Particle Simulations for Nanoplasmonic Laser Induced Fusion Experiment

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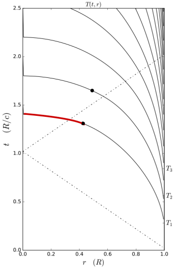
László P. Csernai [1,2,3,6], Norbert Kroó [1,2,12] (part of NAPLIFE Collaboration)



Simultaneous volume ignition happens only up to 12% in an irradiated target

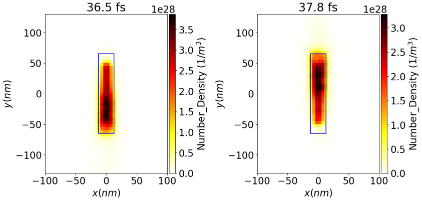
NAno-**P**lasmonic **L**aser **I**nduced **F**usion **E**xperiment was proposed to overcome instabilities and **increase** light **absorption** in the target. **Resonant gold nanoantennas** can be used to **enhance** absorption. [L.P. Csernai, M. Csete, I.N. Mishustin, A. Motornenko, I. Papp, L.M. Satarov, H. Stcker & N. Kroó, Radiation- Dominated Implosion with Flat Target, *Physics and Wave Phenomena*, **28** (3) 187-199 (2020)]

Classically, when simulating gold nanoparticles, electromagnetic responses are described by **bulk permitivity** and Maxwell's equations are solved with Finite Difference Time Domain methods, **without** focusing on **motion of electrons**.

$\epsilon(\omega) = 1 - \frac{\omega_p^2}{(\omega^2+i\gamma\omega)}$ where ω_p is the plasma frequency, γ is the damping factor or collision frequency.

On these scales conduction electrons behave like strongly coupled **plasma**. [Lukas Novotny, Effective Wavelength Scaling for Optical Antennas, Phys. Rev. Lett. **98**, 266802 (2007).]

We simulated nanoantennas with colliding electrons around heavy gold ions using **Partcle-In-Cell** method (EPOCH). [T.D. Arber et al 2015 Plasma Phys. Control. Fusion 57 113001]

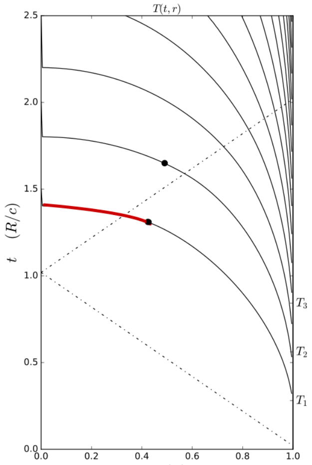


Result in vacuum for 25x130 nm nanorod orthogonal to the beam direction, x. The electro-magnetic field drives the conduction electrons into fluctuations.

The nanorod here has a light absorption cross section **66.5** times bigger than its geometrical cross section.

The model is **idealized**, however, it shows **qualitative potential** for future use in plasma simulations.

From Relativistic Fluid Dynamics



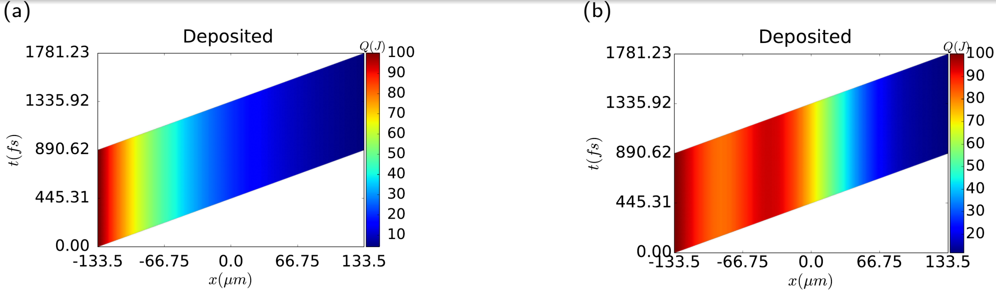
[L.P. Csernai & D.D. Strottman, Laser and Particle Beams 33, 279 (2015)]

$$\alpha_{k_{middle}} = \alpha_{k_{edge}}$$

Simultaneous volume ignition is only up to 12%

See presentation of **Lászlo P. Csernai** titled: **Development in Nano Fusion** on **February 3, 18:00 PM**, Session 12

Varying absorptivity

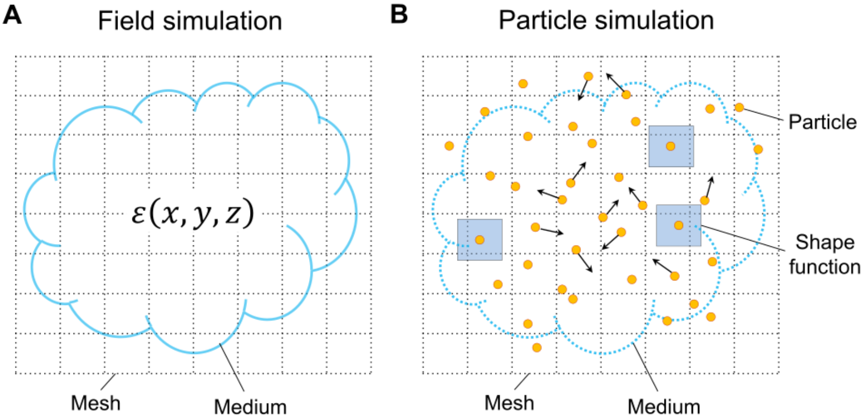


Deposited energy per unit time in the space-time plane across the depth, *h*, of the flat target. **(a) constant** absorptivity **(b) changing** absorptivity

To increase central absorption we used the following distribution:

$$\alpha_{ns}(s) = \alpha_{ns}^{C} + \alpha_{ns}(0) \cdot \exp\left[4 \times \frac{\left(\frac{s}{100}\right)^{2}}{\left(\frac{s}{100} - 1\right)\left(\frac{s}{100} + 1\right)}\right].$$

Nanorod



[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 ω_p is the plasma frequency: $\sqrt{\frac{n_e e^2}{m' \epsilon_0}}$

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

Particle simulation:

$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\mu_0 \epsilon_0} \nabla \times \boldsymbol{B} - \frac{\boldsymbol{J}}{\epsilon_0}, \ \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}$$

$\gamma_i m_i \boldsymbol{v}_i = q_i(\boldsymbol{E}_i + \boldsymbol{v}_i \times \boldsymbol{B}_i)$, γ_i is the relativistic factor

Metal Nanoparticles as Plasmas

The conduction band electrons in metals behave as strongly coupled plasmas.
For golden nanorods of 25nm diameter in vacuum this gives an effective wavelength of $\lambda_{eff} = 266\text{nm}$

$$\frac{\lambda_{eff}}{2R\pi} = 13.74 - 0.12[\varepsilon_\infty + 141.04] - \frac{2}{\pi} + \frac{\lambda}{\lambda_p} 0.12\sqrt{\varepsilon_\infty + 141.04}$$

[Lukas Novotny, Effective Wavelength Scaling for Optical Antennas, Phys. Rev. Lett. **98**, 266802 (2007).]

Particle In Cell methods

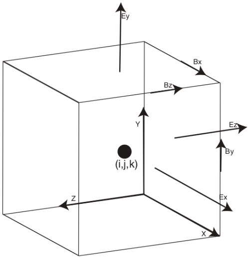


Figure 1. Yee staggered grid used for the Maxwell solver in *EPOCH*.

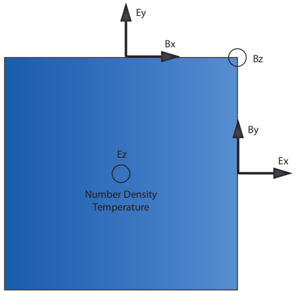


Figure 2: The Yee grid in 2D

[F.H. Harlow (1955). A Machine Calculation Method for Hydrodynamic Problems. Los Alamos Scientific Laboratory report LAMS-1956]

[T.D. Arber et al 2015 Plasma Phys. Control. Fusion 57 113001]

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

FDTD in EPOCH

- $\boldsymbol{E}_{n+\frac{1}{2}} = \boldsymbol{E}_n + \frac{\Delta t}{2}\left(c^2\nabla \times \boldsymbol{B}_n - \frac{\boldsymbol{j}_n}{\epsilon_0}\right)$
- $\boldsymbol{B}_{n+\frac{1}{2}} = \boldsymbol{B}_n - \frac{\Delta t}{2}\left(\nabla \times \boldsymbol{E}_{n+\frac{1}{2}}\right)$
- Call particle pusher which calculates j_{n+1}
- $\boldsymbol{B}_{n+1} = \boldsymbol{B}_{n+\frac{1}{2}} - \frac{\Delta t}{2}\left(\nabla \times \boldsymbol{E}_{n+\frac{1}{2}}\right)$
- $\boldsymbol{E}_{n+1} = \boldsymbol{E}_{n+\frac{1}{2}} + \frac{\Delta t}{2}\left(c^2\nabla \times \boldsymbol{B}_{n+1} - \frac{\boldsymbol{j}_{n+1}}{\epsilon_0}\right)$

Particle pusher

- Solves the relativistic equation of motion under the Lorentz force for each marker-particle

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_n + q\Delta t \left[\boldsymbol{E}_{n+\frac{1}{2}}\left(\boldsymbol{x}_{n+\frac{1}{2}}\right) + \boldsymbol{v}_{n+\frac{1}{2}} \times \boldsymbol{B}_{n+\frac{1}{2}}\left(\boldsymbol{x}_{n+\frac{1}{2}}\right)\right]$$

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

- Villasenor and Buneman current deposition scheme [Villasenor J & Buneman O 1992 Comput. Phys. Commun. 69 306], always satisfied: $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$, where ρ is the charge density.

Particle shape

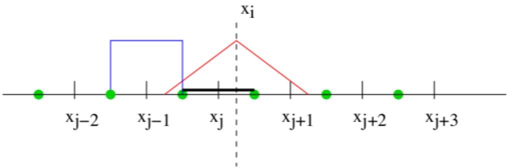


Figure 3: Second order particle shape function

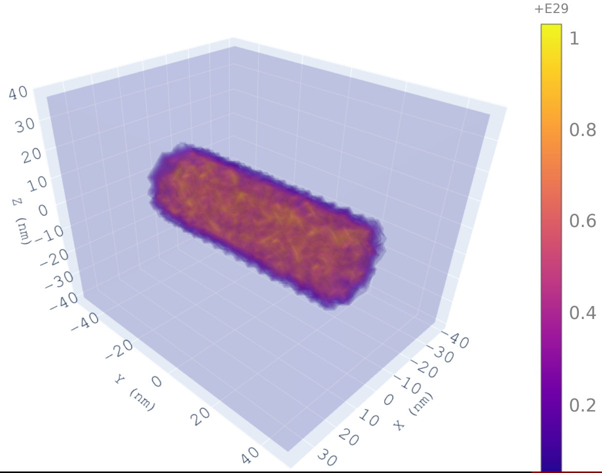
First order approximations are considered

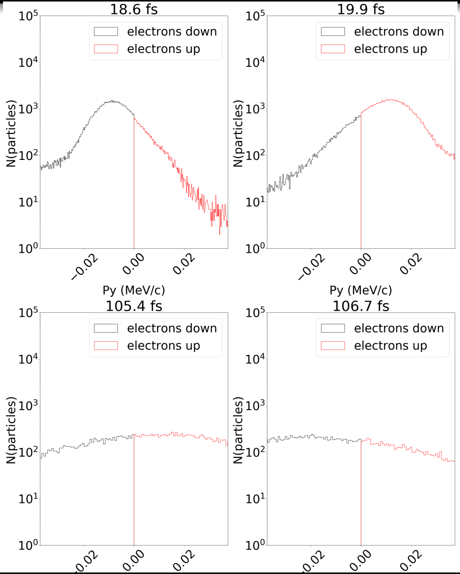
$$F_{part} = \frac{1}{2}F_{i-1}\left(\frac{1}{2} + \frac{x_i - X}{\Delta x}\right)^2 + \frac{1}{2}F_i\left(\frac{3}{4} - \frac{(x_i - X)^2}{\Delta x^2}\right)^2 + \frac{1}{2}F_{i+1}\left(\frac{1}{2} + \frac{x_i - X}{\Delta x}\right)^2$$

[EPOCH 4.0 dev manual]

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 $L_{CB} = 795\text{nm}$

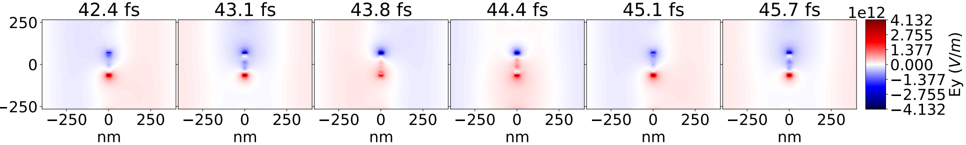
beam crosses the box in
$T = 795\text{nm}/c = 2.65\text{fs}$

Nanorod size: 25 nm diameter with 75 nm length

Pulse length: $40 \times \lambda / c = 106$ fs
Intensity: 4×10^{15} W/cm^2

Kinetic Modelling of the Nanorod

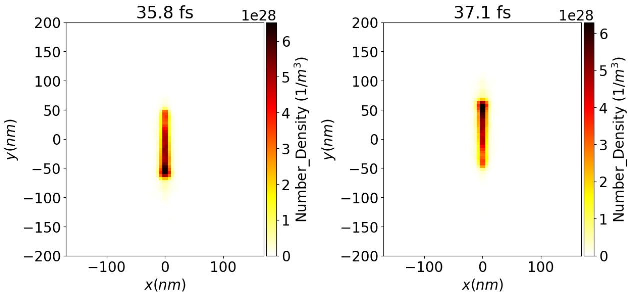
Evolution of the fields



- Evolution of the *E* field's *y* component from 42.4 till 45.7 fs, around a nanorod of 25x130 nm.
- The direction of the *E* field at the two ends of the nanorod does not change.

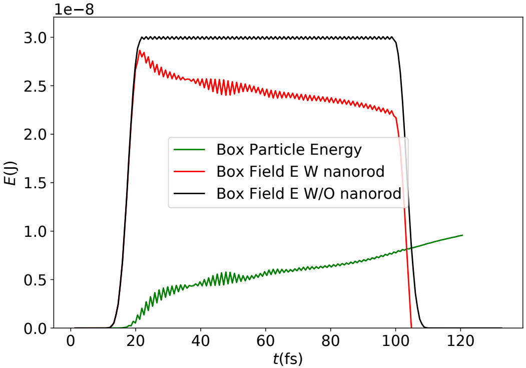
Kinetic Modelling of the Nanorod

Evolution of the nanoantenna



Number density of electrons in the middle of a nanorod of size 25x130 nm at different times. The nanorod is orthogonal to the beam direction, *x*.

Kinetic Modelling of the Nanorod



energy in the box **without nanorod** antenna 3×10^{-8} J (black line)
nanorod absorbs EM energy reducing it to 2.3×10^{-8} J (red line)
deposited energy in the nanorod (green line)
results in light absorption cross section nearly 66.5 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 embedding nanorods in non-vacuum medium
- Fully dedicated software for the project is required
- Next step is estimating the target pre-compression

Thank you!