Istituto Nazionale di Fisica Nucleare
Laboratori Nazionali di Frascati

Workshop computing@CSN5
Applications and innovations at INFN

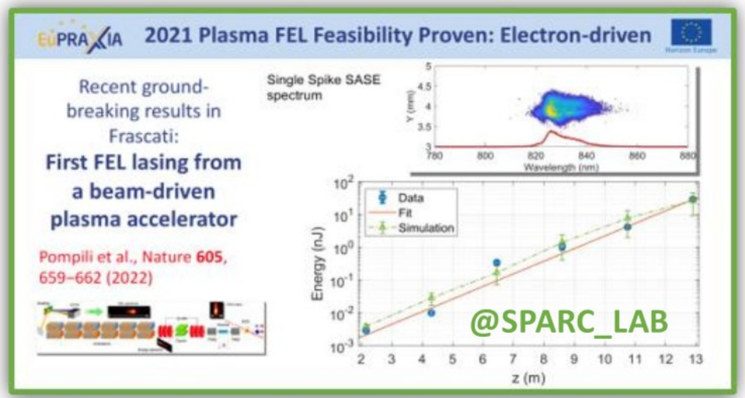
Bari, 14-16 Oct 2024

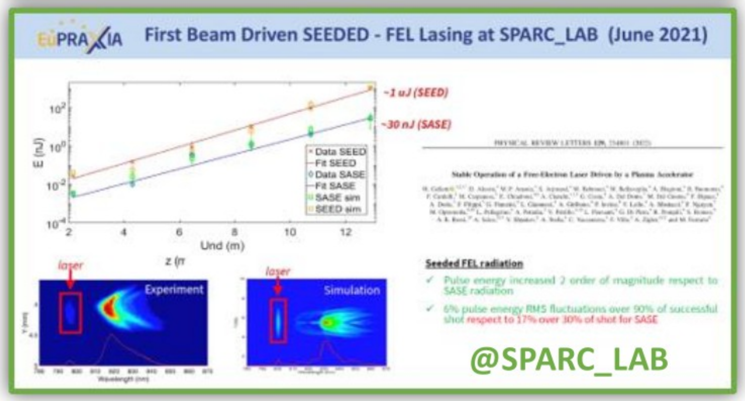
Large scale computing for designing plasma-based particle accelerators

Alessio Del Dotto
INFN -LNF
on behalf of the collaboration

Outline

- An **intense cutting edge activity on plasma acceleration** at LNF and MI






FEATURE EuPRAXIA

Surf's up *Simulation of electron-driven plasma wakefield acceleration, showing the drive electron beam (orange/purple), the plasma electron wake (grey) and wakefield-ionised electrons forming a witness beam (orange).*

EUROPE TARGETS A USER FACILITY FOR PLASMA ACCELERATION

Ralph Assmann, Massimo Ferrario and Carsten Welsch describe the status of the ESFRI project EuPRAXIA, which aims to develop the first dedicated research infrastructure based on novel plasma-acceleration concepts.

Energetic beams of particles are used to explore the fundamental forces of nature, produce known and unknown particles such as the Higgs boson at the LHC, and generate new forms of matter, for example at the future FAIR facility. Photon science also relies on particle beams: electron beams that emit pulses of intense synchrotron light, including soft and hard X-rays, in either circular or linear machines. Such light sources enable time-resolved measurements of biological, chemical and physical structures on the molecular down to the atomic scale, allowing a diverse global community of users to investigate systems ranging from viruses and bacteria to materials science, planetary science, environmental science, nanotechnology and archaeology. Last but not least, particle beams for industry and health support many societal applications ranging from the X-ray inspection of cargo containers to food sterilisation, and from chip manufacturing to cancer therapy.

This scientific success story has been made possible through a continuous cycle of innovation in the physics and technology of particle accelerators, driven for many decades by exploratory research in nuclear and particle physics. The invention of radio-frequency (RF) technology in the 1920s opened the path to an energy gain of several tens of MeV per metre. Very-high-energy accelerators were constructed with RF technology, entering the GeV and finally the TeV energy scales at the Tevatron and the LHC. New collision schemes were developed, for example the mini "beta squeeze" in the 1970s, advancing luminosity and collision rates by orders of magnitudes. The invention of stochastic cooling at CERN enabled the discovery of the W and Z bosons 40 years ago.

However, intrinsic technological and conceptual limits mean that the size and cost of RF-based particle accelerators are increasing as researchers seek higher beam energies. Colliders for particle physics have reached a

THE AUTHORS
Ralph Assmann *DESY and INFN*, **Massimo Ferrario** *INFN*, **Carsten Welsch** *University of Liverpool/INFN.*

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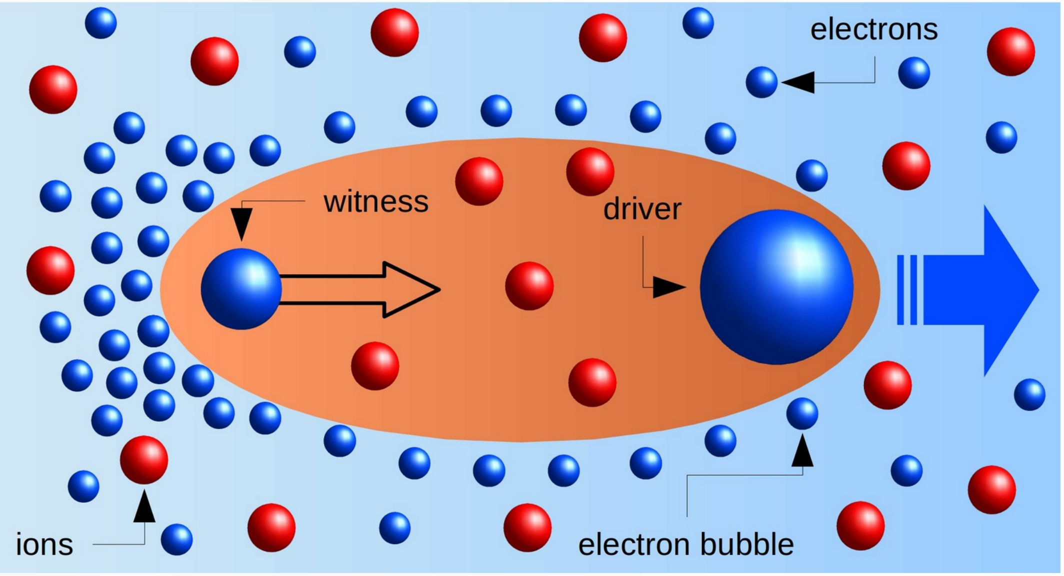
Frascati`s future facility

- > 130 M€ invest funding
- Beam-driven **plasma accelerator** - PWFA
- Europe`s **most compact** and most southern FEL
- The world`s most compact RF accelerator **X band** with CERN

Plasma acceleration



The field **driver**:

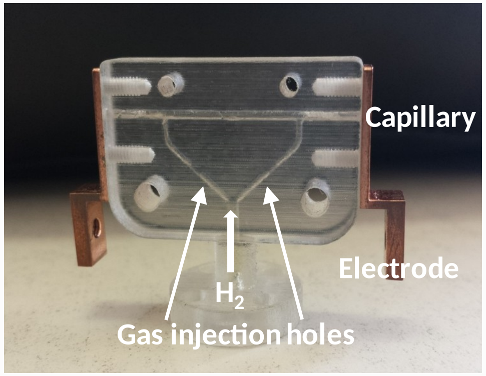
- Particle bunch (PWFA)
- Laser pulse (LWFA)

The **witness** can be:

- Self injected
- Externally injected

$$E_0 = \frac{m_e c \omega_p}{e} \simeq 96\sqrt{n_0(cm^{-3})} \rightarrow E_0 \approx 10\frac{GV}{m} @ n_0 = 10^{16} cm^{-3}$$

From conventional Cavity ~ meter to capillary ~ cm



Computer simulations: why?

- **Plasma acceleration experiments try to investigate multidimensional problems (plasma is an active media)**
- **Phenomenology:** try to capture the essential features by reducing the degrees of freedom of the theory
- **Computers simulations:** provide numerical experiments

The Maxwell-Vlasov model of plasma

- The kinetic description of a collisionless plasma is based on the **Vlasov-Maxwell system of equations**, which characterizes the various species ***s*** of particles in the plasma through their respective distribution functions. The distribution $\mathbf{f_s(t,x,p)}$ satisfies Vlasov's equation.

$$\left(\partial_t + \frac{\mathbf{p}}{m_s\gamma} \cdot \nabla + \mathbf{F}_L \cdot \nabla_{\mathbf{p}}\right) f_s = 0$$

$$\mathbf{F}_L = q_s \left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$$

$$\gamma = \sqrt{1 + \mathbf{p}^2/m_s^2}$$

- The force follows from the existence, in the plasma, of **collective (macroscopic) electromagnetic** field that fulfills **Maxwell equations**.

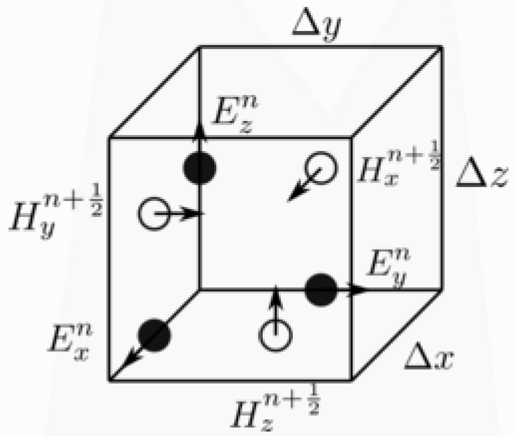
$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \rho$$

$$\nabla \times \mathbf{B} = \mathbf{J} + \partial_t \mathbf{E}$$

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B}$$

The problem we want to solve

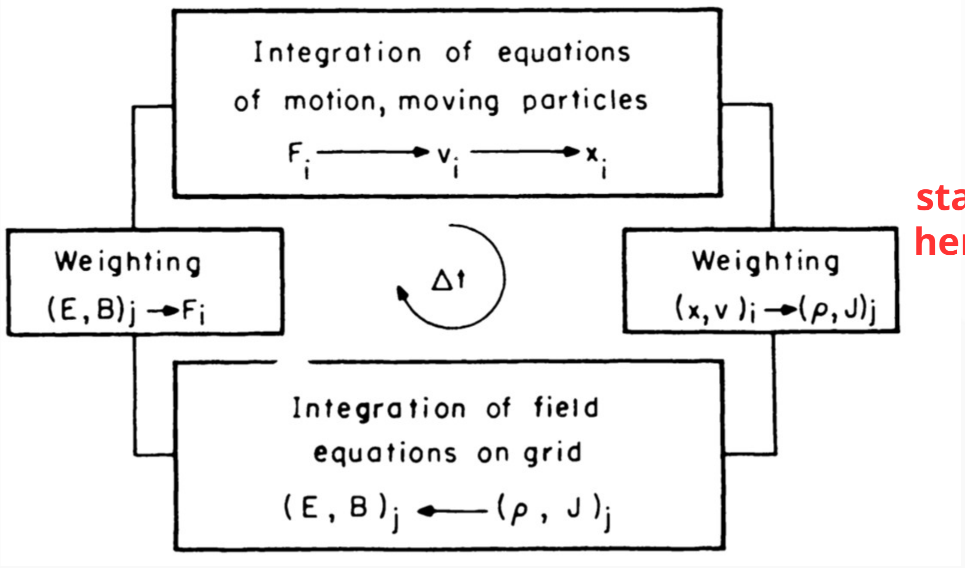


The Particle-In-Cell method owes its name to the discretization of the particles distribution function as a sum of quasi-particles:

$$f_s(t,\mathbf{x},\mathbf{p}) = \sum_{p=1}^{N_s} \frac{w_p}{V_c}\, S\big(\mathbf{x}-\mathbf{x}_p(t)\big)\,\delta\big(\mathbf{p}-\mathbf{p}_p(t)\big)$$

$$\rho(t,\mathbf{x}) = \sum_s q_s \int d^3p\, f_s(t,\mathbf{x},\mathbf{p})$$

$$\mathbf{J}(t,\mathbf{x}) = \sum_s q_s \int d^3p\, \mathbf{v} f_s(t,\mathbf{x},\mathbf{p})$$

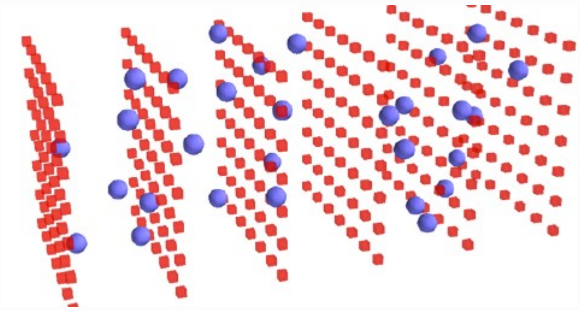


start here!

- ***it is possible to simulate highly non-linear systems***

- ***temperature effects poorly described***
- ***noisy***

(L)PWFA simulations



- Represent the gas/plasma/beam by a set of macro-particles
- Solve the equations of motion for each macro-particle

$$\frac{d\mathbf{x}_p}{dt} = \frac{\mathbf{u}_p}{\gamma_p}$$

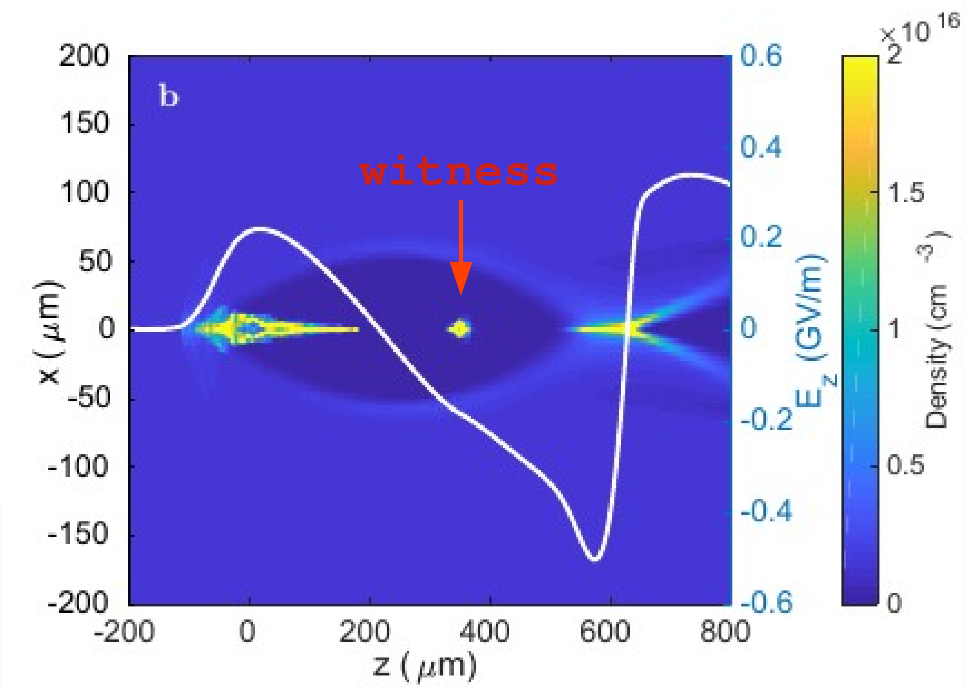
$$\frac{d\mathbf{u}_p}{dt} = r_s\left(\mathbf{E}_p + \frac{\mathbf{u}_p}{\gamma_p} \times \mathbf{B}_p\right)$$

- Self-consistently solve the Maxwell equations on a discrete space-time

- Reduced option: **hybrid/fluid codes**

  Hybrid code = Beam Particles / Laser (3D) + Fluid Plasma Electron Background

Micrometric bunch in a tiny bubble → small variations large instability



Computational costs

3D PIC

- Large requirements in **memory and computational power**: typically several hours on hundreds of CPU/ GPUs

Hybrid/fluid codes

- **Faster** several hours on a limited number of CPU/GPU (assume some kind of symmetry, fluid models, ...)

Electromagnetic particle-in-cell computational applications [edit]

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]	GPLv3	Open Repo:[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]	GNU AGPL	Open Repo [27]	doi:10.1007/3-540-47789-6_36
PhotonPlasma	[28]	Unknown	Open Repo:[29]	doi:10.1063/1.4811384
PICCANTE	[30]	GPLv3+	Open Repo:[31]	doi:10.5281/zenodo.48703
PICLas	[32]	GPLv3+	Open Repo:[33]	doi:10.1016/j.crme.2014.07.005 doi:10.1063/1.5097638
PICMC	[34]	Proprietary	Available from Fraunhofer IST	
PIConGPU	[35]	GPLv3+	Open Repo:[36]	doi:10.1145/2503210.2504564
SMILEI	[37]	CeCILL-B	Open Repo:[38]	doi:10.1016/j.cpc.2017.09.024
iPIC3D	[39]	Apache License 2.0	Open Repo:[40]	doi:10.1016/j.matcom.2009.08.038
The Virtual Laser Plasma Lab (VLPL)	[41]	Proprietary	Unknown	doi:10.1017/S0022377899007515
Tristan v2	[42]	3-Clause-BSD	Open source,[43] but also has a private version with QED/radiative[44] modules	doi:10.5281/zenodo.7566725 [45]
VizGrain	[46]	Proprietary	Commercially available from Esgee Technologies Inc.	
VPIC	[47]	3-Clause-BSD	Open Repo:[48]	doi:10.1063/1.2840133
VSim (Vorpal)	[49]	Proprietary	Available from Tech-X Corporation	doi:10.1016/j.jcp.2003.11.004
Warp	[50]	3-Clause-BSD-LBNL	Open Repo:[51]	doi:10.1063/1.860024
WarpX	[52]	3-Clause-BSD-LBNL	Open Repo:[53]	doi:10.1016/j.nima.2018.01.035
ZPIC	[54]	AGPLv3+	Open Repo:[55]	
ultraPICA		Proprietary	Commercially available from Plasma Taiwan Innovation Corporation.	

Software setup

Several different codes to be tested and wrapped

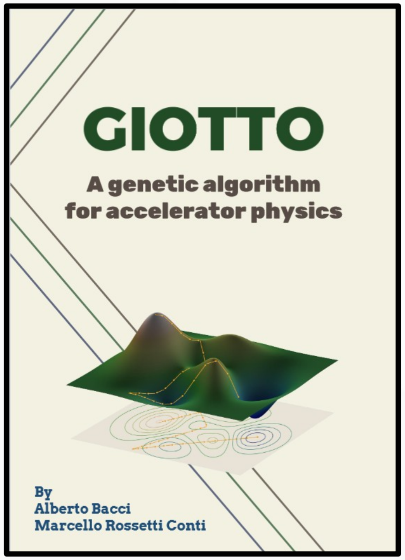
Particle trackers *(CPU)*

Plasma PIC/Hybrid *(CPU , GPU)*

Artificial Intelligence

(a network within INFN-A)

- **GIOTTO (INFN-MI) solves complex multi-objective problems** (correlated parameters, space-charge like) & statistical analysis (machine jitters studies)
- **Bayesian Optimization** on the plasma side



Optimas → Optimization at scale, powered by libEnsamble https://github.com/optimas-org/optimas

<u>Plasma PICs running in IBM PowerAC922 nodes at LNF and MI</u>

3D PIC:

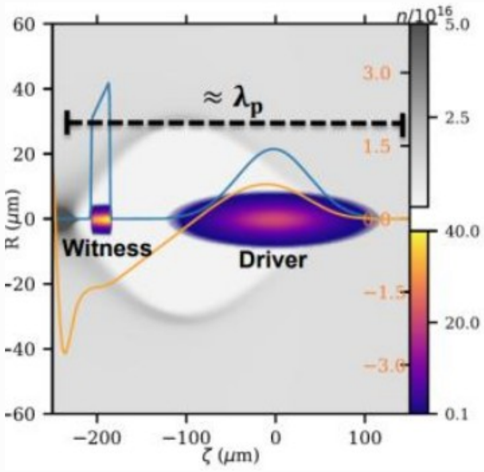
- ~1000h-CPU mm of plasma

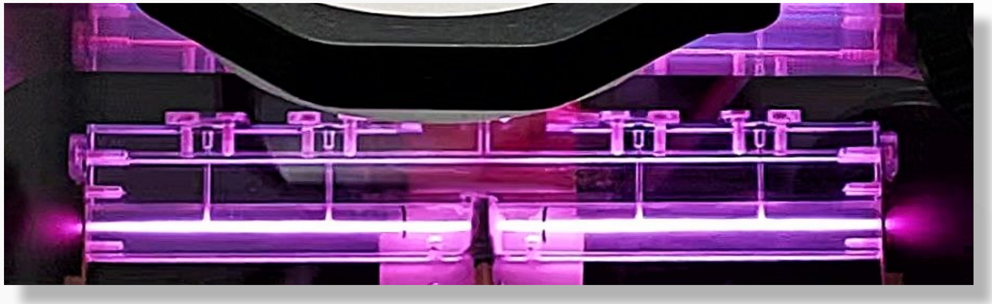
- ~100h-GPU mm of plasma

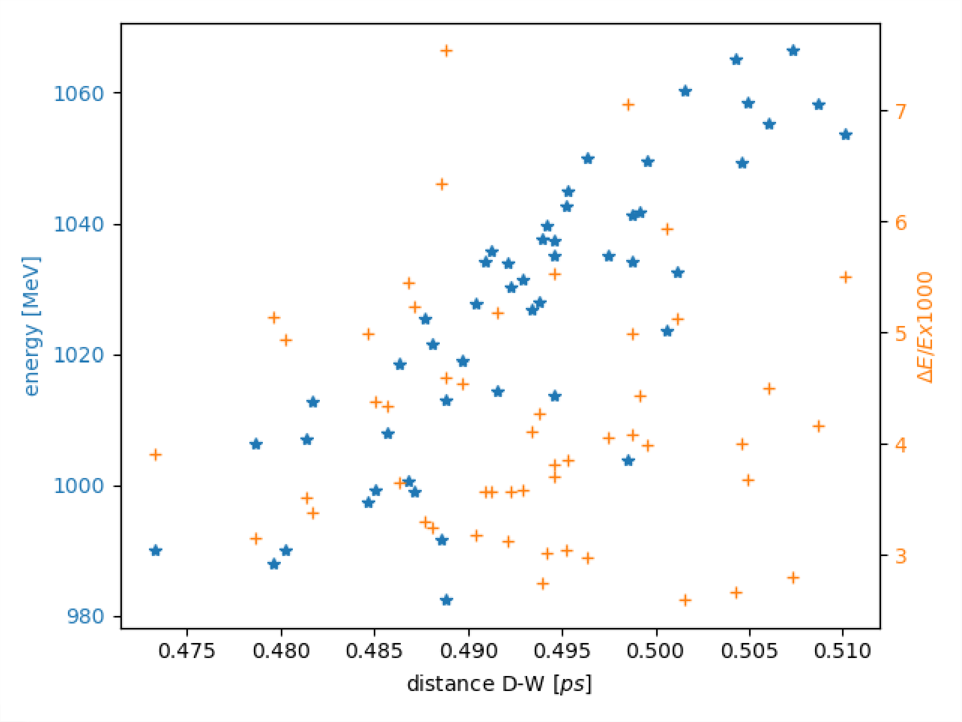
We went for a dedicated hardware for development and TDR related R&Ds!

Beam driven: EuPRAXIA case

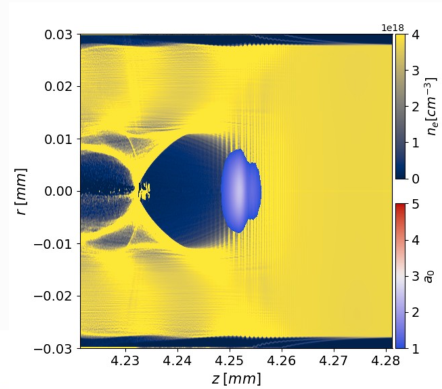
- **TDR** under completion
- FEL requires **high quality** beams
- Simulations must take into account all the relevant jitters
- **Hundreds of runs** on tens of cm plasma channels

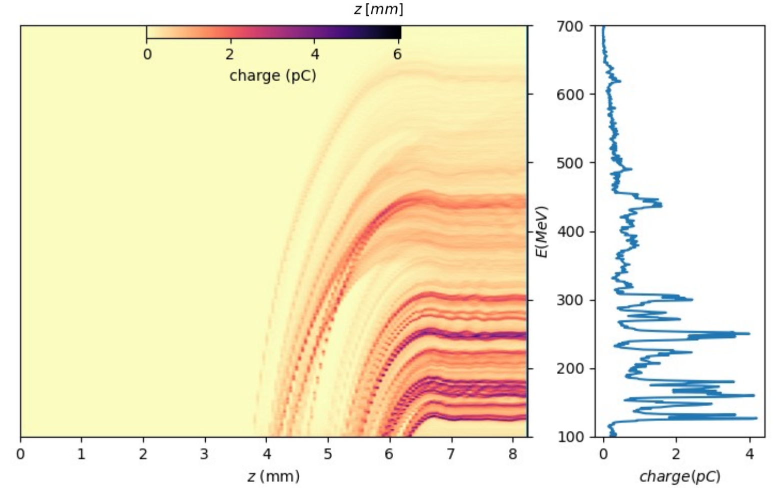






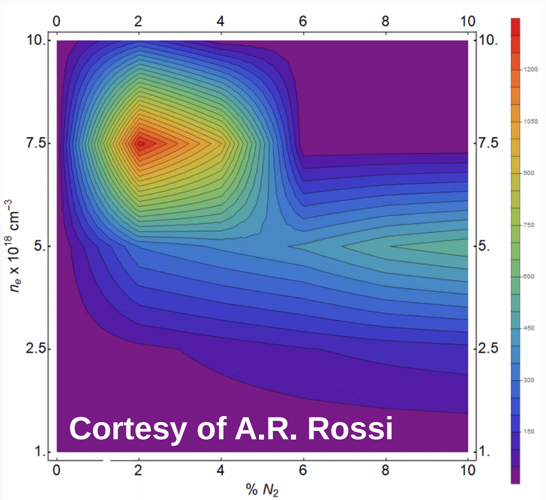
Laser driven: EuAPS case

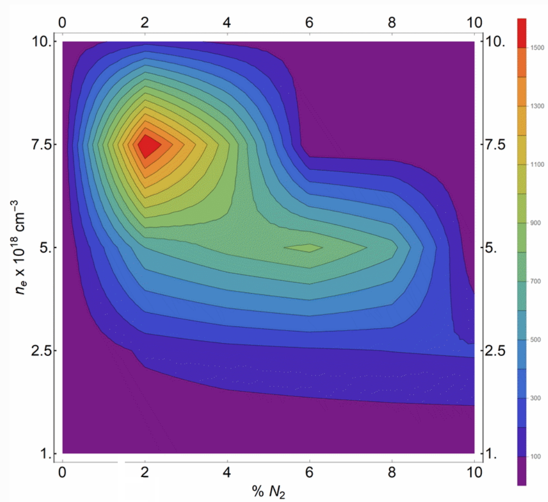




- EuPRAXIA Advanced Photon Source (**EuAPS**) (PNRR project)
- Simulations goal: optimize source photons yield around few keV
- PICs codes coupled with (in kind developed) codes for calculating radiation

parameter space scan: plasma density (He), dopant density (N_2) and laser energy scanned, resulting in **114 runs, each 8 to 10 hours long and up to 1.2 TB data each**.






Thank for your attention