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

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Overview of the presentation

- 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 present LPA experiments @ BELLA (BErkeley Lab Laser Accelerator): ~4.3 GeV e-beam in a 9 cm capillary

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

Laser driver:
- ultra-short ($T_0 \sim$ tens of fs $\sim \lambda_p$)
- ultra-intense (Ti:Sa laser $I_0 > 10^{18}$ W/cm²)

\[ a_0 = eA_0^{\text{laser}}/mc^2 \]
\[ \approx 8.5 \cdot 10^{-10} I_0^{1/2}[W/cm^2] \lambda_0[\mu m] \sim 1 \]

Wakefield excitation due to charge separation: ions at rest VS electrons displaced by ponderomotive force

\[ E_z \sim mc\omega_p/e \sim 100 [V/m] \times (n_0[cm^{-3}])^{1/2} \]

e.g.: for $n_0 \sim 10^{17} \text{ cm}^{-3}$, $a_0 \sim 1 \rightarrow E_z \sim 30 \text{ GV/m},
\sim 10^2-10^3$ larger than conventional RF accelerators

*Esarey et al., RMP (2009)
Scalings for e-beam energy in LPAs

Limits to single stage energy gain:

- **laser diffraction** (∼ Rayleigh range)
  → mitigated by transverse plasma density tailoring (plasma channel) and/or self-focusing: (self-)guiding of the laser

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

- **laser energy depletion** → energy loss into plasma wave excitation (\( L_{pd} \sim n_0^{-3/2} \))

Energy gain (single stage) \( \sim n_0^{-1} \)
Interaction length (single stage) \( \sim n_0^{-3/2} \)
Example of LPA experiment: 1 GeV high-quality beams from ~3 cm plasma

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 4x10^{18} cm^{-3])*

E=1012 MeV
dE/E = 2.9%
1.7 mrad

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laser wavelength ($\lambda_0$)</td>
<td>$\sim \mu$m</td>
</tr>
<tr>
<td>Laser length (L)</td>
<td>$\sim$ few tens of $\mu$m</td>
</tr>
</tbody>
</table>
| Plasma wavelength ($\lambda_p$)            | $\sim 10 \mu$m @ $10^{19}$ cm$^{-3}$  \\
|                                            | $\sim 30 \mu$m @ $10^{18}$ cm$^{-3}$  \\
|                                            | $\sim 100 \mu$m @ $10^{17}$ cm$^{-3}$ |
| Interaction length (D)                     | $\sim$ mm @ $10^{19}$ cm$^{-3}$ → 100 MeV  \\
|                                            | $\sim$ cm @ $10^{18}$ cm$^{-3}$ → 1 GeV  \\
|                                            | $\sim$ m @ $10^{17}$ cm$^{-3}$ → 10 GeV   |

Simulation complexity:

$\propto \left( \frac{D}{\lambda_0} \right) \times \left( \frac{\lambda_p}{\lambda_0} \right)$

$\propto \left( \frac{D}{\lambda_0} \right)^{4/3}$  [if D is deph. length]

3D explicit PIC simulation:

✓ $10^4$–$10^5$ CPUh for 100 MeV stage
✓ $\sim 10^6$ CPUh for 1 GeV stage
✓ $\sim 10^7$–$10^8$ CPUh for 10 GeV stage

![Image from Shadwick et al.](image.png)
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]

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

* Vay, PRL (2007)

# Mora & Antonsen, Phys. Plas. (1997) [WAKE]
% Huang, et al., JCP (2006) [QuickPIC]
^ Lifshitz, et al., JCP (2009) [CALDER-circ]
& Cowan, et al., JCP (2011) [VORPAL/envelope]
+ Mehrling, et al., PPCF (2014) [HiPACE]
INF&RNO ingredients:

- envelope model for the laser
  - no $\lambda_0$
  - 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 w/laser envelope to describe laser-plasma interaction
  - (analytical) averaging over fast oscillations in the laser field
  - scales @ $\lambda_0$ are removed from the plasma model $\rightarrow$ # of time steps
    reduced by $\sim \lambda_p / \lambda_0$

- 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; Benedetti et al., Proc. of ICAP12

INF&RNO* is orders of magnitude faster than full PIC codes still retaining physical fidelity
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)**
  \[
  a_\perp = \frac{\hat{a}(\xi, r)}{2} e^{i(k_0/k_p)\xi} + c.c. \rightarrow \left( \nabla_\perp^2 + 2i \frac{k_0}{k_p} \frac{\partial}{\partial \tau} + 2 \frac{\partial^2}{\partial \xi \partial \tau} - \frac{\partial^2}{\partial \tau^2} \right) \hat{a} = \frac{\delta}{\gamma_{\text{fluid}}} \hat{a}
  \]

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

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

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

- **longitudinal derivatives (no staggering in space):**
  - 2\textsuperscript{nd} order **upwind** FD scheme $\to (\partial_{\xi} f)_{i,j} = (-3f_{i,j} + 4f_{i+1,j} - f_{i+2,j}) / 2\Delta\xi$
  - B.C. easy to implement (unidirectional information flux in $\xi$ from R to L)

- **transverse (radial) derivatives (no staggering in space):**
  - 2\textsuperscript{nd} order **centered** FD scheme $\to (\partial_r f)_{i,j} = (f_{i,j+1} - f_{i,j-1}) / 2\Delta r$
  - fields are not singular in $r=0$, from symmetry we have

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

- RK\textsuperscript{2} [fluid]/RK\textsuperscript{4} [PIC] for time integration of particles/fields (no staggering)

- **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\*: $\beta F_{i-1} + F_i + \beta F_{i+1} = \sum_{k=0,2} a_k(\beta) (f_{i+k} + f_{i-k}) / 2$

- **Langdon-Marder** method for charge conservation

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

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

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

$$a_0 = 1.5, \ k_0/k_p = 20, \ L_{\text{env}} = 1$$

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)
Zhu et al., POP (2012)
The INF&RNO framework: improved laser envelope solver/2

- envelope evolution equation is discretized in time using a 2nd order Crank-Nicholson scheme

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

- FD form for \( \partial/\partial \xi \) → unable to deal with unresolved structures in \( \hat{a} \)

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

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

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

“smoother” behavior compared to \( \Re[\hat{a}] \) and \( \Im[\hat{a}] \)

The INF&RNO framework: improved laser envelope solver/3

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

\[ t = 0.8 \cdot L_{pd} \]

Pump depletion length (resonant pulse): $L_{pd} \approx \frac{\lambda_p^3}{\lambda_0^2} \approx 80 \text{ cm}$
The INF&RNO framework: quasi-static solver*

• QS approximation:
  → neglect the $\partial / \partial t$ in wakefields/plasma quantities

for a given driver configuration solve ODE/PDE for plasma and wakefield →

\[
\frac{dr}{d\xi} = -\frac{ur}{1+\psi}
\]
\[
\frac{d\psi}{d\xi} = \frac{ur}{1+\psi} (Er - B_\phi) - E_z
\]
\[
\gamma - u_z - \psi = 1
\]
\[
\nabla^2_{\perp} E_z = \frac{1}{r} \frac{d}{dr} (rJ_r)
\]
\[
\frac{\partial (Er - B_\phi)}{d\xi} = J_r
\]
\[
\frac{1}{r} \frac{d}{dr} (rB_\phi) = J_z - \frac{\partial E_z}{\partial \xi}
\]

→ retain $\partial / \partial t$ for the driver (laser or particle beam)

driver is frozen while plasma is passed through the driver and wakefields are computed

wakefield is frozen while driver is advanced in time

$\Delta t$ set according to driver evolution (much bigger than conv. PIC)

*Mehrling, Benedetti, et al., PPCF (2014)*
Quasi-static solver allows for significant speed-ups in simulations of underdense plasmas

- Reduction in # of time steps compared to full PIC simulations (laser driver) \( \rightarrow \sim (\lambda_p/\lambda_0)^2 \)

- Reduction in # of time steps compared to a PIC code w/ ponderomotive approx (laser driver) \( \rightarrow \sim \lambda_p/\lambda_0 \)

- QS solver cannot model some aspects of kinetic physics like particle self-injection

BELLA laser propagating in uniform plasma (gas-cell)

- INF&RNO QS (< 1 hour on 1 CPU)
- INF&RNO non-QS (several hours on ~100 CPUs)

\[ n_0 = 4 \times 10^{17} \text{ e/cm}^3 \]
\[ n_0 = 3 \times 10^{17} \text{ e/cm}^3 \]
\[ n_0 = 2 \times 10^{17} \text{ e/cm}^3 \]

\( U_{\text{laser}} = 40 \text{ J} \)
\( T_{\text{laser}} = 30 \text{ fs} \)
\( w_0 = 64 \mu\text{m} \)
The INF&RNO framework: Lorentz Boosted Frame* (LBF) modeling

- 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>$\lambda'<em>0 = \gamma</em><em>(1 + \beta_</em>) \lambda_0 &gt; \lambda_0$</td>
</tr>
<tr>
<td>$\ell \rightarrow$ laser length</td>
<td>$\ell' = \gamma_<em>(1 + \beta_</em>) \ell &gt; \ell$</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>$\Rightarrow t'_{simul} \sim (L'<em>p + \ell')/(c(1 + \beta</em>*))$</td>
</tr>
<tr>
<td>$\Rightarrow t'_{simul} \sim (L'<em>p + \ell')/(c(1 + \beta</em>*))$</td>
<td>$\lambda_0 \gamma_<em>^2 (1 + \beta_</em>)^2$</td>
</tr>
<tr>
<td>$#$ steps = $\frac{t'_{simul}}{\Delta t} \propto \frac{L_p}{\lambda_0} \gg 1$</td>
<td>$#$ steps' = $\frac{t'<em>{simul}}{\Delta t'} \propto \frac{L_p}{\lambda_0 \gamma</em><em>^2 (1 + \beta_</em>)^2}$</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

$\Rightarrow$ sim. in LBF is shorter (optimal frame is the one of the wake $\gamma_* \sim k_0 / k_p$)

$\Rightarrow$ comp. savings if backwards propagating waves are negligible!

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

* Vay, PRL (2007); Vay, et al., JCP (2011)
The INF&RNO framework: Lorentz Boosted Frame* (LBF) 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)
  - 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'  

$\omega_p(t=200, 600, 1000)$

* Vay, JCP (2011)
# Benedetti, et al., Proc. of PAC2011
INF&RNO validated by comparing simulation results with analytical solutions and by performing benchmarks with other PIC codes.*

- Testing the propagation velocity of a low intensity laser pulse\(^*\) \((a_0=0.01)\) in vacuum or plasma:

  plasma profile → \(n(r) = n_0 + \left(\frac{\pi r r_m}{r_m}\right)^{-1} \left(\frac{r}{r_m}\right)^2\)

  laser pulse → \(\hat{a}_\parallel \approx L_m^0 \left(\frac{2r^2}{w_0^2}\right) e^{-r^2/w_0^2}\)

  laser pulse velocity → \(\beta_g = 1 - \frac{k_p^2}{2k_0^2} \left(1 + 2m\right) \left(1 + \frac{r_i^4}{r_m^4}\right)\)

  (theory in black)

- Testing wakefield amplitude in the nonlinear regime: benchmark w/ VORPAL and OSIRIS*

\[E_z/E_0\]

\[a_0=2, k_p w_0=5.7, k_0/k_p=12\]
\[k_p \Delta \xi=1/30, k_p \Delta r=1/10, 20 \text{ ppc}\]

\[E_z/E_0\]

\[a_0=4, k_p w_0=5.7, k_0/k_p=12\]
\[k_p \Delta \xi=1/30, k_p \Delta r=1/10, 20 \text{ ppc}\]

*S. Schroeder, et al., POP (2011)

* Paul et al., Proc. of AAC08 (2008)
INF&RNO validated by comparing simulation results with analytical solutions and by performing benchmarks with other PIC codes/2

- Comparison with 3D PIC code ALaDyn* (INF&RNO sim. is ~150x faster)

<table>
<thead>
<tr>
<th>$n_0$ [e/cm$^3$]</th>
<th>$k_0/k_p$</th>
<th>$a_0$</th>
<th>$\tau$ [fs]</th>
<th>$w_0$ [μm]</th>
<th>$L_{sym}$ [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

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

- code written in C/C++ & parallelized with MPI (1D longitudinal domain decomp.) → typically we run on a few 100s to a few 1000s CPUs
- 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>0.7 μs / (grid point * time step)</td>
<td>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 model current BELLA experiments at LBNL

- Modeling of multi-GeV e-beam production from 9 cm-long capillary-discharge-guided sub-PW laser pulses (BELLA) in the self-trapping regime*

Understanding laser evolution (effect of laser mode and background plasma density on laser propagation): limit cap damage & provide “best” wake for acceleration

Interpreting post-interaction laser spectra as an in situ density diagnostic: knowledge of density is crucial but difficult

Model e-beam production & acceleration

→ features of INF&RNO allowed to run several simulations for detailed parameters scan at a reasonable computational cost

* Leemans et al., PRL (2014)
BELLA laser pulse evolution has been characterized studying the effect of transverse laser mode and plasma density profile.

- An accurate model of the BELLA laser pulse ($U_{\text{laser}} = 15$ J) has been constructed based on measured longitudinal laser intensity profile and transverse intensity profile based on experiment data.

\[
\frac{I}{I_0} = \left[ \frac{2J_1(r/R)}{(r/R)} \right]^2
\]

- Propagation in plasma of Gaussian and top-hat is different.

Propagation distance (cm)

- FWHM = 63.5 μm
- top-hat near field: $\frac{I}{I_0} = \left[ \frac{2J_1(r/R)}{(r/R)} \right]^2$
- Gaussian

Graphs and figures illustrating the intensity profiles and propagation distances for Gaussian and top-hat modes under different plasma densities.
Post-interaction laser optical spectra have been used as an independent diagnostic of the on-axis density.

- Comparison between measured and simulated post-interaction (after 9 cm plasma) laser optical spectra ($U_{\text{laser}} = 7.5 \text{ J}$)

→ good agreement between experiment and simulation: independent (in situ) diagnostic for the plasma density
INF&RNO full PIC simulation allows for detailed investigation of particle self-injection and acceleration.

Simulation cost: (1-3)x10^5 CPUh (gain ~ 1000)
Conclusions

The **INF&RNO** computational framework has been presented

- features: improved laser-envelope solver, ponderomotive, 2D cylindrical, PIC/Fluid integrated, LBF, quasi-static, parallel

- the code is **several orders of magnitude faster compared to “full” PIC**, while still retaining physical fidelity → possible to perform large parameters scan at a reasonable computational cost

- the code has been **widely benchmarked and validated**

- **INF&RNO** used to model current (and future) BELLA experiments at LBNL