

# Xfields physics manual

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# 1 FFT method

We illustrate the method in a single dimension then extend to multiple dimensions.

## 2 Space charge

We assume that the bunch travels rigidly along  $s$  with velocity  $\beta_0 c$ :

$$\rho(x, y, s, t) = \rho_0(x, y, s - \beta_0 c t) \quad (1)$$

$$\mathbf{J}(x, y, s, t) = \beta_0 c \rho_0(x, y, s - \beta_0 c t) \hat{\mathbf{i}}_s \quad (2)$$

We define an auxiliary variable  $\zeta$  as the position along the bunch:

$$\zeta = s - \beta_0 c t. \quad (3)$$

We call  $K$  the lab reference frame in which we have defined all equations above, and we introduce a boosted frame  $K'$  moving rigidly with the reference particle. The coordinates in the two systems are related by a Lorentz transformation [3]:

$$ct' = \gamma_0 (ct - \beta_0 s) \quad (4)$$

$$x' = x \quad (5)$$

$$y' = y \quad (6)$$

$$s' = \gamma_0 (s - \beta_0 ct) = \gamma_0 \zeta \quad (7)$$

The corresponding inverse transformation is:

$$ct = \gamma_0 (ct' + \beta_0 s') \quad (8)$$

$$x = x' \quad (9)$$

$$y = y' \quad (10)$$

$$s = \gamma_0 (s' + \beta_0 ct') \quad (11)$$

The quantities  $(c\rho, J_x, J_y, J_s)$  form a Lorentz 4-vector and therefore they are transformed between  $K$  and  $K'$  by relationships similar to the Eqs. 4-6 [3]:

$$c\rho'(\mathbf{r}', t') = \gamma_0 [c\rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) - \beta_0 J_s(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t'))] \quad (12)$$

$$J'_s(\mathbf{r}', t') = \gamma_0 [J_s(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) - \beta_0 c\rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t'))] \quad (13)$$

where the transformations  $\mathbf{r}(\mathbf{r}', t')$  and  $t(\mathbf{r}', t')$  are defined by Eqs. 8 and 11 respectively. The transverse components  $J_x$  and  $J_y$  of the current vector are invariant for our transformation, and are anyhow zero in our case.

Using Eq. 2 these become:

$$\rho'(\mathbf{r}', t') = \frac{1}{\gamma_0} \rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) \quad (14)$$

$$J'_s(\mathbf{r}', t') = 0 \quad (15)$$

Using Eqs. 1 and 8-10, we obtain:

$$\rho(x', y', s(s', t'), t(s', t')) = \rho_0(x', y', s(s', t') - \beta_0 c t(s', t')) \quad (16)$$

From Eq. 7 we get:

$$s(s', t') - \beta_0 c t(s', t') = \frac{s'}{\gamma_0} \quad (17)$$

where the coordinate  $t'$  has disappeared.

We can therefore write:

$$\rho'(x', y', s', t') = \frac{1}{\gamma_0} \rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \quad (18)$$

The electric potential in the bunch frame is solution of Poisson's equation:

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{\rho'(x', y', s')}{\epsilon_0} \quad (19)$$

From Eq. 18 we can write:

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{1}{\gamma_0 \epsilon_0} \rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \quad (20)$$

We now make the substitution:

$$\zeta = \frac{s'}{\gamma_0} \quad (21)$$

obtained from Eq. 7, which allows to rewrite Eq. 20 as:

$$\frac{\partial^2 \phi'}{\partial x^2} + \frac{\partial^2 \phi'}{\partial y^2} + \frac{1}{\gamma_0^2} \frac{\partial^2 \phi'}{\partial \zeta^2} = -\frac{1}{\gamma_0 \epsilon_0} \rho_0(x, y, \zeta) \quad (22)$$

Here we have dropped the "'" sign from  $x$  and  $y$  as these coordinates are unaffected by the Lorentz boost.

The quantities  $\left(\frac{\phi}{c}, A_x, A_y, A_s\right)$  form a Lorentz 4-vector, we can show that the  $s$  component of the vector potential in the lab frame vanishes:

$$\phi = \gamma_0 (\phi' + \beta_0 c A'_s) \quad (23)$$

$$A_s = A'_s + \beta_0 \frac{\phi'}{c} \quad (24)$$

In the bunch frame the charges are at rest therefore  $A'_x = A'_y = A'_z = 0$  therefore:

$$\phi = \gamma_0 \phi' \quad (25)$$

$$A_s = \beta_0 \frac{\phi'}{c} = \frac{\beta_0}{\gamma_0 c} \phi \quad (26)$$

Combining Eq. 25 with Eq. 22 we obtain the equation in  $\phi$ :

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{1}{\gamma_0^2} \frac{\partial^2 \phi}{\partial \zeta^2} = -\frac{1}{\epsilon_0} \rho_0(x, y, \zeta) \quad (27)$$

### 3 Lorentz force

We stay in the thin lens approximation so we approximate the velocity vector of the particle as:

$$\mathbf{v} = \beta c \hat{\mathbf{i}}_s \quad (28)$$

We want to compute the Lorentz force acting on the particle:

$$\begin{aligned} \mathbf{F} &= q \left( -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \beta c \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) \right) \\ &= q \left( -\nabla\phi - \frac{\beta_0}{\gamma_0 c} \frac{\partial \phi}{\partial t} \hat{\mathbf{i}}_s + \beta c \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) \right) \end{aligned} \quad (29)$$

We compute the vector product:

$$\begin{aligned} \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) &= \left( \frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s} \right) \hat{\mathbf{i}}_x + \left( \frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s} \right) \hat{\mathbf{i}}_y \\ &= \left( \frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s} \right) \hat{\mathbf{i}}_x + \left( \frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s} \right) \hat{\mathbf{i}}_y + \underbrace{\left( \frac{\partial A_s}{\partial s} - \frac{\partial A_s}{\partial s} \right)}_{=0} \hat{\mathbf{i}}_s \\ &= \nabla A_s - \frac{\partial \mathbf{A}}{\partial s} \end{aligned} \quad (30)$$

We replace:

$$\mathbf{F} = q \left( -\nabla\phi - \frac{\beta_0}{\gamma_0 c} \frac{\partial \phi}{\partial t} \hat{\mathbf{i}}_s + \beta \beta_0 \nabla\phi - \frac{\beta \beta_0}{\gamma_0} \frac{\partial \phi}{\partial s} \hat{\mathbf{i}}_s \right) \quad (31)$$

The potentials will have the same form as the sources (this can be shown explicitly using the Lorentz transformations):

$$\phi(x, y, s, t) = \phi \left( x, y, t - \frac{s}{\beta_0 c} \right) \quad (32)$$

For a function in this form we can write:

$$\frac{\partial \phi}{\partial s} = \frac{\partial}{\partial \zeta} = -\frac{1}{\beta_0 c} \frac{\partial \phi}{\partial t} \quad (33)$$

obtaining:

$$\mathbf{F} = q \left( -\nabla\phi + \frac{\beta_0^2}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s + \beta \beta_0 \nabla\phi - \frac{\beta \beta_0}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s \right) \quad (34)$$

Reorganizing:

$$\mathbf{F} = -q(1 - \beta \beta_0) \nabla\phi - \frac{\beta_0(\beta - \beta_0)}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s \quad (35)$$

Explicit dependencies:

$$F_x(x, y, \zeta(t)) = -q(1 - \beta \beta_0) \frac{\partial \phi}{\partial x}(x, y, \zeta(t)) \quad (36)$$

$$F_y(x, y, \zeta(t)) = -q(1 - \beta \beta_0) \frac{\partial \phi}{\partial y}(x, y, \zeta(t)) \quad (37)$$

$$F_z(x, y, \zeta(t)) = -q \left( 1 - \beta \beta_0 - \frac{\beta_0(\beta - \beta_0)}{\gamma_0} \right) \frac{\partial \phi}{\partial \zeta}(x, y, \zeta(t)) \quad (38)$$

Over the single interaction we neglect the particle slippage:

$$\beta = \beta_0 \quad (39)$$

$$\zeta(t) = \zeta \quad (40)$$

(in any case one would need to take into account also the dispersion in order to have the right slippage).

gives the following simplification:

$$F_x(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial \phi}{\partial x}(x, y, \zeta) \quad (41)$$

$$F_y(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial \phi}{\partial y}(x, y, \zeta) \quad (42)$$

$$F_z(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial \phi}{\partial \zeta}(x, y, \zeta) \quad (43)$$

In this way the force over the single interaction becomes independent on time and therefore we can compute the kicks simply as:

$$\Delta \mathbf{P} = \frac{L}{\beta_0 c} \mathbf{F} \quad (44)$$

from which we can compute the kicks on the normalized momenta ( $P_0 = m_0 \beta_0 \gamma_0 c$ ):

$$\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2 c^2} \frac{\partial \phi}{\partial x}(x, y, \zeta) \quad (45)$$

$$\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2 c^2} \frac{\partial \phi}{\partial y}(x, y, \zeta) \quad (46)$$

$$\Delta \delta \simeq \Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2 c^2} \frac{\partial \phi}{\partial \zeta}(x, y, \zeta) \quad (47)$$

Of your beam includes particles of different species (tracking of fragments), note that heree  $q$  is the charge of the kicked particle while  $m_0$  is the mass of the reference particle.

### 3.1 2.5D approximation

For large enough values of  $\gamma_0$ , Eq. 22 can be approximated by:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{1}{\varepsilon_0} \rho_0(x, y, \zeta) \quad (48)$$

which means that we can solve a simple 2D problem for each beam slice (identified by its  $\zeta$ ).

### 3.2 Modulated 2D

Often the beam distribution can be factorized as:

$$\rho_0(x, y, \zeta) = Nq_0\lambda_0(\zeta)\rho_\perp(x, y) \quad (49)$$

where:

$$\int \lambda_0(z) dz = 1 \quad (50)$$

$$\int \rho_\perp(x, y) dx dy = 1 \quad (51)$$

In this case the potential can be factorized as:

$$\phi(x, y, \zeta) = q_0\lambda_0(\zeta)\phi_\perp(x, y) \quad (52)$$

where  $\phi_\perp(x, y)$  is the solution of the following 2D Poisson equation:

$$\frac{\partial^2 \phi_\perp}{\partial x^2} + \frac{\partial^2 \phi_\perp}{\partial y^2} = -\frac{1}{\epsilon_0} \rho_\perp(x, y) \quad (53)$$

The kick can be expressed as:

$$\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{qq_0NL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2} \lambda_0(\zeta) \frac{\partial \phi}{\partial x}(x, y) \quad (54)$$

$$\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{qq_0NL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2} \lambda_0(\zeta) \frac{\partial \phi}{\partial y}(x, y) \quad (55)$$

$$\Delta \delta \simeq \Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = -\frac{qq_0NL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2} \frac{d\lambda_0}{d\zeta}(\zeta) \phi(x, y) \quad (56)$$

## 4 FFT solver

We will use the following notation for the Discrete Fourier Transform of a sequence of length  $M$ :

$$\hat{a}_k = \text{DFT}_M(a_m) = \sum_{m=0}^{M-1} a_m e^{-j2\pi \frac{km}{M}} \quad \text{for } k \in 0, \dots, M \quad (57)$$

The corresponding inverse transform is defined as:

$$a_n = \text{DFT}_M^{-1}(\hat{a}_k) = \frac{1}{M} \sum_{k=0}^{M-1} \hat{a}_k e^{j2\pi \frac{km}{M}} \quad \text{for } m \in 0, \dots, M \quad (58)$$

Multidimensional Discrete Fourier Transforms are obtained by applying sequentially 1D DFTs.. For example, in two dimensions:

$$\begin{aligned} \hat{a}_{k_x k_y} &= \text{DFT}_{M_x M_y} \{a_{m_x m_y}\} = \text{DFT}_{M_y} \left\{ \text{DFT}_{M_x} \{a_{m_x m_y}\} \right\} \\ &= \sum_{m_x=0}^{M_x-1} e^{-j2\pi \frac{k_x m_x}{M_x}} \sum_{m_y=0}^{M_y-1} e^{-j2\pi \frac{k_y m_y}{M_y}} a_{m_x m_y} \end{aligned} \quad (59)$$

$$\begin{aligned}
a_{n_x n_y} &= \text{DFT}_{M_x M_y}^{-1} \left\{ a_{k_x k_y} \right\} = \text{DFT}_{M_y}^{-1} \left\{ \text{DFT}_{M_x}^{-1} \left\{ \hat{a}_{k_x k_y} \right\} \right\} \\
&= \frac{1}{M_x M_y} \sum_{k_x=0}^{M_x-1} e^{j2\pi \frac{k_x m_x}{M_x}} \sum_{k_y=0}^{M_y-1} e^{j2\pi \frac{k_y m_y}{M_y}} \hat{a}_{k_x k_y}
\end{aligned} \tag{60}$$

We start from a 1D case for illustration and then we generalize.

#### 4.1 1D case

We assume free space. The potential can be written as the convolution of a Green function with the charge distribution:

$$\phi(x) = \int_{-\infty}^{+\infty} \rho(x') G(x - x') dx' \tag{61}$$

We assume that the source is limited to the region  $[0, L]$ :

$$\rho(x) = \rho(x) \Pi_{[0, L]}(x) \tag{62}$$

where  $\Pi_{[a, b]}(x)$  is a rectangular window function defined as:

$$\Pi_{[a, b]}(x) = \begin{cases} 1 & \text{for } x \in [a, b] \\ 0 & \text{elsewhere} \end{cases} \tag{63}$$

We are interested in the electric potential only the region occupied by the sources, so we can compute:

$$\phi_L(x) = \phi(x) \Pi_{[0, L]} \left( \frac{x}{L} \right) \tag{64}$$

We replace Eq. (62) and Eq. (64) into Eq.(61), obtaining:

$$\phi_L(x) = \Pi_{[0, L]}(x) \int_{-\infty}^{+\infty} \Pi_{[0, L]}(x) \rho(x') G(x - x') dx' \tag{65}$$

We change variable into  $x'' = x - x'$ :

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0, L]}(x) \Pi_{[0, L]}(x - x'') \rho(x - x'') G(x'') dx'' \tag{66}$$

The integrand vanishes outside the set of the  $(x, x'')$  defined by:

$$\begin{cases} 0 < x < L \\ 0 < (x - x'') < L \end{cases} \tag{67}$$

We flip the signs in the second equation, obtaining:

$$\begin{cases} 0 < x < L \\ -L < (x'' - x) < 0 \end{cases} \tag{68}$$

Combining the two equations we obtain:

$$-L < -L + x < x'' < x < L \quad (69)$$

i.e. the integrand is zero for  $-L < x'' < L$ . Therefore in equation (66) we can replace the  $G(x'')$  with its truncated version:

$$G_{2L}(x'') = G(x'') \Pi_{[-L,L]}(x'') \quad (70)$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]} \left( \frac{x}{L} \right) \Pi_{[0,L]} \left( \frac{x-x''}{L} \right) \rho(x-x'') G_{2L}(x'') dx'' \quad (71)$$

Since the two window function force the integrand to zero outside the region  $|x''| < L$  we can replace  $G_{2L}(x'')$  with its replicated version:

$$G_{2LR}(x'') = \sum_{n=-\infty}^{+\infty} G_{2L}(x'' - 2nL) = \sum_{n=-\infty}^{+\infty} G(x'' - 2nL) \Pi_{[-L,L]} \left( \frac{x'' - 2nL}{2L} \right) \quad (72)$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]} \left( \frac{x}{L} \right) \Pi_{[0,L]} \left( \frac{x-x''}{L} \right) \rho(x-x'') G_{2LR}(x'') dx'' \quad (73)$$

We can go back to the initial coordinate by substituting  $x'' = x - x'$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_{-\infty}^{+\infty} \rho(x') G_{2LR}(x - x') dx' \quad (74)$$

This is a cyclic convolution, so we can proceed as followd. We split the integral:

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_{2nL}^{2(n+1)L} \rho(x') G_{2LR}(x - x') dx' \quad (75)$$

In each term I replace  $x''' = x' + 2nL$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_0^{2L} \rho(x''' - 2nL) G_{2LR}(x - x''' - 2nL) dx' \quad (76)$$

But  $G_{2LR}$  is periodic:

$$\begin{aligned} \phi_L(x) &= \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_0^{2L} \rho(x''' - 2nL) G_{2LR}(x - x''') dx''' \\ &= \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_0^{2L} \sum_{n=-\infty}^{+\infty} \rho(x''' - 2nL) G_{2LR}(x - x''') dx''' \end{aligned} \quad (77)$$



I can define a replicated version of  $\rho(x)$ :

$$\rho_{2LR}(x) = \sum_{n=-\infty}^{+\infty} \rho(x - 2nL) \quad (78)$$

noting that this implies:

$$\rho_{2LR}(x) = 0 \quad \text{for } x \in [L, 2L] \quad (79)$$

We obtain:

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') dx' \quad (80)$$

The function:

$$\phi_{2LR}(x) = \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') dx' \quad (81)$$

is periodic of period  $2L$ . From it the potential of interest can be simply calculated by selecting the first half period  $[0, L]$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \phi_{2LR}(x) \quad (82)$$

We expand  $\phi_{2LR}(x)$  in Fourier series:

$$\phi_{2LR}(x) = \sum_{k=-\infty}^{+\infty} \tilde{\phi}_k e^{j2\pi k \frac{x}{2L}} \quad (83)$$

where the Fourier coefficient are given by:

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \phi_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (84)$$

We replace Eq. (81) into Eq. (84) obtaining:

$$\hat{\phi}_k = \frac{1}{2L} \int_0^{2L} \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') e^{-j2\pi k \frac{x}{2L}} dx' dx \quad (85)$$

With the change of variable  $x'' = x - x'$  we obtain:

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x') e^{-j2\pi k \frac{x'}{2L}} dx' \int_0^{2L} G_{2LR}(x'') e^{-j2\pi k \frac{x''}{2L}} dx'' \quad (86)$$

where we recognize the Fourier coefficients of  $\rho_{2LR}(x)$  and  $G_{2LR}(x)$ :

$$\tilde{\rho}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (87)$$

$$\tilde{G}_k = \frac{1}{2L} \int_0^{2L} G_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (88)$$

obtaining simply:

$$\hat{\phi}_k = 2L \tilde{G}_k \tilde{\rho}_k \quad (89)$$

I assume to have the functions  $\rho_{2LR}(x)$  and  $G_{2LR}(x)$  sampled (or averaged) with step:

$$h_x = \frac{2L}{M} = \frac{L}{N} \quad (90)$$

I can approximate the integrals in Eqs. (87) and (88) as:

$$\tilde{\rho}_k = \frac{1}{M} \sum_{n=0}^{M-1} \rho_{2LR}(x_n) e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{\rho}_k \quad (91)$$

$$\tilde{G}_k = \frac{1}{M} \sum_{n=0}^{M-1} G_{2LR}(x_n) e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{G}_k \quad (92)$$

where we recognize the Discrete Fourier Transforms:

$$\hat{\rho}_k = \text{DFT}_M \{ \rho_{2LR}(x_n) \} \quad (93)$$

$$\hat{G}_k = \text{DFT}_M \{ G_{2LR}(x_n) \} \quad (94)$$

Using Eq. (83) we can obtained a sampled version of  $\phi(x)$ :

$$\phi_{2LR}(x_n) = \sum_{k=0}^{M-1} \tilde{\phi}_k e^{j2\pi \frac{kn}{M}} \quad (95)$$

where we have assumed that  $\phi(x)$  is sufficiently smooth to allow truncating the sum. Using Eqs. (91) and (92)

$$\phi_{2LR}(x_n) = 2L \sum_{k=0}^{M-1} \tilde{G}_k \tilde{\rho}_k e^{j2\pi \frac{kn}{M}} = \frac{2L}{M^2} \sum_{k=0}^{M-1} \hat{G}_k \hat{\rho}_k e^{j2\pi \frac{kn}{M}} \quad (96)$$

This can be rewritten as:

$$\phi_{2LR}(x_n) = \frac{1}{M} \sum_{k=0}^{M-1} (h_x \hat{G}_k) \hat{\rho}_k e^{j2\pi \frac{kn}{M}} = \text{DFT}_M^{-1} \{ \phi_k \} \quad (97)$$

where

$$\hat{\phi}_k = h_x \hat{G}_k \hat{\rho}_k \quad (98)$$

We call “Integrated Green Function” the quantity:

$$G_{2LR}(x_n) = h_x G_{2LR}(x_n) \quad (99)$$

we introduce the corresponding Fourier transform:

$$\hat{G}_k^{\text{int}} = \text{DFT}_M \{ G_{2LR}^{\text{int}}(x_n) \} \quad (100)$$

Eq. (98) can be rewritten as:

$$\hat{\phi}_k = \hat{G}_k^{\text{int}} \hat{\rho}_k \quad (101)$$

### Algorithm - 1D

In summary the potential at the grid nodes can be computed as follows:

1. We compute the Integrated Green function at the grid points in the range  $[0, L]$ :

$$G_{2LR}^{\text{int}}(x_n) = \int_{x_n - \frac{h_x}{2}}^{x_n + \frac{h_x}{2}} G(x) dx \quad (102)$$

2. We extend to the interval  $[L, 2L]$  using the fact that in this interval:

$$G_{2LR}^{\text{int}}(x_n) = G_{2LR}^{\text{int}}(x_n - 2L) = G_{2LR}^{\text{int}}(2L - x_n) \quad (103)$$

where the first equality comes from the periodicity of  $G_{2LR}^{\text{int}}(x)$  and the second from the fact that  $G(x)$  is an even function (i.e.  $G(x) = G(-x)$ ). Note that for  $x_n \in [L, 2L]$  we have that  $2L - x_n \in [0, L]$  so we can reuse the values computed at the previous step.

3. We transform it:

$$\hat{G}_k^{\text{int}} = \text{DFT}_{2N} \{G_{2LR}^{\text{int}}(x_n)\} \quad (104)$$

4. We assume that we are given  $\rho(x_n)$  in the interval  $[0, L]$ . From this we can obtaining  $\rho_{2LR}(x_n)$  over the interval  $[0, 2L]$  simply extending the sequence with zeros (see Eq. (79)).

5. We transform it:

$$\hat{\rho}_k = \text{DFT}_{2N} \{\rho_{2LR}(x_n)\} \quad (105)$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_k = G_k^{\text{int}} \rho_k \quad \text{for } k \in [0, 2N] \quad (106)$$

7. We inverse-transform:

$$\phi_{2LR}(x_n) = \text{DFT}_{2N}^{-1} \{\hat{\phi}_k\} \quad (107)$$

which provides the physical potential in the range  $[0, L]$ :

$$\phi(x_n) = \phi_{2LR}(x_n) \quad \text{for } x_n \in [0, L] \quad (108)$$

## 4.2 Extension to 3D

The procedure described can be extended to multiple dimensions by applying the same reasoning for all coordinates. Obtaining the following procedure:

1. We compute the Integrated Green function at the grid points in the volume  $[0, L_x] \times [0, L_y] \times [0, L_z]$ :

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x} - \frac{h_x}{2}}^{x_{n_x} + \frac{h_x}{2}} dx \int_{y_{n_y} - \frac{h_y}{2}}^{y_{n_y} + \frac{h_y}{2}} dy \int_{z_{n_z} - \frac{h_z}{2}}^{z_{n_z} + \frac{h_z}{2}} dz G(x, y, z) \quad (109)$$

2. We extend to the region  $[0, 2L_x] \times [0, 2L_y] \times [0, 2L_z]$  using the fact that:

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n - 2L_x, y_n, z_n) = G_{2LR}^{\text{int}}(2L_x - x_n, y_n, z_n) \\ \text{for } x_n \in [L_x, 2L_x], y_n \in [0, 2L_y], z_n \in [0, 2L_z] \quad (110)$$

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n, y_n - 2L_y, z_n) = G_{2LR}^{\text{int}}(x_n, 2L_y - y_n, z_n) \\ \text{for } y_n \in [L_y, 2L_y], x_n \in [0, 2L_x], z_n \in [0, 2L_z] \quad (111)$$

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n, y_n, z_n - 2L_z) = G_{2LR}^{\text{int}}(x_n, y_n, 2L_z - z_n) \\ \text{for } z_n \in [L_z, 2L_z], x_n \in [0, 2L_x], y_n \in [0, 2L_y] \quad (112)$$

This allows reusing the values computed at the previous step.

3. We transform it:

$$\hat{G}_{k_x k_y k_z}^{\text{int}} = \text{DFT}_{2N_x 2N_y 2N_z} \{G_{2LR}(x_n, y_n, z_n)\} \quad (113)$$

4. We assume that we are given  $\rho(x_n, y_n, z_n)$  in the region  $[0, L_x] \times [0, L_y] \times [0, L_z]$ . From this we can obtain  $\rho_{2LR}(x_n)$  over the region  $[0, 2L_x] \times [0, 2L_y] \times [0, 2L_z]$  simply extending the matrix with zeros (see Eq. (79)).

5. We transform it:

$$\hat{\rho}_{k_x k_y k_z}^{\text{int}} = \text{DFT}_{2N_x 2N_y 2N_z} \{\rho_{2LR}(x_n, y_n, z_n)\} \quad (114)$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_{k_x k_y k_z} = G_{k_x k_y k_z}^{\text{int}} \rho_{k_x k_y k_z} \quad \text{for } k_x/y/z \in [0, 2N_{x/y/z}] \quad (115)$$

7. We inverse-transform:

$$\phi_{2LR}(x_n, y_n, z_n) = \text{DFT}_{2N_x 2N_y 2N_z}^{-1} \{\hat{\phi}_{k_x k_y k_z}\} \quad (116)$$

which provides the physical potential in the region  $[0, L_x] \times [0, L_y] \times [0, L_z]$ :

$$\phi(x_n, y_n, z_n) = \phi_{2LR}(x_n, y_n, z_n) \quad \text{for } (x_n, y_n, z_n) \in [0, L_x] \times [0, L_y] \times [0, L_z] \quad (117)$$

In summary in 1D what one needs to do is:

Transform the sources and the Green function:

$$\hat{\rho}_k = \frac{1}{M} \sum_{n=0}^{M-1} \rho_{2LR}(x_n) e^{j2\pi \frac{kn}{M}} \quad (118)$$

$$\hat{G}_k = \frac{1}{M} \sum_{n=0}^{M-1} G_{2LR}(x_n) e^{j2\pi \frac{kn}{M}} \quad (119)$$

Do the product and antitransform:

$$\phi_{2LR}(x_n) = 2L \sum_{n=0}^{M-1} \hat{G}_k \hat{\rho}_k e^{-j2\pi \frac{kn}{M}} \quad (120)$$

Repeating the same reasoning along all directions one obtains:

$$\hat{\rho}_{k_x k_y k_z} = \frac{1}{M_x M_y M_z} \sum_{n_x=0}^{M_x-1} e^{j2\pi \frac{k_x n_x}{M_x}} \sum_{n_y=0}^{M_y-1} e^{j2\pi \frac{k_y n_y}{M_y}} \sum_{n_z=0}^{M_z-1} e^{j2\pi \frac{k_z n_z}{M_z}} \rho_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) \quad (121)$$

$$\hat{G}_{k_x k_y k_z} = \frac{1}{M_x M_y M_z} \sum_{n_x=0}^{M_x-1} e^{j2\pi \frac{k_x n_x}{M_x}} \sum_{n_y=0}^{M_y-1} e^{j2\pi \frac{k_y n_y}{M_y}} \sum_{n_z=0}^{M_z-1} e^{j2\pi \frac{k_z n_z}{M_z}} G_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) \quad (122)$$

$$\begin{aligned} \phi_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) = \\ (2L_x)(2L_y)(2L_z) \sum_{k_x=0}^{M_x-1} e^{-j2\pi \frac{k_x n_x}{M_x}} \sum_{k_y=0}^{M_y-1} e^{-j2\pi \frac{k_y n_y}{M_y}} \sum_{k_z=0}^{M_z-1} e^{-j2\pi \frac{k_z n_z}{M_z}} \hat{G}_{k_x k_y k_z} \hat{\rho}_{k_x k_y k_z} \end{aligned} \quad (123)$$

The continuous convolution in 3D is written as

$$\phi(x, y, z) = \iiint_{-\infty}^{+\infty} \rho(x', y', z') G(x - x', y - y', z - z') dx' dy' dz' \quad (124)$$

where:

$$G(x, y, z) = \frac{1}{4\pi\epsilon_0} \frac{1}{\sqrt{x^2 + y^2 + z^2}} \quad (125)$$

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