Integration of ML models into GEANT4 to simulate plasma acceleration

Use case : PALLAS experiment

ARNAUD HUBER[1]

A. SYTOV[2], K. CASSOU[3], V. KUBYTSKYI[3], M. LENIVENKO[3]

Context and Objectives

Context:

Laser-plasma accelerators are compact sources of high-energy electrons (**PALLAS experiment** & **LWFA**)

Simulations are needed to understand and optimize these systems

Problems:

Full-scale simulations are very resource-intensive (PIC models)

Objective:

Integrate ML-based models into Geant4 to efficiently simulate experiments

PALLAS use case

PALLAS is laser-plasma accelerator test facility under construction at IJClab.

- Aiming for *"high-quality beam"* **laser-plasma injector (LPI)** facility working in **Continuous 10 Hz operation**
- Achieve **reliability** and **control** comparable to conventional RF accelerators standards

LPI PALLAS beamline

Parameters	phase 1	phase 2	unit
energy	150	**200**	MeV
charge	15-30	**30**	pC
frep	1-5	10	Hz
energy spread	<5%	**< 3%**	rms
$\epsilon_{n,rms}$	1	**<1**	μm
stability	5%	**<3%**	-
reproductibility	5%	**3%**	-

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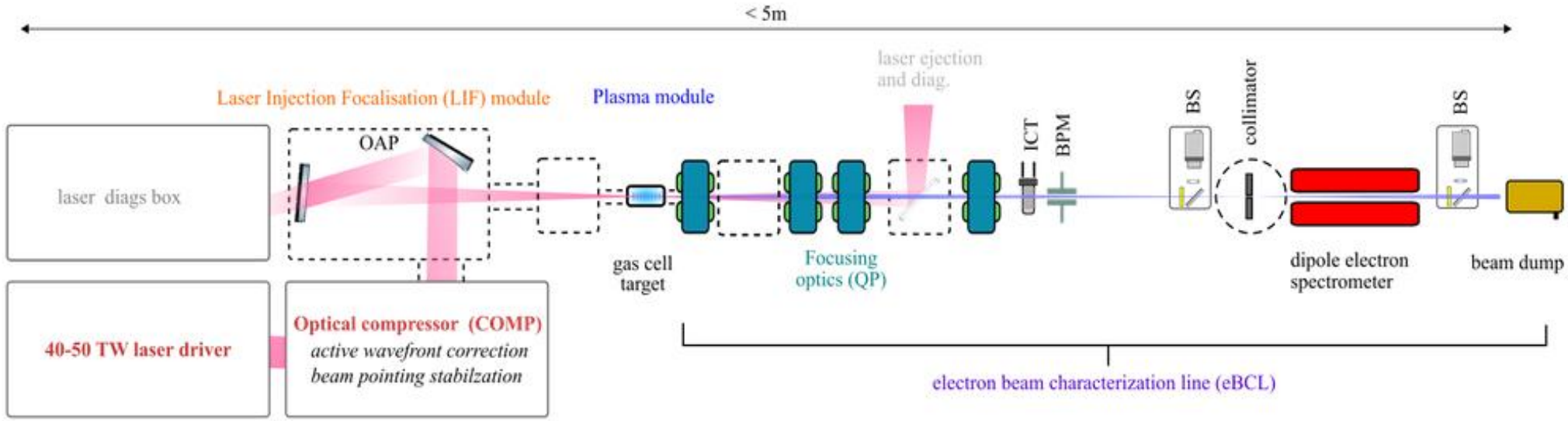


Plasma target development :

- P.Drobniak et al. PRAB 26, 091302 (2023)

Beam Transport :

- Coline Guyot. PhD Thesis, Université Paris-Saclay, 2025.

e- beam compact characterization :

- Down to 500 keV energy
- Resolution emittance
- Longitudinal phase space

LWFA

Principle :

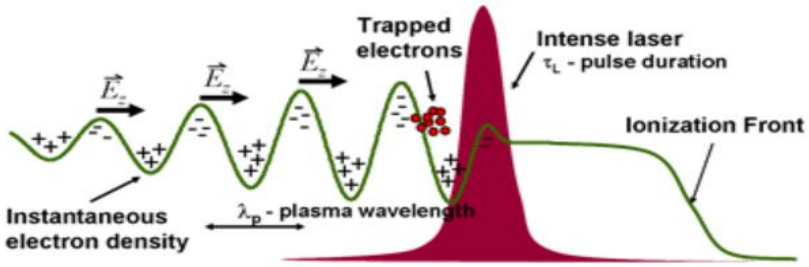
A laser travels through a gas → creating a plasma

- The laser pushes electrons aside, forming a wave
- Injected electrons "surfing" on this wave are accelerated

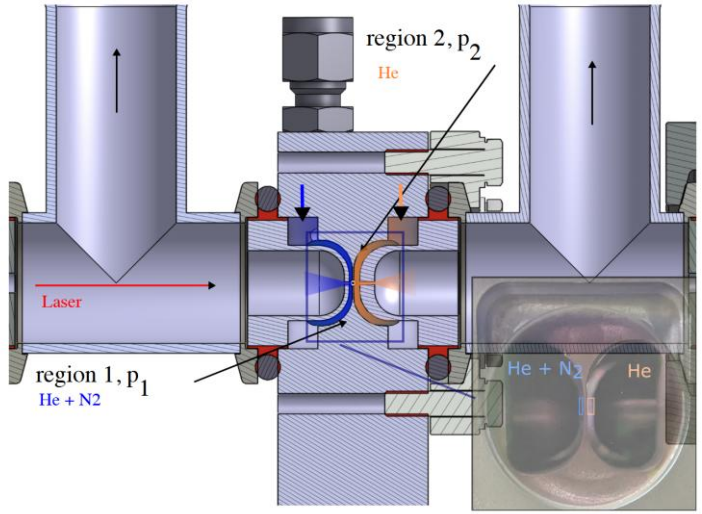
Key facts :

- Acceleration gradients > 100 GeV/m
- Experiments are **highly sensitive** to the **laser/plasma configuration**

Parameters	phase 1	phase 2	phase 3	unit
laser strengh, a_0	1.15-1.4	1.15-1.4	**>1.8**	
laser duration, t_L	40	**30**	**30**	fs (FWHM)
laser waist, w_0	18	18	18	um
Strehl ratio, S_r	**> 0.8**	**> 0.8**	**> 0.8**	-
beam pointing, δu_i	**<0.5**	**<0.5**	**<0.5**	urad
stability	1%	**<1%**	**<1%**	-
frep	10	10	10	Hz
target type	multi-cell	multi-cell	multi-cell	-
injection	ionisation	ionisation	ionisation	-
electron beamline	*CL1*	*CL1*	*TBD*	-



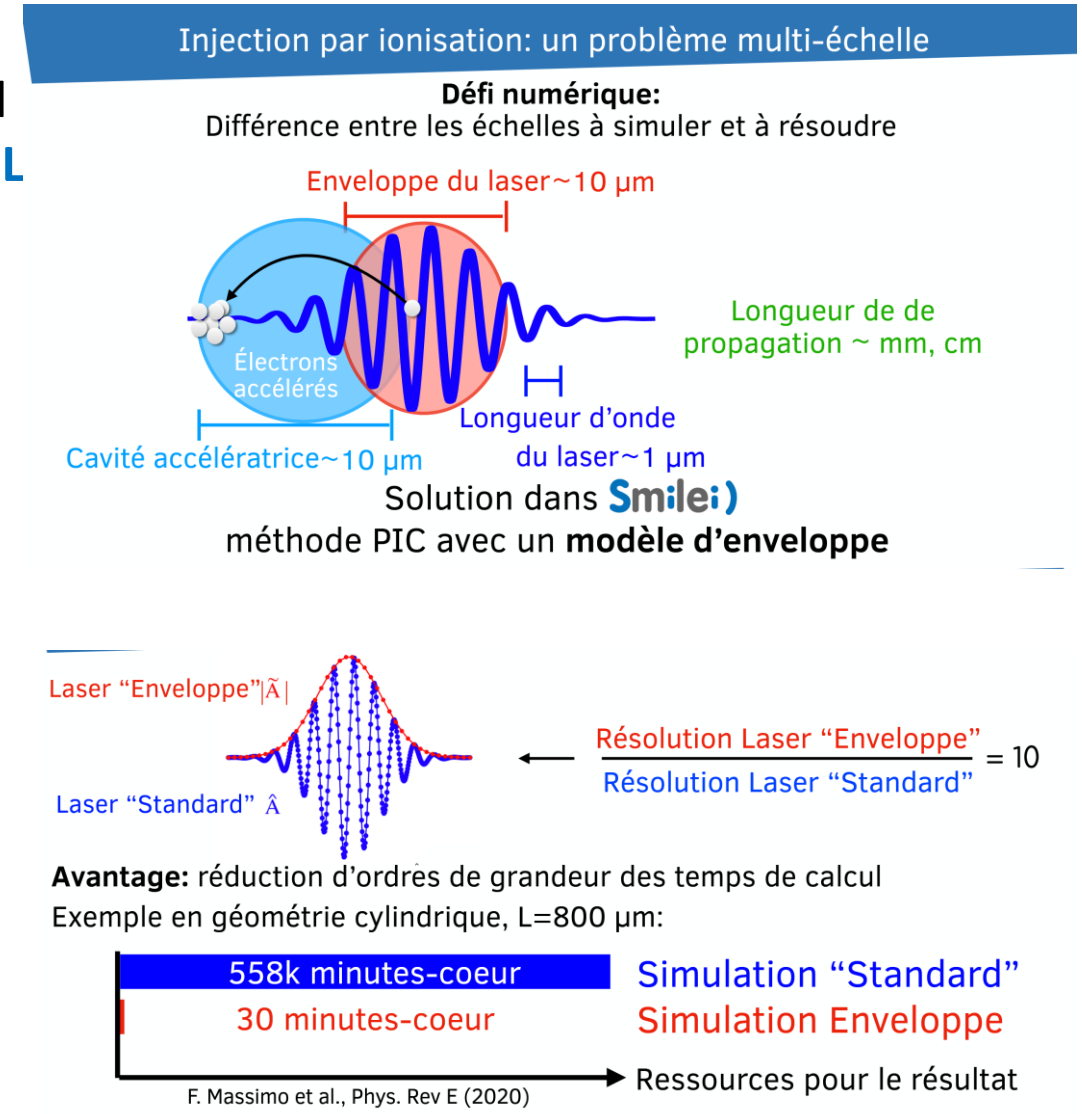
https://cuos.engin.umich.edu/researchgroups/hfs/research/laser-wakefield-acceleration/



Challenges of plasma simulations

PIC simulations (Particle-In-Cell) :

- **Very accurate** but **substantial** computational resources needed
- Numerical challenge (**slides Francesco Massimo – GdR APPEL 2022**)



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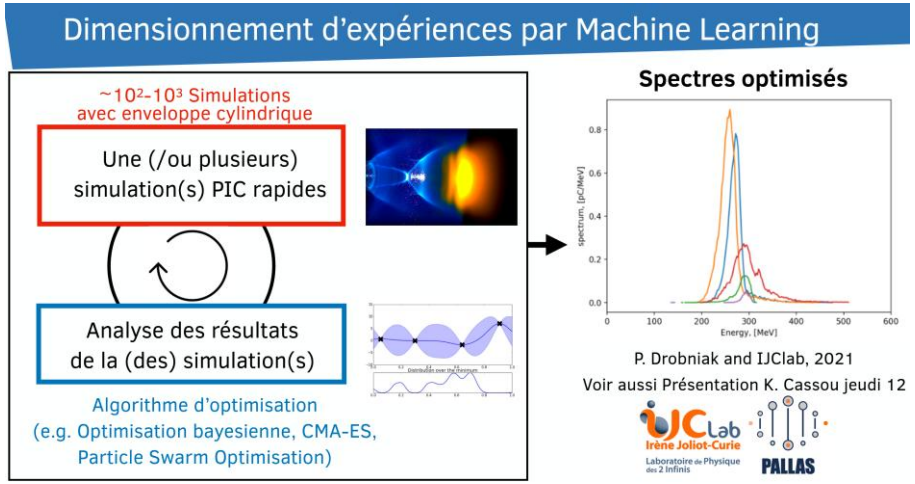
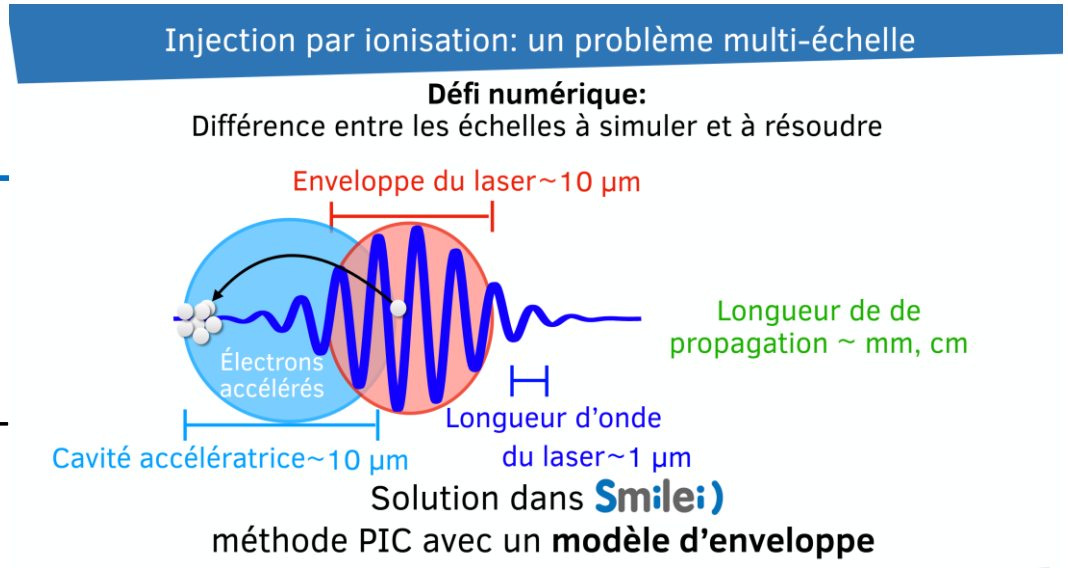
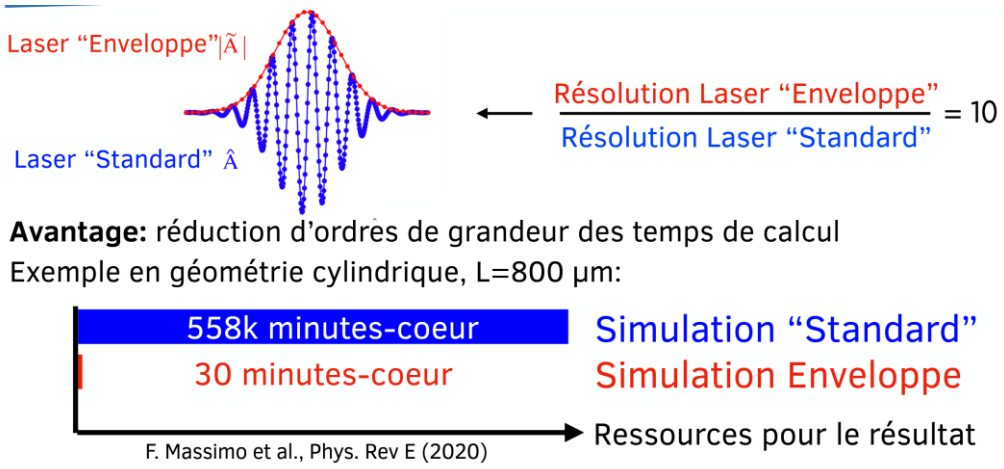
Consequences :

- Difficult to explore **large parameter spaces** (nonlinear, multi-parametric, coupled physical processes)
- Not viable for full *start-to-end* simulations
- **Machine Learning** use case !!!







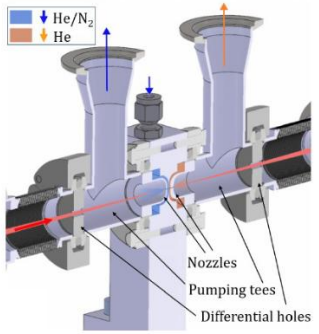
Solution : ML surrogate model

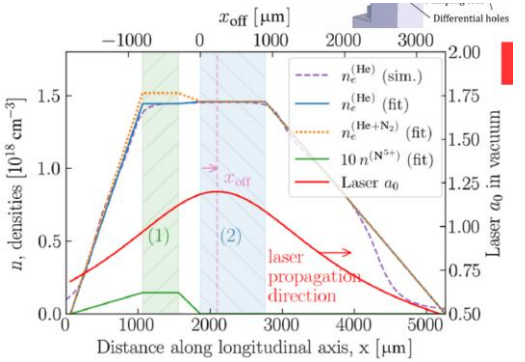
Idea :

- Train an ML model on the results of **Fast PIC simulations**
- **Predict** beam characteristics from input parameters

PALLAS gas cells[4]

Gas density profile generated[4] using **OpenFOAM[5]** code





1. V. Kubytskyi, Optimisation and surrogate models for PALLAS project, Journée modélisation LWFA GdR APPEL 2023
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5. https://www.openfoam.com/
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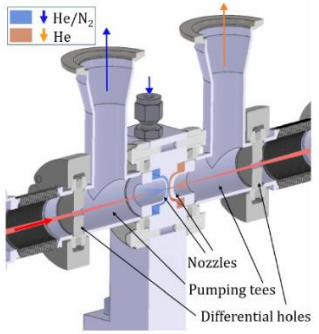
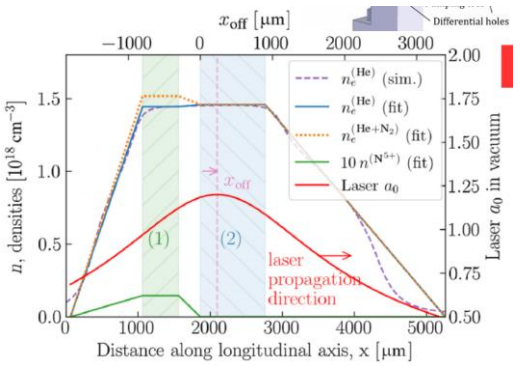
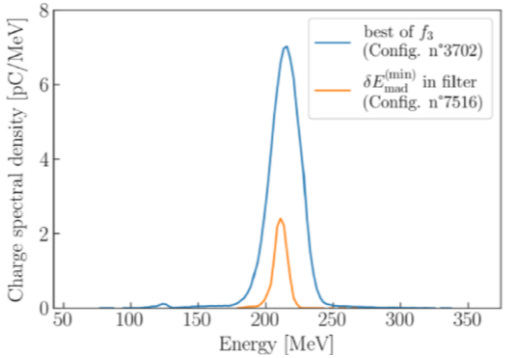




Numerical setup

- target configuration $x = [\, a_0, x_{of}, p_1 = p_2, c_{N_2} \,]$
- Smilei open source PIC code with envelop approximation coupled to ionization[1], azimuthal modes[2] and low ppc :
  ~ 12-24 h.cores/mm.(*running with 240 cores on 96k computing-core HPC SKL*)
- simplified profiles from CFD simulations and confined high-Z dopant.

PIC simulations with SMILEI[6]



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- Train an ML model on the results of **Fast PIC simulations**
- **Predict** beam characteristics from input parameters
- (re)use knowledge of already computed configurations -> construct **surrogate model of the accelerator**[1,2]
- New configuration can be estimated from the surrogate model and validated with SMILEI.

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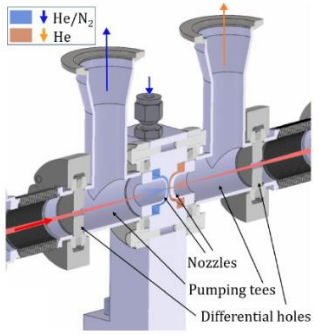

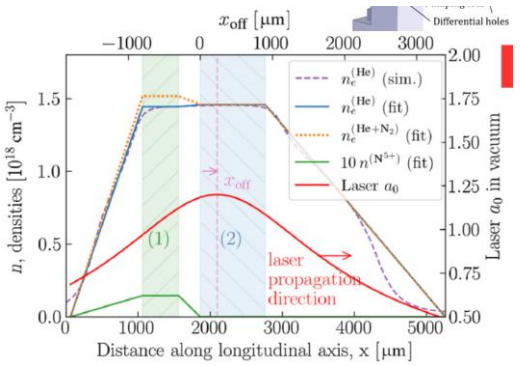

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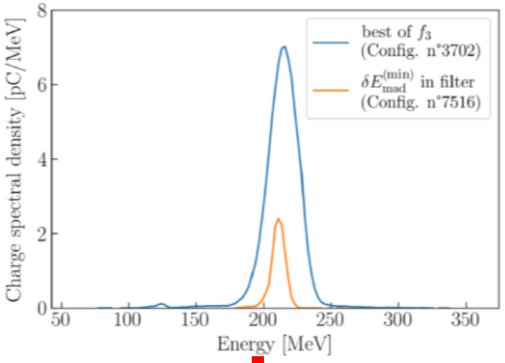

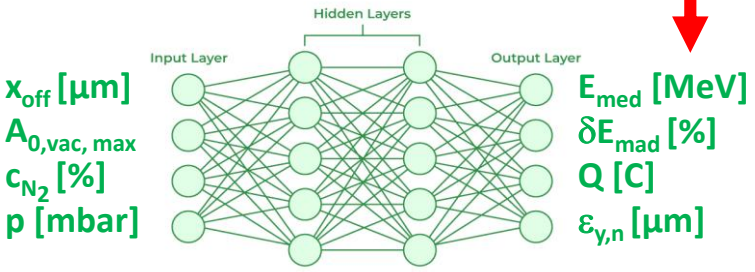

ML surrogate model[2,4,7]

Layer (type)	Output Shape	Param #
Input Layer (InputLayer)	(None, 4)	0
Hidden Layer 1 (Dense)	(None, 100)	500
PReLU activation 1 (PReLU)	(None, 100)	100
Hidden Layer 2 (Dense)	(None, 100)	10,100
PReLU activation 2 (PReLU)	(None, 100)	100
Hidden Layer 3 (Dense)	(None, 100)	10,100
PReLU activation 3 (PReLU)	(None, 100)	100
Output Layer (Dense)	(None, 4)	404

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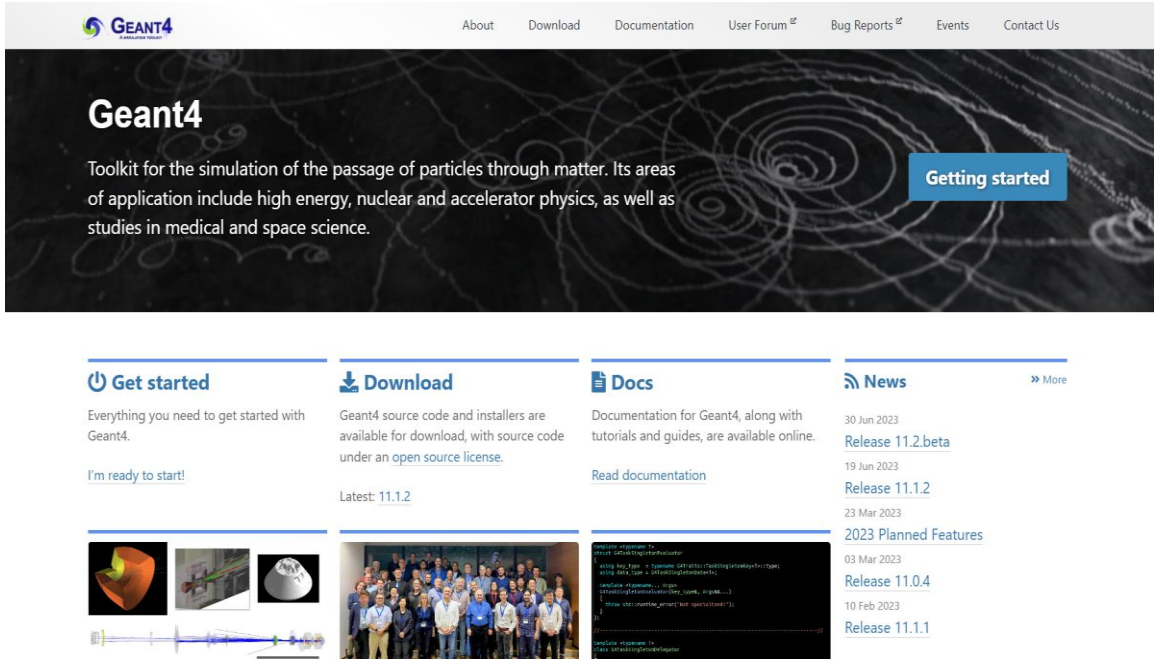
Overview :

- C++
- Object oriented
- Open Source
- **Toolkit** i.e. collection of tools
  - **Geant4 defaults model DOES NOT EXIST !!!**
  - **MUST** provide the **necessary information**, choose the GEANT4 tools

GEANT4 provides some features (building blocks)



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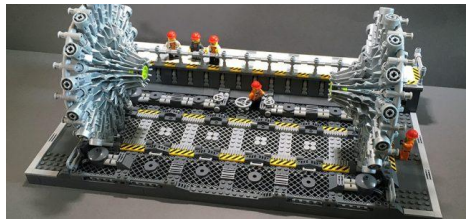

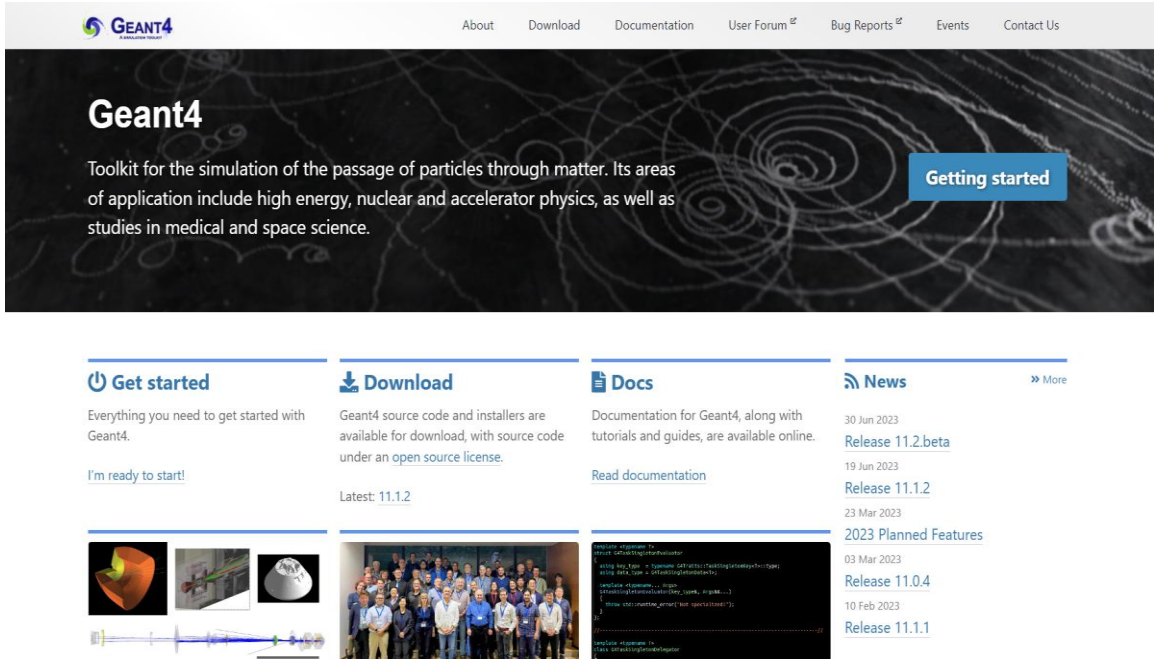

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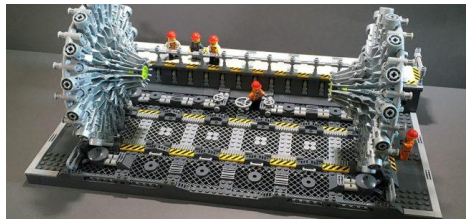

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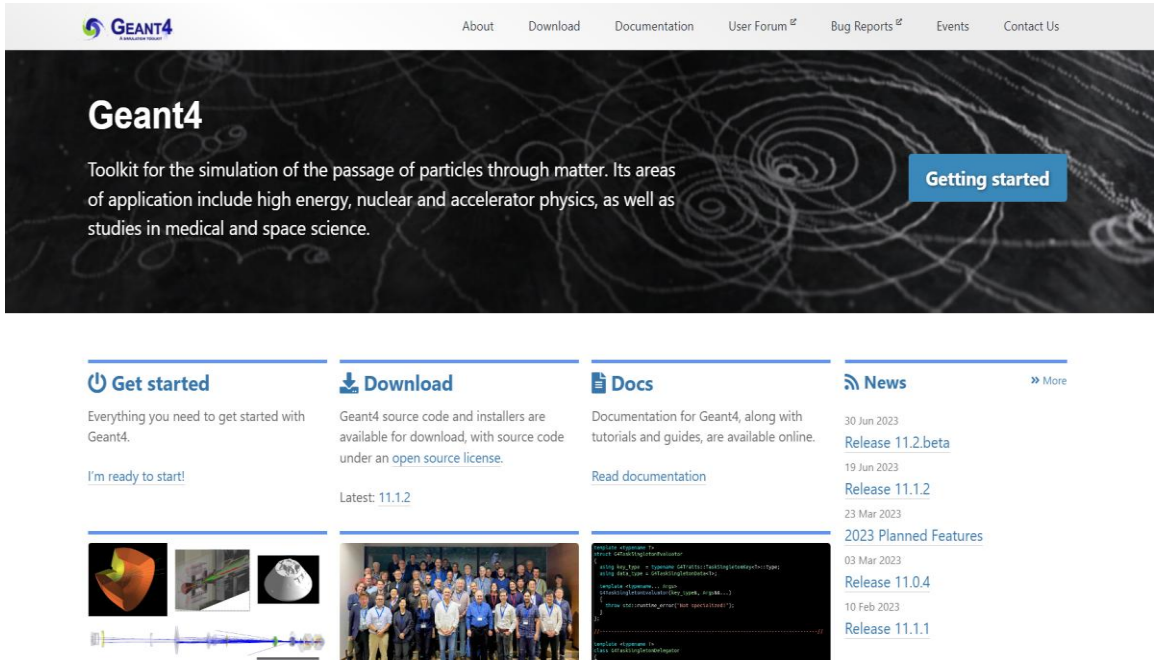

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MC methods :

- Independant particles ✓
- No collective behaviour ✗

⇒ Does **not** model the plasma acceleration itself

⇒ **Link SMILEI – ML surrogate – GEANT4**

ML integration on GEANT4

Requirements :

- Full simulation of the experiment (from acceleration to detection)
- Adaptable to different experimental scenarios

Needs :

- Use of GEANT4's « ParticleGun »
- Data from the ML model (spectrum, direction, position, …)

```
/gun/SetStatusONNX true
/laser/SetOffsetLaserFocus 1680 ## um
/laser/SetNormVecPotential 1.23
/laser/SetFracDopTargetChamber 0.0617 # %(/100)
/laser/SetPressure 47.8 #mbar
```

```
G4double fXof_min = -399.8247;
G4double fXof_max = 1798.325;
G4double fXof_rescaled = fXof / (fXof_max - fXof_min) - fXof_min/(fXof_max - fXof_min);

G4double fA0_min = 1.100516;
G4double fA0_max = 1.849792;
G4double fA0_rescaled = fA0 / (fA0_max - fA0_min) - fA0_min/(fA0_max - fA0_min);

G4double fCN2_min = 0.002064164;
G4double fCN2_max = 0.1199827;
G4double fCN2_rescaled = fCN2 / (fCN2_max - fCN2_min) - fCN2_min/(fCN2_max - fCN2_min);

G4double fP1_min = 10.09451;
G4double fP1_max = 99.95741;
G4double fP1_rescaled = fP1 / (fP1_max - fP1_min) - fP1_min/(fP1_max - fP1_min);
```

```
#ifndef B1PrimaryGeneratorAction_h
#define B1PrimaryGeneratorAction_h 1

#include "G4VUserPrimaryGeneratorAction.hh"
#include "globals.hh"
#include "G4GeneralParticleSource.hh"
#include "G4ParticleGun.hh"
#include <memory>
#include <onnxruntime_c_api.h>
#include <onnxruntime_cxx_api.h>
class G4ParticleGun;
class G4Event;
```

Keras function (Python) -> **tf2onnx.convert.from_keras** -> ONNX file (C++)

```
PrimaryGeneratorAction::PrimaryGeneratorAction(): G4VUserPrimaryGeneratorAction(),
    fParticleGun(0),
    fEnvelopeBox(0)
{
    G4int n_particle = 1;
    fParticleGun  = new G4ParticleGun(n_particle);

    // default particle kinematic
    fParticleGun->SetParticleDefinition(
        G4ParticleTable::GetParticleTable()->FindParticle("e-"));

    //Neural network: create onnx session
    Ort::Env env(ORT_LOGGING_LEVEL_WARNING, "plasma");
    Ort::SessionOptions session_options;
    session_options.SetIntraOpNumThreads(1);
    auto sessionLocal =
        std::make_unique<Ort::Session>(env, "model2.onnx", session_options);
    fSession = std::move(sessionLocal);

    // Get input node information
    fMemory_info = Ort::MemoryInfo::CreateCpu(
        OrtAllocatorType::OrtArenaAllocator, OrtMemTypeDefault);
```

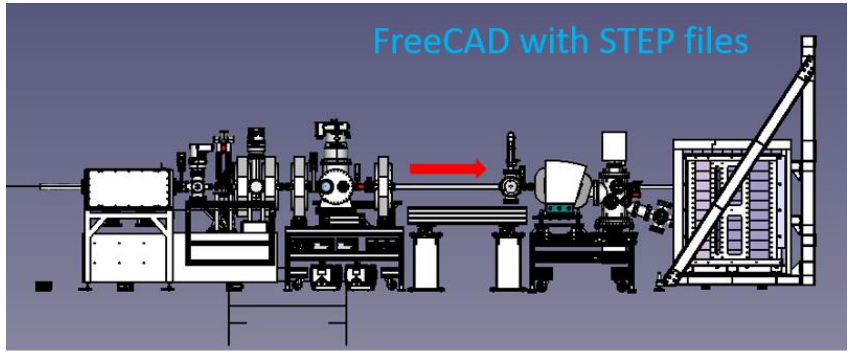
Results and benefics

Key points :

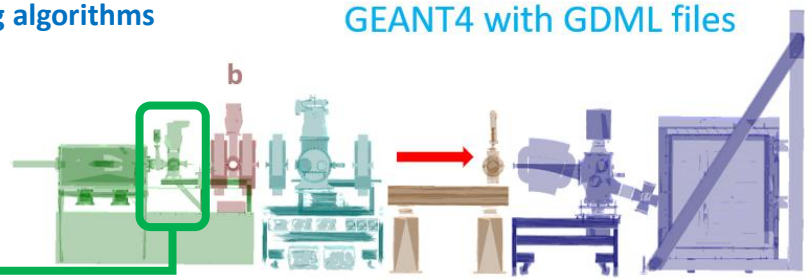
- **Full geometry** of the PALLAS beamline using **GDML**
- **MT** on CPU possible
- Easy exploration of **varied scenarios**

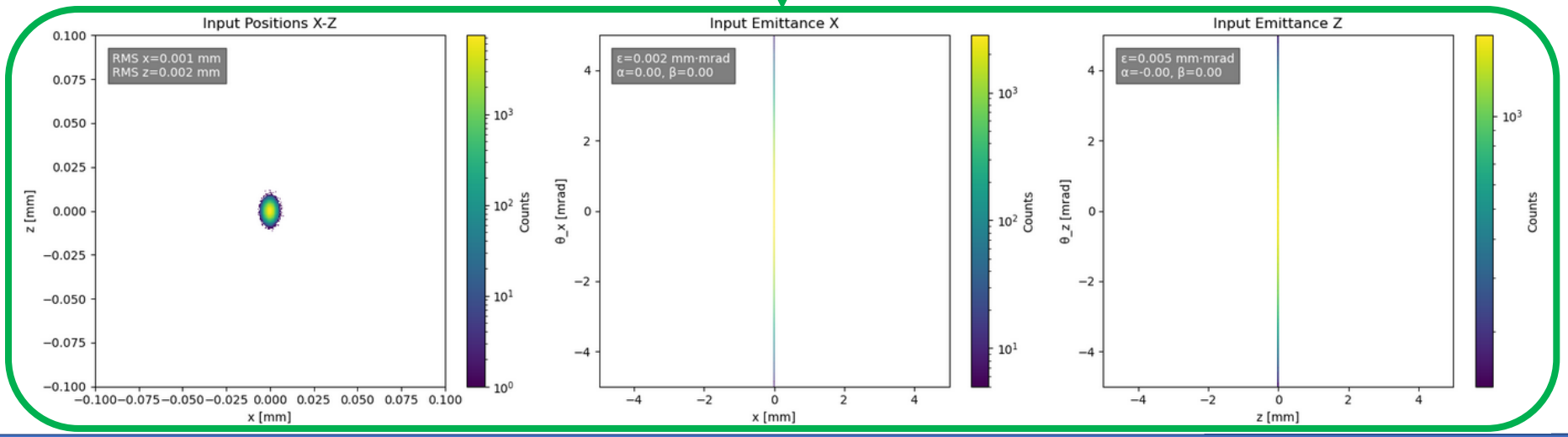
Results :

- **Particle generation consistent with PIC model**
- Complete implementation of beam transport in GEANT4 (quadrupoles)



Meshing algorithms





Particle generation

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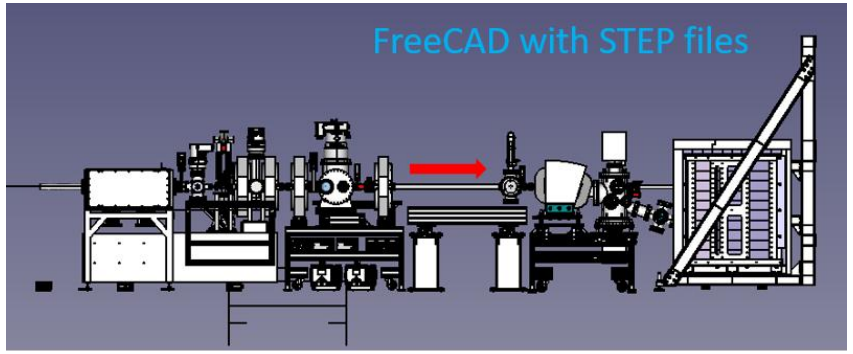

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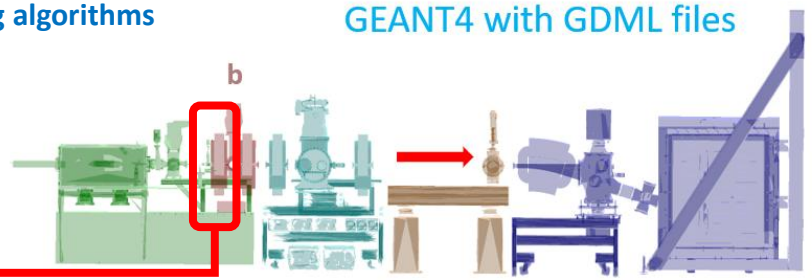

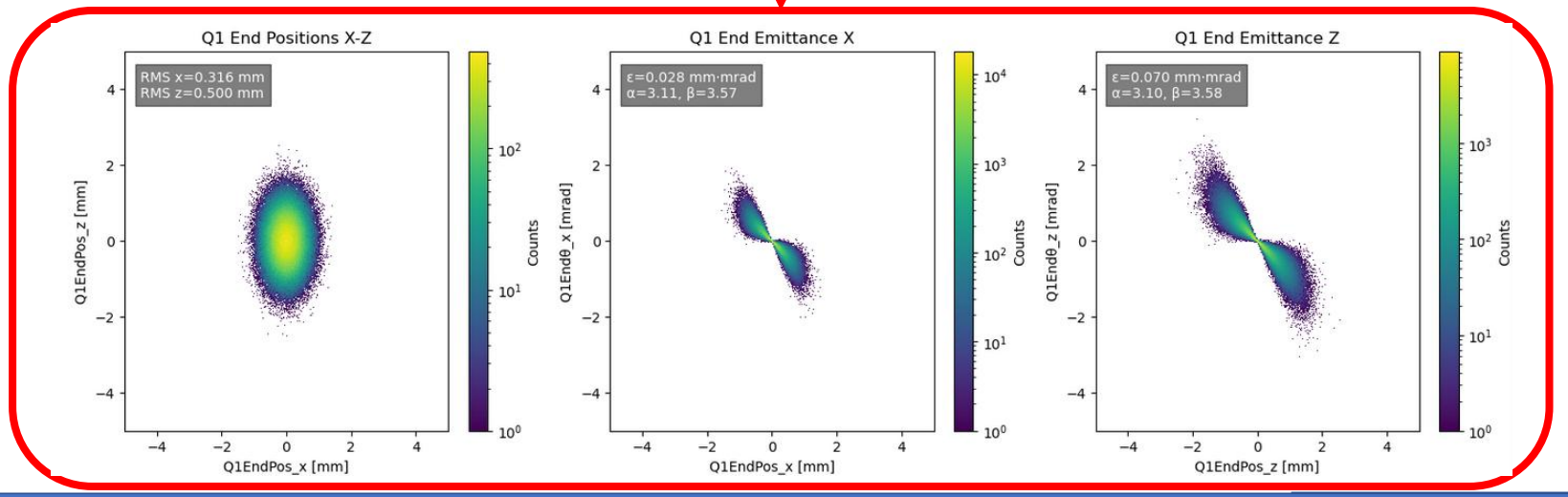

Q1 exit

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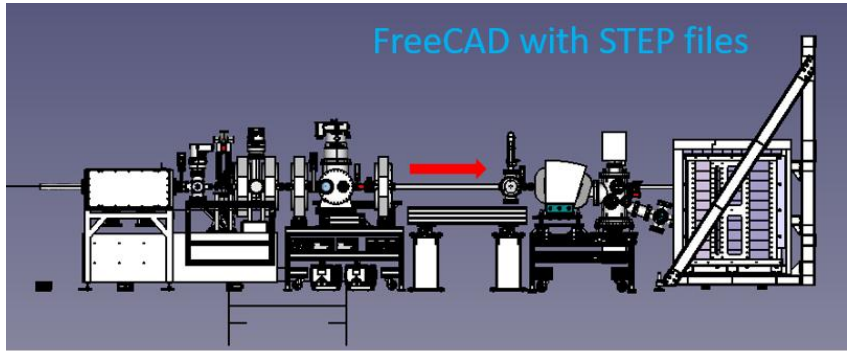
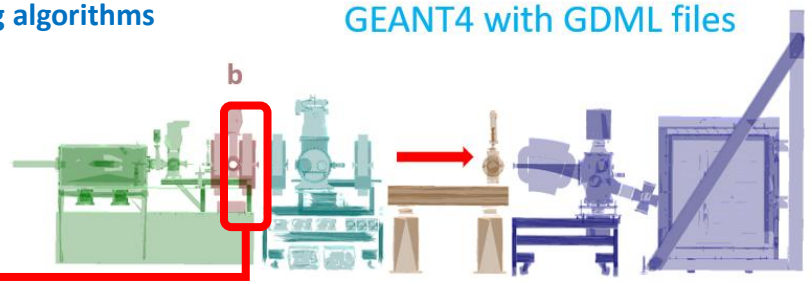
- **MT** on CPU possible
- Easy exploration of **varied scenarios**

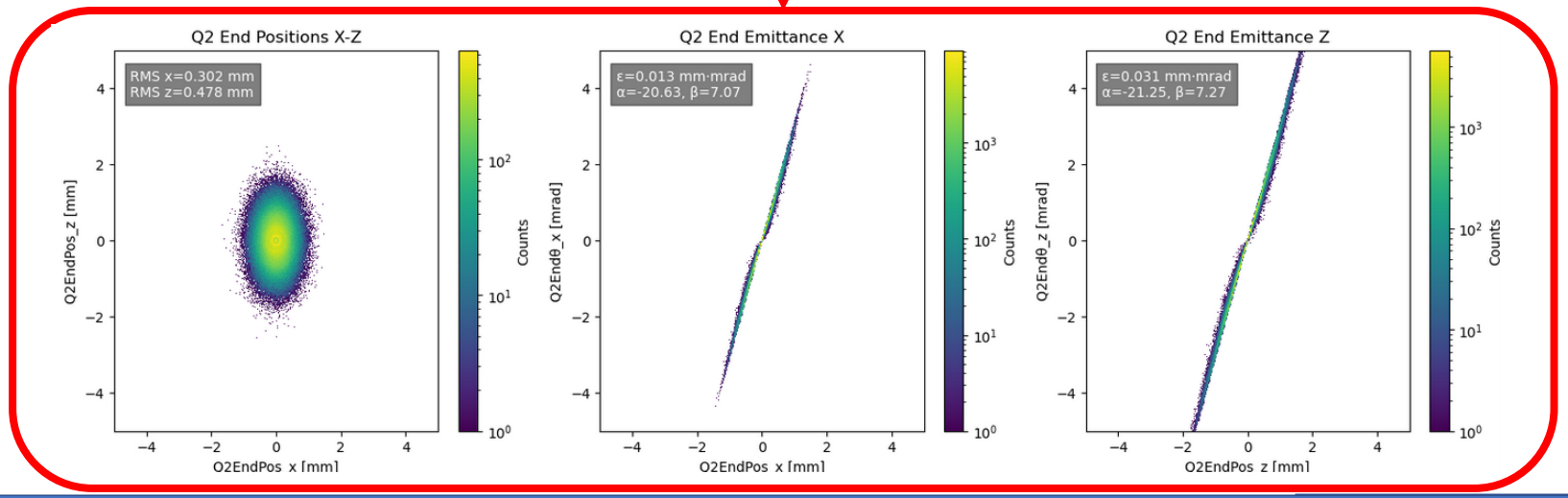
Results :

- Particle generation consistent with PIC model
- **Complete implementation of beam transport in GEANT4 (quadrupoles)**



Meshing algorithms





Q2 exit

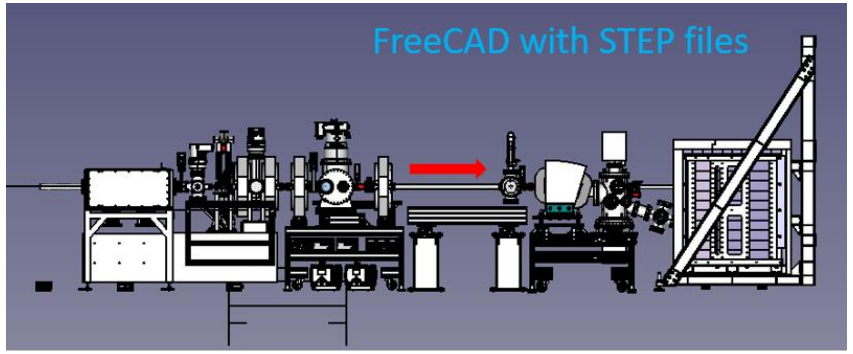
Results and benefics

Key points :

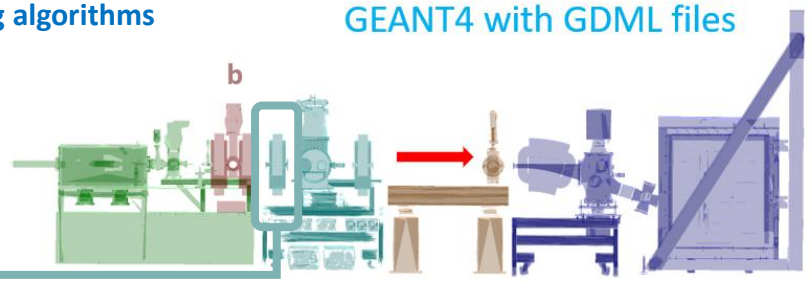
- **Full geometry** of the PALLAS beamline using **GDML**
- **MT** on CPU possible
- Easy exploration of **varied scenarios**

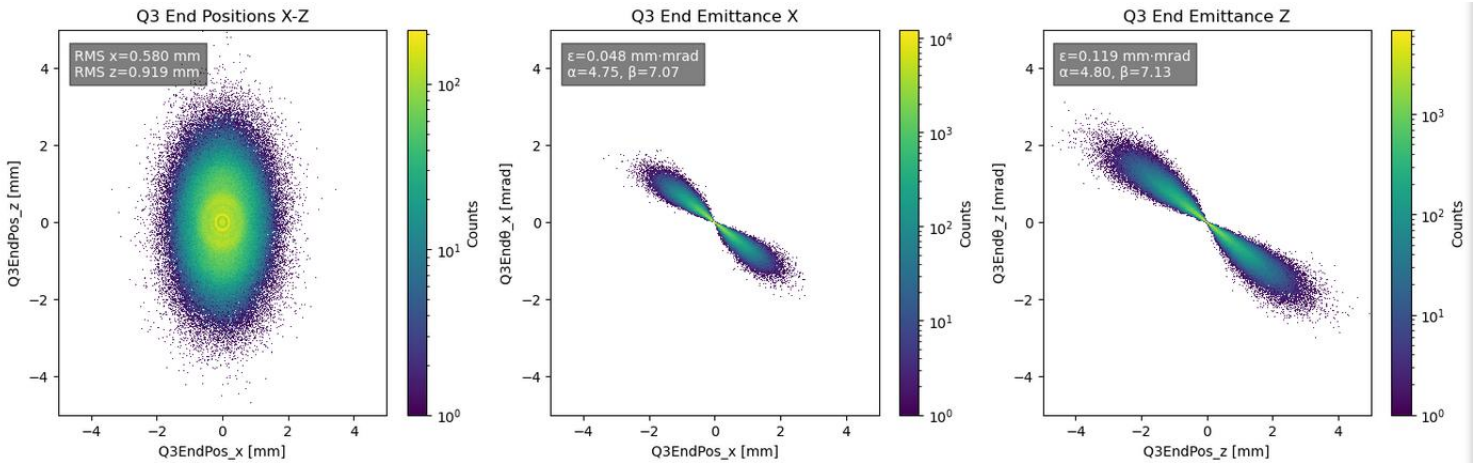
Results :

- Particle generation consistent with PIC model
- **Complete implementation of beam transport in GEANT4 (quadrupoles)**



Meshing algorithms





Q3 exit

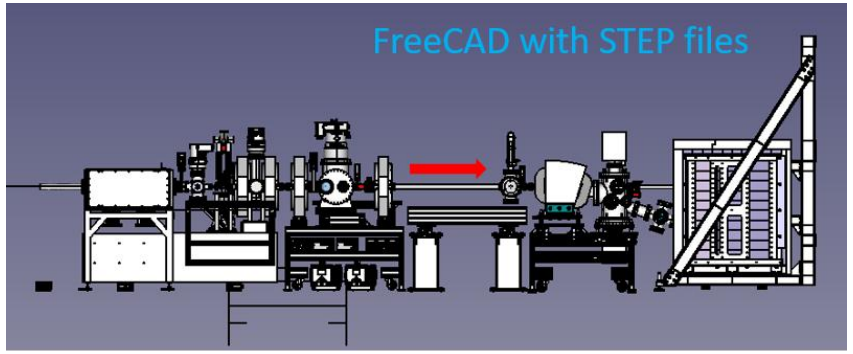
Results and benefics

Key points :

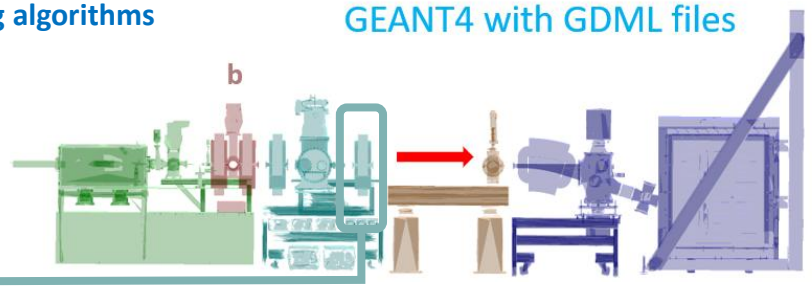
- **Full geometry** of the PALLAS beamline using **GDML**
- **MT** on CPU possible
- Easy exploration of **varied scenarios**

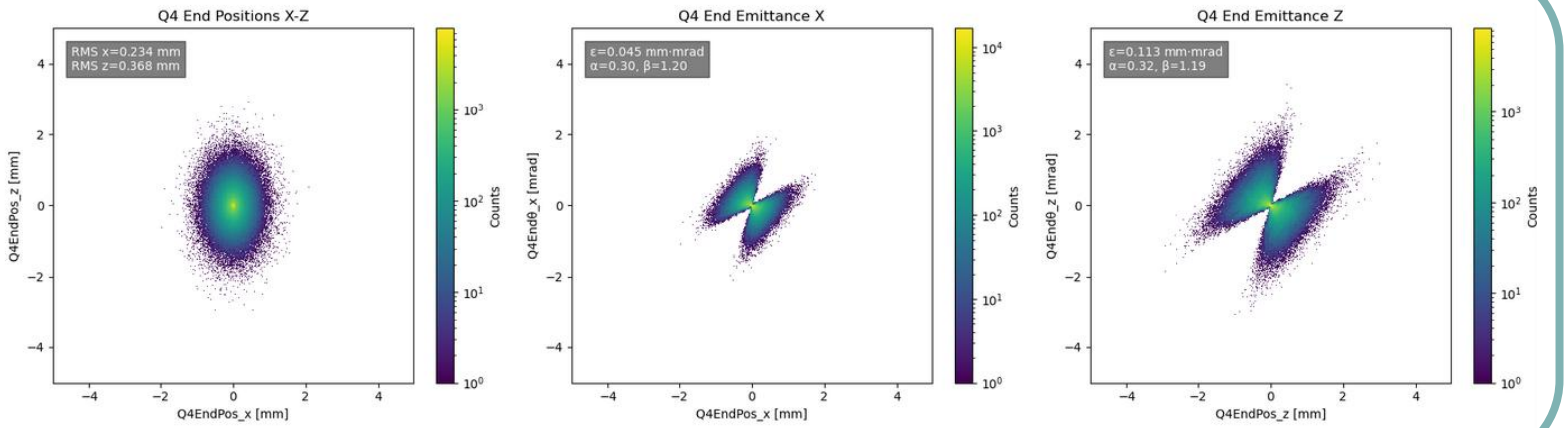
Results :

- Particle generation consistent with PIC model
- **Complete implementation of beam transport in GEANT4 (quadrupoles)**



Meshing algorithms





Q4 exit

Results and benefics

Key points :

- **Full geometry** of the PALLAS beamline using **GDML**
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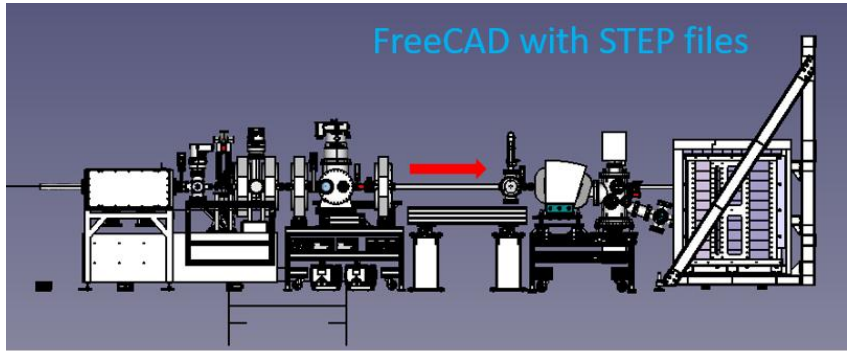
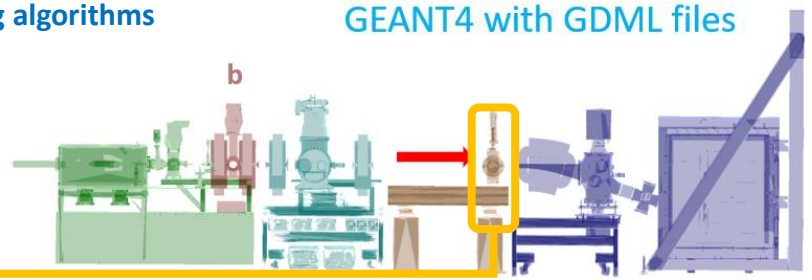
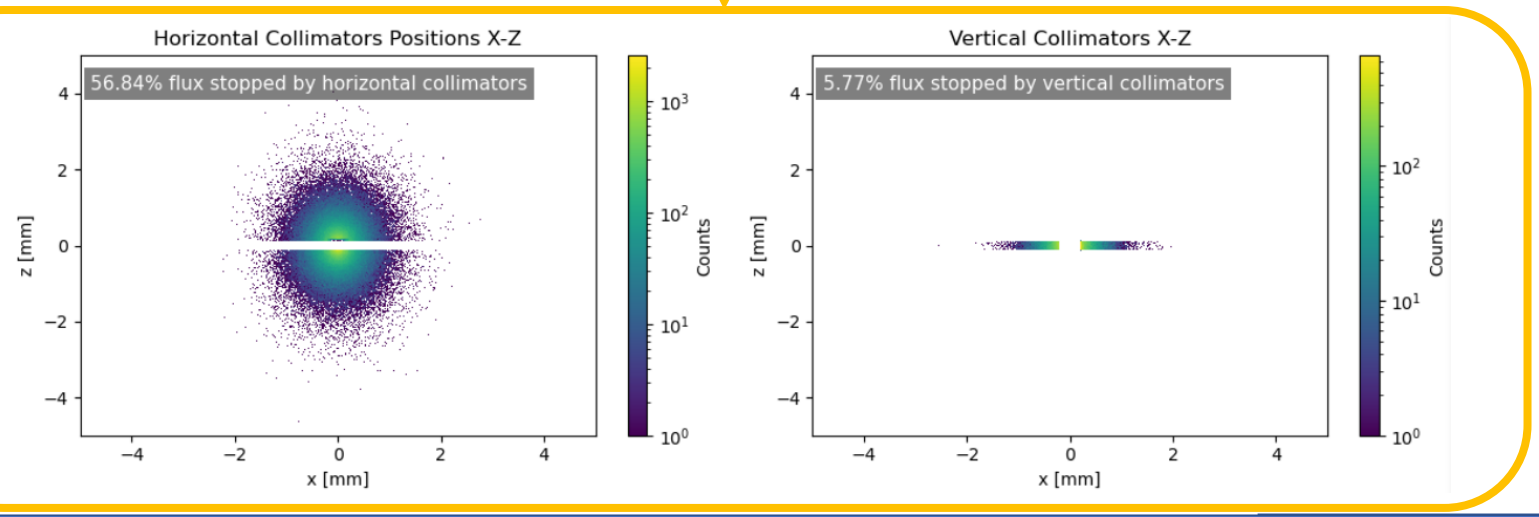
Results :

- Particle generation consistent with PIC model
- **Complete implementation of beam transport in GEANT4 (quadrupoles)**



Meshing algorithms





Collimators

Results and benefics

Key points :

- **Full geometry** of the PALLAS beamline using **GDML**
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Results :

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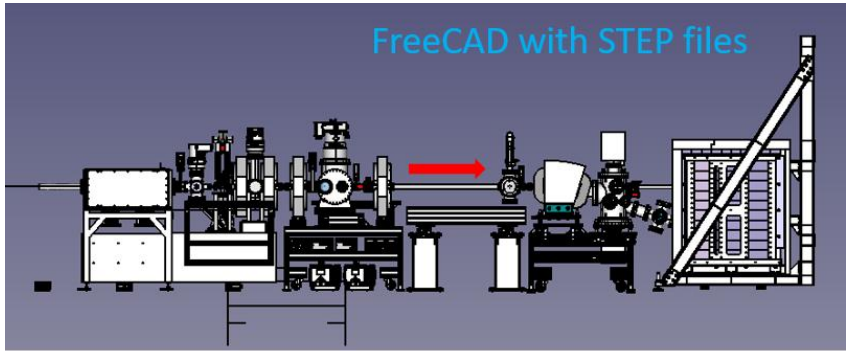
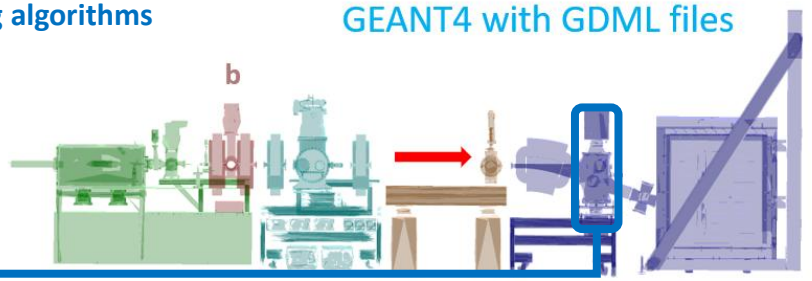
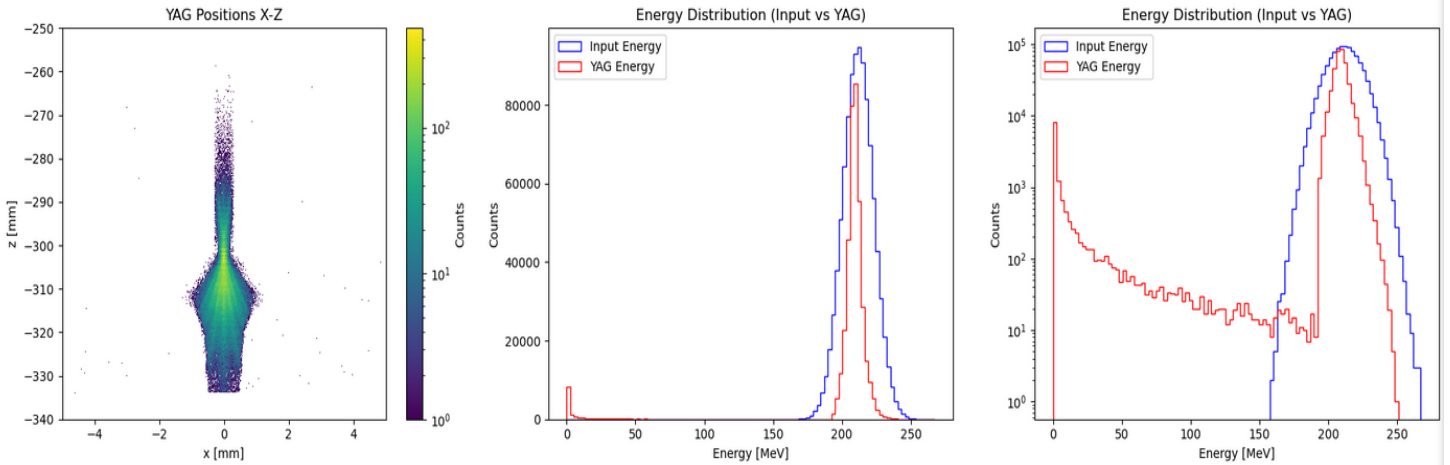
- **Complete implementation of beam transport in GEANT4 (quadrupoles)**



Meshing algorithms





YAG screen

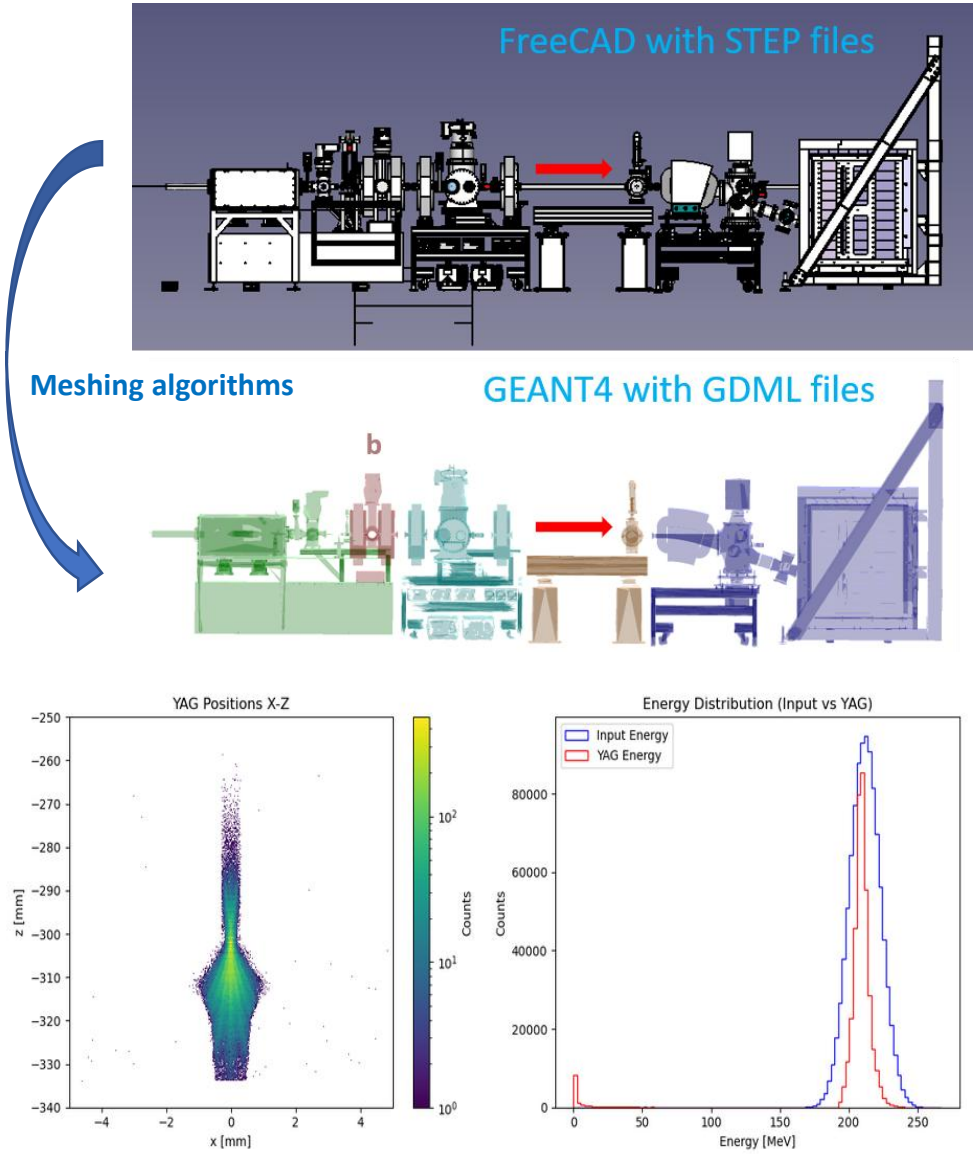
Results and benefics

Key points :

- **Full geometry** of the PALLAS beamline using **GDML**
- **MT** on CPU possible
- Easy exploration of **varied scenarios**

Results :

- Particle generation consistent with PIC model
- Complete implementation of beam transport in GEANT4 (quadrupoles)
- **ML analysis with (Laser parameters, Qx values, Qx distances, slits openings) in order to maximise Charge and/or Energy beam**



Results and benefics

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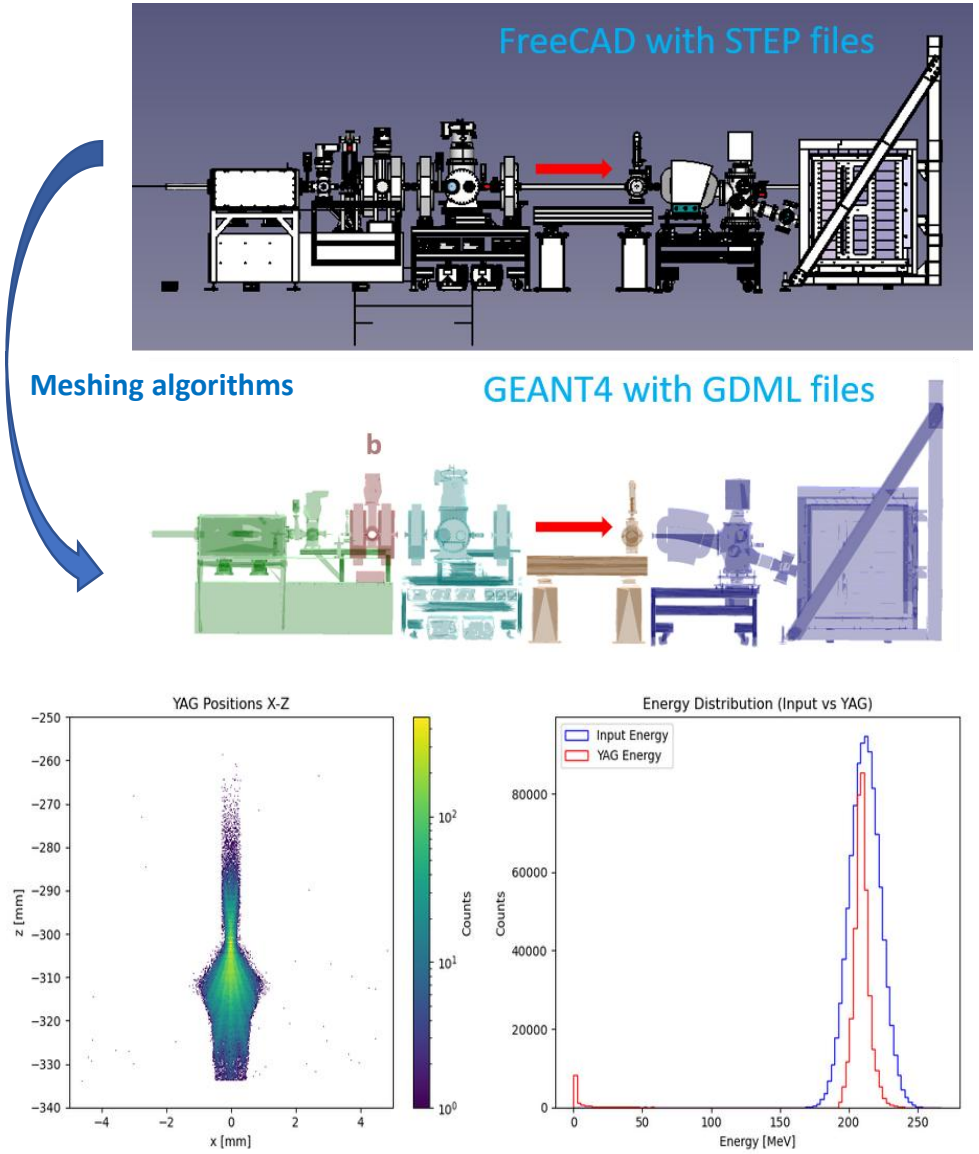
- Complete implementation of beam transport in GEANT4 (quadrupoles)
- ML analysis with (Laser parameters, Qx values, Qx distances, slits openings) in order to maximise Charge and/or Energy beam

- Soon available as an “advanced example”
  - **ML model trained on particle-in-cell simulations of laser-driven plasma wakefield acceleration as a particle source and entire experimental setup implemented using GDML**



Conclusion & Perspectives

- ✓ **Reduced complexity and computational cost**, while maintaining high-fidelity simulation accuracy.
- ✓ **ML model used**: multilayer perceptron (MLP) trained on PIC simulation data of laser-plasma interactions
- ✓ **ONNX framework** enabled seamless translation of the ML model from Python to C++ for integration into Geant4.
- ✓ **Implementation in Geant4**, centered on the PALLAS facility, enabling start-to-end simulations combining plasma acceleration physics with Monte Carlo modeling.
- ✓ **Full experimental setup of PALLAS** implemented in Geant4 using GDML files, including beam transport and detector systems.


Official example of GEANT4 collaboration

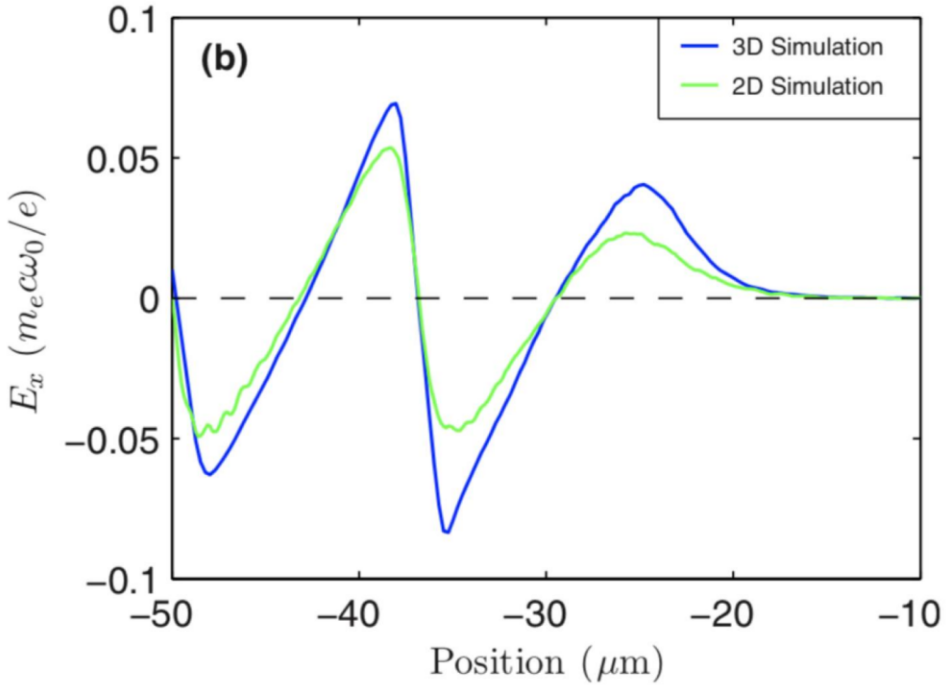

Scalable and adaptable framework for future experiments and applications.


Potential applications: synchrotron light sources, free electron lasers, nuclear physics, and advanced radiotherapy.

The LWFA 3D PIC simulation problem is enormous

!!! SLIDE FRANCESO MASSIMO !!!

2D cartesian simulations:
Not accurate enough



X. Davoine et al., Phys. Plasmas 15, 113102 (2008)

Example of 3D simulation scale
with "classic" electromagnetic PIC loop
and "classic" numerical schemes

- Laser wavelength **λ_0=0.8 µm** -> 0.016 µm , Δx=0.016 µm, cΔt=0.99Δx
- Laser duration: 30 fs -> Window size Lx = 40 µm = 2500 * Δx
- w_0=12 µm -> Δy=Δz=0.5µm , Window size Ly = Lz = 125 µm = 192 * Δy
- Acceleration length = **1 mm** ~ 60000 c* Δt
- 8 macro-particles per cell -> ~2500*250*250*8 =

10^9 macro-particles, pushed for 60k timesteps!

Smallest scale to sample [space and time]

Largest scale to simulate [space and time] (Note: current LWFA studies require several mm, up to 10s of cm, or even m)