Particle-in-cell simulations for Nanoplasmonic Laser Induced Fusion Experiments

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Fusion does not happen spontaneously on Earth

Total fusion energy \( E_f = \frac{1}{4} n^2 \tau \epsilon \langle \nu \sigma \rangle \)

\( \eta E_f \) is the usable energy

The loss is \((1 - \eta)(E_0 + E_b)\)

\( E_0 = 3nkT, \ E_b = bn^2 \tau \sqrt{T} \) (thermal bremsstralung)

Giving the gain factor: \( Q = \frac{\eta\epsilon n^2 \tau \nu \sigma}{4(1-\eta)(3kT+bn\tau \sqrt{T})} \)

\( Q \) must be \( Q > 1 \) for energy production

This also means \( n\tau > \frac{3kT(1-\eta)}{\frac{1}{4} \epsilon \eta \langle \nu \sigma \rangle - b(1-\eta) \sqrt{T}} \rightarrow \text{LC} \)

Fulfilling the Lawson criterion

-Magnetically confined plasmas: increase confinement time

-Inertial confinement fusion: increase density of fusion plasma
Direct vs Indirect drive

LLE OMEGA Laser
60 beam direct drive

NIF Laser
Indirect drive

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Rayleigh-Taylor instabilities

Energy must be delivered as symmetric as possible!

Different levels of corrugation of the shell surfaces:

- **Left:** same roughness of inner and outer surface as specified for the NIF target
- **Center:** outer surface roughness is twice the NIF level
- **Right:** DT inner surface roughness three times larger than NIF specifications

[S. Atzeni et al., Nucl. Fusion 54, 054008 (2014).]
Figure 5.10: Smooth change from spacelike to timelike detonation

Constant absorptivity

\[ \alpha_{k_{\text{middle}}} = \alpha_{k_{\text{edge}}} \]

Simultaneous volume ignition is only up to 12%

[L.P. Csernai & D.D. Strottman, Laser and Particle Beams 33, 279 (2015)]
(a) Left: Single core-shell nano-sphere. Right: Rectangular lattice of nano-spheres in a transverse layer of the target.
(b) Optical cross-section of an individual core-shell nano-sphere optimized to absorb light at 800 nm wavelength and optical response of the same core-shell nano-spheres composing a rectangular lattice.
Changing absorptivity


\[ \alpha_{k_{\text{middle}}} \approx 4 \times \alpha_{k_{\text{edge}}} \]

Simultaneous volume ignition is up to 73%
Flat target

Schematic view of the cylindrical, flat target of radius, $R$, and thickness, $h$.

$V = 2\pi R^3$, $R = \frac{3\sqrt{V}}{2\pi}$, $h = \frac{3\sqrt{4V}}{\pi}$.

[L.P. Csernai, M. Csete, I.N. Mishustin, A. Motornenko, I. Papp, L.M. Satarov, H. Stcker & N. Kroó, Radiation-Dominated Implosion with Flat Target, Physics and Wave Phenomena, 28 (3) 187-199 (2020)]
Deposited energy per unit time in the space-time plane across the depth, $h$, of the flat target. (a) without nano-shells (b) with nano-shells

To increase central absorption we used the following distribution:

$$\alpha_{ns}(s) = \alpha_{ns}^c + \alpha_{ns}(0) \cdot \exp \left[ 4 \times \frac{\left( \frac{s}{100} \right)^2}{\left( \frac{s}{100} - 1 \right) \left( \frac{s}{100} + 1 \right)} \right].$$
Introduction
Simulations and software
Modelling the Nanorod
Conclusions and the future
PIC methods in general
Laser Wake Field Collider

Particle In Cell methods


A super-particle (marker-particle) is a computational particle that represents many real particles.

Particle mover or pusher algorithm as standard Boris algorithm.

Finite-difference time-domain method for solving the time evolution of Maxwell’s equations.

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## Available software

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<th>Computational application</th>
<th>Web site</th>
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<td>Open to academic users but signup required [21]</td>
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<td>Closed (Collaborators with MoU)</td>
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(a) Old and new strategies. $G = 64$ group of tasks and $F = N/128$ master tasks.  
(b) Time spent for **writing particle positions** blue, time spent for **grid based outputs** (EM fields, densities) marked with red.  
General layout of the EPOCH code

- **update_eb_fields_half**
  - $E_n$
  - $B_n$
  - $E_{n+1/2}$
  - $B_{n+1/2}$

- **push_particles**
  - $X^n$
  - $P^n$
  - $J^n$
  - $X^{n+1/2}$

- **update_eb_fields_full**
  - $E_{n+1/2}$
  - $B_{n+1/2}$
  - $E_{n+1}$
  - $B^{n+1}$

$t = t(n)$

- **Code execution flow**

- **EPOCH 4.0 dev manual**
  - (input) deck
  - housekeeping
  - io
  - parser
  - physics_packages
  - user_interaction

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FDTD in EPOCH

- \( E_{n+\frac{1}{2}} = E_n + \frac{\Delta t}{2} \left( c^2 \nabla \times B_n - \frac{j_n}{\varepsilon_0} \right) \)
- \( B_{n+\frac{1}{2}} = B_n - \frac{\Delta t}{2} \left( \nabla \times E_{n+\frac{1}{2}} \right) \)
- Call particle pusher which calculates \( j_{n+1} \)
- \( B_{n+1} = B_{n+\frac{1}{2}} - \frac{\Delta t}{2} \left( \nabla \times E_{n+\frac{1}{2}} \right) \)
- \( E_{n+1} = E_{n+\frac{1}{2}} + \frac{\Delta t}{2} \left( c^2 \nabla \times B_{n+1} - \frac{j_{n+1}}{\varepsilon_0} \right) \)
Solves the relativistic equation of motion under the Lorentz force for each marker-particle

\[ p_{n+1} = p_n + q \Delta t \left[ E_{n+\frac{1}{2}} \left( x_{n+\frac{1}{2}} \right) + v_{n+\frac{1}{2}} \times B_{n+\frac{1}{2}} \left( x_{n+\frac{1}{2}} \right) \right] \]

\( p \) is the particle momentum, \( q \) is the particle’s charge, \( v \) is the velocity.
\( p = \gamma m v \), where \( m \) is the rest mass, \( \gamma = \left[ (p/mc)^2 + 1 \right]^{1/2} \)

Villasenor and Buneman current deposition scheme [Villasenor J & Buneman O 1992 Comput. Phys. Commun. 69 306], always satisfied: \( \nabla \cdot E = \rho/\varepsilon_0 \), where \( \rho \) is the charge density.
Particle shape

Figure 3: Second order particle shape function

First order approximations are considered

\[ F_{part} = \frac{1}{2} F_{i-1} \left( \frac{1}{2} + \frac{x_i - X}{\Delta x} \right)^2 + \frac{1}{2} F_i \left( \frac{3}{4} - \frac{(x_i - X)^2}{\Delta x^2} \right)^2 + \frac{1}{2} F_{i+1} \left( \frac{1}{2} + \frac{x_i - X}{\Delta x} \right)^2 \]

[EPOCH 4.0 dev manual]
Laser parameters:

wavelength of $\lambda = 1\mu m$, full pulse length $\Delta t = 52fs$, focus diameter is $2R = 40\mu m$, $3.0 \cdot 10^{19}$ W/cm$^2$ top intensity.

EPOCH includes a number of ionisation models by which electrons ionise in both the field of an intense laser and through collisions.

Epoch also includes Coulomb collisions

Nanorod

Field simulation

Particle simulation

$\varepsilon(x, y, z)$

Mesh
Medium

Particle
Shape function

Mesh
Medium

[W. J. Ding, et al., Particle simulation of plasmons Nanophotonics, vol. 9, no. 10, pp. 3303-3313 (2020)]
Nanorod

**Field solver:**

\[ \epsilon(\omega) = 1 - \frac{\omega_p^2}{(\omega^2 + i\gamma\omega)} \]

where \( \omega_p \) is the plasma frequency: \( \sqrt{\frac{n_e e^2}{m'\epsilon_0}} \)

\( \gamma \) is the damping factor or collision frequency: \( \gamma = \frac{1}{\tau} \) and \( \tau \) is the average time between collisions

**Particle simulation:**

\[ \frac{\partial E}{\partial t} = \frac{1}{\mu_0 \epsilon_0} \nabla \times B - \frac{J}{\epsilon_0}, \quad \frac{\partial B}{\partial t} = -\nabla \times E \]

\[ \gamma_i m_i v_i = q_i (E_i + v_i \times B_i), \quad \gamma_i \] is the relativistic factor
Kinetic Modelling of the Nanorod

Nanorod inside a PIC simulation box
Considerations for the simulation box:

\[ S_{CB} = 530 \times 530\text{nm}^2 = 2.81 \times 10^{-9}\text{cm}^2 \] and length of 

\[ L_{CB} = 795\text{nm} \]

beam crosses the box in 

\[ T = 795\text{nm/c} = 2.65\text{fs} \]

Nanorod size: 25 nm diameter with 75 nm length

Pulse length: \( 40\times\lambda/c = 106 \text{ fs} \)

Intensity: \( 4 \times 10^{15} \text{ W/cm}^2 \)
Kinetic Modelling of the Nanorod

Evolution of the fields

$E_y$ evolution video
energy in the box **without nanorod** antenna $3 \times 10^{-8}$ J (black line) **nanorod** absorbs EM energy reducing it to $2.3 \times 10^{-8}$ J (red line) **deposited** energy in the nanorod (green line) results in light absorption cross section nearly 35 times higher than its geometrical cross section
Conclusions, Looking forward

- The model returns the analytical calculations regarding the absorption cross section
- The model is highly idealized
- Next step is material around the nanorods
- Fully dedicated software for the project is required
- Next step is estimating the target pre-compression
Pre-compression
Fourier-Bessel PIC method

[Rémi Lehe et al., A spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm, Computer Physics Communications Volume 203]