1 Lattice simulation

1.1 Introduction

In this chapter, we studied the latticeasy article and reproduced it. The content of this chapter is mainly divided into two parts. The first part contains subsections 2.2-2.4, the second part contains subsections 2.5-2.7, and some content is included in the appendix. In the first part, we recalibrate the variables (7)

$$f_{\rm pr} = Aa^r f \quad \mathbf{x}_{\rm pr} = B\mathbf{x} \quad \mathrm{d}t_{\rm pr} = Ca^s \mathrm{d}t \sim Ba^s \mathrm{d}t$$
 (1)

The purpose of this treatment is to make the program calculation simpler by selecting appropriate parameters (like (12)(16)). At the same time, the selection of parameters can avoid the instability and inaccuracy caused by the second-order derivative being the first-order derivative function in the leapfrog method. We also use the average one-order derivative instead of the endpoint (24). This gives a reasonable form of the field equations (17) (29). In this part, we also discussed the selection of initial values of the field, scale factor and their derivatives (30). Note that only the homogeneous part is discussed here.

Although the field equations are solved in configuration space with each lattice point representing a position in space, the initial conditions of fluctuations are set in momentum space and then Fourier transformed to give the initial values of the fields and their derivatives at each grid point. In the second part, we derive distribution of fluctuations on a discrete lattice (42) and show how to set these values randomly (46).. Then, We discuss derivative quations and initial values (51).

1.2 Leapfrog Method

To solve the field equations, including the scalar field f and its derivatives \dot{f} , \ddot{f} , the leapfrog method is appropriate. It looks like:

$$f(t_0 + dt) = f(t_0) + dt \dot{f}(t_0 + \frac{dt}{2})$$
(2)

$$\dot{f}(t_0 + \frac{\mathrm{d}t}{2}) = \dot{f}(t_0 - \frac{\mathrm{d}t}{2}) + \mathrm{d}t \ddot{f}[f(t_0)] \tag{3}$$

$$f(t_0 + 2dt) = f(t_0 + dt) + dt \dot{f}(t_0 + \frac{3dt}{2})$$
(4)

$$\dots$$
 (5)

Compared to the simple Euler method, which takes derivatives at the endpoints(or stratpoints), the leapfrog method takes derivatives at the midpoints. Therefore, Leapfrog method has higher order accuracy and greater stability than a simple Euler method. After choosing the appropriate initial values $f(t_0)$

, $\ddot{f}[f(t_0)]$ and $\dot{f}(-\mathrm{d}t/2) = \dot{f}(t_0) - \ddot{f}[f(t_0)]\mathrm{d}t$, the field values and derivatives are done in full, staggered, desynchronized steps. However, the method relies on being able to calculate \ddot{f} in terms of f at the time t and the value of \dot{f} is always calculated at the midpoint $(t+\mathrm{d}t/2)$, so both accuracy and stability are generally lost if \ddot{f} depends on the first derivative \dot{f} . Therefore, we will rescale the quantities later in order to eliminate first derivative terms in the equations of motion.

1.3 Field Equations and Coordinate Rescalings

The equation of motion for a scalar field f is:

$$\ddot{f} + 3\frac{\dot{a}}{a}\dot{f} - \frac{1}{a^2}\nabla^2 f + \frac{\partial V}{\partial f} = 0 \tag{6}$$

We consider the canonical kinetic form. To begin with we will assume a general form for the variable rescalings

$$f_{\rm Dr} = Aa^r f \quad \mathbf{x}_{\rm Dr} = B\mathbf{x} \quad \mathrm{d}t_{\rm Dr} = Ca^s \mathrm{d}t \sim Ba^s \mathrm{d}t$$
 (7)

where pr means programs rescaling. The position coordinates shouldn't be modified by any powers of the scale factor so that the same comoving wavelengths stay in the box throughout the run. We set B = C to make our program and calculation simpler and ensure that the initial sound speed is 1 $(c_s dt = a(t)dx)$. Then, we get

$$\dot{a} = Ba^{s}a'$$
 $\dot{f} = Ba^{s}f' = \frac{B}{A}(a^{s-r}f'_{pr} - ra^{s-r-1}a'f_{pr})$ (8)

$$\ddot{f} = \frac{B^2}{A} \left[a^{2s-r} f_{\text{pr}}^{"} + (s-2r)a^{2s-r-1}a' f_{\text{pr}}^{"} - r(s-r-1)a^{2s-r-2}a'^2 f_{\text{pr}} - ra^{2s-r-1}a'' f_{\text{pr}} \right]$$
(9)

The equation of motion becomes:

$$f_{\rm pr}^{"} + (s - 2r + 3)\frac{a'}{a}f_{\rm pr}^{"} - a^{-2s - 2}\nabla_{\rm pr}^{2}f_{\rm pr} - \left(r(s - r + 2)\left(\frac{a'}{a}\right)^{2} + r\frac{a''}{a}\right)f_{\rm pr} + \frac{\partial V_{\rm pr}}{\partial f_{\rm pr}} = 0$$
 (10)

where we define $V_{\rm pr}$ in order to consistent with $\rho_{\rm pr}\sim 1/2f_{\rm pr}'^2+V_{\rm pr}\sim A^2/B^2a^{-2s-2r}\rho$

$$V_{\rm pr} = \frac{A^2}{R^2} a^{-2s+2r} V \tag{11}$$

As we mentioned earlier, for the stability and accuracy of the leapfrog method, we need to eliminate the first-order derivative of (10) (mandatory in latticeasy):

$$s - 2r + 3 = 0 (12)$$

To make the code simpler, one can also set (optional)

- $A = f_0^{-1}$ in order to set the scale of the field variables $f_{pr} = Aa^r f$ to be of order unity, at least initially. Note that if the model has multiple fields, where f represents inflaton.
- To make the coefficient of the dominant potential term to include no powers of the scale factor and to be of order unity, we set

$$B = \sqrt{\text{cpl}} f_0^{-1+\beta/2}, \qquad r = \frac{6}{2+\beta}, s = 3\frac{2-\beta}{2+\beta}$$
 (13)

One can find a dominant term of the potential by expand it in a Taylor series:

$$V = \frac{\text{cpl}}{\beta} f^{\beta} + o(f^{\beta}) \tag{14}$$

where cpl represents the coefficient, we get:

$$\frac{dV_{pr}}{df_{pr}} = cplA^{2-\beta}B^{-2}a^{-2s+r(2-\beta)}f^{\beta-1}$$
(15)

we want to scale factor disappear and coefficient becomes one

$$cplA^{2-\beta}B^{-2} = 1 -2s + r(2-\beta) = 0 (16)$$

Then, the EOM becomes:

$$f_{\rm pr}^{"} - a^{-4(4-\beta)/(2+\beta)} \nabla_{\rm pr}^2 f_{\rm pr} - \left(6 \frac{4-\beta}{(2+\beta)^2} \left(\frac{a'}{a} \right)^2 + \frac{6}{2+\beta} \frac{a''}{a} \right) f_{\rm pr} + \frac{\mathrm{d}V_{\rm pr}}{\mathrm{d}f_{\rm pr}} = 0$$
 (17)

$$V_{\rm pr} = \frac{1}{\text{cpl}f_0^{\beta}} a^{6\beta(2+\beta)} V \tag{18}$$

1.4 Scale Factor Evolution

The equation for the scale factor a is derived from the Friedmann equations

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi}{3}\rho\tag{19}$$

$$\ddot{a} = -\frac{4\pi}{3}(\rho + 3p) = -2\frac{{a'}^2}{a} + \frac{8\pi}{a} \left(\frac{1}{3}|\nabla f_i|^2 + a^2V\right)$$
(20)

where:

$$\rho = \frac{1}{2}\dot{f}_i^2 + \frac{1}{2a^2}|\nabla f_i|^2 + V \qquad p = \frac{1}{2}\dot{f}_i^2 - \frac{1}{3} \cdot \frac{1}{2a^2}|\nabla f_i|^2 - V \tag{21}$$

For multiple fields (not coupled), the sum should be calculated for i. To convert to program variables note that

$$\dot{a} = Ba^{s}a' \qquad \ddot{a} = B^{2}(a^{2s}a'' + sa^{2s-1}a'^{2})$$
 (22)

Bringing into (20), we get the scale factor equation:

$$a'' = (-s - 2)\frac{a'^2}{a} + \frac{8\pi}{A^2}a^{-2s - 2r - 1}\left(\frac{1}{3}|\nabla_{pr}f_{i,pr}|^2 + a^{2s + 2}V_{pr}\right) = -C_1\frac{a'^2}{a} + C_2$$
(23)

The second-order derivative(at t) is a function of the first-order derivative. Since we only have the value of the first-order derivative at the midpoint $t \pm dt/2$, this will break the accuracy of the leapfrog algorithm. We use the following method to deal with it:

$$a'_{+} \approx a'_{-} + a'' dt \qquad a' \approx \frac{1}{2} (a'_{+} + a'_{-})$$
 (24)

where $a'_{+}(t + dt/2)$ and $a'_{-}(t - dt/2)$ are from leapfrog, we redefine a'(t), so that a''[a(t), a'(t)]. Bringing (23) into (24) in order to eliminating a:

$$a'_{+} = -\frac{\mathrm{d}tC_{1}}{4a}a'_{+}^{2} - \frac{\mathrm{d}tC_{1}}{2a}a'_{+}a'_{-} - \frac{\mathrm{d}tC_{1}}{4a}a'_{-}^{2} + \mathrm{d}tC_{2} + a'_{-}$$
(25)

The accuracy of the Leapfrog is guaranteed by the redefined a', and it does not cause any problems here. We will not discuss this later. Using the Root-Finding Algorithms, we get:

$$a'_{+} = -a'_{-} - \frac{2a}{\mathrm{d}tC_{1}} \pm \frac{2a}{\mathrm{d}tC_{1}} \sqrt{1 + \frac{2\mathrm{d}tC_{1}}{a}a'_{-} + \frac{(\mathrm{d}t)^{2}C_{1}C_{2}}{a}}$$
 (26)

Taylor expansion at $dt \sim 0$

$$a'_{+} = a'_{-} - \frac{2a}{\mathrm{d}tC_{1}} \pm (\frac{2a}{\mathrm{d}tC_{1}} + 2a'_{-})$$
 (27)

This suggests that the plus sign must be used in order to reduce to the limit $a'_{+} \approx a'_{-}$. Therefore, (23) becomes:

$$a'_{+} = -a'_{-} - \frac{2a}{\mathrm{d}tC_{1}} - \frac{2a}{\mathrm{d}tC_{1}} \sqrt{1 + \frac{2\mathrm{d}tC_{1}}{a}a'_{-} + \frac{(\mathrm{d}t)^{2}C_{1}C_{2}}{a}}$$
(28)

$$a'' = \frac{a'_{+} - a'_{-}}{dt} = \frac{1}{d} \left[-2a'_{-} - \frac{2a}{dC_{1}} \left(1 - \sqrt{1 + \frac{2dtC_{1}a'_{-}}{a} + (dt)^{2} \frac{8\pi}{A2} a^{-C_{3}} \left(\frac{1}{3} |\nabla_{pr} f_{i,pr}|^{2} + a^{C_{4}} V_{pr} \right) \right) \right]$$
(29)

where $C_1 = s + 2$, $C_3 = 2s + 2r$ and $C_4 = 2s + 2$.

So far, we have finished dealing with the background part of fields. The codes recommend inflation $f_{0,pr} = M_P$, and all other fields and fields derivatives initially are zero. The scale factor initially $a_0 = 1$, and combine (19), (8) and (21), a'_0 initially:

$$a_0' = H_{\text{pr},0} = \frac{1}{\frac{3A^2}{4\pi} + r^2 f_{\text{pr}}^2} \left[-r f_{\text{pr}} f_{\text{pr}}' + \sqrt{\frac{3A^2}{4\pi} f_{\text{pr}}' + 2V_{\text{pr}} \left(\frac{3A^2}{4\pi} - r^2 f_{\text{pr}}^2 \right)} \right]$$
(30)

Note, we assume all inhomogeneities are small and ignore the $\nabla_{pr} f_{pr}$ terms. For multiple fields models, one should sum over the fields

1.5 Fourier transformation on lattice

We discuss initial conditions for field derivative fluctuations. The Fourier transforma F_k in three diemensions is defined by:

$$f(x) = \frac{1}{(2\pi)^3} \int d^3k F_k e^{ikx}$$
 (31)

The probability distribution for the ground state of field in FRW universe is Gaussian Distribution [4, 1]:

$$P(F_k) \propto e^{-2a^2 \omega_k |F_k|^2} \qquad \omega_k^2 = k^2 + a^2 m^2 \qquad m^2 = \frac{\partial^2 V}{\partial f^2}$$
 (32)

Field f is always complex under the Fourier transform. The phase of F_k whose real and imaginary components are independently and identically distributed Gaussian with equal variance and zero mean is distributed according to the Rayleigh distribution:

$$P(|F_k|) \propto |F_k|e^{-2a^2\omega_k|F_k|^2} \tag{33}$$

The means-squared value of this distribution is:

$$\langle |F_k|^2 \rangle = \frac{1}{2a^2\omega_k} \tag{34}$$

To derive the expressions used for setting field values on the lattice we must modify equation (33) to account for a finite, discrete space, then account for the rescalings of field and spacetime variables, and finally discuss how to implement the Rayleigh distribution. Consider (31)

$$\langle f^2 \rangle = \frac{1}{L^3 (2\pi)^6} \int \int d^3x d^3k' d^3k F_k F_{k'} e^{i(k+k')x} = \frac{1}{L^3} \int d^3k |F_k|^2$$
 (35)

where L^3 is the volume of the region of integration. $|F_k|^2 \sim L^3$ in order to ensure $\langle f^2 \rangle$ constant. One can also consider the discrete Fourier transform in three dimensions*:

$$f_k = \frac{1}{\mathrm{d}x^3} F_k \tag{36}$$

The spacing between the lattices avoids divergence. We define rms magnitudes

$$W_k = \sqrt{\langle |f_k|^2 \rangle} = \sqrt{\frac{L^3}{2a^2\omega_k(\mathrm{d}x)^6}}$$
 (37)

At a point (i_1, i_2, i_3) on Fourier tansformed lattice the value of k is given by:

$$|k| = \frac{2\pi}{L} \sqrt{i_1^2 + i_2^2 + i_3^2} \tag{38}$$

At this point, we can rewrite (33) to make it suitable for lattice simulation. But before that, let's rescale the parameters, considering (7) and (32):

$$f_{\rm pr} = Aa^r f$$
, $dx_{\rm pr} = Bdx \rightarrow L_{\rm pr} = BL \quad k_{\rm pr} = \frac{k}{B} \quad \omega_{\rm k,pr}^2 = \sqrt{k_{\rm pr}^2 + m_{\rm pr}^2} = \frac{\omega_k}{B} \quad m_{\rm pr} = \frac{am}{B} = a^{2s+2} \frac{d^2 V_{\rm pr}}{df_{\rm pr}^2}$ (39)

(37) becomes:

$$W_{k,\text{pr}}^2 = \langle |f_{k,\text{pr}}|^2 \rangle = \frac{A^2 B^2 a^{2r-2} L_{\text{pr}}^4}{2\omega_{k,\text{pr}} dx_{\text{pr}}^6}$$
(40)

Considering (36) (40), Rayleigh distribution (33) can be expressed as:

$$P(|f_{k,\mathrm{pr}}|) \propto |f_{k,\mathrm{pr}}| \exp\left(-|f_{k,\mathrm{pr}}|^2/W_{k,\mathrm{pr}}^2\right) \tag{41}$$

Don't care about the coefficients, we normalize this equation then:

$$P(|f_{k,\text{pr}}|) = \frac{2}{W_{k,\text{pr}}^2} |f_{k,\text{pr}}| \exp\left(-|f_{k,\text{pr}}|^2 / W_{k,\text{pr}}^2\right)$$
(42)

1.6 Initial conditions of field fluctuations

Now, we discuss how to implement the Rayleigh distribution, consider continuous uniform distributions:

$$X = \int_0^{|f_{k,\text{pr}}|} \frac{2}{W_{k,\text{pr}}^2} |g_{k,\text{pr}}| \exp\left(-|g_{k,\text{pr}}|^2 / W_{k,\text{pr}}^2\right) d|g_{k,\text{pr}}|$$
(43)

$$= \int_0^{|f_{k,\text{pr}}|} \exp\left(-|g_{k,\text{pr}}|^2/W_{k,\text{pr}}^2\right) d\frac{|g_{k,\text{pr}}|^2}{W_{k,\text{pr}}^2} = 1 - \exp\left(-|f_{k,\text{pr}}|^2/W_{k,\text{pr}}^2\right)$$
(44)

Take the inverse:

$$|f_{k,\mathrm{pr}}| = W_{k,\mathrm{pr}} \sqrt{-\ln(1-X)} \sim W_{k,\mathrm{pr}} \sqrt{-\ln X}$$
(45)

X randomly selects points between (0,1), and the last step of equation above is valid. So far, through the program's selection of X, we can generate $|f_{k,pr}|$ that conforms to the distribution (42). The phase of modes are random and uncorrelated. Therefore, the field mode can be expressed as:

$$f_{k,\text{pr}} = e^{i\theta} W_{k,\text{pr}} \sqrt{-\ln X} \qquad \theta \in (0, 2\pi)$$
 (46)

We hereby remind ((40),(38)), (39) and $a = a_0 = 1$:

$$W_{k,\text{pr}} = \frac{ABL^{3/2}}{\sqrt{2\omega_{k,\text{pr}}dx_{\text{pr}}^3}} \qquad \omega_{k,\text{pr}}^2 = \left(\frac{2\pi}{L_{\text{pr}}}\right)^2 (i_1^2 + i_2^2 + i_3^2) + \frac{d^2V_{\text{pr}}}{df_{\text{pr}}^2}$$
(47)

One should read (51).

1.7 Initial conditions of field derivative fluctuations

time dependence of the modes comes from their explicit time dependence $f_{k,\mathrm{pr}} \propto e^{\pm i\omega_k t}$, from factors of the scale factor, and from the time dependence of ω_k itself:

$$f_{k,\text{pr}} \propto \frac{1}{\sqrt{\omega_k}} a^{r-1} e^{\pm i\omega_k t}$$
 $f'_{k,\text{pr}} = \frac{\omega_k}{B} \left[\pm i - \frac{1}{2} \frac{\dot{\omega}_k}{\omega_k^2} + (r-1) \frac{\dot{a}}{\omega_k} \right] f_{k,\text{pr}}$ (48)

Some studies[1] have shown that $\dot{\omega}_k \ll \omega_k^2$, that is $\frac{1}{\sqrt{\omega_k}}$ can be ignored. If this condition is not satisfied in the late stages of inflation then gravitational particle production will occur and it will no longer make sense to take the vacuum fluctuations of equation (32) as initial conditions:

$$f_{k,\mathrm{pr}} \propto a^{r-1} e^{\pm i\omega_k t}$$
 $f'_{k,\mathrm{pr}} = \left(\pm ia^{-s}\omega_{k,\mathrm{pr}} + (r-1)H\right) f_{k,\mathrm{pr}}$ (49)

Prime means taking the derivative with respect to $t_{\rm pr}$. The initial value of $H_{\rm pr}$ is from (30). The symmetry of the Fourier transform suggests that a real field f:

$$f_{-k} = f_k^* \qquad \dot{f}_{-k} = \dot{f}_k^* \tag{50}$$

where the star represents conjugation. Because there is no physically preferred direction on the lattice, the signs of $\pm i\omega_k t$ are not important, choosing the plus sign for a given momentum k necessarily means using the minus sign for the momentum -k. Some studies[1] showed even if every mode is initialized to be same sign, the total momentum this imparts to the field is unnoticeable by the late stages of the evolution in every problem we have considered. We set the initial values:

$$f_k = \frac{1}{\sqrt{2}}(f_{k,1} + f_{k,2}) \qquad \dot{f}_k = \frac{1}{\sqrt{2}}i\omega_k(f_{k,1} - f_{k,2}) - Hf_k \tag{51}$$

where $f_{k,1}$ and $f_{k,2}$ are two modes with separate random phases but equal amplitudes determined by (46).

2 Appendix

2.1 Discrete Fourier transform

Continuous Fourier Transform

$$F(k) = \int d^3x f(x)e^{-ikx} \approx \sum_{n=0}^{N-1} \Delta \mathbf{x} \cdot f(n)e^{-ikn}$$
(52)

where $x_n^1 \to n\Delta x = n\frac{L}{N}$, $f(x) \to f(n \cdot \Delta x)$. Defination of DFT:

$$f(k) = \sum_{n=0}^{N-1} f(n)e^{-ikn} = \frac{\sum_{n=0}^{N-1} \Delta \mathbf{x} \cdot f(n)e^{-ikn}}{\Delta \mathbf{x}} = \frac{1}{\Delta \mathbf{x}} F(k)$$
 (53)

Note, we consider three dimensions.

2.2 Parseval's Theorem

$$\sum_{k=0}^{N-1} |f_k|^2 = \sum_{k=0}^{N-1} f_k f_k^* \tag{54}$$

$$=\sum_{k=0}^{N-1} f_k \left[\frac{1}{N} \sum_{k=0}^{N-1} f_n^* e^{\frac{2\pi i}{N} kn} \right]$$
 (55)

$$= \frac{1}{N} \sum_{k=0}^{N-1} f_n^* \left[\sum_{k=0}^{N-1} f_k e^{\frac{2\pi i}{N} k n} \right]$$
 (56)

$$=\frac{1}{N}\sum_{k=0}^{N-1}|f_n|^2\tag{57}$$

This is a one-dimensional case. The three-dimensional case is easy to prove.

$$\sum_{\mathbf{x}} f(\mathbf{x})^2 = \frac{1}{N^3} \sum_{\mathbf{k}} |f_{3k}|^2 \tag{58}$$

2.3 Initial values in one or two dimensions

Averaging over the lattice position space gives:

$$\langle f(\mathbf{x})^2 \rangle = \frac{1}{N^3} \sum_{\mathbf{x}} f(\mathbf{x})^2 = \frac{1}{N^6} \sum_{\mathbf{k}} |f_{3k}|^2$$

$$\tag{59}$$

Given that the field distribution in Fourier space is on average isotropic this sum can be approximated as a one dimensional sum. In other words, we only need to consider the k shell.

$$|k| = \frac{2\pi}{L} \sqrt{i_1^2 + i_2^2 + i_3^2} = \frac{2\pi}{L} |i| \qquad \langle f(\mathbf{x})^2 \rangle \approx \frac{2\pi}{N^6} \sum_{k} |i|^2 |f_{3k}|^2 = \frac{L^2}{2\pi N^6} \sum_{k} |k| |f_{3k}|^2$$
 (60)

Note, 4π divided by 2 because negative and positive k. The relationship between 3d and 2d:

$$|f_{2k}|^2 \approx \frac{\mathrm{d}x^2}{\pi L} |k| |f_{3k}|^2 \qquad |f_{1k}|^2 \approx \frac{\mathrm{d}x^4}{2\pi L^2} k^2 |f_{3k}|^2$$
 (61)

2.4 speed of sound

consider a volume dV = Avdt the density of medium ρ , mass flow is $\dot{m} = \rho Av$, mass flux conservation requirements

$$\partial j = \partial(\rho v) = \rho dv + v d\rho = 0 \tag{62}$$

Per Newton's second law, the pressure-gradient force provides the acceleration:

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{\rho} \frac{\mathrm{d}P}{\mathrm{d}\mathbf{x}} \to \mathrm{d}P = (-\rho \mathrm{d}v) \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = (v \mathrm{d}\rho)v \to v^2 = c_s^2 = \frac{\mathrm{d}P}{\mathrm{d}\rho}$$
 (63)

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