Efficient modeling of laser-plasma accelerators with INF&RNO

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Overview

- Requirements & challenges for an end-to-end modeling of an LPA-based linear collider [or a driver for an advanced light source (e.g., LPA-based FEL)]

- Development of efficient numerical tools to model LPAs: new features of INF&RNO (quasi-static module, improved laser solver, independent grid for laser envelope and wakefields, ADK ionization module)

- Examples of application of INF&RNO to current and future BELLA experiments (with emphasis on computational savings)

- Summary and future research directions
End-to-end simulation of a plasma-based linear collider is an extremely challenging problem (multi-physics, multi-scale)

LPA-based collider* →

Injector:
- gas dynamics
- bunch self-injection

LPA-stage:
- gas dynamics
- MHD
- laser-plasma interaction

Driver in-coupling

Beam transport
- vacuum propag.
- lenses
- interaction w/plasma mirror

Final focus

Positron generation
- Montecarlo code

All-optical setup (injection+acceleration)
100x10 GeV LPA modules (staging)
Length: \( \leq 1 \) Km (1-10 GV/m) VS ~30 Km of ILC (RF, ~50 MV/m)

Leemans, Esarey, Physics Today (2009)
Schroeder et al., PRSTAB (2010)
LBNL is developing a suite of tools to address the diverse physics of interest to model an LPA-based collider: modeling 3D LPI is (currently) the most challenging task.

<table>
<thead>
<tr>
<th>Time scale</th>
<th>Physics</th>
<th>Codes</th>
<th>Examples</th>
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</thead>
<tbody>
<tr>
<td>~ms</td>
<td>Gas target formation: capillaries and gas jets</td>
<td><strong>Gas dynamics:</strong> ANSYS, OpenFOAM, Collab. w/ John Bell’s group @ CRD, LBNL</td>
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<tr>
<td>~1 ns ↓ ~100 ns</td>
<td>Plasma formation in capillary discharges</td>
<td><strong>MHD:</strong> Bobrova's code (1D, Keldysh) Marple (3D, Keldysh) Hydra (3D, LLNL)</td>
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<tr>
<td>~fs ↓ ~ns</td>
<td>Laser-plasma interaction in 3D (laser evolution, wake formation, particle dynamics)</td>
<td><strong>Vlasov-Maxwell:</strong> WARP, INF&amp;RNO</td>
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Understanding the physics of LPAs requires detailed numerical modeling

We need:

- run 3D simulations (dimensionality matters!) of cm/m-scale LPI in a reasonable time (a few hours/days) [N.B., 10 GeV stage in 3D (~10⁹ grid points, >10⁹ particles, 10⁷ time steps) requires $10^7$ - $10^8$ CPUh → unfeasible with conventional 3D PIC codes]

- perform, for a given problem, several simulations (exploration of the parameter space, optimization, convergence check, experiment ↔ modeling feedback, etc.)

**Reduced Models**

→ Reducing the computational complexity by carefully selecting the amount of information/physics to compute (e.g., quasi-static, ponderomotive, etc.)

Mora & Antonsen, Phys. Plas. (1997) [WAKE]
Huang, et al., JCP (2006) [QuickPIC]
Lifshitz, et al., JCP (2009) [CALDER-circ]
Mehrling, et al., PPCF (2014) [HiPACE]

**Lorentz Boosted Frame**

→ Different spatial/temporal scales in an LPA simulation do not scale the same way changing the reference frame. Simulation length can be greatly reduced going to an optimal (wake) reference frame.

→ Backward propagating waves are neglected.

Vay, PRL (2007)
INF&RNO is a modular framework tailored to efficiently model LPA problems: it is several orders of magnitude faster than full 3D PIC codes still retaining physical fidelity.

**INF&RNO framework**

- Full wave operator for laser + averaged plasma response + axisymmetric envelope
- Analytical averaging over fast laser oscillations: laser → plasma force via averaged ponderomotive force (scales @ $\lambda_{\text{laser}}$ are removed from simulation)
- 2D-cylindrical geometry (same field structure/laser evolution as in 3D at a 2D computational cost)
- “Time-explicit” PIC or fluid description for the plasma (hybrid simulations are possible)
- Quasi-static PIC & fluid modality (neglect time derivative in plasma evolution, retained for laser evolution)

Other features: moving window, parallel, boosted Lorentz frame (fluid), independent grid for laser driver and wakefield, ADK ionization module, etc.
INF&RNO supports PIC and fluid description of the plasma, each modality has a time-explicit or a quasi-static implementation.

**Time-explicit wakefield modality**

Wakefields → \( \frac{\partial E_r}{\partial \tau} = \frac{\partial (E_r - B_\phi)}{\partial \xi} - J_r \) \( \frac{\partial E_z}{\partial \tau} = \frac{\partial (E_z + \frac{1}{r} \frac{\partial (rB_\phi)}{\partial r})}{\partial \xi} - J_z \) \( \frac{\partial B_\phi}{\partial \tau} = -\frac{\partial (E_r - B_\phi)}{\partial \xi} + \frac{\partial E_z}{\partial \tau} \)

Plasma → PIC →

\[ \begin{align*}
  \forall j = 1, \ldots, N_p \\
  \frac{d\xi_j}{d\tau} &= \beta z_j - 1 \\
  \frac{d\eta_j}{d\tau} &= \beta r_j \\
  \gamma_j &= \sqrt{1 + |\beta|^2 + u^2_{z,j} + u^2_{r,j}} \\
\end{align*} \]

Fluid →

\[ \begin{align*}
  \frac{\partial \delta}{\partial \tau} &= \frac{\partial \delta}{\partial \xi} - \nabla \cdot (\vec{B} \delta) \\
  \frac{\partial (\delta u_j)}{\partial \tau} &= \frac{\partial (\delta u_j)}{\partial \xi} - \nabla \left( \vec{B} \delta u_j \right) + \delta \left( -(\vec{E} + \vec{B} \times \vec{B}) - \frac{1}{2 \gamma_{\text{fluid}}} \nabla |\beta|^2 \right)_j \\
  \gamma_{\text{fluid}} &= \sqrt{1 + |\beta|^2 + u^2_{z,j} + u^2_{r,j}} \\
\end{align*} \]

**Quasi-static wakefield modality**:

\( \partial \tau \ll \partial \zeta \rightarrow \text{neglecting } \partial \tau \text{ derivatives in wake & plasma} \)

- Based on upwind operators (e.g., 5th order Adams-Bashforth scheme for particle trajectory in PIC);
- Uses tridiagonal solvers to solve Poisson-like equation in radial space;

![Graph showing the behavior of a_0 = 3, k_p L = 2, k_p w = 4 with N_iter = 2, 5, 10, 20, 500](attachment:graph.png)
Discretized form of laser envelope solver unable to correctly describe strongly depleted laser pulse at finite resolution

Envelope description: 

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

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

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

Benedetti et al., AAC2010
Cowan et al., JCP (2011)
Zhu et al., POP (2012)
Laser model performance considerably improved when a polar representation for the laser envelope is used.

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

\[
\frac{3n+1 - 2 \xi^n + \xi^{n-1}}{\Delta^2} + 2 \left[ i \frac{k_0}{k_p} + \frac{\partial}{\partial \xi} \right] \frac{3n+1 - \xi^{n-1}}{2 \Delta^2} = -\nabla^2_{\perp} \frac{3n+1 + \xi^{n-1}}{2} + \frac{\gamma^n_{\text{fluid}}(\xi^n)}{2}
\]

- FD form for \( \partial / \partial \xi \rightarrow \text{unable to deal} \) with unresolved structures in \( \xi \).

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

Improved laser solver in INF&RNO shows fast convergence rate even in strongly depleted regimes

Quasi-linear regime (1D)

- $a_0 = 1$, $L_{rms} = 1$
- $k_0/k_p = 100$

Nonlinear regime (3D)

- $a_0 = 3$, $L_{rms} = 1$
- $k_0/k_p = 20$

(plasma channel)

- standard $L_{rms}/\Delta\xi = 15$
- standard $L_{rms}/\Delta\xi = 20$
- standard $L_{rms}/\Delta\xi = 30$
- standard $L_{rms}/\Delta\xi = 80$

... improved $L_{rms}/\Delta\xi = 15$
... improved $L_{rms}/\Delta\xi = 20$

~ $43\%$ energy depletion
~ $15\%$ energy depletion
> $65\%$ energy depletion
INF&RNO framework adopts different computational grids and time steps for laser driver and wakefield allowing for significant computational savings.

Spatial/temporal **resolution requirements** and **size** of the computational box for wakefield and laser driver are in general different.

<table>
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<tr>
<th></th>
<th>longitudinal resolution</th>
<th>transverse resolution</th>
<th>temporal resolution</th>
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<tbody>
<tr>
<td>Laser driver</td>
<td>$\Delta \zeta \ll L_{\text{env}}$</td>
<td>$\Delta r &lt; \ll w$</td>
<td>$\Delta s \ll Z_{\text{Rayleigh}}$</td>
</tr>
<tr>
<td>Wakefield</td>
<td>$\Delta \zeta \ll k_p^{-1}$ (linear) $\Delta \zeta \ll \text{sharp feat. (nonlinear)}$</td>
<td>$\Delta r \ll \text{transv. wake} \sim w$ (linear) $\Delta r \sim \Delta \zeta$ (nonlinear)</td>
<td>$\Delta s \leq \Delta \zeta$ (expl.) $\Delta \varphi$ (quasi-static)</td>
</tr>
</tbody>
</table>

→ separate grids (with different resolutions and boundaries) allows for significant computational saving in particular LPI regimes (e.g., strongly depleted regimes, etc.)
A new (simplified) ADK ionization module (with full 3D dynamics) has been included in the 2D-cylindrical INF&RNO framework.

Implementation of the ionization module requires introduction of a (very) fine grid able to represent the fast laser oscillations.

- Fine 2D grid (able to represent structures $< \lambda_{\text{laser}}$)
- Coarse 2D grid (no $\lambda_{\text{laser}}$)
- Interpolate $\hat{a}$ from coarse grid $\rightarrow$ fine grid
- Retrieved laser field $E_{\perp}(\zeta,r)$, $B_{\perp}(\zeta,r)$, $E_{\parallel}(\zeta,r)$
- $x\exp[\text{i}k_0(z-ct)]$

- all ionization calculations (e.g., ionization rates) are done in the fine grid
- ionized electrons are pushed (in 3D) in the complete laser field (quiver motion) + wakefield using sub-cycling: $\Delta s_{\text{ioniz}} << \Delta s_{\text{wake}}$

Limitations:
- assumes the existence of a pre-ionized background, only few transitions are modeled
- valid only if the charge density produced by ionization is a small perturbation of the pre-ionized plasma (ionization process is a “perturbation” of the main LPI)
- beamloading taken into account assuming it is axisymmetric
The ADK ionization module has been validated with analytical theory.*

**RMS width of ionized electrons**

- $\lambda_i = 0.8 \, \mu\text{m}$
- Nitrogen gas [$U_i = 552 \, \text{eV}$]

- $\lambda_i = 0.4 \, \mu\text{m}$, $a_i = 0.14$
- Kripton gas [$U_i = 230 \, \text{eV}$]

**RMS momentum distribution of ionized electrons**

- $\lambda_i = 0.8 \, \mu\text{m}$
- Nitrogen gas [$U_i = 552 \, \text{eV}$]

*C. B. Schroeder et al., PRST-AB (2014)
INF&RNO is used to design and help the interpretation of the results of the STAGING experiment*

Modeling of e-bunch transport $LPA_1 \rightarrow LPA_2 +$ spectrum modulation after $LPA_2$ as a function of the delay between e-bunch and laser2 at the entrance of $LPA_2$.

Challenges/requirements:

- large range of Laser2 delays (-700 fs → +100 fs) with ~fs steps
- large delay → large sim. box in $LPA_2$ sim ($\sim 10 \lambda_p$)
- scanning bunch length (5 values)
- feedback with experiments (different runs w/ and wo/ cap lens, etc.)
- investigate sensitivity to parameters (laser energy, etc.)

→ thousands of simulations required!
Good agreement between INF&RNO modeling and staging experimental results

Experimental demonstration of STAGING: +100 MeV energy gain, 3% capturing efficiency in LPA2

Measurement

INF&RNO modeling (550 simulation runs)

Staging simulation cost with INF&RNO: \(~15\) CPUh (reduction \(~60,000\) compared to 3D PIC)

- separate grid for laser and wake
- quasi-static fluid for wake
- 3D PIC for bunch
INF&RNO is used to model current BELLA experiments: study of laser evolution in a 9 cm capillary* using realistic model for laser pulse

**Accurate model of the BELLA laser has been constructed based on measurements**

- **2013 measured long. laser intensity profile**
- **transverse intensity profile based on exp data**
  - top-hat near field: \( \frac{I}{I_0} = \left[ \frac{2J_1(r/R)}{(r/R)} \right]^2 \)
  - Gaussian

**9 cm LPA (nonlinear regime) simulation cost with INF&RNO:**
- \( \sim 10 \text{ CPUh} \) (reduction \( \sim 10^6 \))
- opt. laser solver
- quasi-static PIC for wake

\( U_{\text{laser}} = 15 \text{ J} \)

*Leemans, et al., PRL (2014)*
Comparison between experimental and simulated post-interaction laser optical spectra is routinely used in current BELLA experiments as independent density diagnostic.

- 80 simulations (density scan) of a 9 cm LPA for each value of the laser energy
- simulated spectra account for geometry and spectral sensitivity of spectrometer
- modeling reproduces key features in laser spectra at different energies
INF&RNO time-explicit PIC simulations allow for detailed investigation of particle self-injection and acceleration.

Simulation cost w/ INF&RNO: 300,000 CPUh (reduction >400) [explicit PIC + opt. laser solver] → will benefit from separate grid laser/wake

Leemans, et al., PRL (2014)

$U_{\text{laser}} = 16 \text{ J}$

$n_0 = 7 \times 10^{17} \text{ cm}^{-3}$

$R_m = 70 \mu\text{m}$

Simulated spectrum

* details very sensitive to laser-plasma param.

$E_{\text{max}} = 4.3 \text{ GeV}$

$Q[E>3\text{GeV}] = 80\text{pC}$

$x' = 0.4 \text{ mrad}$

$E = 4.2 \text{ GeV}$

$dE/E = 6\%$

$Q = 6\text{pC}$

$x' = 0.3 \text{ mrad}$

*best beam
INF&RNO is used to design future BELLA experiments: 10 GeV-class LPA with ionization-induced injector

Laser: $U=36$ J, $w_0=60$ μm, $T=66$ fs + realistic description of the pulse

Plasma target: capillary discharge + laser heater (MHD) $\rightarrow n_0=1.6\times10^{17}$ cm$^{-3}$, $R_{\text{matched}}=70$ μm

Simulation cost w/ INF&RNO: $\sim$50 CPUh (reduction $\sim$10$^6$) [quasi-static PIC wake + ADK ionization module for bunch generation + opt. laser solver]

* Several (~10s) simulations performed to optimize laser guiding and bunch propagation.

* Bobrova et al., POP (2013)

**Graphs:**
- Normalized laser strength, $a_0(s)$
- Energy [GeV], $dE/E$ [%], $\text{div}=0.33$ mrad
- Ionization region (2 cm, 1%N+99%H)

$Q=96$ pC
$E=8.4$ GeV
$dE/E=7.0$ %
$\text{div}=0.33$ mrad

$s=43$ cm
Summary and future research directions

INF&RNO is an accurate and efficient framework to model LPAs
- Validated with experiments at BELLA
- Several order of magnitude faster compared to standard “full” 3D PIC

Modeling with INF&RNO helps the interpretation of current experiments and guides the design of future experiments at BELLA + test new ideas

Future research directions:
- Exploring and developing reduced models to capture relevant physics
- Continue developing numerical schemes for improved efficiency/fidelity
- Combine different approaches to increase speedup
- Improving the parallel efficiency exploiting new hardware (GPUs, many-cores)