Overview of the presentation

- The benchmarking project of the ALaDyn code
- Comparing PIC and HoPIC for error estimates:
  - Maxwell equations
  - Particles motion
  - Fully selfconsistent system
- Charge conservation in HoPIC
The PIC numerical modeling of the Maxwell-Vlasov system

Maxwell equations:

\[
\begin{align*}
\partial_t \mathbf{B} &= -\nabla \times \mathbf{E} \\
\partial_t \mathbf{E} &= \nabla \times \mathbf{B} - \tilde{\omega}_p^2 \mathbf{J} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{E} &= \tilde{\omega}_p^2 \rho
\end{align*}
\]

use particles positions and velocities to construct current and charge density fields \((\rho, \mathbf{J})\):

\[
\partial_t \rho + \nabla \cdot \mathbf{J} = 0
\]

interpolate fields on particle positions \(i = 1, 2, \ldots, N_p\)

\[
\mathbf{E}_i \mathbf{B}_i \\
\downarrow
\]

Particle motion:

\[
\begin{align*}
\frac{d\mathbf{p}_i}{dt} &= \alpha [\mathbf{E}_i + \mathbf{v}_i \times \mathbf{B}_i] \\
\frac{d\mathbf{x}_i}{dt} &= \frac{\mathbf{p}_i}{\gamma_i} = \mathbf{v}_i \\
\gamma &= \sqrt{1 + \mathbf{p}^2}
\end{align*}
\]
The discretization procedures

The general PIC framework is based on a hybrid Lagrangian-Eulerian model:

- Eulerian variables are integrated in space-time using a \( N_g \) grid points;
- Particle motion is described by a set of \( N_p \) numerical particles;
- Discretized fields \((E, B)\) are interpolated on the particle positions using B-splines, local polynomials of compact support.
- The grid defined charge and currents densities are constructed using the same shape functions to collect particle positions on the system grid.
The classical PIC algorithms

Most existing codes are implemented on the basis of classical schemes (Birdsall and Langdon, Eastwood and Hockney):

- Time integration: the leap-frog scheme;
- Space derivatives: the second-order finite difference on staggered mesh (Yee’s module);
- Shape functions: linear or quadratic.

Charge conservation usually implemented by the Esirkepov procedure.

Much has been done for code optimization, parallelization and high level language formulation.

Only recently new high order code design has been proposed (Jacobs and Hesthaven, JCP, 2006) using DG on unstructured grids.
The **ALaDyn** project: a PIC code with high order schemes

The Bologna group started a new project for improving accuracy and efficiency (in the framework of the standard PIC):

- compact finite difference on structured cartesian grid
- high order time integration by Runge Kutta algorithm
- second or third order shape functions
- charge conservation by a proper extension of the Esirkepov procedure

Consolidated results have been implemented on the code ALaDyn and tested (Benedetti *et al* 2008)
I.1 - numerical schemes and features

**ALaDyn** = **A**cceleration by **L**aser and **D**ynamics of charged particles

- developed since January 2007
- fully self-consistent, relativistic EM-PIC code
- “virtual-lab”: laser pulse(s) + injected bunch(es) + plasma ⇒ defined by the user
- written in *C* (*F*95), parallelized with MPI, organized as a LIBRARY
- the (same) code works in 1D, 2D and 3D Cartesian geometry
- relevant features: high order schemes in space/time + moving window + stretched grid + boosted Lorentz frame + hierarchical/adaptive particle sampling
- devel. & maintain. @ Dep. of Phys. - UniBo for the INFN-CNR PlasmonX collaboration
- a version specially designed for benchmarking is also implemented using the classical 2nd order algorithms
Why high order schemes

In PIC framework computational parameters controlling accuracy are given by:

- space-time resolution measured by the number of grid point per wavelength $ppw = \frac{\lambda}{\Delta x}$ ($\lambda$ is the smallest physical space scale)
- the number of representative numerical particles per cell $ppc$
- the order of the shape functions

Numerical experiment using classical (second order) PIC codes show a very slow convergence to high accuracy results by increasing the control parameters.

High Order integration is expected to allow

- improved efficiency: an accuracy level of a 2nd order PIC using less grid points
- a gain factor $g$ (say $g = 2$) entails a reduction of the computational work a factor $g^{\text{dimension}+1}$ which already in 2D largely compensate the increased operation counts.
- grid convergence: high intensity laser plasma interactions pose new challenging accuracy needs.
- in most problems HoPIC show faster grid convergence rate
The numerical behaviours of an algorithm that integrates the Maxwell equations come from:

- space differentiation scheme
- time integration scheme
- the combination of the two

A well documented numerical experience in the contest of linear acoustics, electromagnetism and optics.
Compact schemes for space differentiation

In a one-dimensional grid with uniform spacing $h$ and node points $x_j = jh, \ j = 0, 1, N - 1$, the discretized first derivative $u'(x_j)$ of a $u(x_j)$ function

$$u' \equiv \hat{D}[u] = [\hat{P}^{-1}\hat{C}\Delta u]$$  \hspace{1cm} (1)

where $\hat{P} = [\alpha, 1, \alpha]$ and $\hat{C} = [b, (a + b), b]$ are tridiagonal matrix and $\Delta[u]$ is the two-point second order explicit derivative.

- For function $u_j = u(x_j)$ and first derivative $u'_j = u'(x_j)$ collocated at the node points $x_j$

  $$[\Delta u]_j = \frac{1}{2h}[u_{j+1} - u_{j-1}] \hspace{1cm} a = \frac{2}{3}(\alpha + 2), \hspace{0.5cm} b = \frac{1}{6}(4\alpha - 1).$$

  $\alpha = 1/3$ gives a sixth-order ($C6$) scheme, $\alpha = 1/4$ gives a forth-order ($C4$) scheme.

- For function $u_j = u(x_j)$ and first derivative $u'_j = u'(x_{j+1/2})$ collocated at staggered points

  $$[\Delta u]_i = \frac{1}{h}[u_{i+1/2} - u_{i-1/2}] \hspace{1cm} a = \frac{3}{8}(3 - 2\alpha), \hspace{0.5cm} b = \frac{1}{24}(22\alpha - 1).$$  \hspace{1cm} (2)

  $\alpha = 9/62, \Rightarrow$ gives a sixth-order ($SC6$) scheme. $\alpha = 1/22, \Rightarrow$ gives a fourth-order ($SC4$) scheme. $\alpha = 0, \Rightarrow$ gives a fourth-order explicit ($SE4$) scheme.

The classical second order derivative ($SE2$) is expressed by the limiting case $\alpha = b = 0$ and $a = 1$. 

High order schemes in PIC codes – p. 10
-1- Conservation:

\[ u' \equiv \hat{D}[u] = [\hat{P}^{-1} \hat{C} \Delta u] = \Delta \hat{u} \]

where \( \Delta \hat{u} \) is the numerical primitive of the \( u(x) \) function.

All the global and local conservation laws of the Maxwell equations are then exactly fulfilled as in FD framework.

-2- The inverse of the derivative operator \( \hat{A} = \hat{C}^{-1} \hat{P} \) provides a high order approximation of the cell average \([\hat{v}]_j\). In fact the cell average of the \( v(x) = u'(x) \) function is

\[
[\hat{v}]_j \equiv \frac{1}{h} \int_{x_{j-1/2}}^{x_{j+1/2}} v(x) = \frac{1}{h} [u_{j+1/2} - u_{j-1/2}] = [\Delta u]_j
\]

In the one-dimensional continuity equation:

\[
\partial_t \rho(x, t) = -\partial_x J(x, t) \quad \Rightarrow \quad \frac{d[\hat{A}\rho]_j}{dt} = -\frac{1}{h} [J_{j+1/2} - J_{j-1/2}]
\]
-3- **Spectral like resolution**: the eigenvalue problem of the derivative operator \( \hat{D} \equiv \hat{P}^{-1} \hat{C} \Delta \) provides resolution and stability properties of compact (CFD) schemes. By expressing \( u(x, t) \) in terms of Fourier modes \( e^{i k x_j - \omega(k)t} \) where \( k \) is the discretized wavenumber, the numerical dispersion relation of a 1D wave equation is \( \omega(k) = \frac{1}{h} Z(k) \) where \( Z(k) \) (modified wavenumber) is the purely imaginary eigenvalues of the \( \hat{D} \) matrix. The numerical phase speed, in the continuous time limit, is given by \( v_{ph} = \omega(k)/k = Z(w)/w \), where \( w = kh \). The difference \( R = v_{ph} - 1 \) provides then a measure of the accuracy of the derivative schemes.

The phase speed error for CFD and explicit FD schemes
Numerical time integration

We shall consider the classical forth order, four stages Runge-Kutta scheme (RK4), a forth order three stage symplectic Runge-Kutta (LPF4) and the second order leap frog (LPF2).

In a fourth-order time stepping from time level $t^n$ to time level $t^{n+1} = t^n + \Delta t$, with $\Delta t = \sigma h$ $\sigma$ being the Courant number.

The discretized one-dimensional wave equation in Fourier space takes the form:

$$E^{n+1} = G^R(w)E^n + iG^I(w)B^n, \quad B^{n+1} = G^R(w)B^n + iG^I(w)E^n$$

where $G(w) = [G^R, G^I]$ is the complex amplification factor of the fully discrete algorithm, with real and immaginary parts

$$G^R(w) = 1 - \frac{1}{2}(\sigma Z)^2 + \frac{1}{24}(\sigma Z)^4, \quad G^I(w) = \sigma Z - \frac{1}{6}(\sigma Z)^3.$$

In terms of the wave frequency

$$E^{n+1} = e^{(i\omega+\gamma)\Delta t} E^n, \quad B^{n+1} = e^{(i\omega+\gamma)\Delta t} B^n$$

the complex dispersion relation of the fully discretized system is

$$e^{\gamma \Delta t} = |G| = \sqrt{G^2_R + G^2_I}, \quad \omega(k) = \frac{k}{\sigma w} \sin^{-1} \frac{G_I}{|G|}.$$
The corresponding dispersion relation for a LPF2 scheme is

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

with local stability conditions

$$\sigma Z(w) < 2$$

Coupling a second order integrator with high order space differentiation yealds to superluminal numerical phase speed $v_{ph} > 1$
Isotropy properties in multi dimensional case

In multi dimensional cases, high order schemes having spectral-like behaviours along each direction $Z_x(w) \approx w_x$, $Z_y(w) \approx w_y$, $Z_z(w) \approx w_z$ give accurate isotropy properties of the numerical Laplacian operator.

$$Z^2 = Z_x^2 + Z_y^2 + Z_z^2$$

The reference LPF2 scheme has the dispersion relation strongly dependent on the polar angle $\theta = \tan^{-1}(w_y/w_x)$
Isotropy properties: RK4+SC4 RK4+SC6

The RK4 combined with high order CFD shows a very good isotropy.
The reference analytical model is a linear polarized wave packet:

\[ E_x(z, t) = B_y(z, t) = E_0 \cos(\omega(z - ct)) \cos^2(\beta(z - ct)) \]

\[ \omega = \frac{2\pi}{\lambda}, \quad \beta = \frac{\pi}{2\tau} \]
Error as pointwise difference for increasing space-time resolution.
\[ \Delta t = \sigma \Delta z = \sigma \lambda / n_p \text{ for } n_p = 16, 24, 32, 48, \sigma = 0.6. \]
- upper left: Leap-frog scheme
- upper right: RK4 scheme
- bottom left: Leap-frog 4
The corresponding reference scaling law is also plotted.
Efficient implementation of open boundary conditions

Stretched grid: **high accuracy in the centre** (sub-μm resolution in transv. plane) VS low accuracy in the borders (not interesting!)

\[ x_i \rightarrow \text{“physical” transv. coordinate} / \xi_i \rightarrow \text{“rescaled” transv. coordinate} \]

\[ x_i = \alpha_x \tan \xi_i, \quad \xi_i \text{ unif. distributed} \]

\[ \alpha_x \rightarrow \text{“stretching parameter”} \ (\alpha_x \rightarrow \infty \text{ unif. grid, } \alpha_x \rightarrow 0 \text{ super-stretched grid}) \]

⇒ Adopting a transverse stretched grid we (considerably) **reduce the number of grid points** allowing to **save memory** (keeping fixed the accuracy) compared to an uniform grid.

⇐

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Particles motion

- integration of test particles in freely propagating EM fields
- self consistent problems with source term in Maxwell equation given by collective particle motion
Analytical solution are available only for 1D problems.
Particles moving on freely propagating \((E_z, B_y)\) fields preserve the two integrals of motion:

\[
h_1 = \frac{p_x^2}{2} - p_z \quad h_2 = P_x = A_x - p_x
\]

We compare the \((LPf2 - SE2)\) the \((RK4 - SC4)\) space-time integrators.

Scaling of the max error \(|h(t) - h(0)|\) of the particle invariants of motion for increasing space-time resolution \(\Delta t = \sigma \Delta z = \sigma \lambda / n_p \ n_p = 16, 24, 32, 48, \ \sigma = 0.6\).
Scaling of the max $|h_1(t) - h_1(0)|$ difference for increasing space-time resolution

$\Delta t = \sigma \Delta z = \sigma \lambda / n_p$

$n_p = 24, 32, 48, \sigma = 0.6$.

Left: LPf2 versus RK4

Right: RK4 scheme using second and third order shape functions.
Self consistent case: heating problem

A careful investigation of the numerical heating problem in PIC schemes has been recently published (Estelle et al, PRE 2008)

A 1D cold plasma interacting with a laser pulse should always remain perfectly cold. However, a numerical experiment shows anomalous heating which can be interpreted as consequence of:

- interpolation inaccuracy
- errors in the time integration of the particles motion

Residual transverse momentum ($\langle p_x^2 \rangle^{1/2}$) after the interaction with the laser with $a_0 = 4$ (no self consistency) as a function of the resolution $\#$points/$\lambda_0$ (the time step is fixed according to $c \Delta t = 0.9 \Delta z$) for low order (LF2) and high order (HO) schemes.
The numerical heating problem

Plasma wave excitation in the wake of a laser pulse. Wave breaking arise due to numerical heating

Upleft: LPF2 36 ppw
Upright: RK4 32ppw 2nd order shape-function
Downleft: RK4 25ppw 3rd order shape-function
Convergence difference between PIC and HOPIC schemes

Increasing the laser intensity ($a_0$ → 4) the differences between LPF2 and RK4 become more evident:

- left: LPF2 scheme shows slow convergence in the plasma wave length due to “not so correct” description of the particle motion in the laser field
- right: RK4 shows much faster convergence and correct description with 20ppw
The interpolation problem in a PIC code

- In 1D particle density on grid is defined as

\[ n(x_j, t) = \frac{1}{n} \sum_p S \left( \frac{x_p - x_j}{h} \right) \]

- A grid defined acceleration field \( F_j = F(x_j, t) \) is assigned to the particle position by the same spline technique:

\[ \tilde{F}(x_p) = \sum_j F_j S \left( \frac{x_p - x_j}{h} \right) \]

in particular:

- \( S2: \tilde{F}(x_p) = F_j + \frac{h^2}{8} \Delta^2 F_j + P_2(\xi) \)
- \( S3: \tilde{F}(x_p) = F_j + \frac{h^2}{6} \Delta^2 F_j + P_3(\xi) \)

where \( \xi = (x_p - x_j)/h \) and \( P_2, P_3 \) are second and third order local Lagrange polynomials.
In the continuous space-time limit, Poisson equation, once given as initial condition, can be satisfied at any time by combining Ampere law and the continuity equation.

The same holds trues in the discretized case, if the continuity equation is exact even for approximated variables.

The only way to assure this condition, is to use the numerical continuity equation, for assigned charge density

$$\hat{D} \cdot \mathbf{J} = -\Delta t[\rho]$$

as a definition of the numerical current density $\mathbf{J}$:

- In a one-dimensional case, the problem is straightforward.
- In the multidimensional case, the Esirkepov procedure allows to split the continuity equation as three independent onedimensional differential equations, each defining a proper $J_i$ current component.
Charge preserving scheme in HOPIC

Runge Kutta 4
Longitudinal electric field in 2D test problem (right)
and difference $\delta \rho = \nabla E - \rho$ for charge preserving (bottom left) and non-charge preserving (bottom right)

For LPF4 charge conservation results to be exact!
Ion acceleration in the RPA regime

2D ALaDyn simulation: HO in space [6] + RK4 in time (4 points/skin depth + 15 particles/cell)

See A. Macchi on Tuesday
Ion acceleration in the RPA regime

Medium/low resolution \((n = 4)\) with HO schemes is comparable (or better?) to medium/high resolution \((n = 10)\) with LO schemes.

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Conclusions

1. High order space time integration proved to be effective on improving accuracy and efficiency for both Maxwell equations and particles motion

2. In the fully self-consistent case some problems still remain open, in particular the control of numerical heating

3. A general scheme for extending charge conservation has been proposed