Simulating gold resonant nano-antennas for nano-fusion

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Nanoplasmonic Laser Fusion Research Laboratory

Kőszeg, September 14, 2019 - Int. Workshop on Collectivity
First meeting on the NAPLIFE project (12 people)

Nanoplasmonic Laser Fusion Research Laboratory

NAPLIFE collaboration - participants - ELKH Nat.Res.Labs
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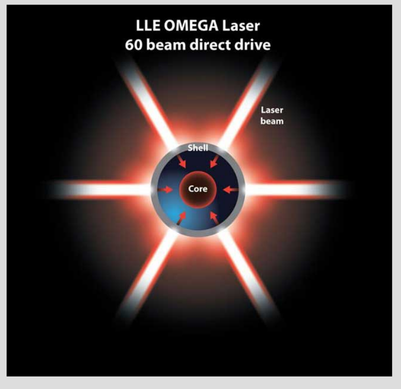
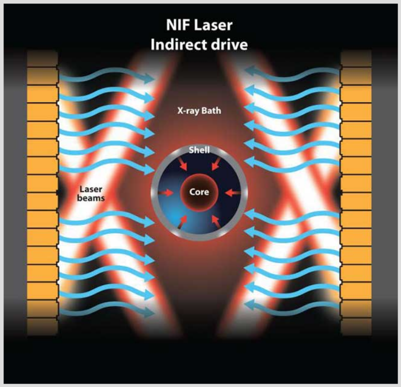
Thermonuclear Fusion

- Fusion does not happen spontaneously on Earth
- Total fusion energy $E_f = \frac{1}{4} n^2 \tau \epsilon \langle v\sigma \rangle$
- ηE_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: $Q = \frac{\eta \epsilon n \tau v \sigma}{4(1-\eta)(3kT + bn\tau\sqrt{T})}$
- Q must be $Q > 1$ for energy production
- This also means $n\tau > \frac{3kT(1-\eta)}{\frac{1}{4}\epsilon\eta\langle v\sigma\rangle - b(1-\eta)\sqrt{T}} \rightarrow$ LC
- Options for fulfilling the Lawson criterion
  - Magnetically confined plasmas: increase confinement time
  - Inertial confinement fusion: increase density of fusion plasma

Direct vs Indirect drive

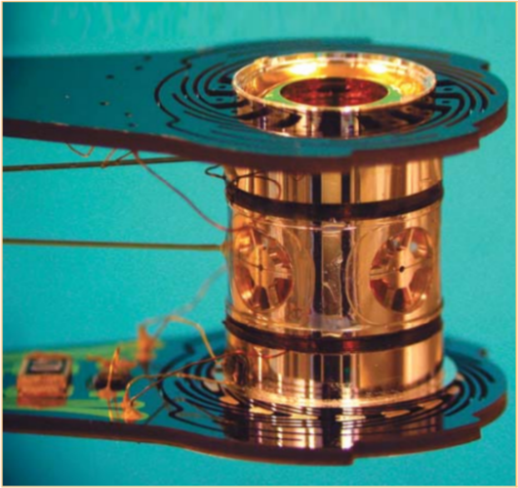




PHOTONICS MEDIA photonics.com

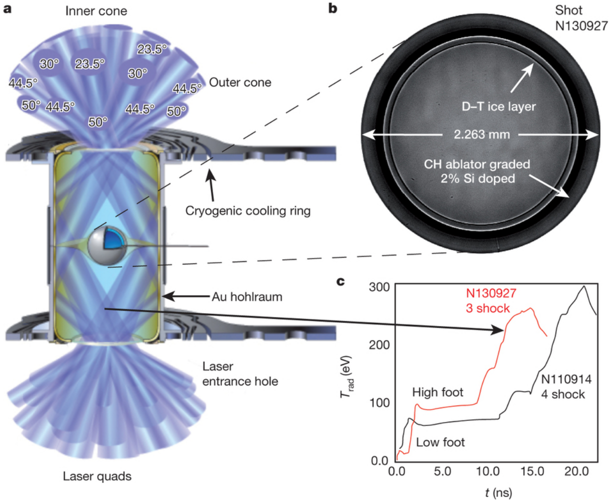
Hohlraum 2014

LAWRENCE LIVERMORE NATIONAL LABORATORY



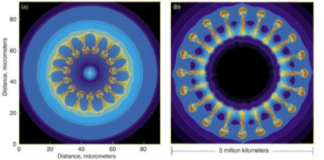
A hohlraum made from gold and 1 cm tall contains the fusion fuel capsule used in experiments at the National Ignition Facility. Light from the laser enters the ends of the cylinder and is converted to x rays, which implode the capsule.

Hohlraum 2014



[O.A. Hurricane et al., Nature, 506, 343 (2014)]

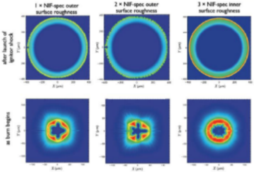
Rayleigh-Taylor instabilities



Striking similarities exist between hydrodynamic instabilities in (a) inertial confinement fusion capsule implosions and (b) core-collapse supernova explosions. [Image (a) is from Sakagami and Nishihara, *Physics of Fluids B* **2**, 2715 (1990); image (b) is from Hachisu et al., *Astrophysical Journal* **368**, L27 (1991).]

Energy must be delivered as sysmmetric 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).] 25

Latest (August 2021) news 1.3MJ kinetic energy at NIF with burning time of 89-137 ps

RFD

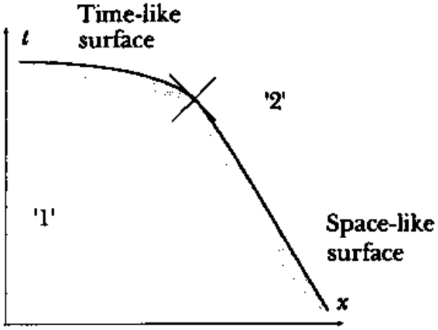
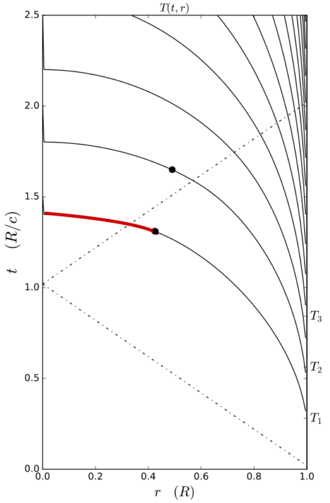


Figure 5.10: Smooth change from spacelike to timelike detonation

[Csernai, L.P. (1987). Detonation on a time-like front for relativistic systems. Zh. Eksp. Teor. Fiz. 92, 379-386.]

Constant absorptivity



[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%

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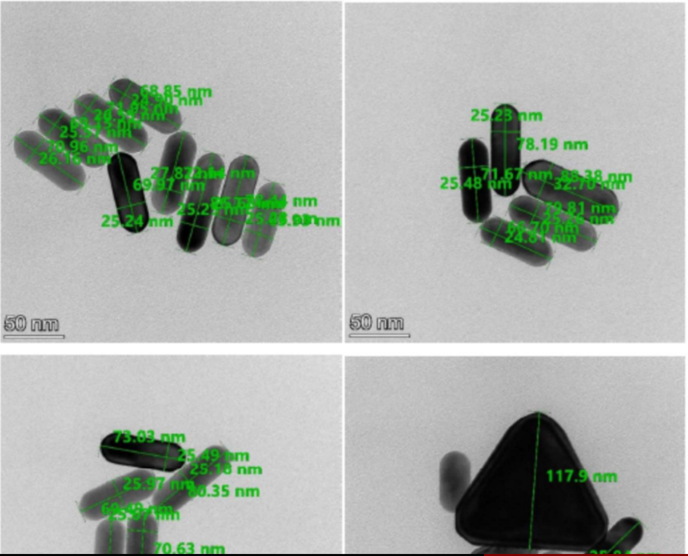
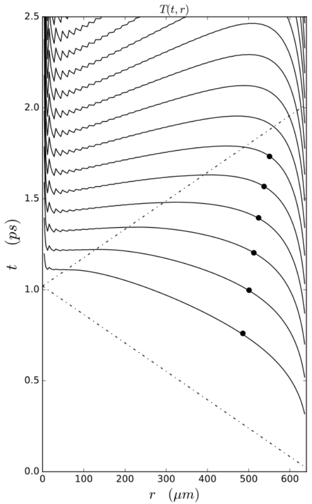


Transmission Electron-microscopy photos of 75x25 nm gold nano-rod antennas

[Judit Kámán, A. Bonyár et al. (NAPLIFE Collab.)., Gold nanorods ..., 10th ICNFP 2021, **Kolymbari]**

Changing absorptivity

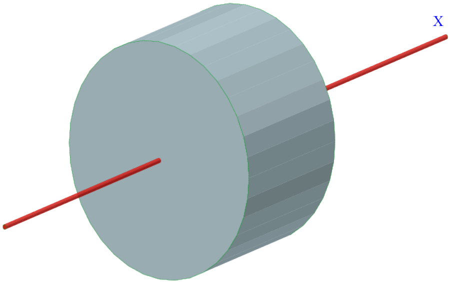


[Csernai, L.P., Kroo, N. and Papp, I. (2017). Procedure to improve the stability and efficiency of laser-fusion by nano-plasmonics method. Patent P1700278/3 of the Hungarian Intellectual Property Office.]

$\alpha_{k_{middle}} \approx 4 \times \alpha_{k_{edge}}$

Simultaneous volume ignition is up to 73%

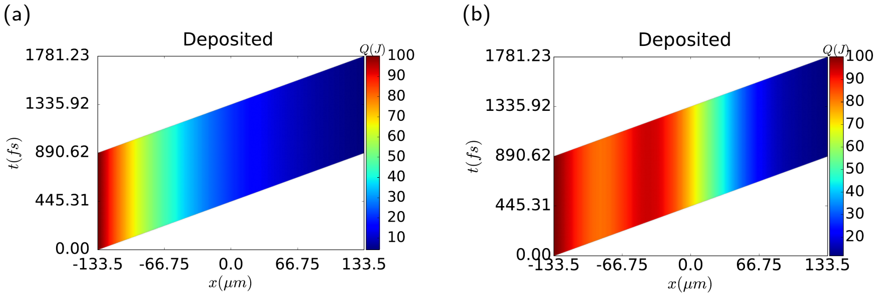
Flat target



Schematic view of the cylindrical, flat target of radius, R, and thickness, h.
$V = 2\pi R^3$, $R = \sqrt[3]{V/(2\pi)}$, $h = \sqrt[3]{4V/\pi}$.

[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)]

Varying absorptivity



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:

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

Particle In Cell methods

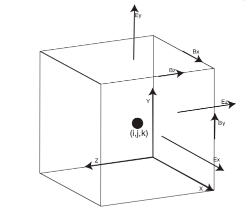


Figure 1. Yee staggered grid used for the Maxwell solver in *EPOCH*.

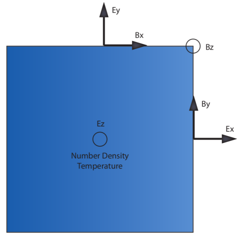


Figure 2: The Yee grid in 2D

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

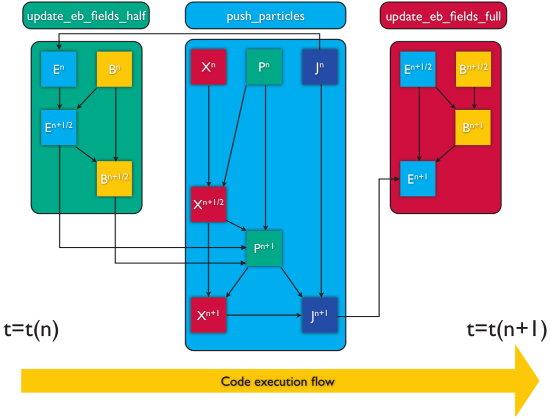
[T.D. Arber et al 2015 Plasma Phys. Control. Fusion 57 113001]

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 **Maxwell's equations**.

General layout of the EPOCH code



[EPOCH 4.0 dev manual]

- (input) deck
- housekeeping
- io
- parser
- physics_packages
- user_interaction

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

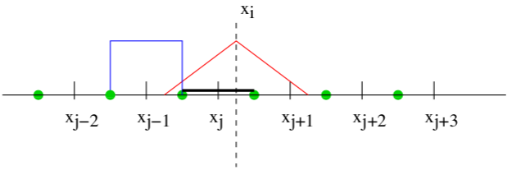


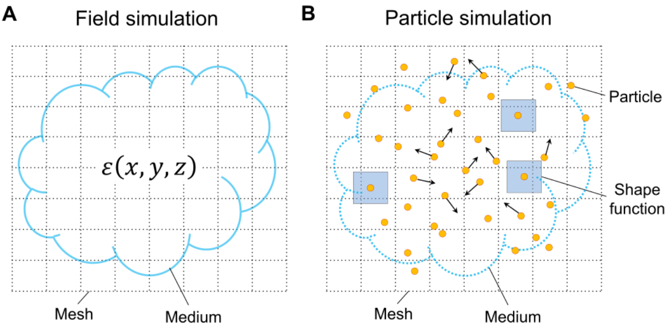
Figure 3: Second order particle shape function

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]

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

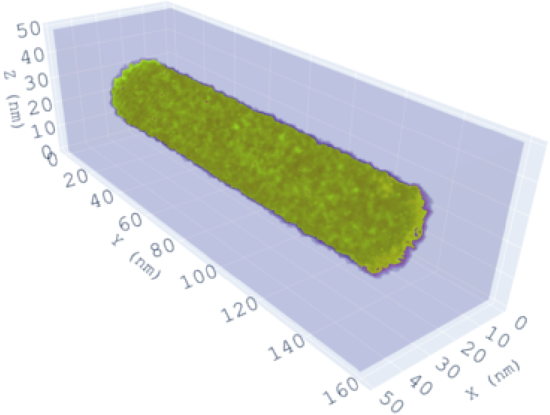
The conduction band electrons in metals behave as strongly coupled plasmas.
For golden nanorods of 25nm diameter in vacuum this gives an effective wavelength of $\lambda_{eff} = 266$nm

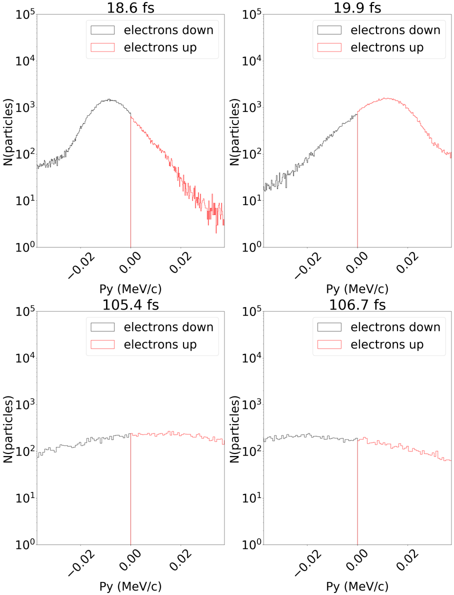
$$\frac{\lambda_{eff}}{2R\pi} = 13.74 - 0.12[\varepsilon_\infty + 141.04] - \frac{2}{\pi} + \frac{\lambda}{\lambda_p} 0.12\sqrt{\varepsilon_\infty + 141.04}$$

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

Kinetic Modelling of the Nanorod

Nanorod inside a PIC simulation box





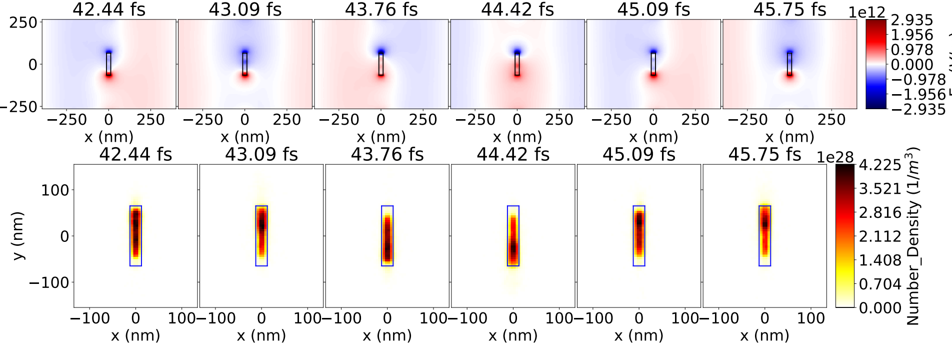
Considerations for the simulation box: $S_{CB} = 530 \times 530\text{nm}^2 = 2.81 \times 10^{-9}\text{cm}^2$ and length of $L_{CB} = 795\text{nm}$

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

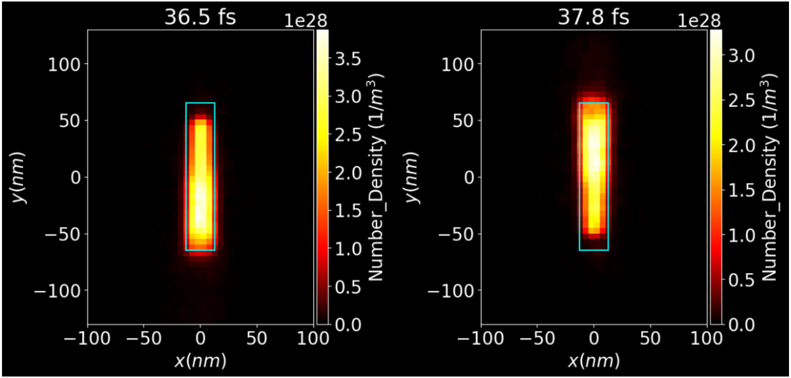
Kinetic Modelling of the Nanorod



- Evolution of the 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.

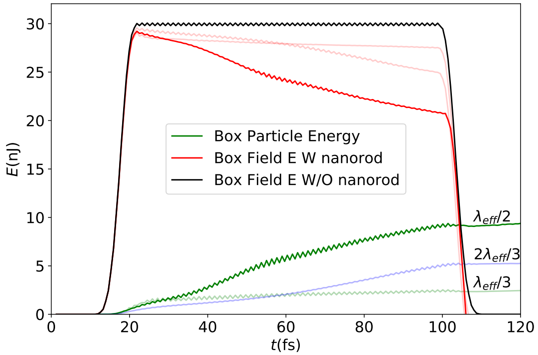
Kinetic Modelling of the Nanorod

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.

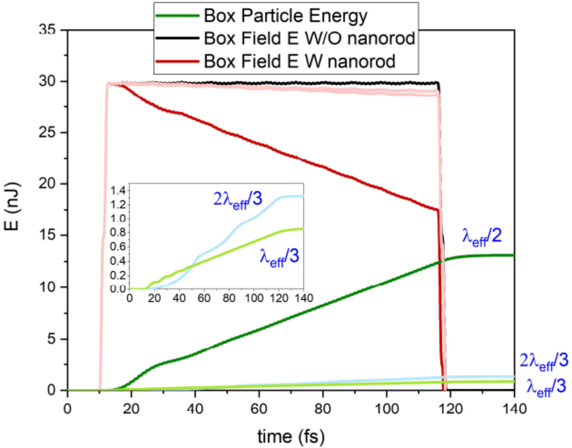
In vacuum



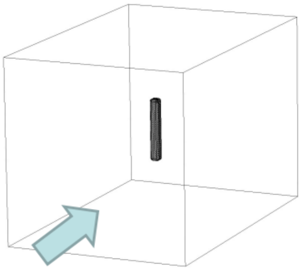
energy in the box **without nanorod** antenna 3×10^{-8} J (black line)
nanorod absorbs EM energy reducing it to 2.3×10^{-8} J (red line)
deposited energy in the nanorod (green line)
results in light absorption cross section highest

Comparison with other methods (Csernai, Csete et al.)

Resilience of Nanorod Antenna with COMSOL



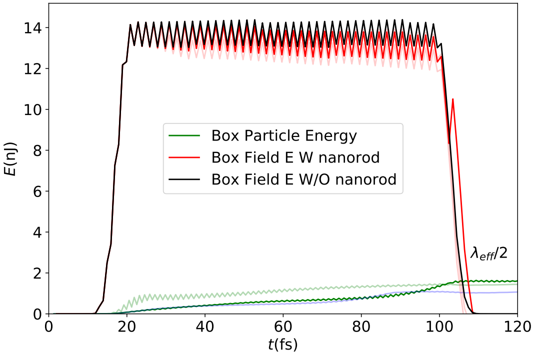
FEM computations with the same model parameters



Good qualitative agreement between FEM and EPOCH/PIC methods

Quantitative difference:

In UDMA



deposited energy in the nanorod (green line)

Conclusions, Looking forward

- The model is in good agreement with currently available widely accepted methods
- The model is highly idealized
- Ionization in the medium must be included alongside nuclear reactions
- Target pre-compression in the next step can be estimated