Advanced multi-stage simulations of laser-driven ion sources for materials science applications

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erc ERC-2014-CoG No. 647554 **ENSURE**

Laser-driven Ion Sources main features

(energy & number of accelerated ions):

- ✓ Match **requirements** of many **materials characterization techniques** (i.e. **Ion Beam Analysis**).
- ✓ Easily achievable with **near critical double-layer targets** and reduced laser requirements.
- ✓ **Peculiar** with respect to conventional accelerators properties (ions delivered in **bunches**, **broad energy spectra**).

NB!

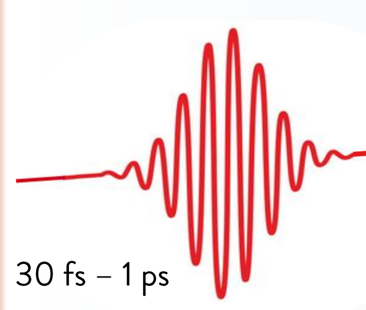
...but these applications are almost completely unexplored...

Assessment with a **multi-stage** approach to **numerical simulations**.

Multi-stage simulation scheme

PIC

Superintense laser pulse (~ 10s TW)



30 fs – 1 ps

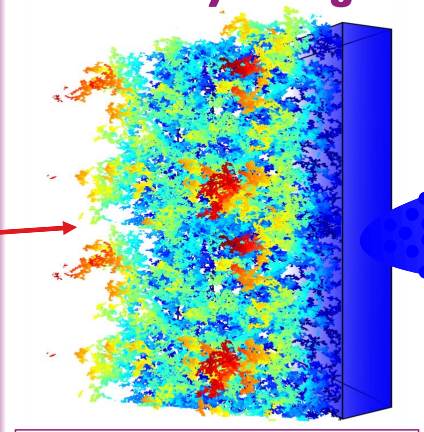
0.1 J – 10 J

10^{18} -10^{22} W/cm^2

I. Prencipe et. al., *Plasma Phys. Control. Fusion* 58 (2016), no. 3, 034019

DLCCA

Double layer target



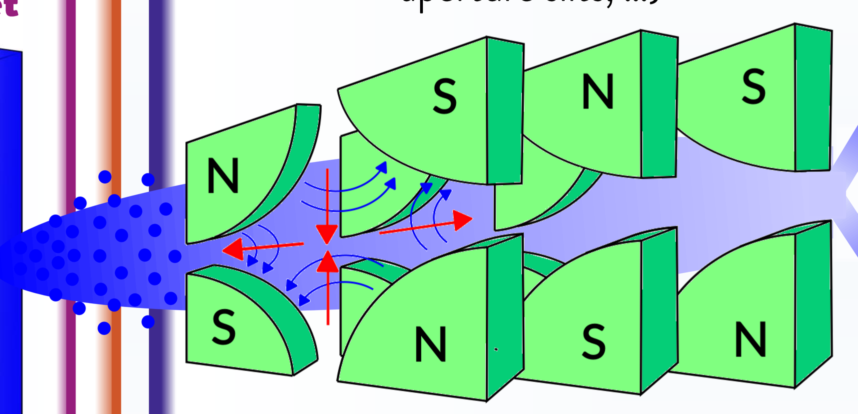
M. Passoni et al, Phys. Rev. Accel. Beams. 19 (2016), no. 6, 061301.

A. Zani et al., Carbon 56 (2013), 358 – 365

Monte Carlo simulation

Beam Handling system

(magnetic dipole, quadrupole magnets, aperture slits, ...)



Accelerated ions

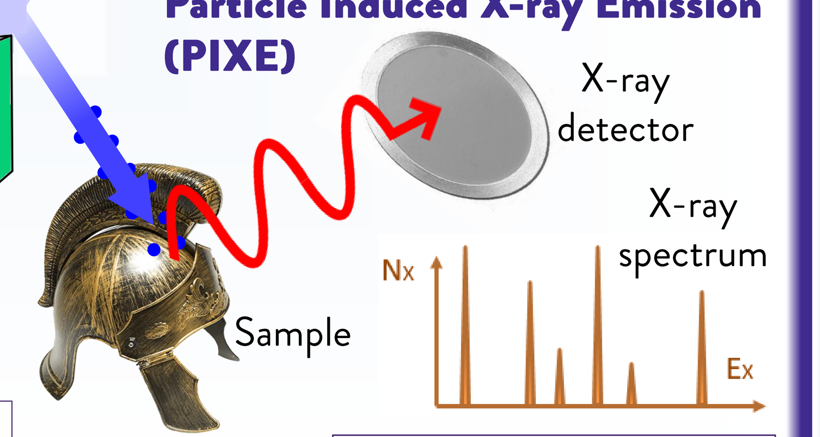
M Scisci`o et al *Sci. Rep.* 8 (2018), no. 1, 6299.

V. Scuderi et al. Nuclear Instruments and Methods in Physics Research Section A, 740 (2014), 87 – 93.

Neutron source

CM Brenner et al. *Plasma Phys. Control. Fusion* 58 (2015), no. 1, 014039

Particle Induced X-ray Emission (PIXE)



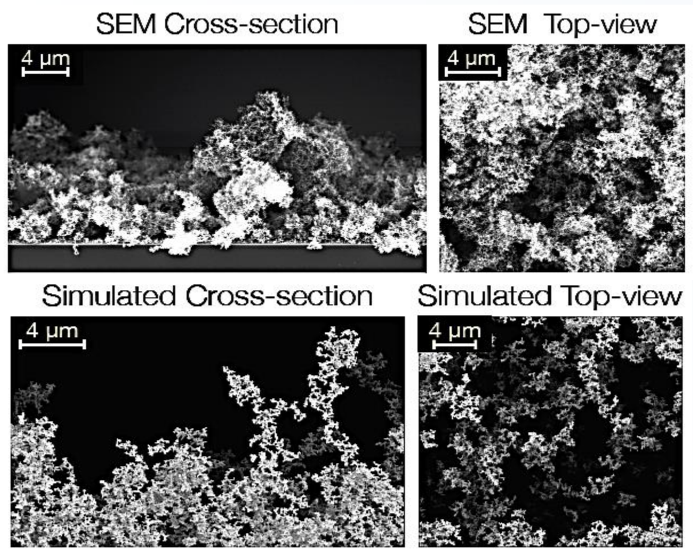
M. Barberio, et al. *Sci. Rep.* 7. (2017).

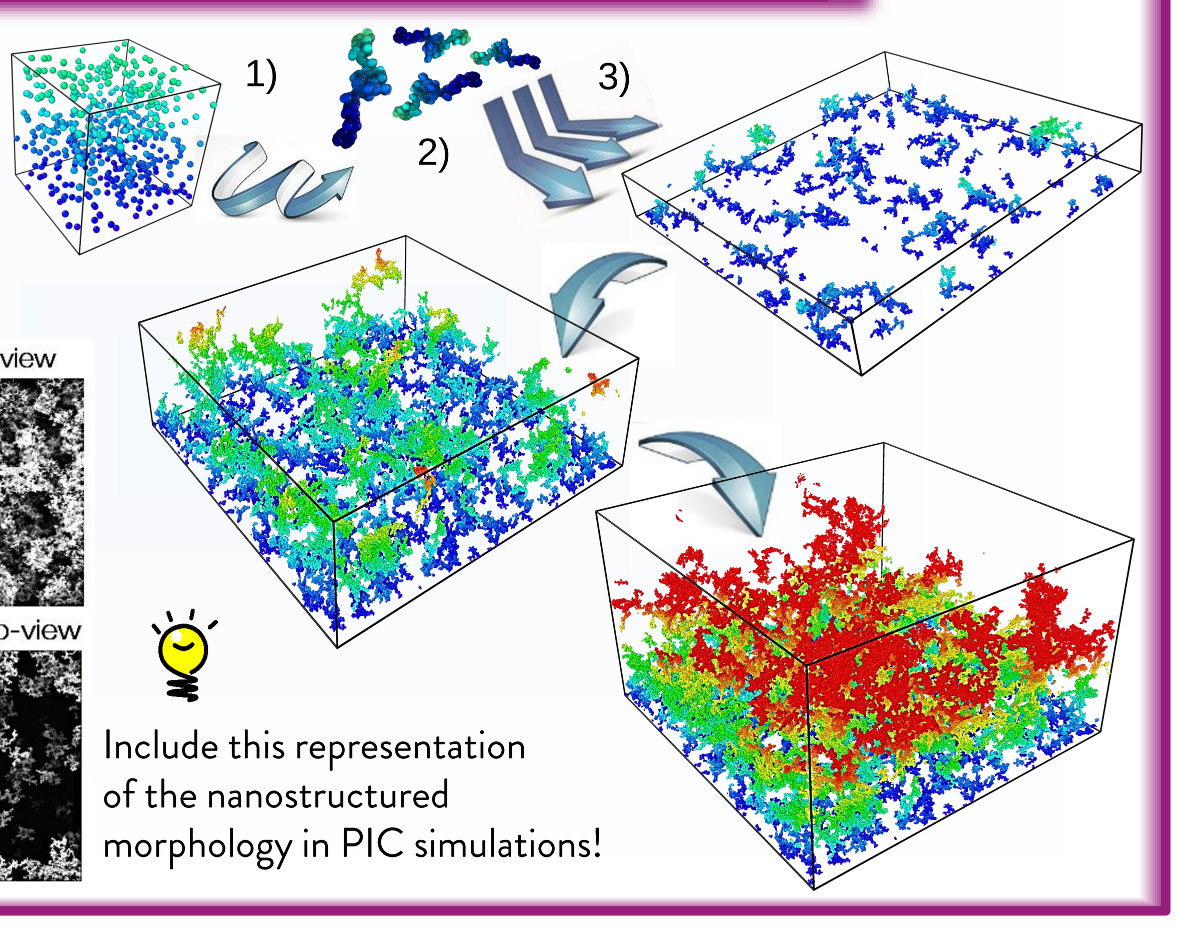
Diffusion Limited Cluster-Cluster Aggregation

Steps to **simulate** the **foam growth**:

1) Brownian motion of nanoparticles
2) Particle aggregation in clusters by irreversible sticking
3) Clusters deposition on substrate

Comparison with SEM images:





Include this representation of the nanostructured morphology in PIC simulations!

Particle-In-Cell Simulation

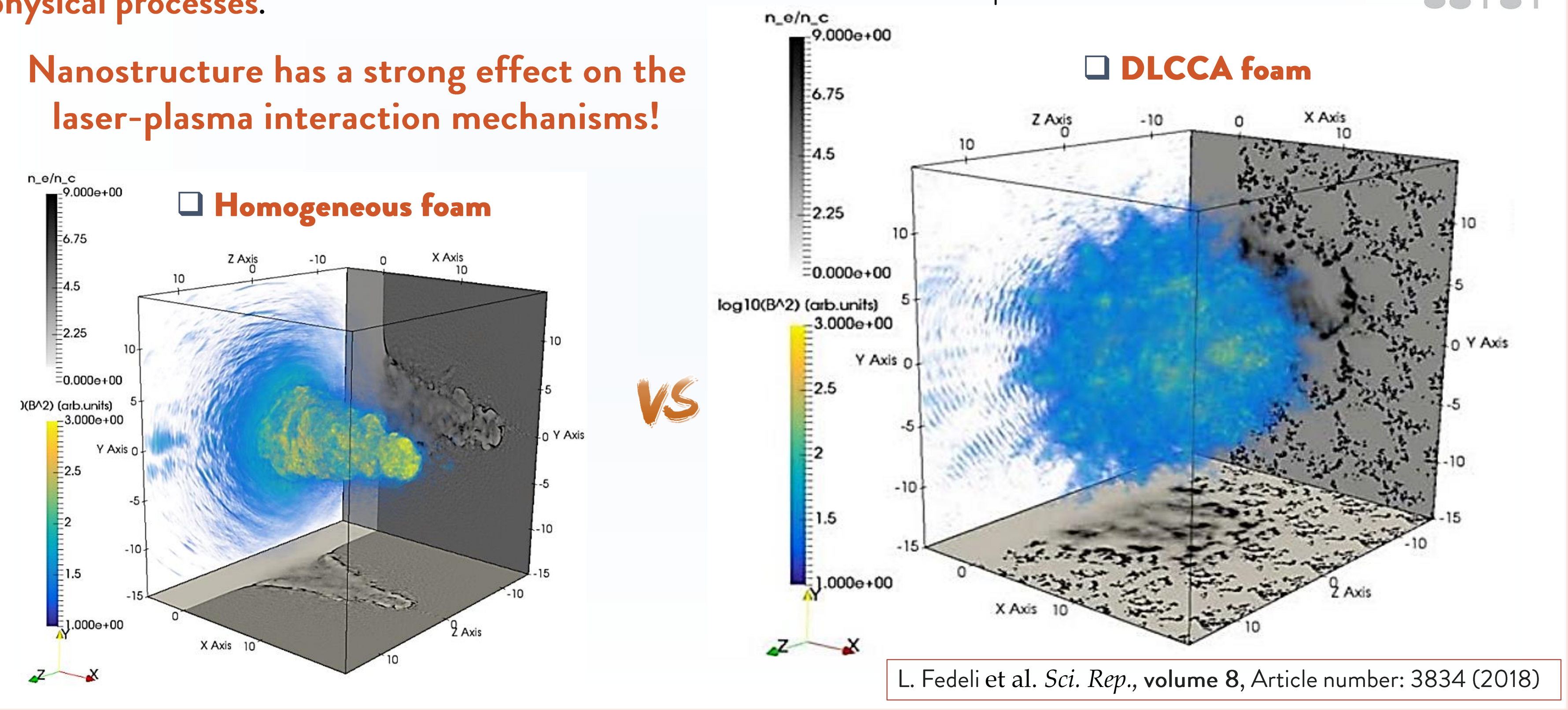
Include **nanostructure morphology** to properly **model physical processes**.

Laser pulse:

- Ultra-short (~30 fs)
- relativistic (a0 = 5–45)
- λ = 0.8 µm

piccante CINECA

Nanostructure has a strong effect on the laser-plasma interaction mechanisms!



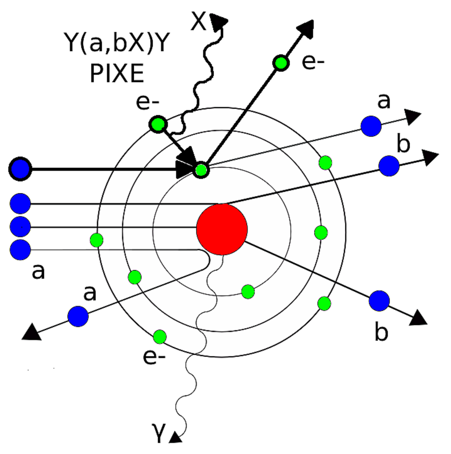
L. Fedeli et al. *Sci. Rep.*, volume 8, Article number: 3834 (2018)

PIXE, general aspects

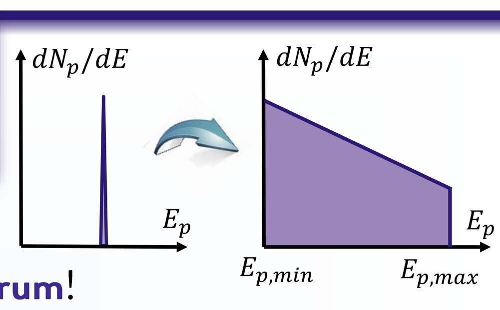
Ion Beam Analysis (**IBA**) technique → Retrieve the elemental composition of unknown samples.

- ❑ **2-5 MeV** monoenergetic **protons**.
- ❑ Elemental **concentrations** & **Depth profiles**
- ❑ **Cultural heritage**, environmental, biological and medical studies.
- ❑ Quantitative analysis → commercial codes

GUPIX



Proper model for PIXE with a laser-driven proton source



PIXE theory developed only for monoenergetic protons → Necessary to **include** a **broad** energy **spectrum**!

$$Y_j = N_p \frac{\Delta\Omega}{4\pi} \varepsilon_j W_j \frac{N_{Av}}{M_j} \int_{E_p}^{0} \sigma_j(E)\, \omega_j exp\left(-\mu_j \int_{E_p}^{E} \frac{dE'}{S(E')} \frac{\cos(\varphi)}{cos(\theta)}\right) \frac{dE}{S(E)}$$

$$Y_j = \frac{\Delta\Omega}{4\pi} \varepsilon_j W_j \frac{N_{Av}}{M_j} \int_{E_{p,min}}^{E_{p,max}} f_p(E_p) \int_{E_p}^{0} \sigma_j(E)\, \omega_j exp\left(-\mu_j \int_{E_p}^{E} \frac{dE'}{S(E')} \frac{\cos(\varphi)}{cos(\theta)}\right) \frac{dE}{S(E)} dE_p$$

Y_j: X-ray yields, $\Delta\Omega$: detector solid angle, ε_j: detector efficiency, W_j: element concentration, N_{Av}: Avogadro's number, M_j: atomic weight, E_p: proton energy, σ_j: ionization cross section, ω_j: fluorescence yield, μ_j: X-ray attenuation coefficient, S: proton stopping power, φ: proton impact angle, $f_p(E_p)$: proton energy distribution ($E_{p,min}$ & $E_{p,max}$: upper and lower energy cutoff).

Sensitivity analysis

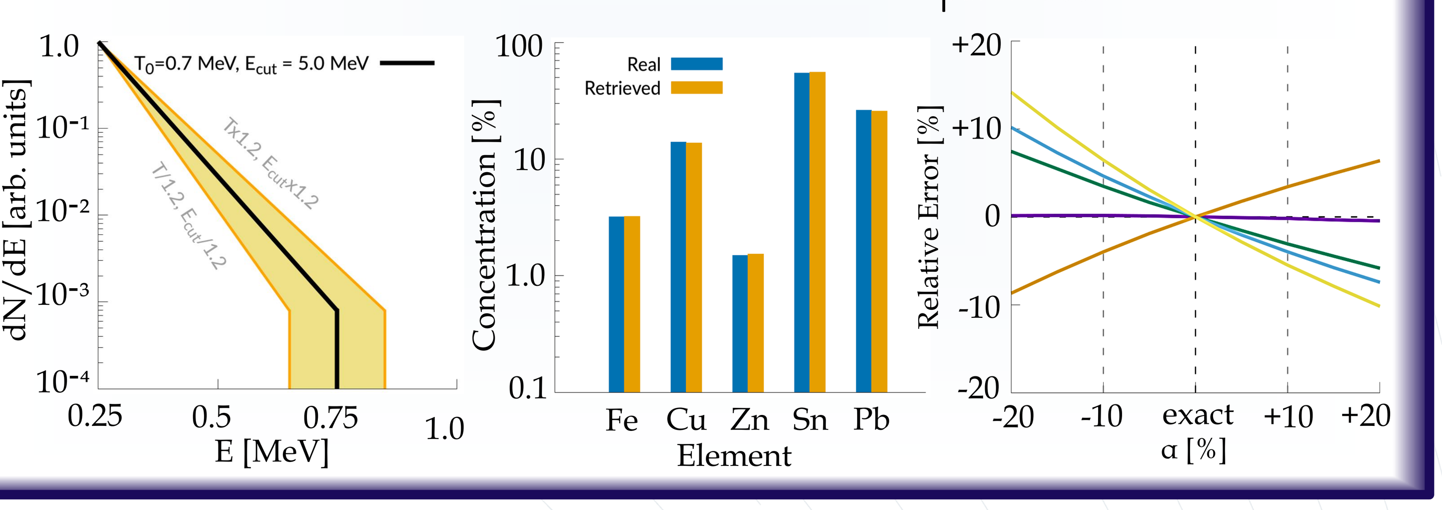
Homogeneous sample **analysis.** VS **Uncertainty** about the proton **spectrum shape.**

Proton energy spectra:

- Monte Carlo (—).
- Iterative code (▭).

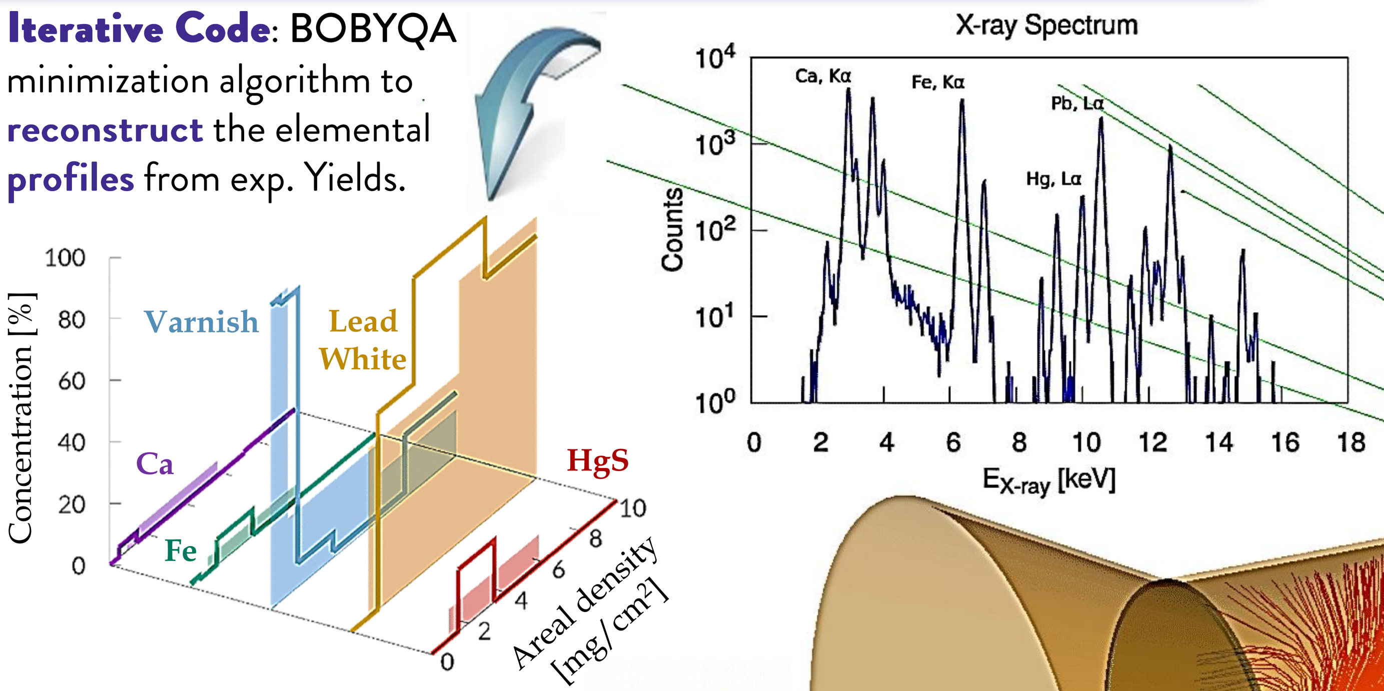
Retrieved elemental concentrations vs **Real** ones.

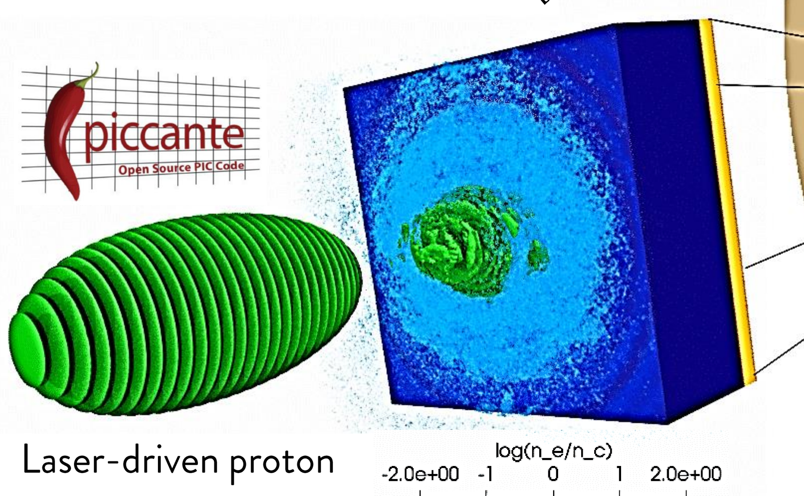
Relative error as a function of the fluctuation parameter.

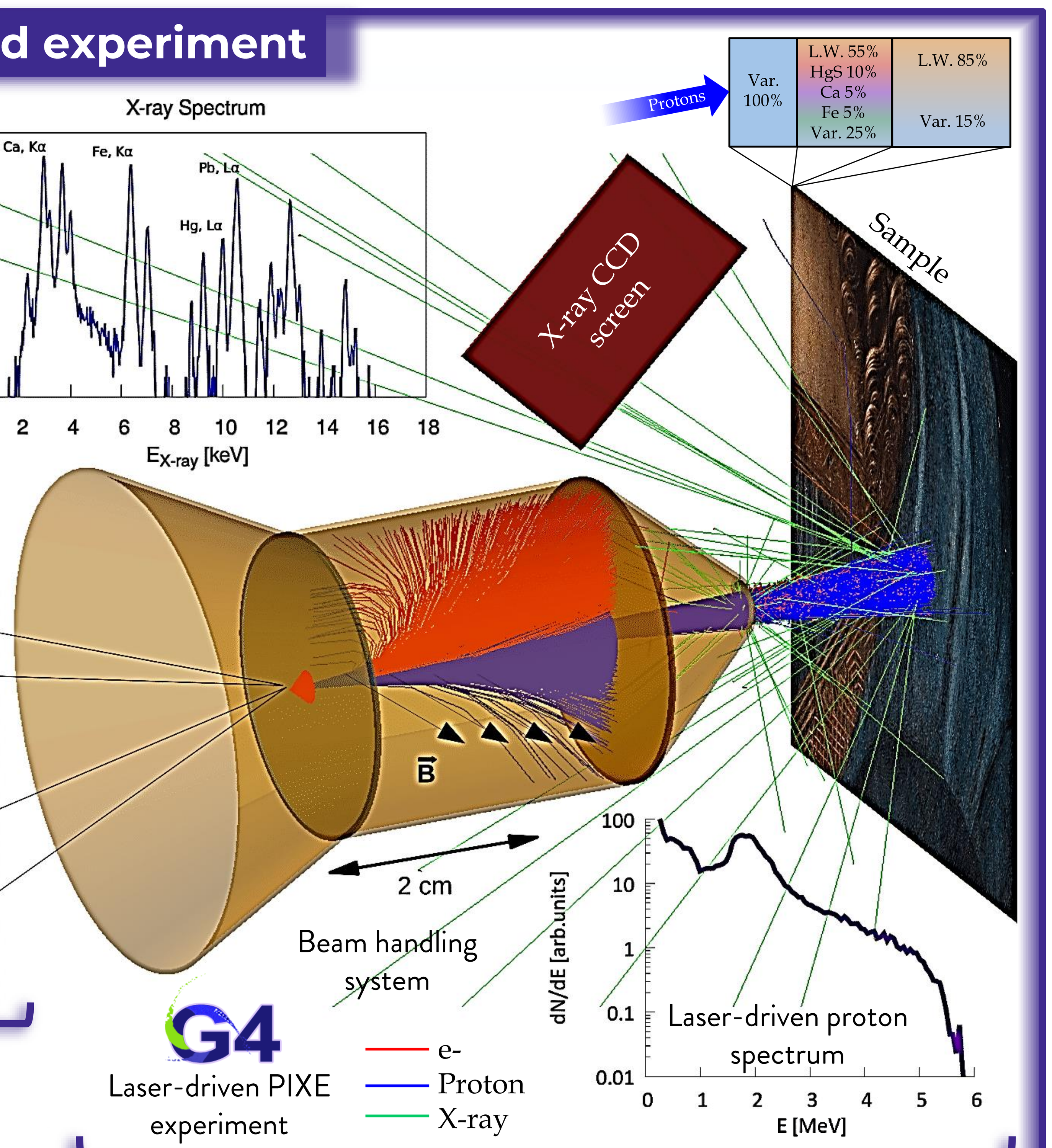


Laser-Driven PIXE simulated experiment

Iterative Code: BOBYQA minimization algorithm to **reconstruct** the elemental **profiles** from exp. Yields.







3D Particle-In-Cell (PIC) Simulation: 30 fs laser pulse interacting with uniform-foam coated targets (5 µm, 1 nc + 0.8 µm, 40 nc) at a₀ = 2 – 4.5

M. Passoni, L. Fedeli, F. Mirani. Superintense Laser-driven Ion Beam Analysis. *Sci. Rep.* (2018) under review

Geant4 Monte Carlo Simulation: performed using ~10^{10} protons with momenta extracted from the PIC simulations output.

Conclusion and perspectives

DLCCA – PIC	Nanostructure has a strong influence on the interaction of an ultra-intense laser with a near critical plasma	Exploit the effect of nanostructure on the accelerated ions spectrum
PIC – Monte Carlo	Assessment of the possibility of reconstructing the composition of complex samples with Laser-Driven PIXE	Particle Induced Gamma Ray & Portable Neutron Sources (under development)

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