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:

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

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

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

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

The corresponding inverse transform is defined as:

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

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

$$\begin{aligned}\hat{a}_{k_xk_y} &= \mathrm{DFT}_{M_xM_y}\left\{a_{m_xm_y}\right\} = \mathrm{DFT}_{M_y}\left\{\mathrm{DFT}_{M_x}\left\{a_{m_xm_y}\right\}\right\}\\ &= \sum_{m_x=0}^{M_x-1} e^{-j2\pi\frac{k_xm_x}{M_x}} \sum_{m_y=0}^{M_y-1} e^{-j2\pi\frac{k_ym_y}{M_y}}\,a_{m_xm_y}\end{aligned} \tag{59}$$

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

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 $x'' = x - x'$:

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

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:

$$-L < -L + x < x'' < x < L \tag{69}$$

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

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

obtaining:

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

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:

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

obtaining:

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

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

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

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

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

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

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

But G_{2LR} is periodic:

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

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

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

noting that this implies:

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

We obtain:

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

The function:

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

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

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

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

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

where the Fourier coefficient are given by:

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

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

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

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

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

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

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

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

obtaining simply:

$$\hat{\phi}_k = 2L\, \hat{G}_k\, \hat{\rho}_k \tag{89}$$

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

$$h_x = \frac{2L}{M} = \frac{L}{N} \tag{90}$$

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

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

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

where we recognize the Discrete Fourier Transforms:

$$\hat{\rho}_k = \mathrm{DFT}_M \left\{\rho_{2LR}(x_n)\right\} \tag{93}$$

$$\hat{G}_k = \mathrm{DFT}_M \left\{G_{2LR}(x_n)\right\} \tag{94}$$

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

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

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

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

This can be rewritten as:

$$\phi_{2LR}(x_n) = \frac{1}{M} \sum_{n=0}^{M-1} (h_x \hat{G}_k)\, \hat{\rho}_k\, e^{j2\pi\frac{kn}{M}} = \mathrm{DFT}_M^{-1} \left\{\phi_k\right\} \tag{97}$$

where

$$\hat{\phi}_k = h_x \hat{G}_k\, \hat{\rho}_k \tag{98}$$

We call "Integrated Green Function" the quantity:

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

we introduce the corresponding Fourier transform:

$$\hat{G}_k^{\mathrm{int}} = \mathrm{DFT}_M \left\{ G_{2LR}^{\mathrm{int}}(x_n) \right\} \tag{100}$$

Eq. (98) can be rewritten as:

$$\hat{\phi}_k = \hat{G}_k^{\mathrm{int}}\, \hat{\rho}_k \tag{101}$$

The 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 $[0, L]$:

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

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

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

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:

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

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:

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

6. We compute the potential in the transformed domain:

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

7. We inverse-transform:

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

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

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

4.2 Extension to multiple dimensionss

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 $[0, L_x] \times [0, L_y] \times [0, L_z]$:

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

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

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

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

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

This allows reusing the values computed at the previous step.

3. We transform it:

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

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 obtaining $\rho_{2LR}(x_n)$ 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:

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

6. We compute the potential in the transformed domain:

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

7. We inverse-transform:

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

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

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

4.3 Green functions

3D Poisson problem in free space

For the equation:

$$\nabla^2 \phi(x, y, z) = -\frac{1}{\varepsilon_0} \rho(x, y, z) \tag{118}$$

where:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \tag{119}$$

the solution can be written as

$$\phi(x,y,z) = \iiint_{-\infty}^{+\infty} \rho(x',y',z')\, G(x-x', y-y', z-z')\, dx'\, dy'\, dz' \tag{120}$$

where:

$$G(x,y,z) = \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{x^2+y^2+z^2}} \tag{121}$$

The corresponding integrated Green function can be written as:

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x}-\frac{h_x}{2}}^{x_{n_x}+\frac{h_x}{2}} dx \int_{y_{n_y}-\frac{h_y}{2}}^{y_{n_y}+\frac{h_y}{2}} dy \int_{z_{n_z}-\frac{h_z}{2}}^{x_{n_z}+\frac{h_z}{2}} dz\, G(x,y,z) \tag{122}$$

$$= +F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{123}$$

$$-F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{124}$$

$$-F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{125}$$

$$+F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{126}$$

$$-F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{127}$$

$$+F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{128}$$

$$+F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{129}$$

$$-F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{130}$$

where $F(x,y,z)$ is a primitive of $G(x,y,z)$, which can be obtained as:

$$F(x,y,z) = \int_{x_0}^{x} dx \int_{y_0}^{y} dy \int_{z_0}^{x} dz\, G(x,y,z) \tag{131}$$

where (x_0, y_0, z_0) is an arbitrary starting point.

An expression for $F(x, y, z)$ is the following

$$F(x,y,z) = \iiint \frac{1}{\sqrt{x^2+y^2+z^2}} dxdydz \tag{132}$$

$$= -\frac{z^2}{2}\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right) - \frac{y^2}{2}\arctan\left(\frac{xz}{y\sqrt{x^2+y^2+z^2}}\right) \tag{133}$$

$$- \frac{x^2}{2}\arctan\left(\frac{yz}{x\sqrt{x^2+y^2+z^2}}\right) + yz\ln\left(x+\sqrt{x^2+y^2+z^2}\right) \tag{134}$$

$$+ xz\ln\left(y+\sqrt{x^2+y^2+z^2}\right) + xy\ln\left(z+\sqrt{x^2+y^2+z^2}\right) \tag{135}$$

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