Parallel Kinetic Simulations Of Laser And Electron Transport Through High Energy Density Plasmas

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What is high energy density plasma?

- The kinetic energy density of a plasma is its pressure. The dimensionless parameter $N_D$ is related to the plasma pressure via the following relation:

\[
\frac{4\pi}{3} n\lambda_d^3 \equiv N_D = 2.1 \times 10^3 \frac{T_{keV}^2}{P_{MBar}^{1/2}}
\]

- When the plasma pressure exceeds $>1\text{MBar}$, then $N_D$ is large but finite so kinetic effects are important so is and the discrete nature of the plasma.

- Discreteness makes the underlying plasma physics, and the modeling of these plasmas difficult with a single code, and a wide range of models are needed, including:
  - particle-in-cell (PIC) models for nearly collisionless plasmas
  - collisional PIC models
  - Vlasov Fokker Planck (VFP) models.
Summary/Highlights of our research activities

- 2D OSIRIS simulations of laser plasma interactions in IFE plasmas
  - Suppression of BSRS using bandwidths under NIF relevant conditions. (see poster by Dr. Wen)
  - Suppression of HFHI using bandwidths under shock ignition relevant conditions (poster by me)
  - Simulation of BSRS in magnetized plasmas, understanding the roles magnetic fields (\// or \\perp to the laser) have on LPI’s under NIF relevant conditions. (work submitted to PRL)

- Evolution of nonlinear plasma waves in magnetic fields and other HED physics via the VFP code OSHUN (see poster by Dr. Joglekar)

- Through our NSF center PICKSC, we maintain several open source codes (including multi-level parallelization for running on the largest supercomputers) which can model HED plasmas with various levels of discrete effects:
  - OSIRIS (EM-PIC) —— Available through an MoU
  - OSHUN (VFP)
  - UPIC (PIC with EM, ES and Darwin field models)
  - UPIC-EMMA (EM-PIC)

- Training experimental and simulation students and post-docs in HED science and advanced computing.
Understanding LPI is critical to the success of the IFE program

~2 MJ into hohlraum, ~ 200KJ turns into x-ray, but just ~10’s KJ is converted to compress the target

Requires very symmetric compression

Requires exact timing

Lasers must hit where and when they are aimed! Laser plasma interactions, where the incident laser decays into two daughter waves, can deflect and reflect the incident laser, causing it to miss the target (and therefore degrades symmetry) The plasma wave produced can accelerate electrons which can pre-heat the target and making it harder to compress.

To push towards breakeven w.r.t. the 2MJ laser drive, or even ignition, will require better understanding and control of laser plasma interactions inside the Hohlraum
Laser and electron transport is important to IFE and NIF, and it is also rich in basic science: excellent for graduate students and post-doctoral researchers.

- In underdense plasmas, the laser undergo LPI (e.g., SRS), where the laser is converted into a nonlinear plasma wave and a backward going scattered light, often in a density gradient. In this scenario, the LPI problem is rich in basic science, including:
  - propagation of a single wave packet up (or down) a density gradient.
  - wave-wave interactions (e.g., excitation of ion waves from multiple EPW’s)
  - wave-particle interactions (generation of energetic electrons through nonlinear EPW’s)

All of these topics are of fundamental interest to the general plasma physics community.
OSIRIS 4.0

osiris framework
- Massively Parallel, Fully Relativistic Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium
  ⇒ UCLA + IST

OPEN ACCESS THROUGH MoU

code features
- Scalability to ~ 1.6 M cores
- SIMD hardware optimized
- Parallel I/O
- Dynamic Load Balancing
- Relativistic binary collisions
- Field ionization
- QED module
- Particle splitting/merging
- Quasi-3D
- Boosted frame
- GPGPU support
- Xeon Phi support

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OSIRIS, UPIC, and OSHUN access and use is international: Used in both HEDP and plasma based accelerator research
Simulations of LPI’s under IFE conditions are computationally challenging.

- Although the SRS problem is 1D (i.e., the instability grows along the direction of laser propagation). Higher dimensional effects in SRS is important -- each “beam” (right) is made up of 4 lasers, called a NIF “quad,” and each laser is not a plane wave but contains “speckles,” each one a few microns in diameter, and the 4 lasers can have same or different polarizations. And the LPI’s inside these hotspots can trigger LPI activities elsewhere via the following mechanisms, and therefore the multi-speckle problem is inherently 2D and even 3D.
  - “seeding” from backscatter light from neighboring speckles
  - “seeding” from plasma wave seeds from a neighboring speckle.
  - “inflation” where hot electrons from a neighboring speckle flatten the distribution function and reduce plasma wave damping.

- Polarization smoothing and external magnetic fields can introduce additional higher dimensional effects.

- 2D multi speckle simulations and 3D simulations with only 2 speckles will take up to 10’s of millions of hours, and 3D multi-speckle simulations will take ~ 1 billion CPU hours! (> 2 months on the largest supercomputer today)
As mentioned previously, static speckle patterns can be destabilizing. However, simulations have shown that adding bandwidth via ISI, SSD, and STUD can control & even suppress SRS growth. We have generalized our antenna module now to include:

- ISI — (using a script provided by NRL)
- SSD
- STUD
- etc...

Our simulations showed that, for “sufficiently large” bandwidth, SRS can be suppressed by the addition of temporal bandwidth.

**ISI (time dependent speckles, bandwidth = 3THz)**

**RPP (static speckles)**

**longitudinal e-field**

**transverse e-field**

**slope \( f_e(v) \) near the phase velocity**
Large scale 2D simulations of SRS with bandwidth (see poster by Dr. Han Wen at this meeting)

- In all of our large simulations using typical NIF parameters showed that SRS can be suppressed by temporal bandwidth. Below is one example from our collection of 2D SRS simulations. The simulation parameters are:
  - \( n \in [0.125, 0.135]n_c \)
  - \( T_o = 3 \) keV
  - Box size = 500 x 80 microns
  - \( I_{14} = 5 \)
  - \( L_n = 450 \) microns
  - \( G = 56 \)

<table>
<thead>
<tr>
<th></th>
<th>RPP</th>
<th>ISI (3 THz)</th>
<th>STUD (pulse length = 1/3 ps)</th>
<th>AP (1/3 ps)</th>
<th>STUD+AP</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I_{14} = 5 )</td>
<td>28%</td>
<td>18%</td>
<td>11%</td>
<td>0.2%</td>
<td>0.5%</td>
</tr>
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</table>

We have performed a large number of 2D simulations, ranging from 120 microns to 750 microns long, which is roughly \( \frac{1}{2} \) of the total length of the NIF inner beam. Typical width of the simulation box is 40 microns, which covers \(~14\) laser speckles. Simulations of this scale takes 1-10 million core hours each.

Linear background density
Immobile ions
Simulations of SRS in magnetized plasmas under NIF relevant conditions (Dr. B. Winjum, submitted for Phys. Rev. Lett.)

• A parallel B-field transversely constrains trapped particles
  - Yin et al* (with results for B = 114T) hypothesized that such fields would limit the collective SRS cascades in multiple speckles due to the interaction of multiple speckles, also the magnetic field can increase the plasma temperature, and Landau damp the driven plasma waves.

\[ \text{\textbf{B}}_{\text{ext}} \parallel \text{\textbf{k}}_{\text{EPW}} \]

• A perpendicular B-field can detrap particles in both physical space and velocity space, which can change the growth and the saturation mechanism of electron plasma waves. This mechanism is much more complicated and require PIC simulations.

\[ \text{\textbf{B}}_{\text{ext}} \perp \text{\textbf{k}}_{\text{EPW}} \]


1D OSIRIS simulations showed reflectivity is reduced when a perpendicular B field is included.

1D simulations show that external magnetic fields can reduce the SRS reflectivity, and also delay the intensity onset of the SRS instability.
Large 2D Multi-Speckle SRS simulations with external magnetic fields:

- **Plasma:**
  - Simulation Box: 120 microns x 40 microns (using 26 million grids and 7 billion particles)
  - Electron temperature: 3keV.
  - Plasma density: linear density gradient, $0.128n_c < n < 0.132n_c$

- **Laser:**
  - $I_{\text{avg}} = 8 \times 10^{14} \text{W/cm}^2$ (3 $\omega$ light)
  - polarized in the plane of the simulation.

- **External magnetic field:**
  - 0, 20T, 50T, bot perpendicular and parallel to laser propagation.
2D Multi-speckle SRS simulations showed that SRS can be limited by external $\mathbf{B}$ fields both parallel and perpendicular to laser propagation.

### Averaged reflectivity with external magnetic fields (no field: 13.2%)

<table>
<thead>
<tr>
<th>$B_{\text{ext}}$ (T)</th>
<th>$\parallel$</th>
<th>$\perp$</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>11.3%</td>
<td>4.6%</td>
</tr>
<tr>
<td>50</td>
<td>10.1%</td>
<td>0%</td>
</tr>
</tbody>
</table>

- $B \parallel k_{\text{EPW}}$ decreases SRS by limiting speckle interactions
- $B \perp k_{\text{EPW}}$ decreases SRS by altering the growth and saturation of EPWs by $(\mathbf{v} \times \mathbf{B})$
- In simulations with an external magnetic field of 50T perpendicular to laser propagation, SRS is completely eliminated.
The mission of the Particle-in-Cell and Kinetic Simulation Software Center (PICKSC) at UCLA is to support an international community of PIC and plasma kinetic software developers, users, and educators, and to increase the use of this software for accelerating the rate of scientific discovery. It aims to make available and document illustrative software programs for different computing hardware, a flexible Framework for rapid construction of parallelized PIC programs, and several distinct production programs. It will also include activities on developing and comparing different PIC algorithms and documenting best practices for developing and using PIC programs. The Center will also develop educational software for undergraduate and graduate courses in plasma physics and computer science. It will also sponsor an annual workshop to help build of community of developers and users. The PI is W.B. Mori and the co-PIs are V.K. Decyk, and F.S. Tsung.

http://picksc.idre.ucla.edu
UCLA develops and uses a set of PIC and fully kinetic codes to study high energy density plasma physics: Inertial confinement fusion, relativistic shocks, and plasma based acceleration: go to http://picksc.idre.ucla.edu or contact us if want access.

- OSHUN (open source, on GitHub)
  - Vlasov Fokker Planck
  - Expands distribution function into spherical harmonics with arbitrary anisotropy
- UPIC Framework (open source, on GitHub)
  - parallel Spectral solvers (ES, EM, Darwin)
  - Collisions
  - Gridless code
- UPIC-EMMA (to be open source soon)
  - EM PIC code optimized for the LWFA problem
  - binary collisions
  - open boundaries for fields & particles to study HED plasmas.

Optimized and scale well on largest computers
Dynamic Load Balancing
Works on GPUs/SIMD units

The codes at PICKSC serves a large number of users and a large number of communities (including space physics, advanced accelerators, and HED plasmas). We feel that having a large base of users and developers will enhance the quality of our production codes (e.g., OSIRIS). For the rest talk, I will show you an example where development done on OSIRIS for the AA community (LWFA) can have an impact on the HED community.
Quasi-3D Algorithm

- Field quantities are 2D in \((r,z)\) and azimuthally expanded in \(\phi\). (particles are in full 3D)
- First introduced by Lifschitz et al \([1]\) in 2009. Davidson et al \([2]\) added charge conservation in this algorithm.

\[
\mathbf{F}(r, z, \phi) = \Re\left\{ \sum_{m=0} \mathbf{F}^m(r, z)e^{im\phi} \right\}
= \mathbf{F}^0(r, z) + \Re\{\mathbf{F}^1\} \cos(\phi) - \Im\{\mathbf{F}^1\} \sin(\phi)
+ \Re\{\mathbf{F}^2\} \cos(2\phi) - \Im\{\mathbf{F}^2\} \sin(2\phi)
+ \cdots .
\]

\[
\begin{align*}
\partial_t B_r^m &= \frac{im}{r} E_z^m + \partial_z E_\theta^m \\
\partial_t B_\theta^m &= \partial_z E_r^m + \partial_r E_z^m \\
\partial_t B_z^m &= -\frac{1}{r} \partial_r (r E_\theta^m) + \frac{im}{r} E_r^m
\end{align*}
\]

The 3D field values \((\mathbf{E}, \mathbf{B}, \mathbf{J})\) are decomposed into azimuthal modes \((E^m, B^m, J^m)\)

\[
\begin{align*}
\partial_t E_r^m &= -\frac{im}{r} E_z^m - \partial_z E_\theta^m - J_\theta^m \\
\partial_t E_\theta^m &= \partial_z B_r^m - \partial_r E_z^m - J_z^m \\
\partial_t E_z^m &= \frac{1}{r} \partial_r (r B_\theta^m) - \frac{im}{r} B_r^m - J_z^m
\end{align*}
\]

up to now, the quasi-3D code has been primarily used to study the LWFA problem, as shown above.

(evolution of the nonlinear wake for full 3D(left) compared to the quasi-3D (right) under identical conditions)


We have applied quasi-3D code on HED plasma problems (preliminary results of laser solid interactions using quasi-3D OSIRIS)

We have added new boundary conditions for fields and particles to allow for the study of HED plasmas in quasi-3D. On the left is a quasi-3D simulation of laser solid interactions of the experiments performed on the TRIDENT laser.
Publications: Published or submitted
Many more in preparation

Publications:


Publications Submitted:


B. J. Winjum, F. S. Tsung, W. B. Mori, “Quenching of stimulated Raman scattering in the kinetic regime by external magnetic fields”.

A. Joglekar, B. J. Winjum, A. Tableman, H. Wen, M. Tzoufras, W. B. Mori, “Validation of OSHUN against collisionless and collisional plasma physics”, submitted to Plasmas Physics and Controlled Fusion

This project has trained many students and post-docs in HED science, both in theory/computation and experiments, including:

- C. Huang 2006 LANL
- J. Fahlen 2010 Arete Associates
- B. Winjum 2010 UCLA
- J. Ralph 2010 LLNL
- T. Wang 2011 Raytheon
- A. Pak 2012 LLNL
- D. Haberberger 2012 LLE
- I. Ellis 2014 Northrup Grumman
- A. Davidson 2016 UCLA
- J. Shaw 2016 LLE
- P. Yu 2016 Snapchat
- J. May 2017 UCLA
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Azimuthal Modal Decomposition
(Ref: Davidson et al, JCP (2015))

• Following Lifschitz et al, we developed the ability to model plasmas with a truncated Fourier decomposition in the \( \phi \) dimension

\[
F(r, z, \phi) = \Re \left\{ \sum_{m=0}^{\infty} F^m(r, z)e^{im\phi} \right\} \\
= F^0(r, z) + \Re\{F^1\} \cos(\phi) - \Im\{F^1\} \sin(\phi) \\
+ \Re\{F^2\} \cos(2\phi) - \Im\{F^2\} \sin(2\phi) \\
+ \cdots.
\]

• The 3D field values \((E, B, J)\) are decomposed into azimuthal modes \((E^m, B^m, J^m)\)

• This representation allows us to retain important 3D physics at the expense of a typical modest 2D simulation. This allows for the exploration of parameter space which was not possible before.

• Up to now the main application of the quasi-3D code is plasma based accelerators.
\[ E(x, y, t) = A(t) \sum_{mn} \hat{e}_{mn}(t) \sin[\omega_0 t + \psi_{mn} - (m-N_x/2)\Delta k_x x - (n-N_y/2)\Delta k_y y + \phi_{mn}(t)] \]

\( m, n \) refer to beamlet
\( N_x \) and \( N_y \) are number of beamlets in directions
\( A(t) \) is the amplitude envelope (on and off spikes for STUD pulses)
\( \hat{e}_{mn}(t) \) is the polarization unit vector
\( \psi_{mn} \) is the phase shift due to static phase plate
\( \phi_{mn}(t) \) is the phase modulation that corresponds

Differences between STUD pulses, FM SSD, RPM SSD, ISI for \( \phi_{mn}(t) \)

STUD pulses: \( \phi_{mn}(t) \) and \( \phi_{mn}(t+T) \) are uncorrelated (they can be constant when on). \( T \) is the “on+off” time of one spike

FM SSD: \( \phi_{mn}(t) = \sum_i \beta_i \sin(2\pi\Delta v_i[t - ms_x \Delta x']) + \sum_j \beta_j \sin(2\pi\Delta v_j[t - ns_y \Delta y']) \)

RPM SSD: \( \phi_{mn}(t) = \phi_m(t - ms_x \Delta x') + \phi_n(t - ns_y \Delta y') \), \( \phi_m \) and \( \phi_n \) are random processes

ISI: for any \( m \) and \( n \), \( \phi_{mn} \) are uncorrelated
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  - UPIC (PIC with EM, ES and Darwin field models)
  - UPIC-EMMA (EM-PIC)

- Training experimental and simulation students and post-docs in HED science and advanced computing.
The particle-in-cell method treats plasma as a collection of computer particles. The interactions do not scale as $N^2$ due to the fact the particle quantities are deposited on a grids and the interactions are calculated on the grids only. Because (# of particles) $>>$ (# of grids), the timing is dominated by the particle calculations and scales as $N$ (orbit calculation + current & charge deposition).

The code spends over 90% of execution time in only 4 routines.

These routines correspond to less than 2% of the code, optimization and porting is fairly straightforward, although not always trivial.
OSHUN: A relativistic Vlasov and a non-relativistic linearized Fokker-Planck

VLASOV

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + q \left( \mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0 \]

- **2D3P relativistic + multispecies**
- **Parallel**: decomposition in 2D configuration space
- **Explicit**: Maxwell’s equations
  - plasma and EM waves, instabilities, basic plasma physics
- **or implicit**: \( \mathbf{J} = \nabla \times \mathbf{B} \)
  - non-local transport, full target simulations

FOKKER-PLANCK

\[ \left( \frac{\delta f^0(v)}{\delta t} \right)_{ee} = \frac{4\pi}{3} \frac{\Gamma_{ee}}{v^2} \frac{\partial}{\partial v} \left[ \frac{1}{v} \frac{\partial W(f^0_0(v), v)}{\partial v} \right] \]

- **Explicit**, nonlinear sub-cycling for the isotropic part of \( f(p) \)
- **Conserves** energy and number density

\[ \left( \frac{\delta f}{\delta t} \right)_{ee} = \frac{4\pi}{\mu} F_f + \left( \frac{\mu - 1}{\mu + 1} \right) \nabla h(F) \cdot \nabla f + \frac{\nabla \nabla G(F) : \nabla f}{2} \]

- **Implicit**

**Spitzer heat conduction**

<table>
<thead>
<tr>
<th>( Z = 1 )</th>
<th>( Z = 2 )</th>
<th>( Z = 4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \kappa = 3.20 )</td>
<td>( \kappa = 4.96 )</td>
<td>( \kappa = 6.98 )</td>
</tr>
</tbody>
</table>

**VFP simul.**

| 3.21 | 4.93 | 7.00 |

*M. Tzoufras et al., JCP 270 (11) 6475-6494 (2011)*
Applications – Electron Plasma Waves

Non-linear electron plasma wave in the presence of an external magnetic field

- Particles are accelerated in the transverse direction
- Eventually become untrapped when parallel force becomes strong enough
- Distribution function becomes Maxwellian again, and Landau damping is reestablished.
Applications – Electron Plasma Waves

- Detrapping mechanism results in a re-emergence of Landau damping
  - Electron plasma wave is damped
- 50 T field is adequate for
  - $n = 0.128 \, n_c$
  - $T = 3 \, \text{keV}$

\[
\frac{\omega_B}{\gamma_{LD}} \approx 12 \\
\frac{\omega_c}{\omega_p} \approx 5 \times 10^{-4} \\
\omega_B > \gamma_{LD} \gg \omega_c
\]
UCLA Particle-in-Cell and Kinetic Simulation Software Center (PICKSC), NSF funded center whose Goal is to provide and document parallel Particle-in-Cell (PIC) and other kinetic codes.

http://picksc.idre.ucla.edu/

github: UCLA Plasma Simulation Group

Planned activities

- Provide parallel skeleton codes for various PIC codes on traditional and new parallel hardware and software systems.
- Provide MPI-based production PIC (& VFP!!) codes that will run on desktop computers, mid-size clusters, and the largest parallel computers in the world.
- Provide key components for constructing new parallel production PIC codes for electrostatic, electromagnetic, and other codes.
- Provide interactive codes for teaching of important and difficult plasma physics concepts
- Facilitate benchmarking of kinetic codes by the physics community, not only for performance, but also to compare the physics approximations used
- Documentation of best and worst practices, which are often unpublished and get repeatedly rediscovered.
- Provide some services for customizing software for specific purposes (based on our existing codes)

Key components and codes will be made available through standard open source licenses and as an open-source community resource, contributions from others are welcome.
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