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High-order integration schemes for Particle In Cell (PIC) method

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Summary. — The detailed numerical investigation of the highly nonlinear physics involved in the interaction of a laser-pulse with a plasma and/or an externally injected beam requires suitable simulation tools which are able to retain the basic features of the process without increasing too much the computational needs. In our group at the University of Bologna we developed an electromagnetic PIC code using high-order schemes (explicit/compact finite differences derivatives and a 4th-order Runge-Kutta) instead of the most used second-order accurate algorithm, this allows to reach higher accuracy with similar number of grid-points or to use coarser grid and relax the computer load without compromising the accuracy. Here we present some validation tests and comparisons for the different schemes.

PACS 52.38.kd – Laser-plasma acceleration of electrons and ions.
PACS 52.65.-y – Plasma simulation.
PACS 02.60.Jh – Numerical differentiation and integration.

1. – Introduction

Most existing PIC codes to study the interaction of ultra intense and short laser pulse with plasma are implemented on the basis of classical schemes [1, 2], where: i) time integration is discretized by second-order leap-frog schemes and space derivatives by the second-order finite difference on staggered mesh (Yee's module) [1, 2]; ii) shape functions for charge weighting and field interpolation are linear or quadratic B-splines, and iii) charge conservation is usually implemented by the Esirkepov procedure [3]. To improve this basic numerical framework on accuracy and efficiency, as needed by the challenging new physical phenomena arising in high-intensity laser-plasma interaction, the Bologna group started a new project aimed at developing a PIC code based on high-order integration schemes (HOPIC). Consolidated results of this numerical activity have been implemented and tested on the new code `ALaDyn` [4,5]. Main features of the `ALaDyn` code are i) a fourth-order Runge-Kutta (RK4) algorithms for time integration, ii) a high-order (up to eighth) compact/explicit finite differences scheme for space integration; iii) a stretched

computational grid in the transverse direction in order to ensure a high resolution where needed (usually around the propagation axis) together with substantially far boundaries; iv) a hierarchical numerical particles sampling that allow to put more particles in the "dynamically interesting" zones and, at the same time, decrease the particles in the outlying regions. In the PIC framework computational parameters controlling accuracy are given by: i) space-time resolution measured by the number of grid points which sample the smallest relevant spatial scale to be resolved ($n_\lambda = \lambda/\Delta x = \sigma\lambda/\Delta t$, where λ is the relevant spatial scale, Δx is the grid size, Δt is the related time step and σ is the Courant number); ii) the number of representative numerical particles per cell n_c and iii) the order of the shape functions. Numerical experiments using classical (second-order) PIC schemes show a very slow convergence to high-accuracy results by increasing the control parameters [6]. HOPIC are expected to allow: i) lower numerical errors, for fixed space-time resolution and the number of particle per cell (ppc); ii) faster convergence rate when increasing space-time resolution. In the following, we document on the improved accuracy of a HOPIC approach by considering 1D non-trivial test problems where some reference analytical solution is available.

2. – Numerical integration of Maxwell equations

Compact finite differences schemes for space differentiation [7], coupled to a RK4 scheme for time integration assure efficient and highly accurate numerical solution for the Maxwell equations. In a one-dimensional grid with uniform spacing h and node points $x_j = jh$, $j = 0, 1, N-1$, the compact first derivative $u'(x_j)$ of a $u(x_{j+1/2})$ function with staggered collocation is expressed by

$$u' \equiv \hat{D}[u] = \left[\hat{P}^{-1}\hat{C}\Delta u\right], \tag{1}$$

where $\hat{P} = [\alpha, 1, \alpha]$ and $\hat{C} = [b, (a+b), b]$ are tridiagonal matrix with coefficients $a = 3(3-2\alpha)/8$, and $b = (22\alpha-1)/24$ and $[\Delta u]_j = [u_{j+1/2} - u_{j-1/2}]/h$ is the two-point second-order explicit derivative. This one-parameter (α) family of compact schemes gives for $\alpha = 9/62$, a sixth-order scheme ($SC6$) and for $\alpha = 1/22$, $b = 0$ a fourth-order scheme ($SC4$). Using the same formula, the $\alpha = 0$ case reproduces the fourth-order explicit scheme ($SE4$). The classical second-order derivative ($SE2$) is here expressed by the limiting case $\alpha = b = 0$ and $a = 1$. By expressing $u(x)$ in terms of Fourier modes e^{ikx}, where k is the discretized wave number, the derivative $\hat{D}$ matrix has purely imaginary eigenvalues $iZ(w)/h$ where $w = kh$, and $Z(w)$ is the numerical or modified wave number, replacing the spectral (exact) ik numerical derivative. The one-dimensional wave equation in semi-discrete form reads $\partial_t u(x,t) + \hat{D}u(x,t) = 0$ gives a dispersion relation $\omega(k) = Z(w)/h$ and a numerical wave speed $v_{ph} = \omega/k = Z(w)/w$. The difference $R = Z(w)/w - 1$ provides then a measure of the resolution property of a derivative scheme. There are significant differences between the $SE2$ and high-order compact derivative (SC): to keep the phase error below some tolerance value, say $R \leq 10^{-4}$, a value of points per wavelength (PPW) larger than 40 is necessary for $SE2$, while a number of PPW in the range 10–12 is already sufficient for $SC4$ and $SC6$. In a fully discretized wave equation, 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

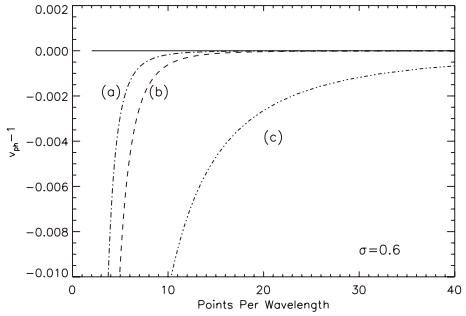

Fig. 1. – The error in phase speed in the 1D wave equation as a function of PPW parameter, using composite schemes: (a) $(RK4 + SC6)$, (b) $(RK4 + SC4)$, (c) $(LP2 + SE2)$.

$$e^{\gamma \Delta t} = |G| = \sqrt{G_R^2 + G_I^2}\,, \qquad \omega(k) = \frac{k}{\sigma w} \sin^{-1} \frac{G_I}{|G|}\,, \tag{2}$$

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

$$G_R(w) = 1 - \frac{1}{2}(\sigma Z(w))^2 + \frac{1}{24}(\sigma Z(w))^4, \qquad G_I(w) = \sigma Z(w) - \frac{1}{6}(\sigma Z(w))^3. \tag{3}$$

The stability condition $|G| \leq 1$ entails an upper limit for the Courant number $\sigma \simeq 1$ for compact schemes $SC4$ and $SC6$. The corresponding dispersion relation for a Leap-Frog scheme (LPF2) is given by $\omega(k) = \frac{2k}{\sigma w} \sin^{-1} \sigma Z(w)/2$ with local stability conditions $\sigma Z(w) < 2$, where now $Z(w)$ is the modified wave number of the $SE2$ derivative scheme. In fig. 1 we plot the phase speed of a 1D wave freely propagating *versus* the number of points per wavelength.

2˙1. *Multidimensional issues.* – In the multidimensional case, high-order compact schemes having spectral-like behaviors along each coordinate direction $Z_s(w) \approx w_s\, s = x, y, z$ give accurate isotropy properties of the numerical Laplacian operator

$$Z^2 = Z_x^2 + Z_y^2 + Z_z^2, \tag{4}$$

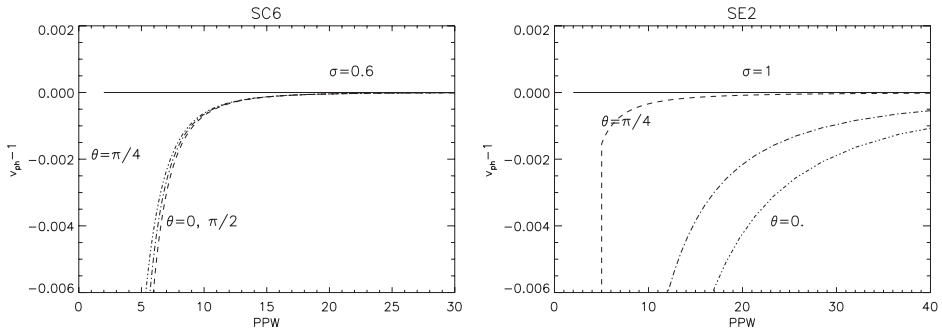

Fig. 2. – The error in phase speed in the 2D wave equation as a function of PPW, for different polar angle θ. Left: $(RK4 + SC6)$ scheme; right: $(LPF2 + SE2)$ scheme.

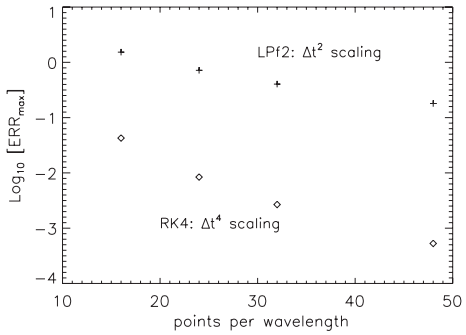

Fig. 3. – The maximum error in the numerical wave solution of the $(LPF2+SE2)$ and $(RK4+SC4)$ schemes, for different resolution $PPW = \lambda/\Delta z$ parameter. The corresponding reference scaling laws in the $\Delta t = \sigma \Delta z$ grid size are also reported.

while the reference $(LPF2+SE2)$ scheme has dispersion relation strongly dependent on the polar angle with respect to the propagation direction. This can be appreciated in fig. 2 where we have plotted the dispersion relations at different angles.

2˙2. *Testing 1D wave propagation.* – Together with the analytical consideration, we tested the different schemes in propagating a 1D wave packet. To measure the error in phase speed for different numerical schemes, we consider a linear polarized wave packet propagating along the z-axis, defined by the vector potential $A_x(z,t)$ with analytical form

$$(5)\quad A_x(z,t) = a_0 \cos(\omega_0(z-ct))\cos^4(\beta(z-ct)), \quad E_x(z,t) = B_y(z,t) = -\frac{1}{c}\partial_t A_x(z,t),$$

with $\omega_0 = \frac{2\pi}{\lambda}$, $\beta = \frac{\pi}{2\tau}$, where λ and τ are, respectively, the wavelength and the duration of the pulse. We compare then the cumulative error, by considering $\max_z |E_x^{\mathrm{num}}(z,t) - E_x(z,t)|$ after a fixed evolution time $T = 50\lambda/c$. Figure 3 shows the maximum error for different integration schemes, when increasing the resolution parameter PPW.

3. – Integration of particles motion

To test accuracy in the particle motion, we consider test particles in the freely propagating (E_x, B_y) fields given in eq. (5), with cold $p_x = p_z = 0$ initial conditions. In the reference analytical model, each particle preserves the two integrals of motion: $h_1(t) = p_x^2/2 - p_z$ $h_2(t) = P_x = A_x - p_x$ giving $h_k(t) = h_k(0) = 0$, $k = 1, 2$. In the discretized problem, the total numerical error results as a combination of: i) the error induced by the time integration scheme of the particle motion; ii) the numerical error induced by the space-time integration scheme wave equation; iii) the interpolation error to evaluate (A_x, E_x, B_y) fields at the particle position $z_i(t)$.

We compare the $LPF2 - SE2$ and the $RK4 - SC4$ space-time integrators. The comparison, see fig. 4, shows significantly different errors and very different scaling laws with respect to the resolution.

3˙1. *Fully self-consistent problem.* – When considering the fully self-consistent problem, the errors in the particle motions manifest themselves as an anomalous numerical

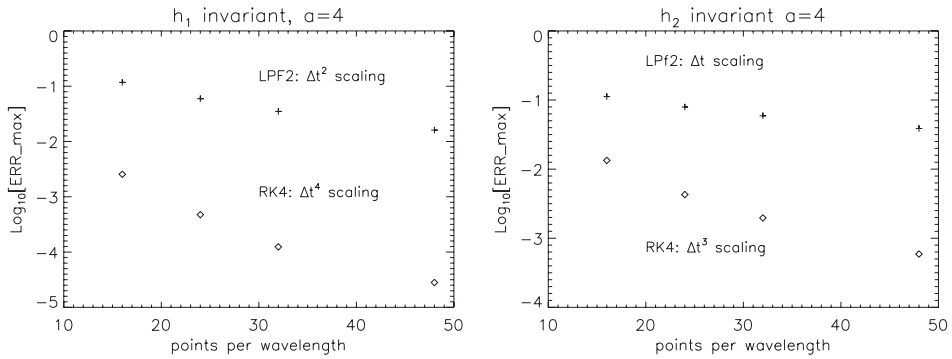

Fig. 4. – Scaling of the maximum error $|h(t) - h(0)|$ of the particle invariants of motion at increasing space-time resolution $\Delta t = \sigma \Delta z$ for $PPW = 16, 24, 32, 48$, $\sigma = 0.6$.

heating causing spurious injections of electrons in the plasma wave (numerical wave breaking), another consequence is the incorrect value of the plasma wavelength. Figure 5 shows the nonlinear generation of 1D plasma wave by an intense laser pulse, as can be seen, at low resolution both, high- and low-order algorithms show spurious wave breaking (the high spike in the phase space) that disappears increasing the resolution. While Runge-Kutta results show a very fast conversion rate, the Leap-Frog results show a much slower one and the need of a high number of grid points. This results in a reward for the increased number of operation per time step needed for the Runge-Kutta: the possibility to relax the resolution by a factor of roughly 2 in each dimension, *i.e.* a factor 8 in 2D and a factor 16 in 3D less operation (the time step is related to the spacial grid-step) gives a significant advance to higher-order scheme.

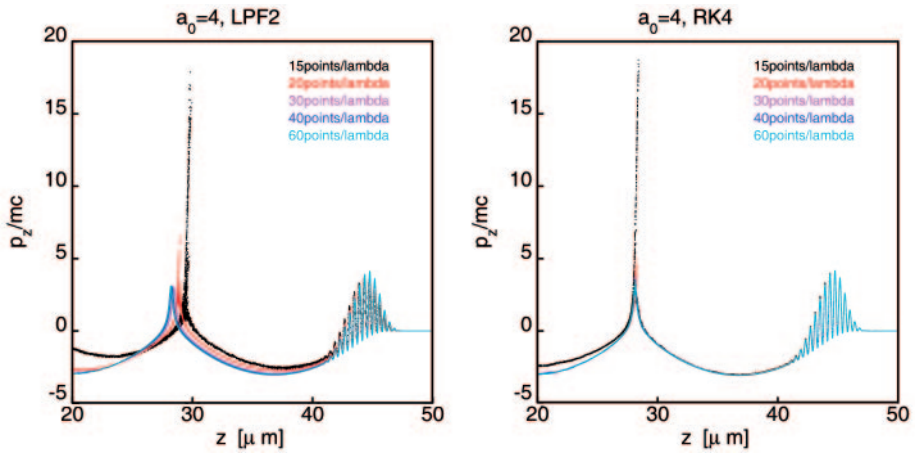

Fig. 5. – Longitudinal phase space of the electrons in the wake of a 1D wave packet. Left: leap-frog with different spatial/temporal resolution. Right: RK4+SE6. The figure shows the plasma wave generated in the wake of the pulse. For LPF at least 40 PPW are needed to get a correct phase space, while for RK4 20 PPW give already a good accuracy.

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