

# How precise can Geant4 be for protontherapy, without G4QGSP\_BIC\_HP

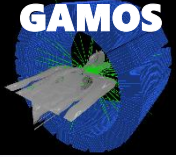
P. Arce<sup>1</sup>, A. Viñals<sup>2</sup>, J.D. Azcona<sup>2</sup>

(1)

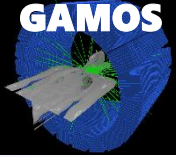
**Ciemat**  
Centro de Investigaciones  
Energéticas, Medioambientales  
y Tecnológicas

(2)

The logo of the Clínica Universidad de Navarra, featuring a circular emblem with a figure and the text "UNIVERSITAS NAVARRENSIS" and "CLINICA UNIVERSIDAD DE NAVARRA".  
Clínica  
Universidad  
de Navarra



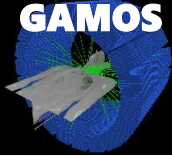
- Monte Carlo vs. Treatment Planning System precision
- To simulate or not to simulate nozzle?
- Position-direction distribution for each beam energy (Transversal profiles in air)
- Energy distribution for each beam energy (Integrated Depth Dose profiles)
- Transversal profiles in water: check Geant4 scattering and position-direction distribution
- Absolute dose
- More complex checks
  - SOBP in water
  - SOBP different materials
  - SOBP oblique
  - SOBP with peculiar shapes
  - patients



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- In protontherapy Monte Carlo commissioning it is common that fit to experimental data reaches **a few mm and a few % precision**
- But today Treatment Planning systems are improving
  - They use what they call Monte Carlo simulation
  - Can also reach **a few mm and a few % precision**
- **Geant4 simulation precision should improve if it wants to be an alternative to TPS “Monte Carlo” simulation**



# Fast Monte Carlo (RayStation MC)

- Based on the Monte Carlo technique of propagating particles in matter

## Energy Loss:

- ❖ Energy loss and straggling is computed **on density and voxel specific material composition**
  - **Bethe-Bloch formula** to calculate absolute energy loss
  - Discretized energy spectra with adaptive energy bin sizes, which provide an **accurate, within 0.2 mm, estimation of the range** as predicted by the continuous slowing down approximation (CSDA)

## Multiple scattering:

- ❖ Elastic multiple and plural scattering is included through the **Goudsmit-Saunderson theory**
  - ❖ Based on voxel specific elemental compositions
- ❖ Elastic proton-hydrogen scattering and inelastic nuclear reactions leading to secondary protons, deuterons, tritons and alphas particles are **modelled based on voxel specific elemental compositions**

# Fast Monte Carlo (RayStation MC)

## Secondary particle transport:

- ❖ **Secondary protons** are transported **like primary protons**
- ❖ **Heavier secondaries** are transported taking **only energy loss** into account
- ❖ Neutral reaction products (**neutrons and gammas**) **are not transported**, but given fractions of the absorbed energy are considered
- ❖ **Delta electrons are not considered**

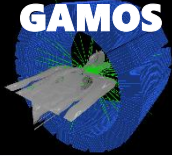
**Optimizes the beam model based on measured IDDs**



# To simulate or not to simulate nozzle?

There are two common ways to simulate a protontherapy treatment:

1. With phase space files after nozzle (one for each beam energy)
  - a) Fit position-direction distribution before nozzle
  - b) For the optimised distribution store phase space file after nozzle with protons (and other particles)
  - c) Read back phase space files to simulate the patient dose
  
2. With proton energy distribution after nozzle (one for each beam energy)
  - a) Fit position-direction distribution after nozzle
  - b) Simulate nozzle and get the energy distribution of protons after it
    - ❖ Fit the beam energy + energy sigma
  - c) Simulate beam after nozzle with energy distribution after nozzle and fitted position-direction distribution



# Do not simulate nozzle

- We opted for option 2
  - ✓ Much easier to simulate position-direction distribution after nozzle (only in air)
  - ✓ Faster simulate only protons with a given energy distribution than reading phase space files
  - ✓ Avoid huge disk space needs to store phase space files

But we have then to guarantee two things:

**1. Contributions of other particles than protons after nozzle are negligible:**

NPARTICLES	70.2	150.2	228.7
proton	1	1	1
e-	0.030606	0.0242768	0.0236784
gamma	0.000431289	0.000301094	0.000280263
neutron	0.00021727	0.000222505	0.000256866
deuteron	8.50657e-05	8.14682e-05	7.06914e-05
triton	4.06365e-06	6.63259e-06	6.75635e-06
He3	8.66912e-06	1.1388e-05	1.01345e-05
alpha	3.98238e-05	4.41755e-05	4.12888e-05

**N particles  
after nozzle**

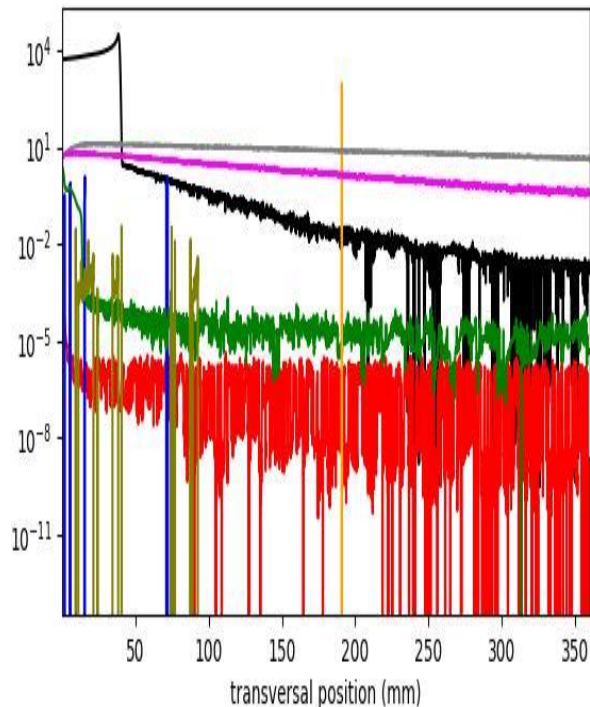


# Do not simulate nozzle

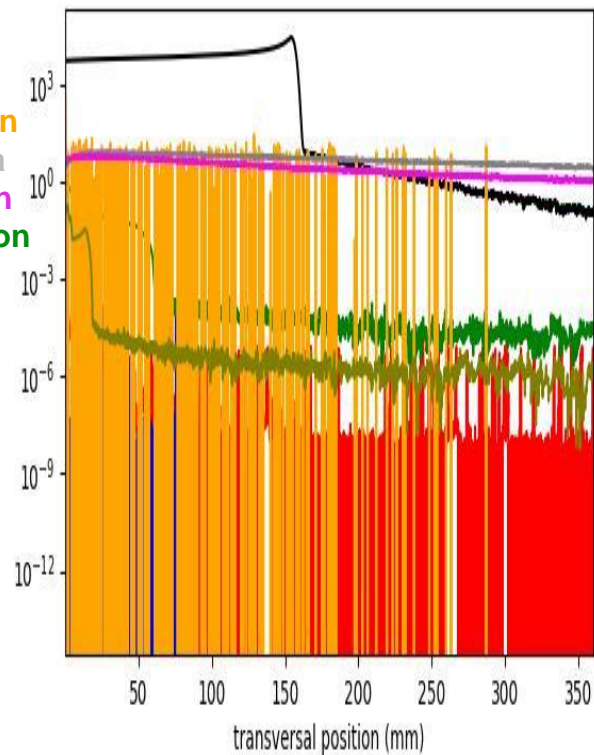
## 1. Contributions of other particles than protons after nozzle are negligible:

Dose from each particle type reading phase space files

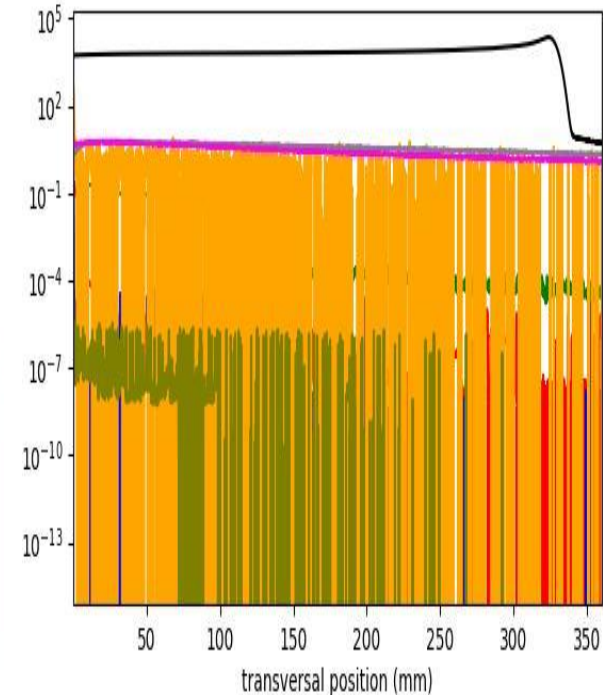
070.2 MeV

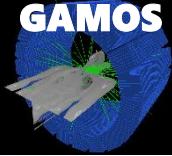


150.2 MeV



228.7 MeV



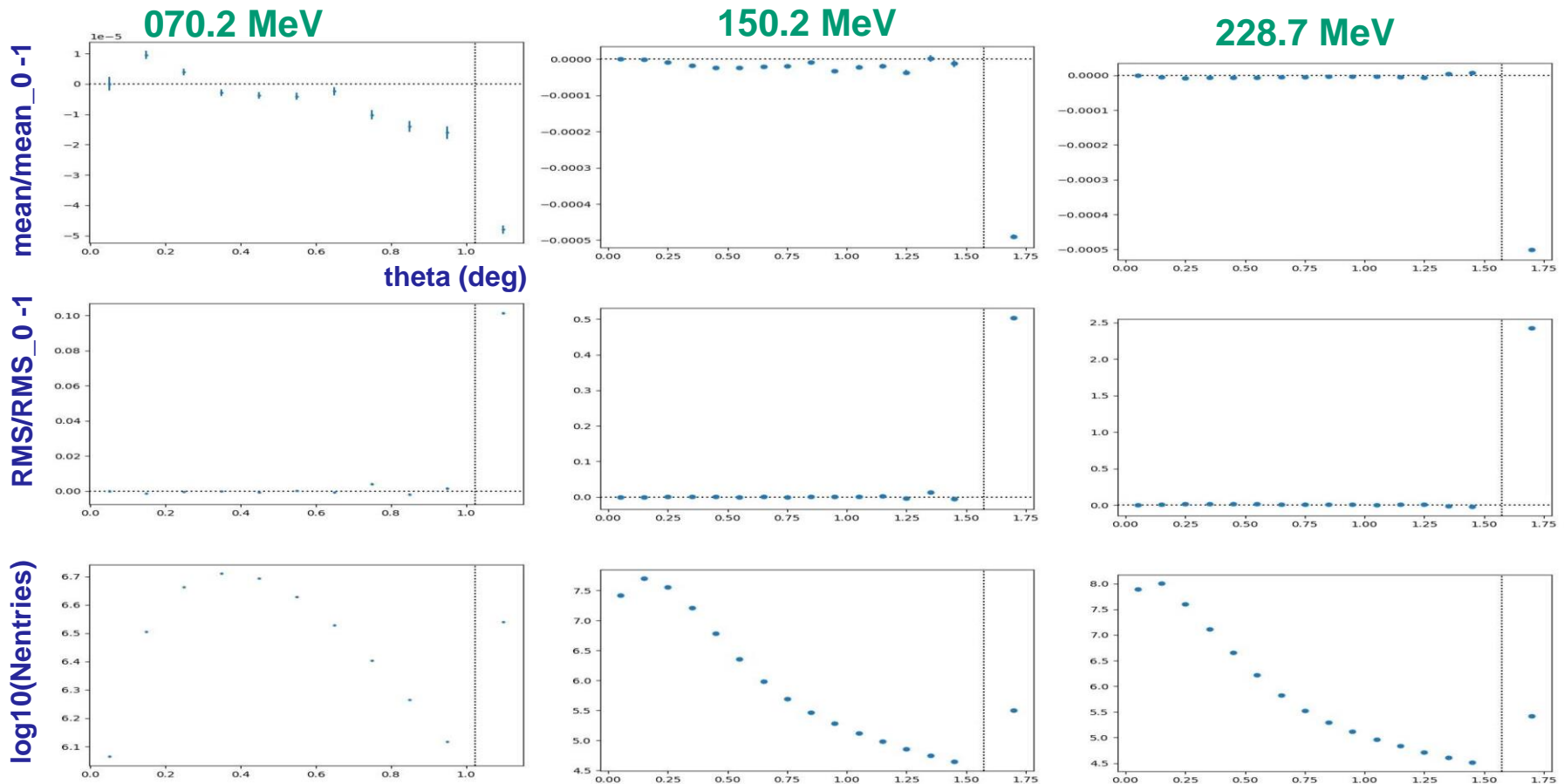


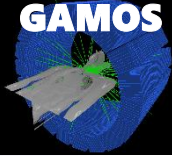
# Do not simulate nozzle

## 2. Angle and position dependence with energy is negligible:

- Simulate nozzle with approximate position/direction distribution and get the dependency of proton energy with the position and direction angle

Mean and RMS of direction theta distribution after nozzle



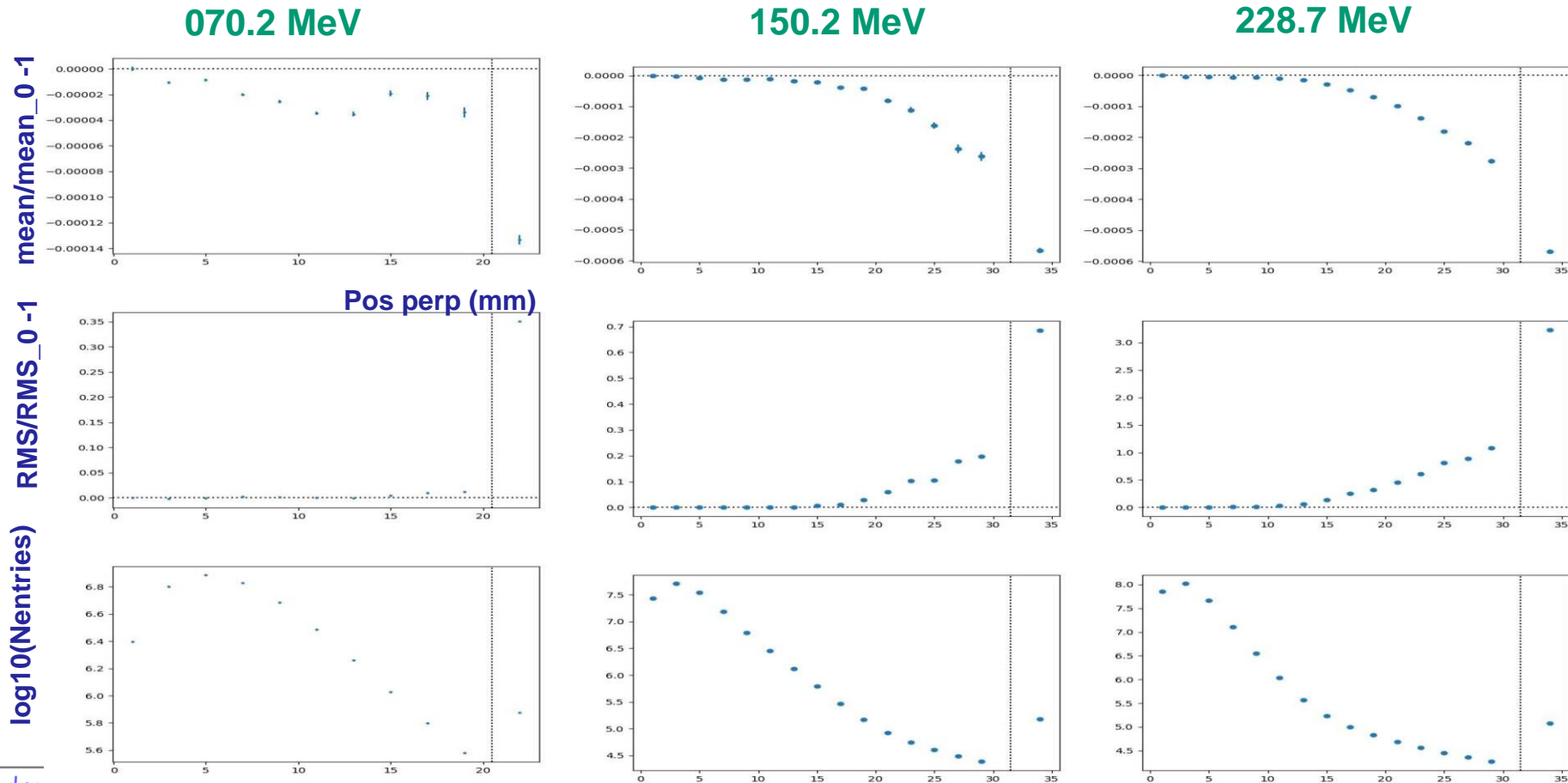


# Do not simulate nozzle

## 2. Angle and position dependence with energy is negligible:

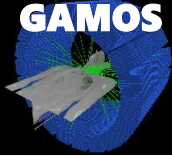
- Simulate nozzle with approximate position/direction distribution and get the dependency of proton energy with the position and direction angle

Mean and RMS of perpendicular position  $\sqrt{x^2+y^2}$  distribution after nozzle



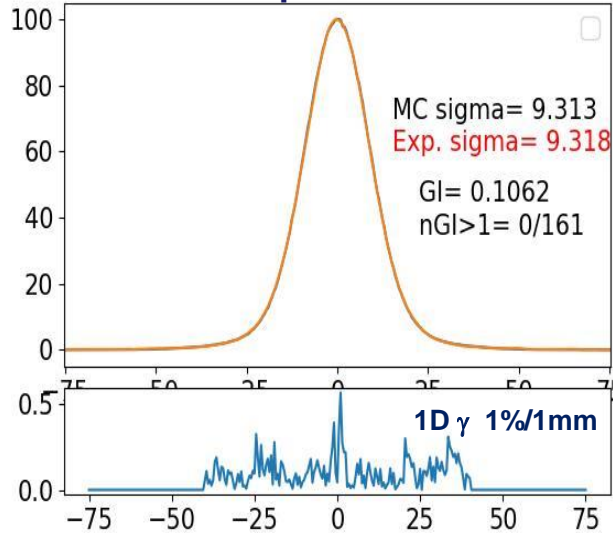


- ❖ Hitachi provides Twiss parameters to describe transverse profiles
  - ☹ They only give an approximate distribution
- We have simulated transversal profiles using the initial Twiss parameters to define a **double 2D Gaussian with position-angle and 1st Gaussian-2nd Gaussian correlation, plus XY phase rotation**
- We have defined an **automatic method to adjust the 16 parameters** with a few iterations
  - ✓ For each of the **98 energies**
  - ✓ Request a **difference in sigma  $\lesssim 50 \mu\text{m}$**
  - ✓ Request a **1D  $\gamma$  index 1%/1mm  $\lesssim 0.25$**

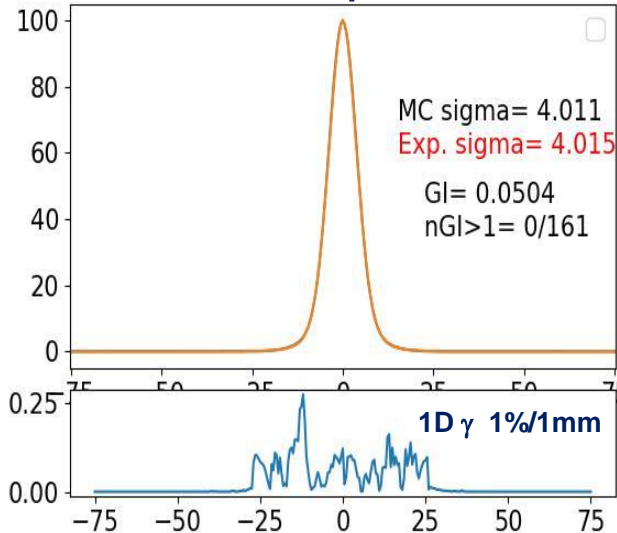


# Transversal profiles in air

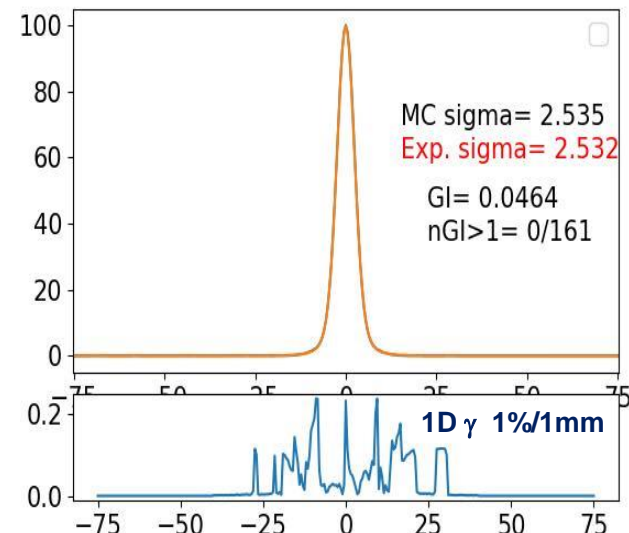
### 70.2 MeV X profile isoc+200mm



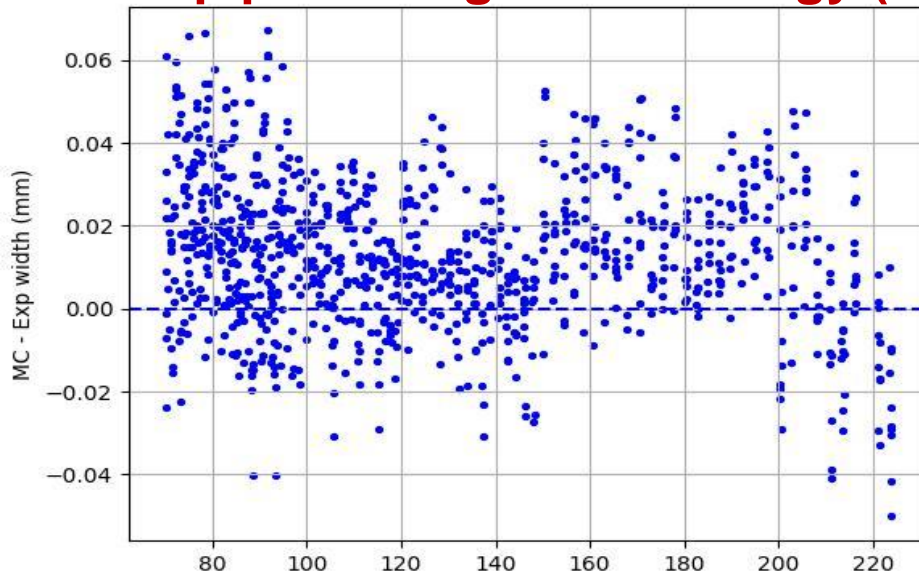
### 150.2 MeV Y profile isoc



### 228.7 MeV X profile isoc-200mm

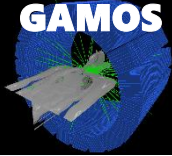


## MC-Exp profile sigma vs. Energy (980 fits)



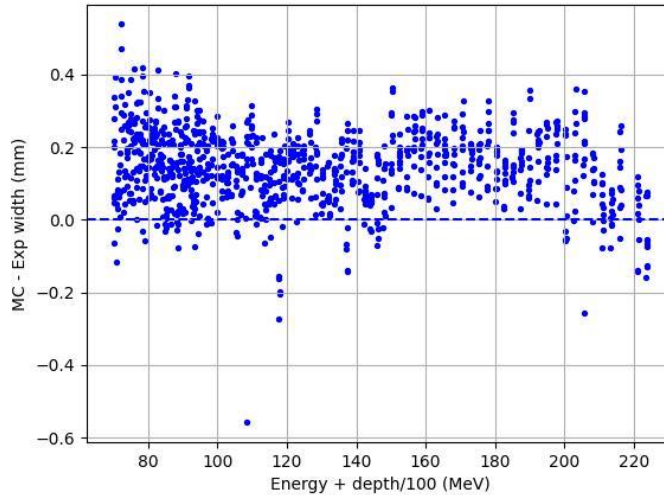
X -Y profile width  
difference  $\sim$  0.1 mm





# Transversal profiles in air

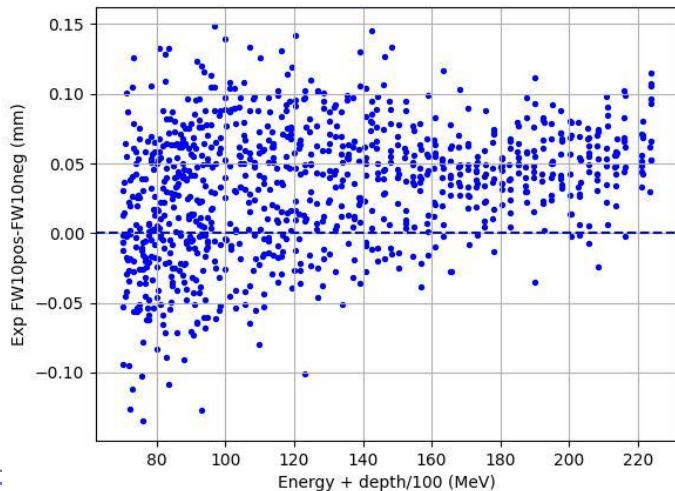
## MC-Exp profile FW10 vs. Energy (980 fits)



**Tails should be improved for some energies!**

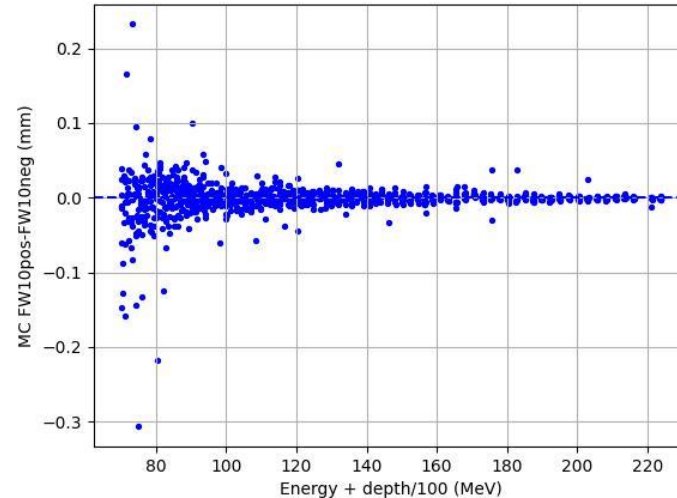
Compare 10% in positive and negative X:

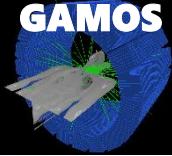
- **Exper:**  $0.15 \cdot \sqrt{2}$  can be due to measurement errors



Compare 10% in positive and negative X:

- **MC:**  $0.2 \cdot \sqrt{2}$  can be due to MC statistics

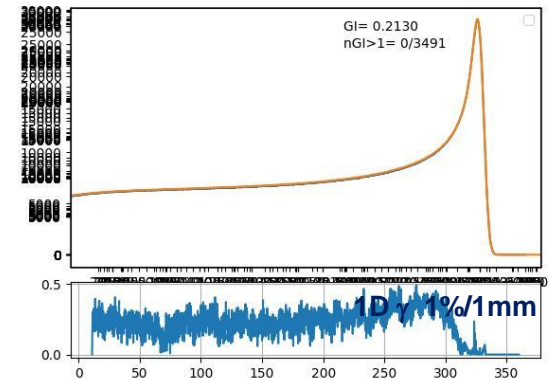
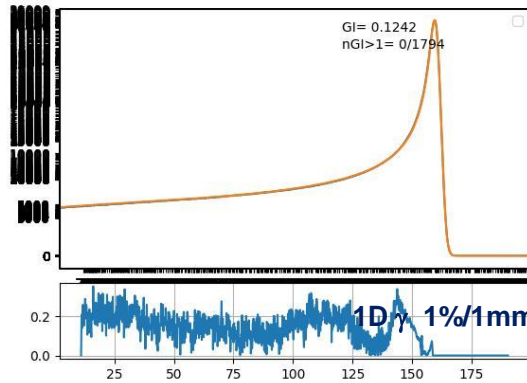
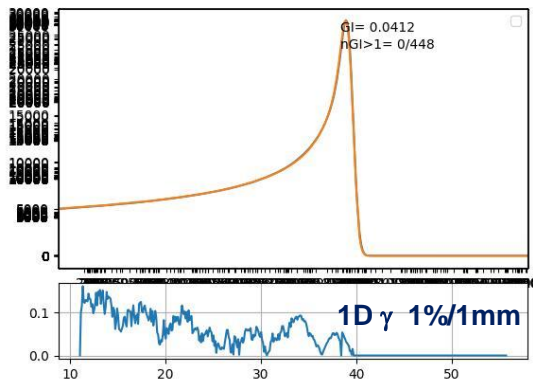




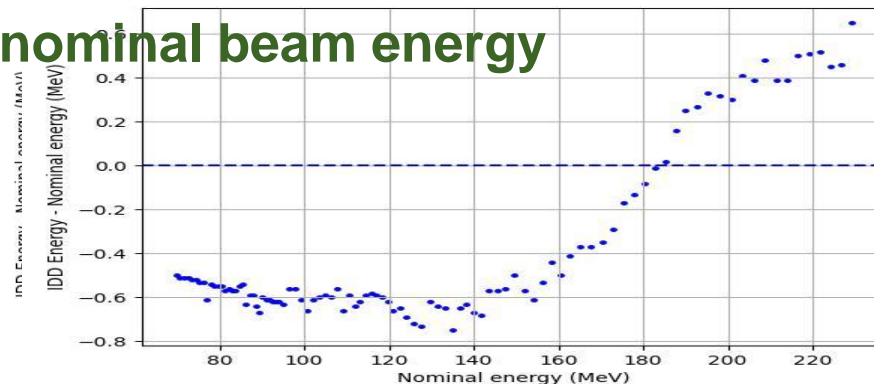
# Energy+energy sigma: Integrated Depth Dose (IDD)

- ❖ We have adjusted the IDD range (R80) and width (at 80%) for the 98 energies
  - ❖ Optimize energy and energy sigma (%) to fit RANGE80, RANGE9010 (difference 90% and 10% after peak) and WIDTH80
  - ❖ Allow not best RANGE80 if average GI improves
- ❖ Optimal energies are slightly different than nominal ones (also for the Raystation TPS)

IDD 70.2 MeV E\_fit = 069.7 s=0.2)    IDD 150.2 MeV E\_fit = 149.7, s=0.0)    IDD 228.7 MeV E\_fit = 229.35, s=0.0)



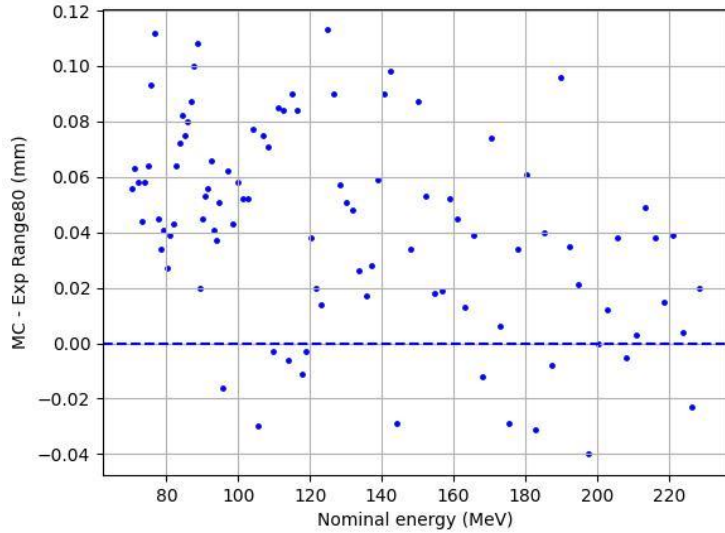
## MC-nominal beam energy



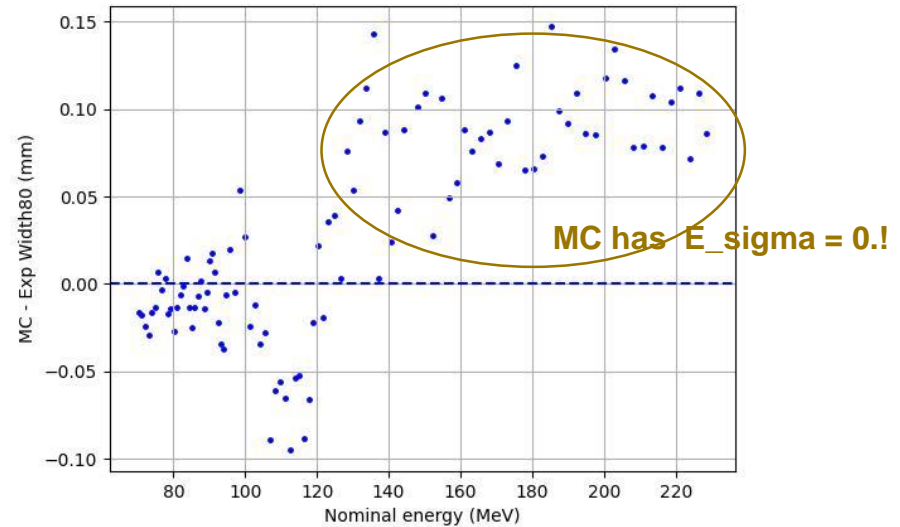
# Integrated Depth Dose (IDD)



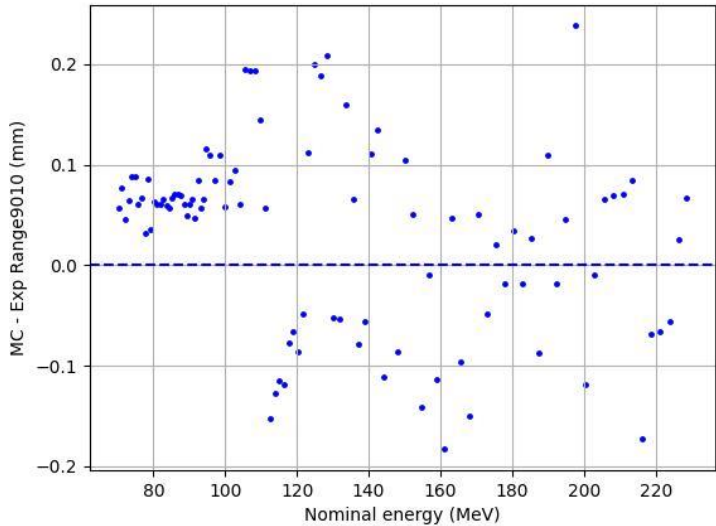
## MC-Exp RANGE\_80 vs. Energy



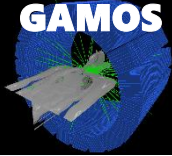
## MC-Exp WIDTH\_80 vs. Energy



## MC-Exp RANGE\_90-RANGE\_10 vs. Energy



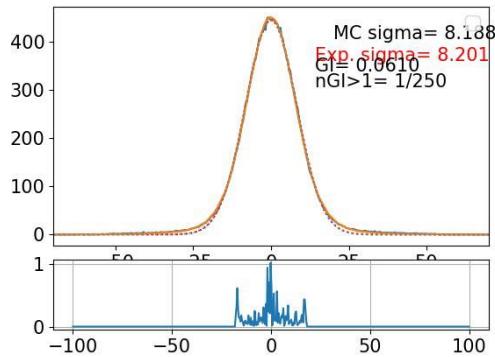




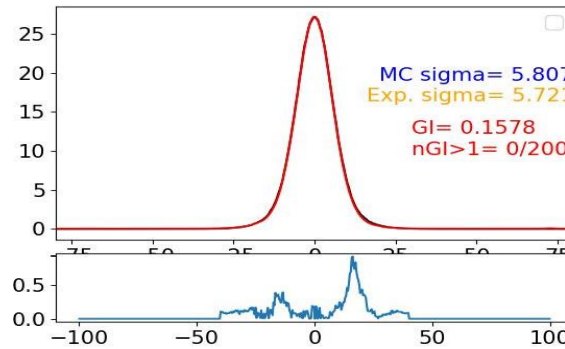
# Transversal profiles in water

- ❖ Measurements of X and Y dose profiles in water for 3 beam energies at 3 depths each

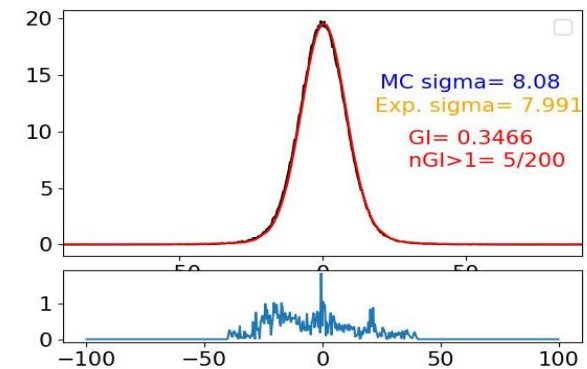
70.2 MeV X profile at 23.28 mm



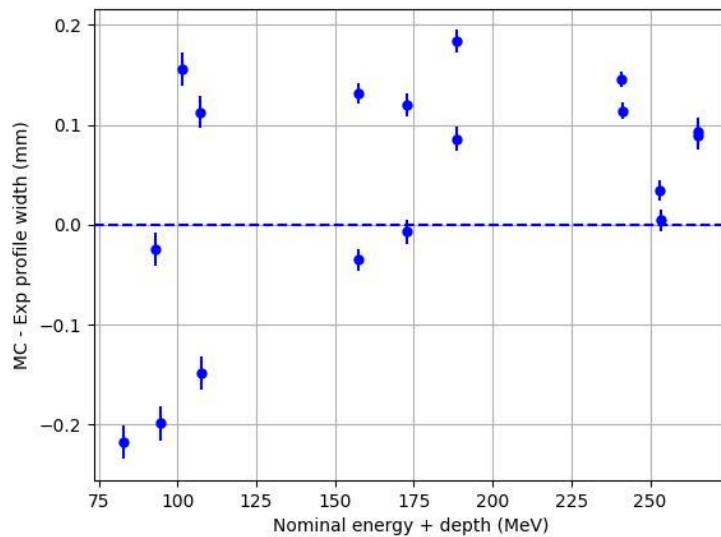
142.5 MeV Y profile at 140 mm



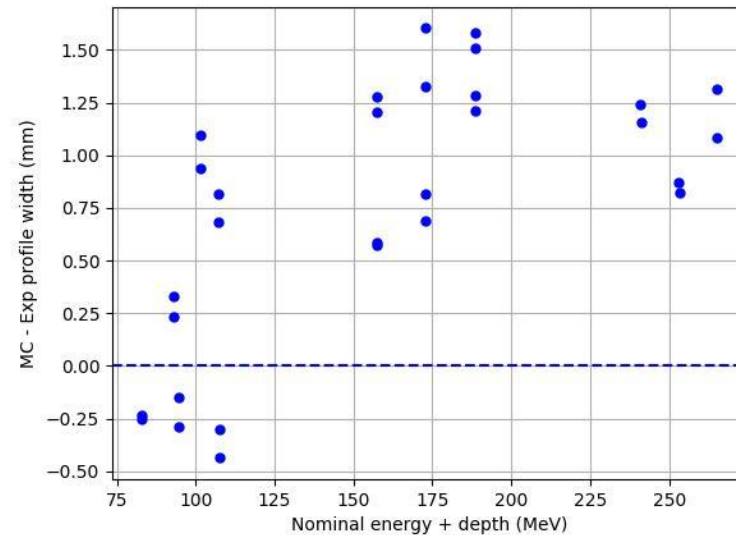
228.7 MeV X profile at 324 mm

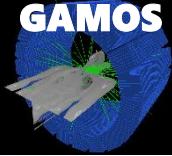


MC-Exper. Profile: sigma vs. Energy



MC-Exper. Profile: FW10 vs. Energy





# Transversal profiles in water: FW10

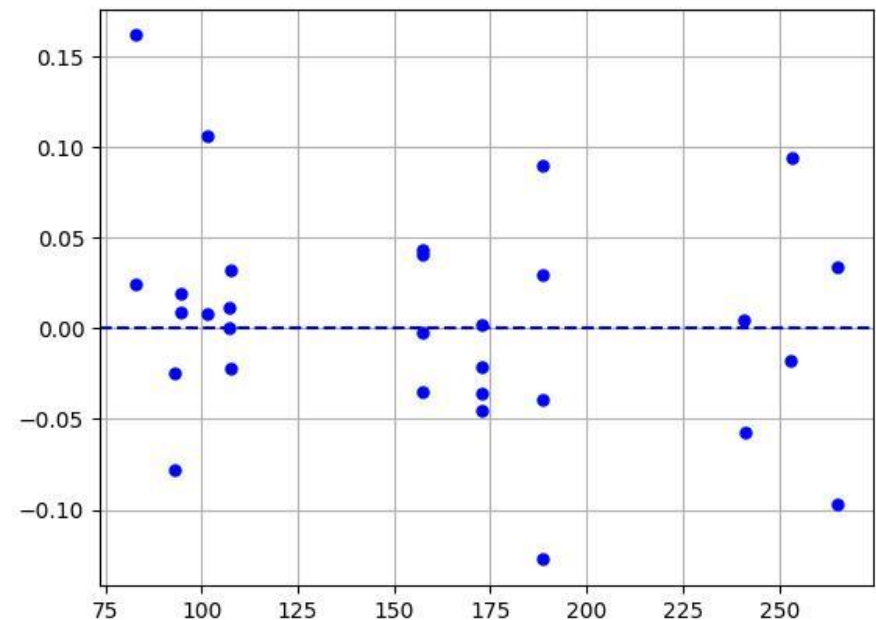
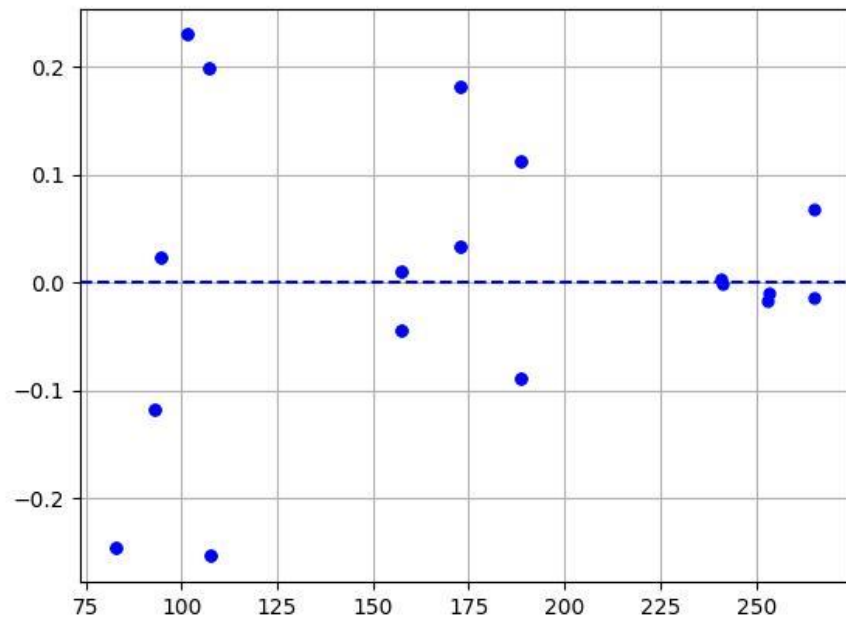
**Diff FW10 >1. mm cannot be explained by errors in measurements or MC**

**FW10: Compare 10% in positive and negative X:**

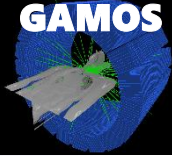
- Exper: 0.25 mm can be due to measurement errors

**FW10: Compare 10% in positive and negative X:**

- MC: 0.1 mm can be due to MC statistics



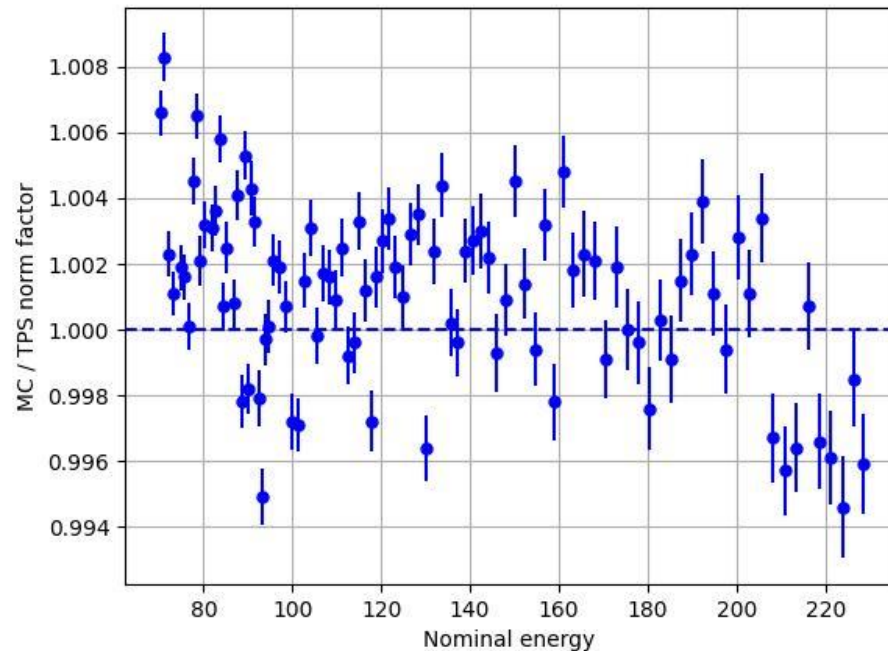
**Tails should be improved (specially for high energies)!**



# Absolute dose

- ❖ For each energy, adjust number of events in MC to get dose in a point equal to measurement of an Advanced Markus chamber in water => number of protons per MU for each E
- ❖ Instead of using point where measurement is taken, correct it by differences in peak MC/Exper (as IDD's are adjusted at peak)

**MC norm factor /  
TPS norm factor**

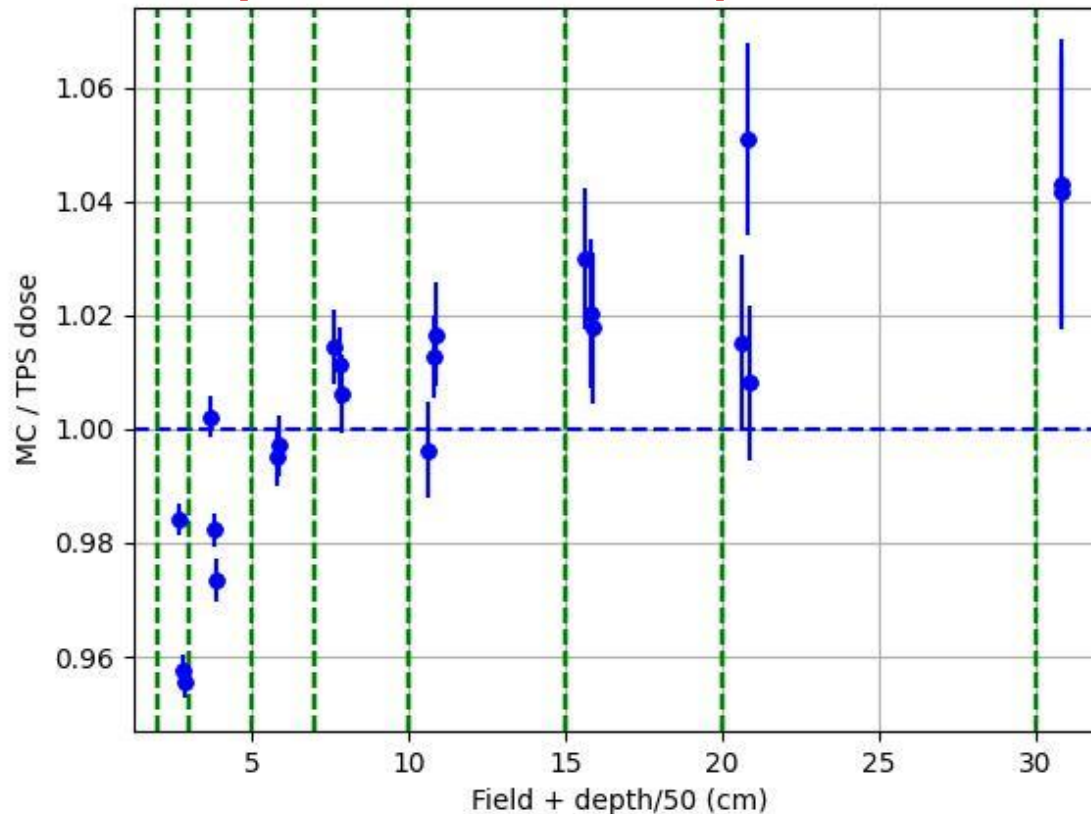


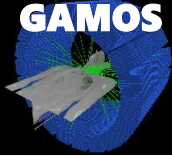
- ❖ Differences w.r.t. values provided by vendor: > 0.5-1.8%

# SOBP measurements in water

- ❖ SOBP for different fields (2x2 cm<sup>2</sup> to 30x30 cm<sup>2</sup>)
- ❖ Compare GAMOS with dose measurements at some points along the central line

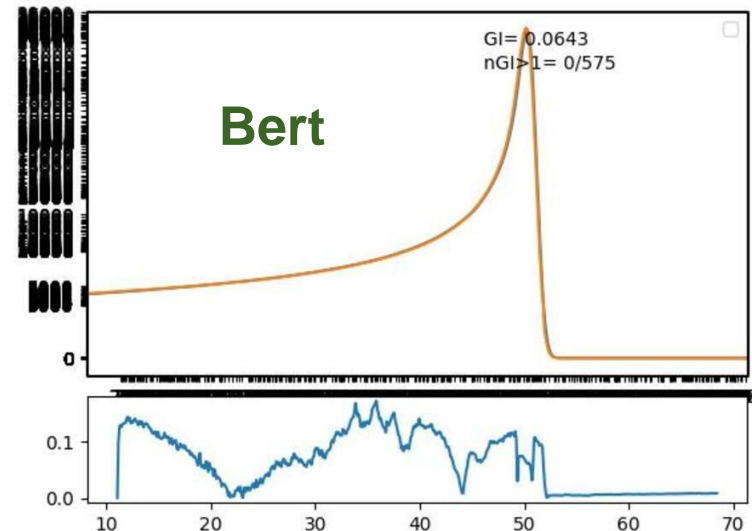
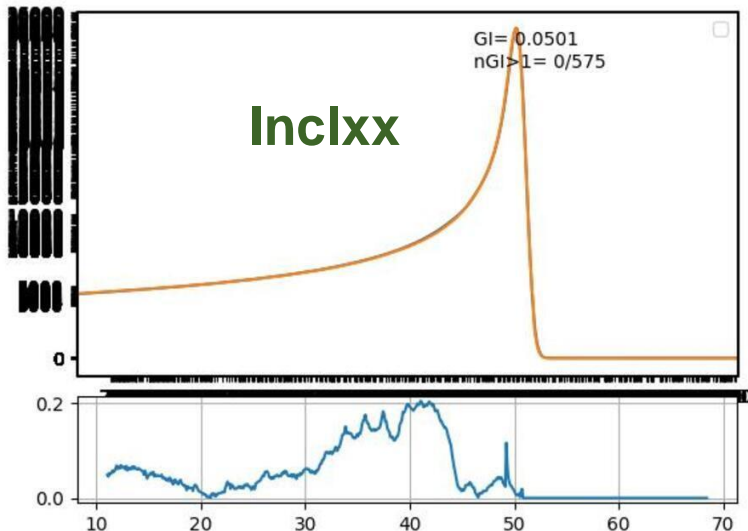
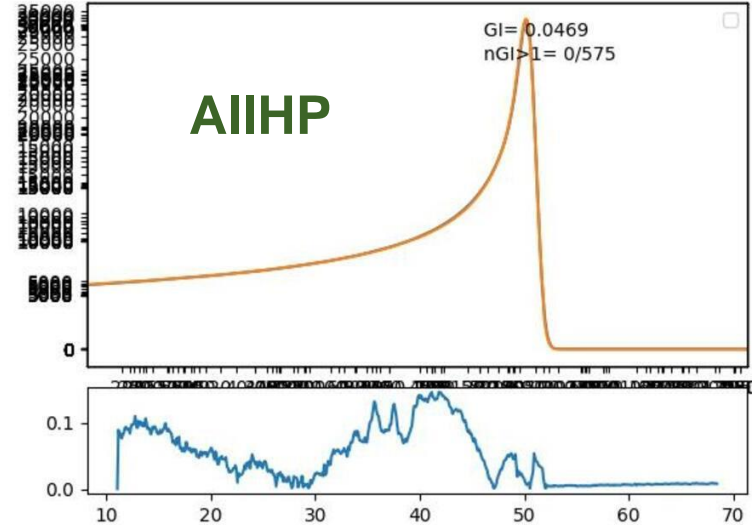
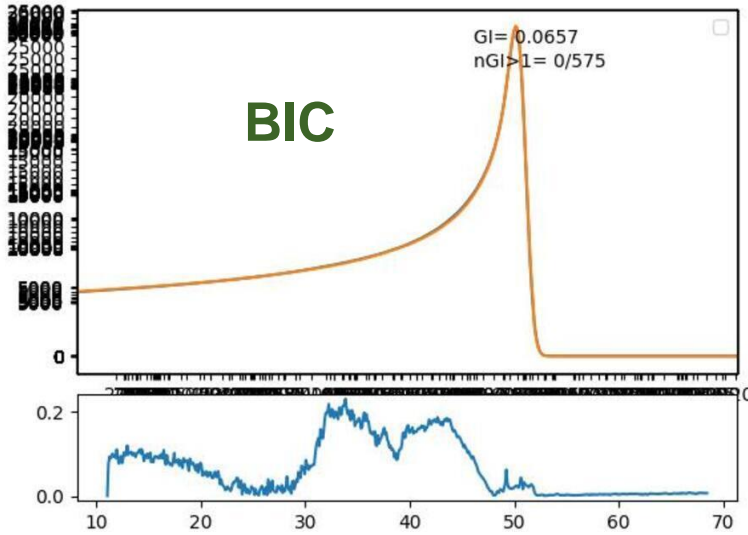
## MC / Exper. dose at SOBP point vs field width



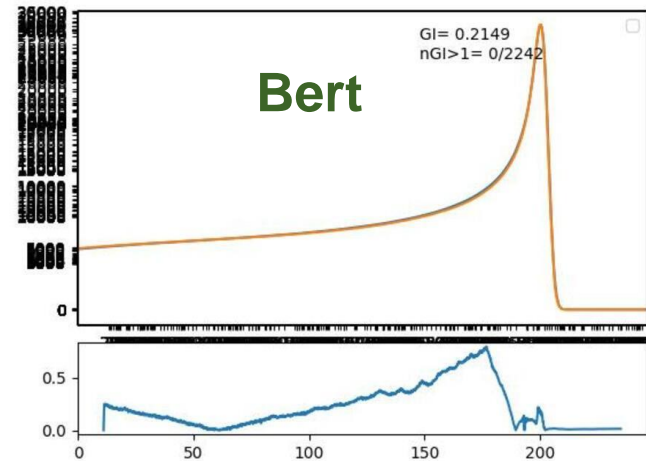
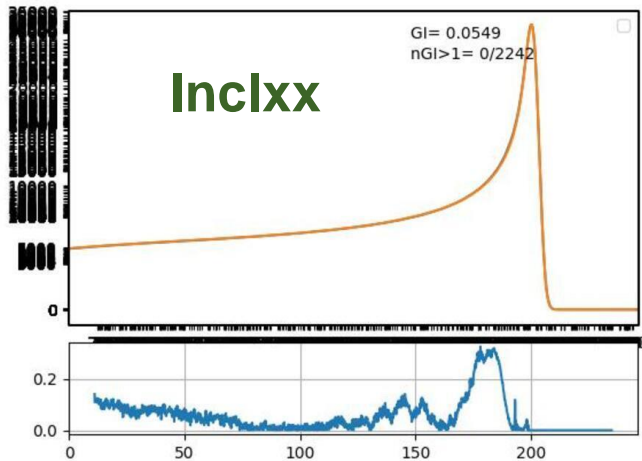
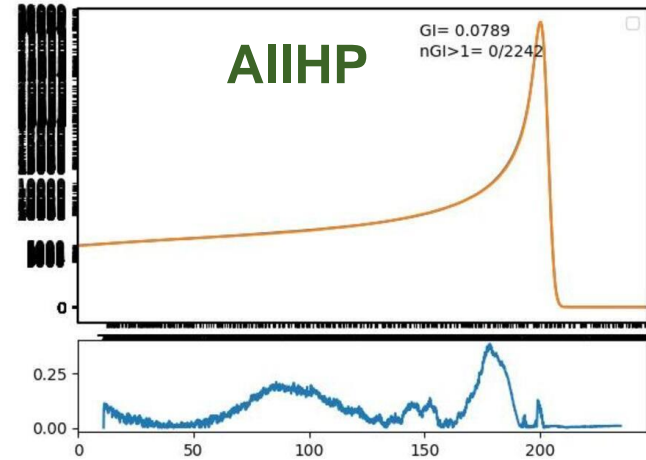
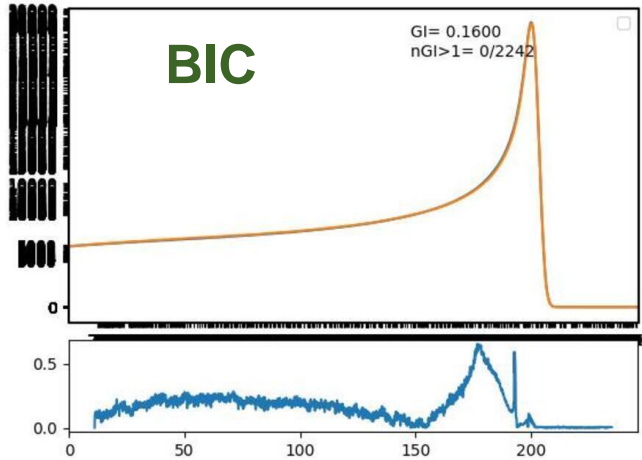


# Best physics list: is it QGSP\_BIC\_HP?

## 79.6 MeV



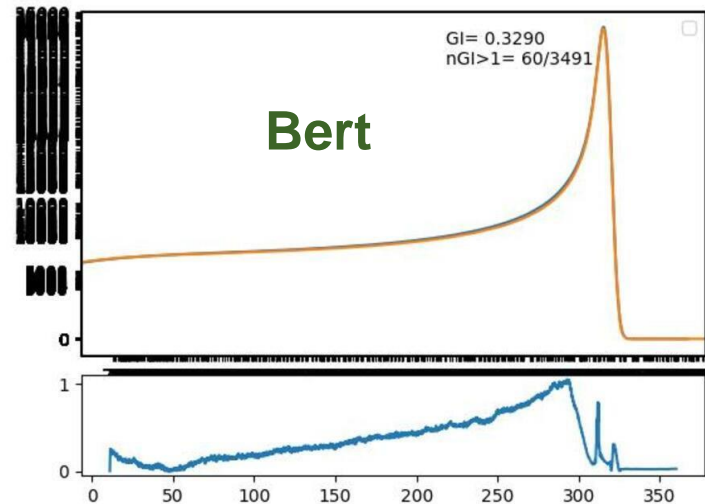
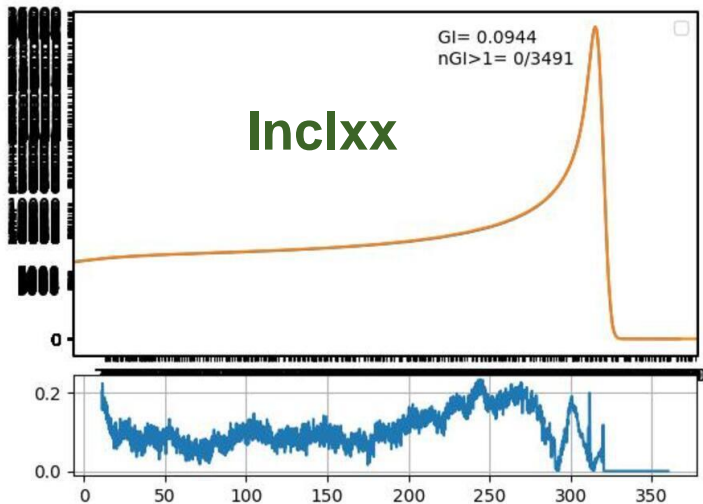
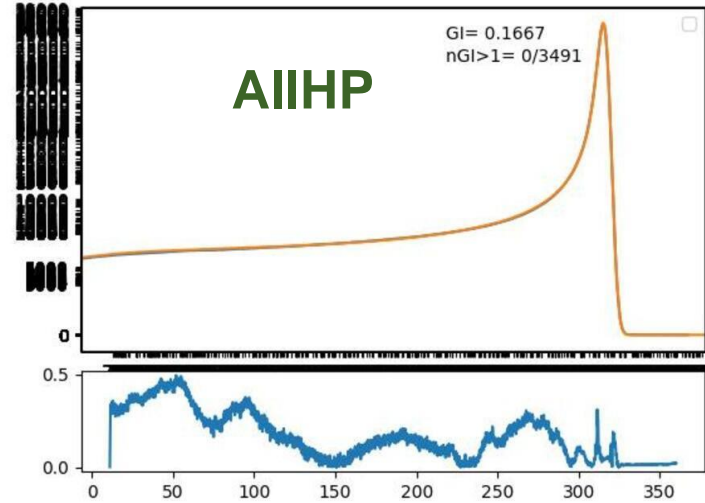
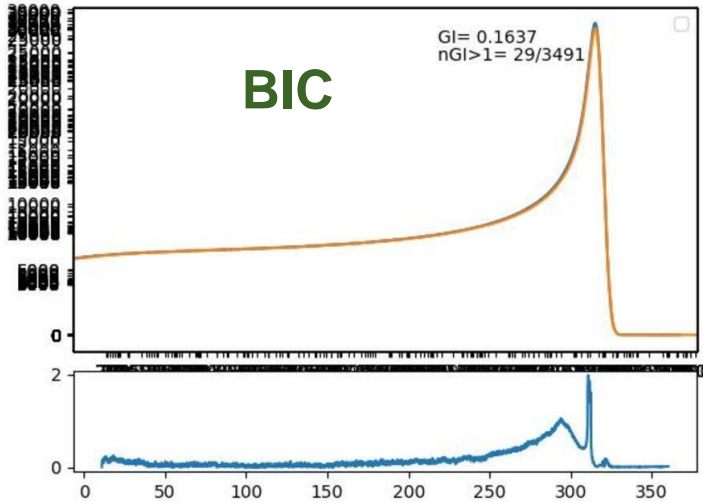
## 170.2 MeV



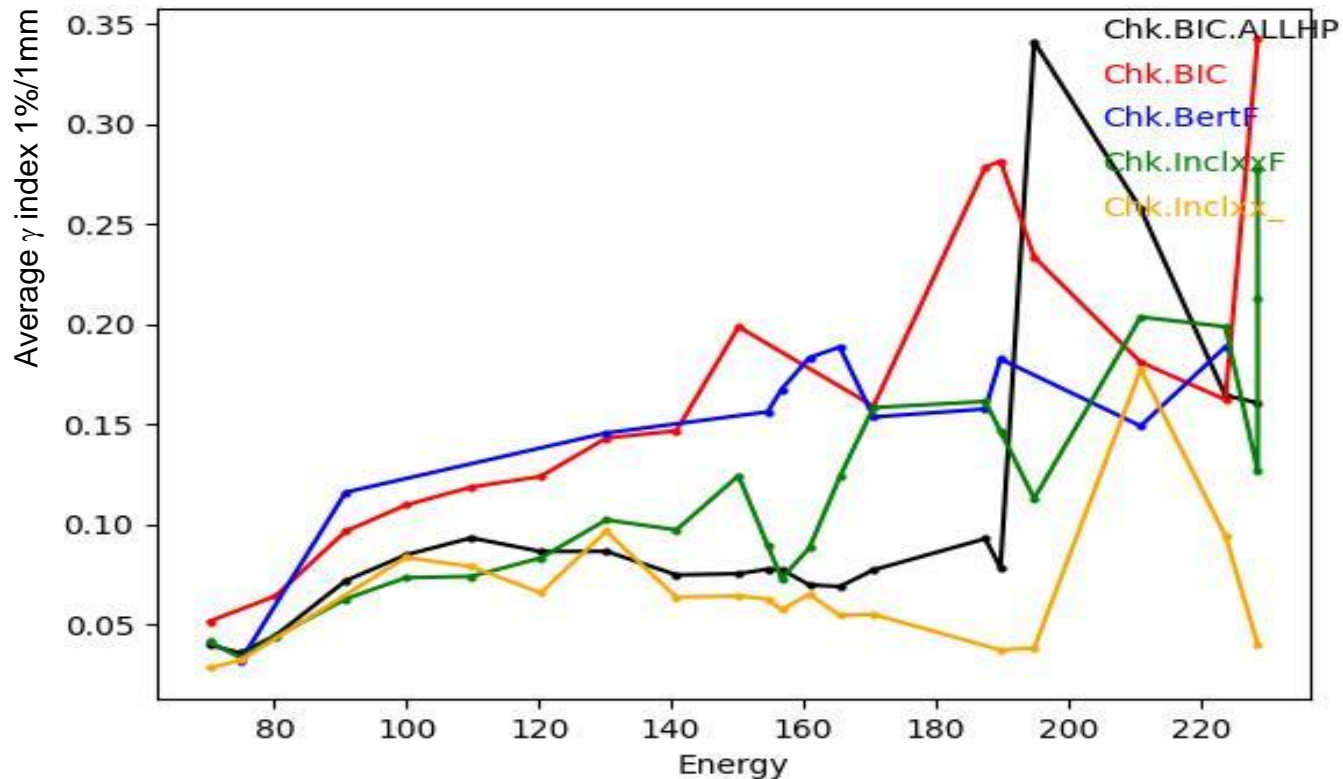


# Best physics list

## 224.2 MeV

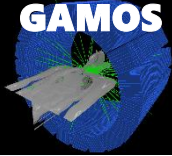


**Compare IDD for four physics lists: QGSP BIC HP, QGSP BIC AllHP, QGSP INCLXX HP, QGSP BERT HP**



➤ INCLXX is best. AllHP is as good, but has problems at  $E > 190$  ??





# Time of different physics lists

**stud.timeCPU.physList/run.patient\_MAMA\_9991\_200\_2\_1**

neutron	HP:	14.070	AllHP:	0.978	Bert:	0.684	Inclxx:	0.991
proton	HP:	401.760	<b>AllHP:</b>	<b>2.888</b>	Bert:	0.768	Inclxx:	0.767
e-	HP:	858.050	AllHP:	1.147	Bert:	0.187	Inclxx:	0.183
ALL	HP:	1712.830	AllHP:	1.565	Bert:	0.433	Inclxx:	0.430

(similar for other 3 patients tested)

HP/AllHP are EMZ, Bert/Inclxx are EMY, that's why e- time is much bigger and proton time slightly bigger

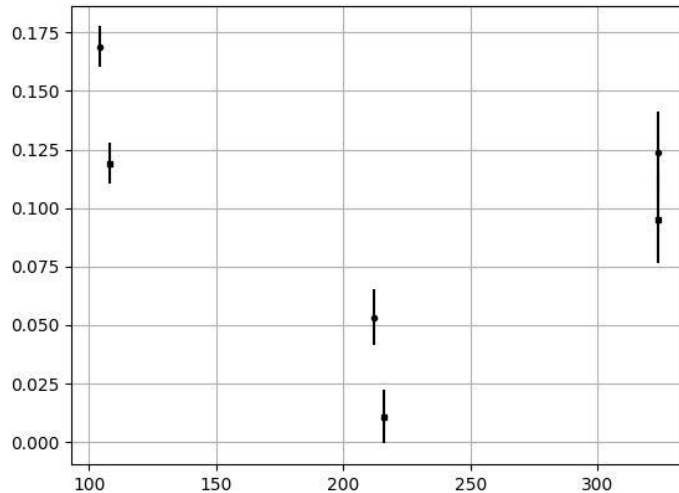
Cut is 0.05

**AllHP takes too much time in protons**

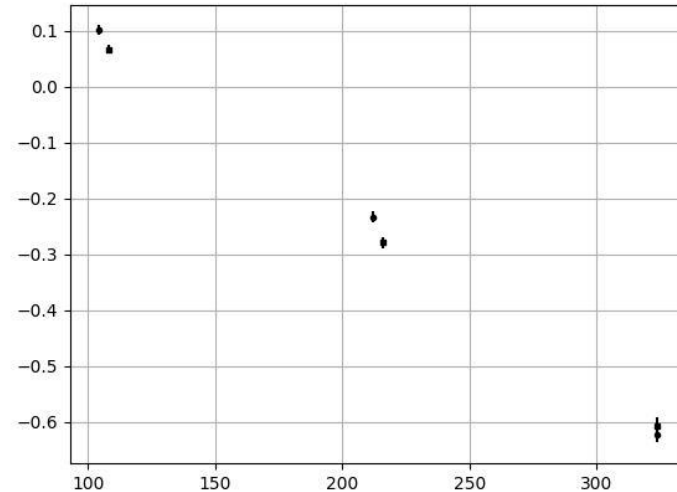
# Optimized physics list: EMY vs EMZ



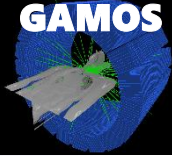
**EMZ:** MC-Exper. Sigma of profile in water  
Energy = 229.35 MeV



**EMY:** MC-Exper. Sigma of profile in water  
Energy = 229.35 MeV



- EMY EMZ is  $\sim 1.45$  slower than EMY, but gives better waterProf
- Get which physics parameters and physics models makes EMZ better, but optimizing the CPU



# EMY+ physics models

- ❖ Make changes in EMY EMZ is ~45 slower than EMY, but gives better waterProf

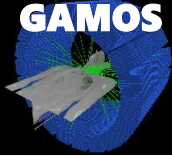
PARAMETER	EMY	EMZ	CPU EMY/EMZ	Optim
/process/eLoss/minKinEnergy	10 eV	100 eV	+2%	<b>100 eV</b>
/process/msc/RangeFactor	0.03	0.08	+7%	<b>0.08</b>
/process/eLoss/StepFunction	0.2 0.1	0.2 0.01	-10%	<b>0.2 0.1</b>
/process/eLoss/StepFunctionMuHad	0.2 0.05	0.1 0.05	=	<b>0.2 0.05</b>
/process/msc/Skin	1	3	=	<b>3</b>



PHYSICS PROCESS	MODEL EMY	MODEL EMZ	CPU EMY/EMZ	MODELOptim
gamma Compton	KleinNishina	LowEPCompton +KleinNishina	=	<b>LowEPCompton +KleinNishina</b>
gamma pair conversion	BetheHeitlerLPM	BetheHeitler5D	=	<b>BetheHeitler5D</b>
e-/e+ msc	UrbanMsc	GoudsmitSaund. +WentzelVIUni	+56%	<b>GoudsmitSaund. +WentzelVIUni</b>
proton msc	UrbanMsc	WentzelVIUni	=	<b>WentzelVIUni</b>
mu & hadron msc	UrbanMsc	WentzelVIUni		<b>WentzelVIUni</b>
e-/e+ Coulomb scattering	NO	YES	+21%	<b>NO</b>
e-/e+ ionisation	MollerBhabha	Penloni +MollerBhabha	=	<b>Penloni +MollerBhabha</b>

## Optimised physics list:

- = EMZ
- /process/eLoss/StepFunction 0.2 0.1 (not 0.2 0.01)
- **No Coulomb scattering**
- **~ 25% faster than EMZ**



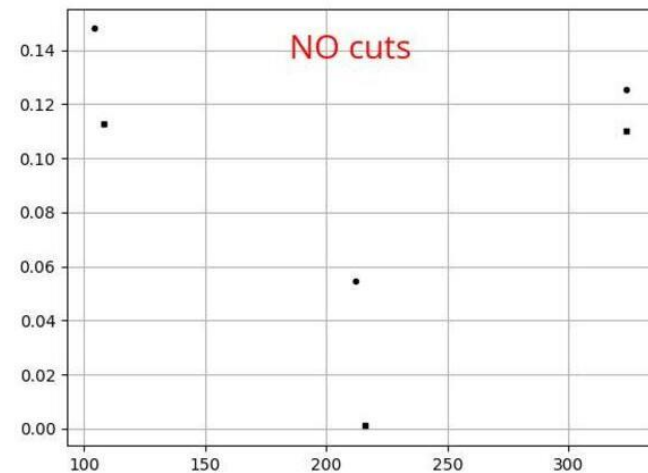
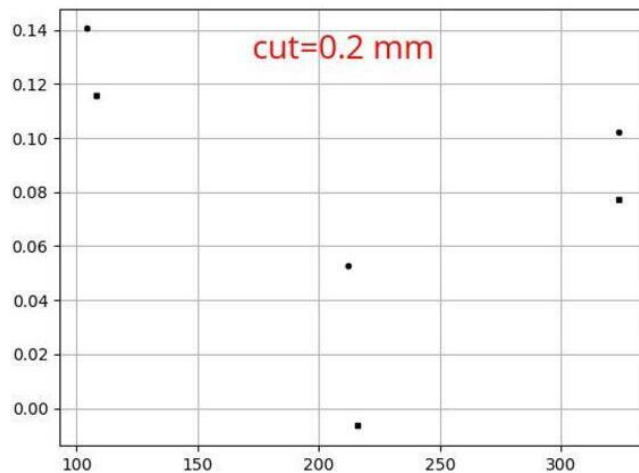
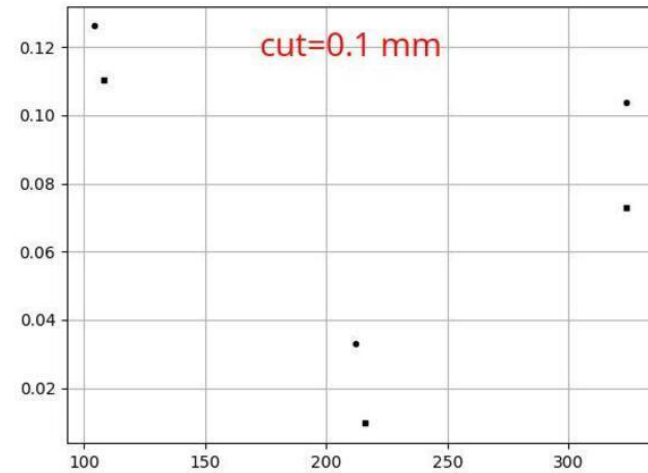
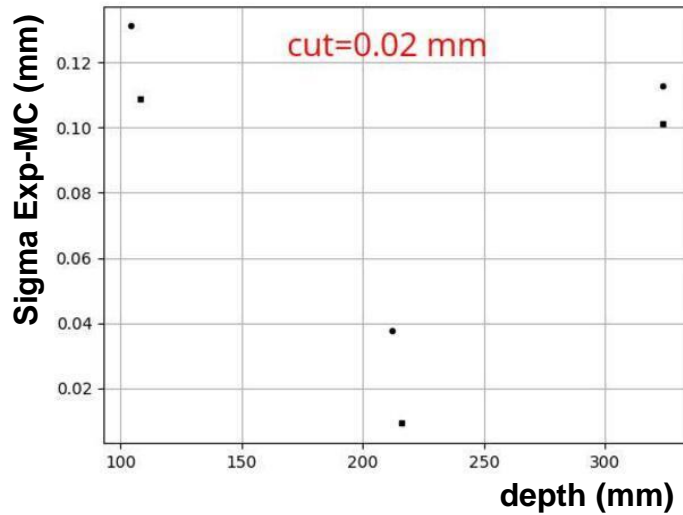
# Optimization of production cuts: Time

Production cut	CPU time (s)	Relative Time
INCLXX_EMZ	11,906	1.
0.005 mm	29,530	2.47
0.02 mm	8,833	0.74
0.05 mm	6,285	0.53
0.1 mm	4,737	0.40
0.2 mm	3,692	0.30
NO e-/e+	3,005	0.25

# Optimization of production cuts: Transversal profiles

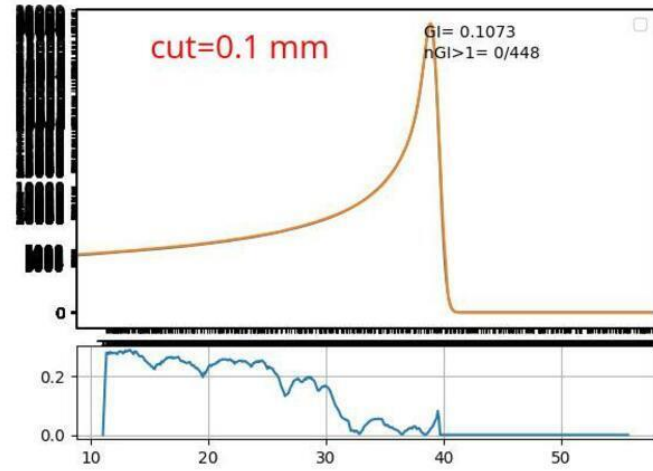
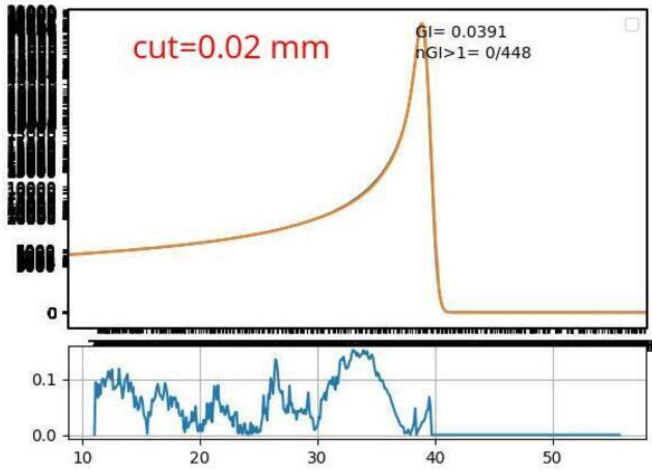


## Water profiles for the highest energy, 228.7 MeV

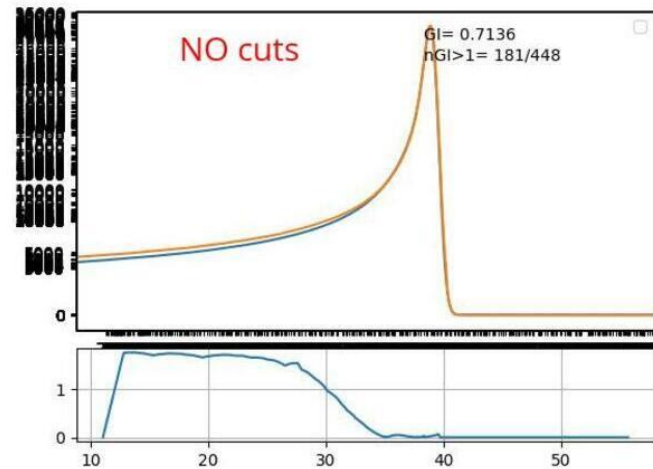
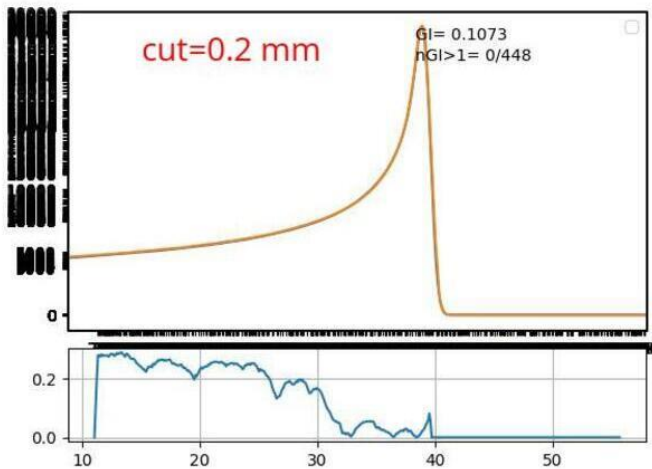


# Optimization of production cuts: IDD

70.2 MeV



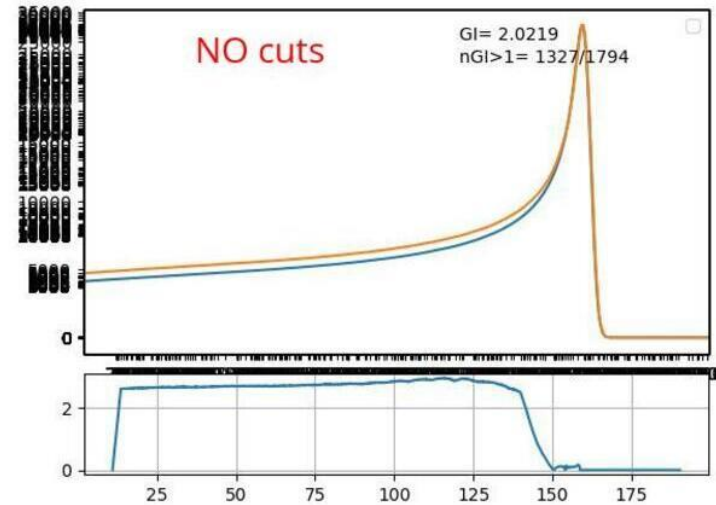
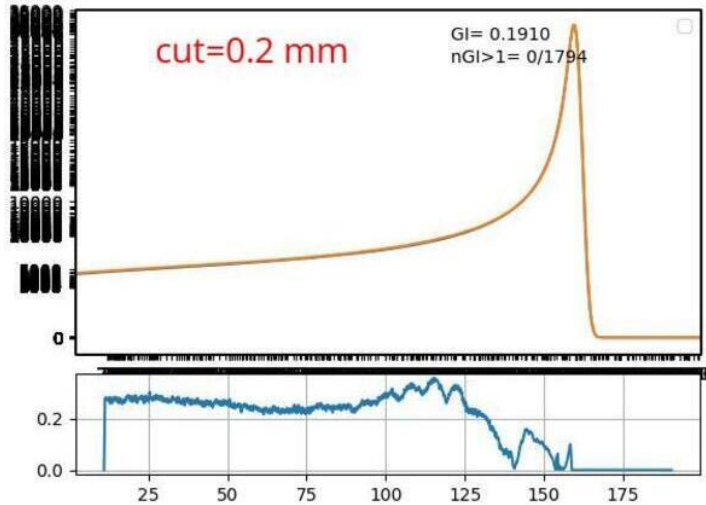
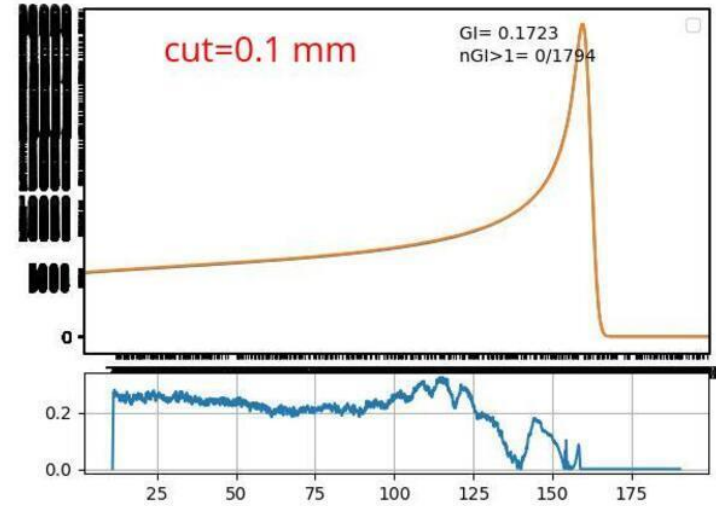
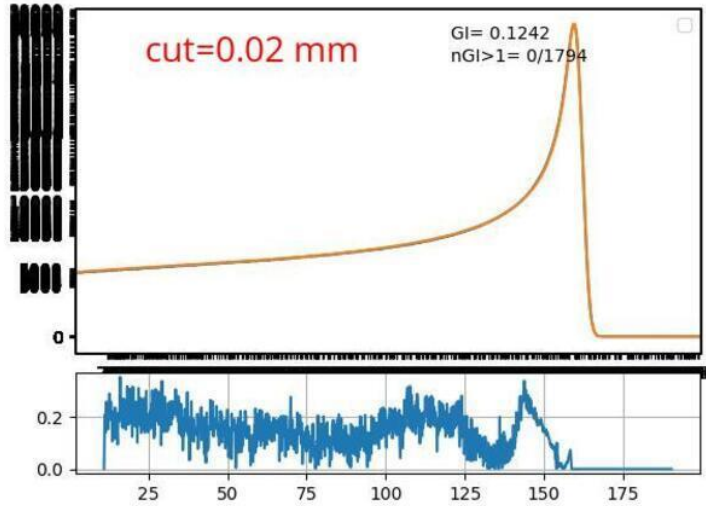
depth (mm)



# Optimization of production cuts: IDD



150.2 MeV

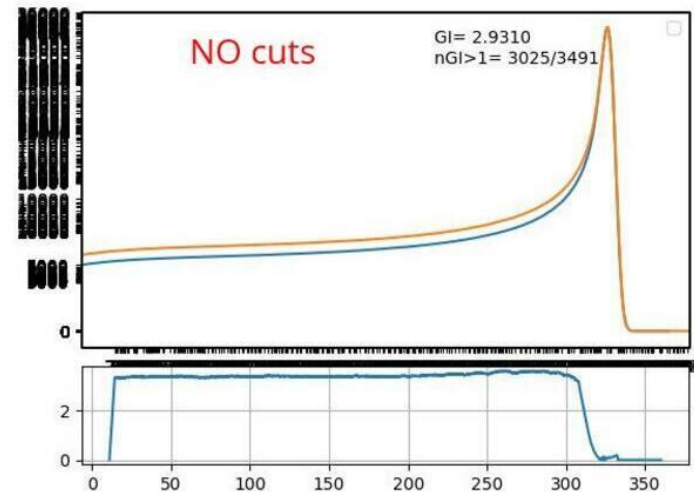
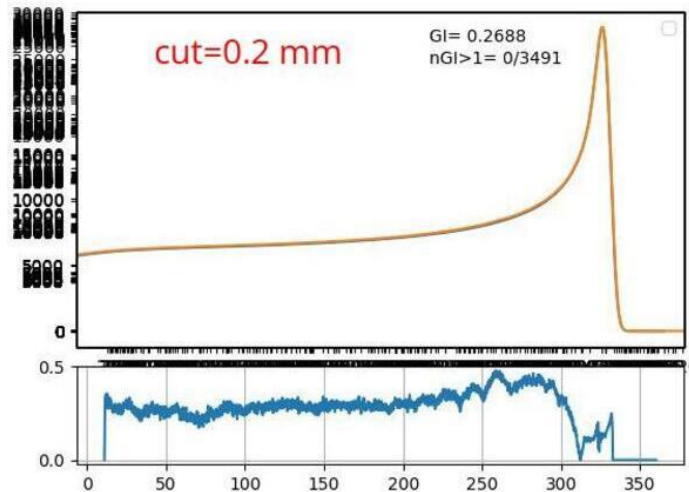
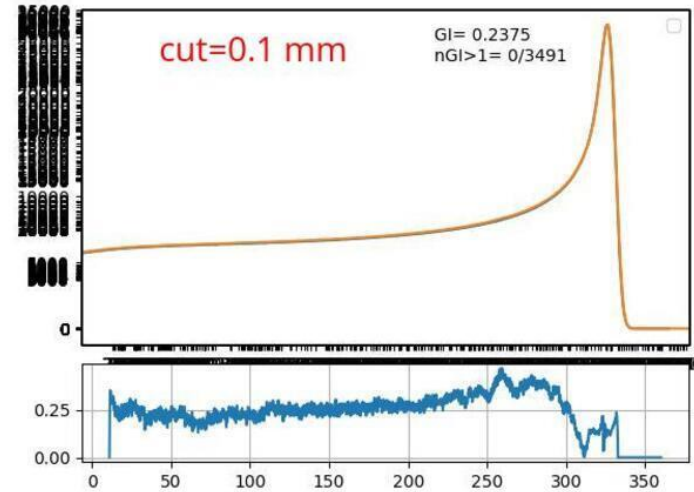
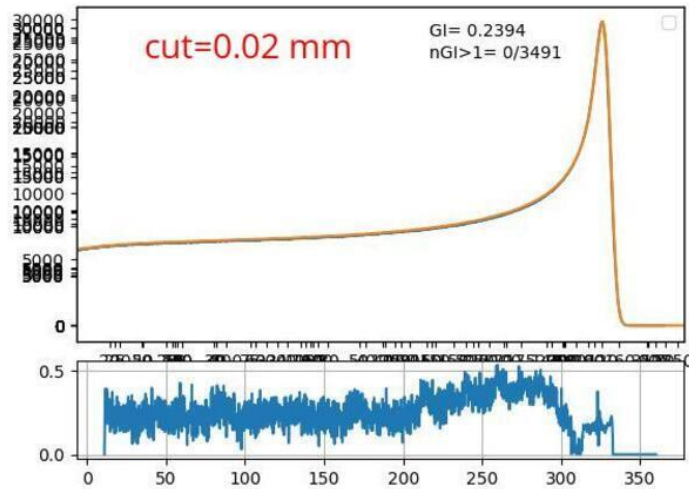




# Optimization of production cuts: IDD

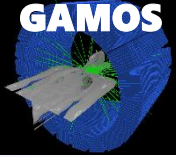


228.7 MeV





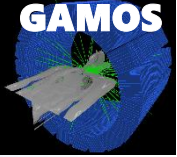
- ❑ We have made a of detailed fig of GAMOS to cun protontherapy experimental data
  - Profiles in air width  $< y$  1%/1mm 0.25
  - IDD proton range  $< y$  1%/1mm 0.5
  - Profiles in water  $< y$  1%/1mm 0.5
  - Absolute dose
  - SOBP measurements  $< 5\%$
  - Patient dose  $< y$  2%/2mm 3
    - HU to material conversion?
- ❑ We have compared GAMOS to RayStation v.12 TPS  
LET<sub>D</sub> unrestricted
  - ❑ Significant measurements found
- ❑ Differences GAMOS – TPS have to be better understood



- We have made a of detailed fit of GAMOS to CUN protontherapy experimental data
  - Profiles in air width  $< y$  1%/1mm 0.25
  - IDD proton range  $< y$  1%/1mm 0.5
  - Profiles in water  $< y$  1%/1mm 0.5
  - Absolute dose  $\sim$  TPS
  - SOBP measurements  $< 5\%$



- ❑ We have optimized the Geant4 physics list
  - ❑ Hadronic models
    - ❑ **QGSP\_INCLXX\_HP\_EMZ** and QGSP\_BIC\_AllHP (EMZ) better than QGSP\_BIC\_HP (EMZ)
    - ❑ QGSP\_BERT\_HP\_EMZ better than QGPS\_BIC\_HP
  - ❑ Electromagnetic models
    - ❑ EMY not good
    - ❑ EMZ but
      - ❑ /process/eLoss/StepFunction 0.2 0.1 (not 0.2 0.01)
      - ❑ No Coulomb scattering
      - ❑ **~ 25% faster than EMZ**
  - ❑ Production cuts
    - ❑ **0.2 60% faster than EMZ**



## TO DO:

- ✓ Add tilt in ellipse describing profiles in air
- ✓ Better understand FW10 discrepancies  $> 1\text{mm}$ 
  - Include energy distribution dependence with position and direction?
  - Play with multiple scattering?
  
- ✓ Modify Mean Excitation Energy of Schneider materials to fit experimental Stopping Power Ratios
- ✓ Adjust VirtualAxisDistance to fit experimental data (instead of nominal value provided by DICOM files)
- ✓ Simulate SOBP of increasing complexity
  
- Simulate patients