

NOTE:

Let Us Become Familiar with the UT/IFS Simulation Codes -- I

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One of the tedious parts of learning for the beginning user of simulation is to familiarize oneself with the detailed listing of the code, in light of simulation theory, perhaps, in particular that of normalization. This note intends to close that gap.

The basic principles of particle simulation codes are well documented and oft-discussed subjects. It may be assumed that these are already "theoretically well understood:" for example, finite-differencing, the leap-frog scheme, finite-sized particles, FFT's, dipole approximations, the Courant-Friedrichs-Lewy condition, the aliases, and so on. It is, however, still quite natural for the beginning student in the field to feel at a loss as to how to begin after all those theories. Although it may take a kinesiology Ph.D. to figure out the theory of running, while a three year-old child can run, it has still taken that child three years to learn how to run in practice. It is this kind of gap which I wish to bridge. What smart simulators can do in two months took this author two years to learn, so do not be discouraged by seemingly tedious, meaningless arrays of names. This note may still contain errors or derivations which can be improved. Please let me know of any corrections which will improve it.

### 1. Equation of Motion

The equation of motion due to electrostatic field is

$$\frac{dv_j}{dt} = \frac{e}{m} E , \quad (1)$$

where  $j$  specifies the  $j$ -th particle (electron),  $e$  is the electron charge (which is usually, and here taken as, positive), and  $m$  the electron mass. With finite particle size,

$$\frac{dv_j}{dt} = \frac{e}{m} \int_0^L E(r) S(r - r_j) dr , \quad (2)$$

where  $L$  is the system length ( $L \equiv N_c \Delta$ ) and  $S(r)$  is the form (shape) factor of particle charge. Ideally, we wish to take the system length as infinite, but we are satisfied with finite  $L$  with  $N_c$  large enough for the periodic boundary condition. On the other hand, we define the form factor as normalized in an infinite system. In case of Gaussian choice of the form factor, this introduces a small amount of error, because the Gaussian is not really periodic at large  $r$ .

$$\begin{aligned} S(r) &= \frac{1}{\sqrt{2\pi}a} \exp\left(-\frac{1}{2} \frac{r^2}{a^2}\right), \\ S(k) &= \frac{1}{L} \exp\left(-\frac{1}{2} k^2 a^2\right). \end{aligned} \quad (3)$$

As far as  $a \ll L$ , the error due to this should be exponentially small.

Since our system is finite and periodic, we use a discretized Fourier transform as follows:

$$\begin{aligned} G(k) &= \frac{1}{L} \sum_{g=1}^{N_c} G(r_g) \exp(-ikr_g) \\ G(r_g) &= \sum_{m=1}^{N_c} G(k) \exp(ikr_g) \end{aligned} \quad (4)$$

where  $r_g = g\Delta$ ,  $k = 2\pi m/L$ , and  $N_c \Delta = L$ . Every quantity with dimensions is normalized in terms of  $\omega_p^{-1}$  for the temporal dimensionality and  $\Delta$  for the spatial dimensionality. In the following we explicitly show these normalizations.

Equation (2) becomes:

$$\frac{d\tilde{v}_j}{d\tilde{t}} = \frac{e}{m\omega_p^2\Delta} \int_0^L E(r) f(r - r_j) dr, \quad (5)$$

where  $\tilde{v}_j = v_j/\omega_p\Delta$  and  $\tilde{t} = t\omega_p$ . From here on, quantities with a tilda are normalized. Here, the plasma frequency is defined as  $\omega_p^2 = 4\pi n_0 e^2/m$ , using the real particle quantities as usual. It can be defined in terms of normalized simulation quantities as well.

Equation (5) becomes:

$$\begin{aligned} \frac{d\tilde{v}_j}{d\tilde{t}} &= \frac{e}{m\omega_p^2\Delta} \int_0^L \sum_{k'} E(k') \exp(ik' \cdot r) \sum_{k''} S(k'') \exp[ik''(r - r_j)] dr \\ &= \frac{e}{m\omega_p^2\Delta} \sum_{k'} \sum_{k''} E(k') S(k'') \exp(-ik'' \cdot r_j) \int_0^L \exp[i(k' + k'')r] dr \\ &= \frac{e}{m\omega_p^2\Delta} \sum_{k'} \sum_{k''} E(k') S(k'') \exp(-ik'' \cdot r_j) L \left\{ \frac{1}{L} \int_0^L \exp[i(k' + k'')r] dr \right\} \\ &= \frac{e}{m\omega_p^2\Delta} \sum_{k'} \sum_{k''} E(k') S(k'') \exp(-ik'' \cdot r_j) L \delta_{k', -k''}, \end{aligned}$$

where  $\delta_{k', -k''}$  is Kronecker's delta. We now have

$$\begin{aligned} \frac{d\tilde{v}_j}{dt} &= \frac{eL}{m\omega_p^2\Delta} \sum_{k'} E(k') S(-k') \exp(ik' \cdot r_j) \\ &= \frac{eL}{m\omega_p^2\Delta} \sum_{k'} E(k') S(k') \exp(ik' \cdot r_j) , \end{aligned}$$

since  $S(r)$  is real and symmetric. Explicitly using Eq. (3), this is cast into

$$\begin{aligned} \frac{d\tilde{v}_j}{dt} &= \frac{e}{m\omega_p^2\Delta} \sum_k E(k) \exp\left(-\frac{1}{2} k^2 a^2\right) \exp(ik \cdot r_j) \\ &= \text{FFT}^{-1} \left[ \frac{e}{m\omega_p^2\Delta} E(k) \exp\left(-\frac{1}{2} k^2 a^2\right) \right] \\ &= \text{FFT}^{-1}[F(k)] \end{aligned} \tag{6}$$

where

$$F(k) \equiv \frac{e}{m\omega_p^2\Delta} E(k) \exp\left(-\frac{1}{2} k^2 a^2\right) . \tag{7}$$

## 2. Poisson's Equation

Poisson's equation is

$$\nabla \cdot \mathbf{E} = 4\pi en = 4\pi\rho \quad . \quad (8)$$

To count charge in the computer, we have to assign a certain amount of charge to a sheet of particle in the simulation. This is done by assigning a macro (or super) charge (as well as a macro mass) to a single simulational particle (sheet):

$$\rho_p = \frac{en_0L}{N} \quad ,$$
$$m_p = \frac{mn_0L}{N} \quad , \quad (9)$$

where  $n_0$  is the real particle density and  $N$  is the total number of simulational macro particles. Now the charge density is given by

$$\rho(\mathbf{r}_j) = \rho_p \int G(\mathbf{r})S(\mathbf{r} - \mathbf{r}_j)dr \quad , \quad (10)$$

where  $G(\mathbf{r})$  is the number of macroscopic simulational particles in a cell. Equation (8) becomes:

$$ik \cdot \mathbf{E}(k) = 4\pi\rho_p G(k)S(k) \quad . \quad (11)$$

Explicitly,

$$\mathbf{E}(k) = \exp\left(-\frac{1}{2}k^2a^2\right) \frac{4\pi\rho_p}{ik} G(k) \quad . \quad (12)$$

Combining Eqs. (12) and (7), we obtain,

$$F(k) = \frac{L}{N} \frac{\exp(-k^2 a^2)}{ik} G(k) \quad (13)$$

This equation is what is employed in the code as

$$\begin{cases} EX(I2) = -G1X(I1)*GKX(I) \\ EX(I1) = G1X(I2)*GKX(I) \end{cases} \quad (14)$$

where

$$\begin{cases} G1X(I1) = \text{Re}[G(k)] \\ G1X(I2) = \text{Im}[G(k)] \end{cases} \quad (15)$$

$$GKX(I) = FGK*EXK/WAK \quad (16)$$

with identification of

$$GKX(I) \rightarrow \frac{L}{N} \frac{\exp(-k^2 a^2)}{k}$$

### 3. Energy Conservation and Scaling of Potential Energy vs. Kinetic Energy

Any decent code should satisfy at least approximate energy conservation if the simulated physical system is closed. In particular, the electrostatic code should satisfy

$$\sum_{j=1}^{\mathcal{N}} \frac{m}{2} v_j^2 + \int_0^L \frac{E(r)^2}{8\pi} dr = K = \text{constant}, \quad (17)$$

where  $\mathcal{N} \equiv$  total number of (micro) particles  $= n_0 L$ . The second term is the total electrostatic energy in the system of length  $L$  in unit area. This term is expressed as

$$\begin{aligned} \int_0^L \frac{E(r)^2}{8\pi} dr &= \sum_{k'} \sum_{k''} \int_0^L dr \exp[i(k' + k'')r] E(k')E(k'') \\ &= L \sum_{k'} \sum_{k''} \delta_{k', -k''} E(k')E(k'') \\ &= L \sum_k |E(k)|^2. \end{aligned} \quad (18)$$

Now recall that in the simulation the code is allotted a macroscopic mass  $m_p$  instead of the original mass  $m$  allotted to a simulated particle:

$$\sum_{j=1}^{\mathcal{N}} m v_j^2 = \sum_{j=1}^N m_p v_j^2. \quad (19)$$

Therefore, the energy conservation relation, Eq. (17), is cast into

$$\frac{1}{2} \left( \sum_{j=1}^N m_p v_j^2 + \frac{1}{4\pi} \sum_{\{k\}}^{N_c} E_k^2 L \right) = K. \quad (20)$$



Rewriting Eq. (20), we obtain

$$\begin{aligned}
 \frac{K}{1/2m_p\omega_p^2\Delta^2} &= \sum_{j=1}^N \tilde{v}_j^2 + \frac{1}{4\pi m_p\omega_p^2\Delta^2} \sum_{\{k\}}^{N_c} E_k^2 L \\
 &= \sum_{j=1}^N \tilde{v}_j^2 + \frac{\Delta^2}{4\pi m_p\omega_p^2\Delta^2} (4\pi n_0 e)^2 \sum_{\{k\}}^{N_c} \tilde{E}_k^2 L \\
 &= \sum_{j=1}^N \tilde{v}_j^2 + N \sum_{\{k\}}^{N_c} \tilde{E}_k^2, \tag{21}
 \end{aligned}$$

where we used Eq. (9) and

$$\tilde{E}_k = \frac{1}{4\pi n_0 e \Delta} E_k. \tag{22}$$

Equation (21) is just the relation used to calculate the total energy in the code. When the fast Fourier transform routine called FFT2 (instead of the more conventional FFT) is used, there is a factor 2 in the field calculation, because the FFT2 folds the k space. The kinetic energy is calculated for N macroscopic simulational particles in the normalized unit:  $\sum_{j=1}^N \tilde{v}_j^2$ . On the other hand, to calculate the total potential energy, the code uses F(k). That is,

$$\tilde{E}_k = F(k) \exp\left(\frac{1}{2} k^2 a^2\right). \tag{23}$$

Therefore, to calculate, the code does

$$N \sum_{\{k\}}^{N_c} \tilde{E}_k^2 = \sum_{I=1}^{N_c} AK(I) * |EX(I)|^2, \tag{24}$$

where

$$AK(I) = N \exp(k^2 a^2)$$

$$|EX(I)|^2 = |F(k)|^2 .$$

In the actual simulation experiments, the value  $K/(1/2m_p \omega_p^2 \Delta^2)$  conserves within -0.1 per cent. See Table 1.

In addition, theory for thermal equilibrium plasma tells that the total potential energy should be the plasma parameter times the total kinetic energy.<sup>1</sup> This means that the second term in Eq. (21) is smaller than the first term by a factor of  $n_0 \lambda_D$ . The first term of Eq. (21) is

$$\sum_{j=1}^N \tilde{v}_j^2 = N \tilde{v}_T^2 , \quad (25)$$

while the second term is roughly

$$\frac{1}{4\pi m_p^2 \omega_p^2 \Delta^2} \sum_k^{N_c} \langle E_k^2 L \rangle \cong \frac{1}{m_p \omega_p^2 \Delta^2} \sum_k^{N_c} m_p v_{Tx}^2$$

$$\cong \frac{m_p \omega_p^2 \Delta^2}{m_p \omega_p^2 \Delta^2} \sum_k^{N_c} \tilde{v}_{Tx}^2$$

$$\cong \chi \sum_k^{N_c} \tilde{v}_T^2 , \quad (26)$$

where the relation  $\langle E_k^2 L / 8\pi \rangle = m_p^2 v_{Tx}^2 / 2$ , with  $\chi = [1 + k^2 \lambda_D^2 \exp(k^2 a^2)]^{-1}$  is used. This last relation is examined in the next section. Thus, we find the plasma parameter in the simulation system is related to kinetic and potential energies as

$$g_{\text{simul}} \approx \frac{P.E.}{K.E.} \lesssim \frac{N_c}{N} . \quad (27)$$

The actual simulational results are listed also in Table 1.

#### 4. Energy Partition

In thermal equilibrium, a plasma sustains fluctuations of various modes of (electrostatic) oscillations. An individual mode  $E_k$  can be regarded as a system (a canonical ensemble system) in contact with a thermal bath of many modes with wavenumber other than  $k$   $\{E_{k'}, k' \neq k\}$ . The contact of  $E_k$  with thermal bath  $\{E_{k'}, k' \neq k\}$  is through the nonlinear mode-mode interaction. According to statistical physics, the probability of taking a certain energy level in canonical ensemble is proportional to the Boltzman factor:

$$P(E_k) dE_k \propto \exp\left[\frac{-\psi(E_k)}{\kappa T}\right] dE_k , \quad (28)$$

(see Ref. 2) where  $\psi(E_k)$  is the energy required to create fluctuations  $E_k$  :

$$\psi(E_k) = \frac{1}{8\pi} E_k^2 L[1 + k^2 \lambda_D^2 \exp(k^2 a^2)] . \quad (29)$$

Since the probability function  $P(E_k)$  should be normalized to 1 (i.e.,  $\int_{-\infty}^{\infty} P(E_k) dE_k = 1$ ), the normalization of Eq. (28) is

$$P(E_k) =$$

$$\frac{1}{\sqrt{2\pi}} \left\{ \frac{L}{4\pi\kappa T} [1 + k^2\lambda_D^2 \exp(k^2 a^2)] \right\}^{1/2} \exp \left\{ -\frac{E_k^2 L}{8\pi\kappa T} \exp[1 + k^2\lambda_D^2 \exp(k^2 a^2)] \right\} . \quad (30)$$

With Eq. (30), we immediately have

$$\left\langle \frac{E_k^2 L}{8\pi} \right\rangle = \frac{1}{2} \frac{\kappa T}{1 + k^2\lambda_D^2 \exp(k^2 a^2)} . \quad (31)$$

We can derive Eq. (31) through another way. According to the fluctuation and dissipation theorem<sup>3,4</sup>, the spectral intensity<sup>1</sup> of the fluctuations in thermal equilibrium is given as

$$S_{\left\{ \frac{p}{f} \right\}}(k, \omega) = -\frac{N}{\pi\omega} \frac{k^2}{\lambda_D^2} \text{Im} \frac{1}{D_{\left\{ \frac{p}{f} \right\}}(k, \omega)} , \quad (32)$$

where subscripts p and f refer to point and finite-size cases, respectively. Using Krammers-Krönig's relation<sup>4,5,6,7</sup>, we obtain

$$\begin{aligned} S_{\left\{ \frac{p}{f} \right\}}(k) &\equiv -\frac{k^2}{\pi k_D^2} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \text{Im} \frac{1}{D_{\left\{ \frac{p}{f} \right\}}(k, \omega)} \\ &= \frac{k^2}{k_D^2} \left[ 1 - \text{Re} \frac{1}{D_{\left\{ \frac{p}{f} \right\}}(k, 0)} \right] \end{aligned} \quad (33)$$

From the expression of  $D_p(k,0) = 1 + k_D^2/k^2$ , we obtain

$$S_p(k) = \frac{k^2}{k^2 + k_D^2} .$$

On the other hand,

$$S_{\left\{ \frac{p}{f} \right\}}(k) = \frac{1}{N} \left\langle |\delta\rho_k|^2 \right\rangle .$$

Therefore,

$$\left\langle \rho_k^2 \right\rangle_{\left\{ \frac{p}{f} \right\}} = \frac{k^2}{4\pi} T \left[ 1 - \frac{1}{D_{\left\{ \frac{p}{f} \right\}}(k,0)} \right]$$

and at the same time

$$\left\langle \rho_k^2 \right\rangle = \frac{k^2}{16\pi^2} \left\langle E_k^2 \right\rangle_L .$$

Thus,

$$\frac{\left\langle E_k^2 L \right\rangle_p}{8\pi} = \frac{1}{2} T \frac{1}{1 + k^2 \lambda_D^2} ,$$

and

$$\frac{\left\langle E_k^2 L \right\rangle_f}{8\pi} = \frac{1}{2} T \frac{1}{1 + k^2 \lambda_D^2 |S(k)|^2} .$$

Thus, we reproduced Eq. (31) through the fluctuation dissipation theorem.

Now let us think about the case for the simulation. Can we expect

$$\frac{1}{1/2\kappa T} \left\langle \frac{E_k^2 L}{8\pi} \right\rangle = \frac{1}{1 + k^2 \lambda_D^2 \exp(k^2 a^2)}$$

in the simulation? If we can, what does  $\kappa T$  in the simulation mean? Is it  $\kappa T = mv_T^2$  or  $\kappa T = m_p v_T^2$ ?

If we think the statistical-physics basis of Eq. (31), what matters is the freedom of kinetic motion. In the simulation the free random motion is not assigned to a particle energy  $1/2v_j^2$ , but to a macroscopic particle's energy  $1/2m_p v_j^2$ . Therefore, we should interpret  $\kappa T = m_p v_j^2$ . In the simulation

$$\begin{aligned} \frac{\langle E_k^2 L \rangle / 8\pi}{m_p v_T^2 / 2} &= \frac{L / 8\pi (\omega_p^2 \Delta / e)^2 \langle F(k)^2 \rangle \exp(k^2 a^2)}{1/2 m_p v_T^2} \\ &= \frac{L}{8\pi} \frac{(4\pi n_0 e \Delta)^2}{1/2 m_p \omega_p^2 \Delta^2 v_T^2} \langle F(k)^2 \rangle \exp(k^2 a^2) \\ &= N \frac{1}{v_T^2} \langle F(k)^2 \rangle \exp(k^2 a^2) \quad , \end{aligned} \tag{34}$$

where we used Eq. (7). According to the present argument,

$$\frac{\langle E_k^2 \rangle / 8\pi}{m_p v_T^2 / 2} = \frac{1}{1 + k^2 \lambda_D^2 \exp(k^2 a^2)} \quad (35)$$

Therefore,

$$\langle F(k)^2 \rangle \exp(k^2 a^2) = \frac{\bar{v}_T^2}{N} \frac{1}{1 + k^2 \lambda_D^2 \exp(k^2 a^2)} \quad (36)$$

In the actual computational runs, we made  $F(k,t)$  the correlation function, i.e.,  $F(k)^2$  and multiplied by  $\exp(k^2 a^2)$ . We plot the simulational values of  $N \bar{v}_T^{-2} [F(k)^2] \exp(k^2 a^2)$  in Fig. 1. The theoretical prediction, i.e., the right-hand side of Eq. (35), is superimposed on the experimental curve. The fit is excellent in the higher  $k$  region. In the lower  $k$  region, there is some deviation from perfect thermal equilibrium; presumably this is because the long wavelength mode is less susceptible to damping or decay and, therefore, does not reach thermal equilibrium as quickly as the short wavelength modes. Note that the correlation is taken over only a finite span of time in the actual simulation, in contrast to theory.

### 5. Summary of Normalization

We summarize the normalization of the codes.

$$(1) \text{ Time}^{-1} : \omega_{pe} + 1, \text{ if } FGK = \frac{NCX \times NCY}{NO} = \frac{\# \text{ grids}}{\# \text{ particles}}$$

as is customarily done.

(ii) Length :

$$\Delta \rightarrow 1, \lambda_{De} = \frac{v_{th}}{\omega_{pe}},$$

Therefore,

$$\tilde{v} = \text{code velocities} = \frac{v}{\Delta \cdot \omega_{pe}}.$$

(iii) Acceleration :

$$\frac{dv}{dt} = \frac{e}{m} E, \quad v = \tilde{v} \cdot \Delta \cdot \omega_{pe}, \quad t = \tilde{t} \omega_{pe}^{-1}.$$

Then,

$$\frac{d\tilde{v}}{dt} \cdot \frac{\Delta \omega_{pe}}{\omega_{pe}^{-1}} = \frac{d\tilde{v}}{dt} \Delta \omega_{pe}^2$$

$$\frac{d\tilde{v}}{dt} = \frac{eE}{m\Delta \omega_{pe}^2} = \tilde{E}.$$

More generally,  $d\tilde{v}/d\tilde{t} = \tilde{E} + \tilde{v}/c \times \tilde{B}$ . Normalization of  $\tilde{E}, \tilde{B}$  is the same in electromagnetic codes. Thus,

$$E = \tilde{E} \frac{m\Delta \omega_{pe}^2}{e} = \tilde{E} (4\pi n e \Delta), \quad B = \tilde{B} \frac{m\Delta \omega_{pe}^2}{e},$$

and

$$\tilde{c} = \frac{c}{\Delta \cdot \omega_{pe}}.$$



(iv) Cyclotron frequencies :

$$\omega_{ce} = \frac{eB}{mc} = \frac{e}{m} \frac{\tilde{B}}{c} \frac{m\Delta\omega_{pe}^2}{e\Delta\omega_{pe}} = \frac{\tilde{B}}{c} \cdot \omega_{pe}$$

$$\tilde{\omega}_{ce} = \frac{\omega_{ce}}{\omega_{pe}} = \frac{\tilde{B}}{c}$$

(v) Ion cyclotron :

$$\omega_{ci} = \frac{eB}{Mc} = \left(\frac{m}{M}\right) \frac{eB}{mc} = \frac{m}{M} \frac{\tilde{B}}{c} \omega_{pe}$$

$$\omega_{pi} = \left(\frac{4\pi ne^2}{m}\right)^{1/2} = \left(\frac{m}{M}\right)^{1/2} \cdot \left(\frac{4\pi ne^2}{m}\right)^{1/2} = \left(\frac{m}{M}\right)^{1/2} \omega_{pe}$$

(vi) Plasma  $\beta$  :

$$\beta = \frac{n\kappa T}{B^2/8\pi} = \frac{nmv_{th}^2}{B^2/8\pi} = \frac{8\pi nm_e (v^2 \cdot \Delta \cdot \omega_{pe})^2}{[ \tilde{B} (m\Delta\omega_{pe}^2/e) ]^2}$$

$$\beta = \frac{\tilde{v}^2}{\tilde{B}^2} \cdot \frac{8\pi nm\Delta^2\omega_{pe}^2 e^2}{m^2\Delta^2\omega_{pe}^4} = 2 \frac{\tilde{v}^2}{\tilde{B}^2}$$

Alternate :

$$\beta = \frac{v_e^2}{c^2} \frac{8\pi nm}{B^2/c^2} = \left( \frac{e^2 8\pi nm}{m^2 e^2 B^2/c^2 m^2} \right) \left( \frac{v_e}{c} \right)^2 = 2 \frac{\omega_{pe}^2}{\omega_{ce}^2} \left( \frac{v_e}{c} \right)^2$$

(vii) Gyroradius :

$$\rho_e = \frac{v_e}{\omega_{ce}} = \frac{\tilde{v} \Delta \omega_{pe}}{(\tilde{B}/c) \omega_{pe}} = \frac{\tilde{v} c}{\tilde{B}} \cdot \Delta$$

$$\rho_i = \left(\frac{M}{m}\right)^{1/2} \frac{v_e}{\omega_{ce}}$$

$$\rho_i = \frac{v_i}{\omega_{ci}} = \frac{\sqrt{T_i/T_e} \sqrt{m/M}}{(m/M) \omega_{ce}} = \left(\frac{T_i}{T_e}\right)^{1/2} \left(\frac{M}{m}\right)^{1/2} \underbrace{\left(\frac{\tilde{v}}{\tilde{B}} \cdot \Delta \tilde{c}\right)}_{\rho_e} .$$

(ix) Skin depth :

$$\frac{c}{\omega_{pe}} = \frac{\tilde{c} \cdot \Delta \cdot \omega_{pe}}{\omega_{pe}} = \tilde{c} \cdot \Delta .$$

(x) If the parameter FGK (we write this through  $g$  as below) is taken other than  $NCX \times NCY / NO$ , the normalization changes accordingly. However, different FGK choices are not recommended for beginning. Let

$$FGK = g \times \left(\frac{NCX \times NCY}{NO}\right) .$$

Then this will scale the individual simulation charge as

$$\omega_{pe} \rightarrow g , \quad \Delta \rightarrow 1 .$$

That is, all the current and change-related numbers are scaled accordingly. This includes fields  $\tilde{E}, \tilde{B}$  and frequencies.

6. The Fourier Transform and the FFT2 Algorithm

In the code quantities are defined on discrete points and the Fourier transform needs according care. The quantity  $f = f(r,s)$  that is only defined at the discrete points  $(r,s)$  and periodic in the directions of  $r$  and  $s$  can be transformed by the discrete Fourier transform defined by

$$\tilde{f}_{lm} \equiv \frac{1}{N_x N_y} \sum_{r,s=0}^{N_x-1, N_y-1} f_{rs} \exp\left(-\frac{2\pi i l r}{N_x}\right) \exp\left(-\frac{2\pi i m s}{N_y}\right)$$

$$\Leftrightarrow f_{rs} \equiv \sum_{l,m=0}^{N_x-1, N_y-1} \tilde{f}_{lm} \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right)$$

The Fourier coefficients  $\tilde{f}_{lm}$  span complete space. If  $f_{rs}$  is real, then one can show from the complex conjugency that:

$$\begin{aligned} \tilde{f}_{N_x-l, m} &= \frac{1}{N_x N_y} \sum_{r,s=0}^{N_x-1, N_y-1} f_{rs} \exp\left[\frac{i 2\pi (N_x-l)r}{N_x}\right] \exp\left(-\frac{2\pi i m s}{N_y}\right) \\ &= \left\{ \frac{1}{N_x N_y} \sum_{r,s=0}^{N_x-1, N_y-1} f_{rs} \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left[\frac{2\pi i (N_y-m)S}{N_y}\right] \right\} = \tilde{f}_{l, N_y-m}^* \end{aligned}$$

and similarly,

$$\begin{aligned} \tilde{f}_{N_x-l, N_y-m} &= \frac{1}{N_x N_y} \sum_{r,s=0}^{N_x-1, N_y-1} f_{rs} \exp\left[-\frac{i 2\pi (N_x-l)r}{N_x}\right] \exp\left[-\frac{2\pi i (N_y-m)S}{N_y}\right] \\ &= \left\{ \frac{1}{N_x N_y} \sum_{r,s=0}^{N_x-1, N_y-1} f_{rs} \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right) \right\} = \tilde{f}_{lm}^* \end{aligned}$$

Thus, we see that we need to know only half of the terms  $\tilde{f}_{lm}$  in order to reconstruct  $f_{rs}$  if  $f_{rs}$  is real, since the other half are related by a complex conjugation.

The algorithm FFT2 takes advantage of this result in calculating the discrete transform of a real array. In this algorithm, the index of  $l$  of  $\tilde{f}_{l,m}$  runs from zero to  $N_x/2-1$ . The components of  $\tilde{f}_{l,m}$  with a higher value of  $l$  are reconstructed by complex conjugation, except for  $l = N_x/2$ .

For  $l = N_x/2$ , we find that

(1)  $\tilde{f}_{N_x/2,m} = \tilde{f}_{N_x/2,N_y-m}^*$ , so that except for  $m=0, N_y/2$ , we can express the terms with index  $1 < m < N_y/2 - 1$  as complex conjugates of terms with  $N_y/2 + 1 < m < N_y - 1$ .

Similarly, for  $l=0$ , we find that (2)  $\tilde{f}_{0,m} = \tilde{f}_{0,N_y-m}$ , so that we can express terms with index  $N_y/2 + 1 < m < N_y - 1$  in terms of the complex conjugate of terms with  $1 < m < N_y/2 - 1$ . Thus, we can suppress terms of  $\tilde{f}_{l,m}$  with index  $l=N_x/2$ , if we eliminate those terms of  $\tilde{f}_{0,m}$  with  $N_y/2 < m < N_y - 1$  (which can be reconstructed) in favor of terms of  $\tilde{f}_{N_x/2,m}$  with  $N_y/2 < m < N_y - 1$ .

The only terms remaining are those  $\tilde{f}_{N_x/2,0}$  and  $\tilde{f}_{N_x/2,N_y/2}$ . However, each of these terms have vanishing imaginary parts, and so do the terms  $\tilde{f}_{0,0}$ ,  $\tilde{f}_{0,N_x/2}$ . Thus, we can place  $\text{Re } \tilde{f}_{N_x/2,0}$  and  $\text{Re } \tilde{f}_{N_x/2,N_y/2}$  in place of  $\text{Im } \tilde{f}_{0,0}$  and  $\text{Im } \tilde{f}_{0,N_y/2}$ , which had vanished.

Table 2 summarizes which indices are kept and which are left out. Note that everything with  $l > N_x/2 + 1$  can be suppressed, since it can be expressed as a conjugate of some term with  $l \leq N_x/2 - 1$ . The only terms which then have to be shuffled are those with  $l=0$ , and  $l=N_x/2$ . Table 3 shows the FFT2 components.

$$(1) \quad f_{N_x/2, N_y/2} = f_{N_x/2, N_y/2}^*$$

$$(2) \quad f_{0, N_y/2} = f_{0, N_y/2}^*$$

$$f_{l, 0} = f_{N_y-l, 0}^* \quad f_{0, 0} = f_{N_x, N_y}$$

$$f_{N_y/2, 0} = f_{N_y/2, 0}^* = f_{0, 0}^*$$

One can also show this result as a summation:

$$\begin{aligned} f_{rs} &= \sum_{m=0}^{N_y-1} \sum_{l=0}^{N_x-1} \tilde{f}_{lm} \exp\left(\frac{2\pi i m s}{N_y}\right) \exp\left(\frac{2\pi i l r}{N_x}\right) \\ &= \sum_{m=0}^{N_y-1} \tilde{f}_{0m} + \tilde{f}_{N_x/2, m} (-1)^r \exp\left(\frac{2\pi i m s}{N_y}\right) \\ &\quad \times \sum_{m=0}^{N_y-1} \sum_{l=1}^{N_y/2-1} \tilde{f}_{nm} \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right) + \sum_{l=N_x/2+1}^{N_x-1} \\ &\quad \times \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right) , \end{aligned}$$

which can be written:

$$\begin{aligned}
 f_{rs} = & \tilde{f}_{00} + \tilde{f}_{0, N_y/2} (-1)^S + \tilde{f}_{N_x/2, 0} (-1)^r + \tilde{f}_{N_x/2, N_y/2} (-1)^r (-1)^S \\
 & + \sum_{m=1}^{N_y/2-1} \left[ \tilde{f}_{0m} + (-1)^r \tilde{f}_{N_x/2, N_y-m}^* \right] \exp\left(\frac{2\pi i m s}{N_y}\right) \\
 & + \sum_{m=N_y/2-1}^{N_y-1} \left[ \tilde{f}_{0, N_y-m}^* + (-1)^r \tilde{f}_{N_x/2, m} \right] \exp\left(\frac{2\pi i m s}{N_y}\right) \\
 & + \sum_{m=0}^{N_y-1} \left[ \sum_{l=1}^{N_x-1} \tilde{f}_{lm} \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right) \right. \\
 & \left. + \sum_{l=N_x/2+1}^{N_x-1} \tilde{f}_{N_x-l, N_y-m}^* \exp\left(\frac{2\pi i l r}{N_x}\right) \exp\left(\frac{2\pi i m s}{N_y}\right) \right].
 \end{aligned}$$

This expression shows explicitly which terms need to be known. Suppose we wish to calculate

$$f(x, y) = \sum_{l=-(N_x/2-1)}^{+(N_x/2-1)} \sum_{m=-(N_y/2-1)}^{+(N_y/2-1)} \tilde{f}_{lm} \exp(ik_l x) \exp(ik_m y)$$

where the indices are related by

$$\tilde{f}_{l, -m} = \tilde{f}_{-l, m}^* \quad \text{and} \quad \tilde{f}_{-l, -m} = \tilde{f}_{lm}^* .$$

This is an approximation to the infinite Fourier series:

$$f(x, y) \approx \sum_{m, l=-\infty}^{+\infty} \tilde{f}_{lm} \exp(ik_l x) \exp(ik_m y)$$

for the case where  $f(x,y)$  is a real function. We can write the sum over positive indices:

$$\begin{aligned}
 f(x,y) &= \tilde{f}_{00} + \sum_{m=1}^{N_y/2-1} \tilde{f}_{0m} \exp(ik_m y) + \sum_{m=1}^{N_y/2-1} f_{0,-m} \exp(-ik_m y) \\
 &+ \sum_{l=1}^{N_x/2-1} \tilde{f}_{l0} \exp(ik_l x) + \sum_{l=1}^{N_x/2-1} \tilde{f}_{-l0} \exp(-ik_l x) \\
 &+ \sum_{m=1}^{N_y/2-1} \sum_{l=1}^{N_x/2-1} \tilde{f}_{lm} \exp(ik_l x) \exp(ik_m y) + \tilde{f}_{l,-m} \exp(ik_l x) \exp(-ik_m y) \\
 &+ \tilde{f}_{-l,m} \exp(-ik_l x) \exp(ik_m y) + f_{-l,-m} \exp(-ik_l x) \exp(-ik_m y) .
 \end{aligned}$$

Then we can use the relations among indices to write:

$$\begin{aligned}
 f(x,y) &= \tilde{f}_{00} + \sum_{m=1}^{N_y/2-1} \tilde{f}_{0m} \exp(ik_m y) + \sum_{m=1}^{N_y/2-1} \tilde{f}_{0m}^* \exp(-ik_m y) \\
 &+ \sum_{l=1}^{N_x/2-1} \tilde{f}_{l0} \exp(ik_l x) + \sum_{l=1}^{N_x/2-1} \tilde{f}_{l0}^* \exp(-ik_l x) \\
 &+ \sum_{m=1}^{N_y/2-1} \sum_{l=1}^{N_x/2-1} \left\{ \tilde{f}_{lm} \exp(ik_l x) \exp(ik_m y) \right. \\
 &+ \tilde{f}_{l,-m} \exp(ik_l x) \exp(-ik_m y) + \tilde{f}_{l,-m}^* \exp(-ik_l x) \exp(ik_m y) \\
 &\left. + \tilde{f}_{lm}^* \exp(-ik_l x) \exp(-ik_m y) \right\} .
 \end{aligned}$$

Now let us make the substitution  $m' = N_y - m$ ,  $l' = N_x - l$ , then:

$$\exp(-ik_m y) = \exp(-2\pi i y) \exp(ik_{m'} y)$$

and

$$\exp(-ik_l x) = \exp(-2\pi i x) \exp(ik_{l'} x) .$$

So, if we limit ourselves to evaluating  $f(x,y)$  at integer values of  $x$  and  $y$ , we can write:

$$\begin{aligned}
 f(x,y) &= \tilde{f}_{00} + \sum_{m=1}^{N_y/2-1} \tilde{f}_{0m} \exp(ik_m y) + \sum_{m=N_y/2+1}^{N_y/2-1} \tilde{f}_{0,N_y-m}^* \exp(ik_m y) \\
 &+ \sum_{l=1}^{N_x/2-1} \tilde{f}_{l0} \exp(ik_l x) + \sum_{l=N_x/2+1}^{N_x/2-1} \tilde{f}_{N_x-l,0}^* \exp(ik_l x) + \sum_{l=1}^{N_x/2-1} \left\{ \sum_{m=1}^{N_y/2-1} \tilde{f}_{lm} \exp(ik_l x) \right. \\
 &\times \exp(ik_m y) + \left. \sum_{m=N_y/2+1}^{N_y-1} \tilde{f}_{l,-(N_y-m)} \exp(ik_l x) \exp(ik_m y) \right\} \\
 &+ \sum_{l=N_x/2+1}^{N_x-1} \left\{ \sum_{m=1}^{N_y/2-1} \tilde{f}_{N_x-l,-m}^* \exp(ik_l x) \exp(ik_m y) \right. \\
 &\left. + \sum_{m=N_y/2+1}^{N_y-1} \tilde{f}_{N_x-l,N_y-m}^* \exp(ik_l x) \exp(ik_m y) \right\}
 \end{aligned}$$

We can see that this expression is not the same as that given by FFT2. For one thing, this expression involves knowledge of coefficients  $\tilde{f}_{lm}$  with negative subscripts, whereas FFT2 does not handle such terms. Secondly, FFT2 involves knowledge of the coefficients  $\tilde{f}_{lm}$ , with  $m$  in the range  $N_y/2 + 1 < m < N_y - 1$ , which are not in our expression for  $f(x,y)$ . However, we can calculate  $f(x,y)$  by using FFT2, if we define the coefficients with  $N_y/2 + 1 < m < N_y - 1$  to be the coefficients with  $-(N_y/2 - 1) < m < -1$ :



$$\tilde{f}_{lm} \equiv \tilde{f}_{l, m-N_y}, \quad \frac{N_y}{2} + 1 < m < N_y - 1, \quad 1 < l < \frac{N_x}{2} - 1$$

$$\tilde{f}_{l, N_y - m} \equiv \tilde{f}_{l, -m} \quad 1 < m < \frac{N_y}{2} - 1, \quad 1 < l < \frac{N_x}{2} - 1$$

Then we obtain:

$$f(x,y) = \tilde{f}_{00} + \sum_{m=1}^{N_y/2-1} \tilde{f}_{0m} \exp(ik_m y) + \sum_{m=N_y/2+1}^{N_y-1} \tilde{f}_{0, N_y - m}^* \exp(ik_m y)$$

$$+ \sum_{m=0}^{N_y-1} \left\{ \sum_{l=1}^{N_y/2-1} \tilde{f}_{lm} \exp(ik_l x) \exp(ik_m y) + \sum_{l=N_y/2+1}^{N_x-1} \tilde{f}_{N_x - l, N_y - m}^* \exp(ik_l x) \exp(ik_m y) \right\}$$

where the prime indicates that  $m = N_y/2$  is omitted. Thus,  $f(x,y)$  is given by FFT2 if we set equal to zero all coefficients with subscripts  $l=N_x/2$  or  $m=N_y/2$ , and  $(x,y)$  are integers.

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Table 1

RUN	TOTAL ENERGY	TOTAL LONGITUDINAL ELECTRIC FIELD ENERGY	SIMULATION $\frac{E_k^2 L / 8\pi}{1/2kT}$ (MODE 1)	THEORY $\frac{E_k^2 L / 8\pi}{1/2kT}$ (MODE 2)
1. Fortran code # of Particles N = 512, Size of Particles a = 2, System length L = 512 ion: moving t <sub>end</sub> = 200ω <sub>p</sub> <sup>-1</sup>	~ 3240 kT	~ 80 kT	~ 0.939	~ 1.0
2. Fortran code N = 1024, a = 4, L = 256 ion: not moving, t <sub>end</sub> = 200ω <sub>p</sub> <sup>-1</sup>	~ 6120	~ 20	~ 0.805	~ 1.0
3. Assembler code N = 512, a = 2, L = 512 ion: moving t <sub>end</sub> = 200ω <sub>p</sub> <sup>-1</sup>	~ 3145	~ 70	~ 0.679	~ 1.0
4. Assembler code N = 5120, a = 2, L = 512 ion: moving t <sub>end</sub> = 600ω <sub>p</sub> <sup>-1</sup>	~ 31300	~ 60	~ 0.564*	~ 1.0

\* Averaged over seven k-modes.

Table 2

0	1	$\rightarrow$	$\frac{N_x}{2} - 1$	$\frac{N_x}{2}$	$\frac{N_x}{2} + 1$	$\rightarrow$	$N_x - 1$	$\frac{N_x - 1}{2}$
(0,0)	(1,0)		$\left(\frac{N_x}{2} - 1, 0\right)$	$\left(\frac{N_x}{2}, 0\right)$	$\left(\frac{N_x}{2} - 1, 0\right)^*$	....	(1,0)*	0
(0,1)	(1,1)	...	$\left(\frac{N_x}{2} - 1, 1\right)$	$\left(\frac{N_x}{2}, N_y - 1\right)^*$	$\left(\frac{N_x}{2} - 1, N_y - 1\right)^*$	....	(1, N <sub>y</sub> -1)*	1
(0,2)	(1,2)		$\left(\frac{N_x}{2} - 1, 2\right)$	$\left(\frac{N_x}{2}, N_y - 2\right)^*$	$\left(\frac{N_x}{2} - 1, N_y - 2\right)^*$		(1, N <sub>y</sub> -2)*	2
.	.						.	
.	.						.	
.	.						.	
$\left(0, \frac{N_y}{2} - 2\right)$	$\left(1, \frac{N_y}{2} - 2\right)$		$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} - 2\right)$	$\left(\frac{N_x}{2}, \frac{N_y}{2} + 2\right)^*$	$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} + 2\right)^*$		$\left(1, \frac{N_y}{2} + 2\right)^*$	$\frac{N_y}{2} - 2$
$\left(0, \frac{N_y}{2} - 1\right)$	$\left(1, \frac{N_y}{2} - 1\right)$		$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} - 1\right)$	$\left(\frac{N_x}{2}, \frac{N_y}{2} + 1\right)^*$	$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} + 1\right)^*$		$\left(1, \frac{N_y}{2} + 1\right)^*$	$\frac{N_y}{2} - 1$
$\left(0, \frac{N_y}{2}\right)$	$\left(1, \frac{N_y}{2}\right)$		$\left(\frac{N_x}{2} - 1, \frac{N_y}{2}\right)$	$\left(\frac{N_x}{2}, \frac{N_y}{2}\right)$	$\left(\frac{N_x}{2} - 1, \frac{N_y}{2}\right)^*$		$\left(1, \frac{N_y}{2}\right)^*$	$\frac{N_y}{2}$
$\left(0, \frac{N_y}{2} + 1\right)^*$	$\left(1, \frac{N_y}{2} + 1\right)$		$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} + 1\right)$	$\left(\frac{N_x}{2}, \frac{N_y}{2} + 1\right)$	$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} - 1\right)^*$		$\left(1, \frac{N_y}{2} - 1\right)^*$	$\frac{N_y}{2} + 1$
$\left(0, \frac{N_y}{2} + 2\right)^*$	$\left(1, \frac{N_y}{2} + 2\right)$		$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} + 2\right)$	$\left(\frac{N_x}{2}, \frac{N_y}{2} + 2\right)$	$\left(\frac{N_x}{2} - 1, \frac{N_y}{2} - 2\right)^*$		$\left(1, \frac{N_y}{2} - 2\right)^*$	$\frac{N_y}{2} + 2$
.	.						.	
.	.						.	
.	.						.	
(0,2)*	(1, N <sub>y</sub> -2)	...	$\left(\frac{N_x}{2} - 1, N_y - 2\right)$	$\left(\frac{N_x}{2}, N_y - 2\right)$	$\left(\frac{N_x}{2} - 1, 1\right)^*$	....	(1,1)*	N <sub>y</sub> -2
(0,1)*	(1, N <sub>y</sub> -1)	...	$\left(\frac{N_x}{2} - 1, N_y - 1\right)$	$\left(\frac{N_x}{2}, N_y - 1\right)$	$\left(\frac{N_x}{2} - 1, 1\right)^*$	....	(1,1)*	N <sub>y</sub> -1

Table 3

FFT2 Components  $g_{nm} = \frac{1}{L_x L_y} \int_0^{L_x} \int_0^{L_y} g(x,y) \exp(-2\pi i L_x/L_x) \exp(-2\pi i m_y/L_y) dx dy$

$G(1,1) = g_{00}$	$G(2,1) = \frac{g_{N_x, 0}}{2}$	$G(3,1) = \text{Re } g_{1,0}$	$G(4,1) = \text{Im } g_{1,0}$	$G(5,1) = \text{Re } g_{2,0}$	$G(6,1) = \text{Im } g_{2,0}$	....	$G(N_x-1,1) = \text{Re } \frac{g_{N_x-1,0}}{2}$	$G(N_x,1) = \text{Im } \frac{g_{N_x-1,0}}{2}$
$G(1,2) = \text{Re } g_{01}$	$G(2,2) = \text{Im } g_{01}$	$G(3,2) = \text{Re } g_{1,1}$	$G(4,2) = \text{Im } g_{1,1}$	$G(5,2) = \text{Re } g_{2,1}$	$G(6,2) = \text{Im } g_{2,1}$	...	$G(N_x-1,2) = \text{Re } \frac{g_{N_x-1,1}}{2}$	$G(N_x,2) = \text{Im } \frac{g_{N_x-1,1}}{2}$
$G(1,3) = \text{Re } g_{02}$	$G(2,3) = \text{Im } g_{02}$	$G(3,3) = \text{Re } g_{1,2}$	$G(4,3) = \text{Im } g_{1,2}$	$G(5,3) = \text{Re } g_{2,2}$	$G(6,3) = \text{Im } g_{2,2}$	...	$G(N_x-1,3) = \text{Re } \frac{g_{N_x-1,2}}{2}$	$G(N_x,3) = \text{Im } \frac{g_{N_x-1,2}}{2}$
$G(1, \frac{N_y}{2} + 1) = g_{0, \frac{N_y}{2}}$	$G(2, \frac{N_y}{2} + 1) = \frac{g_{N_x, \frac{N_y}{2}}}{2}$	$G(3, \frac{N_y}{2} + 1) = \text{Re } g_{1, \frac{N_y}{2}}$	$G(4, \frac{N_y}{2} + 1) = \text{Im } g_{1, \frac{N_y}{2}}$	$G(5, \frac{N_y}{2} + 1) = \text{Re } g_{2, \frac{N_y}{2}}$	$G(6, \frac{N_y}{2} + 1) = \text{Im } g_{2, \frac{N_y}{2}}$	...	$G(N_x-1, \frac{N_y}{2} + 1) = \text{Re } \frac{g_{N_x-1, \frac{N_y}{2}}}{2}$	$G(N_x, \frac{N_y}{2} + 1) = \text{Im } \frac{g_{N_x-1, \frac{N_y}{2}}}{2}$
$G(1, \frac{N_y}{2} + 2) = \text{Re } \frac{g_{N_x, \frac{N_y}{2}-1}}{2}$	$G(2, \frac{N_y}{2} + 2) = \text{Im } \frac{g_{N_x, \frac{N_y}{2}-1}}{2}$	$G(3, \frac{N_y}{2} + 2) = \text{Re } g_{1, \frac{N_y}{2}-1}$	$G(4, \frac{N_y}{2} + 2) = \text{Im } g_{1, \frac{N_y}{2}-1}$	$G(5, \frac{N_y}{2} + 2) = \text{Re } g_{2, \frac{N_y}{2}-1}$	$G(6, \frac{N_y}{2} + 2) = \text{Im } g_{2, \frac{N_y}{2}-1}$	...	$G(N_x-1, \frac{N_y}{2} + 2) = \text{Re } \frac{g_{N_x-1, \frac{N_y}{2}-1}}{2}$	$G(N_x, \frac{N_y}{2} + 2) = \text{Im } \frac{g_{N_x-1, \frac{N_y}{2}-1}}{2}$
$G(1, \frac{N_y}{2} + 3) = \text{Re } \frac{g_{N_x, \frac{N_y}{2}-2}}{2}$	$G(2, \frac{N_y}{2} + 3) = \text{Im } \frac{g_{N_x, \frac{N_y}{2}-2}}{2}$	$G(3, \frac{N_y}{2} + 3) = \text{Re } g_{1, \frac{N_y}{2}-2}$	$G(4, \frac{N_y}{2} + 3) = \text{Im } g_{1, \frac{N_y}{2}-2}$	$G(5, \frac{N_y}{2} + 3) = \text{Re } g_{2, \frac{N_y}{2}-2}$	$G(6, \frac{N_y}{2} + 3) = \text{Im } g_{2, \frac{N_y}{2}-2}$	...	$G(N_x-1, \frac{N_y}{2} + 3) = \text{Re } \frac{g_{N_x-1, \frac{N_y}{2}-2}}{2}$	$G(N_x, \frac{N_y}{2} + 3) = \text{Im } \frac{g_{N_x-1, \frac{N_y}{2}-2}}{2}$
$G(1, N_y) = \text{Re } \frac{g_{N_x, \frac{N_y}{2}-1}}{2}$	$G(2, N_y) = \text{Im } \frac{g_{N_x, \frac{N_y}{2}-1}}{2}$	$G(3, N_y) = \text{Re } g_{1, -1}$	$G(4, N_y) = \text{Im } g_{1, -1}$	$G(5, N_y) = \text{Re } g_{2, -1}$	$G(6, N_y) = \text{Im } g_{2, -1}$	...	$G(N_x-1, N_y) = \text{Re } \frac{g_{N_x-1, -1}}{2}$	$G(N_x, N_y) = \text{Im } \frac{g_{N_x-1, -1}}{2}$

$$\epsilon(k, 0) = \frac{1}{1 + k^2 \lambda_D^2 e^{k^2 a^2}}$$

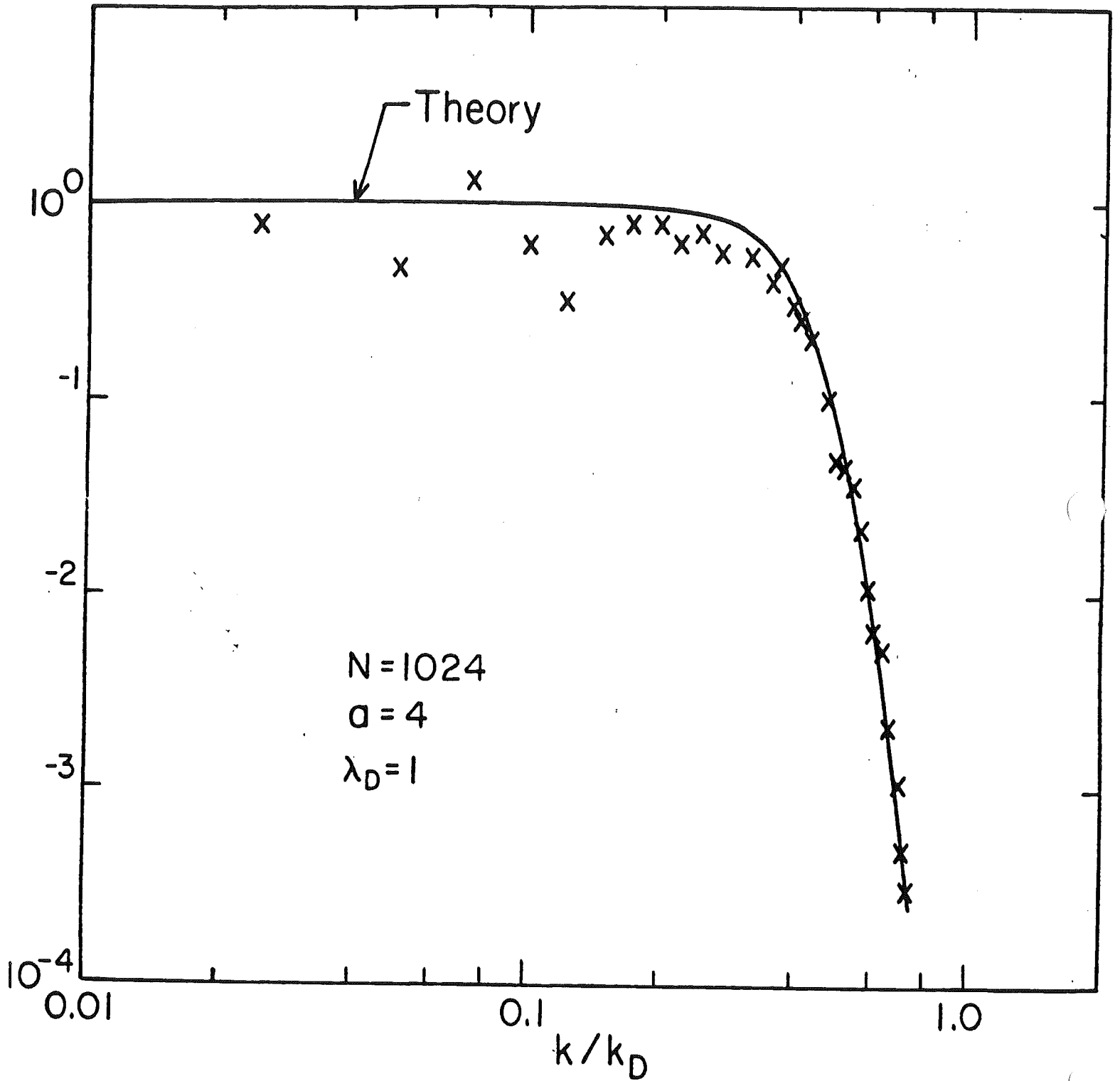


FIGURE 1