of dark energy models.

For precise verification of cosmological models such as dark energy model, precise simulations are required. We focus on the initial condition for cosmological N-body simulations, where Lagrangian linear perturbation, i.e., Zel’dovich approximation has been used for a long time. However, although Zel’dovich approximation describes the evolution of quasi-nonlinear density field, because it is described by linear perturbation, initial conditions fail to take into account higher-order growing modes [14, 15]. Recently, the effect of second-order Lagrangian perturbation (2LPT) on the initial condition for cosmological simulation has been studied [16], which is manifested in the nonlinear structure at low-z era.

We investigated the effect of third-order Lagrangian perturbation (3LPT) on the initial condition for cosmological simulation [17, 18]. In the previous studies, we used $P^3M$ code for cosmological simulations [11]. Although the execution speed of the simulation code is fast, $P^3M$ code can be applied for structure formation of cold dark matter only.

Gadget-2 [13] is a well-known code for cosmological N-body/SPH simulation and can consider not only cold dark matter but also baryonic matter. The code can be executed on parallel computers with distributed memory. Therefore, huge simulations can be implemented with this code [19]. Hence, we have developed 3LPT initial condition code applicable to Gadget-2, which would be quite useful for various analyses considering several situations.

The effect of 3LPT on the initial condition is analysed in terms of statistical quantities for matter density field. Even if the initial condition is given by Gaussian distribution, the matter density field shows non-Gaussian distribution during nonlinear evolution. The difference of non-Gaussianity between the cases of 2LPT and 3LPT appears more than several tens of percents at low-z era. Therefore, for precise prediction of large-scale structures with error of several percents, we would consider the effect of 3LPT on the initial condition for cosmological simulations.

This paper is organized as follows. In Sec. 2 we present Lagrangian perturbations
valid up to the third-order. Then, we discuss the methods and results of the numerical simulations in Sec. 3. In this section, we also introduce statistical quantities for matter distribution. Finally, Sec. 4 presents the conclusions.

2. Lagrangian perturbations

2.1. basic equations

In this section, we briefly introduce Lagrangian perturbation. When the scale of an object is smaller than that of the cosmological horizon, the description of motion of matter by Newtonian dynamics is valid. The cosmological expansion is affected by the scale factor \( a \) in basic equations (continuous equation, Euler’s equation, and Poisson’s equation). The solution \( a \) is derived by Friedmann’s equations or alternative equations. We consider dust fluid, which can ignore the pressure of matter. In the comoving coordinates, the basic equations are described as follows [20, 21, 22, 23, 24]:

\[
\frac{\partial \delta}{\partial t} + \frac{1}{a} \nabla_x \cdot \{ \mathbf{v}(1 + \delta) \} = 0, \tag{1}
\]

\[
\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{a} (\mathbf{v} \cdot \nabla_x) \mathbf{v} + \frac{\dot{a}}{a} \mathbf{v} = -\frac{1}{a} \mathbf{\dot{g}}, \tag{2}
\]

\[
\nabla_x \cdot \mathbf{\dot{g}} = -4\pi G \bar{\rho} a \delta, \tag{3}
\]

where \( \bar{\rho} \) represents background matter density. The density fluctuation \( \delta \) is defined as

\[
\delta \equiv \frac{\rho - \bar{\rho}}{\bar{\rho}}. \tag{4}
\]

\( \mathbf{v} \) denotes peculiar velocity.

In Eulerian perturbation theory, the density fluctuation \( \delta \) is regarded as a perturbation. On the other hand, in Lagrangian perturbation theory, displacement from a homogeneous distribution is considered as a perturbation [24, 25, 26, 27].

\[
\mathbf{x} = \mathbf{q} + s(\mathbf{q}, t), \tag{5}
\]

where \( \mathbf{x} \) and \( \mathbf{q} \) represent comoving Eulerian coordinates and Lagrangian coordinates, respectively. \( s \) denotes the displacement vector, which is regarded as a perturbation quantity. By the Lagrangian perturbation (5), we can solve continuous equation (1) exactly.

\[
\delta = 1 - J^{-1}, J \equiv \det \left( \frac{\partial x_i}{\partial q_j} \right), \tag{6}
\]

\( J \) refers to the Jacobian of the coordinate transformation from Eulerian \( \mathbf{x} \) to Lagrangian \( \mathbf{q} \). Therefore, when we derive the solution of Lagrangian displacement \( s \), we can determine the evolution of the density fluctuation.

The peculiar velocity is given as

\[
\mathbf{v} = a \dot{s}. \tag{7}
\]

We introduce Lagrangian time derivative

\[
\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \frac{1}{a} \mathbf{v} \cdot \nabla_x. \tag{8}
\]
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Taking the divergence and rotation of Euler’s equation (2), we obtain evolution equations for the Lagrangian displacement.

\[ \nabla_x \cdot \left( \ddot{s} + \frac{\dot{a}}{a} \dot{s} \right) = -4\pi G \bar{\rho} \left( J^{-1} - 1 \right), \]
\[ \nabla_x \times \left( \ddot{s} + \frac{\dot{a}}{a} \dot{s} \right) = 0. \]  

Here, superscript dot \( \dot{s} \) refers to Lagrangian time derivative \( t \).

\[ \dot{s} = \frac{ds}{dt}. \]  

To solve the Lagrangian perturbative equations, we decompose the Lagrangian perturbation into its longitudinal and transverse mode.

\[ s = \nabla S + s^T, \]
\[ \nabla \cdot s^T = 0. \]

where \( \nabla \) denotes the Lagrangian spatial derivative.

We convert the spatial derivative from Eulerian coordinates to Lagrangian coordinates in equations (9) and (10).

\[ \frac{\partial}{\partial x_i} = \frac{\partial}{\partial q_i} - s_{j,i} \frac{\partial}{\partial x_j} \]
\[ = \frac{\partial}{\partial q_i} - s_{j,i} \frac{\partial}{\partial q_j} + s_{j,i} s_{k,j} \frac{\partial}{\partial x_k} + \cdots. \]  

where comma indicates Lagrangian spatial derivative.

\[ s_{j,i} = \frac{\partial s_j}{\partial q_i}. \]

2.2. Lagrangian perturbative equations

In this subsection, we derive Lagrangian perturbative equations. The Lagrangian perturbation can be divided into temporal and spatial parts.

\[ S = g^{(1)} S^{(1)} + g^{(2)} S^{(2)} + g^{(3)} S^{(3)} + \cdots, \]
\[ s^T = g^{(1)} T s^{(1)} T + g^{(2)} T s^{(2)} T + g^{(3)} T s^{(3)} T + \cdots, \]  

where superscript \( (n) \) denotes \( n \)-th order perturbation. The description of the perturbative solutions in spatial parts is given by Catelan \[33\].

For the first-order perturbation, i.e., Zel’dovich approximation \[25\], the differential equation for the temporal part is given as follows:

\[ \ddot{g}^{(1)} + 2\frac{\dot{a}}{a} \dot{g}^{(1)} - 4\pi G \bar{\rho} g^{(1)} = 0. \]
When we consider only the growing mode of the temporal parts and set the temporal parts at the initial condition by $g^{(1)}(t_{ini}) = 1$, the Lagrangian displacement is described by the density fluctuation.

$$S^{(1)}_{ii}(q) = -\delta(q).$$

(18)

In other words, the first-order perturbation would be derived by the initial density fluctuation.

If the primordial vorticity does not exist, the vorticity never appears during evolution. Even if the primordial vorticity exists, the transverse mode in the first-order perturbation does not have a growing solution. Therefore, hereafter we ignore the transverse mode.

The second-order perturbation is also divided into spatial and temporal parts [28, 29, 30]. The equations are described as follows:

$$S^{(2)}_{i}(q) = \frac{1}{2} \left( S^{(1)}_{i} S^{(1)}_{jj} - S^{(1)}_{ij} S^{(1)}_{ij} \right) + R_{i}^{(2)},$$

(19)

$$\ddot{g}^{(2)} + 2 \frac{\dot{a}}{a} \dot{g}^{(2)} - 4 \pi G \bar{\rho} g^{(2)} = -4 \pi G \bar{\rho} \left\{ g^{(1)} \right\}^2,$$

(20)

where $R_{i}^{(2)}$ denotes rotation-free vector such that $\varepsilon_{ijk} S_{jk}^{(2)} = 0$.

The third-order perturbation is derived from triplet term of the first-order perturbation and cross-section of the first- and the second-order perturbation [31, 32, 33].

$$S^{(3a)}_{i}(q) = \frac{1}{3} S^{(1)C}_{ij} S^{(1)}_{ji} + R_{i}^{(3a)},$$

(21)

$$S^{(3b)}_{i}(q) = \frac{1}{4} \left[ S^{(1)}_{i} S^{(2)}_{jj} - S^{(1)}_{ij} S^{(2)}_{j} + S^{(2)}_{i} S^{(1)}_{jj} - S^{(2)}_{ij} S^{(1)}_{j} \right] + R_{i}^{(3b)},$$

(22)

$$\ddot{g}^{(3a)} + 2 \frac{\dot{a}}{a} \dot{g}^{(3a)} - 4 \pi G \bar{\rho} g^{(3a)} = -8 \pi G \bar{\rho} \left\{ g^{(1)} \right\}^3,$$

(23)

$$\ddot{g}^{(3b)} + 2 \frac{\dot{a}}{a} \dot{g}^{(3b)} - 4 \pi G \bar{\rho} g^{(3b)} = -8 \pi G \bar{\rho} g^{(1)} \left\{ g^{(2)} - \left(g^{(1)}\right)^2 \right\},$$

(24)

where $S^{(1)C}_{ij}$ represents component of adjoint matrix of the first-order perturbation $S_{ij}$. The adjoint matrix shows the following relation:

$$S^{(1)C}_{ij} S^{(1)}_{ji} = 3 \det (S_{ij}).$$

(25)

When we consider only longitudinal mode in the first-order perturbation, the matrix $s_{ij}$ becomes symmetric.

$$S^{(1)}_{ij} = S^{(1)}_{ji}.$$

$R_{i}^{(3a)}$ and $R_{i}^{(3b)}$ denote rotation-free vector such that $\varepsilon_{ijk} S^{(3a)}_{jk} = \varepsilon_{ijk} S^{(3b)}_{jk} = 0$.

Even if we do not consider transverse mode in the first-order perturbation, the transverse mode in the third-order appears [34]. Because of Kelvin’s circulation theorem, the transverse mode in the third-order perturbation does not imply vorticity. Here, we consider only the longitudinal mode in third-order perturbation.
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In ΛCDM model, the early stage in structure formation is a matter dominant era. Because the effect of cosmological constant seems negligible, the cosmic expansion would be approximated by the solution of Einstein-de Sitter Universe model.

\[ a(t) \propto t^{2/3}. \quad (26) \]

Under this assumption, the perturbative solutions become as follows:

\[ g^{(1)}(t) = t^{2/3}, \quad (27) \]
\[ g^{(2)}(t) = -\frac{3}{7}t^{4/3}, \quad (28) \]
\[ g^{(3a)}(t) = \frac{10}{21}t^2, \quad (29) \]
\[ g^{(3b)}(t) = -\frac{1}{3}t^2, \quad (30) \]

Bouchet et al. \cite{32} derived approximation formula of temporal parts for Λ CDM model. They introduced the logarithmic derivative of the growth factors

\[ f_n = \frac{a g^{(n)}(t)}{g^{(n)}(t)} \quad (31) \]

When the Universe is in the matter dominant era (\( \Omega_m \approx 1 \)), the formula becomes

\[ f_1 \approx \Omega_m^{6/11}, \quad f_2 \approx 2\Omega_m^{153/286}, \quad (32) \]
\[ f_{3a} \approx 3\Omega_m^{146/275}, \quad f_{3b} \approx 3\Omega_m^{9481/17875}. \quad (33) \]

For the case of 0.1 ≤ \( \Omega_m \leq 1 \), the formula becomes

\[ f_1 \approx \Omega_m^{5/9}, \quad f_2 \approx 2\Omega_m^{6/11}, \quad (34) \]
\[ f_{3a} \approx 3\Omega_m^{13/24}, \quad f_{3b} \approx 3\Omega_m^{13/24}. \quad (35) \]

2LPT IC code \cite{16} was implemented with the above formula.

3. Cosmological Simulations

For precise cosmological simulations, we set up precise initial conditions. For execution of Gadget-2, we developed a convert code of the initial conditions from ZA to 3LPT. The convert code is described in Sec 2.2. The rotation-free vectors in \( (19), (21), \) and \( (22) \) have been ignored.

In this study, we set the initial condition at the redshift \( z = 49 \). Because the effect of the cosmological constant is negligible, the temporal components in the convert code are given by solutions of the Einstein–de Sitter model.

We set the cosmological parameters as shown in Table 1. The parameters of simulations are shown in Table 2. These parameters are sample values in the Gadget-2 code, which are slightly different from the recent observation \cite{35}.

Gadget-2 can be executed on many cores by OpenMPI. The simulation code was executed on Linux PC (CentOS 7.5, Core i9 7960X, RAM 64GB), using which the simulation can be executed for approximately 5 h per one sample.
Table 1. Cosmological parameters in the simulations.

| Parameter | Value |
|-----------|-------|
| $\Omega_M$ | 0.25  |
| $\Omega_\Lambda$ | 0.75  |
| $\Omega_b$ | 0.04  |
| $H_0$ [km/s/Mpc] | 70    |
| $\sigma_8$ | 0.8   |
| $n_0$ | 1.0   |

Table 2. Parameters in the cosmological simulation code.

| Parameter          | Value          |
|--------------------|----------------|
| Initial time $z_{in}$ | 49             |
| Box size $L$        | $100h^{-1}$ [Mpc] |
| Number of particles $N$ | $256^3$         |
| $H_0$ [km/s/Mpc]    | 70             |
| Softening Length    | $0.25h^{-1}$ [Mpc] |

Our code was converted from the initial condition generated by ZA to that with 2LPT and 3LPT. Because our code cannot be executed parallelly, we cannot apply the code for huge simulations. For the case of $N = 256^3$, the code requires about 2 GB memory.

For comparison, we also generated the initial conditions by 2LPT.IC code [16]. Therefore, we compared four cases: ZA (1LPT), 2LPT by 2LPT.IC code, 2LPT by our code, and 3LPT. In this simulation, we generated 10 initial conditions for each case. For the analysis of time evolution, we selected 11 time slices ($z = 10, 9, \cdots, 1, 0$) and compared the density distributions. The density field was smoothed over the scale $R$ using the cloud-in-a-cell algorithm. The smoothing scale was set as $100/256h^{-1}, 200/256h^{-1}$ [Mpc], i.e., about $0.4h^{-1}, 0.8h^{-1}$ [Mpc].

First, we set the smoothing scale as about $0.8h^{-1}$ [Mpc]. The distribution function of the density fluctuation is shown in Fig. 1. It is well-known that the distribution function of the density fluctuation approaches to log-normal form during the evolution [36, 37, 38, 39]. At $z = 5$, the effect of higher-order perturbation appeared at the high-density region $\delta > 10$. During the evolution, the high-density region grows rapidly. At $z = 0$, the distribution functions resemble each other.

For a detailed analysis, we apply the non-Gaussianity of the density fluctuation. Even if the primordial density fluctuation is generated by Gaussian distribution, the non-Gaussianity of the density fluctuation would appear through nonlinear evolution. For the analysis of the non-Gaussianity, we introduced higher-order statistical quantities:

\[
\text{skewness} : \gamma = \frac{\langle \delta^3 \rangle}{\sigma^4},
\]

\[
\text{kurtosis} : \eta = \frac{\langle \delta^4 \rangle - 3\sigma^4}{\sigma^6},
\]
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Figure 1. Distribution function of the density fluctuation from N-body simulation ($R \simeq 0.8h^{-1}$ Mpc) with different initial conditions. (a) $z = 5$, (b) $z = 3$, (c) $z = 1$, (d) $z = 0$. The distribution function approaches the log-normal form during the evolution.

where $\sigma$ means dispersion of the density fluctuation.

$$\sigma = \sqrt{\langle \delta^2 \rangle}. \quad (36)$$

In the weakly nonlinear stage, these statistical quantities were derived by second-order perturbation theory [20, 26].

In our previous study, we showed the difference of the non-Gaussianity of the density fluctuation between the initial conditions given by 1LPT, 2LPT, and 3LPT. The difference between the cases of 2LPT (our code) and 3LPT is about several percent.

First, we show the evolution of the non-Gaussianity with error bars. The evolution of the density dispersion is shown in Fig. 2. At $z = 1$, the difference of the density dispersion between the case of ZA and 3LPT becomes larger than 10%. Furthermore, the difference of the density dispersion between the case of 2LPT (our code) and 3LPT is about 5%. Therefore, for accuracy with 1%, we should consider the effect of 3LPT for the initial conditions of cosmological $N$-body simulations.
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Figure 2. Dispersion of the density fluctuation from N-body simulation ($R \simeq 0.8h^{-2}$ Mpc) with different initial conditions. (a) Comparison of the dispersion between the initial conditions. (b) The Difference of the dispersion between ZA and other cases.

Figure 3. Skewness of the density fluctuation from the N-body simulation ($R \simeq 0.8h^{-1}$ Mpc) with different initial conditions. (a) Comparison of the skewness between the initial conditions. (b) The difference in the skewness between ZA and other cases.

Then, we show the evolution of the non-Gaussianity in Figs. 3 and 4. Because variations among samples are very large, in the subsequent analysis, the error bars were omitted. By comparison between the case of ZA and higher-order perturbations, the difference in the non-Gaussianity exceeds 10%. When $z = 0$, the difference in the non-Gaussianity between the cases of 2LPT and 3LPT becomes very small, and we need to consider the effect of 3LPT for the initial conditions at $z > 1$.

We change the smoothing scale to $R \simeq 0.4h^{-1}$ [Mpc]. Even if the smoothing scale is changed, the tendency of the distribution function for the density fluctuation is similar
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Figure 4. Kurtosis of the density fluctuation from the N-body simulation ($R \simeq 0.8h^{-1}$ [Mpc]) with different initial conditions. (a) Comparison of the kurtosis between the initial conditions. (b) The difference in the kurtosis between ZA and other cases.

to the case of $R \simeq 0.8h^{-1}$ [Mpc]. The distribution function is shown in Fig. 5.

Time evolution of dispersion of the density fluctuation is shown in Fig. 6. The non-Gaussianity of the distribution of the density fluctuation is shown in Figs. 7 and 8.

We noticed a distribution of peculiar velocity. Here, we compute the absolute value of the peculiar velocity for each particle. When clusters are formed, the particles in clusters slow down. Therefore, the peculiar velocity does not increase monotonically. The probability of the peculiar velocity for each time is shown in Fig. 9. The effect of higher-order perturbation in the initial conditions appears in fast particles. For a more detailed analysis, we compare the probability of the peculiar velocity between the case of ZA and other cases. The difference in the probability of the peculiar velocity is shown in Fig. 10. The effect of higher-order perturbation appears in fast particles. When we consider higher-order perturbation for the initial conditions of the $N$-body simulation, the peculiar velocity increases. At $z = 5$, the number of fast particles (faster than $500$ [km/s]) in the case of 2LPT is more than that in the case of ZA. Similarly, the number of fast particles in the case of 3LPT is more than that in the case of 2LPT. Although the particles form clusters at low-$z$ era ($z = 3, 1, 0$), the tendency continues afterwards. Therefore, if we consider higher-order perturbation in the initial conditions for cosmological $N$-body simulations, the density distribution in the redshift space would change dramatically.

4. Summary

We analysed the effect of higher-order perturbation for the initial conditions of cosmological $N$-body simulations. Based on our previous studies, we developed an initial condition converter for Gadget-2 code.
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Figure 5. Distribution function of the density fluctuation from the N-body simulation ($R \simeq 0.4h^{-1}$ Mpc) with different initial conditions. (a) $z = 5$, (b) $z = 3$, (c) $z = 1$, (d) $z = 0$. The distribution function approaches the log-normal form during the evolution.

For density fluctuation, the effect of higher-order perturbation appeared in strongly nonlinear region. Although the primordial density fluctuation was generated by the Gaussian distribution, because of nonlinear evolution, the non-Gaussianity of the distribution of the density fluctuation appeared at low-$z$ era. Further, we compared the statistical quantities for the non-Gaussianity. Although it varied significantly depending on the samples, the effect of 3LPT on the initial condition was evident.

With regard to the peculiar velocity, the higher-order perturbation affected fast particles, and during clustering, the effect gradually disappeared. Considering the density distribution in redshift space, the effect of higher-order perturbation would appear in the shape of structures such as finger-of-god [40, 41].

For the 2LPT initial conditions, the results obtained using our code were slightly different from that obtained by the 2LPT IC code. In our code, the spatial differential was calculated by the difference in the Lagrangian space. On the other hand, in the 2LPT IC code, the spatial differential was calculated in the Lagrangian Fourier space.
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Further, in our code, the time evolution from recombination era to the initial time ($z = 49$) was given by the growing factor in the E-dS Universe mode. In the 2LPT IC code, the time evolution was given by an approximated formula for the $\Lambda$CDM model. The difference in the initial set up spread in the nonlinear stage.

Although the results obtained using both the codes varied slightly, we demonstrated that the effect of 3LPT in the initial condition appeared in the nonlinear stage. Therefore, for more precise prediction for a large-scale structure, the effect of 3LPT on the initial condition should be considered for cosmological $N$-body simulations. This

Figure 6. Dispersion of the density fluctuation from the N-body simulation ($R \approx 0.4h^{-1}\text{Mpc}$) with different initial conditions. (a) Comparison of the dispersion between the initial conditions. (b) The difference in the dispersion between ZA and other cases.

Figure 7. Skewness of the density fluctuation from the N-body simulation ($R \approx 0.4h^{-1}\text{Mpc}$) with different initial conditions. (a) Comparison of the skewness between the initial conditions. (b) The difference in the skewness between ZA and other cases.
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Figure 8. Kurtosis of the density fluctuation from the N-body simulation \( R \approx 0.4h^{-1} \) [Mpc]) with different initial conditions. (a) Comparison of the kurtosis between initial conditions. (b) The difference in the kurtosis between ZA and other cases.

Effect would appear in other statistical quantities as well.

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Figure 9. The distribution function of the peculiar velocity from the $N$-body simulation with different initial conditions. (a) $z = 5$, (b) $z = 3$, (c) $z = 1$, (d) $z = 0$. At high-$z$ era, the effect of higher-order perturbation in the initial conditions appears.

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Figure 10. The difference in the distribution function of the peculiar velocity between the case of ZA and other cases. (a) $z = 5$, (b) $z = 3$, (c) $z = 1$, (d) $z = 0$. Owing to the effect of higher-order perturbations, the peculiar velocity increases.

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