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Grid Effects on the Plasma Simulation by the Finite-Sized Particle

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About the so-called usual models, in which the total momentum is conserved, it is well known that the total energy is not conserved due to the nonuniformity of space caused by spatial grids. It fluctuates and increases in time from a stochastic origin. In order to see the accuracy of the plasma simulations, it is important to evaluate the fluctuation K_g, which is more dominant for small errors during the shorter time. We study its standard deviation in t, $\sigma\{K_g\}$, and the correlation time of $dK_g/K \cdot dt$, τ_c, about periodic one-dimensional systems, where K is the kinetic energy. We evaluate $\sigma\{K_g\}$ by invoking the stochastic theory and obtain a scaling law:

$$\sigma\{K_g\}/K \simeq (2/\pi)^{1/2} \cdot \eta \cdot \{(2M)^{1/2} n_s \lambda_D\}^{-1} \cdot (t\tau_c \omega_p^2)^{1/2},$$

where $2M$ is the number of the grids per one period, n_s is the electron density, λ_D is the Debye length, and ω_p is the plasma angular frequency. The coefficient η depends on the magnitude of the unphysical grid force of each model. Our simulations with the usual models (CIC–PIC, modified SUDS, and method 2/2) support this scaling law. We obtain the correlation time empirically. It is found that $\tau_c \simeq \Delta t$ if Δt is sufficiently large, and $\tau_c \simeq \frac{1}{4} \Delta/v_{th}$ if $\Delta/(\Delta t \cdot v_{th}) > 3$, where Δt is the time step, Δ is the grid distance, and v_{th} is the thermal velocity of the electron.

I. INTRODUCTION

From a large number of runs, Hockney has derived empirical laws of the error of total energy [1, 14]. Assuming a linear increase in time, he defined the heating time τ_H, during which the total energy increases by 25%. The conception of the heating time is useful in the case of sufficiently large error (an example is presented in Ref. [1, Fig. 4]), or has a meaning for long periods of time. In the usual simulations, however, the heating time cannot be measured, because the energy increment is much smaller than the energy fluctuation, which is the same kind of numerical error as the energy increment. Accordingly, the measurement of the fluctuation in total energy is useful for monitoring simulations.

In this paper, we evaluate the fluctuation of total energy on simple assumptions and make a comparison between these estimations and the numerical results in

the usual models, which calculate the total momentum conserved. Here we explain the difference between the energy increment and the energy fluctuation along the outline of Hockney's consideration [1, p. 24], because we consider that these two quantities are dominated by the same stochastic process. We define K_g as the difference between the initial total energy H_0, and $\bar{K}_g$ as the energy increment, which is obtained by averaging the fluctuation of K_g during a sufficiently long period of time. Then the energy increment in time t, which is due to the presence of the unphysical grid force δF, is

$$\bar{K}_g = \frac{N_p m}{2} \{\Delta v^2\} = \frac{N_p}{2m} \left\{\int_0^t \delta F \, dt\right\}^2 = \frac{1}{2m} \langle \delta F^2 \rangle \, t\tau_c \,, \tag{1}$$

where $\langle \delta F^2 \rangle$ is a random force fluctuation of square magnitude, m is the particle mass, and N_p is the number of particles. The standard deviation of K_g, $\sigma\{K_g\}$, is considered as follows.

$$\begin{aligned} \sigma\{K_g\} &= \sigma\{N_p m(v \cdot \Delta v)\} = \left\{N_p{}^2 \left(\int_0^t v \cdot \delta F \, dt\right)^2\right\}^{1/2} \\ &= \left\{v_{th}^2 \cdot N_p \left(\int_0^t \delta F \, dt\right)^2\right\}^{1/2} = v_{th} \langle \delta F^2 \rangle^{1/2} (t\tau_c)^{1/2}. \end{aligned} \tag{2}$$

In order to evaluate the fluctuation in total energy both theoretically and experimentally, the following way is more convenient. Using the total energy

$$H (= H_0 + K_g),$$

we express the above considerations in a differential form:

$$dH/dt = A(t) \cdot H, \tag{3}$$

where $A(t)$ is the fluctuated function of t. Its mean value is zero, and so the standard deviation $\sigma\{A(t)\}$ and the correlation time τ_c are characteristic quantities. Namely, the evaluation of $\sigma\{K_g\}$ in t is reduced to the computation of $A(t)$ and τ_c.

Lewis *et al.* also investigated the fluctuation in total energy [6, 11]. They experimentally discovered a relation concerning it: $\Delta H \propto 1/(n_s \lambda_D)$, where

$$\Delta H = (H_{\max} - H_{\min})/(H_{\max} + H_{\min}).$$

Our interests are focused on the problem of how much the spatial interpolation of each model influences the fluctuation of total energy. For convenience, we utilize the Fourier transform in order to solve the Poission equation, and adopt the sharp-cutoff cloud [4] as the gridless shape factor throughout this work. In this paper, we do not compare the spatial resolutions, the execution speeds, and so on, of all the models.

In Section II, we derive $\sigma\{A(t)\}$, applying the one-dimensional periodic system of plasma as a test problem. In Section III, we measure $\sigma\{A(t)\}$ in actual simulations and compare it with the above estimation. As to the correlation time τ_c, we discuss it qualitatively. Experimentally, we calculate the autocorrelation function and measure the correlation time. The results verify the above discussion.

II. The Fluctuation in Total Energy

The Basic Equations of the Gridless Cloud Plasma

We consider a periodic one-dimensional system which is composed of two species of N ions and N electrons. Each species has the equal magnitude of the charge and the system is neutral. The mass and charge densities per unit area of the ith particle are m_i and e_i, respectively. Following Refs. [4, 5], we adopt $S(x)$ as the shape factor of clouds. Then the kinetic equations of the particles are

$$dx_i/dt = v_i, \qquad m_i\, dv_i/dt = F_i, \tag{4}$$

$$F_i = e_i \int_0^L S(x - x_i)\, E(x)\, dx, \tag{5}$$

where L is a period. The electrostatic field is given by

$$E = -d\Phi/dx, \qquad d^2\Phi/dx^2 = -1/\epsilon_0 \sum_{i=1}^{2N} e_i S(x - x_i). \tag{6}$$

The total energy H, which is an invariant of the system, is the sum of the kinetic energy K and the field energy W,

$$H = K + W = \sum_{i=1}^{2N} \left\{ \tfrac{1}{2} m_i v_i^2 + \tfrac{1}{2} e_i \int_0^L \Phi(x)\, S(x - x_i)\, dx \right\}. \tag{7}$$

The shape factor $S(x)$ can be expanded to the Fourier series from the periodic condition and is an even function of x due to the symmetry of space,

$$S(x) = (1/L) \sum_{m=0}^{M_c} S_m \cos 2\pi m x/L, \tag{8}$$

where the coefficient S_m should be satisfied with the normalizing condition and M_c corresponds to the maximum mode number in the system.

Interpolation of the Shape Factor

When we solve the above equations using the digital computer, we commonly introduce the spatial grids in order to save the computer time. We obtain the field quantities at the grid points and with them interpolate the quantities at other points. The shape factor $S(x - x_i)$ for the particle position x_i is approximated to a function $S_g(x, x_i)$, which is a linear combination of $S(x - x_{i0\pm l})$, where $x_{i0\pm l}$ are n nearest grid points of x_i ($l = 0, 1, \ldots, n/2$ for $n = even$ or $(n - 1)/2$ for $n = odd$). The total energy H cannot, however, be conserved in the usual models, because S_g loses the property of the spatial uniformity owing to this approximation. This is the essential cause of the numerical error, if the particles per one Debye length are few. Accordingly, the choice of S_g has been an important problem. Here we analyze the properties of the approximated shape factor S_g of CIC–PIC ($n = 2$) [2, 3], method 2/2 ($n = 3$) [6], and modified SUDS ($n = 3$) [7] in order to estimate the errors of the conserved quantities.

The system is assumed to have $2M$ grids. Then the grid distance Δ and the normalized grid distance Δ_0 are

$$\Delta = L/2M, \qquad \Delta_0 = \pi/M. \tag{9}$$

Generally M is equal to or greater than M_c. The case of $M > M_c$ is equivalent to the higher-mode-cutoff method [8].

Next we define x_{i0} as $x_i = x_{i0} + \delta_i$, where δ_i is measured from the grid points,

$$x_{i0} = [x_i/\Delta] \times \Delta \qquad \text{for } n = even, \tag{10a}$$

$$x_{i0} = [x_i/\Delta + 0.5] \times \Delta \qquad \text{for } n = odd, \tag{10b}$$

where the square brackets denote the Gauss symbol. Then the approximated shape factor $S_g^{(n)}$ is written in the forms:

Interpolation with the values at two grid points.

$$S_g^{(2)}(x, x_i) = (1 - \delta_i/\Delta) \cdot S(x - x_{i0}) + (\delta_i/\Delta) \cdot S(x - x_{i0+1}), \tag{11}$$

Interpolation with the values at three grid points.

$$S_g^{(3)}(x, x_i) = w_{-1}S(x - x_{i0-1}) + w_0 S(x - x_{i0}) + w_{+1}S(x - x_{i0+1}), \tag{12}$$

where w_i is a weight of the interpolation, which is the polynomial of δ_i. The slight modification of the above equations is necessary at the end points of the system, by considering the periodic condition.

As a method of determining w_i, we attempt to set S_g well aproximated to S in the lower modes, which dominate the collective motions of the plasma. In other words, we determine w_i so that the difference $S - S_g^{(3)}$ is $O(\Delta^3)$ except for $\delta_i = \pm\Delta/2$. In

this case, however, the weight function of this method has discontinuties similar to the dipole approximation [7]. As is pointed out [7, 12], these discontinuties enhance the error of total energy. In actual simulations we verified that the error in this method is larger than in CIC–PIC, except for $M_c < \frac{1}{4}M$ (strong higher-mode-cutoff). Accordingly, we obtain w_i from the condition that the difference $S - S_g^{(3)}$ is $O(\Delta^2)$ as in CIC–PIC and that the weight function is continuous (Appendix A) as follows.

$$\{w_{-1}, w_0, w_{+1}\} = \{-(1-2\gamma)(\delta_i/\Delta)^2 - (\delta_i/\Delta)/2 + (1-\gamma)/2, (2-4\gamma)(\delta_i/\Delta)^2 + \gamma, -(1-2\gamma)(\delta_i/\Delta)^2 + (\delta_j/\Delta)/2 + (1-\gamma)/2\}, \quad (13)$$

where γ is an arbitrary constant, the magnitude of which considerably varies the properties of the model. The following two values have the distinguishing features:

$\gamma = 0.50$: Quadric terms vanish to reduce a linear interpolation. It is equivalent to modified SUDS.

$\gamma = 0.75$: The weight function is continuous to the first derivative. It is equivalent to method 2/2.

The shape factor S_g is satisfied with the conditions required for the shape factor, except for the uniformity of space.

Interparticle Forces and Momentum Conservations

Lewis *et al.* derive the interparticle force for each of their models and prove the momentum conservation for the CIP–PIC (method 1/1) [6]. Here we represent the interparticle force in the case of systems where all variable quantities are expanded to the Fourier series or an eigenfunction of the system.

The force $F_j^{(n)}$ acting on the jth particle can be expressed in the form

$$F_j^{(n)} = \sum_{i=1}^{2N} F_{j,i}^{(n)}$$

$$= \frac{e_j}{4\pi\epsilon_0} \sum_{i=1}^{2N} e_i \sum_{m=1}^{M_c} \frac{S_m}{m} \{f_{s,m}^{(n)}(\delta_i, \delta_j) \sin mk\Delta_0 + f_{c,m}^{(n)}(\delta_i, \delta_j) \cos mk\Delta_0\}, \quad (14)$$

where

$$k = (x_{j0} - x_{i0})/\Delta, \quad (15)$$

$f_{s,m}^{(n)}$: *Symmetrical polynomials of* δ_i *and* δ_j ,

$f_{c,m}^{(n)}$: *Alternating polynomials of* δ_i *and* δ_j .

As in the results of Lewis *et al.*, the self-force $F_{i,i}^{(n)}$ vanishes and the total momentum is conserved exactly because $F_{i,j}^{(n)} = -F_{j,i}^{(n)}$. The concrete expressions of $f_{s,m}^{(n)}$ and $f_{c,m}^{(n)}$ are obtained by replacing S with S_g in Eqs. (5) and (6) as follows.

$$f_{s,m}^{(2)} = \{1 - (\delta_i + \delta_j)/\Delta + 2\delta_i\delta_j/\Delta^2\}(1 - \cos m\Delta_0) + \cos m\Delta_0\,, \tag{16a}$$

$$f_{c,m}^{(2)} = \{(\delta_j - \delta_i)/\Delta\} \sin m\Delta_0\,, \tag{16b}$$

$$\begin{aligned} f_{s,m}^{(3)} = {} & (1 - 2\gamma)^2 (6 - 8 \cos m\Delta_0 + 2 \cos 2m\Delta_0)\, \delta_i^2\delta_j^2/\Delta^4 \\ & + (1 - 2\gamma)\{(3\gamma - 1) - 2(2\gamma - 1) \cos m\Delta_0 + (\gamma - 1) \cos 2m\Delta_0\} \\ & \times (\delta_i^2 + \delta_j^2)/\Delta^2 + 0.5(3\gamma^2 - 2\gamma + 1) + 2\gamma(1 - \gamma) \cos m\Delta_0 \\ & + 0.5(1 - \gamma)^2 \cos 2m\Delta_0 + 0.5(1 - \cos 2m\Delta_0)\, \delta_i\delta_j/\Delta^2, \end{aligned} \tag{16c}$$

$$\begin{aligned} f_{c,m}^{(3)} = {} & (\delta_j - \delta_i)/\Delta\{(4\gamma - 2)(\sin m\Delta_0 - 0.5 \sin 2m\Delta_0)\, \delta_i\delta_j/\Delta^2 \\ & + \gamma \sin m\Delta_0 - 0.5(\gamma - 1) \sin 2m\Delta_0\}. \end{aligned} \tag{16d}$$

An Evaluation of the Fluctuation in Total Energy

Except for the energy-conserving codes developed by Lewis *et al.* [6] and Langdon [12], the error of total energy is inevitable for the usual models, even if the time integral is calculated exactly. Here we consider the properties of the error of total energy and estimate the magnitude of it. An origin of the error is that the approximated shape factor S_g loses the uniformity of space or does not depend only on $x - x_i$. In other words, it is considered that the spatial grids exert the unphysical forces on the particles in the system [8]. We assume this unphysical grid force $\delta F_j^{(n)}$ as the difference between the force $F_j{}^*$ acting on the shape factor S^*, which has the uniformity of space, and the force $F_j^{(n)}$ acting on the approximated shape factor $S_g^{(n)}$:

$$\begin{aligned} \delta F_j^{(n)} = F_j^{(n)} - F_j{}^* = {} & \frac{e_j}{4\pi\epsilon_0} \sum_{i=1}^{2N} e_i \sum_{m=1}^{M_c} \frac{S_m}{m} \\ & \times \left[\left\{f_{s,m}^{(n)}(\delta_i\,, \delta_j) - \kappa_m^{(n)} \cos \frac{2\pi m}{L} (\delta_j - \delta_i)\right\} \sin mk\Delta_0 \right. \\ & \left. + \left\{f_{c,m}^{(n)}(\delta_i\,, \delta_j) - \kappa_m^{(n)} \sin \frac{2\pi m}{L} (\delta_j - \delta_i)\right\} \cos mk\Delta_0\right], \end{aligned} \tag{17}$$

where $F_j{}^*$ is not equal to the force F_j acting on the shape factor S generally, because S_g approximates S well in the lower modes but not in the higher modes at all. Accordingly, $\kappa_m^{(n)}$ are correction factors caused by the interpolation, which converge to unity as m decreases. The unphysical energy K_g which flows in or out the system is given by

$$dK_g^{(n)}/dt = \sum_{j=1}^{2N} v_j\, \delta F_j^{(n)}, \tag{18}$$

where we assume that time is continuous. The effects of the finite time step are

discussed in Section III. Although $F_j^{(n)}$ is determined by the kinetic equation which obeys the law of causality, $\delta F_j^{(n)}$ can be considered as a random noise which is almost independent of the history of the system. So the unphysical kinetic energy K_g is evaluated statistically on some assumptions.

In the case of the sufficiently small error, the mean value of dK_g/dt is equal to zero and so the standard deviation, $\sigma\{dK_g/dt\}$, and the correlation time, τ_c, are the quantities required for the evaluation of K_g, where τ_c is a characteristic time during which dK_g/dt varies. Then K_g is obtained statistically at time t. If the error is sufficiently small and t is not long, the random noise theory [13] shows that the mean value of K_g equals zero and the standard deviation $\sigma\{K_g\}$ is

$$\sigma\{K_g\} \simeq \sigma\{dK_g/dt\}(t\tau_c)^{1/2}. \tag{19}$$

Next we evaluate $\sigma\{dK_g/dt\}$ on the following assumptions.

(a) The particles are distributed at random.

(b) The correlation between the unphysical force $\delta F_j^{(n)}$ and the particle velocities v_j does not exist.

(c) The correlations between δ_i, δ_j, and $k\{=(x_{j0} - x_{i0})/\Delta\}$ do not exist.

These assumptions do not involve the effects of the properties of the plasma such as the Debye shielding, the particle-bunching by the potential fluctuations, and so on. Although these effects influence the evaluation of $\sigma\{dK_g^{(n)}/dt\}$, these assumptions are almost correct in the limit of the small fluctuation energy. On the above assumptions, probabilities $p(\delta_i)$ and $q(k)$ are calculated as follows.

$$p(\delta_i) = 1/\Delta, \qquad q(k) = (M - |k|)/M^2, \tag{20}$$

Next we define the fluctuating kinetic energy $K_{g,l}^{(n)}$ which is sampled at time t_l. Then the square of the standard deviation $\sigma\{dK_{g,l}^{(n)}/dt\}$ is

$$\begin{aligned}\sigma^2\{dK_g^{(n)}/dt\} &= \frac{l}{l_s}\sum_{l=1}^{l_s}(dK_{g,l}^{(n)}/dt)^2 \\ &= \frac{1}{l_s}\sum_{l=1}^{l_s}\left\{\sum_{j=1}^{2N} v_j^2(\delta F_j^{(n)})^2 + \sum_{i\neq j}^{2N} v_i v_j\, \delta F_i^{(n)}\, \delta F_j^{(n)}\right\}_l,\end{aligned} \tag{21}$$

where l_s is the number of the samples, which are assumed sufficiently large. In the following we eliminate the subscript l and the notation $(1/l_s)\sum_{l=1}^{l_s}$ in order to avoid complicated expressions. Assumption (b) suggests that the second term of Eq. (21) vanishes. Accordingly we get an approximation

$$\sigma^2\{dK_g^{(n)}/dt\} = \sum_{j=1}^{2N} v_j^2(\delta F_j^{(n)})^2 = \langle v_j^2\rangle \sum_{j=1}^{2N}(\delta F_j^{(n)})^2, \tag{22}$$

where the angle brackets shows the average for the particles. Namely, we conclude that $\sigma^2\{dK_g^{(n)}/dt\}$ is a product of the random force fluctuation of square magnitude, $\sum_{j=1}^{2N}(\delta F_j^{(n)})^2$, and the average of the square of velocity $\langle v_j^2\rangle$, as discussed in Section I. The detailed derivation of $\sum_{j=1}^{2N}(\delta F_j^{(n)})^2$ is shown in Appendix B.

Using the subscripts i and e to denote quantities associated with the ion and electron, we obtain

$$\sigma\left\{\frac{dK_g^{(n)}}{K\,dt}\right\} = \frac{1}{\pi^{1/2}}\,\omega_p{}^2\,\frac{1}{M^{1/2}}\,\frac{1}{N/L}\,\frac{(\langle v_i{}^2\rangle + \langle v_e{}^2\rangle)^{1/2}}{(m_i/\mu)\langle v_i{}^2\rangle + (m_e/\mu)\langle v_e{}^2\rangle}\cdot\eta^{(n)}\left(\frac{M_c}{M}\right), \tag{23}$$

where

$$\omega_p{}^2 = \frac{e^2N}{\epsilon_0\mu L} = (1/m_i + 1/m_e)\,\frac{Ne^2}{\epsilon_0 L}, \tag{24}$$

$$\eta^{(2)}(M_c/M) = \left[\int_0^{(M_c/M)\pi} dx\left(\frac{S_{x/\Delta}^2}{4x^2}\right)\left\{\kappa_{x/\Delta}^2 + \frac{4}{9} + \frac{4}{9}\cos x + \frac{1}{9}\cos^2 x - \frac{8\kappa_{x/\Delta}}{x^4}(1-\cos x)^2\right\}\right]^{1/2}, \tag{25}$$

where $S_{x/\Delta}$ and $\kappa_{x/\Delta}$ are the smooth functions of x, which are equal to S_m and $\kappa_m^{(n)}$, when $x/\Delta = m$, respectively. $\eta^{(3)}$ is too complex to be presented here, although it can be calculated analytically. Therefore, we show the numerical results later. In order to clarify the scaling law about the fluctuation in total energy, we neglect the terms for the ion:

$$\sigma\left\{\frac{dK_g^{(n)}}{Kd(\omega_p t)}\right\} \simeq \frac{1}{\pi^{1/2}}\,\frac{1}{M^{1/2}}\,\frac{1}{n_s\lambda_D}\cdot\eta^{(n)}\left(\frac{M_c}{M}\right). \tag{26}$$

From the experimental results, Lewis *et al.* indicated that the fluctuation is approximately proportional to $(n_s\lambda_D)^{-1}$ for $\Delta/\lambda_D = 1$ [6]. Our evaluation supports their empirical law. Generally it is proportional to $[(2M)^{1/2}\cdot n_s\cdot\lambda_D]^{-1}$ for all methods. The coefficient $\eta^{(n)}$ involves the unknown factor $\kappa_m^{(n)}$, which depends on each model.

Determination of the Unphysical Grid Force or $\kappa_m^{(n)}$

The gridded systems with the shape factor $S_g^{(n)}$ are similar to the gridless systems with the shape factor S^* about the physical properties, whether they have the uniformity of space or not. Therefore, we study the fluctuation spectrum of the electric field. In the gridless system, the fluctuation spectrum of the thermal equilibrium state, $\langle\epsilon_0 E_m{}^2\rangle$ [4, 5], is

$$\langle\epsilon_0 E_m{}^2\rangle = \frac{m_e\langle v_e{}^2\rangle}{L}\,\frac{(S_m{}^*/2)^2}{(S_m{}^*/2)^2 + (k_m\lambda_D)^2}, \tag{27}$$

where $k_m = 2\pi m/L$ and $\lambda_D{}^2 = \frac{1}{2} \cdot \epsilon_0 m_e \langle v_e{}^2 \rangle / n_s e^2 = \frac{1}{2} \cdot \epsilon_0 m_i \langle v_i{}^2 \rangle / n_s e^2$. In the gridded system, the problem is more difficult [10]. When the Debye shielding effect can be neglected or the particles are distributed at random in space, however, we calculate it as well as the evaluation of $\sigma\{dK_g^{(n)}/dt\}$ as follows.

$$\langle \epsilon_0 E_m{}^2 \rangle = \frac{2}{L} \frac{\mu \omega_p{}^2}{k_m{}^2} \xi_m^{(n)} (S_m/2)^2, \tag{28}$$

where

$$\xi_m^{(2)} = \tfrac{2}{3} + \tfrac{1}{3} \cos m\Delta_0 , \tag{29a}$$

$$\begin{aligned} \xi_m^{(3)} = {} & (2 - 4\gamma)^2 (1 - \cos m\Delta_0)^2/12 + (2 - 4\gamma)(1 - \cos m\Delta_0) \\ & \times \{\gamma + (1 - \gamma) \cos m\Delta_0\}/2 + \{\gamma + (1 - \gamma) \cos m\Delta_0\}^2 \\ & + \sin^2 m\Delta_0/12. \end{aligned} \tag{29b}$$

When λ_D is sufficiently large, Eq. (27) can be set equal to Eq. (28). As a result, we conclude the following.

$$\kappa_m^{(n)} = \{\xi_m^{(n)}\}^{1/2}. \tag{30}$$

In Fig. 1, we show $\eta^{(n)}(x)$, which is calculated from Eqs. (25) and (30).

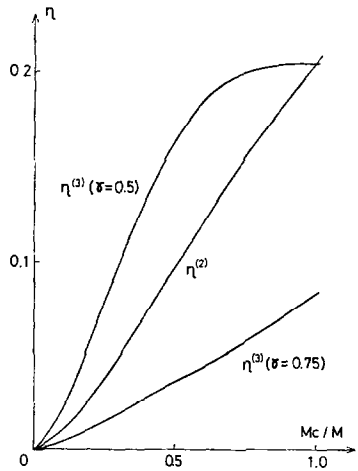

FIG. 1. $\eta^{(n)}$ vs M_e/M.

III. Numerical Results and Comparison with the Theory

We carried out numerical simulations of the system explained in Section II in order to verify the scaling law. Namely we measure the standard deviation $\sigma\{dH/Hdt\}$ and the correlation time τ_c, and compare the estimated value $\sigma\{dK_g/Kdt\}$ with the measured value $\sigma\{dH/Hdt\}$. These two values are expected to be approximately equal because the potential energy W is sufficiently smaller than the kinetic energy K. The algorithm for advancing particles is the standard time-centered leapfrog scheme and Eq. (6) is integrated by using FFT [9]. The total energy H is calculated by the use of the equation which is modified by replacing S by $S_g^{(n)}$ in Eq. (7). As the initial state of plasma, the electron–ion pairs are put uniformly in space and the particle velocities are selected independently from Maxwellian distributions. In spite of the special distribution of space at the initial state, it is confirmed that $\sigma\{dH/Hdt\}$ measured per 40 steps is kept constant within a factor of 3 through each run. In order to avoid the round-off errors, all data are treated with the double precision (1 word = 72 bits).

Numerical Results

We change the differential equation, Eq. (3), into the difference equation

$$(H_{n+1} - H_n)/\Delta t = H_n A_n , \tag{31}$$

where H_n is the total energy at the nth step ($t = n \cdot \Delta t$). Accordingly, we compute the statistical values about N_d data of the following h_n.

$$h_n = A_n \cdot \Delta t = H_{n+1}/H_n - 1 \qquad (n = 1, 2, 3,..., N_d). \tag{32}$$

Then the standard deviation σ is calculated as

$$\sigma^2 = (1/N_d) \sum_{i=1}^{N_d} \left\{ h_i - (1/N_d) \sum_{j=1}^{N_d} h_j \right\}^2 . \tag{33}$$

Using σ, we calculate the empirical value η_{emp} as follows.

$$\eta_{\text{emp}} = \frac{\pi^{1/2}\sigma}{\omega_p^2 \Delta t} \frac{M^{1/2} \cdot N}{L} \frac{(m_i/\mu)\langle v_i^2 \rangle + (m_e/\mu)\langle v_e^2 \rangle}{(\langle v_i^2 \rangle + \langle v_e^2 \rangle)^{1/2}} . \tag{34}$$

In the case of finite Δt, the autocorrelation function, $R(k \cdot \Delta t)$, is defined as

$$R(k \cdot \Delta t) = \frac{1}{N_d - k} \sum_{i=1}^{N_d - k} h_i \cdot h_{i+k} \qquad (k = 0, 1, 2, 3,...), \tag{35}$$

and the correlation time τ_c is calculated by assuming the Markoffian process [13].

As the simulation parameters, the following values are chosen. $S_m = 2$ ($m \gtrsim 1$); $2M = 32 \sim 512$; $N = 160$, 320, and 640; $\lambda_D \cdot (L/2\pi)^{-1} = 0.05$ and 0.2; $\langle v_i^2 \rangle / \langle v_e^2 \rangle = 0.01$; $m_i/m_e = 25$; $\omega_p \cdot \Delta t = 0.2$, 0.1, 0.05, and 0.04; and $N_d \simeq 500$. Figure 2 shows that η_{emp} keeps constant within a factor of 2, when σ varies between 10^{-2} and 10^{-4}. Therefore, it is experimentally confirmed that the scaling law, Eq. (23), holds good about the parameters $2M$, N, Δt, and $\langle v_e^2 \rangle$.

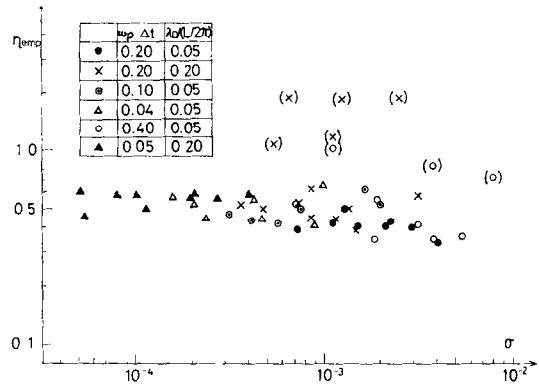

FIG. 2. η_{emp} vs σ for various parameters in CIC–PIC. The round brackets represent runs with the parameters: $\Delta t \cdot v_{th} > \Delta$, in which η_{emp} is greatly enhanced.

Notice that Eq. (23) is obtained under the condition that time is continuous. So the next condition that the fine variation of space is calculated smoothly in time should be required:

$$\langle v_e^2 \rangle^{1/2} \cdot \Delta t < \Delta. \tag{36}$$

Actually, if the above condition is not satisfied, η_{emp} is enhanced, as shown in Fig. 2. However, by setting Δt shorter or Δ longer and satisfying Eq. (32), η_{emp} can be reduced to the usual values.

Table 1 shows η_{emp} for each model in the case of $M_c/M = 1$ and $\frac{1}{2}$. η_{emp} is reduced by 50% for CIC–PIC and method 2/2 but is reduced only 10% for SUDS, when the higher modes are cut off: $M_c/M = \frac{1}{2}$.

Correlation Time

As mentioned above, we replace the differential equations, Eq. (4), by difference equations in actual simulations. This means that the unphysical grid force $\delta F_j^{(n)}$ is kept constant during a time step Δt and the right-hand side of Eq. (18) is a step

TABLE I

Comparisons between the Theoretical and Empirical Values of η

Model	$M_c/M = 1$		$M_c/M = \frac{1}{2}$	
	η_{emp}	η_{emp}/η	η_{emp}	η_{emp}/η
CIC–PIC	0.50	2.4	0.29	2.9
Modified SUDS	0.26	1.3	0.23	1.4
Method 2/2	0.14	1.6	0.06	1.6

function of t. Accordingly, the correlation time τ_c is larger than Δt. If Δt is sufficently large and the particle positions in one grid interval are randomized during one time step, τ_c is nearly equal to Δt. On the contrary, if Δt is sufficiently small and time is considered almost continuous, τ_c is expected to be proportional to Δ/v_{th} and is a characteristic time during which the particle distribution in one grid interval changes continuously.

These features for the correlation time are presented in Fig. 3. It shows the

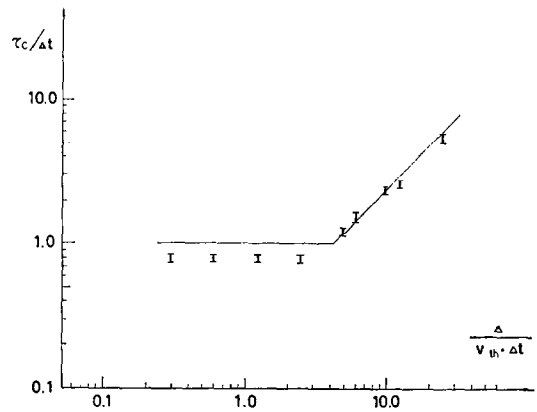

FIG. 3. τ_c/Δ vs $\Delta/(v_{th} \cdot \Delta t)$ in CIC–PIC.

dependence of $\tau_c/\Delta t$ on $\Delta/(\Delta t \cdot v_{th})$, which indicates how many time steps a thermal electron takes to pass one grid interval. If $\Delta/(\Delta t \cdot v_{th})$ is sufficiently small, τ_c is equal to Δt and is independent of the other parameters. When $\Delta/(\Delta t \cdot v_{th})$ is larger than 3, it increases linearly in $\Delta/(\Delta t \cdot v_{th})$. Namely, τ_c becomes independent

of Δt and nearly equal to $\frac{1}{4} \cdot \Delta/v_{th}$. From the above results and Eq. (32), the optimum time step should be satisfied with the condition

$$0.3\Delta/v_{th} < \Delta t < \Delta/v_{th}$$

These results are consistent with Hockney's in [1, Eq. (12)] in the case of the Debye length larger than half of the grid distance, although his evaluation is concerned with the heating time.

VI. Discussions and Conclusions

In Section II, we introduced assumptions (a), (b), and (c) in order to evaluate the energy fluctuation statistically. In these assumptions the dynamical shielding effects of plasma are neglected. If the Debye length is sufficiently large, it is clear that these effects can be neglected. Judging from the properties of the fluctuation spectrum [see Eqs. (27) and (28)], we can expect that our scaling law will give the correct results, if Eq. (36) and the following condition are satisfied:

$$2\pi M_c > L\lambda_D^{-1}. \tag{37}$$

Actually, we observed that the accuracy of the scaling law is rather poor when M_c is reduced to a parameter of $2\pi M_c \simeq 0.5 \cdot L\lambda_D^{-1}$.

Concerning method 2/2 and modified SUDS, η_{emp} agrees with $\eta^{(3)}$ within a factor of 1.6. Especially, it is well explained that η_{emp} for $M_c/M = \frac{1}{2}$ becomes smaller by only 10% than that for $M_c/M = 1$. However, η_{emp} in CIC–PIC is larger by a factor of 2.4 or 2.9 than $\eta^{(2)}$. We could not find the cause within the accuracy of this work. In order to improve the accuracy of the scaling law and the coefficient η, we should consider the dynamical effects of plasma and the error associated with the spatial interpolation of the scalar potential. If we adopt the empirical value for η, however, we believe that our scaling law holds within a factor of 2.

We discuss some applications of our work for other problems. It is well known that Eqs. (6) are solved by transforming them into difference equations. In this case our evaluation can be applied after slight modifications. The scaling law about the heating time τ_H is calculated in the case of $2\pi M_c > L\lambda_D^{-1}$, because the random force fluctuation of square magnitude, $\langle \delta F^2 \rangle$, is obtained. Extensions to the two- or three-dimensional problem are possible for the usual models. Our considerations concerning the interpolation of the shape factor are generally applicable for the system with the more complex boundary conditions and curved spatial grids of the two- and three-dimensions.

APPENDIX A: THE DETERMINATION OF WEIGHTS ($n = 3$)

When $M_c \ll M$, $S(x - x_{i0-1})$, $S(x - x_{i0})$, and $S(x - x_{i0+1})$ can be approximated by the Taylor expansion in the neighborhood of $x - x_i$. From Eq. (12), we obtain

$$S_g^{(3)}(x, x_i) = (w_{-1} + w_0 + w_{+1}) \cdot S(x - x_i) - \{(\Delta + \delta_i) w_{-1} + \delta_i w_0 + (-\Delta + \delta_i) w_{+1}\} \cdot S'(x - x_i) + O(\Delta^2), \tag{A.1}$$

where $S'(x)$ is $dS(x)/dx$. Therefore, we get

$$\begin{aligned} w_{-1} + w_0 + w_{+1} &= 0, \\ (\Delta + \delta_i) w_{-1} + \delta_i w_0 + (-\Delta + \delta_i) w_{+1} &= 0. \end{aligned} \tag{A.2}$$

In addition to the above conditions, we adopt the following condition that the weight function is continuous at $\delta_i = \pm\Delta/2$.

$$\begin{aligned} w_{-1}(\delta_i = -\Delta/2) &= w_0(\delta_i = +\Delta/2), \\ w_{+1}(\delta_i = +\Delta/2) &= w_0(\delta_i = -\Delta/2). \end{aligned} \tag{A.3}$$

Assuming w_i as a quadric polynomial of δ_i and solving Eqs. (A.2) and (A.3), we obtain Eq. (13), which involves the arbitrary constant γ.

When M_c is nearly equal to M, we extend the above definition and use these weights. So one should take notice that $S^{(n)}$ never becomes the approximation of S in higher modes.

APPENDIX B: DERIVATION OF $\sum_{j=1}^{2N} (\delta F_j^{(n)})^2$

We rewrite Eq. (17) for simplicity in the form

$$\delta F_j^{(n)} = \frac{e_j}{4\pi\epsilon_0} \sum_{i=1}^{2N} e_i \sum_{m=1}^{M_c} (g_{s,m}^{(n)} \sin mk\Delta_0 + g_{c,m}^{(n)} \cos mk\Delta_0), \tag{B.1}$$

where

$$\begin{aligned} g_{s,m}^{(n)}(\delta_i, \delta_j) &= (S_m/m)\{f_{s,m}^{(n)}(\delta_i, \delta_j) - \kappa_m^{(n)} \cos(2\pi m/L)(\delta_j - \delta_i)\}, \\ g_{c,m}^{(n)}(\delta_i, \delta_j) &= (S_m/m)\{f_{c,m}^{(n)}(\delta_i, \delta_j) - \kappa_m^{(n)} \sin(2\pi m/L)(\delta_j - \delta_i)\}. \end{aligned}$$

Like the derivation of Eq. (22), averaging over the samples lets the cross terms cancel and yields $\sum_{j=1}^{2N} (\delta F_j^{(n)})^2$ in the form

$$\sum_{j=1}^{2N} (\delta F_j^{(n)})^2 = \sum_{j=1}^{2N} \left(\frac{e_j}{4\pi\epsilon_0}\right)^2 \sum_{i=1}^{2N} e_i^2 \sum_{m=1}^{M_c} (g_{s,m}^{(n)} \sin mk\Delta_0 + g_{c,m}^{(n)} \cos mk\Delta_0)^2. \quad \text{(B.2)}$$

Considering assumption (c), we introduce the probabilities $p(\delta_i)$ and $q(k)$ [Eq. (20)], and replace the summations of i, j, and k by integrations:

$$\sum_{j=1}^{2N} (\delta F_j^{(n)})^2 = \left(\frac{2Ne^2}{4\pi\epsilon_0}\right)^2 \sum_{m=1}^{M_c} (\tilde{g}_{s,m}^2 + \tilde{g}_{c,m}^2)/2, \quad \text{(B.3)}$$

where the notation $\tilde{g}^2$ denotes the integration

$$\int_a^b \int_a^b g^2 p(\delta_i)\, p(\delta_j)\, d\delta_i\, d\delta_j\,,$$

$$\begin{pmatrix} a = 0, & b = \Delta & \text{for} & n = even; \\ a = -\Delta/2, & b = \Delta/2 & \text{for} & n = odd. \end{pmatrix}$$

Replacing the summation of m by an integration yields the numerical factor $\eta^{(n)}$ of Eq. (23), and the random force fluctuation of square magnitude is obtained as follows.

$$\sum_{j=1}^{2N} (\delta F_j^{(n)})^2 = \frac{1}{\pi} \frac{\mu^2 L^2}{2M} \omega_p{}^4 \cdot \left\{\eta^{(n)} \left(\frac{M_c}{M}\right)\right\}^2. \quad \text{(B.4)}$$

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REFERENCES

1. R. W. HOCKNEY, *J. Computational Phys.* **8** (1971), 19.
2. R. L. MORSE AND C. W. NIELSON, *Phys. Fluids* **12** (1969), 2418.
3. C. K. BIRDSALL AND D. FUSS, *J. Computational Phys.* **3** (1969), 494.
4. A. B. LANGDON AND C. K. BIRDSALL, *Phys. Fluids* **13** (1970), 2115.
5. H. OKUDA AND C. K. BIRDSALL, *Phys. Fluids* **13** (1970), 2123.
6. H. R. LEWIS, A. SYKES, AND J. A. WESSON, *J. Computational Phys.* **10** (1972), 85.

7. W. L. KUER, J. M. DAWSON, AND B. ROSEN, *J. Computational Phys.* **13** (1973), 114.
8. A. B. LANGDON, *J. Computational Phys.* **6** (1970), 247.
9. R. C. SINGLETON, *Comm. ACM* **11** (1968), 773.
10. A. B. LANGDON, in "Proceedings of the Fourth Annual Conference on Numerical Simulations of Plasmas" U. S. Government Printing Office, Washington, D. C. 20402, 1970, Stock No. 08510059.
11. D. I. BROWN, S. J. GITOMER, AND H. R. LEWIS, *J. Computational Phys.* **14** (1974), 193.
12. A. B. LANGDON, *J. Computational Phys.* **12** (1973), 247.
13. S. CHANDRASEKHAR, "Reviews of Modern Physics," Vol. 15, Dover, New York, 1954.
14. R. W. HOCKNEY, S. P. GOEL, AND J. W. EASTWOOD, *J. Computational Phys.* **14** (1974), 148.