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 $\beta_0 c$:

$$\rho\left(x, y, s, t\right) = \rho_0\left(x, y, s - \beta_0 ct\right) \tag{1}$$

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

We define an auxiliary variable ζ as the position along the bunch:

$$\zeta = s - \beta_0 ct\,. \tag{3}$$

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]:

$$ct' = \gamma_0\left(ct - \beta_0 s\right) \tag{4}$$

$$x' = x \tag{5}$$

$$y' = y \tag{6}$$

$$s' = \gamma_0\left(s - \beta_0 ct\right) = \gamma_0 \zeta \tag{7}$$

The corresponding inverse transformation is:

$$ct = \gamma_0\left(ct' + \beta_0 s'\right) \tag{8}$$

$$x = x' \tag{9}$$

$$y = y' \tag{10}$$

$$s = \gamma_0\left(s' + \beta_0 ct'\right) \tag{11}$$

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

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

$$J_s'\left(\mathbf{r}', t'\right) = \gamma_0\left[J_s\left(\mathbf{r}\left(\mathbf{r}', t'\right), t\left(\mathbf{r}', t'\right)\right) - \beta_0 c\rho\left(\mathbf{r}\left(\mathbf{r}', t'\right), t\left(\mathbf{r}', t'\right)\right)\right] \tag{13}$$

where the transformations $\mathbf{r}\left(\mathbf{r}', t'\right)$ and $t\left(\mathbf{r}', t'\right)$ 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:

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

$$J_s'\left(\mathbf{r}', t'\right) = 0 \tag{15}$$

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

$$\rho\left(x',y',s(s',t'),t(s',t')\right)=\rho_0\left(x',y',s(s',t')-\beta_0 c\,t(s',t')\right) \tag{16}$$

From Eq. 7 we get:

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

where the coordinate t' has disappeared.
We can therefore write:

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

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

$$\frac{\partial^2\phi'}{\partial x'^2}+\frac{\partial^2\phi'}{\partial y'^2}+\frac{\partial^2\phi'}{\partial s'^2}=-\frac{\rho'(x',y',s')}{\varepsilon_0} \tag{19}$$

From Eq. 18 we can write:

$$\frac{\partial^2\phi'}{\partial x'^2}+\frac{\partial^2\phi'}{\partial y'^2}+\frac{\partial^2\phi'}{\partial s'^2}=-\frac{1}{\gamma_0\varepsilon_0}\rho_0\left(x',y',\frac{s'}{\gamma_0}\right) \tag{20}$$

We now make the substitution:

$$\zeta=\frac{s'}{\gamma_0} \tag{21}$$

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

$$\frac{\partial^2\phi'}{\partial x^2}+\frac{\partial^2\phi'}{\partial y^2}+\frac{1}{\gamma_0^2}\frac{\partial^2\phi'}{\partial\zeta^2}=-\frac{1}{\gamma_0\varepsilon_0}\rho_0\left(x,y,\zeta\right) \tag{22}$$

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:

$$\phi=\gamma_0\left(\phi'+\beta_0 cA'_s\right) \tag{23}$$

$$A_s=A'_s+\beta_0\frac{\phi'}{c} \tag{24}$$

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

$$\phi=\gamma_0\phi' \tag{25}$$

$$A_s=\beta_0\frac{\phi'}{c}=\frac{\beta_0}{\gamma_0 c}\phi \tag{26}$$

Combining Eq. 25 with Eq. 22 we obtain the equation in ϕ:

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{1}{\gamma_0^2}\frac{\partial^2\phi}{\partial\zeta^2}=-\frac{1}{\varepsilon_0}\rho_0\left(x,y,\zeta\right) \tag{27}$$

3 Lorentz force

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

$$\mathbf{v} = \beta c \,\hat{\mathbf{i}}_s \tag{28}$$

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

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

We compute the vector product:

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

We replace:

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

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

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

For a function in this form we can write:

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

obtaining:

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

Reorganizing:

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

Explicit dependencies:

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

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

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

Over the single interaction we neglect the particle slippage:

$$\beta = \beta_0 \tag{39}$$
$$\zeta(t) = \zeta \tag{40}$$

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

$$F_x(x,y,\zeta) = -q(1-\beta_0^2)\frac{\partial\phi}{\partial x}(x,y,\zeta) \tag{41}$$
$$F_y(x,y,\zeta) = -q(1-\beta_0^2)\frac{\partial\phi}{\partial y}(x,y,\zeta) \tag{42}$$
$$F_z(x,y,\zeta) = -q(1-\beta_0^2)\frac{\partial\phi}{\partial \zeta}(x,y,\zeta) \tag{43}$$

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

$$\Delta\mathbf{P} = \frac{L}{\beta_0 c}\mathbf{F} \tag{44}$$

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

$$\Delta p_x = \frac{m_0}{m}\frac{\Delta P_x}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial\phi}{\partial x}(x,y,\zeta) \tag{45}$$
$$\Delta p_y = \frac{m_0}{m}\frac{\Delta P_y}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial\phi}{\partial y}(x,y,\zeta) \tag{46}$$
$$\Delta\delta \simeq \Delta p_z = \frac{m_0}{m}\frac{\Delta P_z}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial\phi}{\partial \zeta}(x,y,\zeta) \tag{47}$$

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 γ_0, Eq. 22 can be approximated by:

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

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

3.2 Modulated 2D

Often the beam distribution can be factorized as:

$$\rho_0(x, y, \zeta) = Nq_0\lambda_0(\zeta)\rho_\perp(x, y) \tag{49}$$

where:

$$\int \lambda_0(z)\, dz = 1 \tag{50}$$

$$\int \rho_\perp(x, y)\, dx\, dy = 1 \tag{51}$$

In this case the potential can be factorized as:

$$\phi(x, y, \zeta) = q_0\lambda_0(\zeta)\phi_\perp(x, y) \tag{52}$$

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

$$\frac{\partial^2\phi_\perp}{\partial x^2} + \frac{\partial^2\phi_\perp}{\partial y^2} = -\frac{1}{\varepsilon_0}\rho_\perp\,(x, y) \tag{53}$$

The kick can be expressed as:

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

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

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

4 FFT solver

We start from a 1D case for illustration and then we generalize.
We assume free space. The potential can be written as the convolution of a Green function with the charge distribution:

$$\phi(x) = \int_{-\infty}^{+\infty} \rho(x')\, G(x - x')dx' \tag{57}$$

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

$$\rho(x) = \rho(x)\,\Pi_{[0,L]}\,(x) \tag{58}$$

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

$$\Pi_{[a,b]}(x) = \begin{cases} 1 & \text{for } a < x < b \\ 0 & \text{elsewhere} \end{cases} \tag{59}$$

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

$$\phi_L(x) = \phi(x)\Pi_+\left(\frac{x}{L}\right) \tag{60}$$

We replace Eq. (58) and Eq. (60) into Eq.(57), obtaining:

$$\phi_L(x) = \Pi_{[0,L]}\left(x\right)\int_{-\infty}^{+\infty}\Pi_{[0,L]}\left(x\right)\rho(x')\,G(x-x')dx' \tag{61}$$

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

$$\phi_L(x) = \int_{-\infty}^{+\infty}\Pi_{[0,L]}\left(x\right)\Pi_{[0,L]}\left(x - x''\right)\rho(x-x'')\,G(x'')dx'' \tag{62}$$

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

$$\begin{cases} 0 < x < L \\ 0 < (x - x'') < L \end{cases} \tag{63}$$

We flip the signs in the second equation, obtaining:

$$\begin{cases} 0 < x < L \\ -L < (x'' - x) < 0 \end{cases} \tag{64}$$

Combining the two equations we obtain:

$$-L < -L + x < x'' < x < L \tag{65}$$

i.e. the integrand is zero for $-L < x'' < L$. Therefore in equation (62) we can replace the $G(x'')$ with its truncated version:

$$G_{2L}(x'') = G(x'')\,\Pi_{[-L,L]}\left(x''\right) \tag{66}$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty}\Pi_{[0,L]}\left(\frac{x}{L}\right)\Pi_{[0,L]}\left(\frac{x-x''}{L}\right)\rho(x-x'')\,G_{2L}(x'')dx'' \tag{67}$$

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:

$$G_{2LR}(x'') = \sum_{n=-\infty}^{+\infty} G_{2L}(x' - 2nL) = \sum_{n=-\infty}^{+\infty} G(x'' - L - 2nL)\,\Pi_{[-L,L]}\left(\frac{x'' - 2nL}{2L}\right) \tag{68}$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty}\Pi_{[0,L]}\left(\frac{x}{L}\right)\Pi_{[0,L]}\left(\frac{x-x''}{L}\right)\rho(x-x'')\,G_{2LR}(x'')dx'' \tag{69}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_{-\infty}^{+\infty} \rho(x')\, G_{2LR}(x - x')dx' \tag{70}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{2nL}^{2(n+1)L} \rho(x')\, G_{2LR}(x - x')dx' \tag{71}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{0}^{2L} \rho(x''' - 2nL)\, G_{2LR}(x - x''' - 2nL)dx' \tag{72}$$

But G_{2LR} is periodic:

$$\begin{aligned}\phi_L(x) &= \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{0}^{2L} \rho(x''' - 2nL)\, G_{2LR}(x - x''')dx''' \\ &= \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_{0}^{2L} \sum_{n=-\infty}^{+\infty} \rho(x''' - 2nL)\, G_{2LR}(x - x''')dx'''\end{aligned} \tag{73}$$

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

$$\rho_{2LR}(x) = \sum_{n=-\infty}^{+\infty} \rho(x - 2nL) \tag{74}$$

obtaining:

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_{0}^{2L} \rho_{2LR}(x')\, G_{2LR}(x - x')dx' \tag{75}$$

The function:

$$\phi_{2LR}(x) = \int_{0}^{2L} \rho_{2LR}(x')\, G_{2LR}(x - x')dx' \tag{76}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \phi_{2LR}(x) \tag{77}$$

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

$$\phi_{2LR}(x) = \sum_{k=-\infty}^{+\infty} \tilde{\phi}_k\, e^{j2\pi k \frac{x}{2L}} \tag{78}$$

where the Fourier coefficient are given by:

$$\tilde{\phi}_k = \frac{1}{2L}\int_0^{2L} \phi_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{79}$$

We replace Eq. (76) into Eq. (79) obtaining:

$$\hat{\phi}_k = \frac{1}{2L}\int_0^{2L}\int_0^{2L} \rho_{2LR}(x')\, G_{2LR}(x-x')\, e^{-j2\pi k \frac{x}{2L}}\, dx'\, dx \tag{80}$$

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

$$\tilde{\phi}_k = \frac{1}{2L}\int_0^{2L} \rho_{2LR}(x') e^{-j2\pi k \frac{x'}{2L}} dx' \int_0^{2L} G_{2LR}(x'') e^{-j2\pi k \frac{x''}{2L}}\, dx'' \tag{81}$$

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

$$\tilde{\rho}_k = \frac{1}{2L}\int_0^{2L} \rho_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{82}$$

$$\tilde{G}_k = \frac{1}{2L}\int_0^{2L} G_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{83}$$

obtaining simply:

$$\hat{\phi}_k = 2L\, \hat{G}_k\, \hat{\rho}_k \tag{84}$$

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

$$h_x = \frac{2L}{M} = \frac{L}{N} \tag{85}$$

I can approximate the integrals in Eqs. (82) and (83) as:

$$\tilde{\rho}_k = \frac{1}{M}\sum_{n=0}^{M-1} \rho_{2LR}(x_n)\, e^{-j2\pi \frac{kn}{M}} = \frac{1}{M}\hat{\rho}_k \tag{86}$$

$$\tilde{G}_k = \frac{1}{M}\sum_{n=0}^{M-1} G_{2LR}(x_n)\, e^{-j2\pi \frac{kn}{M}} = \frac{1}{M}\hat{G}_k \tag{87}$$

where we recognize the Discrete Fourier Transforms:

$$\hat{\rho}_k = \mathrm{DFT}\left\{\rho_{2LR}(x_n)\right\} \tag{88}$$

$$\hat{G}_k = \mathrm{DFT}\left\{G_{2LR}(x_n)\right\} \tag{89}$$

Using Eq. (78) we can obtained a sampled version of $\phi(x)$:

$$\phi_{2LR}(x_n) = \sum_{n=0}^{M-1} \tilde{\phi}_k\, e^{j2\pi \frac{kn}{M}} \tag{90}$$

where we have assumed that $\phi(x)$ is sufficiently smooth to allow truncating the sum. Using Eqs. (86) and (87)

$$\phi_{2LR}(x_n) = 2L\sum_{n=0}^{M-1} \tilde{G}_k\, \tilde{\rho}_k\, e^{j2\pi \frac{kn}{M}} = \frac{2L}{M^2}\sum_{n=0}^{M-1} \hat{G}_k\, \hat{\rho}_k\, e^{j2\pi \frac{kn}{M}} \tag{91}$$

This can be rewritten as:

$$\phi_{2LR}(x_n) = \frac{1}{M}\sum_{n=0}^{M-1}(h_x\hat{G}_k)\,\hat{\rho}_k\,e^{j2\pi\frac{kn}{M}} = \mathrm{DFT}^{-1}\left\{(h_x\hat{G}_k)\,\hat{\rho}_k)\right\} \tag{92}$$

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

1. We sample or average the Green function with step h_x over the interval $[0, L]$, obtaining the sequence $G(x_n)$ for $n = 0, ..., N-1$
2. We build its replicate version in the interval $[L, 2L]$ using the fact that:

$$G_{2LR}(2L - x) = G(-x) = G(x) \tag{93}$$

....

4.1 Extension to 3D

In summary in 1D what one needs to do is:
Transform the sources and the Green function:

$$\hat{\rho}_k = \frac{1}{M}\sum_{n=0}^{M-1}\rho_{2LR}(x_n)\,e^{j2\pi\frac{kn}{M}} \tag{94}$$

$$\hat{G}_k = \frac{1}{M}\sum_{n=0}^{M-1}G_{2LR}(x_n)\,e^{j2\pi\frac{kn}{M}} \tag{95}$$

Do the product and antitransform:

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

Repeating the same reasoning along all directions one obtains:

$$\hat{\rho}_{k_xk_yk_z} = \frac{1}{M_xM_yM_z}\sum_{n_x=0}^{M_x-1}e^{j2\pi\frac{k_xn_x}{M_x}}\sum_{n_y=0}^{M_y-1}e^{j2\pi\frac{k_yn_y}{M_y}}\sum_{n_z=0}^{M_z-1}e^{j2\pi\frac{k_zn_z}{M_z}}\,\rho_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) \tag{97}$$

$$\hat{G}_{k_xk_yk_z} = \frac{1}{M_xM_yM_z}\sum_{n_x=0}^{M_x-1}e^{j2\pi\frac{k_xn_x}{M_x}}\sum_{n_y=0}^{M_y-1}e^{j2\pi\frac{k_yn_y}{M_y}}\sum_{n_z=0}^{M_z-1}e^{j2\pi\frac{k_zn_z}{M_z}}\,G_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) \tag{98}$$

$$\begin{aligned}&\phi_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) = \\ &\qquad(2L_x)(2L_y)(2L_z)\sum_{k_x=0}^{M_x-1}e^{-j2\pi\frac{k_xn_x}{M_x}}\sum_{k_y=0}^{M_y-1}e^{-j2\pi\frac{k_yn_y}{M_y}}\sum_{k_z=0}^{M_z-1}e^{-j2\pi\frac{k_zn_z}{M_z}}\,\hat{G}_{k_xk_yk_z}\hat{\rho}_{k_xk_yk_z}\end{aligned} \tag{99}$$

The continuous convolution in 3D is written as

$$\phi(x, y, z) = \iiint_{-\infty}^{+\infty}\rho(x', y', z')\,G(x - x', y - y', z - z')\,dx'\,dy'\,dz' \tag{100}$$

where:

$$G(x, y, z) = \frac{1}{4\pi\varepsilon_0}\frac{1}{\sqrt{x^2 + y^2 + z^2}} \tag{101}$$

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