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# High Performance Computing for Nanoplasmonic Laser Fusion

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Molnár, Anton Motornenko, Leonid M. Satarov, Horst Stöcker, Daniel D.
Strottman, András Szenes, Dávid Vass, Tamás S. Biró, László P. Csernai,
Norbert Kroó

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## 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 $n\tau > \frac{3kT(1-\eta)}{\frac{1}{4}\epsilon\eta\langle v\sigma \rangle - b(1-\eta)\sqrt{T}} \to$ LC
- Fulfilling the Lawson criterion
    - Magnetically confined plasmas: increase confinement time
    - Inertial confinement fusion: increase density of fusion plasma

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# Direct vs Indirect drive

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# Hohlraum 2014



**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.

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# Hohlraum 2014
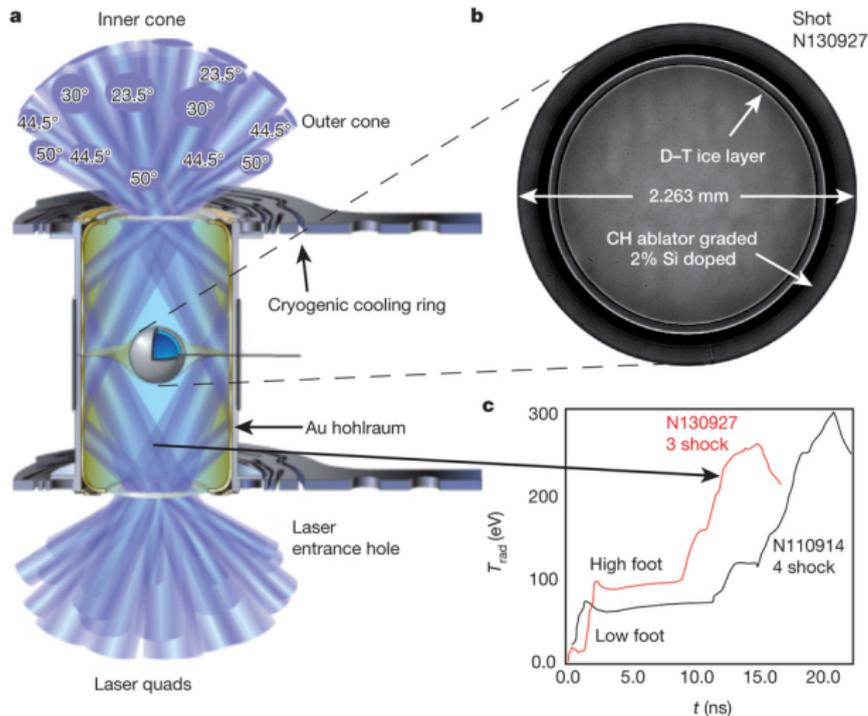


[O.A. Hurricane et al., Nature, 506, 343 (2014)]

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# Laser-Induced



Laser light shines
on the target
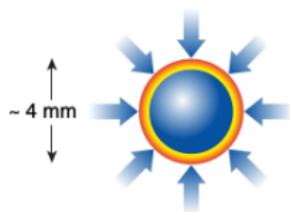
The target
is compressed

~ 4 mm
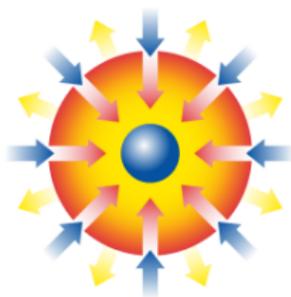
The target is ignited

The target
burns

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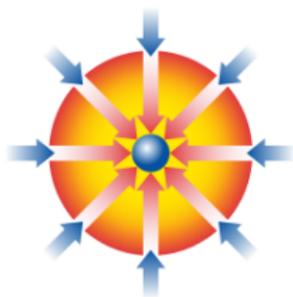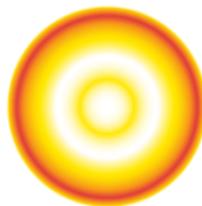
# Rayleigh-Taylor instabilities



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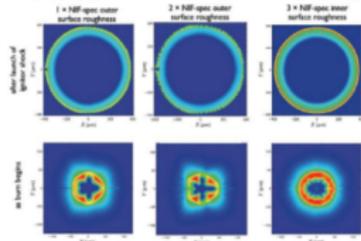
**Left:** same roughness of inner and outer surface as specified for the NIF target
**Center:** outer surface roughness is twice the NIF level
**Right:** DT inner surface roughness three times larger than NIF specifications

[S. Atzeni et al., Nucl. Fusion 54, 054008 (2014).]

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## RFD
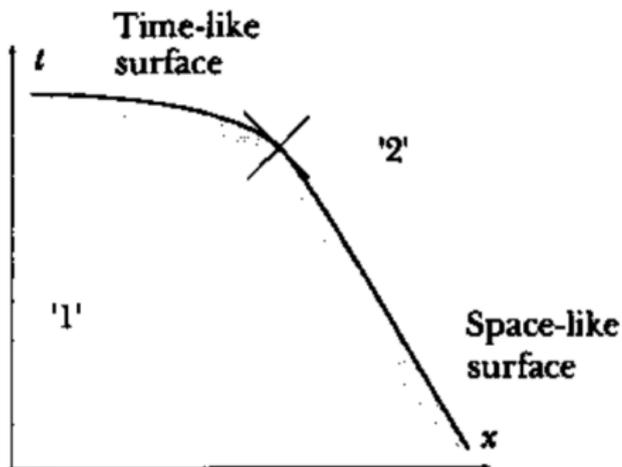


Figure 5.10: Smooth change from spacelike to timelike detonation

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

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# 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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## Doping with gold

(a)
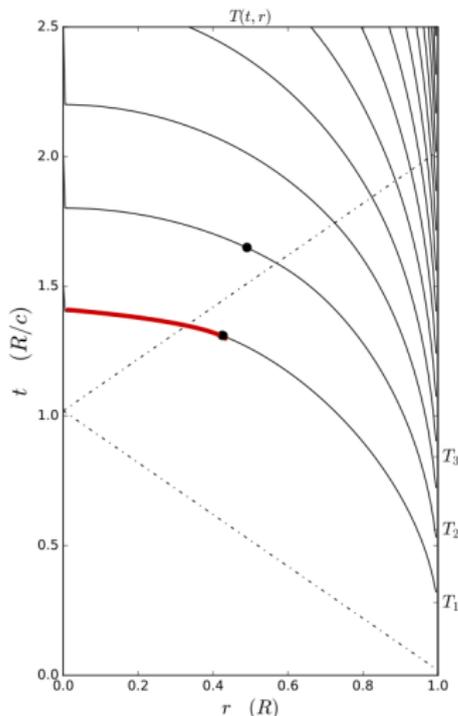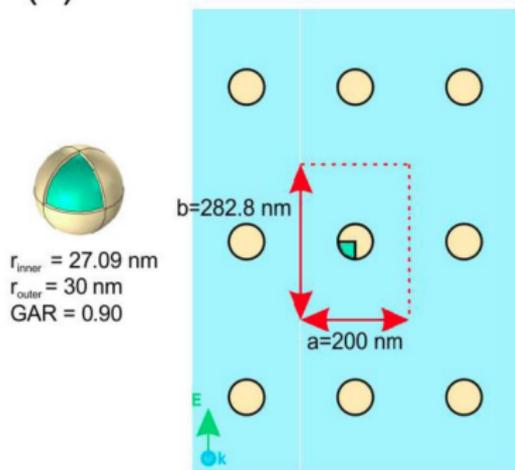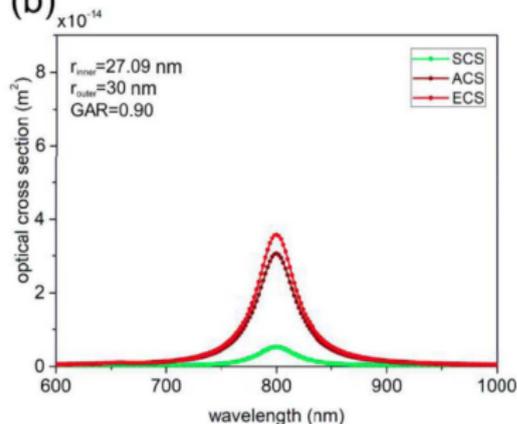


(a) Left: Single core-shell nano-sphere. Right: Rectangular lattice of
nano-spheres in a transverse layer of the target.
(b) Optical cross-section of an individual core-shell nano-sphere optimized to
absorb light at 800 nm wavelength and optical response of the same core-shell
nano-spheres composing a rectangular lattice.

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# Changing absorptivity
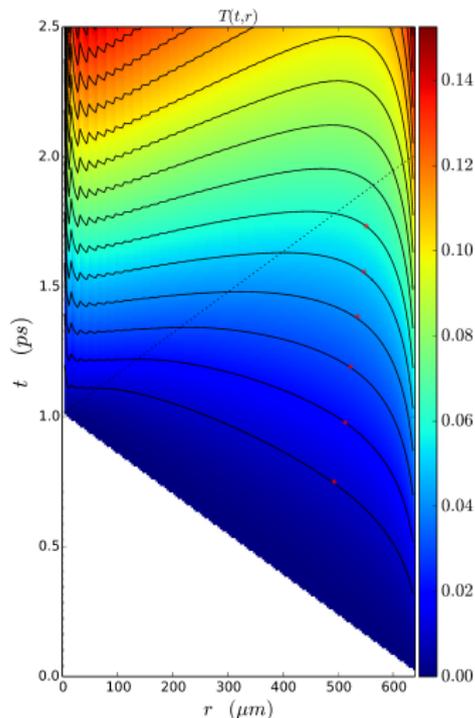


[Csernai, L.P., Kroo, N. and Papp, I. (2017). Procedure to improve the stability and efficiency of laser-fusion by nano-plasmonics method. Patent P1700278/3 of the Hungarian Intellectual Property Office.]

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

Simultaneous volume ignition is up to 73%

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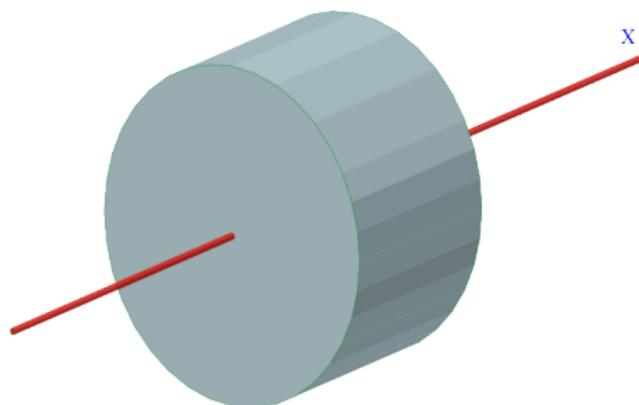
# Flat target



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)]

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# Varying absorptivity

(a)



(b)
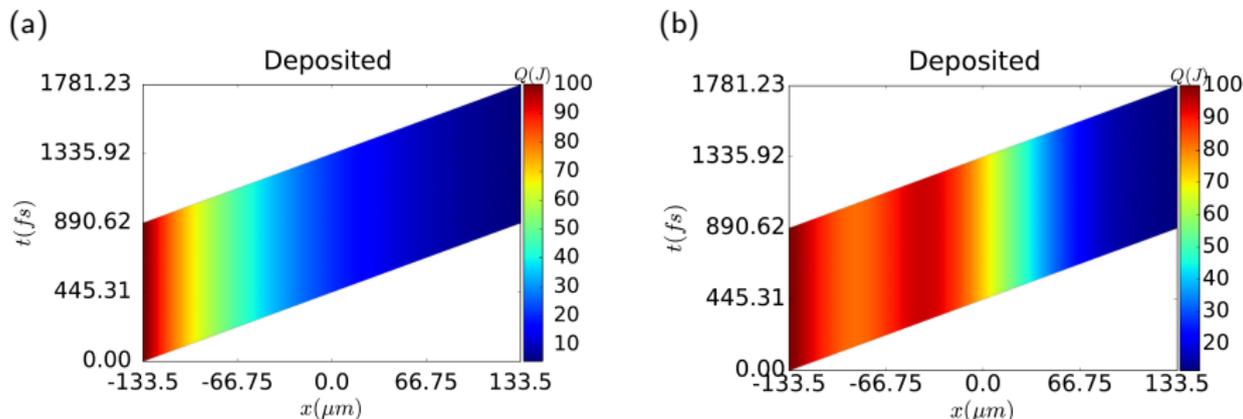
**Deposited energy** per unit time in the space-time plane across the depth, $h$, of the flat target. **(a) without** nano-shells **(b) with** nano-shells
To increase central absorption we used the following distribution:

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

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# Similar configurations

Nuclear probes of an out-of-equilibrium plasma at the highest compression   **Phys. Lett. A  383 (2019) 2285-2289.**

G. Zhang [a,b,*], M. Huang [c], A. Bonasera [d,e,*], Y.G. Ma [f,b,i,*], B.F. Shen [g,h,*], H.W. Wang [a,b], W.P. Wang [g], J.C. Xu [g], G.T. Fan [a,b], H.J. Fu [b], H. Xue [b], H. Zheng [j], L.X. Liu [a,b], S. Zhang [c], W.J. Li [b], X.G. Cao [a,b], X.G. Deng [b], X.Y. Li [b], Y.C. Liu [b], Y. Yu [k], Y. Zhang [b], C.B. Fu [k], X.P. Zhang [k]

4 (up) + 4(down) lasers
Target thickness, h (3.6μm-1mm)
& radius, R, (150-400μm) were varied.

Total pulse energy 1.2kJ (2ns) for 8 beams.
Shortest (250ps) pulses -> 100s MeV ions > non-thermal distr. = directed ion acceleration

Typical fusion neutron energies were measured & used to extract the target density.



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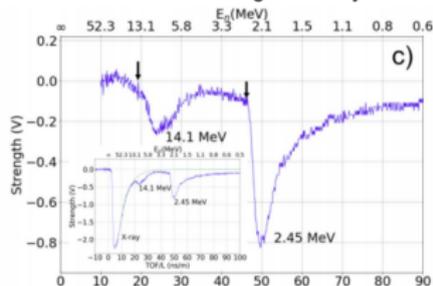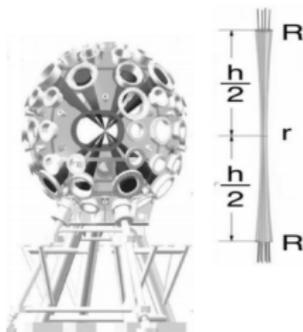
# Similar configurations
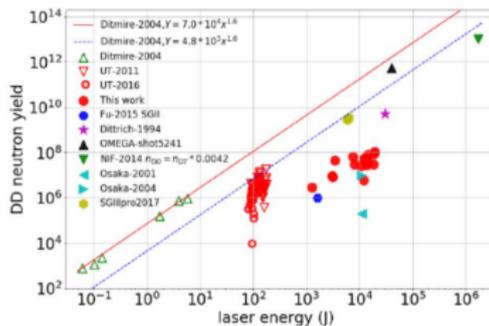


Figure 3: (color online) Fusion yield as function of laser energy. Different experimental results Ditmire-2004[40], UT-2011[20], UT-2016[19], Fu-2015 SGII[45], Dittrich-1994[49] , NIF-2014[48] , Osaka -2001[46], Osaka-2004[47], OMEGA-shot5241[41]and SGIIIpro2017[42] are indicated in the inset.
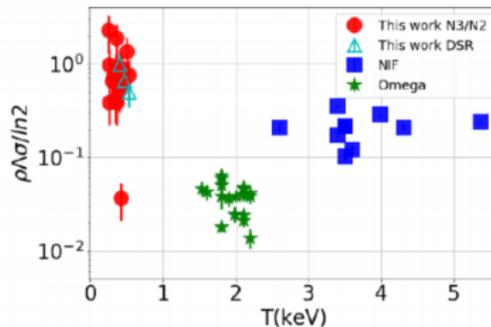


Figure 4: (color online) $\Lambda\rho\sigma/\ln2$ obtained from eq.(4) vs T from eq.(1). Omega and NIF data are derived from the experiments[25], using the Down Scatter Ratio[23, 21]. Our results using the DSR method ($N_4/N_3$) are given by the open triangle symbols in good agreement with the $N_3/N_2$ ratios.

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# Experiment and collaboration

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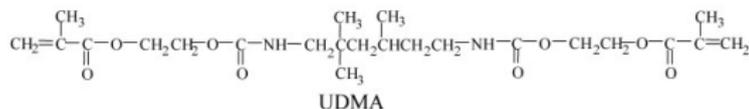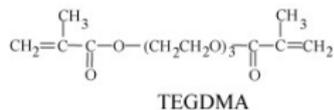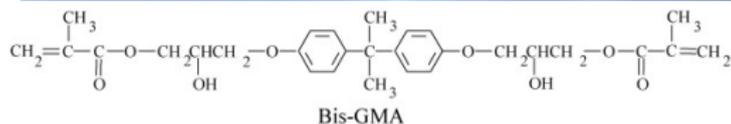
# Available software

| Computational application | Web site | License | Availability | Canonical Reference |
|---|---|---|---|---|
| SHARP | [17] | Proprietary | | doi:10.3847/1538-4357/aa6d13 |
| ALaDyn | [18] | GPLv3+ | | 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] | |

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# Particle In Cell methods
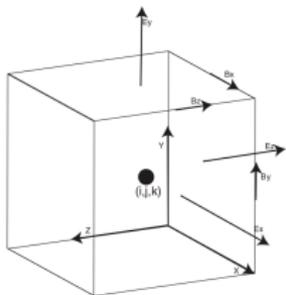


**Figure 1.** Yee staggered grid used for the Maxwell solver in *EPOCH*.
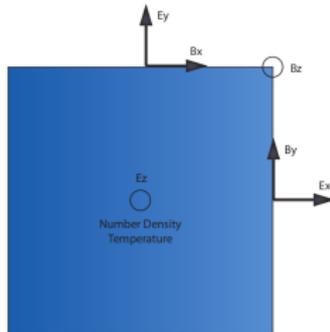


Figure 2: The Yee grid in 2D

[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**.

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# General layout of the EPOCH code
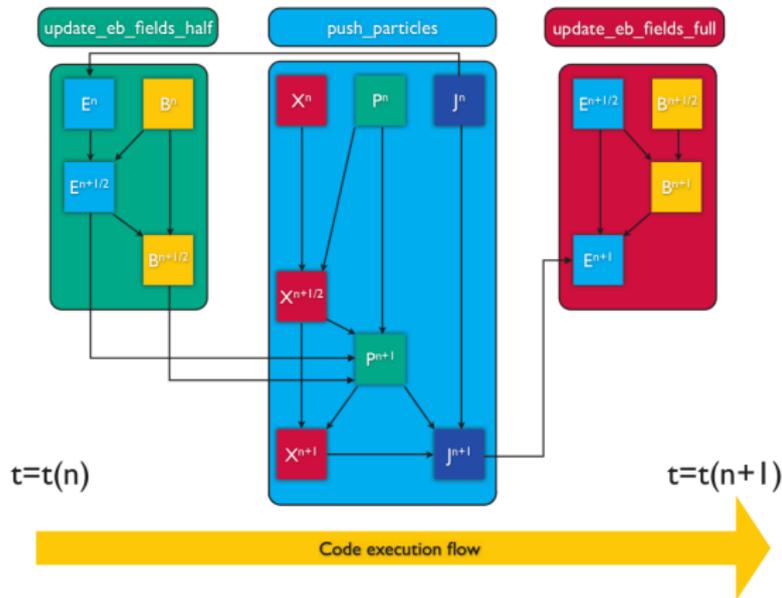


[EPOCH 4.0 dev manual]

- (input) <u>deck</u>
- housekeeping
- io
- parser
- physics_packages
- <u>user_interaction</u>

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# 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 $j_{n+1}$

- $\boldsymbol{B}_{n+1} = \boldsymbol{B}_{n+\frac{1}{2}} - \frac{\Delta t}{2}\left(\nabla\times\boldsymbol{E}_{n+\frac{1}{2}}\right)$

- $\boldsymbol{E}_{n+1} = \boldsymbol{E}_{n+\frac{1}{2}} + \frac{\Delta t}{2}\left(c^2\nabla\times\boldsymbol{B}_{n+1} - \frac{\boldsymbol{j}_{n+1}}{\epsilon_0}\right)$

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# 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.

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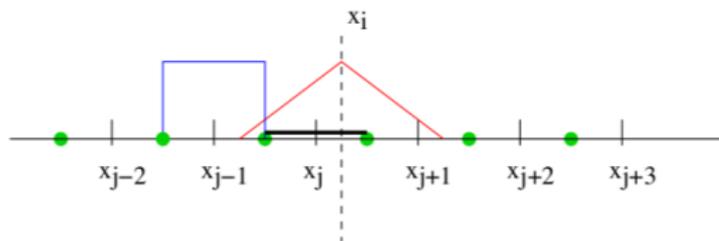
# Particle shape



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]

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# A spicy code
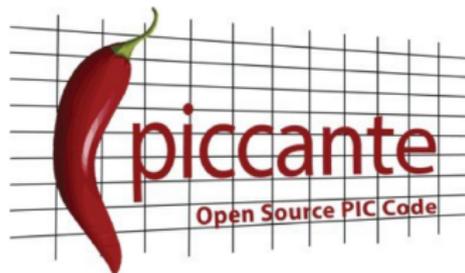
Still beta version Supports:

- rough_box features
- grating
- grid stretching
- highly optimized output

1. A. Sgattoni, et. al., Laser-Driven Rayleigh-Taylor Instability: Plasmonics Effects and Three-Dimensional Structures, Phys. Rev. E, 91, 013106 (2015)

2. A. Sgattoni, et. al., High Energy Gain in Three-Dimensional Simulations of Light Sail Acceleration, Appl. Phys. Lett., 105, 084105 (2014)

3. L. Fedeli, et. al., Electron acceleration by relativistic surface plasmons in laser-grating interaction, Physical Review Letters 116, 015001 (2016)

4. A. Sgattoni, et. al., High field plasmonics and laser-plasma acceleration in solid targets, Plasma Physics and Controlled Fusion 58, 014004 (2015)

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# Benefits of a spicy code



(a)



(b)
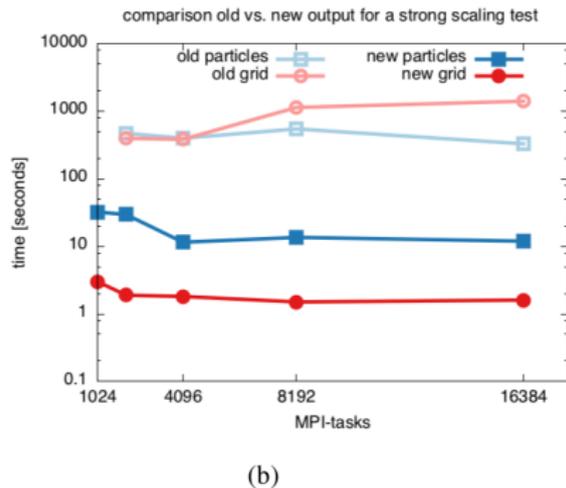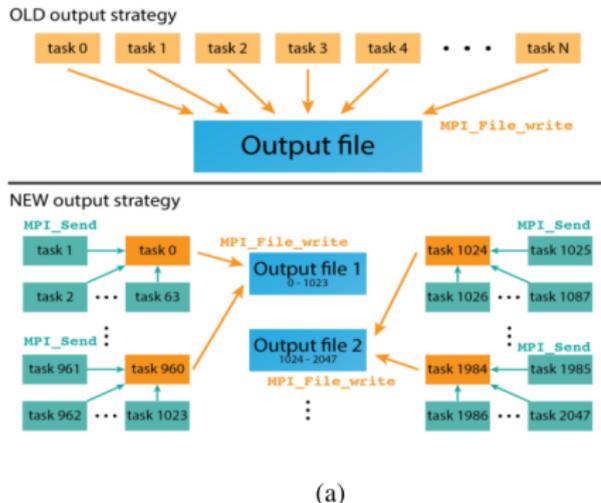
(a) Old and new strategies. G = 64 group of tasks and F = N/128 master tasks.
(b) Time spent for **writing particle positions** red, time spent for **grid based outputs**
(EM fields, densities) marked with blue.

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# Ionisation
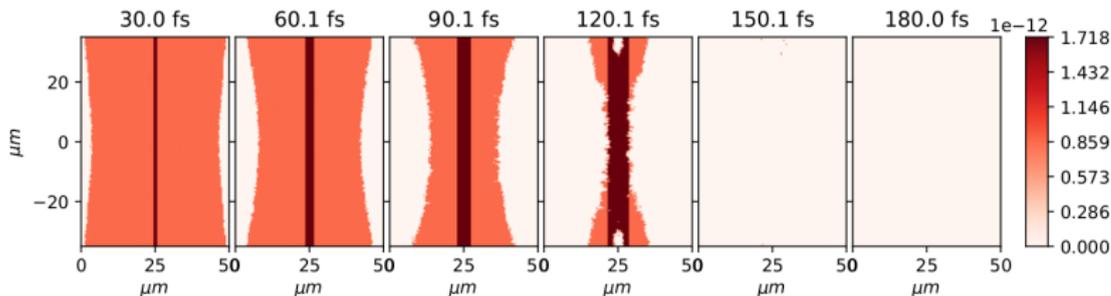


Figure 2: (color online) The ionization of the $H$ atoms in a Laser Wake Field (LWF) wave due to the irradiation from both the $\pm x$- directions, on an initial target density of $n_H = 2.13 \cdot 10^{27}$ atoms/m$^3$ = $2.13 \cdot 10^{21}$ atoms/cm$^3$. The energy of the $H$ atoms in Joule [J] per marker particle is shown. The $H$ atoms disappear as protons and electrons are created. Due to the initial momentum of the colliding $H$ slabs, the target and projectile slabs interpenetrate each other and this leads to double energy density. Several time-steps are shown at 30 fs time difference.

However **PICCANTE** does **not** contain ionisation
**EPOCH includes** a number of ionisation models by which electrons ionise in both the field of an intense laser and through collisions.
[Keldysh L 1965 Sov. Phys.JETP 20 1307]

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## Conclusions, Looking forward

- Mechanical, pressure driven processes are subject to RT instability, while shorter and more energetic irradiation can prevent the possibility of all mechanical instabilities.

- For more realistic estimates relativistic analysis is needed

- First steps include only smaller lasers with monomer targets

- PICCANTE unfinished, but with essential advantages

- For experimental physicists EPOCH is more user friendly