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

István Papp, Larissa Bravina, Mária Csete, Igor N. Mishustin, Dénes Molnár, Anton Motornenko, Leonid M. Satarov, Horst Stöcker, Daniel D. Strottman, András Szenes, Dávid Vass, Tamás S. Biró, László P. Csernai, Norbert Kroó

FIAS Frankfurt Institute for Advanced Studies

NATIONAL RESEARCH CENTER "KURCHATOV INSTITUTE"

# Nanoplasmonic Laser Fusion Research Laboratory

**Theoretical Group**

Csete, Mária, team leader (SZTE)
Papp, István (Wigner FK)
Tóth, Emese (SZTE)
Vass, Dávid (SZTE)
Fekete, Olivér (SZTE)
Szenes, András (SZTE)

**Material Preparation Group**

Bonyár, Attila, team leader (BME ETT)
Borók, Alexandra (BME ETT)
Szalóki, Melinda (DE FOK)
Petrik, Péter (EK)

**Laser Group**

Rácz, Péter, team leader (Wigner FK)
Dombi, Péter (Wigner FK)
Kedves, Miklós (Wigner FK)
Aladi, Márk (Wigner FK)

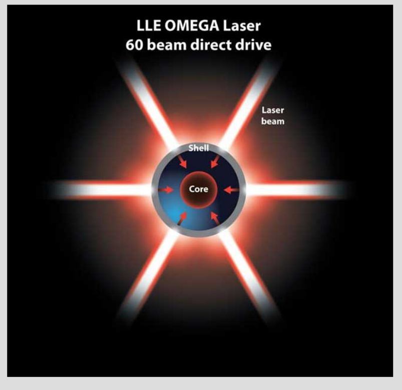
**Spectroscopy Group**

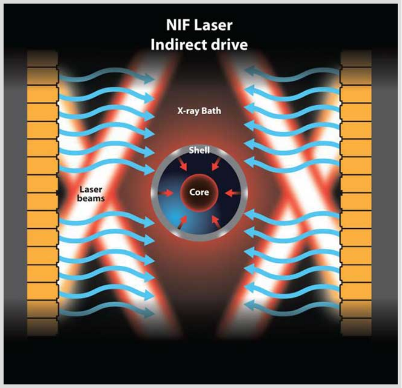
Veres, Miklós, team leader (Wigner FK)
Kámán, Judit (Wigner FK)
Rigó, István (Wigner FK)
Nagyné Szokol, Ágnes (Wigner FK)
Holomb, Román (Wigner FK)

# Thermo-nuclear Fusion

- Fusion does not happen spontaneously on Earth
- Total fusion energy $E_f = \frac{1}{4} n^2 \tau \epsilon \langle v\sigma \rangle$
- $\eta E_f$ 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: $Q = \frac{\eta \epsilon n \tau v \sigma}{4(1-\eta)(3kT + bn\tau\sqrt{T})}$
- $Q$ 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
- Fulfilling the Lawson criterion
  - Magnetically confined plasmas: increase confinement time
  - Inertial confinement fusion: increase density of fusion plasma

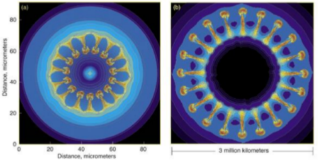
# Direct vs Indirect drive




PHOTONICS MEDIA photonics.com

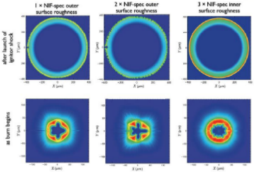
# Rayleigh-Taylor instabilities




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

# RFD

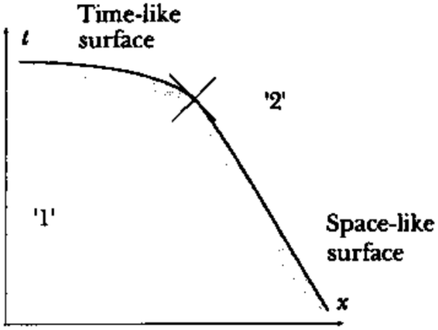
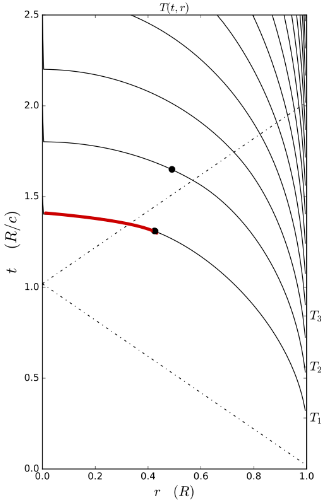



Figure 5.10: Smooth change from spacelike to timelike detonation

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

# Constant absorptivity

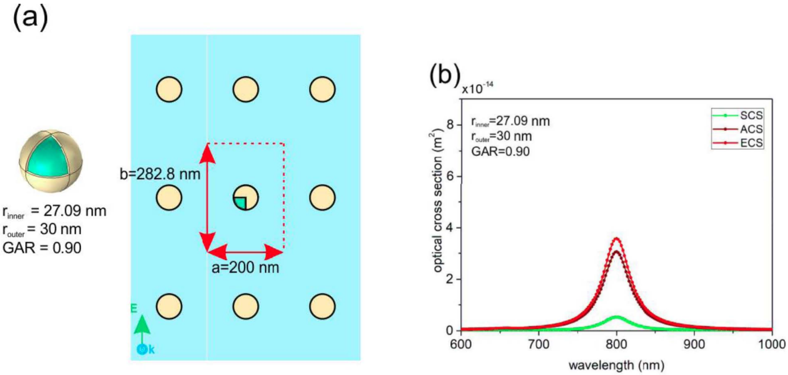



[L.P. Csernai & D.D. Strottman, Laser and Particle Beams 33, 279 (2015)]

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

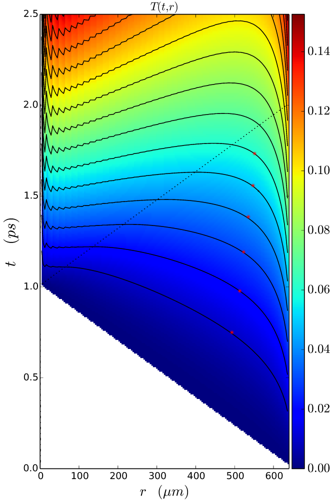
Simultaneous volume ignition is only up to 12%

# Doping with gold




(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

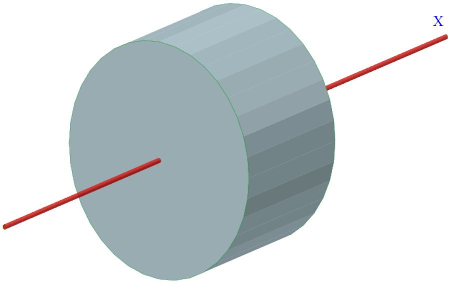



[Csernai, L.P., Kroo, N. and Papp, I. (2017). Procedure to improve the stability and efficiency of laser-fusion by nano-plasmonics method. Patent P1700278/3 of the Hungarian Intellectual Property Office.]

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

Simultaneous volume ignition is up to 73%

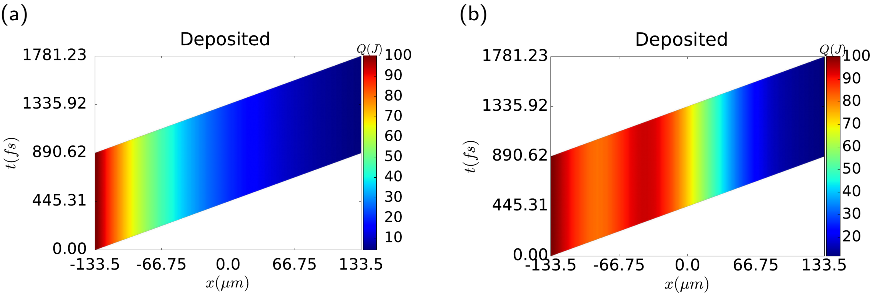
# Flat target




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

[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

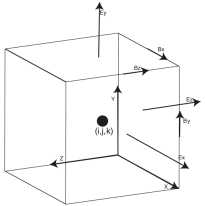



**Figure 1.** Yee staggered grid used for the Maxwell solver in *EPOCH*.

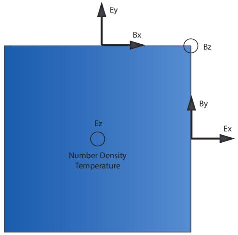



Figure 2: The Yee grid in 2D

[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.

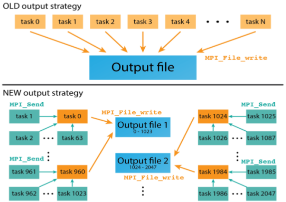
Particle **mover** or **pusher** algorithm as standard **Boris algorithm**.

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

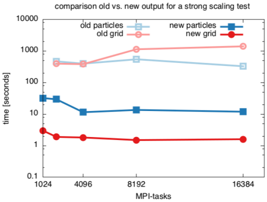
# Available software

| Computational application | Web site | License | Availability | Canonical Reference |
|---|---|---|---|---|
| SHARP | [17] | Proprietary | | doi:10.3847/1538-4357/aa6d13 |
| ALaDyn | [18] | GPLv3+ | Open Repo:[19] | doi:10.5281/zenodo.49553 |
| EPOCH | [20] | GPL | Open to academic users but signup required :[21] | doi:10.1088/0741-3335/57/11/113001 |
| FBPIC | [22] | 3-Clause-BSD-LBNL | Open Repo:[23] | doi:10.1016/j.cpc.2016.02.007 |
| LSP | [24] | Proprietary | Available from ATK | doi:10.1016/S0168-9002(01)00024-9 |
| MAGIC | [25] | Proprietary | Available from ATK | doi:10.1016/0010-4655(95)00010-D |
| OSIRIS | [26] | Proprietary | Closed (Collaborators with MoU) | doi:10.1007/3-540-47789-6_36 |
| PICCANTE | [27] | GPLv3+ | Open Repo:[28] | doi:10.5281/zenodo.48703 |
| PICLas | [29] | Proprietary | Available from Institute of Space Systems and Institute of Aerodynamics and Gas Dynamics at the University of Stuttgart | doi:10.1016/j.crme.2014.07.005 |
| PIConGPU | [30] | GPLv3+ | Open Repo:[31] | doi:10.1145/2503210.2504564 |
| SMILEI | [32] | CeCILL-B | Open Repo:[33] | doi:10.1016/j.cpc.2017.09.024 |
| iPIC3D | [34] | Apache License 2.0 | Open Repo:[35] | doi:10.1016/j.matcom.2009.08.038 |
| The Virtual Laser Plasma Library | [36] | Proprietary | Unknown | doi:10.1017/S0022377899007515 |
| VizGrain | [37] | Proprietary | Commercially available from Esgee Technologies Inc. | |
| VPIC | [38] | 3-Clause-BSD | Open Repo:[39] | doi:10.1063/1.2840133 |
| VSim (Vorpal) | [40] | Proprietary | Available from Tech-X Corporation | doi:10.1016/j.jcp.2003.11.004 |
| Warp | [41] | 3-Clause-BSD-LBNL | Open Repo:[42] | doi:10.1063/1.860024 |
| WarpX | [43] | 3-Clause-BSD-LBNL | Open Repo:[44] | doi:10.1016/j.nima.2018.01.035 |
| ZPIC | [45] | AGPLv3+ | Open Repo:[46] | |

# Piccante



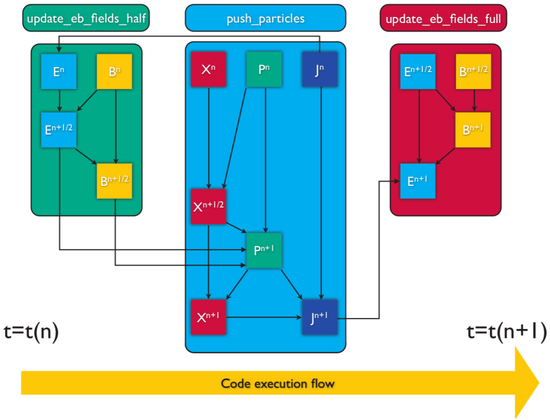

(a)




(b)

(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.
[A. Sgattoni, L. Fedeli, S. Sinigardi, A. Marocchino, A. Macchi, V. Weinberg, A. Karmakar; https://arxiv.org/pdf/1503.02464.pdf]

# 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 $\rho$ is the charge density.

# Particle shape

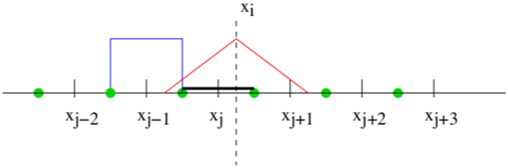


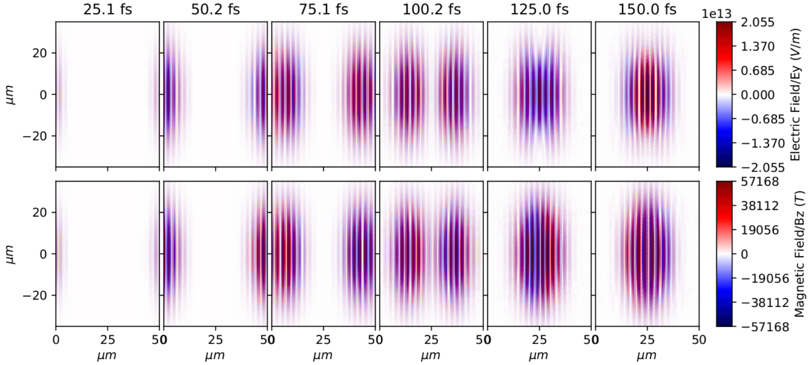

Figure 3: Second order particle shape function

First order approximations are considered

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

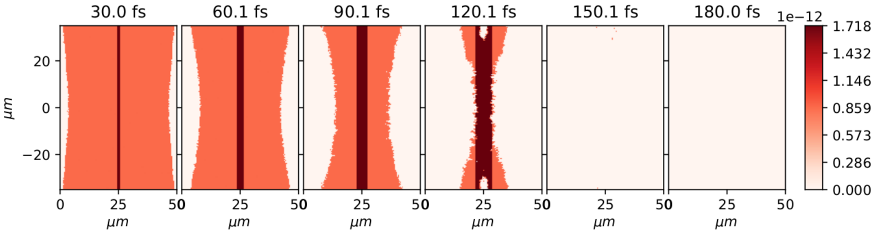
[EPOCH 4.0 dev manual]

# Colliding fields using EPOCH




Laser parameters:
wavelength of $\lambda = 1\mu$m, full pulse length $\Delta_t = 52$fs, focus diameter is $2R = 40\mu$m, $3.0 \cdot 10^{19}$ W/cm$^2$ top intensity.
[Papp, I., et al., NAPLIFE Collaboration, Phys. Lett. A, (2021)]

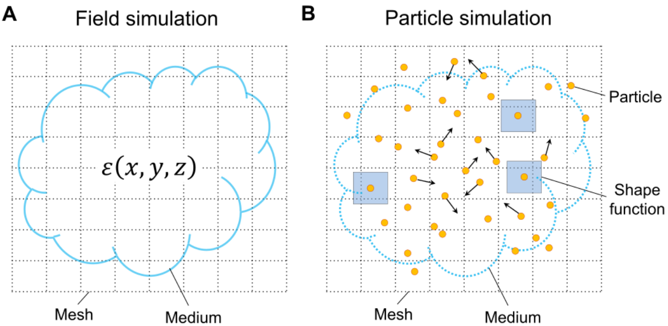
# Multi-photon ionisation




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
[K. Nanbu , S. Yonemura. Weighted particles in Coulomb collision simulations based on the theory of a cumulative scattering angle. *Journal of Computational Physics*, vol. **145**, pp. 639?654 (1998)]

# 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 $\omega_p$ 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

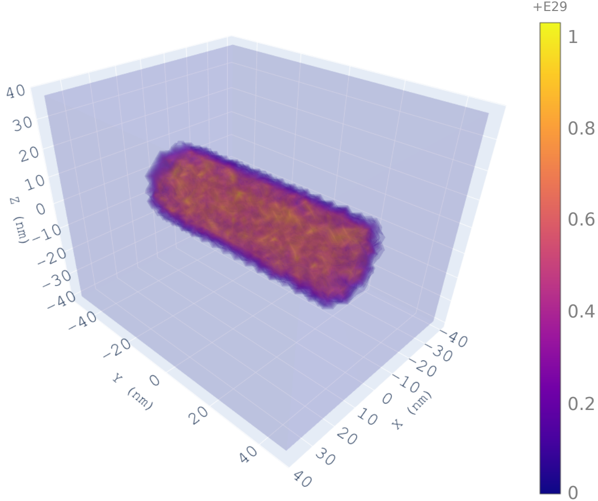
**Particle simulation:**

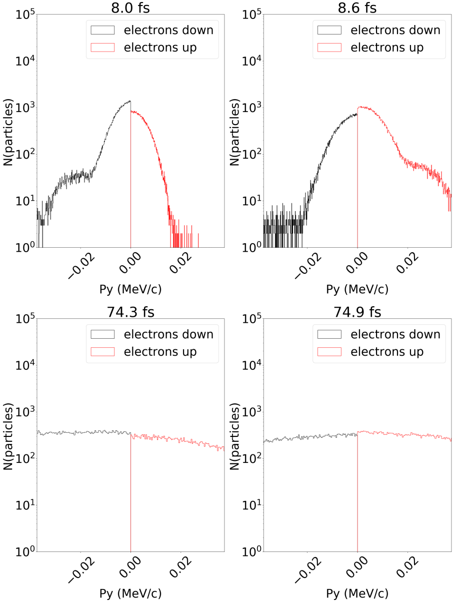
$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\mu_0 \epsilon_0} \nabla \times \boldsymbol{B} - \frac{\boldsymbol{J}}{\epsilon_0}, \ \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}$$

$\gamma_i m_i \boldsymbol{v}_i = q_i(\boldsymbol{E}_i + \boldsymbol{v}_i \times \boldsymbol{B}_i)$, $\gamma_i$ 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 $L_{CB} = 795\text{nm}$

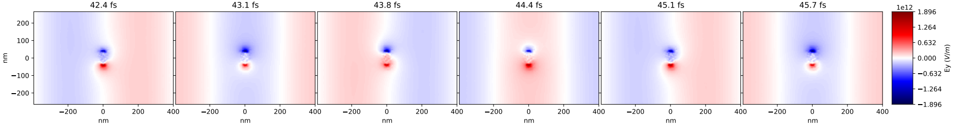
beam crosses the box in $T = 795\text{nm}/c = 2.65\text{fs}$

Nanorod size: 25 nm diameter with 75 nm length

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

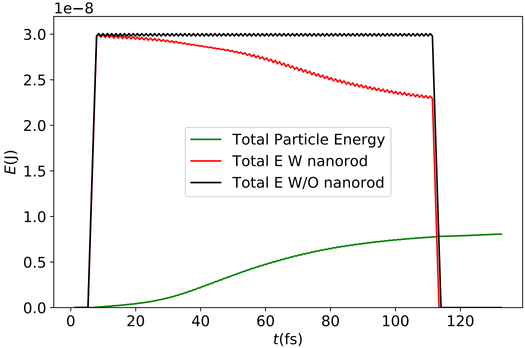
# Kinetic Modelling of the Nanorod

Evolution of the fields




$E_y$ evolution video

# Kinetic Modelling of the Nanorod

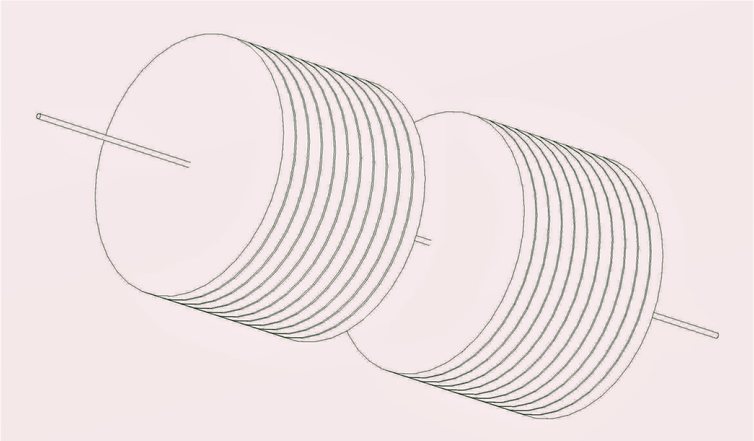



energy in the box **without nanorod** antenna $3\times10^{-8}$ J (black line)
**nanorod** absorbs EM energy reducing it to $2.3\times10^{-8}$ J (red line)
**deposited** energy in the nanorod (green line)
results in light absorption cross section nearly 35 times higher than its geometrical cross section

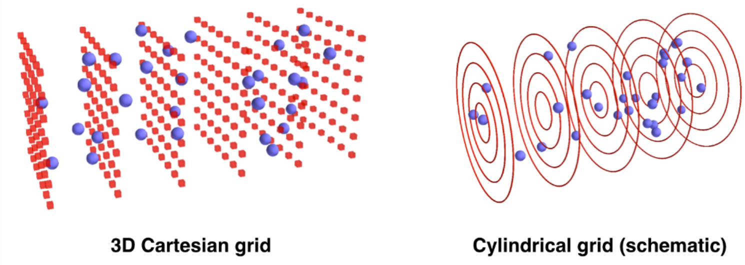
# Conclusions, Looking forward

- 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]