

Enabling Numerical Modeling of Extreme-Intensity Laser Produced Hot Dense Plasma



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2D Simulation Parameters



Simulation box geometry

Ionization wave in silica driven by relativistic laser pulse



Hot electron transport in insulator target

Ionization wave in silica driven by relativistic laser pulse



Hot electron transport in insulator target

Ionization wave in silica driven by relativistic laser pulse





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Fast Electron Beam Preceding Ionization Front



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What physics is necessary in simulation to study HEDP in ultra-intense LPI?



Everything happens in less than a picosecond (10⁻¹²s). (Information is very limited in experiments...)

Summary: Physics in ultra-fast heated solid target



Plasma discharge Kinetic instabilities and wave excitations Collisional energy transport and target heating



The physics in the laser isochoric heating is complicate. The collective effects and the collisional effects are competing inside the target.

We need a kinetic simulation code with the atomic physics models.

Friday, January 7, 2011

What model will be capable of simulating ultra-intense laser produced HEP plasmas?



LPI - target region will not be able to be separated. We need to solve both regions self-consistently.

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Transport region: atomic physics





Energy transport depends on resistive magnetic fields inside solid





Resistive magnetic fields depend on how resistivity evolves during the interaction. Correct resistivity and dynamic ionization are crucial in the modeling. Resistive magnetic field ~ 10 - 100 MG.

Challenges in computational modeling of HEDLP by LPI



- Model requires to resolve extremely large density scales plasmas. (e.g. 10¹⁹ ~ 10²⁶ cm⁻³ for Fast Ignition)
- Model requires the Coulomb collision to simulate the energy transport and heating in HEDLP. (i.e. resistive effects, scattering)
- Model requires the dynamics ionization processes since the plasma electron density and the resistivity depend on the charge state inside the target. (e.g. ultra-fast heated thin metal target by LPI)
- Model should have a strict energy conservation to avoid the numerical heating/numerical ionization in HEDLP.

PICLS is a particle-in-cell simulation code, which is designed to solve the above issues, featuring the binary collisions among charged particles and the ionization processes.



Y. Sentoku, and A. J. Kemp, "Numerical methods for particle simulations at extreme densities and temperatures", J. Comput. Phys. 227, 6846 (2008)

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PICLS: 1, 2, & 3D laser plasma simulation code





Adopting the high order interpolation, PICLS has much less numerical heating with even 40 times larger mesh of Debye length. Drastically reducing PIC cost.



III. Full relativistic collision model for weighted particles

Based on Takizuka & Abe binary collision model (1977).
Extended our early work of weakly relativistic model (Sentoku, 1998) to the full relativistic regime.
Extended the model for weighted particle simulations.
Verified with the theoretical prediction (stopping power, energy exchange).

Basic equations of PIC simulation - non-thermal & non-equilibrium plasma -

• Maxwell's equations (PDE: solved on grids)

$$\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c} \mathbf{J}$$
$$\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

• Equation of particles (ODE)

 $m_i \gamma_i$

dt

$$\frac{d\mathbf{P}_i}{dt} = q_i (\mathbf{E}_i + \frac{\mathbf{P}_i}{m_i c \gamma_i} \times \mathbf{B}_i)$$
$$\frac{d\mathbf{x}_i}{m_i c \gamma_i} = \frac{\mathbf{P}_i}{m_i c \gamma_i}$$



 γ_i : Lorentz factor

Particle-in-Cell (PIC) simulation with Atomic processes (Monte Carlo models)



Finite Differential Time Domain method (FDTD)

Maxwell equations

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

Finite differential equations

$$\frac{\mathbf{E}^{n+1} - \mathbf{E}^n}{\Delta t} = c\nabla \times \mathbf{B}^{n+1/2} - 4\pi \mathbf{J}^{n+1/2}$$

$$\frac{\mathbf{B}^{n+1/2} - \mathbf{B}^{n-1/2}}{\Delta t} = -c\nabla \times \mathbf{E}^n$$

Definition of fields on grid

Both the space and time centered differences.





FDTD: Numerical dispersion

by inserting a plane wave $E(x,t) = E_{\theta} \exp[i(\mathbf{k} \cdot \mathbf{x} - \omega t)]$

$$\left(\frac{\sin\omega\Delta t/2}{c\Delta t}\right)^2 = \left(\frac{\sin k_x \Delta x/2}{\Delta x}\right)^2 + \left(\frac{\sin k_y \Delta y/2}{\Delta y}\right)^2$$

Obviously $\boldsymbol{\omega}$ is real (stable) when

$$c\Delta t < c\Delta t_c = \sqrt{\frac{\Delta x \Delta y}{\Delta x^2 + \Delta y^2}}$$





 $\lambda \Delta x=5, \Delta t=0.7 \Delta t_c$



Waves delay due to the numerical dispersion, since then a fine resolution (small grid&time-step) is necessary to simulate the laser propagation in a long (cm scale) distance.

Directional splitting (DS) method in PICLS



Maxwell equations

P-pol component

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$
$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

$$\frac{\partial}{\partial t} \begin{pmatrix} E_x \\ E_y \\ B_z \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -c \\ 0 & -c & 0 \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} E_x \\ E_y \\ B_z \end{pmatrix} + \begin{pmatrix} 0 & 0 & c \\ 0 & 0 & 0 \\ c & 0 & 0 \end{pmatrix} \frac{\partial}{\partial y} \begin{pmatrix} E_x \\ E_y \\ B_z \end{pmatrix} = - \begin{pmatrix} J_x \\ J_y \\ 0 \end{pmatrix}$$

Step1: x-direction

$$E_{y}^{\pm} = B_{z} \pm E_{y}$$

$$\frac{\partial E_{y}^{+}}{\partial t} + c \frac{\partial E_{y}^{+}}{\partial x} = -\frac{1}{2}J_{y}$$

$$\frac{\partial E_{y}^{-}}{\partial t} - c \frac{\partial E_{y}^{-}}{\partial x} = +\frac{1}{2}J_{y}$$
Step2: y-direction
$$E_{x}^{\pm} = B_{z} \mp E_{x}$$

$$\frac{\partial E_{x}^{+}}{\partial t} - c \frac{\partial E_{x}^{+}}{\partial y} = -\frac{1}{2}J_{x}$$

$$\frac{\partial E_{x}^{-}}{\partial t} - c \frac{\partial E_{x}^{-}}{\partial y} = -\frac{1}{2}J_{x}$$

$$no d/dy \text{ for } (Ey, Bz)$$

$$\frac{\partial E_{x}^{+}}{\partial t} - c \frac{\partial E_{x}^{-}}{\partial y} = -\frac{1}{2}J_{x}$$

$$\frac{\partial E_{x}^{-}}{\partial t} - c \frac{\partial E_{x}^{-}}{\partial y} = -\frac{1}{2}J_{x}$$

$$\frac{\partial A_{y}^{+}}{\partial t} = -\frac{1}{2}J_{x}$$



Equation of wave with constant velocity c (c>0)



Finite difference equation,

 $f(x_i + \Delta x, t_n + \Delta t) = f(x_i, t_n)$



When $\Delta x = c \Delta t$, the numerical solution of this equation is very easy, just copy the grid value to the next grid.

DS: Calculate the numerical dispersion



Step1: x-direction

$$\begin{split} E_{y}^{n+1} &= E_{y0} \exp[k_{x}x_{i} + k_{y}y_{j} - \omega(t_{n} + \Delta t)] \\ &= \frac{B_{z0} + E_{y0}}{2} \exp[k_{x}(x_{i} - \Delta x) + k_{y}y_{j} - \omega(t_{n})] - \frac{1}{2}J_{y,i-1/2,j} \\ &- \frac{B_{z0} - E_{y0}}{2} \exp[k_{x}(x_{i} + \Delta x) + k_{y}y_{j} - \omega(t_{n})] - \frac{1}{2}J_{y,i+1/2,j} \\ B_{z}^{n*} &= B_{z0} \exp[k_{x}x_{i} + k_{y}y_{j} - \omega(t_{n}^{*})] \\ &= \frac{B_{z0} + E_{y0}}{2} \exp[k_{x}(x_{i} - \Delta x) + k_{y}y_{j} - \omega(t_{n})] - \frac{1}{2}J_{y,i-1/2,j} \\ &+ \frac{B_{z0} + E_{y0}}{2} \exp[k_{x}(x_{i} + \Delta x) + k_{y}y_{j} - \omega(t_{n})] + \frac{1}{2}J_{y,i+1/2,j} \end{split}$$



Step2: y-direction

$$\begin{split} E_x^{n+1} &= E_{x0} \exp[k_x x_i + k_y y_j - \omega(t_n + \Delta t)] \\ &= -\frac{B_{z0}}{2} \exp[k_x x_i + k_y (y_j - \Delta y) - \omega(t_n^*)] + \frac{E_{x0}}{2} \exp[k_x x_i + k_y (y_j - \Delta y) - \omega(t_n)] - \frac{1}{2} J_{x,i,j-1/2} \\ &+ \frac{B_{z0}}{2} \exp[k_x x_i + k_y (y_j + \Delta y) - \omega(t_n^*)] + \frac{E_{x0}}{2} \exp[k_x x_i + k_y (y_j + \Delta y) - \omega(t_n)] - \frac{1}{2} J_{y,i,j+1/2} \\ B_z^{n+1} &= B_{z0} \exp[k_x x_i + k_y y_j - \omega(t_n + \Delta t)] \\ &= \frac{B_{z0}}{2} \exp[k_x x_i + k_y (y_j - \Delta y) - \omega(t_n^*)] - \frac{E_{x0}}{2} \exp[k_x x_i + k_y (y_j - \Delta y) - \omega(t_n)] + \frac{1}{2} J_{x,i,j-1/2} \\ &+ \frac{B_{z0}}{2} \exp[k_x x_i + k_y (y_j + \Delta y) - \omega(t_n^*)] + \frac{E_{x0}}{2} \exp[k_x x_i + k_y (y_j + \Delta y) - \omega(t_n)] - \frac{1}{2} J_{y,i,j+1/2} \end{split}$$

Friday, January 7, 2011







Map of phase velocity by DS

Map of phase velocity by FDTD

NO numerical dispersion along the grids.



 $\lambda \Delta x=5, \Delta t=0.7 \Delta t_c$



Waves delay due to the numerical dispersion, since then a fine resolution (small grid&time-step) is necessary to simulate the laser propagation in a long (cm scale) distance.

Wakefield simulation by PIC



PIC solves the Maxwell equations and kinetic equations of charged particles.



Laser: a = 1, pulse length = 5λ



10 mesh is quite enough for one laser wavelength with the DS scheme. The FDTD needs two times more meshes in one direction. numerical modeling of hot dense plasma is challenging due to large scale both in time and space

e.g. • fast ignition in inertial confinement fusion (ICF) time scale ~ ps, spatial scale ~ 100 μm

time step ~ I/ω_p ~ 0.01 fs \rightarrow simulation time scale ~ ps mesh size $\propto T_e^{1/2}/\omega_p$ ~ 0.001 µm \rightarrow simulation scale 100 um

> time step will be >10⁵ number of mesh will be ~10^{5×N_D} impossible by current computers!!

Can we extend grid size greater than debye length without having numerical heating?

High order interpolation to extend grid size ~ plasma skin length >> Debye length

- reduce numerical heating by high order interpolation -

Time evolution of system energy of thermal plasma

demonstration (1d) - *internal energy evolution* -Plasma: solid density (40n_c), T_{e0}=10eV (without a laser pulse)

To resolve the above plasma with standard PIC simulation, 1000 grids/µm resolution is required to suppress the numerical heating!

- reduce numerical heating by high order interpolation -

demonstration (1d) - *internal energy evolution* -Plasma: solid density (40n_c), T_{e0}=10eV (without a laser pulse)

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Time evolution of system energy of thermal plasma

4 order magnitude less computational cost in 2D!!

Long time stability with high order interpolation - demonstration by 2D PIC -



Time evolution of thin plasma after short pulse irradiation

target $40n_c$, thickness 2 um, box:10um x 6um a=2, 30 fs, np=10, Δx =1um/25

Relativistic collision model for weighted particles

 $\frac{T_0}{m_{\rm e}c^2} =$



 $v_{lphaeta} = rac{4\pi (e_lpha e_eta)^2 n_{
m l} L}{p_{
m rel}^2 v_{
m rel}},$

T₀: transition temperature from Spitzer regime to degenerate regime

 $v_{\alpha\beta}=\frac{4m_{\rm e}Ze^4L}{3\pi\hbar^3}$

 $\left(\frac{\sqrt{2}\pi^{3/2}\hbar^3 n_{\rm h}}{m^{3/2}}\right)$

Collision frequency in degenerate regime

Y.T. Lee, R.M. More, Phys. Fluids 27 (1984) 1273.

Y. Sentoku and A. J. Kemp, J. Comp. Phys. 227, 6846 (2008).

Full relativistic kinematic of energy transfer in collision

Binary collision model (Takizuka & Abe, J. Comp. Phys., 1977) Weakly relativistic collision model (Sentoku et al., J. Phys. Soc. Jpn, 1998)





laboratory frame



center of mass frame, γ_{cm}

Perfect energy and momentum conservation!

Full relativistic kinematic of energy transfer in collision



Full relativistic kinematic of energy transfer in collision



Energy transfer rate from hot electrons to ions - test simulation of relativistic collision model -



Electron stopping power in hydrogen plasma - test simulation of e-e collision -



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NIST database: electron stopping power in hydrogen gas

Collision model of weighted particles in PICLS

Rejection method & Partial scattering method -



Perfect energy conservation & statistical momentum conservation

Beam relaxation: benchmark of weighted particle collision model

Bulk e- 90% Beam e- 10% with p_{drift}=0.7m_ec n=10²⁵ 1/cm³ e-e collision

case A (TA77): uniform weighted particle, 500/cell (bulk 450, beam 50) case B (NY98): weighted 250/cell (bulk 125, beam 125) case C (SK07): weighted 250/cell (bulk 125, beam 125)



Rejection method has serious energy violation with small number of particle



Partial scattering method has a perfect energy conservation with small particles.

ionization

Field ionization Collisional ionization (equilibrium model) Collision for partially ionized plasmas

Field ionization in PICLS - Tunneling ionization model -



Ionization Rate (Landau and Lifshitz, Quantum Mechanics)

$$W[E(t)] = 4\omega_a \left(\frac{\varepsilon_i}{\varepsilon_h}\right)^{5/2} \frac{E_a}{E(t)} \exp\left[-\frac{2}{3}\left(\frac{\varepsilon_i}{\varepsilon_h}\right)^{3/2} \frac{E_a}{E(t)}\right]$$

- We use the ADK formula to calculate the ionization rate W(E). Ionization probability R=1-exp[-W(E)△t], E is the electric field.
- Condition of ionization: R > random number [0-1].
- The new electron has the same weight and position as the ionized ion. It is created with no momentum.

$$j_{ion}^{(i)} = \frac{U_p^{eV}}{|E_{norm}|^2 \Delta t} E^{(i)}$$

Ionization current

 ε_i : ionization potential ε_h : potential of hydrogen (13.6eV)

$$\omega_a = \frac{m_e e^4}{\hbar^3} \qquad E_a = \frac{m^2 e^5}{\hbar^4}$$

Field calculation

Field ionization and calculation of the ionization current

Particle movement

Current calculation

S. Kato, Y. Kishimoto, and J. Koga, Phys. Plasmas 5, 292 (1998).

Ionization model in PICLS

Thomas Fermi model (equilibrium model) -

80

70

Bulk electrons are heated up by hot electrons via collisional or collective processes.

collisional PIC.

The heating is calculated by the

1) Average charge state is calculated as function of bulk electron temperature T_e and local mass density ρ . The function $Z(T_e, \rho)$ is obtained by fitting the EOS database.

2) After the ionization is done, new electrons are born, and the bulk electrons will lose the ionization energy (by shrinking momenta to conserve energy).

The field ionization is also implemented for the insulator target.

Friday, January 7, 2011





Proton Image as result of MA current transport in AI, Cu, and Au targets



What makes a modulated transport?

- 1. instabilities at the interface?
- 2. modulation inside target?
- 3. instabilities at the vacuum interface



LULI Experiment



Laser: I=6x10¹⁹ W/cm² duration=350fs, spot=8um



LULI Experiment



Laser: I=6x10¹⁹ W/cm² duration=350fs, spot=8um



Friday, January 7, 2011

Benchmark 2D Code with Collsion&Ionization - MA current transport in AI, Cu, and Au targets-









Resistivity term is a minor term in fixed Z case.

Resistivity evolution in ionizing target - competition between heating and cooling -

Temperature and average Z distribution inside 1um at t=80fs







ionization consumes local energy



Resistive magnetic fields evolution in high Z target - competition between heating and cooling (ionization) -





Resistive magnetic fields evolution in high Z target - competition between heating and cooling (ionization) -





Resistivity η drops by bulk heating, however η recovers in high Z target due to local cooling via ionization. Strong B fields grow in the ionization wave (slower than fast e-).

Friday, January 7, 2011

Ionization affects the resistivity inside target and excites 100MG resistive magnetic fields in Au & Cu



Resistive B-field

$$\frac{\partial \mathbf{B}}{\partial t} = -\left(\eta \nabla \times \mathbf{J} + \nabla \eta \times \mathbf{J}\right)$$

•Al target: ∇×J term is dominant. Resistive magnetic fields is ~ 5MG. Modulated.

- Au target: ∇η term is dominant. Strong resistive magnetic fields ~ 100MG. Single channel.
- •Cu target: η has a twin peak distribution. Strong resistive fields like gold, but twin channel (2D), would be hollow (3D) pattern.

The cyclotron frequency will become ~ ω₀ (laser frequency) under 100MG B-field. The fine resolution of sub-micron, subfemtosecond is required!



Pattern of sheath is consistent with the proton image observed in different material, AI, Cu, and Au in LULI exp.





Fig. Electrostatic potential at the target rear in 1um. Plots observed at the time when the sheath potential has the maximum, and time-averaged during 100 fs.



Proton has a smooth image from thicker Cu target



Ionization driven resistive magnetic fields extend only in the heated region (propagation speed ~ 0.15c, heat diffusion velocity). MeV electrons, which go beyond the strong B fields, are spraying and make a smooth potential at the target rear.

Friday, January 7, 2011



- We had studied the MA current transport in high conductive target by collisional/ionization PICLS code.
- We found that the current term (∇×J) is dominant in low Z target (AI) as a source term of resistive magnetic fields. While the resistivity term (∇η) plays an important role, and produces extremely strong B-fields (~0.1gigagauss) in high Z target (Cu, Au). Important to include ionization in Cu&Au targets.
- The resistive magnetic field structure depends on the resistivity evolution in the heated region. The Cu target has a twin jets (hollow) structure, and the Au has a single channel under the current experiment/simulation conditions.
- Hot electron transport is affected by the strong resistive B fields, and it makes modulation in the sheath potential at target rear, which is recorded in the MeV proton image. PICLS shows a consistent potential profile with the proton images for AI, Cu, and Au targets.















