Charge preserving high order PIC schemes

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Abstract

In this paper we present some new results on our investigation aimed at extending to higher order (HOPIC) the classical PIC framework. After reviewing the basic resolution properties of the Runge-Kutta time integrator, coupled to fourth (sixth) order compact schemes for space derivatives in the Maxwell equations, we focus on the problem of extending charge conservation schemes to a general HOPIC framework. This issue represents the main contribution of the present work. We consider then a few numerical examples of 1D laser-plasma interaction in the under-dense and over-dense regimes relevant for ions acceleration, to test grid convergence and to compare HOPIC results with standard PIC schemes (LOPIC).

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Introduction

The classical PIC numerical modeling (Birdsall and Langdon\textsuperscript{[1]}, Eastwood and Hockney \textsuperscript{[2]}) is a particle-grid method to solve the Vlasov-Maxwell system, whereby the Vlasov fluid in phase space is sampled by a finite number of Lagrangian (macro) particles while Maxwell equations are discretized on a finite-dimensional grid and integrated by finite difference schemes. In this hybrid approach, grid defined fields are related to particles positions by \textit{k}--th order splines of compact support. In a PIC framework, the following computational parameters controlling accuracy can be identified:

1. the space-time resolution measured by the number of grid points per wavelength \( n_{l} = \lambda / \Delta x \), where \( \lambda \) represents the relevant physical space scale to be resolved and \( \Delta x \) is the typical grid size. In relativistic laser-plasma interactions, where \( c \) is the dominant propagation speed, the related time resolution is given by the time step size \( \Delta t = \sigma \Delta x / c \), where \( \sigma \approx 1 \) is the Courant number;

2. the average number of representative numerical particles per cell \( N_{\text{cell}} \). This is a crucial parameter controlling the resolution properties of the charge and current density fields entering as a source terms in the Maxwell equations. In a relativistic laser-plasma interaction, even for large \( N_{\text{cell}} \) numbers, regions of low plasma density and high energy tails in the particle distributions soon form, with a resulting undersampling in terms of numerical particles.

3. the form and order \( k \) of the shape functions used to assign electromagnetic fields at each particle position and to reconstruct charge and current density fields using point-particles. Increasing the spline order helps in reducing statistical noise and aliasing, but too high spline smoothing may produce unphysical effects in regions where the particles number is too low. To date, by taking also into account cost effective implementations, most running PIC codes use routinely quadratic B-splines.

In relevant non-linear problems where analytical solutions are not available, it is possible to check accuracy of a
PIC scheme only by exploiting numerical convergence in the space of these control parameters. This practice is widely pursued in other computational areas, like fluid-dynamics and electro-magnetism, but is rather unusual in the PIC community. Only recently ([3]), an accurate numerical investigation using a standard second-order PIC code has been presented, addressing in particular the numerical heating problem. This work provides extensive numerical evidence that by increasing the indicated control parameters, numerical heating is reduced but convergence is very slow. This implies very demanding computational resources to assure reliable numerical results in multidimensional problems.

To improve on accuracy and, hopefully, to achieve also a faster numerical convergence, our group has developed and tested high order integration schemes for particles and fields equations (HOPIC). In this first part of our investigation, only the space-time resolution parameter, item (1), is of concern, while other building-blocks of a PIC modeling, like spline weighting and interpolation, are left untouched by now.

Consolidated results of this activity have been encoded in the ALaDyn package (Benedetti et al, 2008 [10, 11], Sgattoni et al, 2009 [12]). ALaDyn also includes some other nontrivial features that are not going to be discussed in this paper: a stretched computational grid, hierarchical particles sampling, high order filters and the possibility to run simulation in a boosted Lorentz frame.

In the following, we summarize the main computational steps entering a HOPIC code. To complete our study, we extend the charge preserving algorithms, first designed for LOPIC codes ([9]) to more general numerical modeling. Finally, as preliminary results of a more extended investigation on grid convergence, we apply and compare both LOPIC and HOPIC schemes to a few 1D non-trivial test problems.

1. Numerical integration of Vlasov-Maxwell system

1.1. Fourth-order Runge-Kutta time integration

The non linear system evolving in time particles and fields in a relativistic PIC method has the form:

\[ \frac{du}{dt} = F(u,t) \]  

which can be integrated to order \( K \) approximation by an explicit \( s \)-stage Runge-Kutta scheme. Numerical experiences point out that only schemes with \( K \geq 4 \) may work as a viable alternative to the classical second-order dissipation-free leap-frog integrator. In ALaDyn code we have implemented the classical fourth-order \( RK4 \) scheme and fourth-order, \( s \) stages \( RK4(s) \) schemes proposed by Calvo et al.[4], which are members of a wide class of low-storage, low-dissipation (LSD) Runge-Kutta integrators. The \( RK4 \) scheme advances Eq. (1) from time level \( t^n \) to time level \( t^{n+1} = t^n + \Delta t \) by three first order substeps:

\[ u^{i+1} = u^0 + a_i \Delta t F^i, \quad i = 0, 1, 2 \]  

where \( u^0 = u^e \) and \( F^i \equiv F(u^i, t^i) \), followed by a final step

\[ u^{n+1} = u^0 + \Delta t \tilde{F}, \quad \tilde{F} = \sum_{i=0}^{3} b_i F^i, \]  

with coefficients \( a_i = (1/2, 1/2, 1) \) and \( b_s = (1/6, 1/3, 1/3, 1/6) \). This scheme is faster than other equivalent integrators, but requires a \((3N)\) storage of the \((u^e, u^0, \tilde{F})\) arrays, each of dimension \( N \).

A typical LDS \( RK4(s) \) scheme is given by a sequence of \( s \) sub-steps:

\[ u' = u^{i-1} + b_i \Delta t F(\tilde{u}^{i-1}) \]  

\[ \tilde{u}' = u' + c_i \Delta t F(\tilde{u}^{i-1}) \]  

for \( i = 1, 2, ..., s \), using the auxiliary array \( \tilde{u} \), satisfying \( \tilde{u}_0 = u^0 = u^{(0)} \) and \( \tilde{u}' = u^{(n+1)} \). It requires then a \((2N)\) storage of the \((u, \tilde{u})\) arrays but at least \( s = 5 \) integration sub-steps are required to achieve fourth-order.

1.2. Space derivatives in the Maxwell equation

Compact FD schemes for space differentiation (Lele, 1992,[5]), coupled to a fourth-order Runge-Kutta scheme for time integration assure highly accurate numerical approximations for Maxwell equations, allowing to keep phase errors, dissipative damping and anisotropy in wave propagation at low levels using relatively coarse grid cell size.

In a one dimensional grid with uniform spacing \( h \) and node points \( x_j = jh, \ j = 0, 1, N-1 \), a compact first derivative \( u'(x_j) \) of a \( u(x_{j+1/2}) \) function with staggered collocation is expressed by

\[ u' = \hat{D}_1[u] = [\hat{P}^{-1} \hat{C} \Delta u] \]
where \( \hat{P} = [\alpha, 1, \alpha] \) and \( \hat{C} = [b, (a + b), b] \) are tridiagonal matrix with coefficients \( a = 3(3-2\alpha)/8 \), \( b = (22\alpha-1)/24 \) and \( [\Delta u]_j = [u_{j+1/2} - u_{j-1/2}]/h \) is the two-point second order explicit derivative.

This one-parameter (\( \alpha \)) family of compact schemes gives for \( \alpha = 9/62 \), a sixth-order (\( SC_6 \)) scheme and for \( \alpha = 1/22 \), \( b = 0 \) a fourth-order (\( SC_4 \)) scheme. Within the same formula, the \( \alpha = 0 \) case reproduces the fourth-order explicit (\( SE_4 \)) scheme and \( \alpha = b = 0, a = 1 \) recovers the classical second order derivative (\( SE_2 \)).

### 1.3. Dispersion relations for the numerical Maxwell equation

By expressing \( u(x) \) in terms of Fourier modes \( e^{ikx} \) where \( k \) is the discretized wavenumber, the derivative \( \hat{D} \) matrix has purely immaginary eigenvalues \( iZ(w)/h \) where \( w = k\sigma \) is the adimensional wavenumber and \( Z(w) \) represents the numerical or modified wavenumber, given by

\[
Z(w) = 2a \sin w/2 + b \sin 3w/2 \quad 1 + 2\alpha \cos(w)
\]

(7)
to be compared with \( Z(w) = w \) for exact (spectral) differentiation.

To evaluate the resolution properties of different schemes, we consider a one-dimensional Maxwell equation for fields (\( E, B \)) propagating with unit phase speed. In semi-discrete form, it is expressed by the wave system

\[
\partial_t E(x, t) + \hat{D} B(x, t) = 0, \quad \partial_t B(x, t) + \hat{D} E(x, t) = 0
\]

giving a dispersion relation \( \omega(k) = \pm Z(w)/h \) with wave speed \( v_{ph} = \omega/k = \pm Z(w)/w \). In the continuous time limit, the difference \( R(w) = Z(w)/w - 1 \), as a function of the wavenumber \( w \) or of the points per wavelength \( ppw = 2\pi/w \), provides then a measure of the accuracy of the derivative scheme.

In the fully discretized case, using a fourth-order Runge-Kutta (RK4) scheme for time integration with time step \( \Delta t = \sigma h \), the resulting dispersion relation for the complex frequency \( \Omega = \omega + i\gamma \), takes the form:

\[
e^{i\Omega t} = |G| \Rightarrow G_R^2 + G_I^2 = \frac{k}{\sigma w} \sin^{-1} \frac{G_I}{|G|}
\]

(9)
where \( G(w) = [G_R, G_I] \) is the complex amplification factor, with

\[
G_R(w) = 1 - \frac{1}{2}(\sigma Z(w))^2 + \frac{1}{24}(\sigma Z(w))^4 \tag{10}
\]

\[
G_I(w) = \sigma Z(w) - \frac{1}{6}(\sigma Z(w))^3. \tag{11}
\]

The stability condition \(|G| \leq 1\) entails an upper limit for the Courant number \( \sigma = 1 \) for compact schemes (SC4) and (SC6).

In the classical PIC codes, where the leap-frog scheme in time is coupled to the staggered second order space derivative (SE2), one has a dispersion relation for the real frequency component \((\gamma = 0)\), given by

\[
\sin(\omega \Delta t/2) = \frac{\sigma}{2} Z(w), \quad \omega(k) = \frac{2k}{\sigma w} \sin^{-1} \sigma Z(w)/2. \tag{12}
\]

with a local stability conditions \( \sigma Z(w) < 2 \). In figure 1 the error in phase speed during one time step \( \Delta t = \sigma h_z \) is plotted as a function of the space-time resolution for different schemes. By comparing high order schemes to the classical second order \( LPf/2 \) scheme, it is evident that, to keep phase error below a tolerance level, say \( \epsilon < 10^{-3} \), standard PIC approximations require rather small grid cells, \( \text{ppw} > 35 \), while \( 8-10 \) grid points per wavelength are sufficient in HOPIC schemes. On the same range of values, the HOPIC dissipation rate per time step turns out to be sufficiently small, but to preserve the field energy over long time integration one needs higher resolution.

The leap-frog integrator coupled to a higher order space derivative fails to reduce the dispersive error, and even produces superluminal \( v_{ph} > 1 \) phase speeds. However, it is still possible to reduce the leap-frog dispersive error by taking advantage of that, for Courant number \( \sigma = 1 \), the truncation error of the \( SE2 \) scheme cancels the \( O(\Delta t)^3 \) truncation error of the time integration, and the composite \( (LPf/2 + ES2) \) scheme achieves fifth-order accuracy.

We propose then an optimized four-point derivative scheme \( OS E2 \), having a modified wavenumber

\[
Z^{opt}(w) = 2[a \sin w/2 + b \sin 3w/2] \tag{13}
\]

with coefficients \( a = 1 + (1 - \sigma^2)/8, \quad b = (1 - a)/3 \), reducing to the \( a = 1, b = 0 \) \( SE2 \) case for \( \sigma = 1 \). By construction, even if \( OS E2 \) is formally second order, the composite \( LPf + OS E2 \) scheme shares high order accuracy for any Courant number.

This optimal behaviour can be documented in 1D test problems where analytical solutions are available. To that purpose, we consider the free propagation of a linear polarized laser \((E_x, B_y)\) field generated by the vector potential

\[
A_z(z,t) = a_0 \cos^2[\pi(z - z_f - ct)/l_z] \cos[2\pi(z - ct)/\lambda] \tag{14}
\]

with a \( \cos^2(\beta) \) profile centered at \( z = z_f \) at the initial time and having compact support in the \(-\pi/2 \leq \beta \leq \pi/2\) range of its argument.

We set here \( \lambda = 1 \mu m, a_0 = 4 \) and a pulse length \( l_z = 40 \mu m \). The numerical solution evolved up to some time \( T \) is then compared with the exact solution at \( t = T \), as documented in figure 2 where the maxima of the pointwise numerical errors for different schemes and for different grid resolutions are reported. It is evident that both the \((RK - SC)\) and the optimized leap-frog schemes give the expected \( O(\Delta t)^3 \) scaling of the accumulated numerical error. Moreover, the optimized scheme shows even better resolution properties than the \((RK - SC)\) integrator, mainly because the leap-frog integrator entails no dissipative errors.

In multi-D cases, compact schemes, having spectral-like behaviors along each coordinate direction \( Z(w_s) = w_s + O(w_s)^3 \) \( s = x, y, z \) give also accurate isotropy properties of the numerical Laplacian operator \( \hat{\nabla} \cdot \hat{\nabla} \) with modified wavenumber \( Z^2 = \sum_s Z_s^2(w_s) \).

By contrast, the low-order \( (LPf2 + SE2) \) scheme has a dispersion relation for a \( 2D \) propagation of the form (here \( h_x = h_y = h \))

\[
v_{ph} = \frac{2}{\sigma w} \sin^{-1}[\sigma \sqrt{Z^2(w_x) + Z^2(w_y)}] \tag{15}
\]

where \( w_s = w \cos \theta, w_y = w \sin \theta \). The dominant \( O(w_s^3 + w_y^3) \) truncation error of the numerical Laplacian is then strongly dependent on the polar angle with respect to the propagation direction \( \theta = \tan^{-1} w_y/w_x \). This is documented in figure 3 where the error in phase speed at representative polar angles are plotted and compared.

The favourable properties of the optimized leap-frog met in 1D propagation do not extend directly to the multi-dimensional case. However, the optimisation procedure
Figure 3: The error in phase speed in the 2D wave equation as a function of \(ppw = 2\pi/|w|\) parameter, for different polar angles \(\theta = \tan^{-1}(w_r/w_s)\). Upper- (RK4 + SC4) scheme; Middle- (LPf2 + SE2) scheme; Lower- (LPf2 + OS E2) scheme.

can still provide some help to reduce the anisotropy of the numerical Laplacian in a \((Lp f - SE2)\) scheme. This is shown in the lowest panel of the same figure 3, documenting a 2D dispersion relation obtained by a proper combination of the optimized \(Z^{opt}(w_s)\) scheme along the propagation direction with a standard \(Z(w_s)\) of the \((SE2)\) scheme in the perpendicular \(y\) direction.

1.4. Numerical accuracy in test particles motion

The high order Runge-Kutta integration provides higher accuracy and the expected \(O(\Delta t)^4\) scaling of the numerical errors also in the relativistic equations of motion for Lagrangian particles in a prescribed \((E, B)\) field ([12]), as long as particle orbits and the related invariants depend only on the time integration scheme.

A more challenging problem arises when the fully self-consistent PIC modeling is considered, using splines of compact support for field assignment and for charge and current density reconstruction on a grid. In fact, well known pathologies of particle-grid coupling, like numerical heating and aliasing (not considered in the present investigation), are expected to persist even in a HOPIC methodology.

2. Implementing charge conservation in HOPIC codes

2.1. Enforcing the continuity equation is a multi-step scheme

In a multistep Runge-Kutta integration, the discretized Ampere law advancing the electric field in a time step \(\Delta t\), in adimensional form is expressed by

\[
\mathbf{E}^{n+1} = \mathbf{E}^n + \Delta t \sum_b \mathbf{b}_b [\tilde{\mathbf{D}} \times \mathbf{B}^b - \tilde{\omega}_p^2 \mathbf{J}^b] \tag{16}
\]

where \(\tilde{\mathbf{D}}\) denotes the numerical space derivative and \(\tilde{\omega}_p\) is the adimensional electron plasma frequency. This equation embraces the correct time evolution of the electrostatic \(\mathbf{E}\) component coming from the incremental Poisson equation:

\[
\tilde{\mathbf{D}} \cdot \mathbf{E}^{n+1} = \tilde{\mathbf{D}} \cdot \mathbf{E}^n + \tilde{\omega}_p^2 \rho^{n+1} - \rho^n \tag{17}
\]

as long as the vector identity \(\tilde{\mathbf{D}} \cdot [\tilde{\mathbf{D}} \times \mathbf{B}] = 0\) and the discretized continuity equation

\[
[\rho^{n+1} - \rho^n] + \Delta t \sum_k b_k \tilde{\mathbf{D}} \cdot \mathbf{J}^k = 0 \tag{18}
\]
are exactly fulfilled to within machine accuracy. For centered (explicit or compact) numerical derivatives the first condition is always satisfied. In a particle-grid modeling, where the density field \( \rho (x,t) \) is reconstructed from Lagrangian particles positions \( x_p(t) \), it is possible to enforce the continuity only by using the same equation as a constraint on the definition of the current density field \( \mathbf{J}(x,t) \). The same argument applies, of course, in a one-step leap-frog scheme where:

\[
[\rho^{t+1} - \rho^t] + \Delta t \mathbf{D} \cdot \mathbf{J}^{t+1/2} = 0. 
\]

In fact, in a PIC modeling where the current and density fields are reconstructed as independent variables on a finite-dimensional grid \( x \) using the particles coordinates \( (x_p, v_p) \)

\[
\rho(x, t) = \sum_p \tilde{S}[x - x_p(t)], \quad \mathbf{J}(x, t) = \sum_p v_p(t) \tilde{S}[x - x_p(t)]
\]

(here expressed in the shortland notation where \( \tilde{S}(\cdot) \) denotes tensor product of one-dimensional splines), the discretized continuity equation is never satisfied, even for a 1D grid and for a one-particle system. Moreover, the resulting numerical error, being of \( O(1) \) size, cannot be reduced by increasing the space-time resolution or by changing the integration scheme.

In a number of papers ([1], [6],[7],[8], to cite a few), techniques have been designed to enforce the numerical continuity equation on a grid and for a one-particle system. Moreover, the resulting numerical error, being of \( O(1) \) size, cannot be reduced by increasing the space-time resolution or by changing the integration scheme.

2.2. Enforcing the continuity equation on a grid

To complete our charge preserving design for HOPIC, the main problem left over is then how to extract in a unique way a vector field \( \mathbf{J}(x,t) \) for assigned \( \mathbf{D} \cdot \mathbf{J} = \mathcal{S}(x,t) \).

In a one-dimensional grid \( x_j = jh_x, \ j = 0, 1, \ldots, N_x + 1 \) with particles confined on a bounded domain \( x_1 \leq x \leq x_{N_x} \), charge assignments by a quadratic spline give non zero density variations \( [\Delta \rho]_j = [\rho^t - \rho^0]_j \) in the \( 0 \leq j \leq N_x + 1 \) grid range, with conservation of the total charge for each particle species \( \sum_j [\Delta \rho]_j = 0 \). By setting \( a_k \Delta t \mathbf{J}_k \rightarrow J_s \) for a generic substep, the current component \( J_s \) can be reconstructed by solving the finite differences equation

\[
[\mathcal{D}, J_s]_j = -[\Delta \rho]_j 
\]

where for a compact or explicit scheme the numerical derivative is expressed by \( \mathcal{D}_s J_s \equiv \hat{\mathcal{P}}^{-1} \hat{\mathcal{C}} [\Delta \rho]_j \). By inversion of this matrix equation on a staggered grid, one has then

\[
[J_s]_{j+1/2} - [J_s]_{j-1/2} = \hat{h}_s [\hat{\mathcal{C}}^{-1} \hat{\mathcal{P}} \Delta \rho]_j \equiv S_j 
\]

or

\[
[J_s]_{j+1/2} = \sum_{j=0}^N S_j, \quad j = 0, 1, \ldots, N_x + 1
\]

since, for particles confined on a bounded domain, \( [J_s]_{0-1/2} = 0 \) is a consistent boundary condition.
In a multidimensional case, the reconstruction of the \( \mathbf{J} \) vector components proceeds following two main steps: (i) first, the density increment due to the particles move from old \((x^0, y^0, z^0)\) to new \((x^1, y^1, z^1)\) positions, is decomposed using the algebraic identity ([9]):

\[
\Delta \rho = [\Delta \rho]_x + [\Delta \rho]_y + [\Delta \rho]_z
\]

(27)

where each term \([\Delta \rho]_c\) contains only density differences coming from the particles motion along the corresponding \(c = (x, y, z)\) coordinate axis. By construction, one has

\[
[\Delta \rho]_x = \frac{1}{3} [\Delta_1 \rho]_x + \frac{1}{6} [\Delta_2 \rho]_x
\]

(28)

where, in the shorthand notation \(\rho_{x,p,q} = \rho(x^p, y^q, z^r)\),

\[
[\Delta_1 \rho]_x = [\rho_{1,1,0} - \rho_{1,0,0}] + [\rho_{1,0,0} - \rho_{0,0,0}]
\]

(29)

and

\[
[\Delta_2 \rho]_x = [\rho_{1,0,1} - \rho_{0,1,0} + \rho_{0,1,0} - \rho_{0,0,1}].
\]

(30)

This composition rule extends then under the \(x \to y \to z\) cycling to compute \([\Delta \rho]_y\) and \([\Delta \rho]_z\), variations, respectively. (ii) For assigned density increments \([\Delta \rho]_c\), the current density components \([J_c]_{x,y,z}\) are then defined as solutions of three independent one-dimensional difference equations on a 3D grid \(x_c = \{x_j, y_k, z_l\}\)

\[
\tilde{D}_c J_c = -h_c [\Delta \rho]_c, \quad c = x, y, z.
\]

(31)

In the particular case of a leap-frog scheme, with space differentiation given by the \(S E 2\) scheme \((\tilde{P} = \tilde{C} = \hat{I})\), this extended procedure recovers the Esirkepov[9] reconstruction, the only difference being that here the charge and current densities are related directly as grid defined fields, independently of the adopted integration scheme and of the shape functions used in the charge density weighting.

There are no ‘first-principle’ general reasons to sustain this method of enforcing the continuity equation on a grid. The ansatz expressed in the Eq.(31) can be justified only by consistency arguments: in fact, in the continuous space-time limit \(h \to 0, \Delta t \to 0\), the \(\mathbf{J}(\mathbf{x}_c, t)\) solution of Eq. (31) recovers the native definition based on the particles velocity of the Eq.(20).

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2.3. Documenting charge conservation

To document charge conservation of the proposed scheme, we have considered a 2D problem where a laser pulse with intensity parameter \(a_0 = 4\), focal spot size \(w = 5\mu m\) and pulse duration \(\tau = 50\, fs\) interacts with an electron-proton plasma at subcritical density \(n = n_e/100\), producing strongly non-linear plasma waves. Charge conservation can be diagnosed directly by plotting the residual error in the Poisson equation \(R = \tilde{D} \cdot \mathbf{E} - \omega_{p}\rho\). The figure 4 shows the distribution of residual errors \(R(\zeta, s)\) is accumulated after a sufficiently long integration time. HOPIC and LOPIC give equivalent results in this kind of numerical tests, of course, since the residual \(R\) is just a measure of the zero-machine accuracy of the enforced continuity equation.

3. Testing grid convergence in 1D laser-plasma interaction

In physical regimes where wave propagation (laser fields and plasma waves) are the dominant processes, HOPIC provides a significant advance in terms of accuracy and then of efficiency with respect to the classical PIC schemes. We illustrate this aspect by considering plasma waves in a Laser Wakefield Plasma Acceleration (LWFA) configuration.

In the physical regimes relevant to ions acceleration, when
Figure 5: The wake structure in \((z, P_z/mc)\) phase space at increasing space-time resolution \(ppw = 16, 24, 32, 40\), where \(ppw = \lambda/\Delta z\).

3.1. Non linear electron plasma waves in LWFA regime

We consider first a laser-pulse with initial condition expressed by the vector potential \(A_z(z, t=0)\) as in Eq. (14), with parameters: \(a_0 = 4\), \(\lambda = 1\mu m\) and \(\tau = 25 fs\), interacting with a plasma with initial density profile \(n(z) = n_0/\lambda z \leq \lambda\) and \(n(z) = n_0\) \(z > \lambda\), where \(\lambda = 50\mu m\) and \(n_0 = n_e/100\). We consider then the first wake structures in the particle phase space \((z, P_z/mc)\), as documented in the figure 5. In this problem the HOPIC faster rate of convergence is evident. LOPIC, even in the best resolved range, still shows a phase delay of the plasma waves peaks.

3.2. Protons acceleration in RPA regimes

We consider first a model for proton acceleration in a 1D RPA regime, using a laser pulse with circular polarization (CP). The \((E, B)\) fields initial distributions are generated by the vector potential components with a \(cos^2()\)
3.3. Proton acceleration in TNSA regimes

We now briefly present some results obtained studying the proton acceleration in the TNSA regime. Though the physics associated with this regime can be much richer than what is effectively included in the PIC code (collisions, ionization, etc.), it is still interesting to consider this problem and to study the results of these simulations. In this case we considered a linear polarized laser field of Eq.(14) with $a_0 = 20$, wavelength $\lambda = 1\mu m$ and pulse length $l_z = 20\mu m$ corresponding to a FWHM duration $\tau = 25f/s$, interacting with an electron-proton target with density $n = 10n_e$ and size $d = 0.5$. Within this choice, the reflectivity parameter is $\zeta = \pi(n/n_e)(d/\lambda) \approx 15.7 < a_0$. Diagnostic is provided by the time evolution of protons and electrons energy maxima, as shown in figure 8, and by the time evolution of the $E_z$ field maxima in figure 9. From our analysis it has been difficult to spot a definitive difference in the behaviours of low and high order schemes and to find some clear threshold for the resolution. Here LOPIC seems to assures a better convergence, for $r \geq 8$, while HOPIC shows a non monotonic behavior at increasing resolution.

Conclusions

In this paper we presented in detail the extentsions of the electromagnetic PIC framework to high order schemes using compact finite differences derivations and Runge-Kutta time integration. An extension of the charge preserving scheme of [9] to high order schemes has also been deeply described. The presented schemes have been
Figure 8: The time history of proton energy maxima (upper curves) and electrons energy maxima (lower curves) in the TNSA laser-target interaction, for different values of the resolution parameter $r = d_e/\Delta z$ in the range $6 \leq r \leq 16$: Upper panel- LOPIC scheme; Lower panel- HOPIC scheme.

Figure 9: The maximum in the electrostatic $E_z$ field as a function of time in the TNSA laser-target interaction, for different values of the resolution parameter $r = d_e/\Delta z$ in the range $6 \leq r \leq 16$. In the figures is also reported the mean electron energy (in Mev). Upper panel- LOPIC scheme; Lower panel- HOPIC scheme.

tested and compared in different regimes and the tests show how in most situations the HOPIC schemes give various advantages over the LOPIC, in term of resolution and numerical convergence, giving the possibility, for example, to run multi-dimensional simulations on relatively small machines maintaining an acceptable accuracy.

References


