Report on the implementation of relativistic binary collisions in kinetic plasma codes

Michael J Touati[1]

[1] Plasma simulation group, University of California, Los Angeles

Abstract

UPIC-EMMA is a fully relativistic and fully parallelized spectral electromagnetic PIC code [Yu et al., 2014]. Inherited from the UPIC framework, UPIC-EMMA is coded in layers for convenient extension with different programming styles. The lowest layers are written in Fortran77 for high performance. They can be easily extended to many other languages. On top of this layer exists a library of Fortran90 wrapper functions which hide the complexity of the Fortran77 layer and that provides simpler arguments which enables strict type checking. The code separates the physics procedures from the communication, and utilizes the message-passing interface (MPI) for parallel processing. In addition, a multi-tasking library was implemented to enable mixed multi-tasking and MPI messaging, where multi-tasking is used on a shared memory node with multiple cores, and message-passing is used between such nodes [Decyk, 2007]. UPIC-EMMA also features 3D load balancing where the fields and particles use different partitions. For the field solver, the simulation box is usually partitioned in one dimension in 2D, and two dimensions in 3D, so that each processor holds global information in the dimension to be transformed. As a result, it requires a fast parallel transpose routine for efficient execution of the Fast Fourier Transform (FFT) in multi-dimensions. It scales well on parallel computers if the problem size is large enough [Decyk, 1995]. Scaling stops when the all-to-all transpose used in the FFT becomes latency dominated, which depends on the network being used. In many cases the decomposition for the particles is the same as that for the fields although this does not have to be the case.

Contents

1 Charge and current deposit

In UPIC-EMMA, both the charge density

$$\rho(\mathbf{r}_{i,j,k},\, t_n) = \sum_{a=e,\, i} \sum_{\ell=1}^{N_a} q_a \int_{\mathbb{R}^3} S_a^3[\mathbf{r}] W_{a,\ell}^3 \left[\mathbf{r}_{i,j,k} - \mathbf{r},\, t_n\right] d^3\mathbf{r} \tag{1}$$

and current density

$$\mathbf{j}(\mathbf{r}_{i,j,k},\, t_n) = \sum_{a=e,\, i} \sum_{\ell=1}^{N_a} q_a \mathbf{v}_{a,\ell}(t_n) \int_{\mathbb{R}^3} S_a^3\left[\mathbf{r}\right] W_{a,\ell}^3 \left[\mathbf{r}_{i,j,k} - \mathbf{r},\, t_n\right] d^3\mathbf{r} \tag{2}$$

are deposited at each time step t_n on a spatial mesh

$$\forall i \in [1..N_x],\, j \in [1..N_y],\, k \in [1..N_z],\, \mathbf{r}_{i,j,k} = \begin{pmatrix} x_i \\ y_j \\ z_k \end{pmatrix} = \begin{pmatrix} (i-1)\,\Delta_x \\ (j-1)\,\Delta_y \\ (k-1)\,\Delta_z \end{pmatrix} \tag{3}$$

from the knowledge of macro-particle locations $\mathbf{r}_{a,\ell}(t_n)$ and velocities $\mathbf{v}_{a,\ell}(t_n)$. All macro-particles of same species have the same charge q_a, same mass m_a and same shape

$$S_a^3\left[\mathbf{r}\right] = S_{a,x}[x] S_{a,y}[y] S_{a,z}[z] \tag{4}$$

with

$$\forall \xi \in \{x,\, y,\, z\},\, S_{a,\xi}[\xi] = \frac{1}{\sqrt{2\pi {\lambda_{a,\xi}}^2}} \exp\left(-\frac{\xi^2}{2{\lambda_{a,\xi}}^2}\right)$$

where $\lambda_{a,x}$, $\lambda_{a,y}$ and $\lambda_{a,z}$ represent the macro-particles size in the x, y and z-direction, respectively. Also in UPIC-EMMA, the charge and current deposits are done according to a linear interpolation on the grid in all directions so that

$$W_{a,\ell}^3\left[\mathbf{r}_{i,j,k},\, t_n\right] = W_{a,\ell,x}\left[x_i,\, t_n\right] W_{a,\ell,y}\left[y_j,\, t_n\right] W_{a,\ell,z}\left[z_k,\, t_n\right] \tag{5}$$

where

$$\forall \xi \in \{x,\, y,\, z\},\, W_{a,\ell,\xi}\left[\xi,\, t_n\right] = \max\left\{0,\, \frac{\Delta_\xi - |\xi - \xi_{a,\ell}(t_n)|}{{\Delta_\xi}^2}\right\}.$$

Knowing the charge and current densities in the whole spatial mesh at time t_n, one may perform their Inverse Discrete Fourier Transform (IDFT) in order to solve the Maxwell equations in the Fourier space. Let us note so

$$\forall p \in [1..N_x],\, q \in [1..N_y],\, r \in [1..N_z],\, \mathbf{k}_{p,q,r} = \begin{pmatrix} k_{x,p} \\ k_{y,q} \\ k_{z,r} \end{pmatrix} = 2\pi \begin{pmatrix} (p-1)\,/\Delta_x \\ (q-1)\,/\Delta_y \\ (r-1)\,/\Delta_z \end{pmatrix} \tag{6}$$

the spatial mesh in the Fourier space and

$$\widehat{F}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \frac{1}{N_x N_y N_z} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} F\left(\mathbf{r}_{i,j,n},\, t_n\right) \exp\left[\iota\left(k_{x,p} x_i + k_{y,q} y_j + k_{z,r} z_k\right)\right] \tag{7}$$

where $\iota = \sqrt{-1}$, the IDFT of the field quantity $F \in \{\mathbf{E},\, \mathbf{B},\, \rho,\, \mathbf{j},\, ...\}$. In practice, since the correlation of two distributions in the real domain corresponds to a multiplication of their transforms in the Fourier domain, the charge and current deposits are firstly done without accounting for the macro-particles shape, that is, by computing for $a \in \{e,\, i\}$

$$\widetilde{\rho}_a\left(\mathbf{r}_{i,j,k},\, t_n\right) = \sum_{\ell=1}^{N_a} q_a W_{a,\ell}^3\left[\mathbf{r}_{i,j,k},\, t_n\right] \tag{8}$$

and

$$\widetilde{\mathbf{j}}_a\left(\mathbf{r}_{i,j,k},\, t_n\right) = \sum_{\ell=1}^{N_a} q_a \mathbf{v}_{a,\,\ell}(t_n) W_{a,\ell}^3\left[\mathbf{r}_{i,j,k},\, t_n\right] \tag{9}$$

instead of (1) and (2). Then, the IDFT $\widehat{\widetilde{\rho}}_a$ and $\widehat{\widetilde{\mathbf{j}}}_a$ are then computed to finally get

$$\widehat{\rho}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{S}_e^3[\mathbf{k}_{p,q,r}]\widehat{\widetilde{\rho}}_e\left(\mathbf{k}_{p,q,r},\, t_n\right) + \widehat{S}_i^3[\mathbf{k}_{p,q,r}]\widehat{\widetilde{\rho}}_i\left(\mathbf{k}_{p,q,r},\, t_n\right) \tag{10}$$

and

$$\widehat{\mathbf{j}}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{S}_e^3[\mathbf{k}_{p,q,r}]\widehat{\widetilde{\mathbf{j}}}_e\left(\mathbf{k}_{p,q,r},\, t_n\right) + \widehat{S}_i^3[\mathbf{k}_{p,q,r}]\widehat{\widetilde{\mathbf{j}}}_i\left(\mathbf{k}_{p,q,r},\, t_n\right) \tag{11}$$

where the macro-particles shape simply reads

$$\widehat{S}_a^3[\mathbf{k}_{p,q,r}] = \exp\left(-\frac{k_{x,p}^2\lambda_{a,x}^2 + k_{y,q}^2\lambda_{a,y}^2 + k_{z,r}^2\lambda_{a,z}^2}{2}\right) \tag{12}$$

in the Fourier space.

2 Maxwell solver

As a spectral PIC code, the electric and magnetic fields are solved in the Fourier space in UPIC-EMMA. For this, the electric field $\widehat{\mathbf{E}}$ is separated into its longitudinal and transverse parts $\widehat{\mathbf{E}}_L$ and $\widehat{\mathbf{E}}_T$ defined by

$$\widehat{\mathbf{E}}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{\mathbf{E}}_L\left(\mathbf{k}_{p,q,r},\, t_n\right) + \widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) \tag{13}$$

with $\mathbf{k}_{p,q,r} \times \widehat{\mathbf{E}}_L\left(\mathbf{k}_{p,q,r},\, t_n\right) = \mathbf{0}$ and $\mathbf{k}_{p,q,r} \cdot \widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) = \mathbf{0}$. $\widehat{\mathbf{E}}_L$ is solved at each time step according to the Maxwell-Gauss equation

$$\widehat{\mathbf{E}}_L\left(\mathbf{k}_{p,q,r},\, t_n\right) = -\iota 4\pi \frac{\mathbf{k}_{p,q,r}}{{\mathbf{k}_{p,q,r}}^2}\widehat{\rho}\left(\mathbf{k}_{p,q,r},\, t_n\right). \tag{14}$$

Thus, a charge conserving current deposit or Boris correction to the longitudinal component of the electric field is not required in UPIC-EMMA to maintain that Maxwell-Gauss equation is satisfied. We make use of the equation of continuity coupled with the Maxwell-Gauss equation

$$\frac{1}{4\pi}\frac{\partial \widehat{\mathbf{E}}_L}{\partial t}\left(\mathbf{k}_{p,q,r},\, t_n\right) = -\iota\frac{\mathbf{k}_{p,q,r}}{{\mathbf{k}_{p,q,r}}^2}\frac{\partial \widehat{\rho}}{\partial t}\left(\mathbf{k}_{p,q,r},\, t_n\right) = -\frac{\mathbf{k}_{p,q,r}}{{\mathbf{k}_{p,q,r}}^2}\mathbf{k}_{p,q,r}\cdot\widehat{\mathbf{j}}\left(\mathbf{k}_{p,q,r},\, t_n\right)$$

in order to eliminate the longitudinal electric field from the Maxwell-Ampere equation and solve at each time step the transverse part $\widehat{\mathbf{E}}_T$ according to

$$\frac{\partial \widehat{\mathbf{E}}_T}{\partial t}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \iota c\mathbf{k}_{p,q,r}\times\widehat{\mathbf{B}}\left(\mathbf{k}_{p,q,r},\, t_n\right) - 4\pi\widehat{\mathbf{j}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) \tag{15}$$

where

$$\widehat{\mathbf{j}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{\mathbf{j}}\left(\mathbf{k}_{p,q,r},\, t_n\right) - \frac{\mathbf{k}_{p,q,r}}{{\mathbf{k}_{p,q,r}}^2}\mathbf{k}_{p,q,r}\cdot\widehat{\mathbf{j}}\left(\mathbf{k}_{p,q,r},\, t_n\right). \tag{16}$$

Finally, at each time, the longitudinal component of the magnetic field is set to zero and its transverse part is solved according to the Maxwell-Faraday equation

$$\frac{\partial \widehat{\mathbf{B}}}{\partial t}\left(\mathbf{k}_{p,q,r},\, t_n\right) = -\iota c\mathbf{k}_{p,q,r}\times\widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right). \tag{17}$$

From a numerical point of view, Equations (15) and (17) for the transverse magnetic and transverse electric fields are solved according to the following leap-frog algorithm :

1. The magnetic field is advanced during the first half time step

$$\widehat{\mathbf{B}}(\mathbf{k}_{p,q,r},\, t_n+\Delta_t/2) = \widehat{\mathbf{B}}\left(\mathbf{k}_{p,q,r},\, t_n\right) - \frac{\Delta_t}{2}\iota c\mathbf{k}_{p,q,r}\times\widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) \tag{18}$$

2. The electric field is thus deduced

$$\begin{aligned}\widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n+\Delta_t\right) &= \widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right)\\ &+ \Delta_t\Big[\iota c\mathbf{k}_{p,q,r}\times\widehat{\mathbf{B}}(\mathbf{k}_{p,q,r},\, t_n+\Delta_t/2) - 4\pi\widehat{\mathbf{j}}_T(\mathbf{k}_{p,q,r},\, t_n+\Delta_t/2)\Big]\end{aligned} \tag{19}$$

3. The magnetic field is advanced during the second half time step

$$\widehat{\mathbf{B}}\left(\mathbf{k}_{p,q,r},\, t_n+\Delta_t\right) = \widehat{\mathbf{B}}(\mathbf{k}_{p,q,r},\, t_n+\Delta_t/2) - \frac{\Delta_t}{2}\iota c\mathbf{k}_{p,q,r}\times\widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n+\Delta_t\right) \tag{20}$$

Following the Von-Neumann stability procedure, one find the dispersion relation [Dawson, 1983]

$${\mathbf{k}_{p,q,r}}^2 c^2 = \frac{4}{{\Delta_t}^2}\sin^2\left(\frac{\omega\Delta_t}{2}\right) \tag{21}$$

by looking form solutions of the form

$$\begin{cases} \widehat{\mathbf{E}}_T\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{\mathbf{E}}_0\left(\mathbf{k}_{p,q,r}\right) \exp\left[\iota\omega\left(n+\dfrac{1}{2}\right)\Delta_t\right] \\ \widehat{\mathbf{B}}\left(\mathbf{k}_{p,q,r},\, t_n\right) = \widehat{\mathbf{B}}_0\left(\mathbf{k}_{p,q,r}\right) \exp\left[\iota\omega n\Delta_t\right] \end{cases}.$$

Therefore, the numerical dispersion in UPIC-EMMA is superluminal and the algorithm is stable only if

$$\frac{{\mathbf{k}_{p,q,r}}^2 c^2 {\Delta_t}^2}{4} < 1. \tag{22}$$

From this, we see that the size of the time step is dictated by the largest $\mathbf{k}$-mode or highest-frequency electromagnetic mode resolved by the code, that is, the Nyquist spatial frequency

$$k_{\text{Nyquist}} = \pi\sqrt{\frac{1}{{\Delta_x}^2} + \frac{1}{{\Delta_y}^2} + \frac{1}{{\Delta_z}^2}} \tag{23}$$

corresponding to the half of the sampling rate of the discretized space $\{\mathbf{r}_{i,j,k},\ (i,\ j,\ k) \in [1..N_x] \times [1..N_y] \times [1..N_z]\}$. This gives the Courant-Friedrichs condition

$$\Delta_t \leq \frac{2}{\pi c} \frac{1}{\sqrt{\dfrac{1}{{\Delta_x}^2} + \dfrac{1}{{\Delta_y}^2} + \dfrac{1}{{\Delta_z}^2}}}. \tag{24}$$

3 Macro-particle pusher

Again, since the correlation of two distributions in the real domain corresponds to a multiplication of their transforms in the Fourier domain, the electric and magnetic component of the force acting on the particle denoted by "a, ℓ" at time t_n is obtained by first computing the Discrete Fourier Transform (DFT)

$$\mathbf{E}_s^{i,j,k,n} = \sum_{p=1}^{N_x}\sum_{q=1}^{N_y}\sum_{r=1}^{N_z} \widehat{\mathbf{E}}\left(\mathbf{k}_{p,q,r},\, t_n\right) \widehat{S}_a^3[\mathbf{k}_{p,q,r}] \exp\left[-\iota\left(k_{x,p}x_i + k_{y,q}y_j + k_{z,r}z_k\right)\right] \tag{25}$$

and then by linearly interpolating from the mesh points

$$\begin{array}{rcccll} \mathbf{E}_s(\mathbf{r}_{a,\ell}^n, t_n) & = & (1-\alpha) & (1-\beta) & \left[(1-\gamma)\,\mathbf{E}^{i_\ell,j_\ell,k_\ell,n} + \gamma\,\mathbf{E}^{i_\ell,j_\ell,k_\ell+1,n}\right] \\ & + & (1-\alpha) & \beta & \left[(1-\gamma)\,\mathbf{E}^{i_\ell,j_\ell+1,k_\ell,n} + \gamma\,\mathbf{E}^{i_\ell,j_\ell+1,k_\ell+1,n}\right] \\ & + & \alpha & (1-\beta) & \left[(1-\gamma)\,\mathbf{E}^{i_\ell+1,j_\ell,k_\ell,n} + \gamma\,\mathbf{E}^{i_\ell+1,j_\ell,k_\ell+1,n}\right] \\ & + & \alpha & \beta & \left[(1-\gamma)\,\mathbf{E}^{i_\ell+1,j_\ell+1,k_\ell,n} + \gamma\,\mathbf{E}^{i_\ell+1,j_\ell+1,k_\ell+1,n}\right] \end{array} \tag{26}$$

where

$$\begin{cases} \alpha = \dfrac{x_{a,\ell}(t_n) - x_{i_\ell}}{\Delta_x} \\ \beta = \dfrac{y_{a,\ell}(t_n) - y_{j_\ell}}{\Delta_y} \\ \gamma = \dfrac{z_{a,\ell}(t_n) - z_{k_\ell}}{\Delta_z} \end{cases} \quad \text{and} \quad \begin{cases} i_\ell = 1 + \mathbb{E}\left\{\dfrac{x_{a,\ell}(t_n)}{\Delta_x}\right\} \\ j_\ell = 1 + \mathbb{E}\left\{\dfrac{y_{a,\ell}(t_n)}{\Delta_y}\right\} \\ k_\ell = 1 + \mathbb{E}\left\{\dfrac{z_{a,\ell}(t_n)}{\Delta_z}\right\} \end{cases}$$

(idem for $\mathbf{B}_s(\mathbf{r}^n_{a,\ell}, t_n)$). The position and velocity of macro-particles denoted by "a, ℓ" are finally obtained according to

$$\frac{\mathbf{p}^{n+1/2}_{a,\ell} - \mathbf{p}^{n-1/2}_{a,\ell}}{\Delta_t} = q_a \left[\mathbf{E}_s\left(\mathbf{r}^n_{a,\ell}, t_n\right) + \frac{\mathbf{p}^{n+1/2}_{a,\ell} + \mathbf{p}^{n-1/2}_{a,\ell}}{2\gamma^n_{a,\ell} m_a c} \times \mathbf{B}_s\left(\mathbf{r}^n_{a,\ell}, t_n\right) \right] \tag{27}$$

and

$$\mathbf{r}^{n+1}_{a,\ell} = \mathbf{r}^n_{a,\ell} + \frac{\mathbf{p}^{n+1/2}_{a,\ell}}{m_a \sqrt{1 + \left(\frac{\mathbf{p}^{n+1/2}_{a,\ell}}{m_a c}\right)^2}} \Delta_t. \tag{28}$$

Equation (27) is an implicit equation where the new momentum $\mathbf{p}^{n+1/2}_{a,\ell} = \mathbf{p}_{a,\ell}(t_n + \Delta/2)$ appears on both sides of the equation. The solution is known as the Boris mover. It consists in computing successively

1. The acceleration of macro-particles by the electric field during the first half time step

$$\mathbf{p}^-_{a,\ell} = \mathbf{p}^{n-1/2}_{a,\ell} + q_a \mathbf{E}_s(\mathbf{r}^n_{a,\ell}, t_n)\frac{\Delta_t}{2}$$

2. Their rotation due to the magnetic field

$$\frac{\mathbf{p}^+_{a,\ell} - \mathbf{p}^-_{a,\ell}}{\Delta_t} = q_a \frac{\mathbf{p}^+_{a,\ell} + \mathbf{p}^-_{a,\ell}}{2\gamma^n_{a,\ell} m_a c} \times \mathbf{B}_s(\mathbf{r}^n_{a,\ell}, t_n)$$

   with $\gamma^n_{a,\ell} = \gamma^+_{a,\ell} = \gamma^-_{a,\ell} = \sqrt{1 + \left(\frac{\mathbf{p}^-_{a,\ell}}{m_a c}\right)^2}$ that is solved geometrically according to

$$\begin{cases} \mathbf{p}^*_{a,\ell} &= \mathbf{p}^-_{a,\ell} + \mathbf{p}^-_{a,\ell} \times \dfrac{\boldsymbol{\omega}^n_{c,a}\Delta_t}{2} \\ \mathbf{p}^+_{a,\ell} &= \mathbf{p}^*_{a,\ell} + \mathbf{p}^*_{a,\ell} \times \dfrac{\boldsymbol{\omega}^n_{c,a}\Delta_t}{1 + \left(\dfrac{\boldsymbol{\omega}^n_{c,a}\Delta_t}{2}\right)^2} \end{cases}$$

   where $\boldsymbol{\omega}^n_{c,a} = \dfrac{q_a \mathbf{B}_s(\mathbf{r}^n_{a,\ell}, t_n)}{\gamma^n_{a,\ell} m_a c}$ is the macro-particle cyclotron frequency vector.

3. The acceleration of macro-particles by the electric field during the second half time step

$$\mathbf{p}^{n+1/2}_{a,\ell} = \mathbf{p}^+_{a,\ell} + q_a \mathbf{E}_s(\mathbf{r}^n_{a,\ell}, t_n)\frac{\Delta_t}{2}$$

Let us note here that the macro-particle positions and velocities/momenta (and correspondingly the charge and current densities) are defined at half integer values in time with respect to each other. If positions are defined at whole time steps and velocities (momentum) at half integer values, then the longitudinal and transverse components of the electric field are defined at whole time steps (when particle positions are defined) and the magnetic field is defined at half-integer values. The current at the half integer time are time centered by averaging the new and old positions during the deposit.

Normalized quantity	$\underline{t}$	$\underline{\mathbf{r}}$	$\underline{\mathbf{k}}$	$\underline{\mathbf{v}}_{a,\ell}$	$\underline{m}_a$	$\underline{\mathbf{p}}_{a,\ell}$	$\underline{q}_a$	$\underline{\rho}$	$\underline{\mathbf{j}}$	$\underline{\mathbf{E}}$	$\underline{\mathbf{B}}$
=	$\omega_p t$	$\dfrac{\mathbf{r}}{\Delta}$	$\mathbf{k}\Delta$	$\dfrac{\mathbf{v}_{a,\ell}}{\omega_p\Delta}$	$\dfrac{m_a}{m_e}$	$\dfrac{\mathbf{p}_{a,\ell}}{m_a\omega_p\Delta}$	$\dfrac{q_a}{e}$	$\dfrac{\rho\Delta^3}{e}$	$\dfrac{\mathbf{j}\Delta^2}{e\omega_p}$	$\dfrac{e\mathbf{E}}{m_e{\omega_p}^2\Delta}$	$\dfrac{e\mathbf{B}}{m_e{\omega_p}^2\Delta}$

Table 1: Units used in UPIC-EMMA.

4 Units

Let us note the plasma electron frequency

$$\omega_p = \sqrt{\frac{4\pi n_0 e^2}{m_e}} \tag{29}$$

where

$$n_0 = \frac{N_e d_e}{N_x N_y N_z \Delta_x \Delta_y \Delta_z} = \frac{N_e d_e}{N_x N_y N_z \Delta^3} \frac{1}{\underline{\Delta}_x \underline{\Delta}_y \underline{\Delta}_z}. \tag{30}$$

Here, N_e and N_i are the total number of macro-electrons and macro-ions. d_e is the number of real electrons per macro electron. N_x, N_y and N_z and $\underline{\Delta}_x$, $\underline{\Delta}_y$ and $\underline{\Delta}_z$ are the number of spatial mesh points and their numerical space steps in the x, y and z-direction, respectively. The latter are normalized by a free parameter Δ. In UPIC-EMMA, all quantities are normalized according to **Table 1**. Let us also note the normalized spatial mesh :

$$\forall i \in [1..N_x],\ j \in [1..N_y],\ k \in [1..N_z],\ \underline{\mathbf{r}}_{i,j,k} = \begin{pmatrix} \underline{x}_i \\ \underline{y}_j \\ \underline{z}_k \end{pmatrix} = \begin{pmatrix} (i-1)\,\underline{\Delta}_x \\ (j-1)\,\underline{\Delta}_y \\ (k-1)\,\underline{\Delta}_z \end{pmatrix} \tag{31}$$

in the real space and

$$\forall p \in [1..N_x],\ q \in [1..N_y],\ r \in [1..N_z],\ \underline{\mathbf{k}}_{p,q,r} = \begin{pmatrix} \underline{k}_{x,p} \\ \underline{k}_{y,q} \\ \underline{k}_{z,r} \end{pmatrix} = 2\pi \begin{pmatrix} (p-1)\,/\underline{\Delta}_x \\ (q-1)\,/\underline{\Delta}_y \\ (r-1)\,/\underline{\Delta}_z \end{pmatrix} \tag{32}$$

in the Fourier space. The normalized charge and current density in the Fourier space become

$$\widehat{\underline{\rho}}\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) = \widehat{\underline{S}}^3_e[\underline{\mathbf{k}}_{p,q,r}]\widehat{\underline{\rho}}_e\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) + \widehat{\underline{S}}^3_i[\underline{\mathbf{k}}_{p,q,r}]\widehat{\underline{\rho}}_i\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) \tag{33}$$

and

$$\widehat{\underline{\mathbf{j}}}\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) = \widehat{\underline{S}}^3_e[\underline{\mathbf{k}}_{p,q,r}]\widehat{\widetilde{\underline{\mathbf{j}}}}_e\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) + \widehat{\underline{S}}^3_i[\underline{\mathbf{k}}_{p,q,r}]\widehat{\widetilde{\underline{\mathbf{j}}}}_i\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) \tag{34}$$

with $\forall a \in \{e,\, i\}$,

$$\widehat{\underline{S}}^3_a[\underline{\mathbf{k}}_{p,q,r}] = \exp\left(-\frac{{\underline{k}_{x,p}}^2{\underline{\lambda}_{a,x}}^2 + {\underline{k}_{y,q}}^2{\underline{\lambda}_{a,y}}^2 + {\underline{k}_{z,r}}^2{\underline{\lambda}_{a,z}}^2}{2}\right), \tag{35}$$

$$\widehat{\widetilde{\underline{\rho}}}_a\left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) = \frac{1}{N_x N_y N_z}\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} \widetilde{\underline{\rho}}_a\left(\underline{\mathbf{r}}_{i,j,n},\, \underline{t}_n\right)\exp\left[\iota\left(\underline{k}_{x,p}\underline{x}_i + \underline{k}_{y,q}\underline{y}_j + \underline{k}_{z,r}\underline{z}_k\right)\right] \tag{36}$$

and

$$\widehat{\widetilde{\underline{\mathbf{j}}}}_a \left(\underline{\mathbf{k}}_{p,q,r},\, \underline{t}_n\right) = \frac{1}{N_x N_y N_z} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} \widetilde{\underline{\mathbf{j}}}_a \left(\underline{\mathbf{r}}_{i,j,n},\, \underline{t}_n\right) \exp\left[\iota\left(\underline{k}_{x,p}\underline{x}_i + \underline{k}_{y,q}\underline{y}_j + \underline{k}_{z,r}\underline{z}_k\right)\right] \tag{37}$$

while the charge and current deposit read

$$\widetilde{\underline{\rho}}_a(\underline{\mathbf{r}}_{i,j,k},\, \underline{t}_n) = \sum_{\ell=1}^{N_a} \underline{q}_a \underline{W}^3_{a,\ell}\left[\underline{\mathbf{r}}_{i,j,k},\, \underline{t}_n\right] \tag{38}$$

and

$$\widetilde{\underline{\mathbf{j}}}_a(\underline{\mathbf{r}}_{i,j,k},\, \underline{t}_n) = \sum_{\ell=1}^{N_a} \underline{q}_a \underline{\mathbf{v}}_{a,\ell}(\underline{t}_n) \underline{W}^3_{a,\ell}\left[\underline{\mathbf{r}}_{i,j,k},\, \underline{t}_n\right] \tag{39}$$

with

$$\underline{\mathbf{v}}_{a,\ell}(\underline{t}_n) = \frac{\mathbf{v}_{a,\ell}(t_n)}{\omega_p \Delta} =, \frac{\underline{\mathbf{p}}_{a,\ell}(\underline{t}_n)}{\underline{m}_a \underline{c}\sqrt{1+\left(\dfrac{\underline{\mathbf{p}}_{a,\ell}(\underline{t}_n)}{\underline{m}_a \underline{c}}\right)^2}} \tag{40}$$

$$\underline{W}^3_{a,\ell}\left[\underline{\mathbf{r}}_{i,j,k},\, \underline{t}_n\right] = \underline{W}_{a,\ell,x}\left[\underline{x}_i,\, \underline{t}_n\right] \underline{W}_{a,\ell,y}\left[\underline{y}_j,\, \underline{t}_n\right] \underline{W}_{a,\ell,z}\left[\underline{z}_k,\, \underline{t}_n\right] \tag{41}$$

and

$$\forall \underline{\xi} \in \{\underline{x},\, \underline{y},\, \underline{z}\},\, \underline{W}_{a,\ell,\xi}\left[\underline{\xi},\, \underline{t}_n\right] = \max\left\{0,\, \frac{\underline{\Delta}_\xi - \left|\underline{\xi} - \underline{\xi}_{a,\ell}(\underline{t}_n)\right|}{\underline{\Delta}_\xi{}^2}\right\}. \tag{42}$$

The Maxwell solver become

$$\widehat{\underline{\mathbf{E}}}_L^{p,q,r,n} = -\frac{\iota \underline{\mathbf{k}}_{p,q,r}}{\underline{\mathbf{k}}_{p,q,r}{}^2}\, a_f\, \widehat{\underline{\rho}}^{p,q,r,n} \tag{43}$$

$$\widehat{\underline{\mathbf{j}}}_T^{p,q,r,n} = \widehat{\underline{\mathbf{j}}}^{p,q,r,n} - \frac{\underline{\mathbf{k}}_{p,q,r}}{\underline{\mathbf{k}}_{p,q,r}{}^2} \underline{\mathbf{k}}_{p,q,r} \cdot \widehat{\underline{\mathbf{j}}}^{p,q,r,n} \tag{44}$$

and

$$\left\{\begin{array}{lclcll}
\widehat{\underline{\mathbf{B}}}^{p,q,r,n+1/2} & = & \widehat{\underline{\mathbf{B}}}^{p,q,r,n} & - & \dfrac{\underline{\Delta}_t}{2} & \underline{c}\left(\iota \underline{\mathbf{k}}_{p,q,r}\right) \times \widehat{\underline{\mathbf{E}}}_T^{p,q,r,n} \\
 & & & & & \\
\widehat{\underline{\mathbf{E}}}_T^{p,q,r,n+1} & = & \widehat{\underline{\mathbf{E}}}_T^{p,q,r,n} & + & \underline{\Delta}_t & \underline{c}\left(\iota \underline{\mathbf{k}}_{p,q,r}\right) \times \widehat{\underline{\mathbf{B}}}^{p,q,r,n+1/2} \\
 & & & - & \underline{\Delta}_t & a_f\, \widehat{\underline{\mathbf{j}}}_T^{p,q,r,n+1/2} \\
\widehat{\underline{\mathbf{B}}}^{p,q,r,n+1} & = & \widehat{\underline{\mathbf{B}}}^{p,q,r,n+1/2} & - & \dfrac{\underline{\Delta}_t}{2} & \underline{c}\left(\iota \underline{\mathbf{k}}_{p,q,r}\right) \times \widehat{\underline{\mathbf{E}}}_T^{p,q,r,n+1}
\end{array}\right. \tag{45}$$

where two important parameters

$$a_f = \frac{1}{n_0 \Delta^3} = \frac{N_x N_y N_z}{N_e} \underline{\Delta}_x \underline{\Delta}_y \underline{\Delta}_z \text{ and } \underline{c} = \frac{c}{\omega_p \Delta} \tag{46}$$

have appeared in the equations. The electric and magnetic component of the force acting on the particle denoted by "a, ℓ" at time $\underline{t}_n$ become

$$\begin{array}{rcccll} \underline{\mathbf{E}}_s(\mathbf{r}^n_{a,\ell}, t_n) & = & (1-\alpha) & (1-\beta) & \left[(1-\gamma)\,\underline{\mathbf{E}}^{i_\ell,j_\ell,k_\ell,n} \right. & \left. +\ \gamma\,\underline{\mathbf{E}}^{i_\ell,j_\ell,k_\ell+1,n}\right] \\ & + & (1-\alpha) & \beta & \left[(1-\gamma)\,\underline{\mathbf{E}}^{i_\ell,j_\ell+1,k_\ell,n} \right. & \left. +\ \gamma\,\underline{\mathbf{E}}^{i_\ell,j_\ell+1,k_\ell+1,n}\right] \\ & + & \alpha & (1-\beta) & \left[(1-\gamma)\,\underline{\mathbf{E}}^{i_\ell+1,j_\ell,k_\ell,n} \right. & \left. +\ \gamma\,\underline{\mathbf{E}}^{i_\ell+1,j_\ell,k_\ell+1,n}\right] \\ & + & \alpha & \beta & \left[(1-\gamma)\,\underline{\mathbf{E}}^{i_\ell+1,j_\ell+1,k_\ell,n} \right. & \left. +\ \gamma\,\underline{\mathbf{E}}^{i_\ell+1,j_\ell+1,k_\ell+1,n}\right] \end{array} \tag{47}$$

with

$$\underline{\mathbf{E}}_s^{i,j,k,n} = \sum_{p=1}^{N_x}\sum_{q=1}^{N_y}\sum_{r=1}^{N_z} \widehat{\underline{\mathbf{E}}}\left(\underline{\mathbf{k}}_{p,q,r},\ \underline{t}_n\right) \widehat{\underline{S}}_a^3[\underline{\mathbf{k}}_{p,q,r}] \exp\left[-\iota\left(\underline{k}_{x,p}\underline{x}_i + \underline{k}_{y,q}\underline{y}_j + \underline{k}_{z,r}\underline{z}_k\right)\right] \tag{48}$$

and

$$\left\{\begin{array}{l} \alpha = \dfrac{\underline{x}_{a,\ell}(\underline{t}_n) - \underline{x}_{i_\ell}}{\underline{\Delta}_x} \\ \beta = \dfrac{\underline{y}_{a,\ell}(\underline{t}_n) - \underline{y}_{j_\ell}}{\underline{\Delta}_y} \\ \gamma = \dfrac{\underline{z}_{a,\ell}(\underline{t}_n) - \underline{z}_{k_\ell}}{\underline{\Delta}_z} \end{array}\right. \quad \text{and} \quad \left\{\begin{array}{l} i_\ell = 1 + \mathbb{E}\left\{\dfrac{\underline{x}_{a,\ell}(\underline{t}_n)}{\underline{\Delta}_x}\right\} \\ j_\ell = 1 + \mathbb{E}\left\{\dfrac{\underline{y}_{a,\ell}(\underline{t}_n)}{\underline{\Delta}_y}\right\} \\ k_\ell = 1 + \mathbb{E}\left\{\dfrac{\underline{z}_{a,\ell}(\underline{t}_n)}{\underline{\Delta}_z}\right\} \end{array}\right.$$

(idem for $\underline{\mathbf{B}}_s(\underline{\mathbf{r}}^n_{a,\ell}, \underline{t}_n)$). Finally, the macro-particles pusher becomes

1.
$$\underline{\mathbf{p}}^-_{a,\ell} = \underline{\mathbf{p}}^{n-1/2}_{a,\ell} + \underline{q}_a \underline{\mathbf{E}}_s(\underline{\mathbf{r}}^n_{a,\ell}, \underline{t}_n)\underline{\Delta}_t/2$$

2.
$$\left\{\begin{array}{rcl} \underline{\mathbf{p}}^*_{a,\ell} & = & \underline{\mathbf{p}}^-_{a,\ell} + \underline{\mathbf{p}}^-_{a,\ell} \times \underline{\boldsymbol{\omega}}^n_{c,a}\underline{\Delta}_t/2 \\ \underline{\mathbf{p}}^+_{a,\ell} & = & \underline{\mathbf{p}}^*_{a,\ell} + \underline{\mathbf{p}}^*_{a,\ell} \times \dfrac{\underline{\boldsymbol{\omega}}^n_{c,a}\underline{\Delta}_t}{1 + \left(\underline{\boldsymbol{\omega}}^n_{c,a}\underline{\Delta}_t/2\right)^2} \end{array}\right. \quad \text{with } \underline{\boldsymbol{\omega}}^n_{c,a} = \frac{\underline{q}_a \underline{\mathbf{B}}_s(\mathbf{r}^n_{a,\ell}, t_n)}{\underline{m}_a\underline{c}\sqrt{1 + \left(\dfrac{\underline{\mathbf{p}}^-_{a,\ell}}{\underline{m}_a\underline{c}}\right)^2}}.$$

3.
$$\underline{\mathbf{p}}^{n+1/2}_{a,\ell} = \underline{\mathbf{p}}^+_{a,\ell} + \underline{q}_a \underline{\mathbf{E}}_s(\underline{\mathbf{r}}^n_{a,\ell}, \underline{t}_n)\underline{\Delta}_t/2.$$

and

$$\underline{\mathbf{r}}^{n+1}_{a,\ell} = \underline{\mathbf{r}}^n_{a,\ell} + \frac{\underline{\mathbf{p}}^{n+1/2}_{a,\ell}}{\underline{m}_a\sqrt{1 + \left(\dfrac{\underline{\mathbf{p}}^{n+1/2}_{a,\ell}}{\underline{m}_a\underline{c}}\right)^2}}\underline{\Delta}_t. \tag{49}$$

References

[Dawson, 1983] Dawson, J. M. (1983). Particle simulation of plasmas. *Rev. Mod. Phys.*, 55(2).

[Decyk, 1995] Decyk, V. K. (1995). *Comput. Phys. Commun.*, 97:87–94.

[Decyk, 2007] Decyk, V. K. (2007). *Comput. Phys. Commun.*, 177(95).

[Yu et al., 2014] Yu, P., Xu, X., Decyk, V. K., An, W., Vieira, J., Tsung, F. S., Fonseca, R. A., and Silva, L. O. (2014). Modelling of laser wakefield acceleration in lorentz boosted frame using em-pic code with spectral solver. *Journal of Computational Physics*.