Efficient Modeling of Laser-Plasma Accelerators Using the Ponderomotive-Based Code INF&RNO

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Overview

• challenges in modeling laser-plasma accelerators (LPAs) over distances ranging from cm to m scales

• the code INF&RNO (INtegrated Fluid & paRticle simulatioN cOde)
  ✔ basic equations, numerics and features of the code
  ✔ validation tests and performance

• applications
  ✔ modeling of current LOASIS experiments (tunable LPA)
  ✔ modeling of 10 GeV LPA stage for BELLA (BErkeley Lab Laser Accelerator)

• conclusions
Laser-plasma accelerators*: 1-100 GV/m accelerating gradients

- **Plasma waves**
  - Electron density, \( n/n_0 \)
  - Laser pulse
  - Plasma waves
  - Wakefields

- **Wakefields** (due to charge separation: ion at rest VS displaced electrons)
  \[
  E_z \sim mc\omega_p/e \sim 100 \text{ [V/m]} \times (n_0 \text{[cm}^{-3}])^{1/2}
  \]
  e.g.: for \( n_0 \sim 10^{18} \text{ cm}^{-3}, I_0 \sim 10^{18} \text{ W/cm}^2 \implies E_z \sim 100 \text{ GV/m}, \]
  \~ 10^3 \text{ larger than conventional RF accelerators}

\*Tajima and Dawson, PRL (1979)
Energy gain in a (single stage) LPA

Limits to single stage energy gain:

- **laser diffraction** (~ Rayleigh range)
  → mitigated by transverse plasma density tailoring (plasma channel) and/or self-focusing

- **beam-wave dephasing**
  \[ \beta_{\text{bunch}} \sim 1, \beta_{\text{wave}} \sim 1 - \frac{\lambda_0^2}{2\lambda_p^2} \rightarrow \text{slippage} \quad L_d \propto \frac{\lambda_p}{(\beta_{\text{bunch}} - \beta_{\text{wave}})} \sim n_0^{-3/2} \]
  → mitigated by longitudinal density tailoring

- **laser energy depletion** → energy loss into plasma wave excitation

Energy gain (single stage) \( \sim n_0^{-1} \)
Experimental demonstration: 1 GeV high-quality beam from LPA

GeV e-bunch produced from cm-scale plasma (using 1.5 J, 46 fs laser, focused on a 3.3 cm discharge capillary with a density of $4 \times 10^{18}$ cm$^{-3}$)*

$E=1012 \text{ MeV}$

$dE/E = 2.9\%$

$1.7 \text{ mrad}$

3D full-scale modeling of an LPA over cm to m scales is a challenging task.

Simulation complexity:
\[ \propto \frac{D}{\lambda_0} \times \left( \frac{\lambda_p}{\lambda_0} \right) \]
\[ \propto \left( \frac{D}{\lambda_0} \right)^{4/3} \text{ [if D is deph. length]} \]

<table>
<thead>
<tr>
<th></th>
<th>~ \mu m</th>
</tr>
</thead>
<tbody>
<tr>
<td>laser wavelength ((\lambda_0))</td>
<td></td>
</tr>
<tr>
<td>laser length (L)</td>
<td>~ few tens of (\mu m)</td>
</tr>
<tr>
<td>plasma wavelength ((\lambda_p))</td>
<td>~10 (\mu m) @ 10^{19} (cm^{-3})</td>
</tr>
<tr>
<td></td>
<td>~30 (\mu m) @ 10^{18} (cm^{-3})</td>
</tr>
<tr>
<td></td>
<td>~100 (\mu m) @ 10^{17} (cm^{-3})</td>
</tr>
<tr>
<td>interaction length (D)</td>
<td>~ mm @ 10^{19} (cm^{-3}) → 100 MeV</td>
</tr>
<tr>
<td></td>
<td>~ cm @ 10^{18} (cm^{-3}) → 1 GeV</td>
</tr>
<tr>
<td></td>
<td>~ m @ 10^{17} (cm^{-3}) → 10 GeV</td>
</tr>
</tbody>
</table>

3D explicit PIC simulation:
- \(10^4 - 10^5\) CPUh for 100 MeV stage
- ~10^6 CPUh for 1 GeV stage
- ~10^7 - 10^8 CPUh for 10 GeV stage
The INF&RNO framework: motivations

What we need (from the computational point of view):

- run 3D simulations (dimensionality matters!) of cm/m-scale laser-plasma interaction in a reasonable time (a few hours/days)
- perform, for a given problem, different simulations (exploration of the parameter space, optimization, convergence check, etc.)

Reduced Models

[drawbacks/issues: neglecting some aspects of the physics depending on the particular approximation made]

- Huang, et al., JCP (2006) [QuickPIC]
- Lifshitz, et al., JCP (2009) [CALDER-circ]
- Cowan, et al., JCP (2011) [VORPAL/envelope]
- Benedetti, et al., AAC2010 + submitted (2012) [INF&RNO]

Boosted Lorentz Frame

[drawbacks/issues: control of numerical instabilities, self-injection to be investigated, under-resolved physics (e.g. RBS)]

* Vay, PRL (2007)
INF&RNO* is orders of magnitude faster than full PIC codes still retaining physical fidelity

INF&RNO ingredients:

- envelope model for the laser
  - no $\lambda_{\text{laser}}$
  - axisymmetric

- 2D cylindrical (r-z)
  - self-focusing & diffraction for the laser as in 3D
  - significant reduction of the computational complexity
    ... but only axisymmetric physics

- ponderomotive approximation to describe laser $\rightarrow$ plasma interaction
  - (analytical) averaging over fast oscillations in the laser field
  - $\Rightarrow$ scales @ $\lambda_{\text{laser}}$ are removed from the plasma model

- PIC & (cold) fluid
  - fluid $\rightarrow$ noiseless and accurate for linear/mildly nonlinear regimes
  - integrated modalities (e.g., PIC for injection, fluid acceleration)
  - hybrid simulations (e.g., fluid background + externally injected bunch)

* Benedetti et al., Proc. of AAC10 (2010); Benedetti et al., Proc. of PAC11 (2011); Benedetti et al., JCP, submitted
The **INF&RNO** framework: physical model

The code adopts the “comoving” normalized variables $\xi = k_p (z - ct)$, $\tau = \omega_p t$

- **laser pulse (envelope)**
  \[ a_\perp = \frac{\delta (\xi, r)}{2} e^{i(k_0/k_p)\xi} + c.c. \rightarrow \left( \nabla^2 + 2i \frac{k_0}{k_p} \frac{\partial}{\partial \tau} + 2 \frac{\partial^2}{\partial \xi \partial \tau} - \frac{\partial^2}{\partial \tau^2} \right) \delta = \frac{\delta}{\gamma_{\text{fluid}}} \bar{a} \]

- **wakefield (fully electromagnetic)**
  \[
  \frac{\partial E_r}{\partial \tau} = \frac{\partial (E_r - B_\phi)}{\partial \xi} - J_r \\
  \frac{\partial E_z}{\partial \tau} = \frac{\partial E_z}{\partial \xi} + \frac{1}{r} \frac{\partial (rB_\phi)}{\partial r} - J_z \\
  \frac{\partial B_\phi}{\partial \tau} = - \frac{\partial (E_r - B_\phi)}{\partial \xi} + \frac{\partial E_z}{\partial r}
  \]

- **plasma**
  \[
  \text{PIC} \rightarrow \begin{cases}
  \frac{d\xi_j}{d\tau} &= \beta_{z,j} - 1 \\
  \frac{du_{z,j}}{d\tau} &= -\frac{\partial \gamma_j}{\partial \xi} - E_z - \beta_r B_\phi \\
  \frac{dr_j}{d\tau} &= \beta_{r,j} \\
  \frac{du_{r,j}}{d\tau} &= -\frac{\partial \gamma_j}{\partial r} - E_r + \beta_z B_\phi \\
  \gamma_j &= \sqrt{1 + |\bar{a}|^2 + u_{z,j}^2 + u_{r,j}^2}
  \end{cases}
  \]
  \[
  \text{fluid} \rightarrow \begin{cases}
  \frac{\partial \delta}{\partial \tau} &= \frac{\partial \delta}{\partial \xi} - \nabla \cdot (\bar{\beta} \delta) \\
  \frac{\partial (\delta u_j)}{\partial \tau} &= \frac{\partial (\delta u_j)}{\partial \xi} - \nabla \cdot (\bar{\beta} \delta u_j) + \delta \left( -(E + \bar{\beta} \times B) - \frac{1}{2\gamma_{\text{fluid}}} \nabla |\bar{a}|^2 \right)_j \\
  \gamma_{\text{fluid}} &= \sqrt{1 + |\bar{a}|^2 + u_z^2 + u_r^2}
  \end{cases}
  \]

where $\delta$ is the density and $\mathbf{J}$ the current density.
The INF&RNO framework: numerical aspects

- **longitudinal derivatives:**
  - 2\textsuperscript{nd} order **upwind** FD scheme \( \rightarrow (\partial_\xi f)_{i,j} = (-3f_{i,j} + 4f_{i+1,j} - f_{i+2,j}) / 2\Delta_\xi \)
  - BC easy to implement (unidirectional “information” flux using \( \xi \))

- **transverse (radial) derivatives:**
  - 2\textsuperscript{nd} order **centered** FD scheme \( \rightarrow (\partial_r f)_{i,j} = (f_{i,j+1} - f_{i,j-1}) / 2\Delta_r \)
  - fields are not singular in \( r=0 \), from symmetry we have

\[
\partial_r E_z = 0, \quad E_r = B_\phi = 0, \quad \lim_{r \to 0} E_r / r = \partial E_r / \partial r |_0, \quad \lim_{r \to 0} B_\phi / r = \partial B_\phi / \partial r |_0
\]

- **time integration for plasma / EM wakefield:** \textbf{RK2 [fluid]} / \textbf{RK4 [PIC]}

- **quadratic shape** function for force interpolation/current deposition [PIC]

- **digital filtering** for current and/or fields smoothing [PIC]
  - N*binomial filter (1, 2, 1) + compensator
  - compact low-pass filter\(*:** \( \beta F_{i-1} + F_i + \beta F_{i+1} = \sum_{k=0,2} a_k(\beta) (f_{i+k} + f_{i-k}) / 2 \)

\* Shang, JCP (1999)
The INF&RNO framework: improved laser envelope solver/1

- envelope description: \( a_{\text{laser}} = \hat{a} \exp[i k_0 (z-c t)]/2 + \text{c.c.} \)

- early times: NO need to resolve \( \lambda_0 (\sim 1 \text{ \mu m}) \), only \( L_{\text{env}} \sim \lambda_p (\sim 10-100 \text{ \mu m}) \)

- later times: laser-pulse redshifting \( \rightarrow \) structures smaller than \( L_{\text{env}} \) arise in \( \hat{a} \) (mainly in \( \text{Re}[\hat{a}] \) and \( \text{Im}[\hat{a}] \)) and need to be captured*

\[ a_0=1.5, \frac{k_0}{k_p}=20, L_{\text{env}}=1 \]

Is it possible to have a good description of a depleted laser at a reasonably low resolution?

* Benedetti at al., AAC2010
Cowan et al., JCP (2011)
W. Zhu et al., POP (2012)
The **INF&RNO framework**: improved laser envelope solver

- envelope evolution equation is discretized in time using a 2\(^{nd}\) order Crank-Nicholson scheme

\[\frac{\hat{a}^{n+1} - 2\hat{a}^n + \hat{a}^{n-1}}{\Delta^2} + 2\left(i \frac{k_0}{k_p} + \frac{\partial}{\partial \xi}\right)\frac{\hat{a}^{n+1} - \hat{a}^{n-1}}{2\Delta} = -\nabla^2_{\perp} \frac{\hat{a}^{n+1} + \hat{a}^{n-1}}{2} + \frac{\delta^n}{\gamma_{\text{fluid}}(\hat{a}^n)} \frac{\hat{a}^{n+1} + \hat{a}^{n-1}}{2}\]

- FD form for $\partial/\partial \xi \rightarrow$ unable to deal with unresolved structures in $\hat{a}$

- **INF&RNO** uses a polar representation for $\hat{a}$ when computing $\partial/\partial \xi$

\[
\hat{a} = \Re[\hat{a}] + i\Im[\hat{a}] = |\hat{a}|e^{i\theta}
\]

\[
\partial_\xi \hat{a} = \begin{cases} 
\partial_\xi (\Re[\hat{a}]) + i\partial_\xi (\Im[\hat{a}]) & \text{(cartesian)} \\
\partial_\xi (|\hat{a}|)e^{i\theta} + i(\partial_\xi \theta)\hat{a} & \text{(polar)}
\end{cases}
\]

- smoother behavior compared to $\Re[\hat{a}]$ and $\Im[\hat{a}]$
The INF&RNO framework: improved laser envelope solver/3

1D sim.: $a_0=1$, $k_0/k_p=100$, $L_{rms}=1$ (parameters of interest for a 10 GeV LPA stage)

pump depletion length (resonant pulse): $L_{pd} \approx \frac{\lambda_r^3}{\lambda_0^2} \approx 80 \text{ cm}$
The INF&RNO framework: Lorentz Boosted Frame\(^*\) (LBF) modeling/1

- The spatial/temporal scales involved in a LPA simulation DO NOT scale in the same way changing the reference frame

<table>
<thead>
<tr>
<th>Laboratory Frame</th>
<th>Boosted Lorentz Frame ((\beta_*))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda_0 \rightarrow ) laser wavelength</td>
<td>(\lambda'<em>0 = \gamma</em>* (1 + \beta_*) \lambda_0 &gt; \lambda_0)</td>
</tr>
<tr>
<td>(\ell \rightarrow ) laser length</td>
<td>(\ell' = \gamma_* (1 + \beta_*) \ell &gt; \ell)</td>
</tr>
<tr>
<td>(L_p \rightarrow ) plasma length</td>
<td>(L'<em>p = L_p / \gamma</em>* &lt; L_p)</td>
</tr>
<tr>
<td>(c \Delta t &lt; \Delta z \ll \lambda_0, \lambda_0 &lt; \ell \ll L_p)</td>
<td>(\Rightarrow t_{\text{simul}} \sim (L_p + \ell) / c)</td>
</tr>
<tr>
<td># steps = (\frac{t_{\text{simul}}}{\Delta t} \propto \frac{L_p}{\lambda_0} \gg 1)</td>
<td>(\Rightarrow t'<em>{\text{simul}} \sim \frac{(L'<em>p + \ell')/(c(1 + \beta</em>*))}{t'</em>{\text{simul}}} \propto \frac{L_p}{\lambda_0 \gamma_<em>^2 (1 + \beta_</em>)^2})</td>
</tr>
<tr>
<td>large # of steps</td>
<td># of steps reduced ((1/\gamma_*^2))</td>
</tr>
</tbody>
</table>

\(\Rightarrow\) the LF is not the optimal frame to run a LPA simulation

\(\Rightarrow\) simulation in the LBF is shorter (optimal frame is the one of the wake)

\(\Rightarrow\) OK \textbf{iff} backwards propagating waves are negligible!

\(\Rightarrow\) diagnostic more complicated (LBF \(\leftrightarrow\) LF loss of simultaneity)

\* Vay, PRL (2007); Vay, \textit{et al.}, JCP (2011)
The INF&RNO framework: Lorentz Boosted Frame modeling/2

- LBF modeling implemented in INF&RNO/fluid (INF&RNO/PIC underway):
  - input/output in the Lab frame (swiping plane*, transparent for the user)
  - no instability observed at high $\gamma_{LBF}$ (reported in 2D/3D PIC runs)
  - some of the approx. in the envelope model are not Lorentz invariant (limit $\max \gamma_{LBF}$)

$\gamma_{LBF} = 8$

LF = 16h 47' VS LBF = 15'

* Vay, JCP (2011)
The INF&RNO framework: particle resampling to reduce noise

• “adaptive” particle resampling (useful for “quick” runs)
  - numerical particles loaded \( \sim \) uniformly in the computational domain
  - charge of a particle \( q_i \propto r_{0,i} \) (particles born at large radii are “heavier”)
  - “heavy” particles generate “spikes” in density/current when \( r_i \sim 0 \)
    \( \rightarrow \) particles are split into fragments as \( r_i \rightarrow 0 \)
  - drawbacks: small violation of the local charge/energy conservation (total charge and momentum are conserved), heating of the plasma
Benchmark 1/3: laser pulse velocity

Propagation velocity of a low intensity ($a_0=0.01$) laser pulse* in vacuum or plasma

\[
\begin{aligned}
    n(r) &= n_0 + (\pi r e r_m^2)^{-1} \left( \frac{r}{r_m} \right)^2 \\
    a_\perp &\sim L_m^0 \left( \frac{2r_i^2}{w_0^2} \right) e^{-r^2/w_0^2}
\end{aligned}
\]

\[
\beta_g = 1 - \frac{k_p^2}{2k_0^2} - \frac{1 + 2m}{k_0^2 r_i^2} \left[ 1 + \frac{r_i^4}{r_m^4} + \frac{r_i^2}{r_m^2} \left( \frac{\partial(r_i/r_m)}{\partial(z/Z_m)} \right)^2 \right]
\]

\[
\begin{align*}
    m=0 \text{ (Gaussian), } k_0 r_i &= 80 \\
    m=1 \text{ (LG1), } k_0 r_i &= 80 \\
    m=0 \text{ (matched Gaussian), } k_p r_i &= k_p r_m \\
    m=0 \text{ (mismatched Gaussian), } k_p r_i &= 1.5 k_p r_m \quad \text{plasma channel} \quad \left( k_0/k_p = 25, \quad k_p r_m = 3.14 \right) \\
    m=0 \text{ (Gaussian, converging at the entrance of the channel), } k_p r_i &= \sqrt{2} k_p r_m, \quad dr_i/dz < 0
\end{align*}
\]

Benchmark 2/3: comparison with “full” 3D PIC/1

Comparison with VORPAL and OSIRIS*  

<table>
<thead>
<tr>
<th>$a_0$</th>
<th>$k_p w_0$</th>
<th>$k_0/k_p$</th>
<th>numerics</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4</td>
<td>5.7</td>
<td>11.2</td>
<td>$k_p \Delta \xi = 1/30$, $k_p \Delta r = 1/10$, 20ppc, QSF</td>
</tr>
</tbody>
</table>

* Paul et al., Proc. of AAC08 (2008)
Benchmark 3/3: comparison with “full” 3D PIC/2

Comparison with 3D PIC code ALaDyn*

<table>
<thead>
<tr>
<th>$n_0$ [e/cm$^3$]</th>
<th>$k_0/k_p$</th>
<th>$a_0$</th>
<th>$T$ [fs]</th>
<th>$w_0$ [$\mu$m]</th>
<th>$L_{\text{sym}}$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 $\cdot$ 10$^{18}$</td>
<td>24</td>
<td>5</td>
<td>30</td>
<td>16</td>
<td>3.2</td>
</tr>
</tbody>
</table>

box: $23 \times 20$ - res: $1/30 \times 1/20$ - $\Delta t = 0.25 \Delta z$ - QSF - split [2] - filter [250]

* Benedetti et al., IEEE TPS (2008); Benedetti et al., NIM A (2009)
Performance of INF&RNO

- code written in C/C++ & parallelized with MPI (1D longitudinal domain decomp.)
- code performance on a MacBookPro laptop (2.5GHz, 4GBRAM, 1333MHz DDR3)

<table>
<thead>
<tr>
<th>FLUID (RK2)</th>
<th>PIC (RK4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8 μs / (grid point * time step)</td>
<td>1.1 μs / (particle push * time step)</td>
</tr>
</tbody>
</table>

- Examples of simulation cost
  - 100 MeV stage (~$10^{19}$ cm$^{-3}$, ~mm) / PIC → $\sim 10^2$ CPUh
  - 1 GeV stage (~$10^{18}$ cm$^{-3}$, ~cm) / PIC → $\sim 10^3$–$10^4$ CPUh
  - 10 GeV stage quasi-lin. (~$10^{17}$ cm$^{-3}$, ~m) / FLUID → $\sim 10^3$ CPUh
  - 10 GeV stage quasi-lin. (~$10^{17}$ cm$^{-3}$, ~m) / FLUID + LBF[$\gamma_{LBF}$=10] → $\sim 20$ CPUh
  - 10 GeV stage bubble (~$10^{17}$ cm$^{-3}$, ~10 cm) / PIC → $\sim 10^4$–$10^5$ CPUh

=> gain between 2 and 5 orders of magnitude in the simulation time
INF&RNO is used to successfully model current experiments at LOASIS

Tunable laser plasma accelerator based on longitudinal density tailoring*

Electrons injected at density gradient + coupling of injected electrons to a lower density, separately tunable plasma for further acceleration.

INF&RNO is used to successfully model current experiments at LOASIS

Tunable laser plasma accelerator based on longitudinal density tailoring

Electrons injected at density gradient + coupling of injected electrons to a lower density, separately tunable plasma for further acceleration.

BELLA laser: $T_{\text{laser}} \approx 40 \text{ fs}, E_{\text{laser}} \approx 40 \text{ J} \ (\sim 1 \text{ PW})$

Plasma channel, $n_0 \approx 3 \times 10^{17} \text{ e/cm}^3$

Simulation cost: $< 10^5 \text{ kCPUh} \ (\text{gain } \sim 10^3) \ [\text{NERSC}]$

→ laser diffracts without channel even if $P/P_c \sim 12$
10 GeV-class quasi-monoenergetic beams can be obtained in ~ 10 cm capillary

**Longitudinal phase space @ z = 10 cm**

- $Q \approx 200 \text{ pC}$
- $E_{\text{average}} \approx 9 \text{ GeV}$
- $(dE/E)_{\text{rms}} \approx 7\%$
- $(\sigma_z)_{\text{rms}} \approx 1 \mu \text{m}$
- $(\sigma_x)_{\text{rms}} \approx 2 \mu \text{m}$
- $(\sigma_x')_{\text{rms}} \approx 0.45 \text{ mrad}$

**Plasma density @ z = 10 cm**
Conclusions

The INF&RNO computational framework has been presented

- features: envelope, ponderomotive, 2D cylindrical, PIC/Fluid integrated, LBF, parallel

- the code is several orders of magnitude faster compared to “full” PIC, while still retaining physical fidelity

- the code has been widely benchmarked and validated

- modeling of future BELLA experiments show 10 GeV-class beams in ~ 10 cm
Plasma density

$k_p (z - ct)$